



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:47 PM UTC

PDB ID : 8UGR / pdb_00008ugr
EMDB ID : EMD-42233
Title : In-situ structure of typeX supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-06
Resolution : 6.50 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:

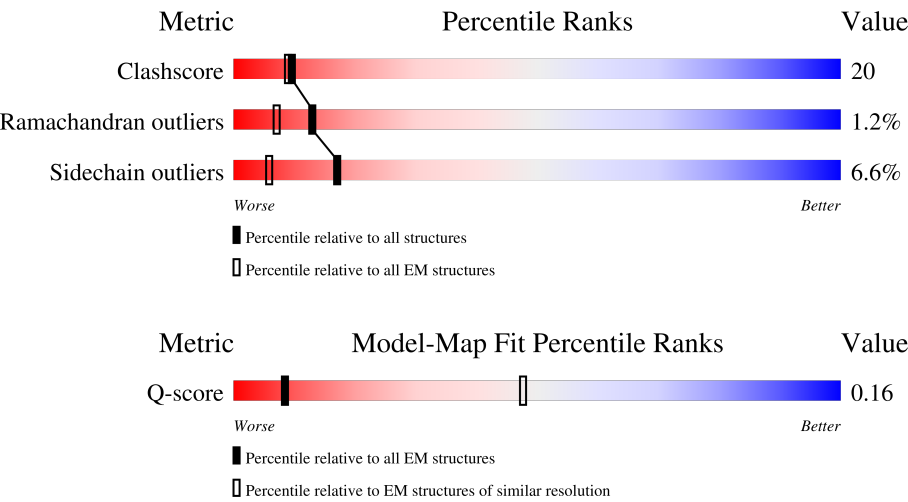
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 6.50 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.



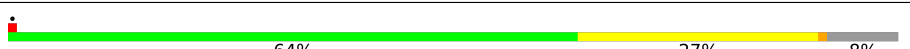
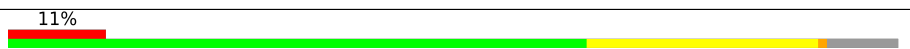
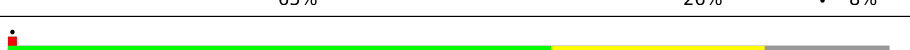
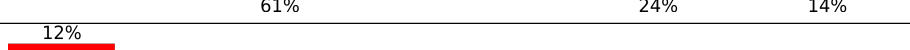
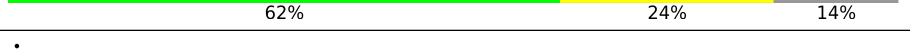
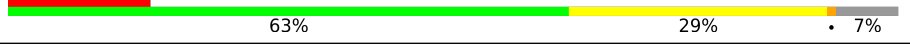
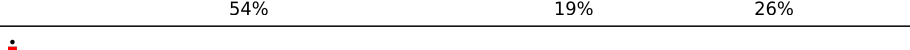
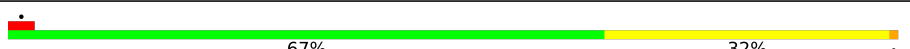
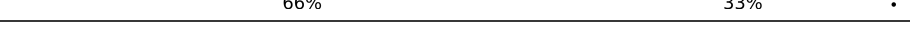
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	556 (6.00 - 7.00)

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	
1	5A	115	
2	1B	258	
2	5B	258	

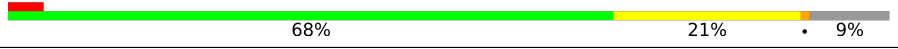
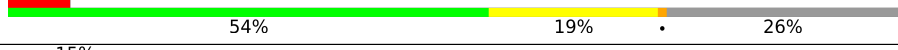
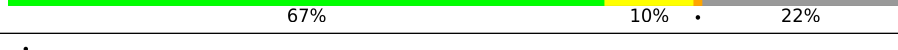
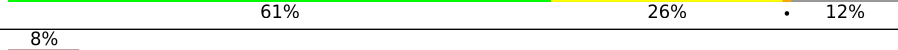
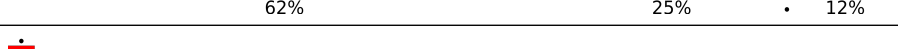
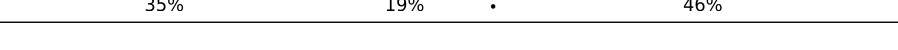
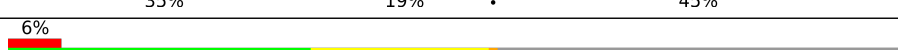
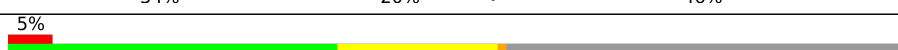
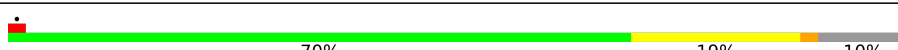
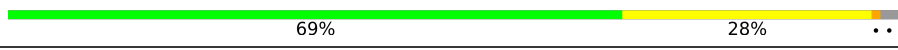
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Mol	Chain	Length	Quality of chain
3	1C	264	
3	5C	264	
4	1D	466	
4	5D	466	
5	1E	249	
5	5E	249	
6	1F	464	
6	5F	464	
7	1G	727	
7	5G	727	
8	1H	318	
8	5H	318	
9	1I	239	
9	5I	239	
10	1J	175	
10	5J	175	
11	1K	98	
11	5K	98	
12	1L	606	
12	5L	606	
13	1M	459	
13	5M	459	
14	1N	347	
14	5N	347	
15	1O	357	

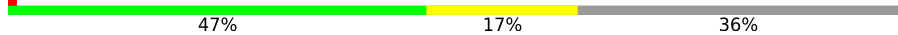
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Mol	Chain	Length	Quality of chain
15	5O	357	
16	1P	377	
16	5P	377	
17	1Q	175	
17	5Q	175	
18	1R	123	
18	5R	123	
19	1S	99	
19	5S	99	
20	1T	156	
20	1U	156	
20	5T	156	
20	5U	156	
21	1V	116	
21	5V	116	
22	1W	128	
22	5W	128	
23	1X	172	
23	5X	172	
24	1Y	141	
24	5Y	141	
25	1Z	144	
25	5Z	144	
26	1a	70	
26	5a	70	

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Mol	Chain	Length	Quality of chain
27	1b	84	
27	5b	84	
28	1c	76	
28	5c	76	
29	1d	122	
29	5d	122	
30	1e	106	
30	5e	106	
31	1f	58	
31	5f	58	
32	1g	154	
32	5g	154	
33	1h	189	
33	5h	189	
34	1i	128	
34	5i	128	
35	1j	105	
35	5j	105	
36	1k	98	
36	5k	98	
37	1l	186	
37	5l	186	
38	1m	129	
38	5m	129	
39	1n	179	

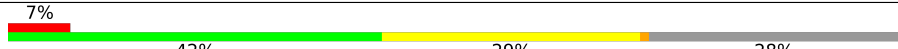
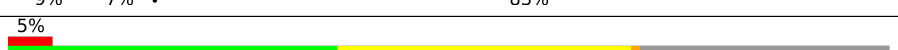
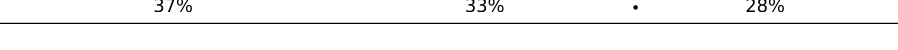
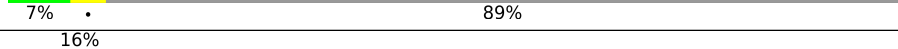
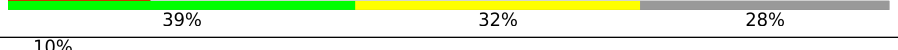
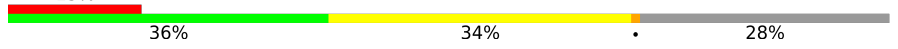
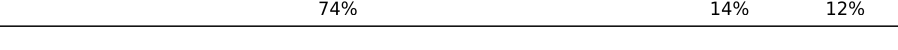
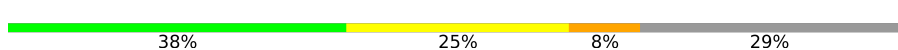
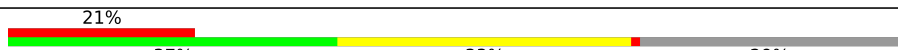
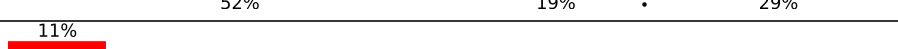
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Mol	Chain	Length	Quality of chain
39	5n	179	
40	1o	136	
40	5o	136	
41	1p	176	
41	5p	176	
42	1q	145	
42	5q	145	
43	1r	113	
43	5r	113	
44	1s	471	
44	5s	471	
45	3A	480	
45	3N	480	
45	6A	480	
45	6N	480	
46	3B	453	
46	3O	453	
46	6B	453	
46	6O	453	
47	3C	379	
47	3P	379	
47	6C	379	
47	6P	379	
48	3D	326	
48	3Q	326	

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Mol	Chain	Length	Quality of chain
48	6D	326	
48	6Q	326	
49	3E	274	
49	3I	274	
49	3R	274	
49	3V	274	
49	6E	274	
49	6I	274	
49	6R	274	
49	6V	274	
50	3F	111	
50	3S	111	
50	6F	111	
50	6S	111	
51	3G	82	
51	3T	82	
51	6G	82	
51	6T	82	
52	3H	91	
52	3U	91	
52	6H	91	
52	6U	91	
53	3J	64	
53	3W	64	
53	6J	64	

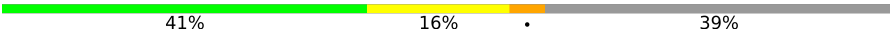
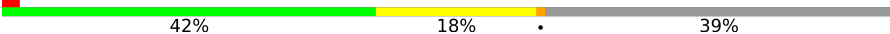
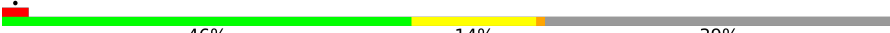
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Mol	Chain	Length	Quality of chain
53	6W	64	
54	3X	56	
54	3Y	56	
54	6X	56	
54	6Y	56	
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	129	
60	8F	129	
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	
63	8I	75	
64	4J	80	
64	8J	80	

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Mol	Chain	Length	Quality of chain
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
70	SF4	1B	201	-	-	X	-
70	SF4	1F	502	-	-	X	-
70	SF4	5B	201	-	-	X	-
70	SF4	5F	502	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	6E	301	-	-	X	-
75	CDL	8A	610	-	-	X	-
88	CUA	4B	302	-	-	X	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 233868 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		
1	5A	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		
2	5B	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
			1746	1128	299	317	2		
3	5C	209	Total	C	N	O	S	0	0
			1746	1128	299	317	2		

- 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		
4	5D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

- 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		
5	5E	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		
6	5F	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		
7	5G	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		
8	5H	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		
9	5I	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		
10	5J	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		
11	5K	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		
12	5L	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		
13	5M	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		
14	5N	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	5O	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		
16	5P	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		
17	5Q	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		
18	5R	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		
19	5S	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		
20	5T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	5U	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		
21	5V	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		
22	5W	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		
23	5X	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		
24	5Y	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		
25	5Z	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		
26	5a	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		
27	5b	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		
28	5c	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		
29	5d	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		
30	5e	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		
31	5f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

- 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		
32	5g	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		
33	5h	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		
34	5i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8
5i	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		
35	5j	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		
36	5k	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		
37	5l	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		
38	5m	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		
39	5n	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		
40	5o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

- 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		
41	5p	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		
42	5q	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		
43	5r	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		
44	5s	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	0	0
			3415	2157	604	635	19		
45	6A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	6N	445	Total	C	N	O	S	0	0
			3415	2157	604	635	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
			3139	1965	556	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3132	1960	555	609	8		
46	6B	418	Total	C	N	O	S	0	0
			3139	1965	556	610	8		
46	6O	417	Total	C	N	O	S	0	0
			3132	1960	555	609	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		
47	6C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	6P	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		
48	6D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	6Q	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		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		
49	6E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	6R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6S	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	72	Total	C	N	O	S	0	0
			616	403	114	97	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	6G	72	Total	C	N	O	S	0	0
			616	403	114	97	2		
51	6T	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		
52	6H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			464	305	82	77		
53	3W	56	Total	C	N	O	0	0
			464	305	82	77		
53	6J	56	Total	C	N	O	0	0
			464	305	82	77		
53	6W	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		
54	6X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	6Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	513	Total	C	N	O	S	0	0
			4016	2687	624	674	31		
55	8A	513	Total	C	N	O	S	0	0
			4016	2687	624	674	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			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		
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		

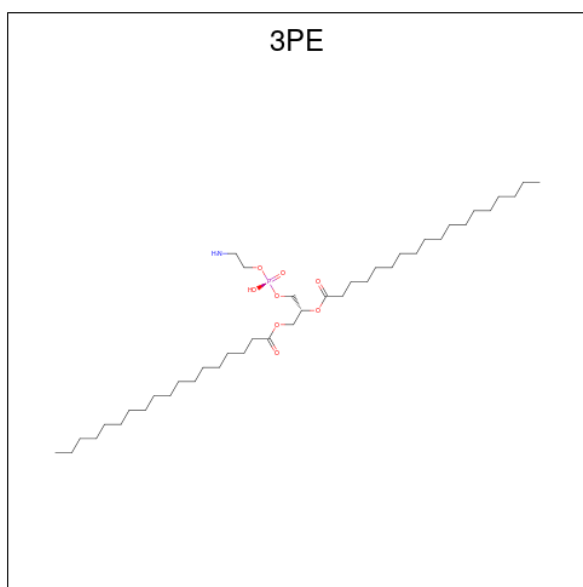
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

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: C₄₁H₈₂NO₈P).



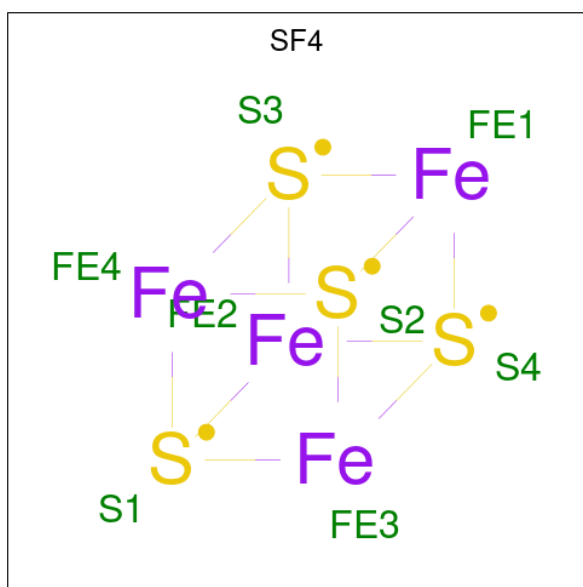
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	1N	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			41	31	1	8	1	

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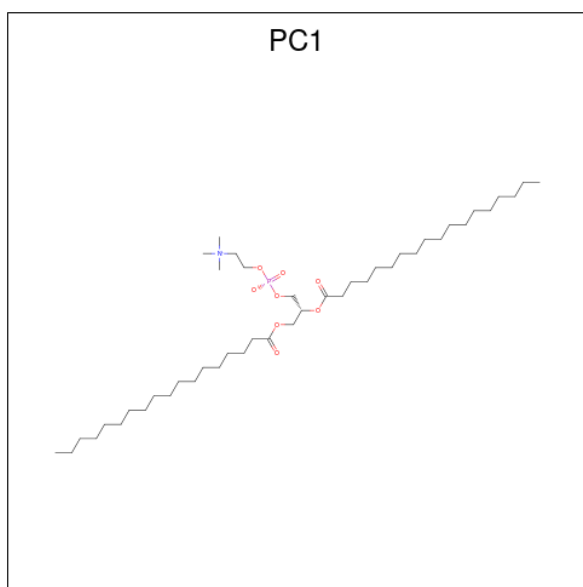
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69	1d	1	Total 48	C 38	N 1	O 8	P 1	0
69	1j	1	Total 44	C 34	N 1	O 8	P 1	0
69	5A	1	Total 47	C 37	N 1	O 8	P 1	0
69	5J	1	Total 44	C 34	N 1	O 8	P 1	0
69	5L	1	Total 46	C 36	N 1	O 8	P 1	0
69	5L	1	Total 45	C 35	N 1	O 8	P 1	0
69	5L	1	Total 31	C 21	N 1	O 8	P 1	0
69	5M	1	Total 45	C 35	N 1	O 8	P 1	0
69	5M	1	Total 50	C 40	N 1	O 8	P 1	0
69	5N	1	Total 49	C 39	N 1	O 8	P 1	0
69	5N	1	Total 51	C 41	N 1	O 8	P 1	0
69	5Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	5Y	1	Total 30	C 20	N 1	O 8	P 1	0
69	5Y	1	Total 33	C 23	N 1	O 8	P 1	0
69	5Y	1	Total 27	C 17	N 1	O 8	P 1	0
69	5Y	1	Total 41	C 31	N 1	O 8	P 1	0
69	5d	1	Total 48	C 38	N 1	O 8	P 1	0
69	5j	1	Total 44	C 34	N 1	O 8	P 1	0

- Molecule 70 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
70	1B	1	Total	Fe	S	0
			8	4	4	
70	1F	1	Total	Fe	S	0
			8	4	4	
70	1G	1	Total	Fe	S	0
			8	4	4	
70	1G	1	Total	Fe	S	0
			8	4	4	
70	1I	1	Total	Fe	S	0
			8	4	4	
70	1I	1	Total	Fe	S	0
			8	4	4	
70	5B	1	Total	Fe	S	0
			8	4	4	
70	5F	1	Total	Fe	S	0
			8	4	4	
70	5G	1	Total	Fe	S	0
			8	4	4	
70	5G	1	Total	Fe	S	0
			8	4	4	
70	5I	1	Total	Fe	S	0
			8	4	4	
70	5I	1	Total	Fe	S	0
			8	4	4	

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



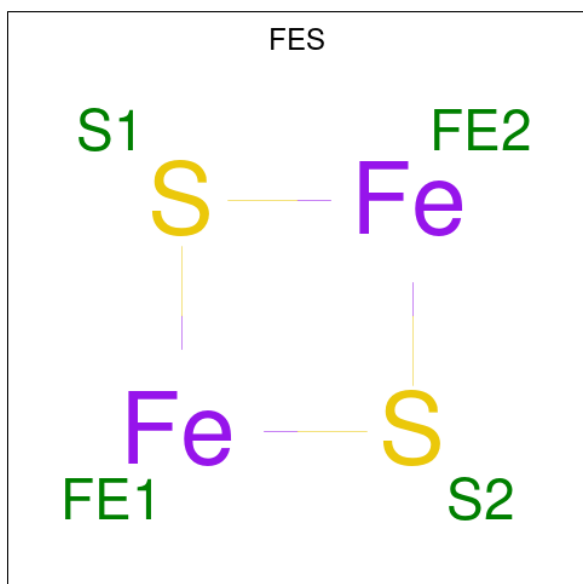
Mol	Chain	Residues	Atoms					AltConf
71	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
71	1m	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	5A	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	5B	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	5H	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	5I	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	5I	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	5M	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	5P	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	5Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	5h	1	Total	C	N	O	P	0
			47	37	1	8	1	
71	5m	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



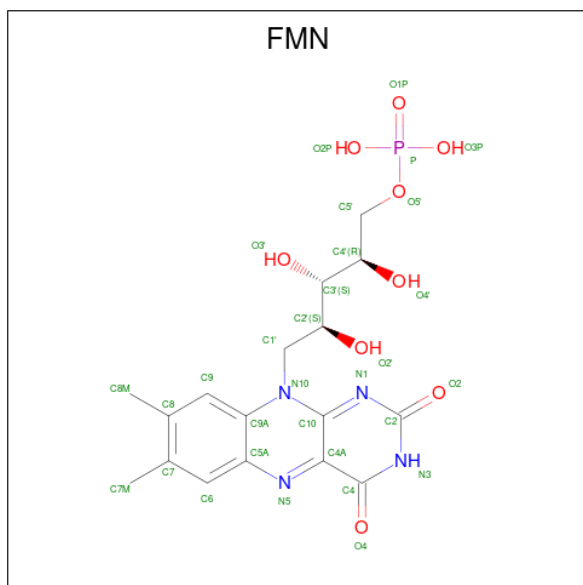
Mol	Chain	Residues	Atoms			AltConf
72	1E	1	Total	Fe	S	0
			4	2	2	
72	1G	1	Total	Fe	S	0
			4	2	2	
72	3E	1	Total	Fe	S	0
			4	2	2	
72	3R	1	Total	Fe	S	0
			4	2	2	
72	5E	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
72	5G	1	Total	Fe	S	0
			4	2	2	
72	6E	1	Total	Fe	S	0
			4	2	2	
72	6R	1	Total	Fe	S	0
			4	2	2	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

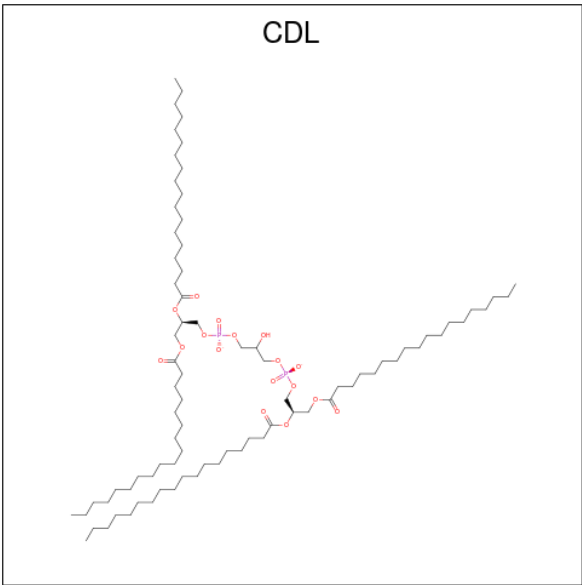


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	
73	5F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

Mol	Chain	Residues	Atoms		AltConf
74	1G	1	Total	K	0
			1	1	
74	5G	1	Total	K	0
			1	1	

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



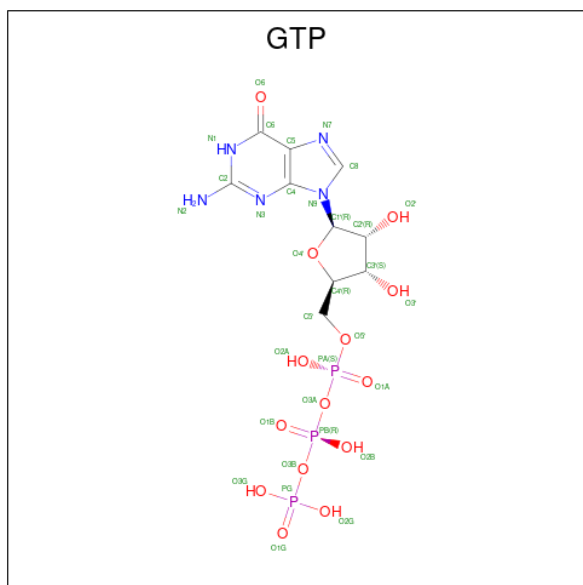
Mol	Chain	Residues	Atoms				AltConf
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1i	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	5L	1	Total	C	O	P	0
			76	57	17	2	
75	5N	1	Total	C	O	P	0
			62	43	17	2	
75	5X	1	Total	C	O	P	0
			86	67	17	2	
75	5d	1	Total	C	O	P	0
			65	46	17	2	
75	5i	1	Total	C	O	P	0
			80	61	17	2	
75	5q	1	Total	C	O	P	0
			61	42	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	8A	1	Total	C	O	P	0
			100	81	17	2	
75	8B	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: $C_{10}H_{16}N_5O_{14}P_3$).

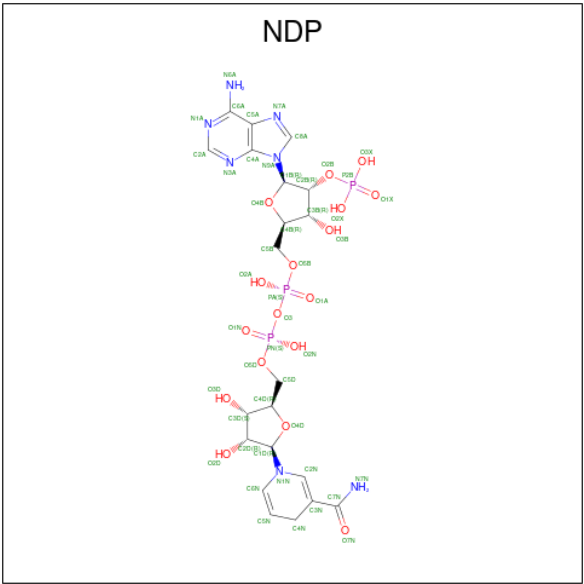


Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	
76	5O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

Mol	Chain	Residues	Atoms		AltConf
77	1O	1	Total	Mg	0
			1	1	
77	4A	1	Total	Mg	0
			1	1	
77	5O	1	Total	Mg	0
			1	1	
77	8A	1	Total	Mg	0
			1	1	

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

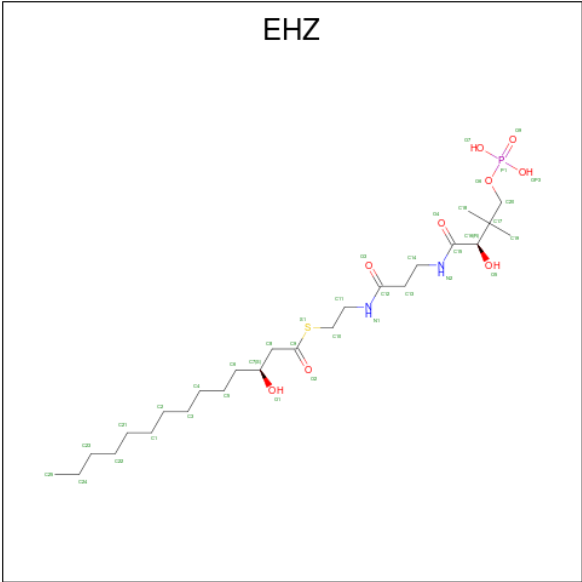


Mol	Chain	Residues	Atoms					AltConf
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	
78	5P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

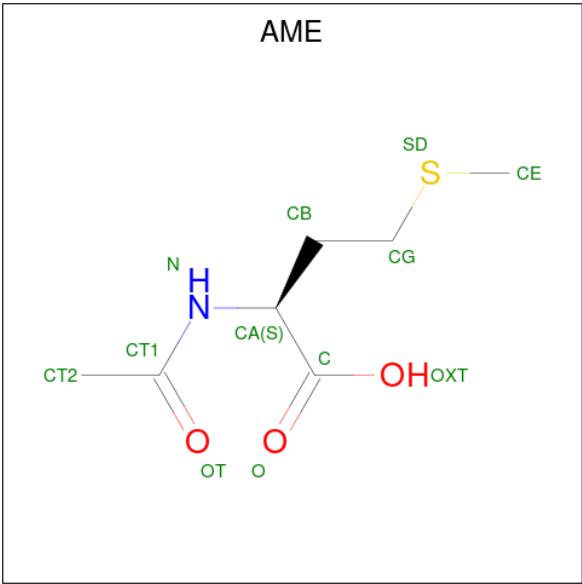
Mol	Chain	Residues	Atoms		AltConf
79	1R	1	Total	Zn	0
			1	1	
79	4F	1	Total	Zn	0
			1	1	
79	5R	1	Total	Zn	0
			1	1	
79	8F	1	Total	Zn	0
			1	1	

- 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).



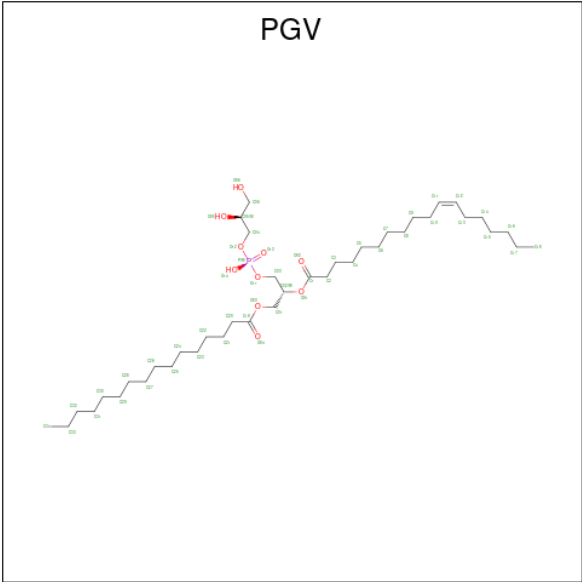
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	5T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	5n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 81 is N-ACETYL METHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



Mol	Chain	Residues	Atoms					AltConf
81	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	
81	5h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 82 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



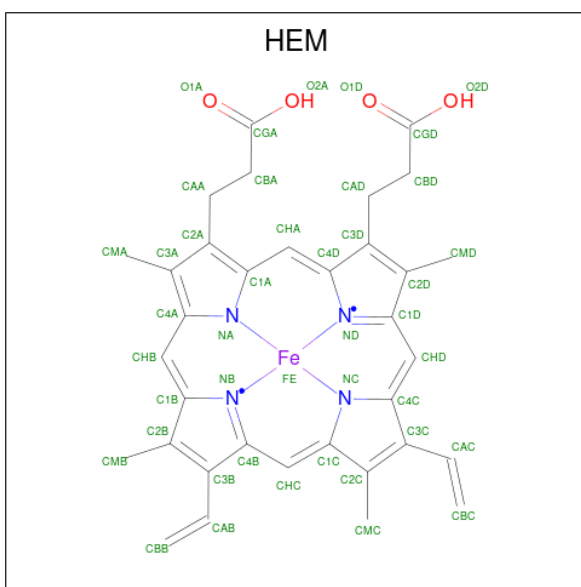
Mol	Chain	Residues	Atoms				AltConf
82	1p	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	

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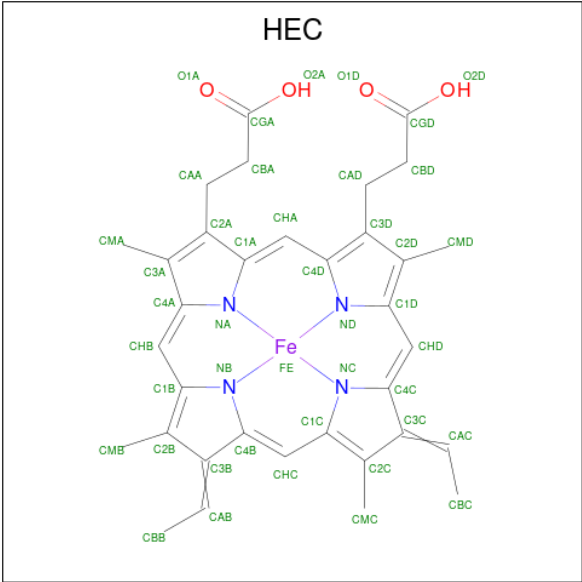
Mol	Chain	Residues	Atoms				AltConf
82	4C	1	Total 51	C 40	O 10	P 1	0
82	4G	1	Total 51	C 40	O 10	P 1	0
82	4J	1	Total 51	C 40	O 10	P 1	0
82	4K	1	Total 51	C 40	O 10	P 1	0
82	4L	1	Total 51	C 40	O 10	P 1	0
82	8A	1	Total 51	C 40	O 10	P 1	0
82	8A	1	Total 51	C 40	O 10	P 1	0
82	8A	1	Total 51	C 40	O 10	P 1	0
82	8A	1	Total 51	C 40	O 10	P 1	0
82	8B	1	Total 51	C 40	O 10	P 1	0
82	8C	1	Total 51	C 40	O 10	P 1	0
82	8C	1	Total 51	C 40	O 10	P 1	0
82	8C	1	Total 51	C 40	O 10	P 1	0
82	8C	1	Total 51	C 40	O 10	P 1	0
82	8C	1	Total 51	C 40	O 10	P 1	0
82	8G	1	Total 51	C 40	O 10	P 1	0
82	8J	1	Total 51	C 40	O 10	P 1	0
82	8K	1	Total 51	C 40	O 10	P 1	0
82	8L	1	Total 51	C 40	O 10	P 1	0

- Molecule 83 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



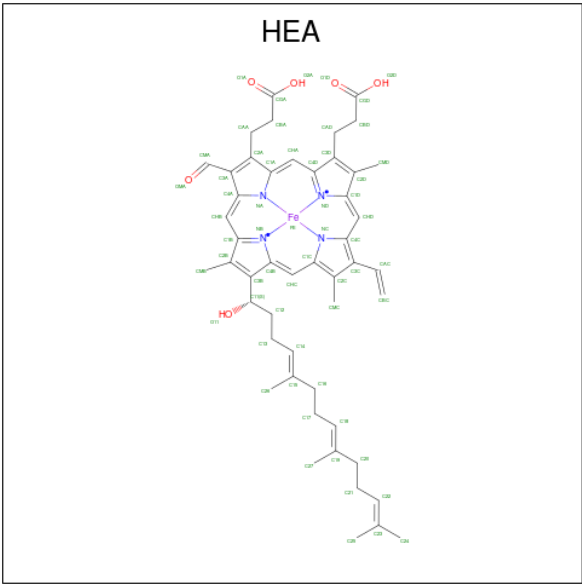
Mol	Chain	Residues	Atoms					AltConf
83	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	6C	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	6C	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	6P	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	6P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 84 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
84	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
84	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	6D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
84	6Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 85 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
85	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
85	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
85	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
85	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

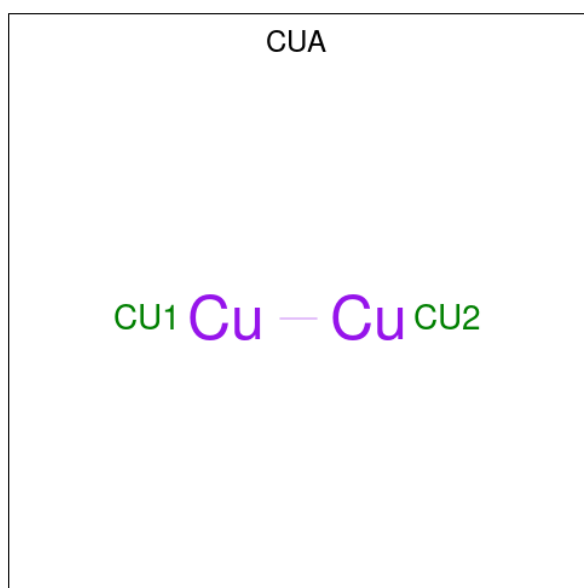
- Molecule 86 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
86	4A	1	Total	Cu	0
			1	1	
86	8A	1	Total	Cu	0
			1	1	

- Molecule 87 is SODIUM ION (CCD ID: NA) (formula: Na).

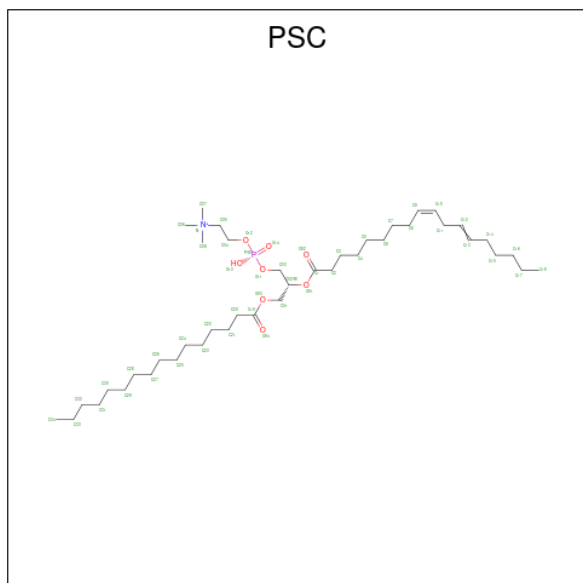
Mol	Chain	Residues	Atoms		AltConf
87	4A	1	Total	Na	0
			1	1	
87	8A	1	Total	Na	0
			1	1	

- Molecule 88 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



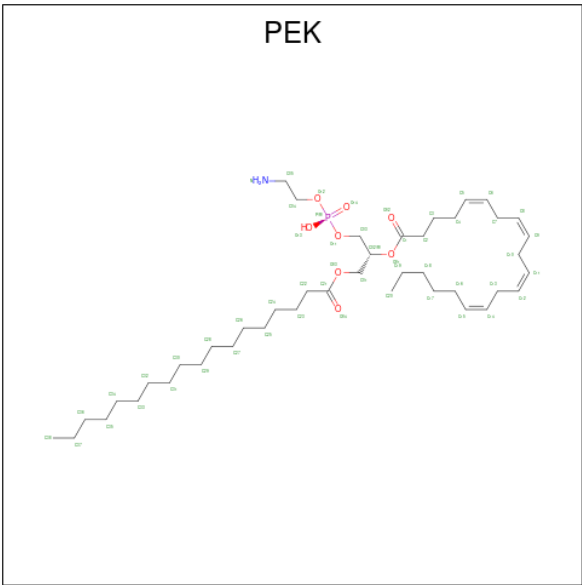
Mol	Chain	Residues	Atoms		AltConf
88	4B	1	Total	Cu	0
			2	2	
88	8B	1	Total	Cu	0
			2	2	

- Molecule 89 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



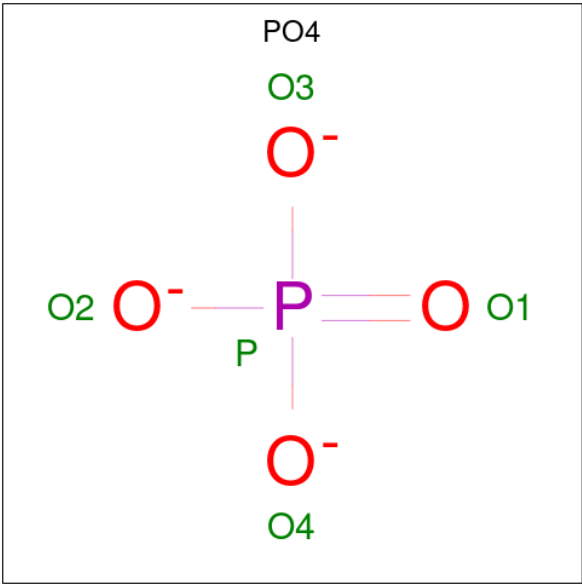
Mol	Chain	Residues	Atoms					AltConf
89	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	
89	8A	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 90 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
90	4C	1	Total	C	N	O	P	0
			53	43	1	8	1	
90	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
90	8C	1	Total	C	N	O	P	0
			53	43	1	8	1	
90	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 91 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

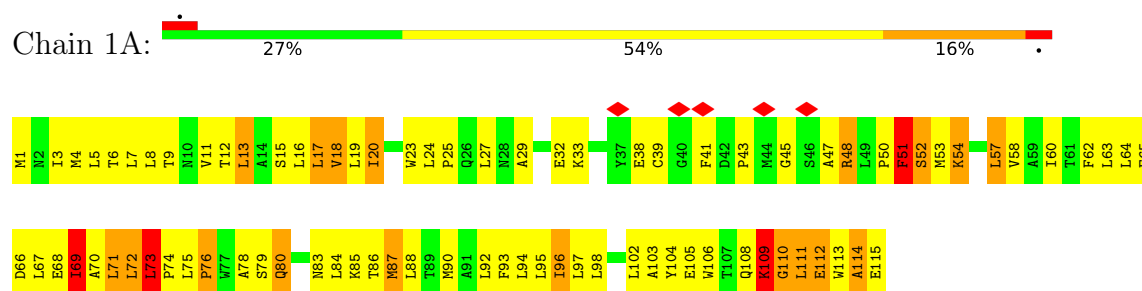


Mol	Chain	Residues	Atoms			AltConf
91	4H	1	Total	O	P	0
			5	4	1	
91	8H	1	Total	O	P	0
			5	4	1	

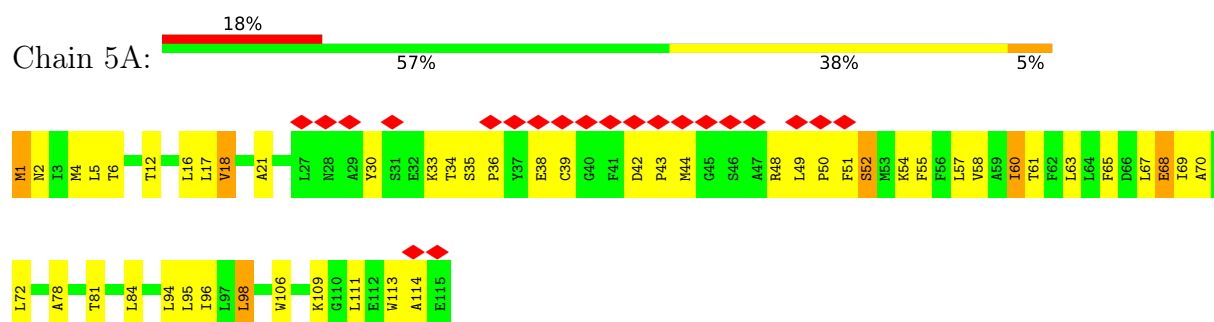
3 Residue-property plots [i](#)

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

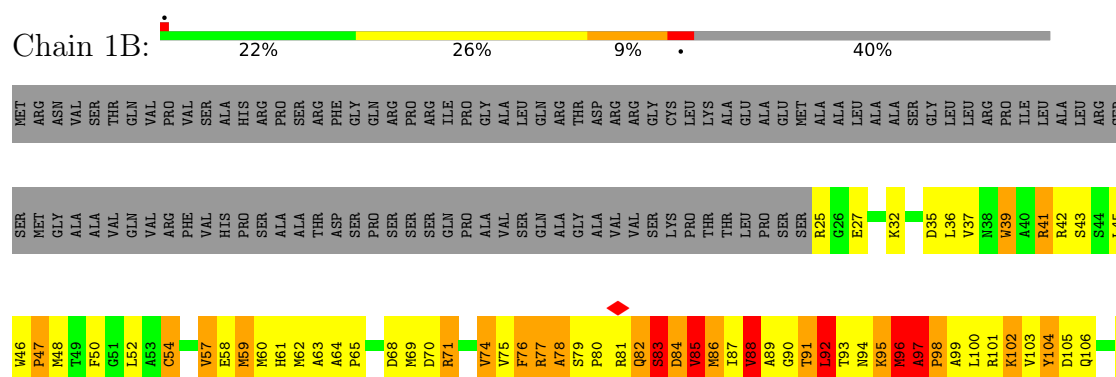
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

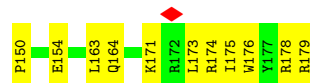
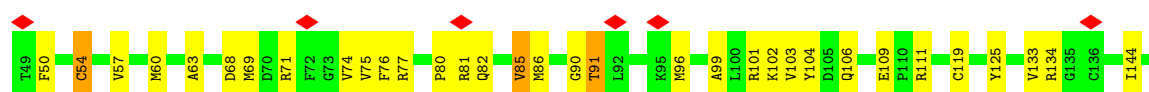
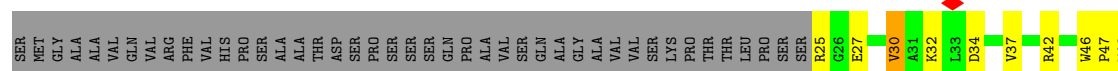


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

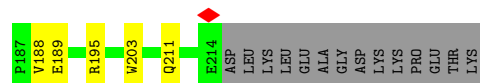
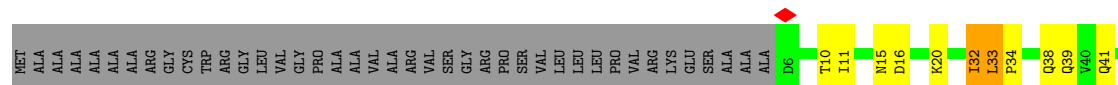




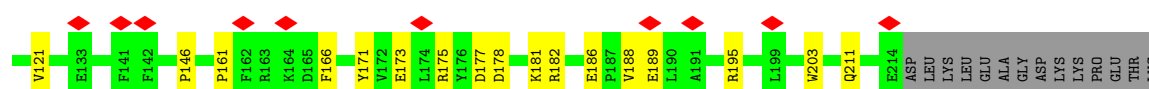
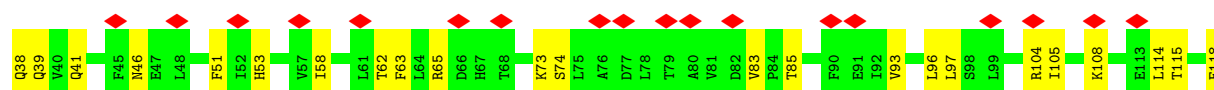
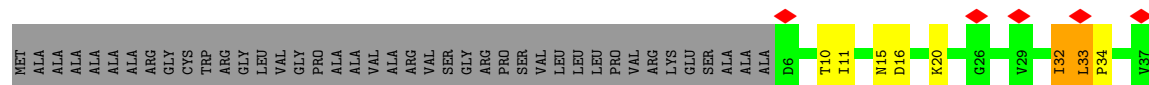
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



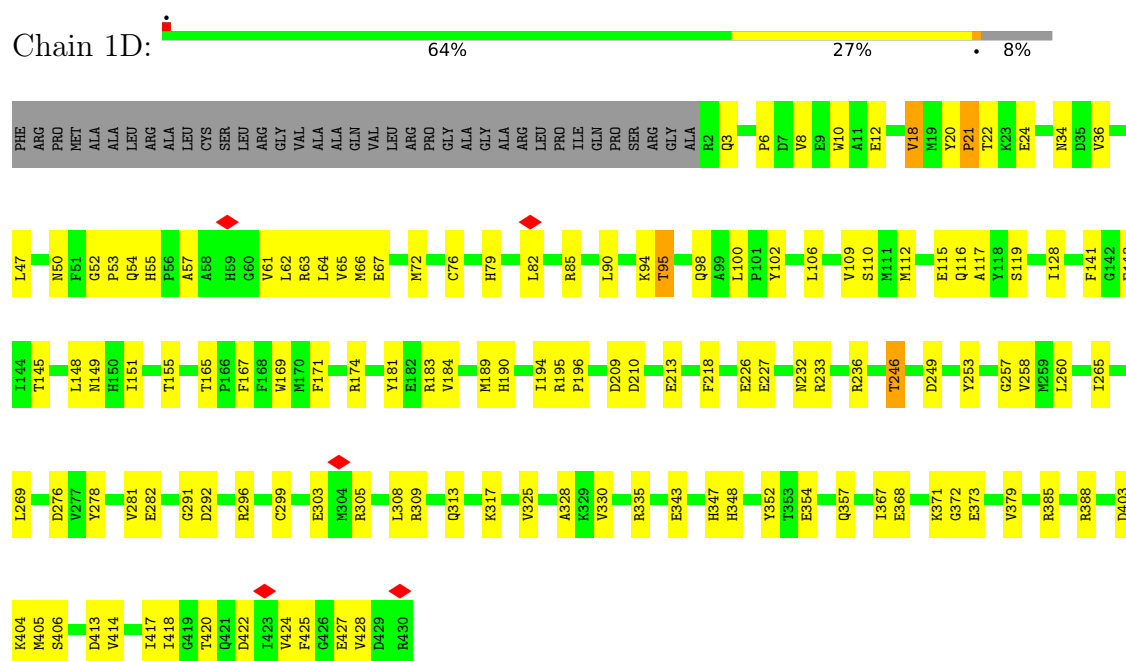
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



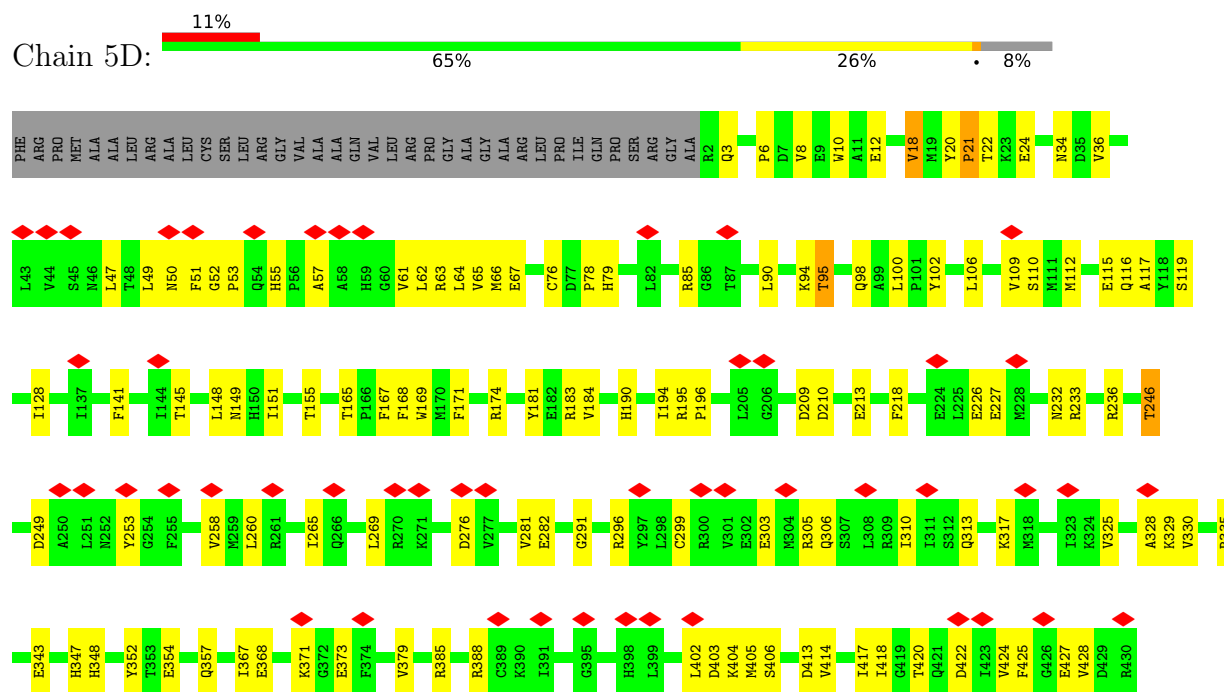
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



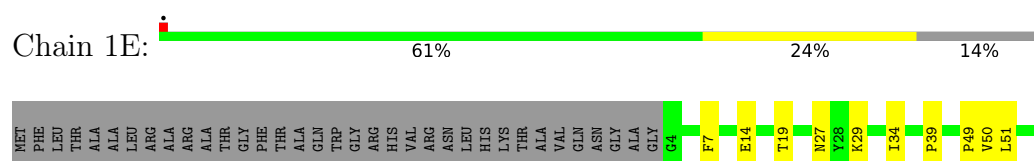
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

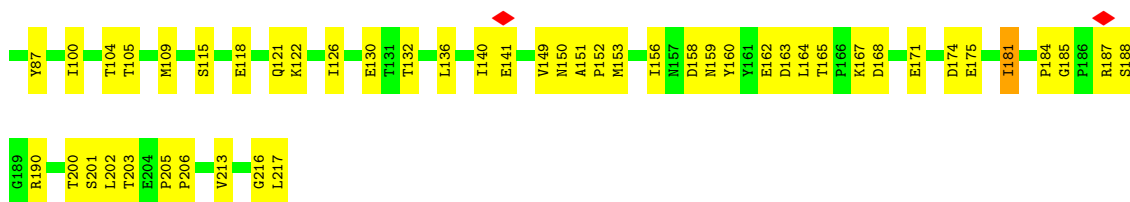


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

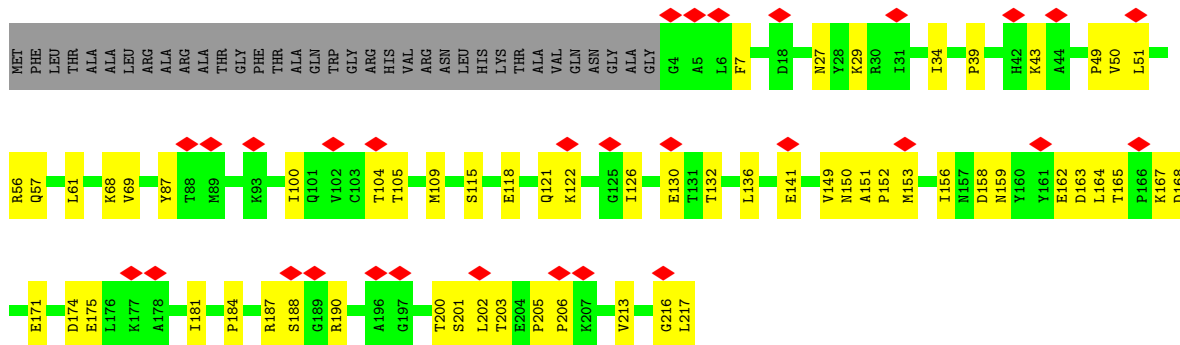


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

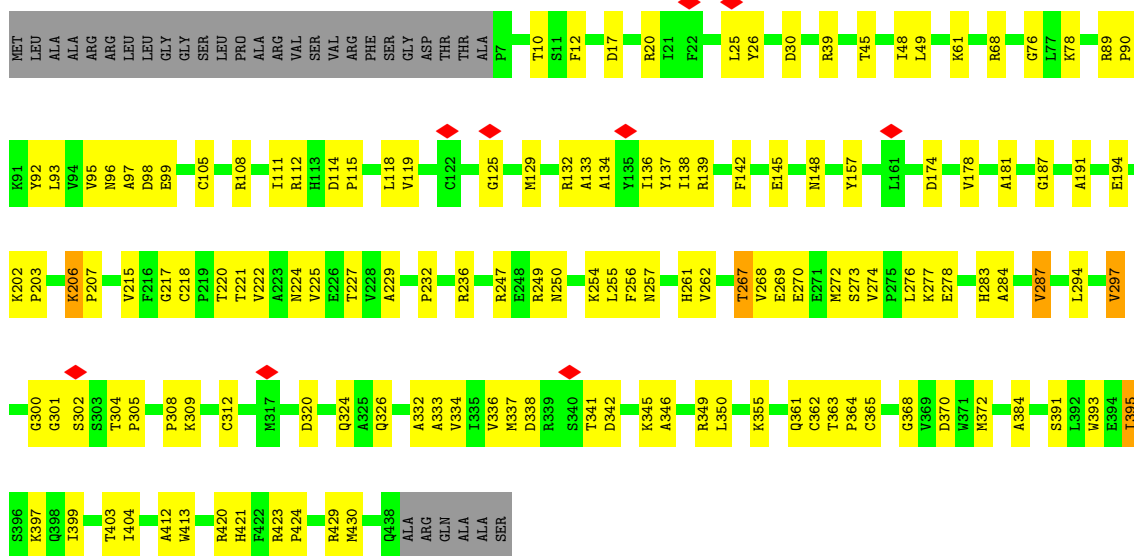




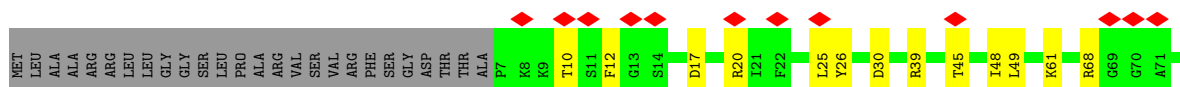
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

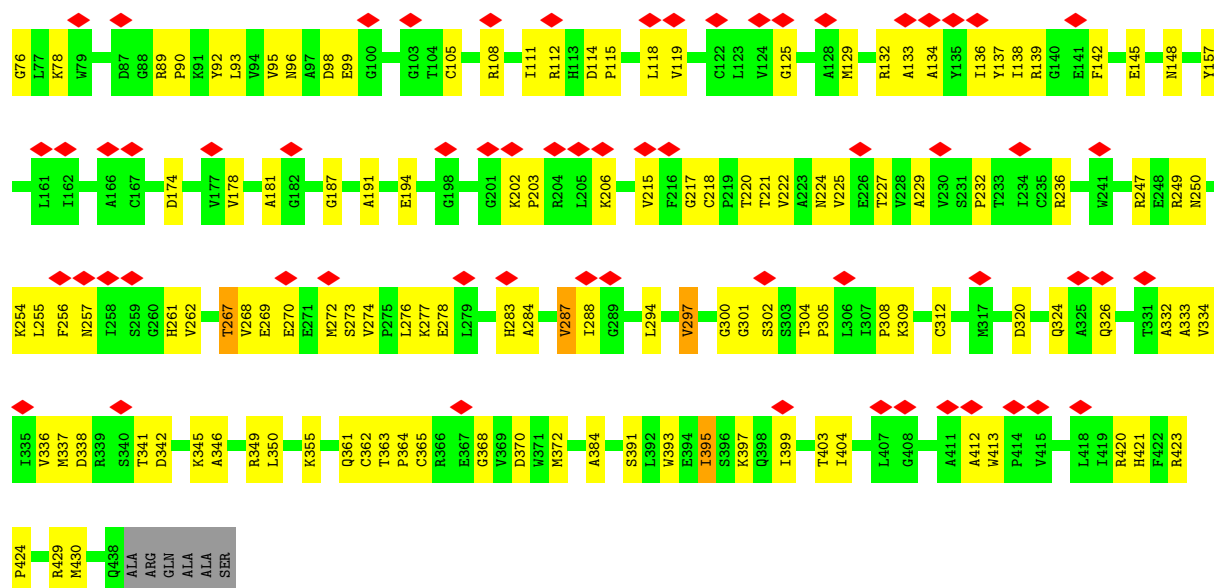


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



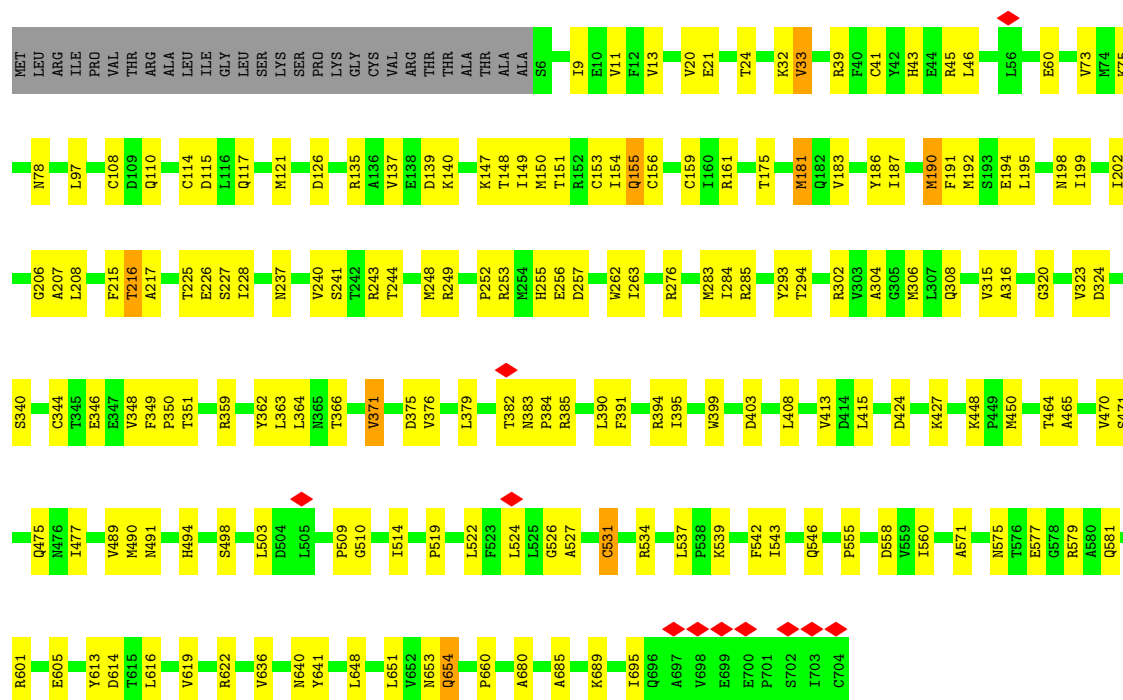
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





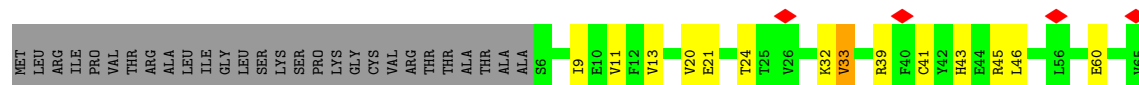
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

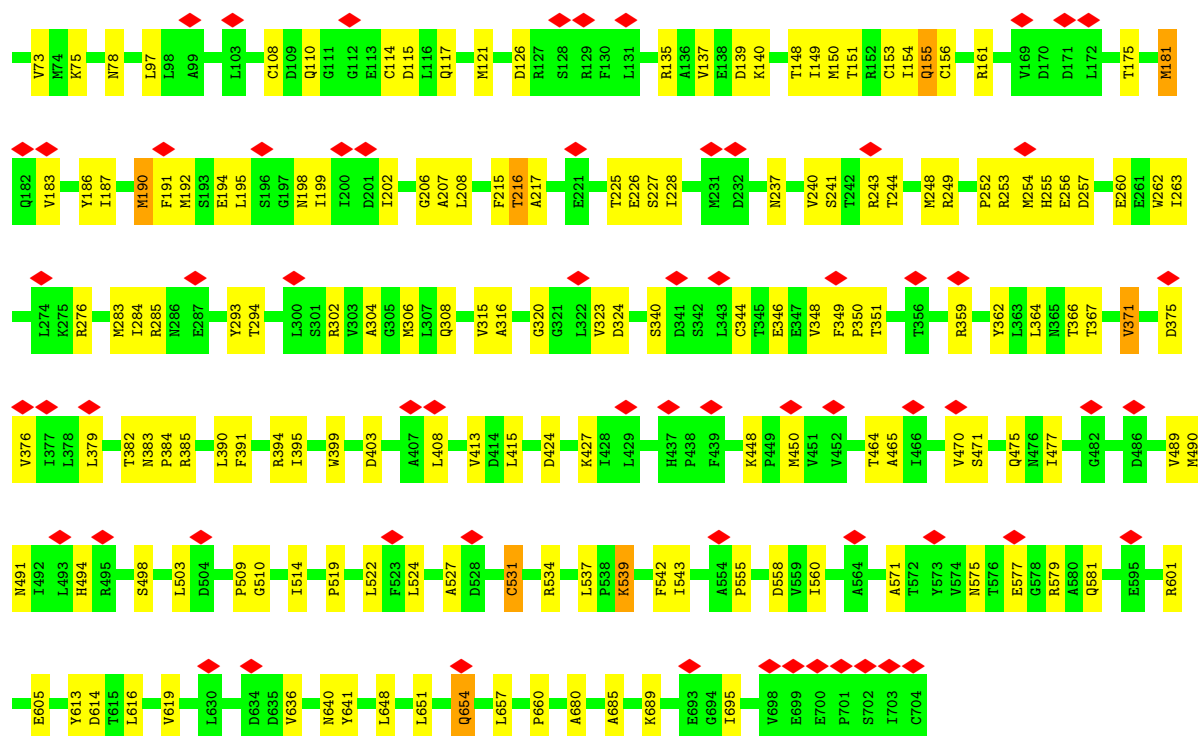
Chain 1G: 72% 24%



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

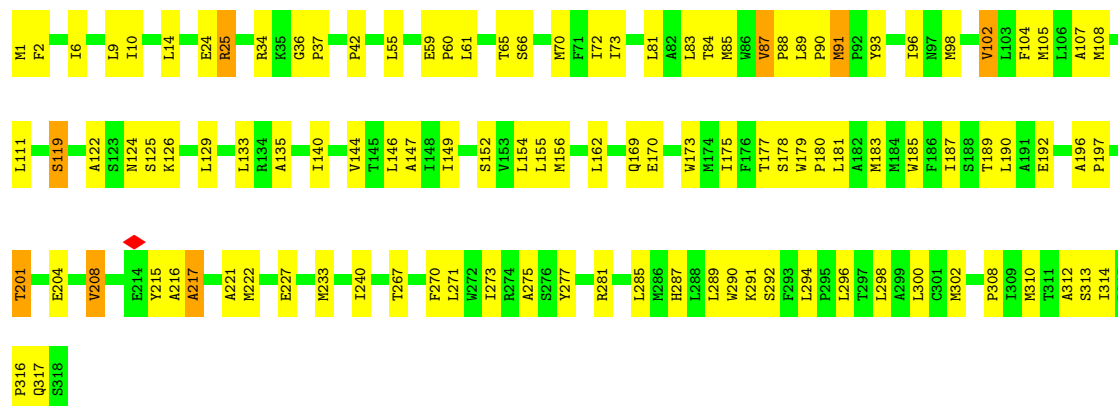
Chain 5G: 9% 72% 23%





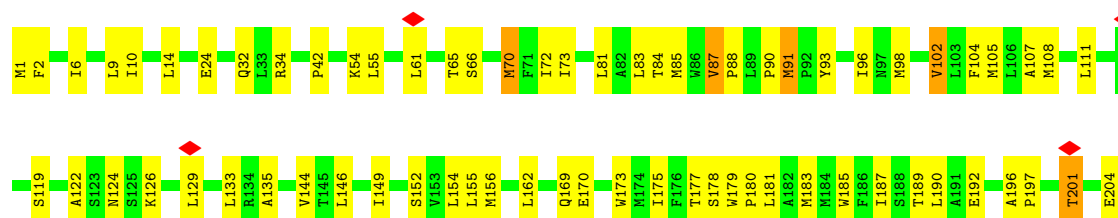
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H: 65% 32% .



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

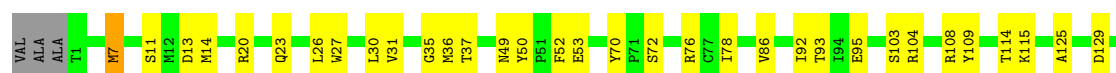
Chain 5H: 68% 30% .





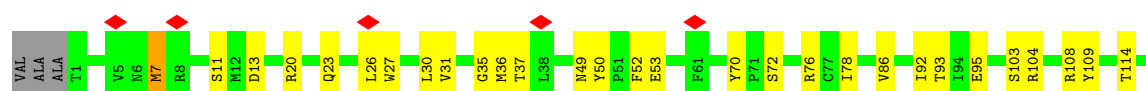
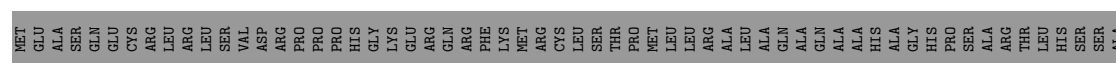
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 53% 20% 26%



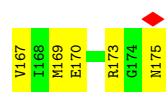
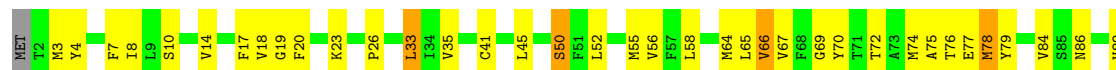
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 5I: 54% 19% 26%



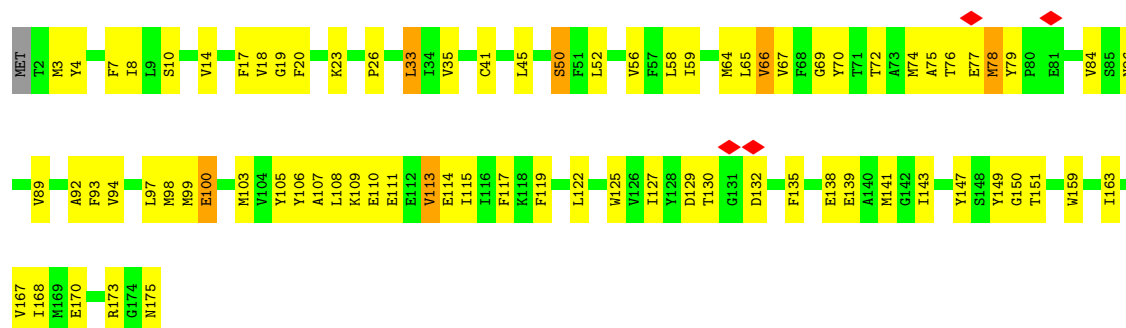
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J: 54% 42% 4%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 5J: 54% 42% 4%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K: 66% 33%



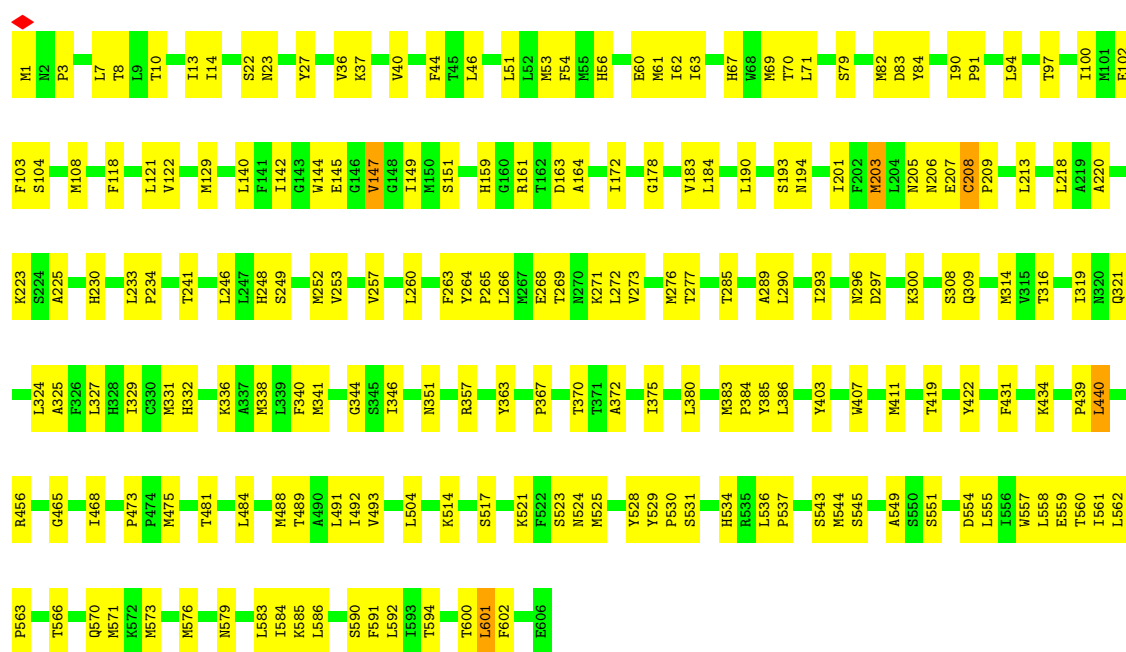
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 5K: 66% 32%



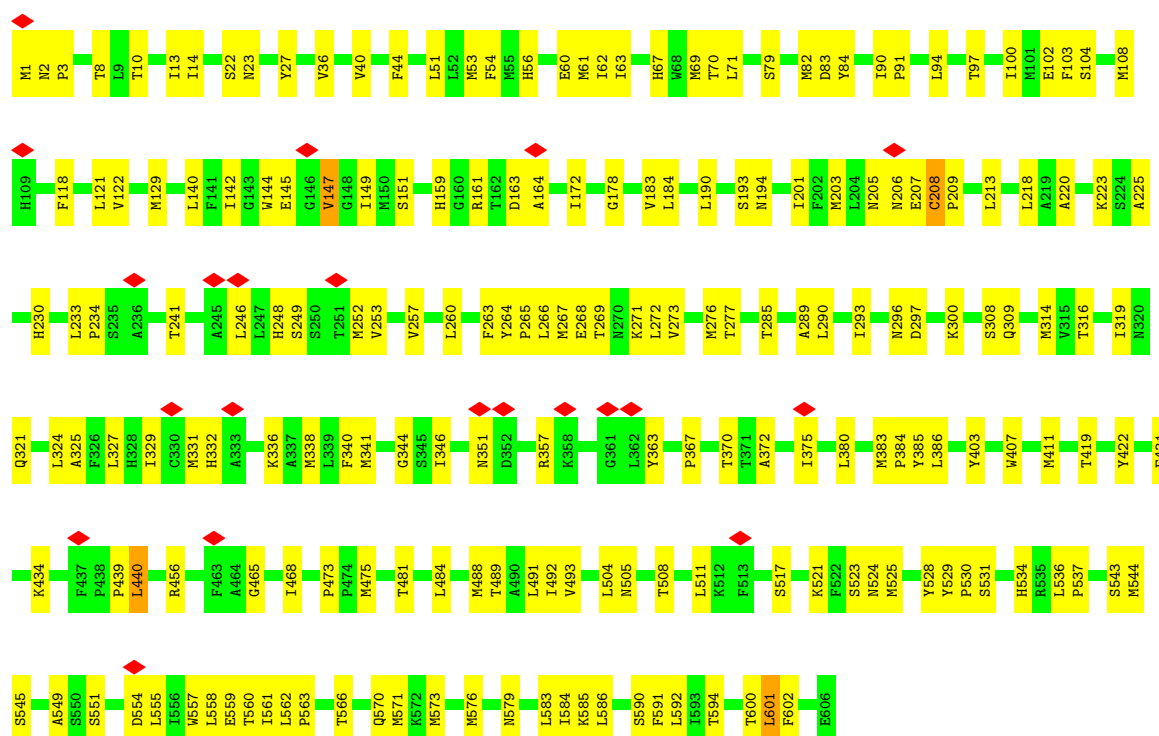
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L: 67% 32%



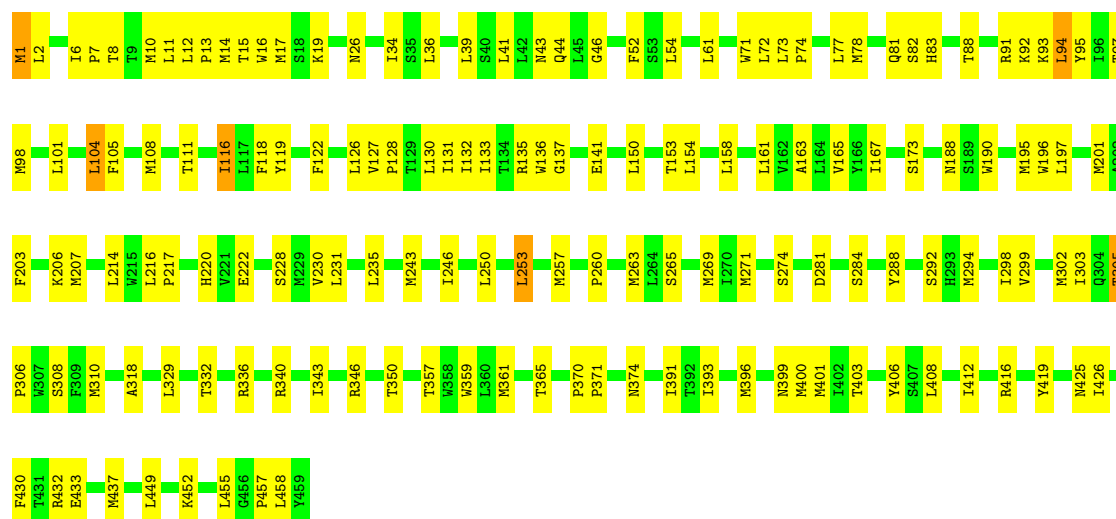
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 5L:  67% 32%



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

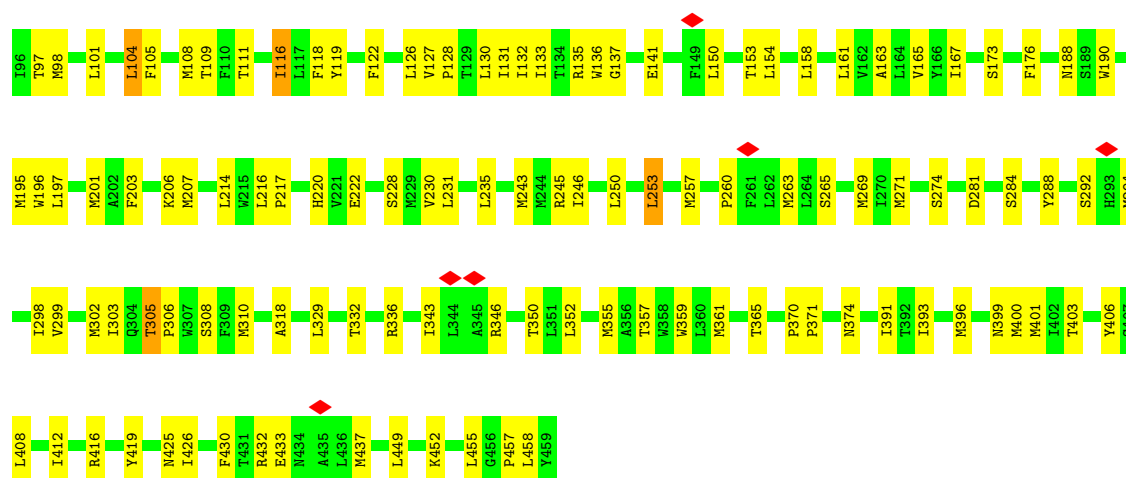
Chain 1M:  67% 32%



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

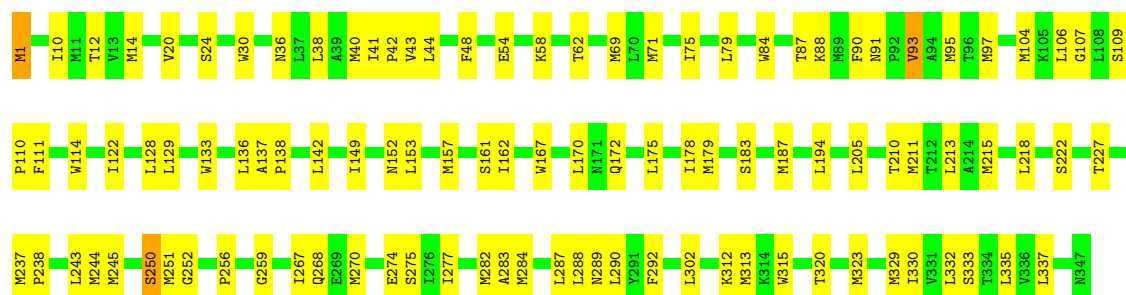
Chain 5M:  66% 33%





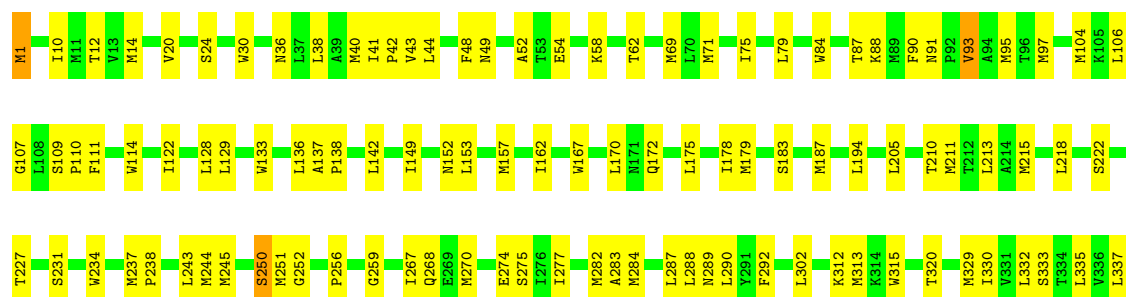
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N: 70% 29%



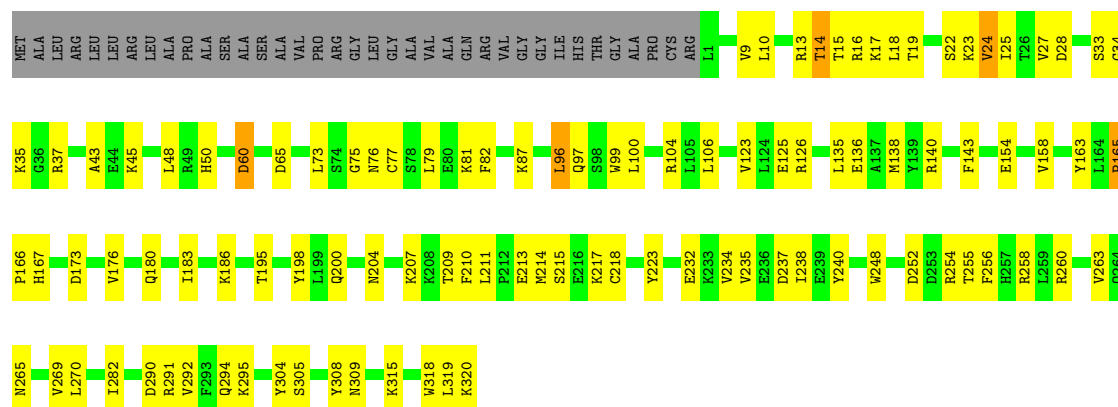
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 5N: 69% 30%

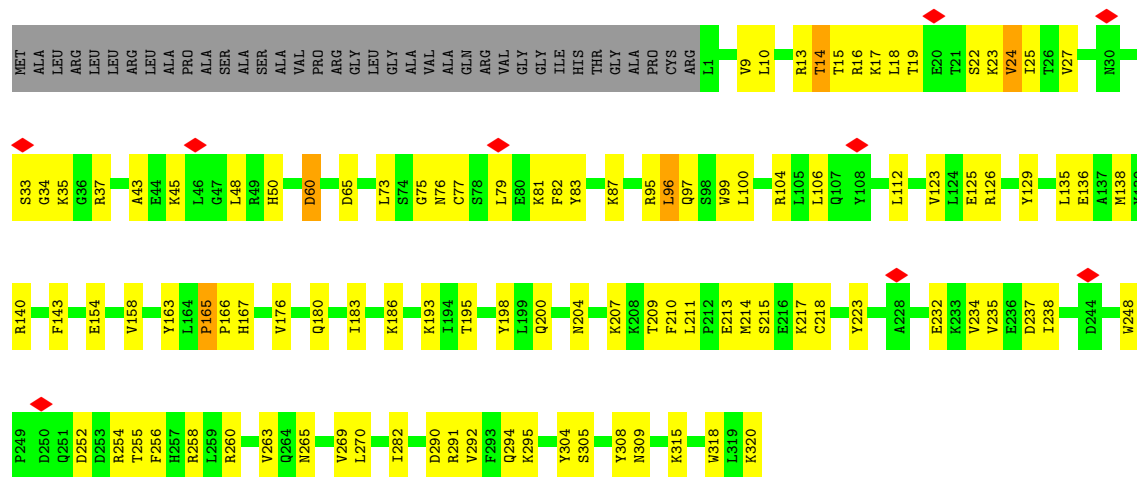


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

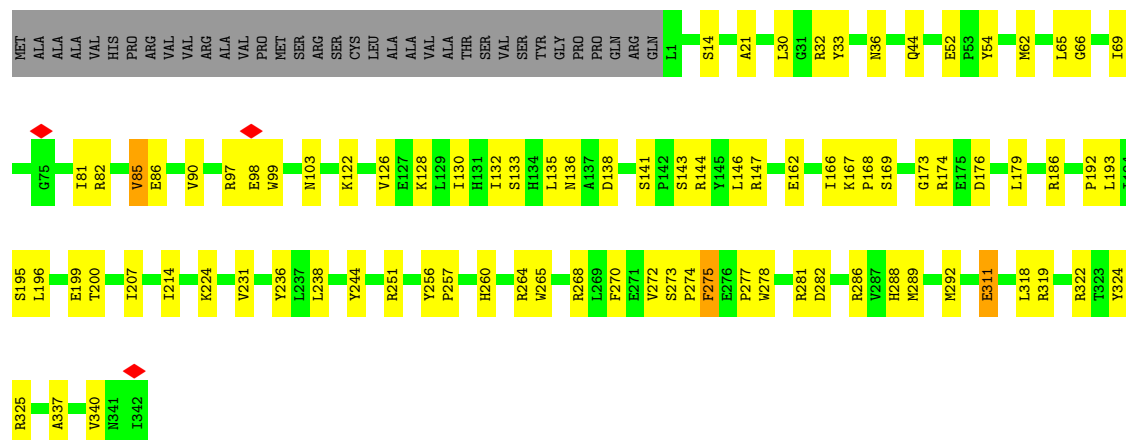
Chain 10: 61% 27% 10%



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

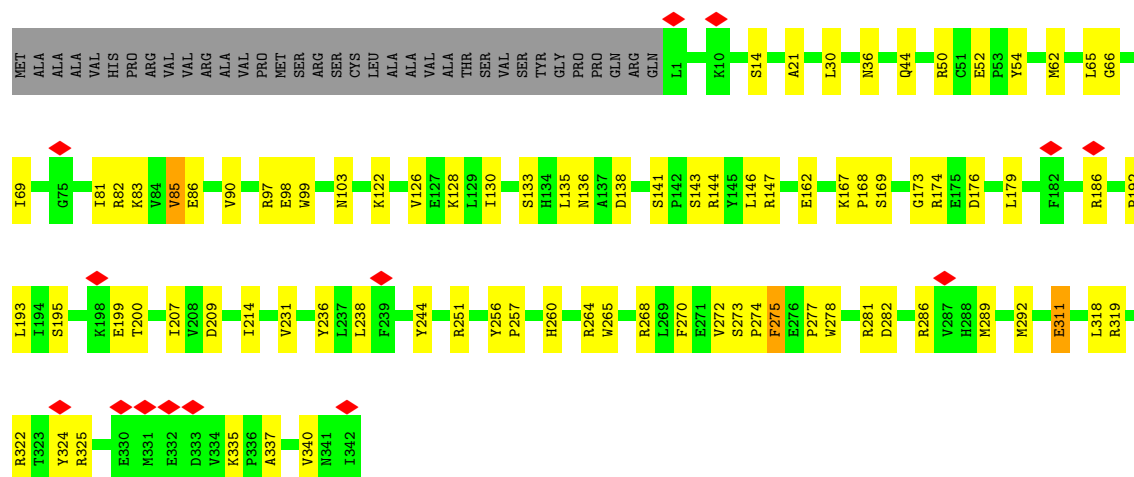


- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



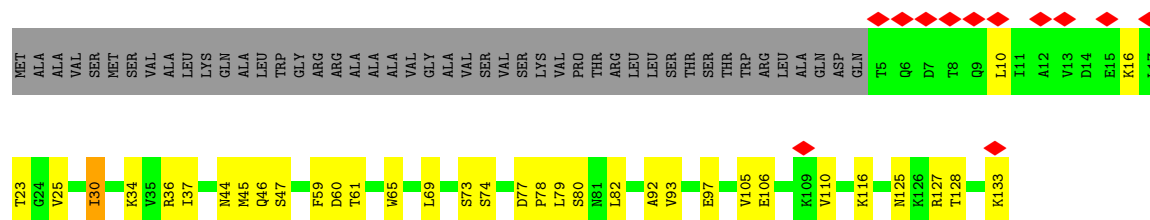
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 5P:  68% 21% 9%



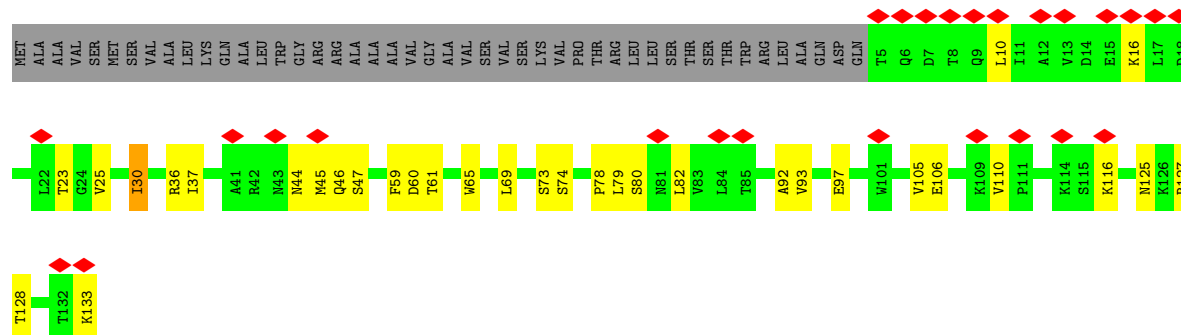
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:  7% 54% 19% 26%



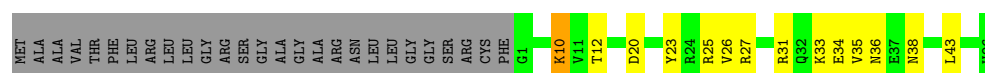
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 5Q:  15% 55% 18% 26%



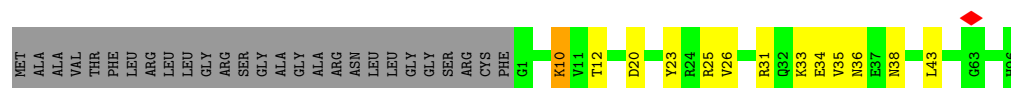
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:  67% 11% 22%



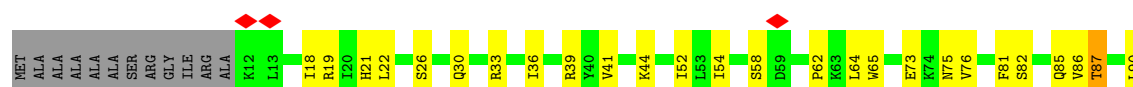
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 5R: 



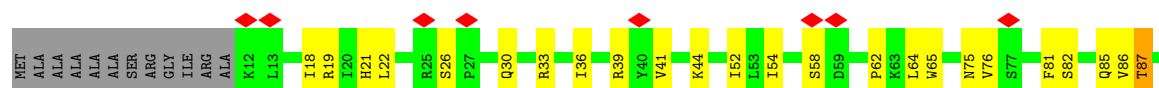
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S: 

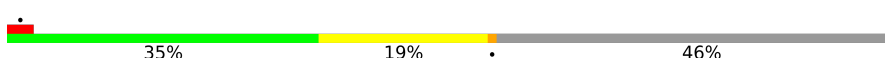


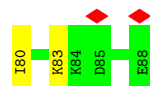
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 5S: 



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

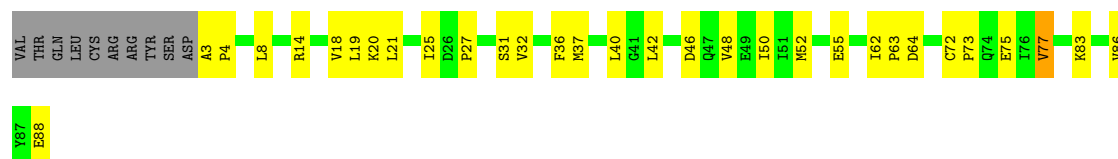
Chain 1T: 



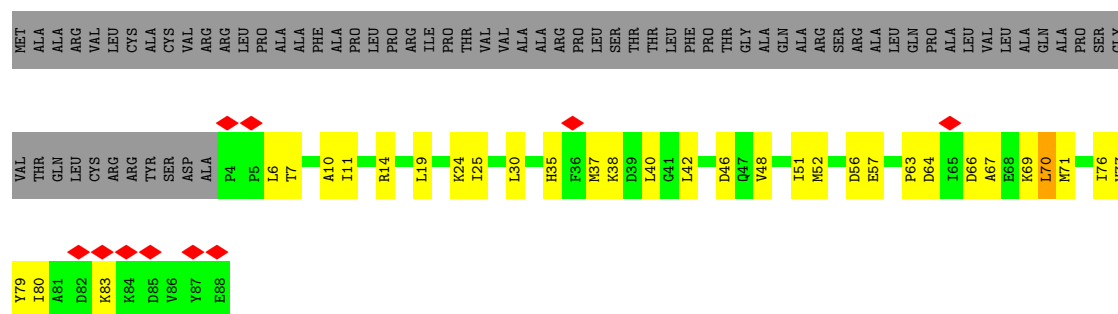
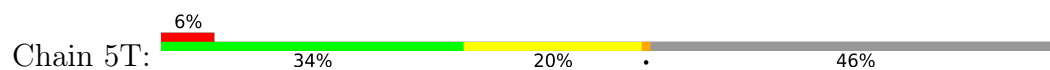
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1U: 

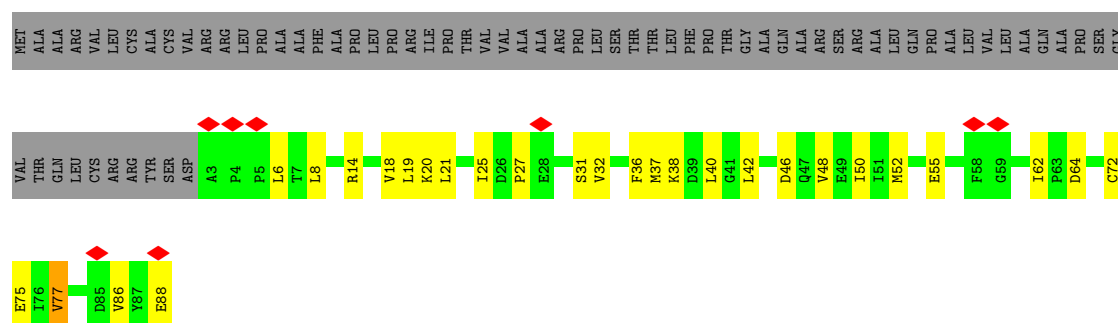
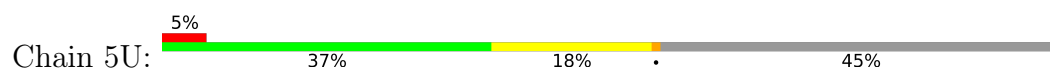




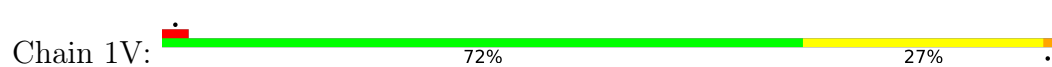
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



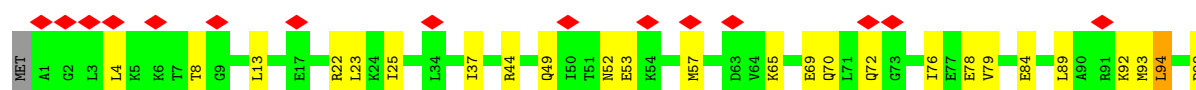
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



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



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





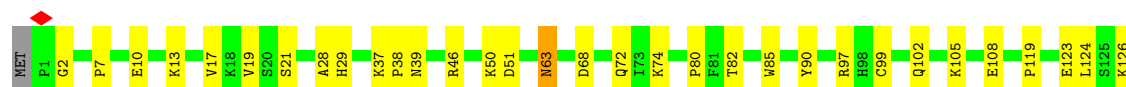
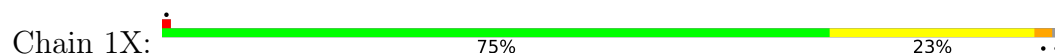
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



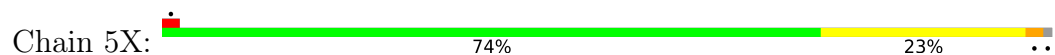
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

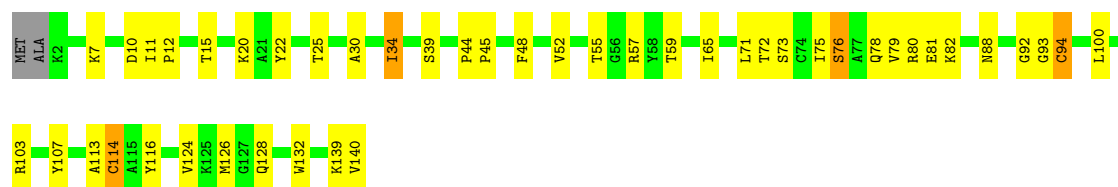


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



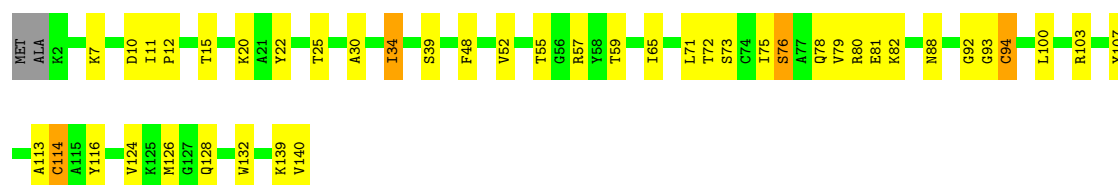
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y:  67% 29% ..



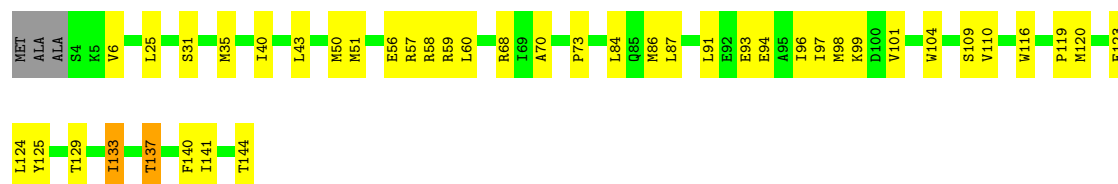
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 5Y:  68% 28% ..



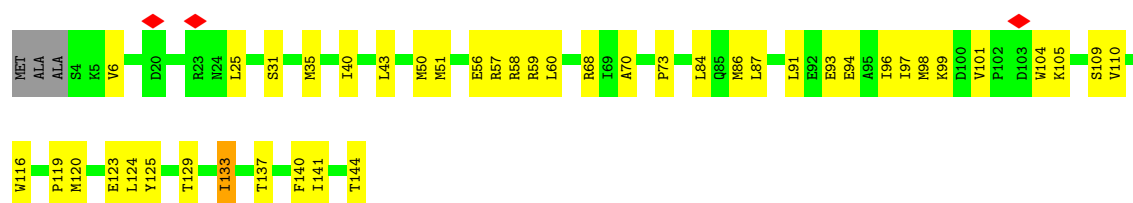
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:  69% 28% ..



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 5Z:  68% 29% ..



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

Chain 1a:  70% 30%

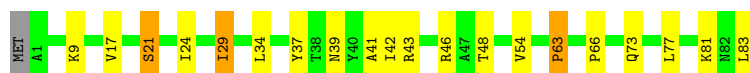


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 5a:  73% 27%



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



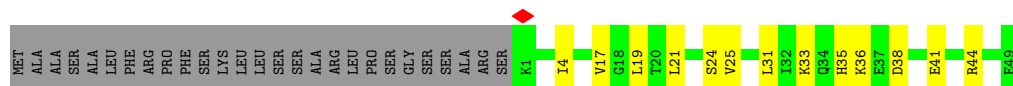
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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



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



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



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



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



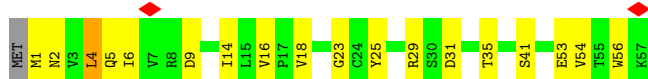
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



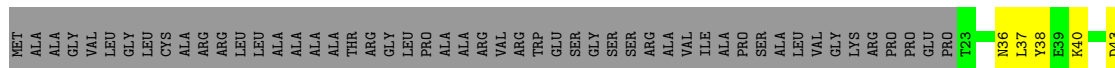
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



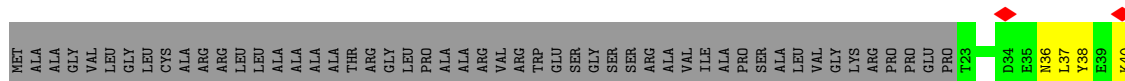
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



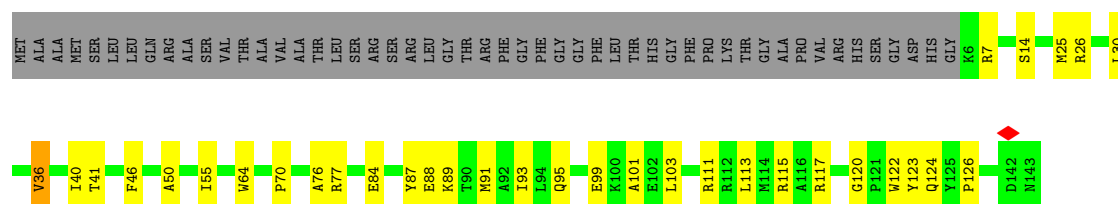
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



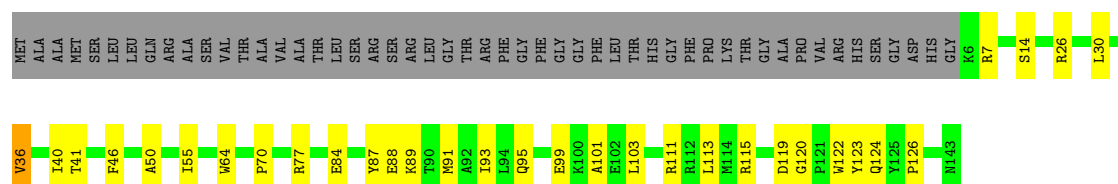
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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



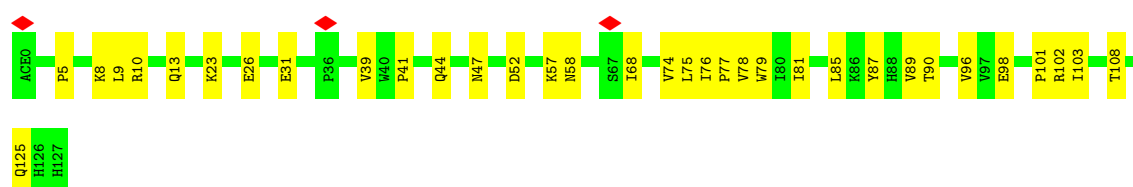
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



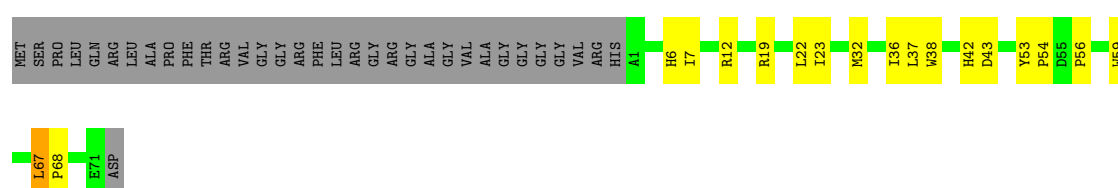
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



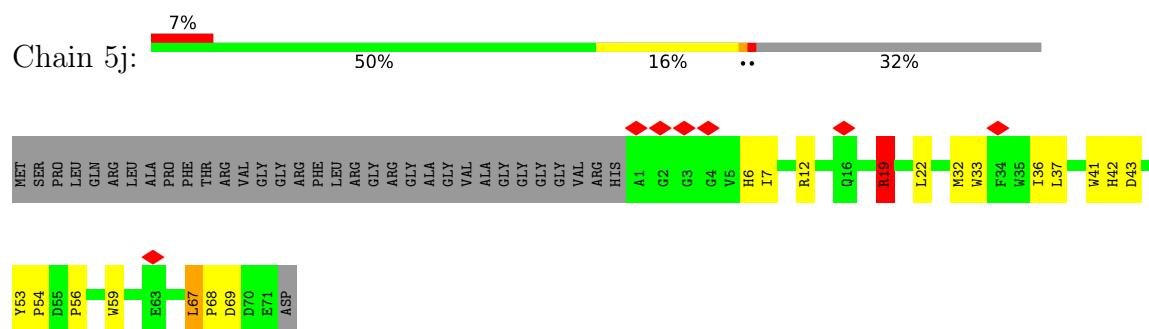
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



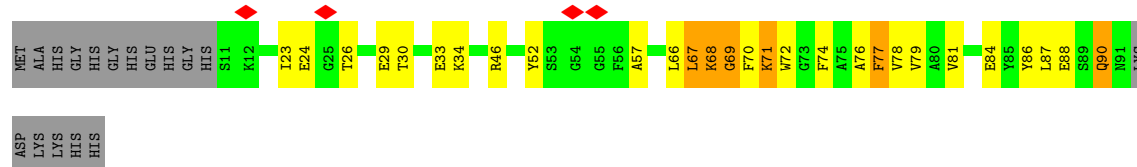
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



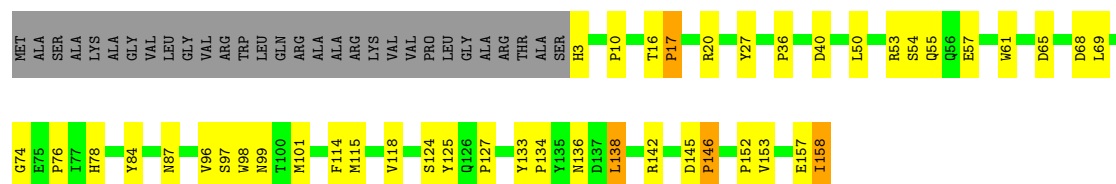
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



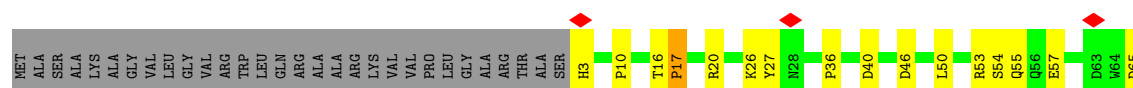
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

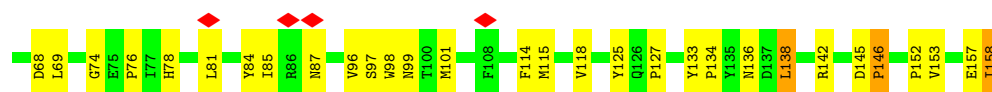


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



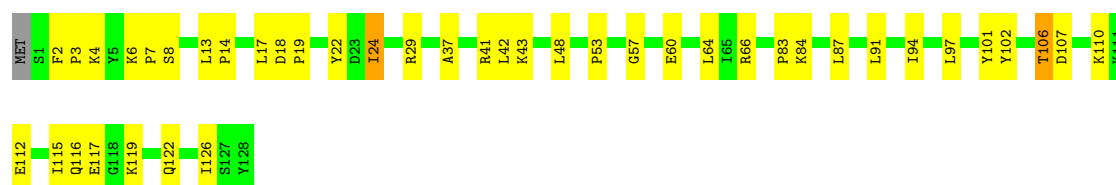
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





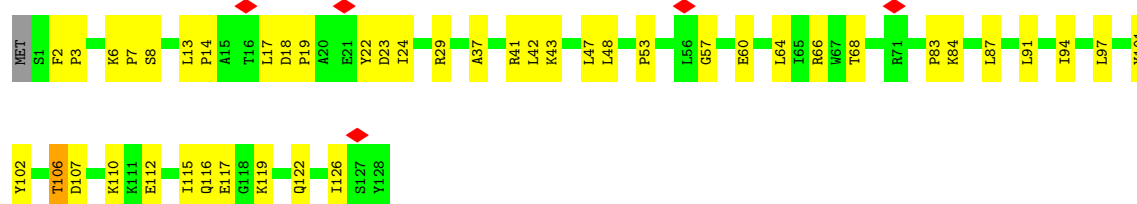
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 67% 31%



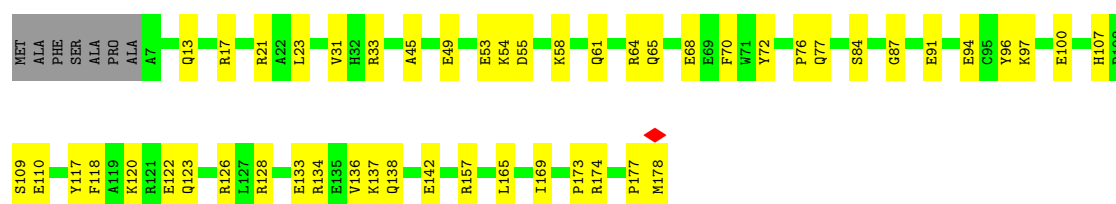
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 5m: 65% 33%



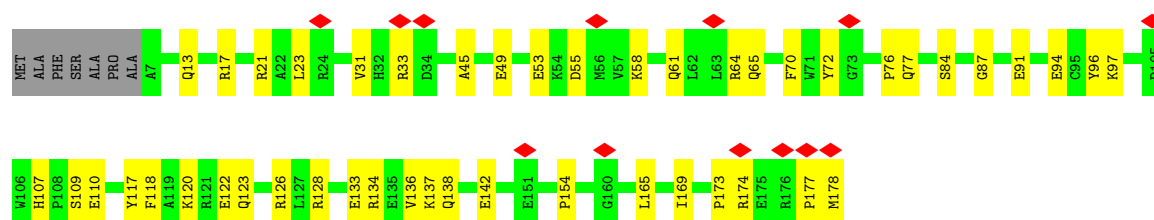
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n: 68% 28%



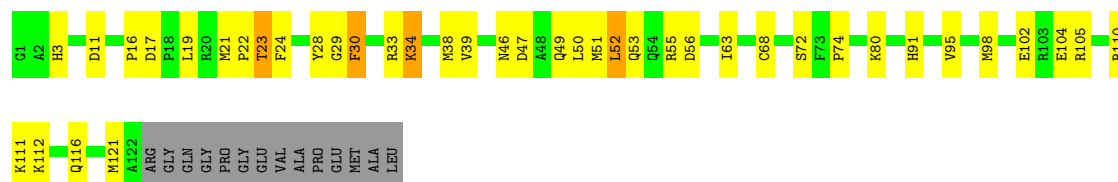
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 5n: 7% 70% 26%

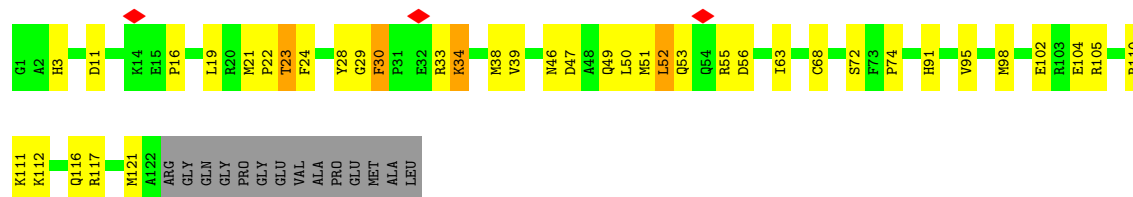


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

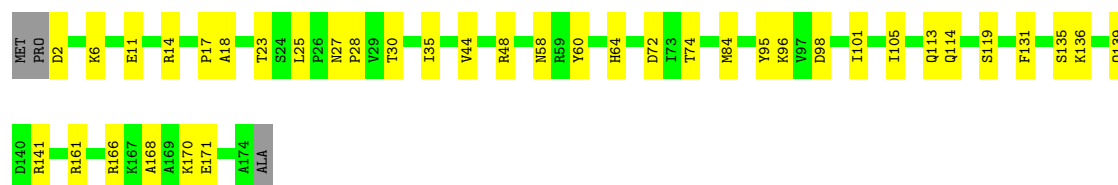
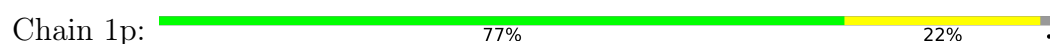
Chain 1o: 60% 27% 10%



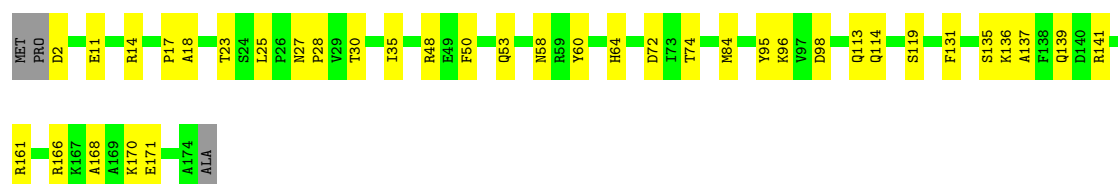
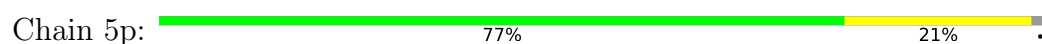
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



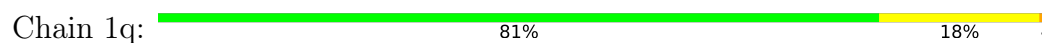
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



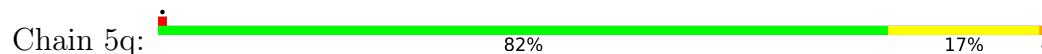
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

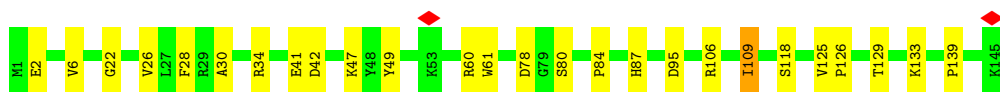


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

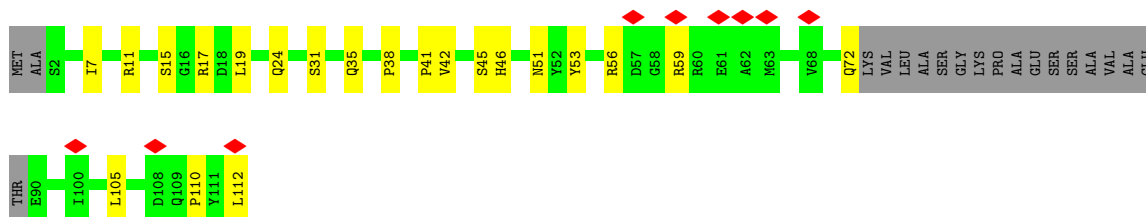




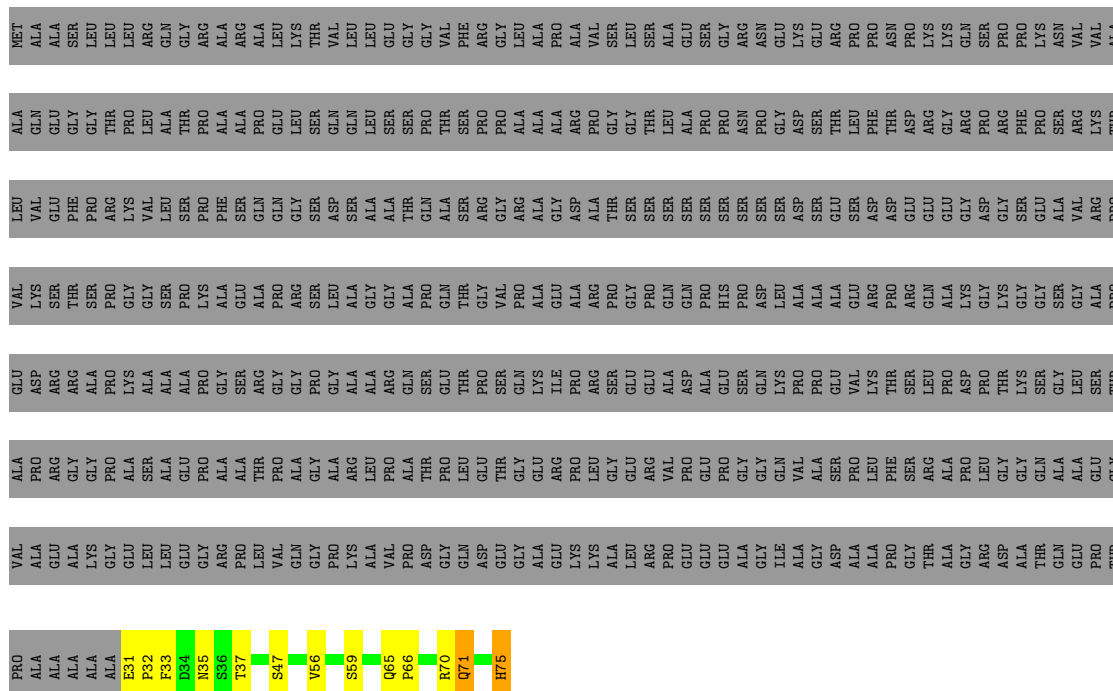
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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

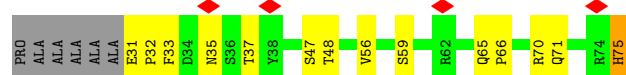


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

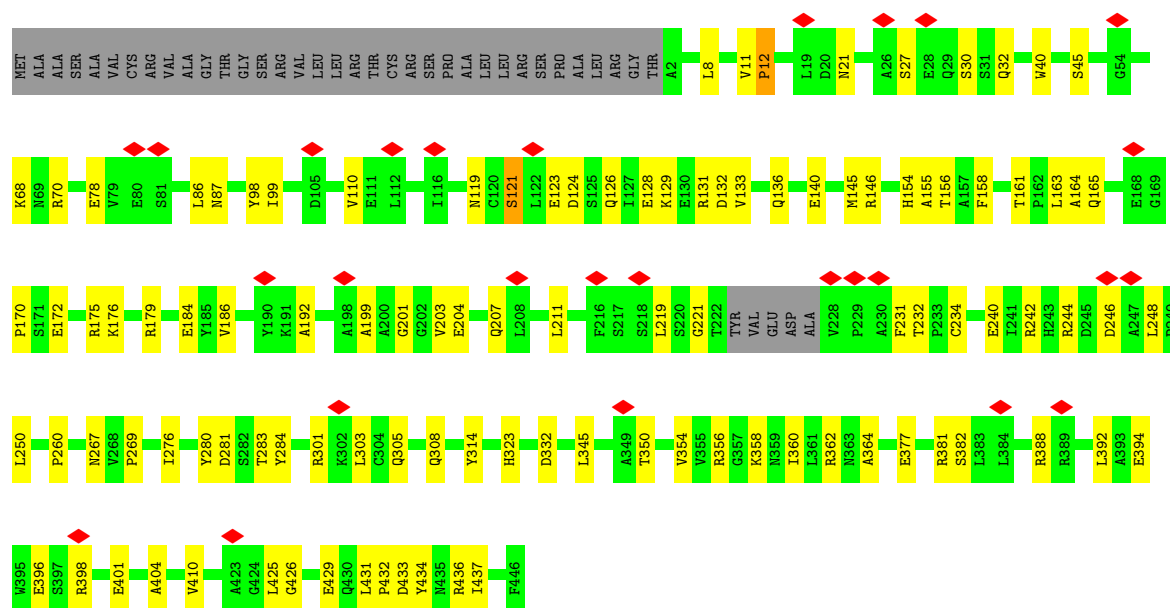


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

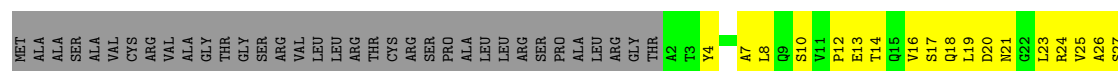


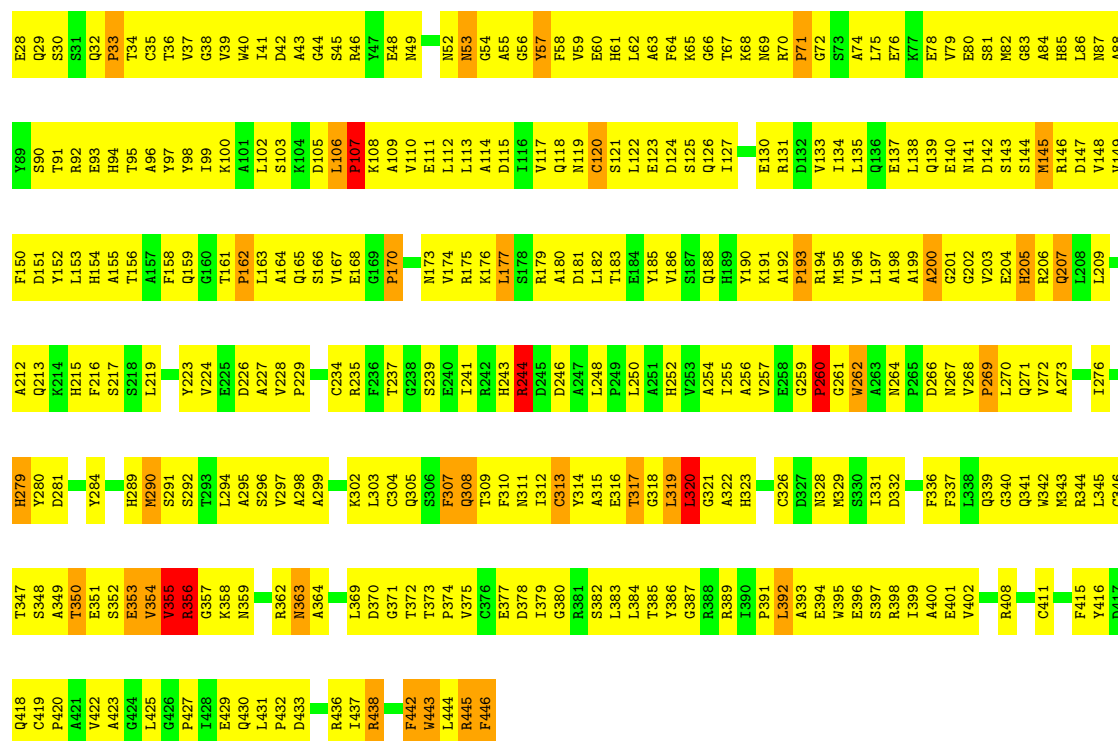


Chain 3A:

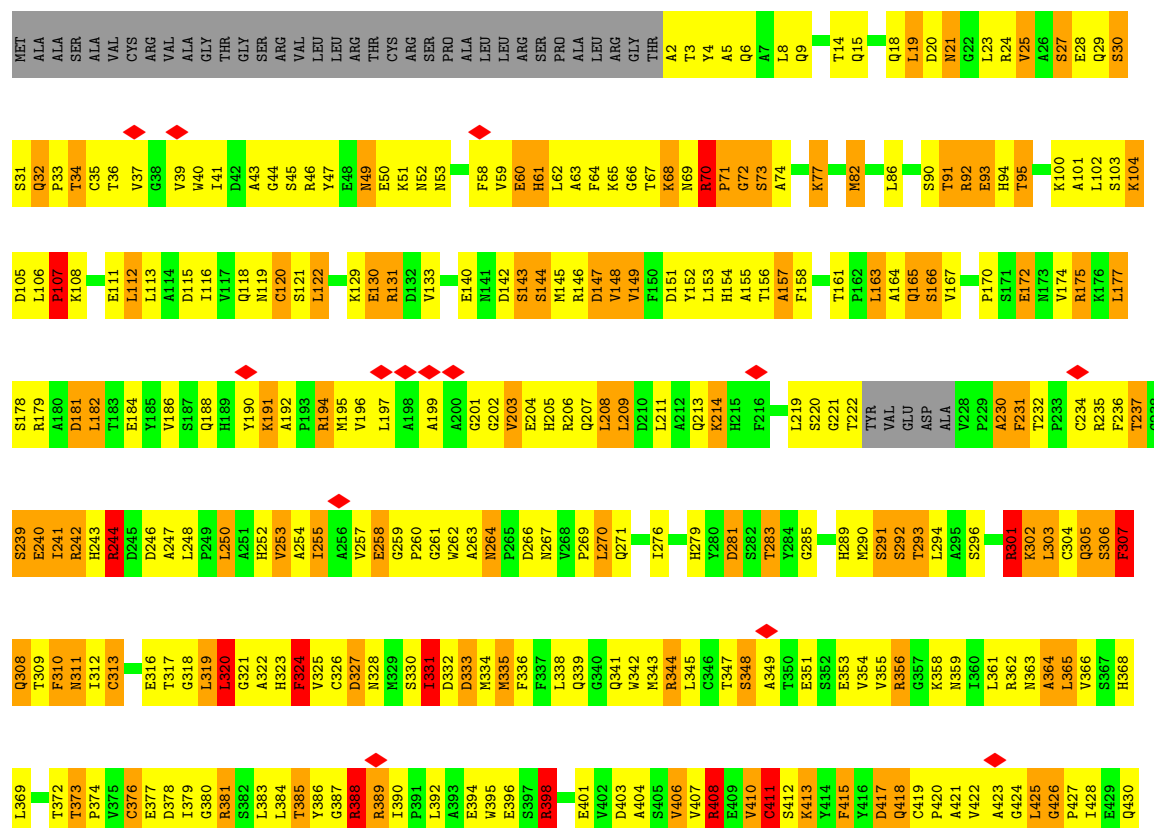
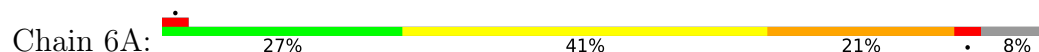


Chain 3N: 22% 62% 7% 7%





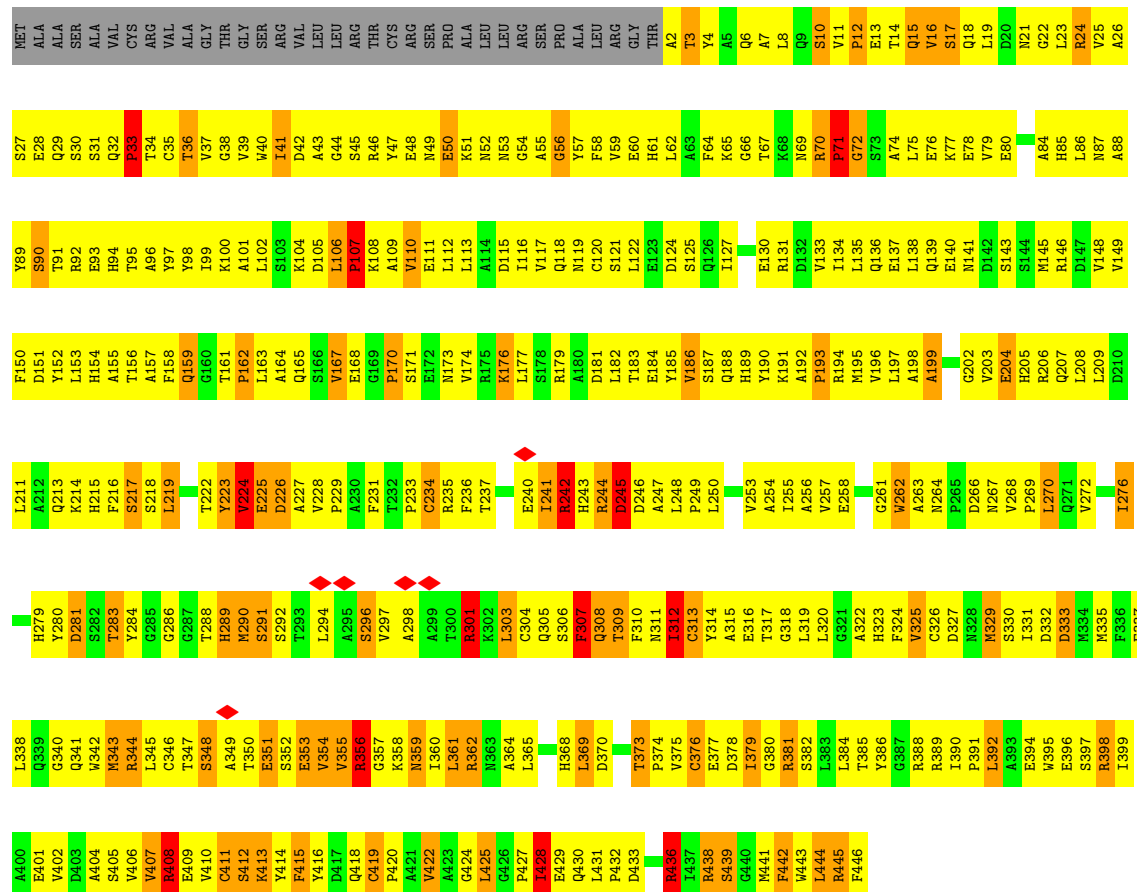
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



L431 P432
D433 Y434
N435 R436
I437 R438
S439 R440
M441 F442
W443 L444
R445 F446

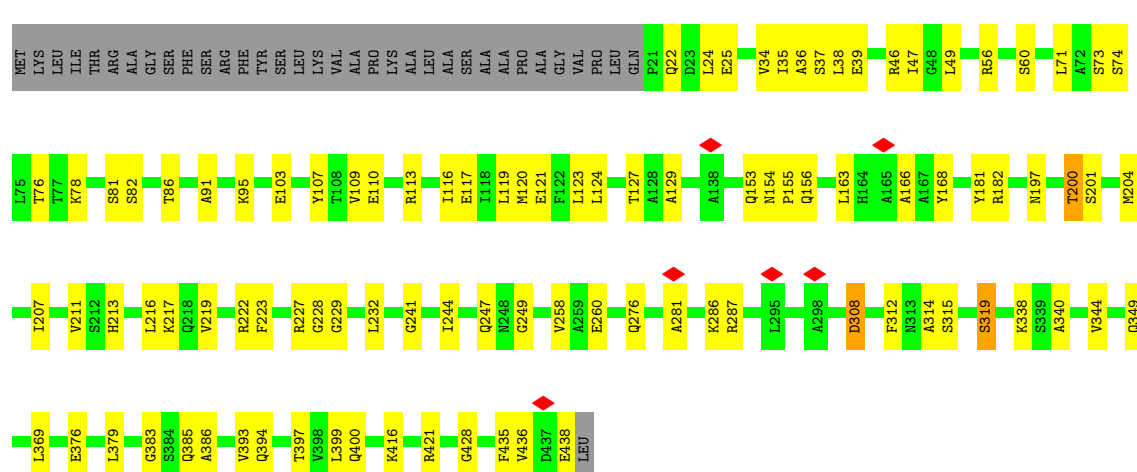
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 6N: 16% 57% 16% 7%

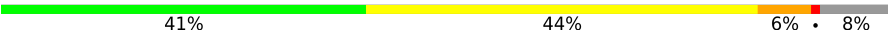


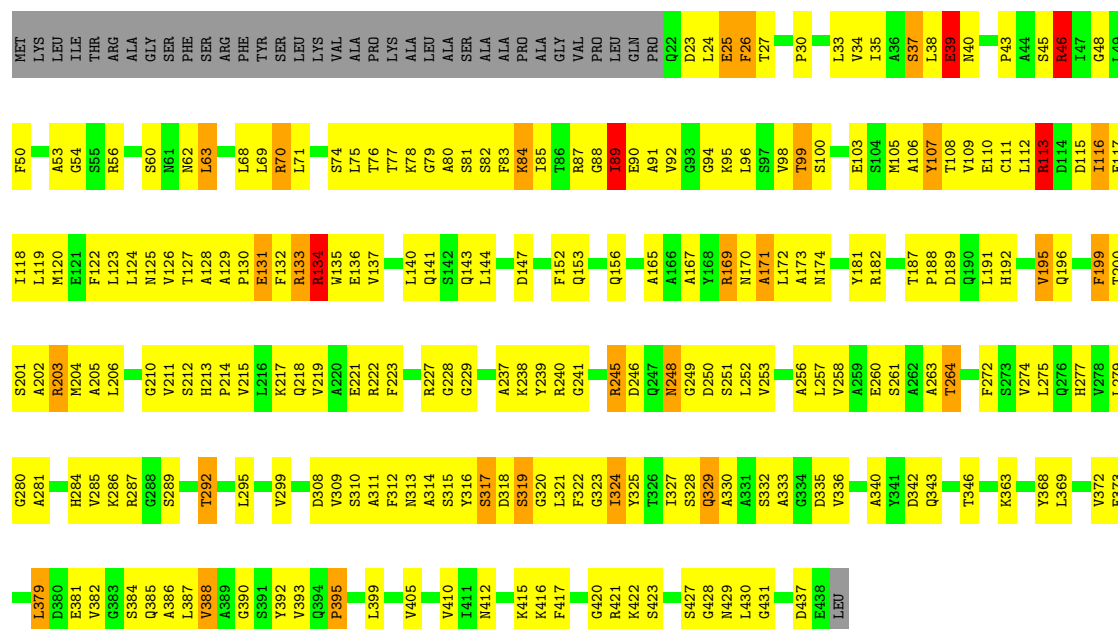
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B: 70% 21% 8%

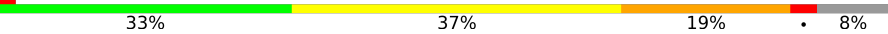


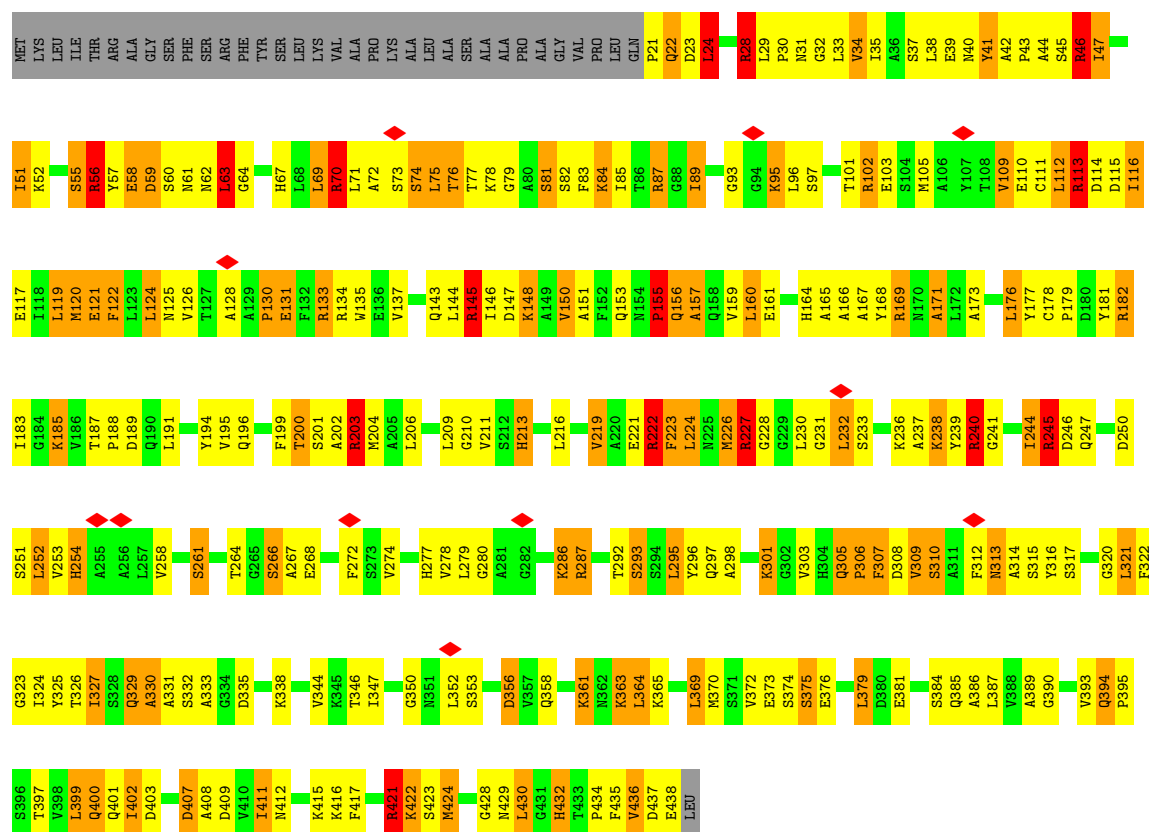
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O: 

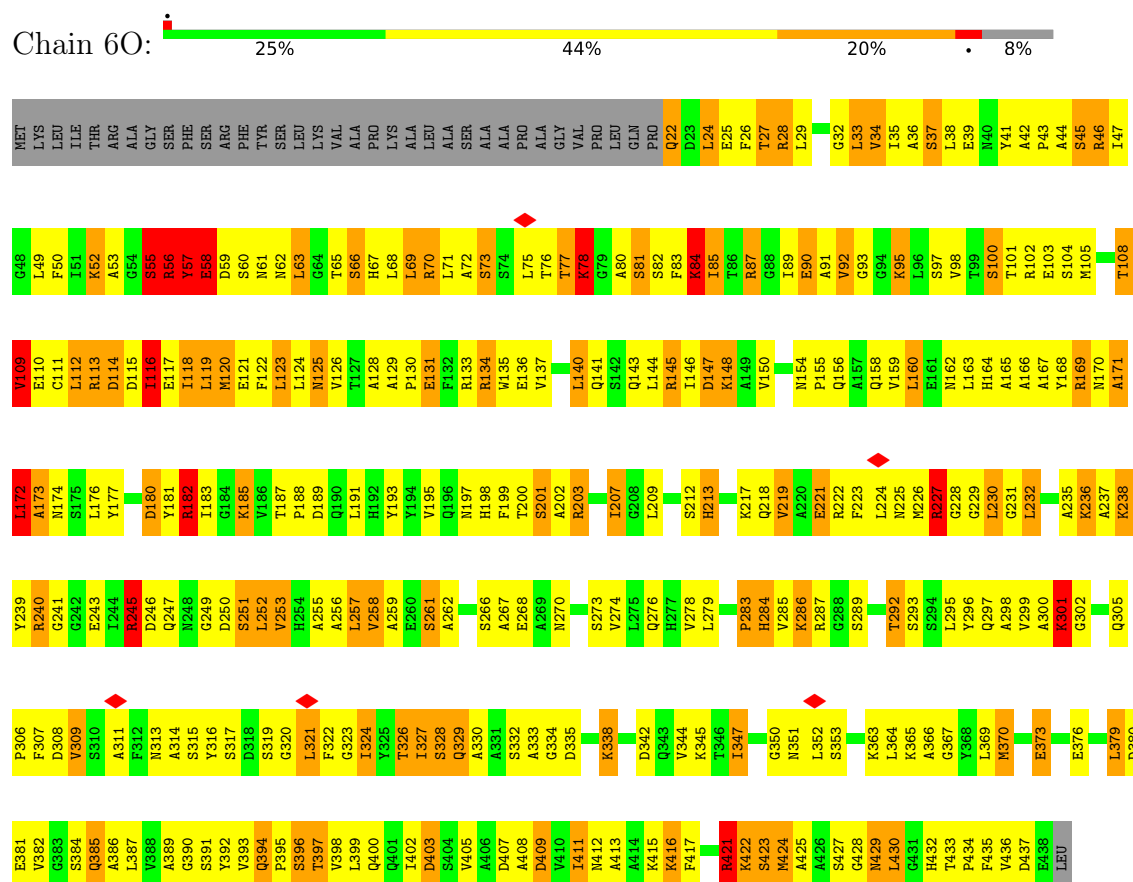


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

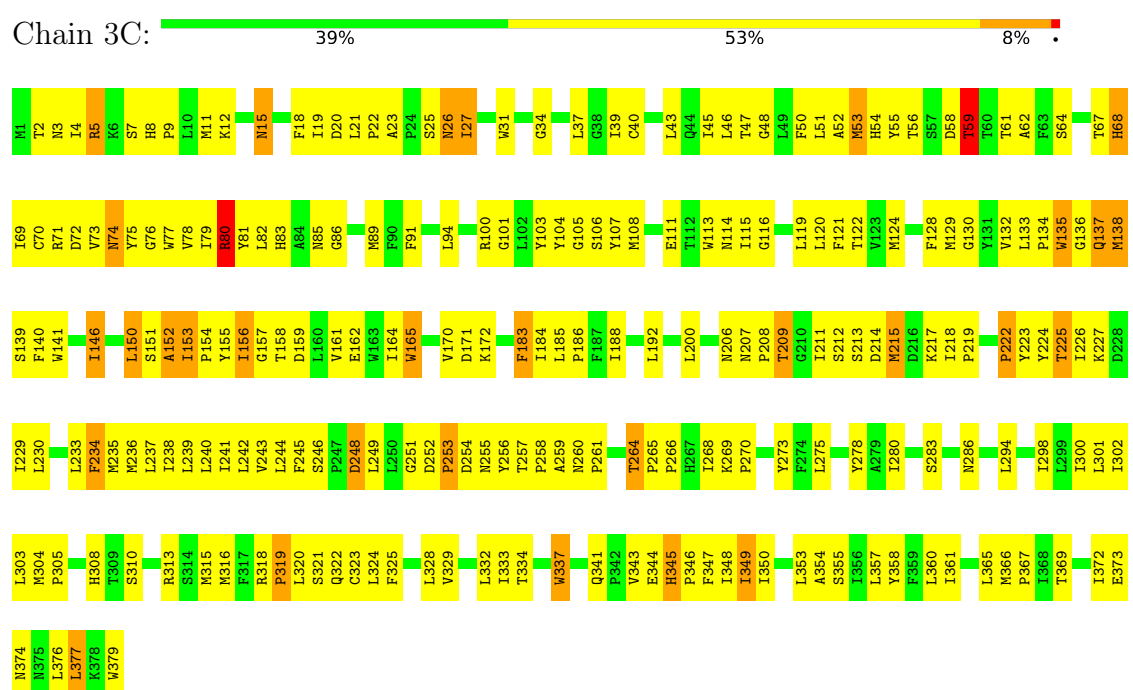
Chain 6B: 



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

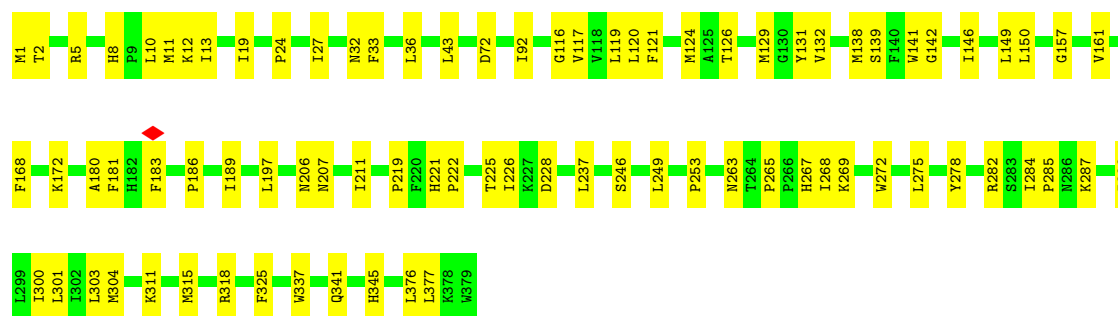


- Molecule 47: Cytochrome b



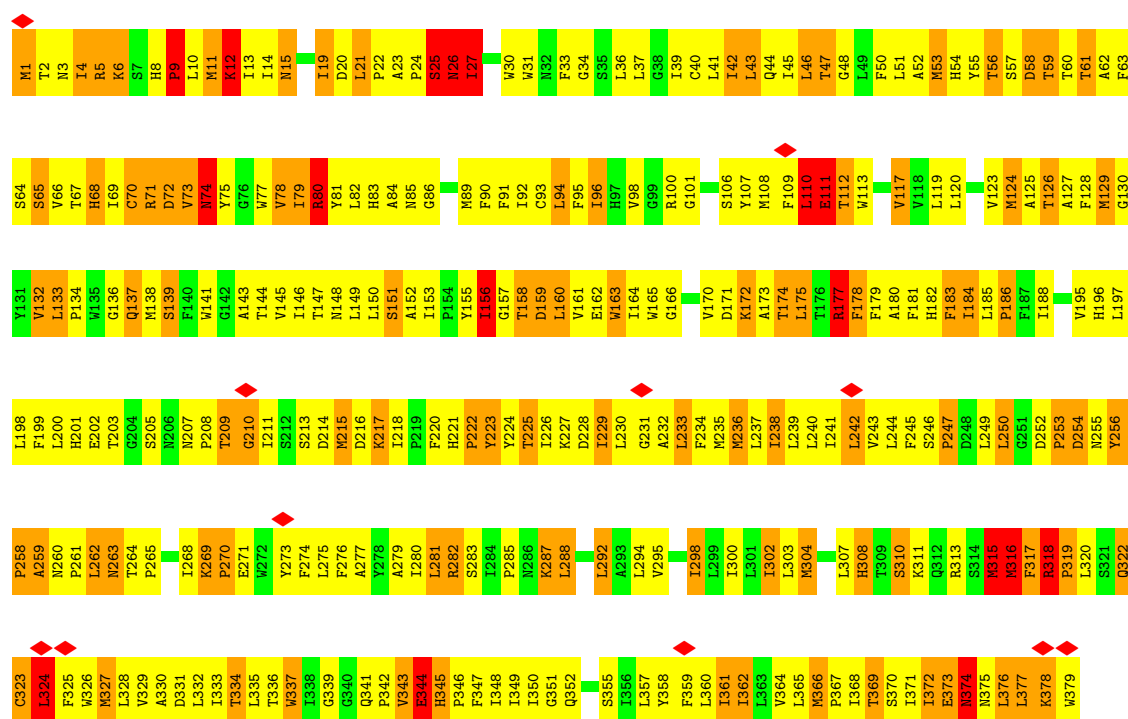
- Molecule 47: Cytochrome b

Chain 3P:  78% 22%



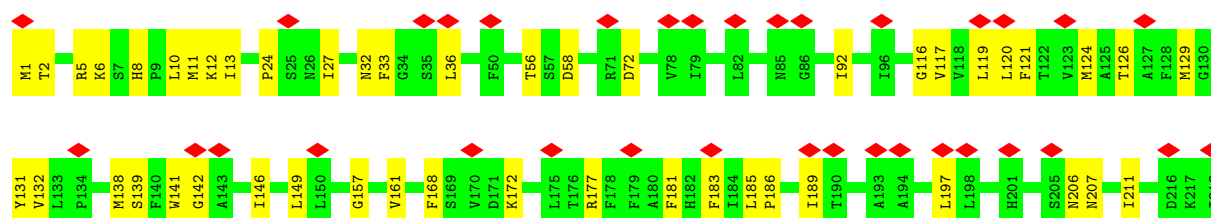
• Molecule 47: Cytochrome b

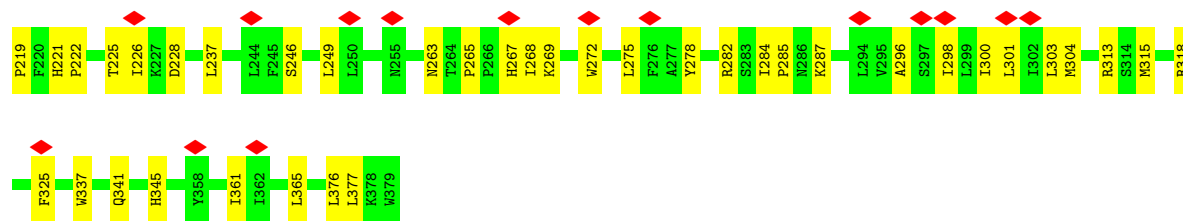
Chain 6C:  19% 50% 26%



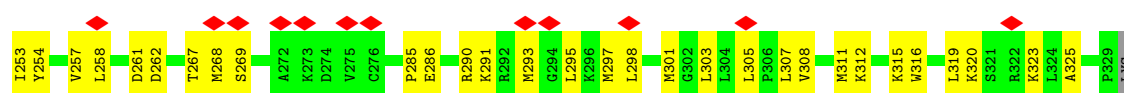
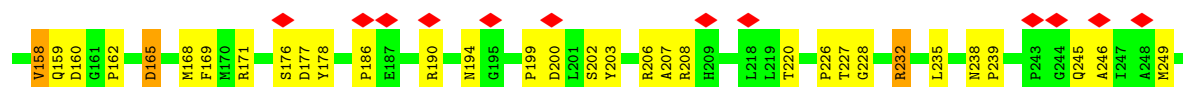
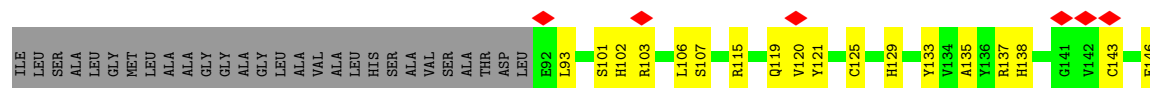
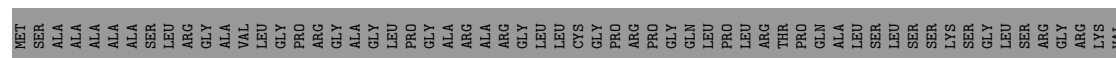
• Molecule 47: Cytochrome b

Chain 6P:  13% 77% 23%

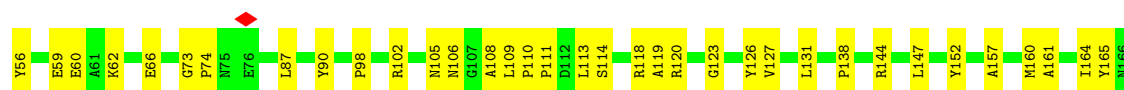
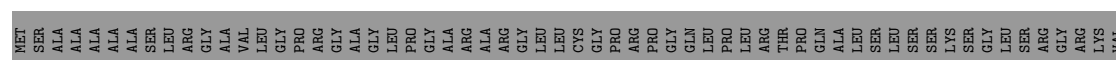




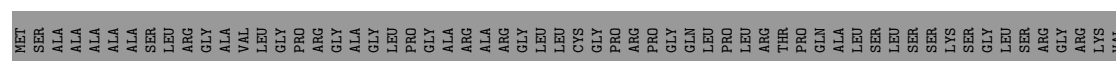
• Molecule 48: Cytochrome c1

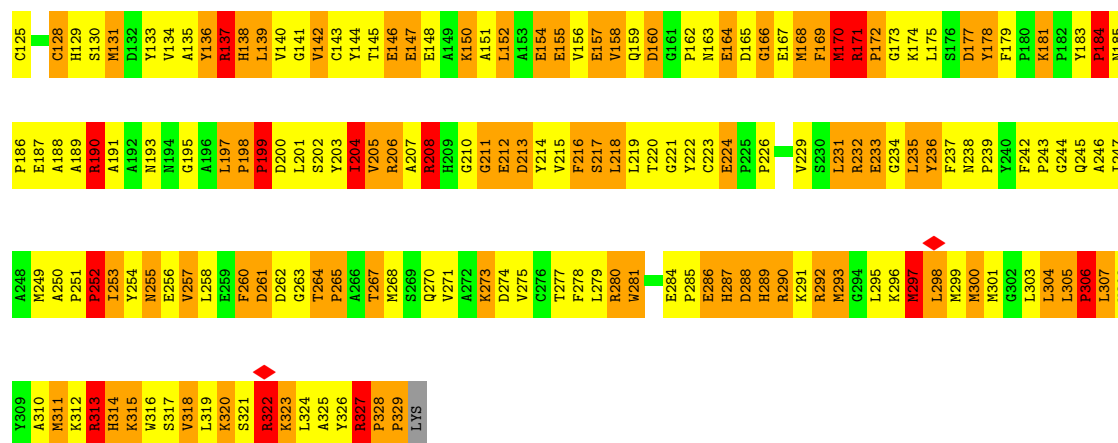


• Molecule 48: Cytochrome c1

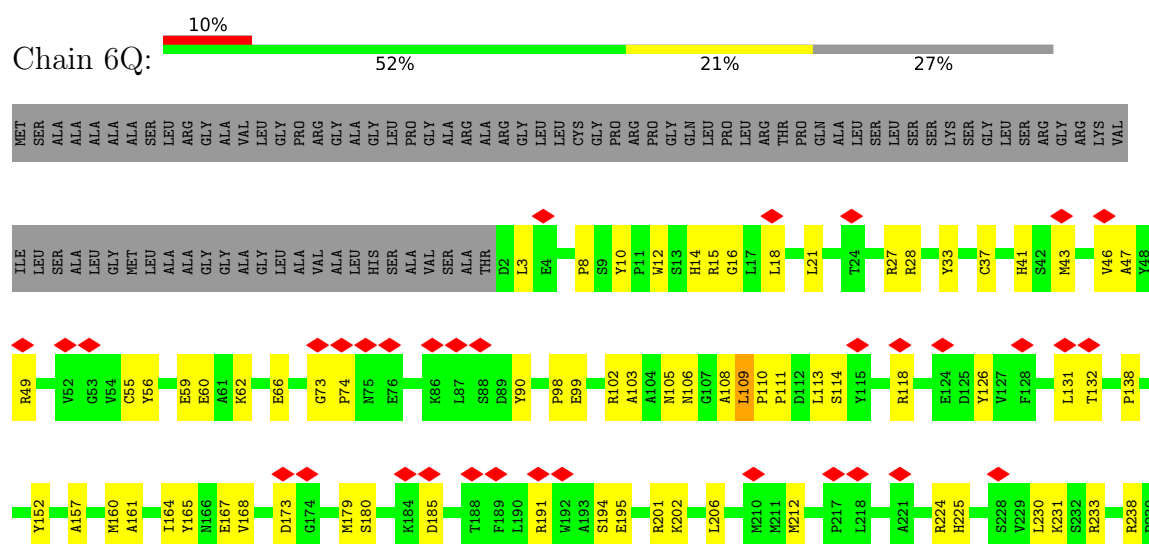


• Molecule 48: Cytochrome c1

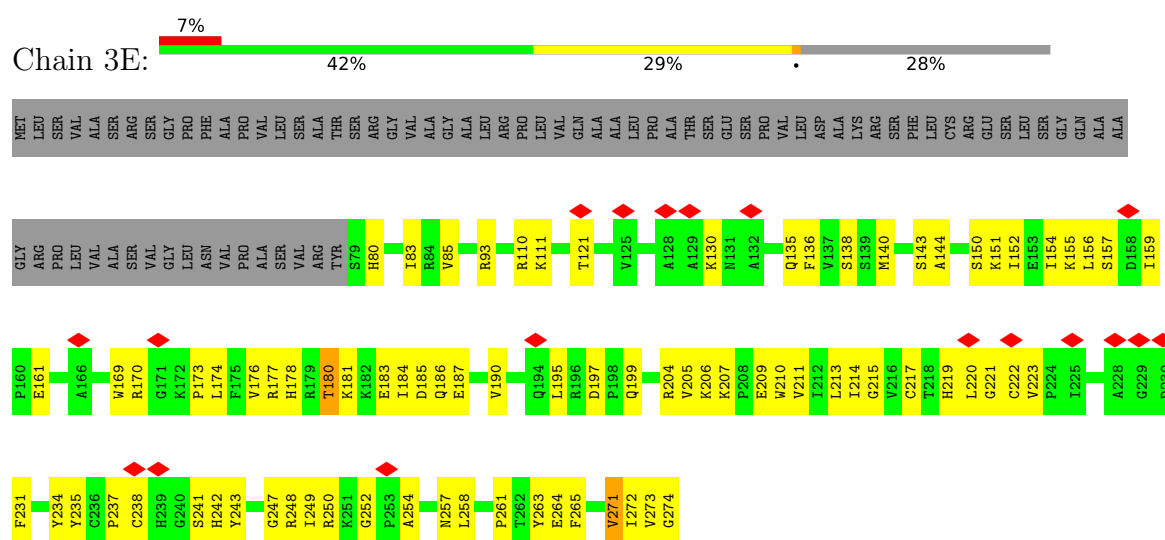




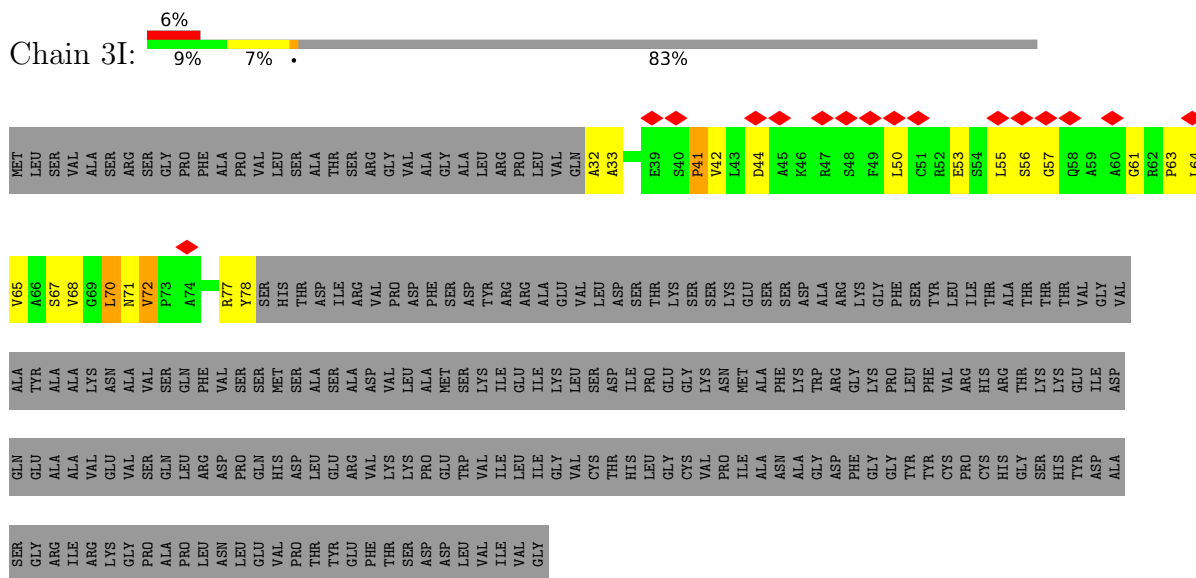
• Molecule 48: Cytochrome c1



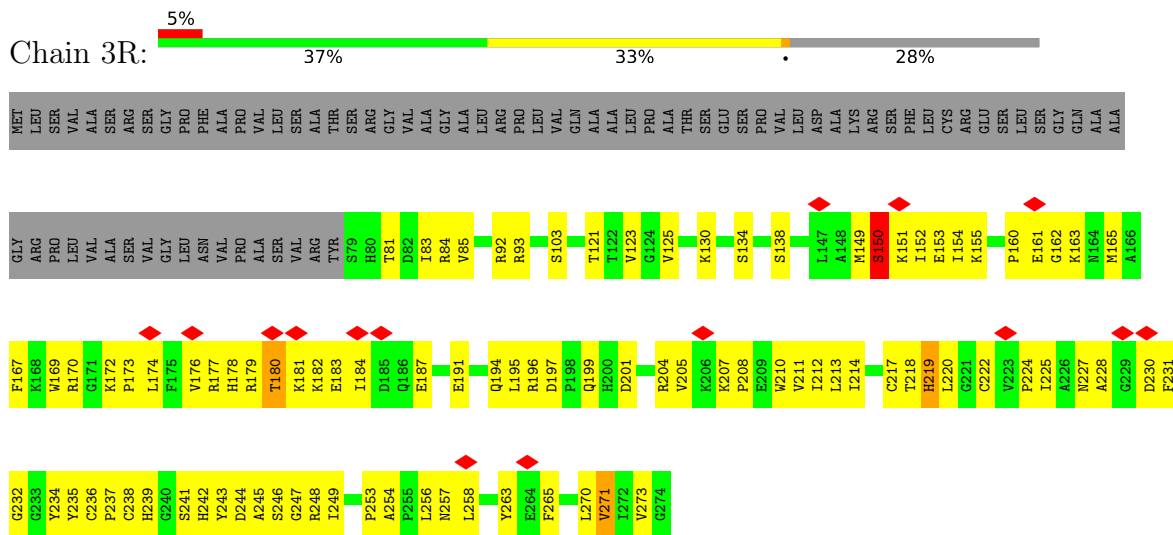
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



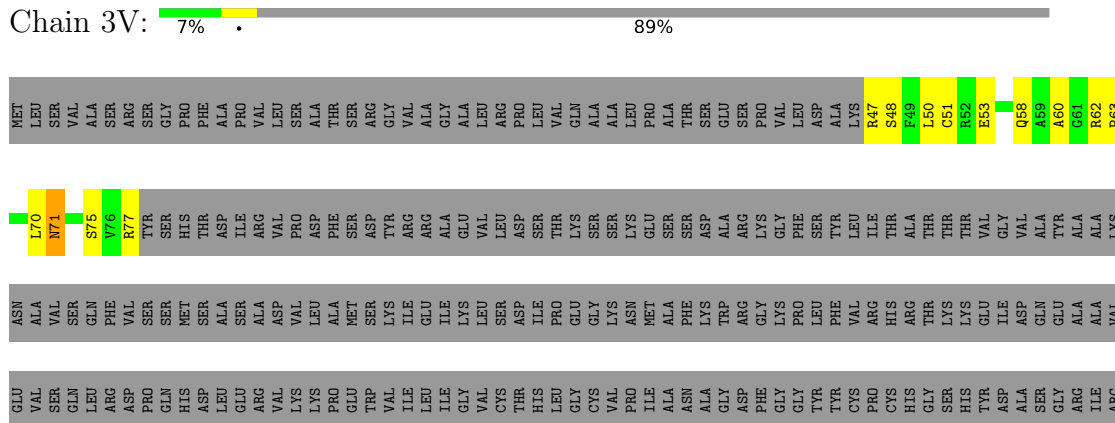
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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



LYS
GLY
PRO
ALA
PRO
LEU
ASN
LEU
GLU
VAL
PRO
THR
THR
GLY
PHE
THR
SER
SER
ASP
ASP
LEU
VAL
ILE
VAL
GLY

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

Chain 6E: 16% 39% 32% 28%

MET
LEU
SER
VAL
VAL
ALA
SER
SER
ARG
SER
GLY
PHE
PHE
ASN
PRO
THR
ALA
PRO
VAL
VAL
LEU
SER
SER
ALA
THR
THR
SER
SER
ARG
GLY
VAL
ALA
ALA
GLY
GLY
ALA
LEU
ARG
PRO
PRO
LEU
VAL
Gln
ALA
ALA
LEU
PRO
ALA
THR
THR
SER
SER
GLY
SER
PRO
VAL
ASP
ALA
LYS
ARG
SER
PHE
LEU
CYS
ARG
GLY
SER
SER
SER
GLY
Gln
ALA
ALA

GLY
ARG
PRO
LEU
VAL
ALA
SER
SER
VAL
VAL
GLY
LEU
ASN
VAL
ALA
PRO
ALA
ALA
TYR
S79
H80
I83
P86
D87
F88
S89
D90
Y91
S99
S107
K111
S114
I117
T118
T121
Y125
A126
Y127
A128
A129
Q135
F136
S139
M140
S143
A144
D145
V146
I147

A148
M149
S150
K151
I152
E153
I154
K155
L156
S157
D158
I159
P160
E161
G162
K163
M164
M165
A166
F167
K168
W169
R170
G171
K172
P173
L174
F175
Y176
R177
H178
R179
T180
K181
K182
E183
I184
D185
Q186
E187
V190
G194
L195
R196
D197
P198
Q199
R204
V205
K206
K207
P208
E209
W210
V211
T212
L213

L214
G215
V216
C217
H219
L220
G221
C222
V223
P224
T225
A226
R227
A228
G229
D230
F231
Y234
Y235
C236
C237
C238
H239
G240
S241
H242
Y243
G247
R248
I249
R250
G251
G252
P253
A254
N257
L258
P261
T262
E263
E264
F265
T266
L270
V271
I272
V273
G274

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

Chain 6I: 10% 9% 7% 83%

MET
LEU
SER
VAL
ALA
SER
SER
ARG
SER
GLY
PHE
PHE
ALA
PRO
VAL
VAL
LEU
SER
SER
ALA
THR
THR
SER
ARG
GLY
VAL
ALA
ALA
GLY
ALA
ALA
LEU
ARG
PRO
PRO
LEU
VAL
Gln
A32
A33
L34
P35
A36
T37
S38
E39
S40
P41
V42
L43
D44
A45
K46
R47
S48
F49
L50
G51
R52
L55
S56
G57
Q58
A59
A60
G61

R62
P63
L64
V65
A66
G68
G69
L70
N71
V72
P73
A74
S75
V76
R77
Y78
HIS
THR
THR
ASP
ILE
VAL
ARG
VAL
LEU
PRO
MET
PHE
SER
SER
SER
SER
HIS
THR
THR
THR
THR
THR

THR
VAL
GLY
VAL
VAL
GLY
TYR
ALA
ALA
ALA
VAL
LYS
LYS
ASN
ALA
VAL
SER
SER
Gln
PHE
VAL
VAL
SER
SER
SER
MET
SER
SER
SER
SER
HIS
THR
THR
THR
THR
LYS

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

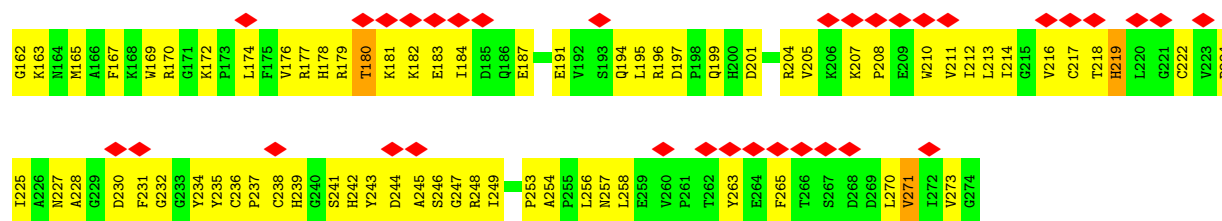
HIS
TYR
ASP
ALA
SER
GLY
ARG
ILE
ARG
LYS
GLY
VAL
ALA
PRO
PRO
ALA
ALA
VAL
SER
ASN
ASN
GLY
VAL
PRO
PHE
THR
THR
SER
ASP
ASP
VAL
LEU
LEU
ILE
ILE
GLY

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

Chain 6R: 15% 36% 34% 28%

MET
LEU
SER
VAL
VAL
ALA
SER
SER
ARG
SER
GLY
PHE
PHE
ASN
PRO
ALA
PRO
VAL
VAL
LEU
SER
SER
ALA
THR
THR
SER
SER
ARG
GLY
VAL
ALA
ALA
GLY
LEU
ARG
PRO
PRO
Gln
ALA
ALA
LEU
PRO
GLY
SER
GLY
VAL
VAL
ASP
ALA
ARG
SER
PHE
LEU
CYS
ARG
GLY
SER
SER
SER
SER
Gln
ALA
ALA

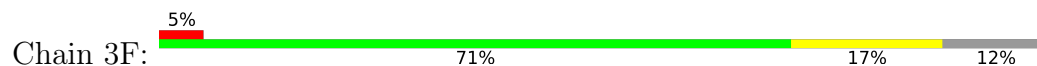
GLY
ARG
PRO
PRO
VAL
VAL
ALA
SER
SER
VAL
VAL
GLY
LEU
ASN
VAL
VAL
PRO
ALA
ALA
TYR
S79
H80
T81
D82
T83
R84
V85
R92
R93
K104
E105
T121
T122
V123
G124
V125
K130
S134
V137
S138
A144
L147
A148
M149
S150
K151
I152
E153
I154
K155
I159
P160
E161



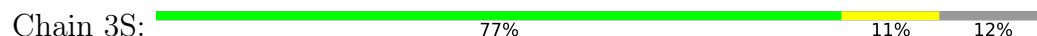
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



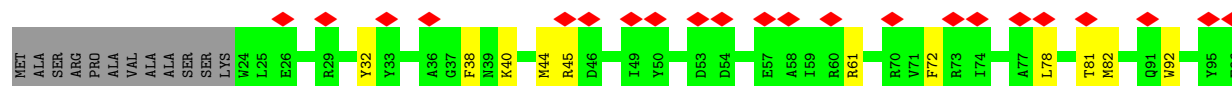
- Molecule 50: Cytochrome b-c1 complex subunit 7

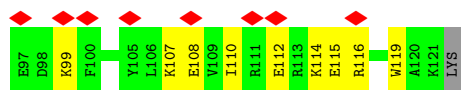


- Molecule 50: Cytochrome b-c1 complex subunit 7

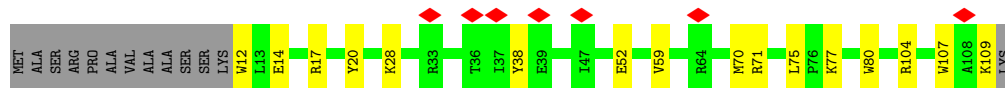
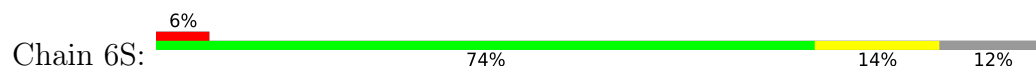


- Molecule 50: Cytochrome b-c1 complex subunit 7

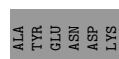
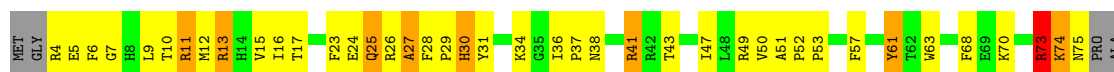




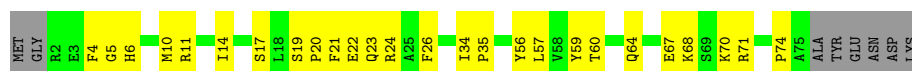
- Molecule 50: Cytochrome b-c1 complex subunit 7



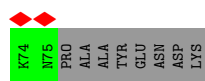
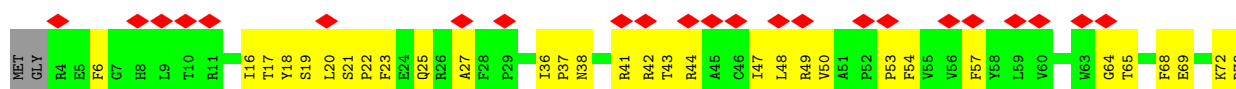
- Molecule 51: Cytochrome b-c1 complex subunit 8



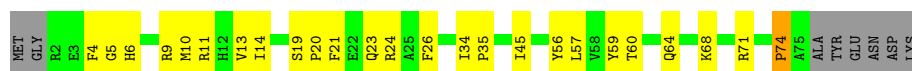
- Molecule 51: Cytochrome b-c1 complex subunit 8



- Molecule 51: Cytochrome b-c1 complex subunit 8



- Molecule 51: Cytochrome b-c1 complex subunit 8



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





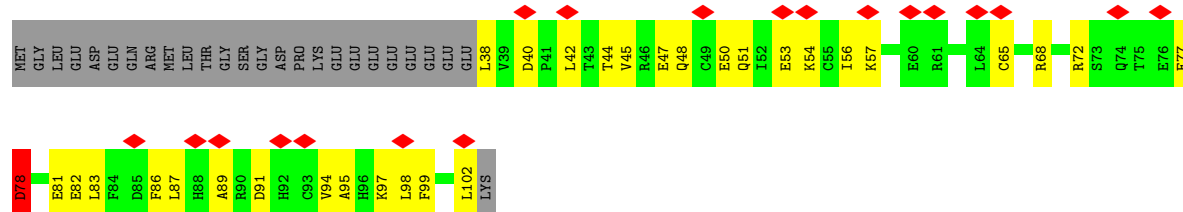
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U: 52% 19% 29%



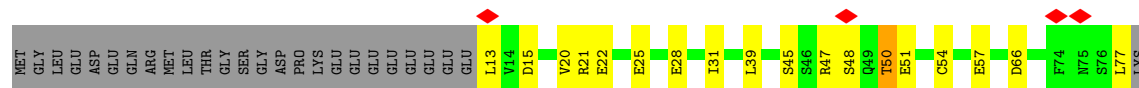
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 6H: 21% 37% 33% 29%



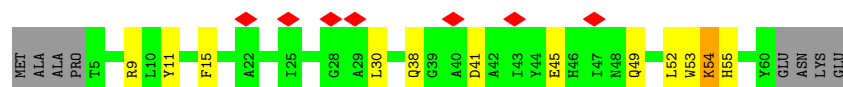
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 6U: 52% 19% 29%



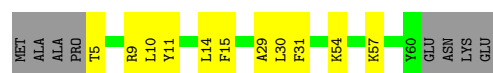
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J: 11% 69% 17% 12%



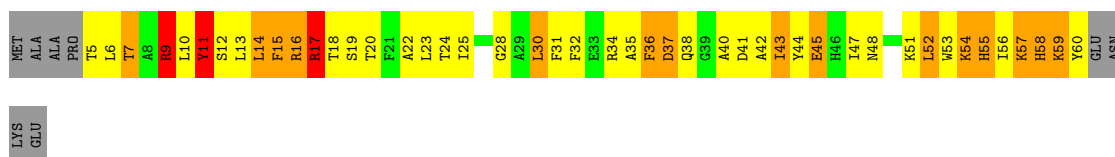
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W: 70% 17% 12%

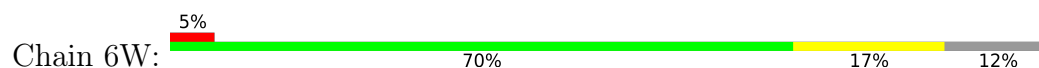


- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 6J: 16% 44% 23% 5% 12%



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



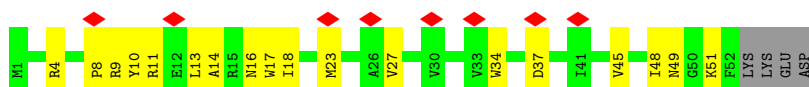
- Molecule 54: Cytochrome b-c1 complex subunit 10



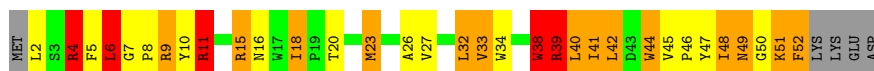
- Molecule 54: Cytochrome b-c1 complex subunit 10



- Molecule 54: Cytochrome b-c1 complex subunit 10

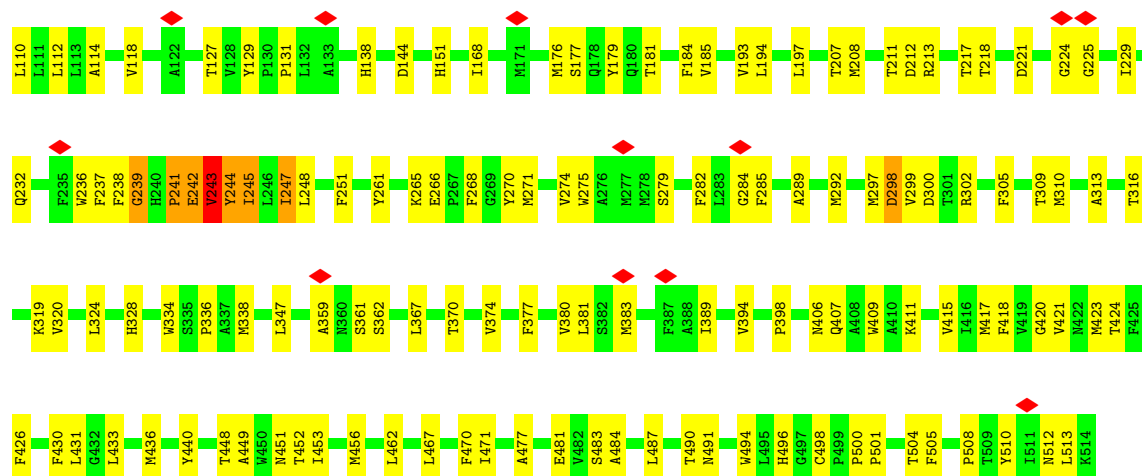


- Molecule 54: Cytochrome b-c1 complex subunit 10

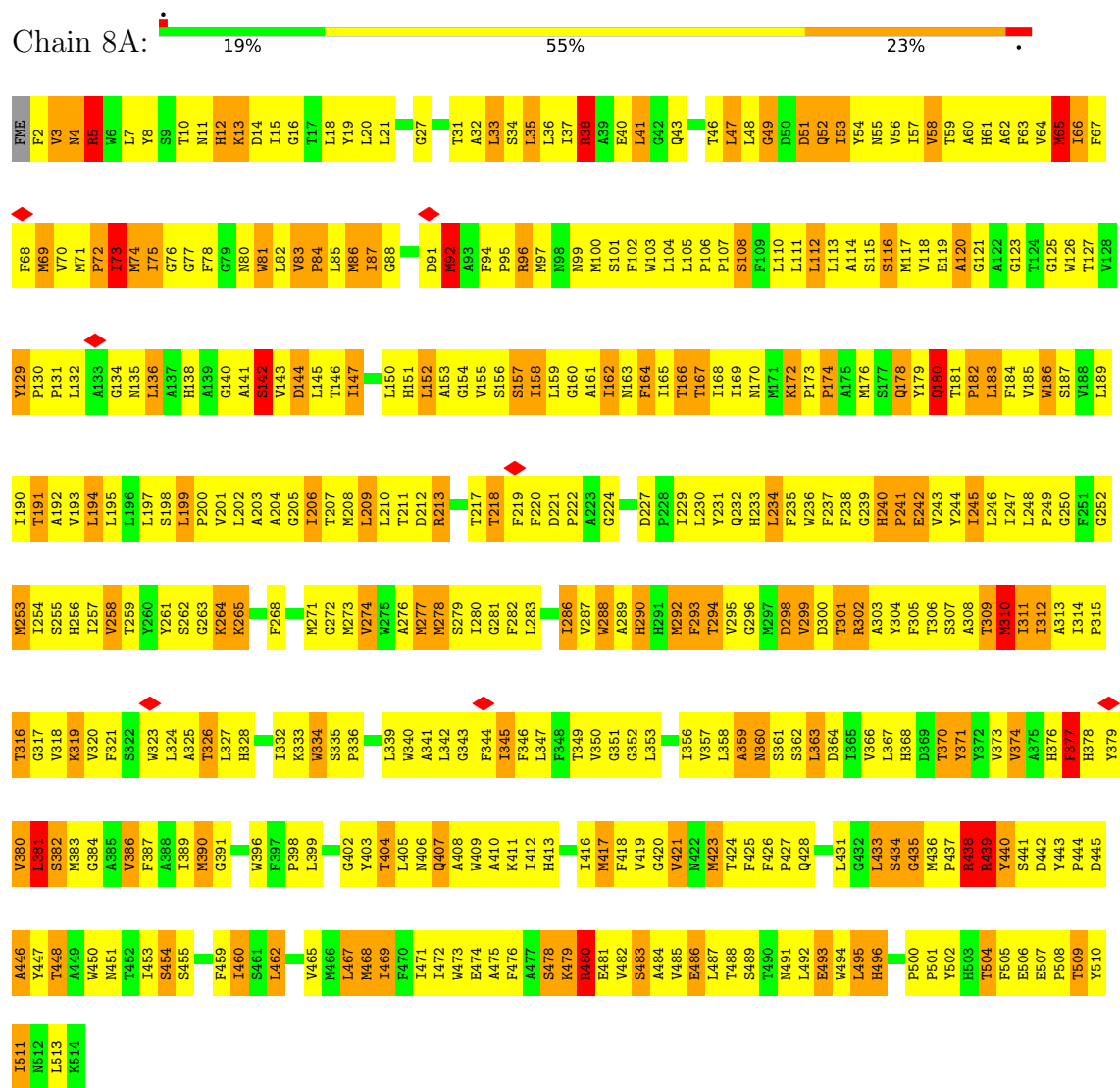


- Molecule 55: Cytochrome c oxidase subunit 1

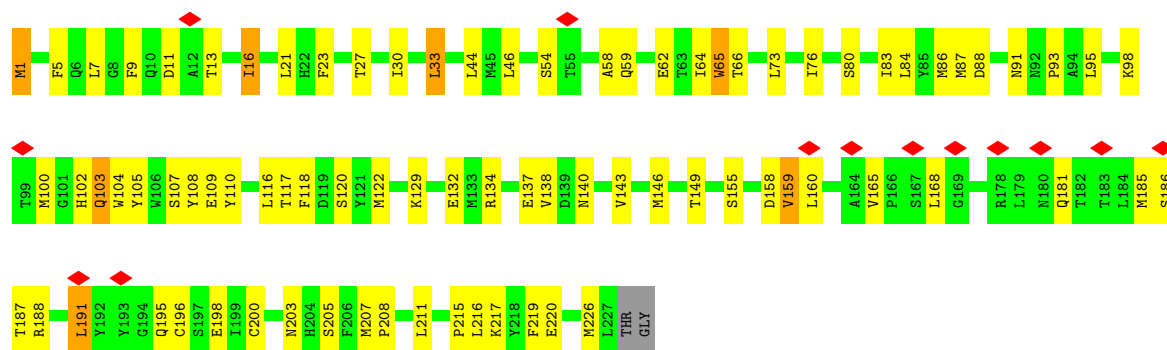




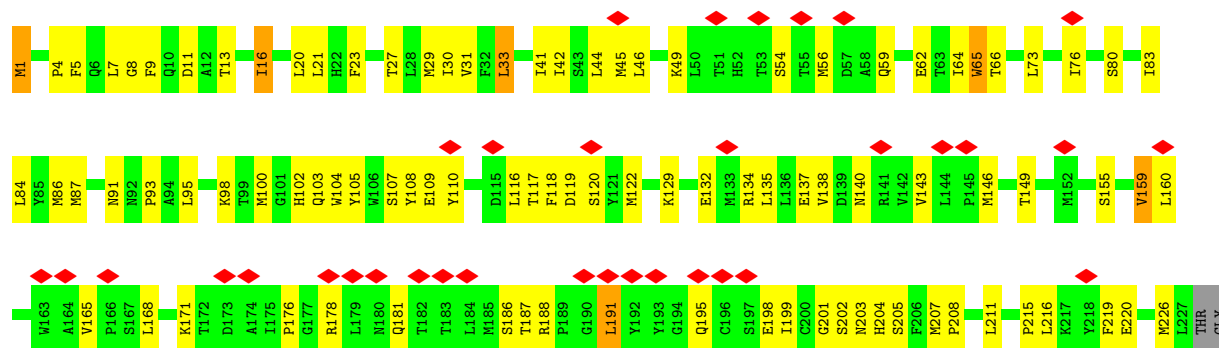
• Molecule 55: Cytochrome c oxidase subunit 1



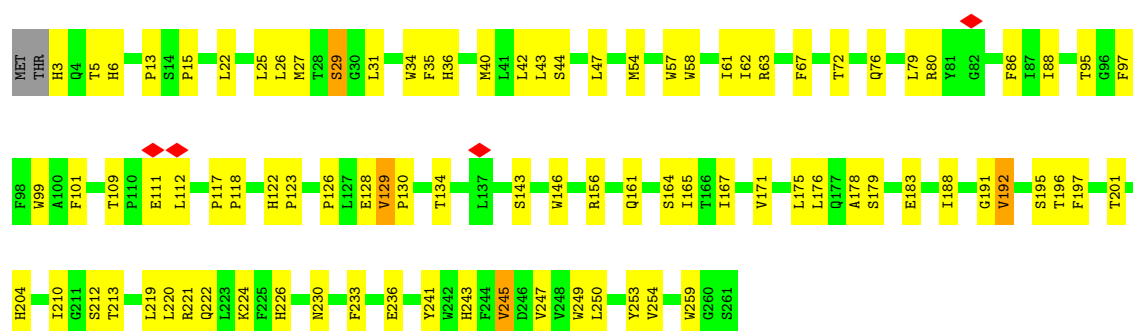
• Molecule 56: Cytochrome c oxidase subunit 2



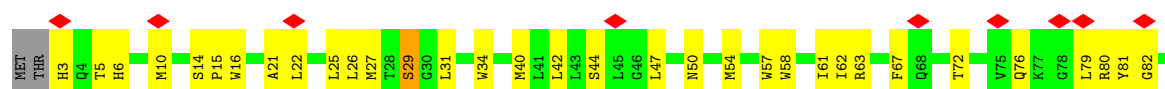
• Molecule 56: Cytochrome c oxidase subunit 2

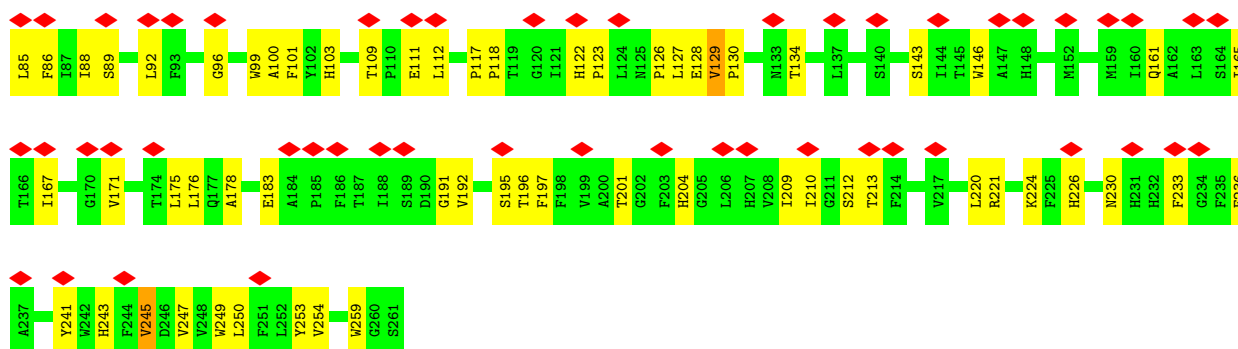


• Molecule 57: Cytochrome c oxidase subunit 3

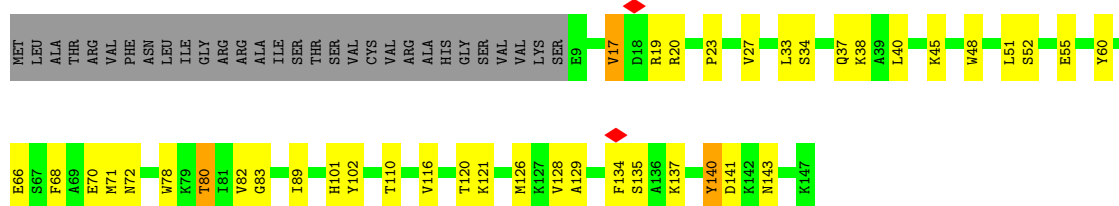


• Molecule 57: Cytochrome c oxidase subunit 3

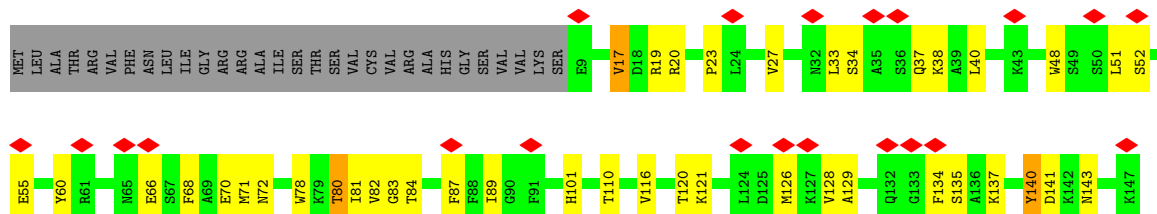




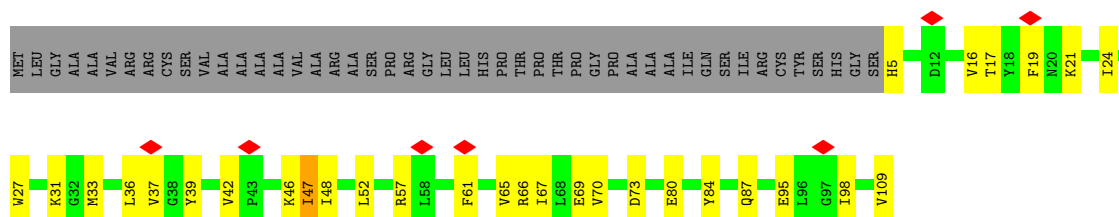
• Molecule 58: Cytochrome c oxidase subunit 4



• Molecule 58: Cytochrome c oxidase subunit 4

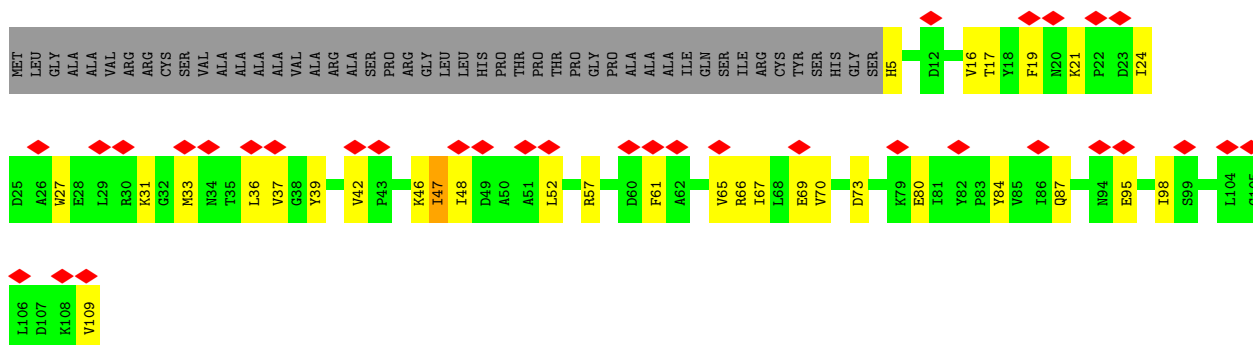


• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

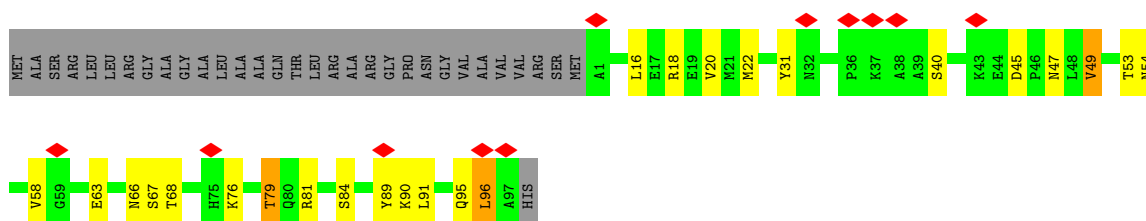


• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

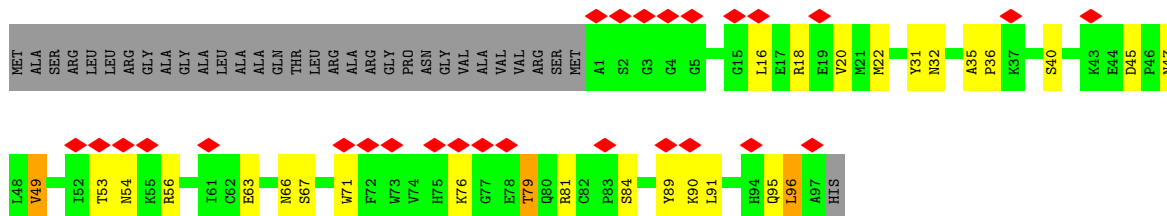




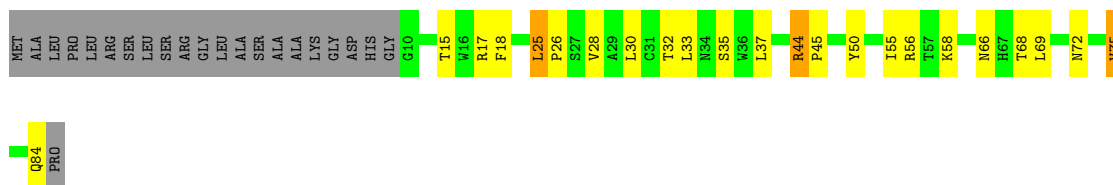
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



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

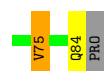


- Molecule 61: Cytochrome c oxidase subunit 6A2

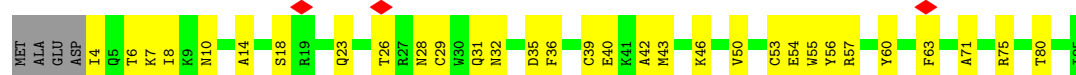


- Molecule 61: Cytochrome c oxidase subunit 6A2





- Molecule 62: Cytochrome c oxidase subunit 6B1



- Molecule 62: Cytochrome c oxidase subunit 6B1



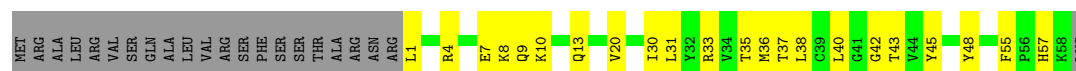
- Molecule 63: Cytochrome c oxidase subunit 6C



- Molecule 63: Cytochrome c oxidase subunit 6C



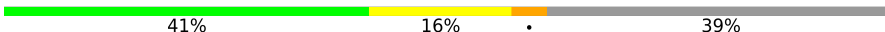
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

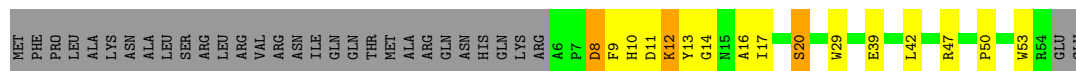


- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

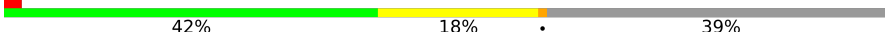


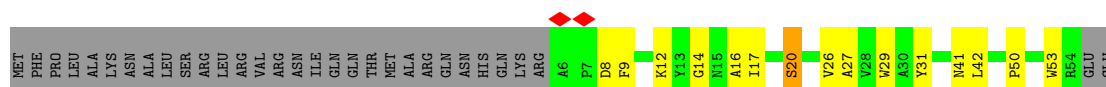
- Molecule 65: Cytochrome c oxidase subunit 7B

Chain 4K: 



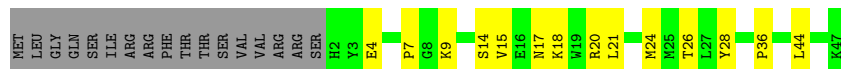
- Molecule 65: Cytochrome c oxidase subunit 7B

Chain 8K: 



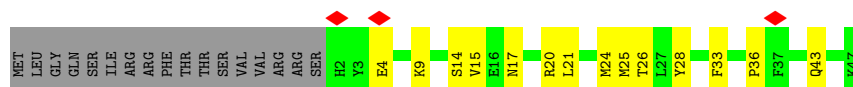
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 4L: 



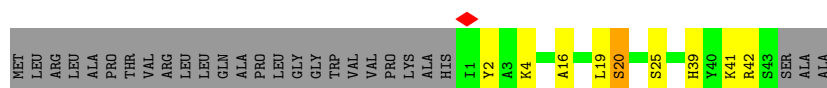
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 8L: 



- Molecule 67: Cytochrome c oxidase subunit 8

Chain 4M: 



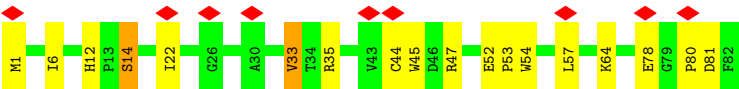
- Molecule 67: Cytochrome c oxidase subunit 8

Chain 8M: 

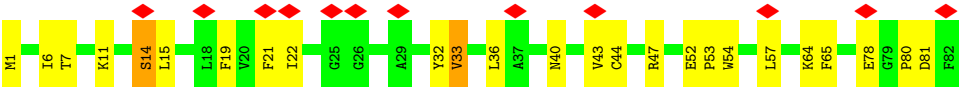


- Molecule 68: Cytochrome c oxidase subunit NDUF4A

Chain 4N: 



• Molecule 68: Cytochrome c oxidase subunit NDUF4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	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	1.533	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	798.72, 798.72, 798.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.87	0/930	1.17	2/1271 (0.2%)
1	5A	0.20	0/930	0.42	0/1271
2	1B	2.15	4/1270 (0.3%)	2.56	17/1713 (1.0%)
2	5B	0.16	0/1273	0.32	0/1722
3	1C	0.13	0/1797	0.33	0/2447
3	5C	0.13	0/1797	0.33	0/2447
4	1D	0.95	1/3545 (0.0%)	0.54	3/4806 (0.1%)
4	5D	0.95	1/3545 (0.0%)	0.53	3/4806 (0.1%)
5	1E	0.14	0/1698	0.35	0/2311
5	5E	0.15	0/1698	0.35	0/2311
6	1F	0.15	0/3401	0.32	0/4595
6	5F	0.15	0/3401	0.32	0/4595
7	1G	0.14	0/5451	0.32	1/7387 (0.0%)
7	5G	0.14	0/5451	0.32	0/7387
8	1H	0.25	0/2566	0.45	0/3509
8	5H	0.17	0/2566	0.37	0/3509
9	1I	0.12	0/1443	0.29	0/1952
9	5I	0.12	0/1443	0.29	0/1952
10	1J	0.27	0/1364	0.54	1/1850 (0.1%)
10	5J	0.25	0/1364	0.50	0/1850
11	1K	0.19	0/751	0.34	0/1018
11	5K	0.19	0/751	0.34	0/1018
12	1L	0.16	0/4939	0.35	0/6718
12	5L	0.16	0/4939	0.35	0/6718
13	1M	0.16	0/3713	0.35	0/5063
13	5M	0.16	0/3713	0.35	0/5063
14	1N	0.16	0/2765	0.35	0/3758
14	5N	0.17	0/2765	0.35	0/3758
15	1O	0.22	1/2650 (0.0%)	0.54	4/3588 (0.1%)
15	5O	0.22	1/2650 (0.0%)	0.54	4/3588 (0.1%)
16	1P	0.15	0/2828	0.33	0/3834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	5P	0.15	0/2828	0.33	0/3834
17	1Q	0.14	0/1070	0.32	0/1446
17	5Q	0.15	0/1070	0.32	0/1446
18	1R	0.12	0/755	0.29	0/1018
18	5R	0.12	0/755	0.29	0/1018
19	1S	0.16	0/711	0.36	0/956
19	5S	0.16	0/711	0.36	0/956
20	1T	0.14	0/701	0.30	0/946
20	1U	0.13	0/706	0.28	0/954
20	5T	0.14	0/701	0.30	0/946
20	5U	0.14	0/706	0.28	0/954
21	1V	0.17	0/946	0.31	0/1281
21	5V	0.17	0/946	0.31	0/1281
22	1W	0.17	0/995	0.30	0/1340
22	5W	0.17	0/995	0.30	0/1340
23	1X	0.13	0/1436	0.34	0/1938
23	5X	0.14	0/1436	0.34	0/1938
24	1Y	0.28	1/1037 (0.1%)	0.45	3/1404 (0.2%)
24	5Y	0.28	1/1037 (0.1%)	0.45	3/1404 (0.2%)
25	1Z	0.16	0/1199	0.30	0/1617
25	5Z	0.16	0/1199	0.30	0/1617
26	1a	0.14	0/577	0.31	0/777
26	5a	0.14	0/577	0.31	0/777
27	1b	1.41	4/664 (0.6%)	1.48	7/912 (0.8%)
27	5b	1.41	4/664 (0.6%)	1.49	7/912 (0.8%)
28	1c	0.13	0/430	0.31	0/581
28	5c	0.14	0/430	0.31	0/581
29	1d	0.13	0/1016	0.25	0/1374
29	5d	0.13	0/1016	0.25	0/1374
30	1e	0.15	0/836	0.34	0/1118
30	5e	0.15	0/836	0.34	0/1118
31	1f	0.14	0/499	0.35	0/673
31	5f	0.15	0/499	0.35	0/673
32	1g	0.13	0/858	0.33	0/1165
32	5g	0.13	0/858	0.34	0/1165
33	1h	0.14	0/1184	0.32	0/1603
33	5h	0.14	0/1184	0.32	0/1603
34	1i	0.14	0/1138	0.33	0/1551
34	5i	0.15	0/1138	0.33	0/1551
35	1j	0.12	0/627	0.28	0/858
35	5j	0.19	0/627	0.41	0/858
36	1k	0.44	0/668	0.67	1/903 (0.1%)
36	5k	0.68	1/668 (0.1%)	0.98	5/903 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	1l	2.70	2/1365 (0.1%)	1.26	11/1867 (0.6%)
37	5l	2.70	2/1365 (0.1%)	1.26	11/1867 (0.6%)
38	1m	0.72	1/1092 (0.1%)	0.48	1/1481 (0.1%)
38	5m	0.72	1/1092 (0.1%)	0.48	1/1481 (0.1%)
39	1n	0.15	0/1549	0.33	0/2098
39	5n	0.15	0/1549	0.33	0/2098
40	1o	0.13	0/1069	0.28	0/1430
40	5o	0.13	0/1069	0.28	0/1430
41	1p	0.17	0/1481	0.33	0/1997
41	5p	0.17	0/1481	0.33	0/1997
42	1q	0.12	0/1253	0.27	0/1704
42	5q	0.12	0/1253	0.27	0/1704
43	1r	0.12	0/777	0.27	0/1051
43	5r	0.13	0/777	0.26	0/1051
44	1s	0.13	0/394	0.30	0/533
44	5s	0.13	0/394	0.30	0/533
45	3A	0.29	1/3481 (0.0%)	0.56	4/4722 (0.1%)
45	3N	0.91	0/3487	1.29	17/4711 (0.4%)
45	6A	0.96	0/3481	1.17	3/4722 (0.1%)
45	6N	0.93	0/3487	1.21	14/4711 (0.3%)
46	3B	0.17	0/3192	0.33	0/4322
46	3O	0.97	0/3184	1.21	2/4311 (0.0%)
46	6B	0.98	0/3192	1.19	1/4322 (0.0%)
46	6O	0.96	0/3184	1.20	4/4311 (0.1%)
47	3C	0.91	0/3123	1.22	2/4269 (0.0%)
47	3P	0.18	0/3122	0.35	0/4269
47	6C	0.91	0/3123	1.18	6/4269 (0.1%)
47	6P	0.18	0/3122	0.36	0/4269
48	3D	0.27	0/1946	0.44	0/2641
48	3Q	1.95	2/1962 (0.1%)	1.07	5/2663 (0.2%)
48	6D	0.93	0/1946	1.22	8/2641 (0.3%)
48	6Q	1.95	2/1962 (0.1%)	1.07	4/2663 (0.2%)
49	3E	0.22	0/1551	0.42	0/2098
49	3I	1.38	4/342 (1.2%)	1.72	5/465 (1.1%)
49	3R	0.17	0/1551	0.40	0/2098
49	3V	0.17	0/225	0.34	0/303
49	6E	0.22	0/1551	0.42	0/2098
49	6I	1.38	4/342 (1.2%)	1.71	5/465 (1.1%)
49	6R	0.18	0/1551	0.40	0/2098
49	6V	0.17	0/225	0.34	0/303
50	3F	0.17	0/888	0.32	0/1193
50	3S	0.14	0/888	0.27	0/1193
50	6F	0.17	0/888	0.33	0/1193

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
50	6S	0.14	0/888	0.27	0/1193
51	3G	0.92	0/636	1.20	0/859
51	3T	0.62	3/649 (0.5%)	1.52	4/878 (0.5%)
51	6G	0.22	0/636	0.41	0/859
51	6T	0.61	3/649 (0.5%)	1.52	4/878 (0.5%)
52	3H	0.90	0/539	1.27	0/724
52	3U	0.24	0/539	0.44	0/724
52	6H	0.44	0/539	0.59	0/724
52	6U	0.23	0/539	0.44	0/724
53	3J	0.19	0/476	0.44	0/641
53	3W	0.19	0/476	0.32	0/641
53	6J	0.88	0/476	1.16	0/641
53	6W	0.19	0/476	0.32	0/641
54	3X	0.16	0/445	0.32	0/608
54	3Y	0.17	0/437	0.37	0/598
54	6X	0.16	0/445	0.33	0/608
54	6Y	0.89	0/437	1.09	0/598
55	4A	0.32	1/4156 (0.0%)	0.66	7/5679 (0.1%)
55	8A	0.88	0/4156	1.26	7/5679 (0.1%)
56	4B	0.32	0/1865	0.51	0/2544
56	8B	0.32	0/1865	0.50	0/2544
57	4C	0.20	0/2179	0.34	0/2981
57	8C	0.21	0/2179	0.34	0/2981
58	4D	0.19	0/1197	0.32	0/1617
58	8D	0.19	0/1197	0.32	0/1617
59	4E	0.20	0/871	0.40	1/1182 (0.1%)
59	8E	0.20	0/871	0.40	1/1182 (0.1%)
60	4F	0.23	0/749	0.40	0/1016
60	8F	0.23	0/749	0.40	0/1016
61	4G	0.18	0/644	0.34	0/881
61	8G	0.18	0/644	0.34	0/881
62	4H	0.30	0/708	0.47	0/956
62	8H	0.30	0/708	0.47	0/956
63	4I	0.20	0/563	0.35	0/748
63	8I	0.20	0/563	0.35	0/748
64	4J	0.20	0/466	0.34	0/631
64	8J	0.20	0/466	0.34	0/631
65	4K	0.40	0/396	0.54	0/543
65	8K	0.18	0/396	0.34	0/543
66	4L	0.21	0/394	0.36	0/528
66	8L	0.22	0/394	0.36	0/528
67	4M	0.18	0/349	0.32	0/477
67	8M	0.18	0/349	0.32	0/477

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	4N	0.19	0/680	0.41	0/921
68	8N	0.19	0/680	0.41	0/921
All	All	0.62	45/233003 (0.0%)	0.67	189/316071 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1B	0	6
6	1F	0	1
6	5F	0	1
8	1H	0	2
8	5H	0	1
35	5j	0	1
45	3N	0	7
45	6A	0	17
45	6N	0	10
46	3O	0	8
46	6B	0	17
46	6O	0	15
47	3C	0	2
47	6C	0	8
48	3D	0	1
48	6D	0	13
51	3G	0	5
52	3H	0	1
52	6H	0	1
53	6J	0	4
54	6Y	0	5
55	8A	0	8
58	4D	0	1
58	8D	0	1
All	All	0	136

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	3Q	74	PRO	N-CD	85.76	2.67	1.47
48	6Q	74	PRO	N-CD	85.70	2.67	1.47
37	5I	17	PRO	N-CD	76.92	2.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1l	17	PRO	N-CD	76.83	2.55	1.47
37	5l	146	PRO	N-CD	63.31	2.36	1.47

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	6Q	74	PRO	N-CD-CG	-47.94	31.30	103.20
48	3Q	74	PRO	N-CD-CG	-47.91	31.34	103.20
2	1B	95	LYS	CA-C-N	-42.09	41.14	121.54
2	1B	95	LYS	C-N-CA	-42.09	41.14	121.54
51	6T	74	PRO	N-CD-CG	-37.36	47.16	103.20

There are no chirality outliers.

5 of 136 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	71	ARG	Sidechain
2	1B	77	ARG	Sidechain
2	1B	81	ARG	Sidechain
2	1B	92	LEU	Mainchain
2	1B	96	MET	Mainchain

5.2 Too-close contacts [i](#)

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	949	67	0
1	5A	916	0	950	49	0
2	1B	1242	0	1241	201	0
2	5B	1242	0	1249	39	0
3	1C	1746	0	1697	35	0
3	5C	1746	0	1697	34	0
4	1D	3452	0	3389	121	0
4	5D	3452	0	3389	93	0
5	1E	1658	0	1662	42	0
5	5E	1658	0	1662	41	0
6	1F	3325	0	3288	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	5F	3325	0	3288	91	0
7	1G	5362	0	5388	127	0
7	5G	5362	0	5388	123	0
8	1H	2504	0	2602	93	0
8	5H	2504	0	2602	86	0
9	1I	1412	0	1366	48	0
9	5I	1412	0	1366	43	0
10	1J	1329	0	1326	88	0
10	5J	1329	0	1326	90	0
11	1K	750	0	798	41	0
11	5K	750	0	798	39	0
12	1L	4818	0	4956	160	0
12	5L	4818	0	4956	159	0
13	1M	3632	0	3836	136	0
13	5M	3632	0	3836	138	0
14	1N	2712	0	2872	84	0
14	5N	2712	0	2872	85	0
15	1O	2590	0	2556	70	0
15	5O	2590	0	2556	72	0
16	1P	2751	0	2776	60	0
16	5P	2751	0	2776	60	0
17	1Q	1047	0	1042	31	0
17	5Q	1047	0	1042	31	0
18	1R	741	0	704	11	0
18	5R	741	0	704	10	0
19	1S	700	0	719	18	0
19	5S	700	0	719	16	0
20	1T	689	0	687	25	0
20	1U	694	0	691	17	0
20	5T	689	0	687	25	0
20	5U	694	0	691	16	0
21	1V	927	0	972	25	0
21	5V	927	0	972	25	0
22	1W	971	0	975	23	0
22	5W	971	0	975	24	0
23	1X	1398	0	1378	34	0
23	5X	1398	0	1378	31	0
24	1Y	1016	0	1020	41	0
24	5Y	1016	0	1020	38	0
25	1Z	1168	0	1161	42	0
25	5Z	1168	0	1161	40	0
26	1a	562	0	557	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	5a	562	0	557	17	0
27	1b	643	0	645	14	0
27	5b	643	0	645	15	0
28	1c	417	0	425	10	0
28	5c	417	0	425	9	0
29	1d	985	0	978	36	0
29	5d	985	0	978	34	0
30	1e	816	0	823	33	0
30	5e	816	0	823	33	0
31	1f	487	0	498	17	0
31	5f	487	0	498	14	0
32	1g	835	0	795	26	0
32	5g	835	0	795	25	0
33	1h	1151	0	1164	29	0
33	5h	1151	0	1164	27	0
34	1i	1100	0	1107	29	0
34	5i	1100	0	1107	25	0
35	1j	601	0	546	29	0
35	5j	601	0	546	35	0
36	1k	649	0	626	21	0
36	5k	649	0	626	46	0
37	1l	1310	0	1204	42	0
37	5l	1310	0	1204	41	0
38	1m	1062	0	1075	44	0
38	5m	1062	0	1075	49	0
39	1n	1495	0	1434	52	0
39	5n	1495	0	1434	51	0
40	1o	1045	0	1016	38	0
40	5o	1045	0	1016	35	0
41	1p	1449	0	1416	42	0
41	5p	1449	0	1416	41	0
42	1q	1212	0	1174	20	0
42	5q	1212	0	1174	19	0
43	1r	759	0	783	16	0
43	5r	759	0	783	14	0
44	1s	382	0	351	11	0
44	5s	382	0	351	12	0
45	3A	3411	0	3309	70	0
45	3N	3415	0	3331	767	0
45	6A	3411	0	3309	235	0
45	6N	3415	0	3326	836	0
46	3B	3139	0	3118	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	3O	3132	0	3110	233	0
46	6B	3139	0	3118	192	0
46	6O	3132	0	3110	278	0
47	3C	3025	0	3090	339	0
47	3P	3024	0	3090	76	0
47	6C	3025	0	3090	322	0
47	6P	3024	0	3090	77	0
48	3D	1888	0	1834	112	0
48	3Q	1904	0	1849	65	0
48	6D	1888	0	1832	230	0
48	6Q	1904	0	1849	62	0
49	3E	1518	0	1498	104	0
49	3I	337	0	347	29	0
49	3R	1518	0	1498	105	0
49	3V	223	0	233	24	0
49	6E	1518	0	1498	113	0
49	6I	337	0	347	33	0
49	6R	1518	0	1498	97	0
49	6V	223	0	233	27	0
50	3F	868	0	857	35	0
50	3S	868	0	857	11	0
50	6F	868	0	857	29	0
50	6S	868	0	857	15	0
51	3G	616	0	620	53	0
51	3T	628	0	634	26	0
51	6G	616	0	622	53	0
51	6T	628	0	634	29	0
52	3H	533	0	513	29	0
52	3U	533	0	513	13	0
52	6H	533	0	513	40	0
52	6U	533	0	513	13	0
53	3J	464	0	467	9	0
53	3W	464	0	467	7	0
53	6J	464	0	467	42	0
53	6W	464	0	467	8	0
54	3X	429	0	430	15	0
54	3Y	421	0	418	10	0
54	6X	429	0	430	17	0
54	6Y	421	0	418	31	0
55	4A	4016	0	3994	148	0
55	8A	4016	0	3994	501	0
56	4B	1828	0	1837	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	8B	1828	0	1836	93	0
57	4C	2096	0	2027	83	0
57	8C	2096	0	2027	110	0
58	4D	1163	0	1143	37	0
58	8D	1163	0	1143	36	0
59	4E	852	0	845	20	0
59	8E	852	0	845	19	0
60	4F	734	0	718	18	0
60	8F	734	0	718	29	0
61	4G	617	0	585	17	0
61	8G	617	0	585	21	0
62	4H	687	0	647	26	0
62	8H	687	0	647	30	0
63	4I	550	0	560	16	0
63	8I	550	0	560	16	0
64	4J	456	0	459	23	0
64	8J	456	0	459	24	0
65	4K	383	0	366	16	0
65	8K	383	0	366	25	0
66	4L	381	0	380	12	0
66	8L	381	0	380	13	0
67	4M	338	0	345	9	0
67	8M	338	0	345	14	0
68	4N	660	0	664	17	0
68	8N	660	0	664	29	0
69	1A	47	0	71	4	0
69	1J	44	0	62	5	0
69	1L	122	0	172	8	0
69	1M	95	0	141	12	0
69	1N	100	0	157	19	0
69	1Y	171	0	218	16	0
69	1d	48	0	73	11	0
69	1j	44	0	65	0	0
69	5A	47	0	71	2	0
69	5J	44	0	62	5	0
69	5L	122	0	172	7	0
69	5M	95	0	141	13	0
69	5N	100	0	157	20	0
69	5Y	171	0	218	17	0
69	5d	48	0	73	12	0
69	5j	44	0	65	0	0
70	1B	8	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	1F	8	0	0	2	0
70	1G	16	0	0	1	0
70	1I	16	0	0	0	0
70	5B	8	0	0	2	0
70	5F	8	0	0	2	0
70	5G	16	0	0	1	0
70	5I	16	0	0	0	0
71	1B	46	0	66	3	0
71	1H	48	0	73	7	0
71	1I	98	0	150	11	0
71	1J	35	0	44	4	0
71	1M	44	0	65	8	0
71	1P	33	0	40	5	0
71	1Y	35	0	44	3	0
71	1h	47	0	71	3	0
71	1m	46	0	66	5	0
71	5A	35	0	44	1	0
71	5B	46	0	66	2	0
71	5H	48	0	73	5	0
71	5I	98	0	150	11	0
71	5M	44	0	65	8	0
71	5P	33	0	40	2	0
71	5Y	35	0	44	3	0
71	5h	47	0	71	3	0
71	5m	46	0	66	5	0
72	1E	4	0	0	1	0
72	1G	4	0	0	1	0
72	3E	4	0	0	4	0
72	3R	4	0	0	1	0
72	5E	4	0	0	1	0
72	5G	4	0	0	1	0
72	6E	4	0	0	4	0
72	6R	4	0	0	1	0
73	1F	31	0	19	2	0
73	5F	31	0	19	1	0
74	1G	1	0	0	0	0
74	5G	1	0	0	0	0
75	1L	76	0	99	3	0
75	1N	62	0	68	4	0
75	1X	86	0	125	12	0
75	1d	65	0	77	7	0
75	1i	80	0	104	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	1q	61	0	66	5	0
75	4B	100	0	156	6	0
75	4C	100	0	156	18	0
75	5L	76	0	99	2	0
75	5N	62	0	68	4	0
75	5X	86	0	125	13	0
75	5d	65	0	77	7	0
75	5i	80	0	104	9	0
75	5q	61	0	66	5	0
75	8A	100	0	156	28	0
75	8B	100	0	156	7	0
75	8D	100	0	156	19	0
76	1O	32	0	12	4	0
76	5O	32	0	12	5	0
77	1O	1	0	0	0	0
77	4A	1	0	0	0	0
77	5O	1	0	0	0	0
77	8A	1	0	0	0	0
78	1P	48	0	26	1	0
78	5P	48	0	26	1	0
79	1R	1	0	0	0	0
79	4F	1	0	0	0	0
79	5R	1	0	0	0	0
79	8F	1	0	0	0	0
80	1T	37	0	0	1	0
80	1n	37	0	0	1	0
80	5T	37	0	0	1	0
80	5n	37	0	0	1	0
81	1h	11	0	12	3	0
81	5h	11	0	12	3	0
82	1p	51	0	76	4	0
82	4A	204	0	304	30	0
82	4C	255	0	380	33	0
82	4G	51	0	76	8	0
82	4J	51	0	76	11	0
82	4K	51	0	76	7	0
82	4L	51	0	76	12	0
82	8A	204	0	304	46	0
82	8B	51	0	76	10	0
82	8C	255	0	380	39	0
82	8G	51	0	76	12	0
82	8J	51	0	76	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	8K	51	0	76	9	0
82	8L	51	0	76	7	0
83	3C	86	0	60	11	0
83	3P	86	0	60	6	0
83	6C	86	0	60	16	0
83	6P	86	0	60	6	0
84	3D	42	0	32	2	0
84	3Q	43	0	32	2	0
84	6D	42	0	32	5	0
84	6Q	43	0	32	2	0
85	4A	120	0	108	8	0
85	8A	120	0	108	16	0
86	4A	1	0	0	0	0
86	8A	1	0	0	0	0
87	4A	1	0	0	0	0
87	8A	1	0	0	0	0
88	4B	2	0	0	3	0
88	8B	2	0	0	0	0
89	4B	52	0	80	7	0
89	8A	52	0	80	7	0
90	4C	105	0	149	7	0
90	8C	105	0	149	9	0
91	4H	5	0	0	0	0
91	8H	5	0	0	0	0
All	All	233868	0	234967	9307	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 20.

The worst 5 of 9307 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)
2:1B:95:LYS:HG2	2:1B:96:MET:SD	1.25	1.68
45:3N:150:PHE:HE1	45:3N:310:PHE:CZ	1.11	1.66
45:6N:148:VAL:HG12	45:6N:152:TYR:CE2	1.17	1.65
45:3N:64:PHE:CE1	45:3N:86:LEU:HD13	1.24	1.63
2:1B:96:MET:HG3	4:1D:82:LEU:CD2	1.26	1.61

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	112/115 (97%)	79 (70%)	27 (24%)	6 (5%)	1	14
1	5A	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	6	34
2	1B	147/258 (57%)	115 (78%)	22 (15%)	10 (7%)	1	11
2	5B	153/258 (59%)	147 (96%)	6 (4%)	0	100	100
3	1C	207/264 (78%)	202 (98%)	5 (2%)	0	100	100
3	5C	207/264 (78%)	202 (98%)	5 (2%)	0	100	100
4	1D	427/466 (92%)	409 (96%)	18 (4%)	0	100	100
4	5D	427/466 (92%)	410 (96%)	17 (4%)	0	100	100
5	1E	212/249 (85%)	199 (94%)	13 (6%)	0	100	100
5	5E	212/249 (85%)	199 (94%)	13 (6%)	0	100	100
6	1F	430/464 (93%)	411 (96%)	17 (4%)	2 (0%)	24	63
6	5F	430/464 (93%)	411 (96%)	17 (4%)	2 (0%)	24	63
7	1G	697/727 (96%)	675 (97%)	19 (3%)	3 (0%)	30	67
7	5G	697/727 (96%)	675 (97%)	19 (3%)	3 (0%)	30	67
8	1H	316/318 (99%)	293 (93%)	21 (7%)	2 (1%)	21	59
8	5H	316/318 (99%)	295 (93%)	20 (6%)	1 (0%)	36	72
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
9	5I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	155 (90%)	15 (9%)	2 (1%)	10	44
10	5J	172/175 (98%)	158 (92%)	12 (7%)	2 (1%)	10	44
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
11	5K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	1L	604/606 (100%)	568 (94%)	33 (6%)	3 (0%)	24	63
12	5L	604/606 (100%)	568 (94%)	33 (6%)	3 (0%)	24	63
13	1M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	5M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	43	78
14	1N	345/347 (99%)	337 (98%)	7 (2%)	1 (0%)	36	72
14	5N	345/347 (99%)	337 (98%)	7 (2%)	1 (0%)	36	72
15	1O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
15	5O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
16	5P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
17	1Q	127/175 (73%)	122 (96%)	5 (4%)	0	100	100
17	5Q	127/175 (73%)	122 (96%)	5 (4%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
18	5R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
19	5S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	83 (100%)	0	0	100	100
20	1U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
20	5T	83/156 (53%)	83 (100%)	0	0	100	100
20	5U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
21	5V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
22	5W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	59
23	5X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	59
24	1Y	137/141 (97%)	136 (99%)	1 (1%)	0	100	100
24	5Y	137/141 (97%)	136 (99%)	1 (1%)	0	100	100
25	1Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
25	5Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
26	5a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
27	5b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1c	47/76 (62%)	47 (100%)	0	0	100	100
28	5c	47/76 (62%)	47 (100%)	0	0	100	100
29	1d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
29	5d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
30	5e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
31	5f	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
32	5g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
33	1h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
33	5h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	1i	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
34	5i	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
35	5j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	77 (98%)	2 (2%)	0	100	100
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
37	5l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	1m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
38	5m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
39	1n	170/179 (95%)	162 (95%)	8 (5%)	0	100	100
39	5n	170/179 (95%)	162 (95%)	8 (5%)	0	100	100
40	1o	120/136 (88%)	120 (100%)	0	0	100	100
40	5o	120/136 (88%)	120 (100%)	0	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
41	5p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
42	5q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	1r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	5r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
44	5s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
45	3A	436/480 (91%)	428 (98%)	6 (1%)	2 (0%)	24	63
45	3N	443/480 (92%)	387 (87%)	44 (10%)	12 (3%)	4	25
45	6A	436/480 (91%)	297 (68%)	110 (25%)	29 (7%)	1	12
45	6N	443/480 (92%)	289 (65%)	113 (26%)	41 (9%)	0	8
46	3B	416/453 (92%)	407 (98%)	9 (2%)	0	100	100
46	3O	415/453 (92%)	366 (88%)	40 (10%)	9 (2%)	5	29
46	6B	416/453 (92%)	302 (73%)	96 (23%)	18 (4%)	2	17
46	6O	415/453 (92%)	288 (69%)	103 (25%)	24 (6%)	1	13
47	3C	377/379 (100%)	333 (88%)	35 (9%)	9 (2%)	4	27
47	3P	377/379 (100%)	370 (98%)	7 (2%)	0	100	100
47	6C	377/379 (100%)	223 (59%)	115 (30%)	39 (10%)	0	6
47	6P	377/379 (100%)	370 (98%)	7 (2%)	0	100	100
48	3D	235/326 (72%)	230 (98%)	5 (2%)	0	100	100
48	3Q	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
48	6D	235/326 (72%)	156 (66%)	47 (20%)	32 (14%)	0	3
48	6Q	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
49	3E	194/274 (71%)	176 (91%)	17 (9%)	1 (0%)	24	63
49	3I	45/274 (16%)	40 (89%)	5 (11%)	0	100	100
49	3R	194/274 (71%)	173 (89%)	17 (9%)	4 (2%)	5	30
49	3V	29/274 (11%)	29 (100%)	0	0	100	100
49	6E	194/274 (71%)	175 (90%)	18 (9%)	1 (0%)	24	63
49	6I	45/274 (16%)	40 (89%)	5 (11%)	0	100	100
49	6R	194/274 (71%)	173 (89%)	17 (9%)	4 (2%)	5	30
49	6V	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%)	95 (99%)	1 (1%)	0	100	100
50	6F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	6S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	3G	70/82 (85%)	59 (84%)	10 (14%)	1 (1%)	9	40
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
51	6G	70/82 (85%)	70 (100%)	0	0	100	100
51	6T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	63/91 (69%)	59 (94%)	2 (3%)	2 (3%)	3	21
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
52	6H	63/91 (69%)	58 (92%)	4 (6%)	1 (2%)	7	38
52	6U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	6	32
53	3W	54/64 (84%)	54 (100%)	0	0	100	100
53	6J	54/64 (84%)	36 (67%)	15 (28%)	3 (6%)	1	14
53	6W	54/64 (84%)	54 (100%)	0	0	100	100
54	3X	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
54	6X	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
54	6Y	49/56 (88%)	32 (65%)	12 (24%)	5 (10%)	0	6
55	4A	511/514 (99%)	493 (96%)	15 (3%)	3 (1%)	21	59
55	8A	511/514 (99%)	329 (64%)	146 (29%)	36 (7%)	1	11
56	4B	225/229 (98%)	215 (96%)	9 (4%)	1 (0%)	30	67
56	8B	225/229 (98%)	215 (96%)	9 (4%)	1 (0%)	30	67
57	4C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
58	4D	137/169 (81%)	131 (96%)	6 (4%)	0	100	100
58	8D	137/169 (81%)	131 (96%)	6 (4%)	0	100	100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
59	8E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
60	4F	95/129 (74%)	92 (97%)	3 (3%)	0	100	100
60	8F	95/129 (74%)	92 (97%)	3 (3%)	0	100	100
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
61	8G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	8H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
63	4I	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
63	8I	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
64	8J	56/80 (70%)	55 (98%)	1 (2%)	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%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	42
68	8N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	42
All	All	28141/33842 (83%)	26038 (92%)	1775 (6%)	328 (1%)	13	44

5 of 328 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1B	59	MET
2	1B	84	ASP
2	1B	98	PRO
2	1B	102	LYS
2	1B	114	VAL

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%)	64 (65%)	35 (35%)	0	1
1	5A	99/99 (100%)	90 (91%)	9 (9%)	9	27
2	1B	131/212 (62%)	112 (86%)	19 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5B	131/212 (62%)	123 (94%)	8 (6%)	17	38
3	1C	191/228 (84%)	187 (98%)	4 (2%)	47	65
3	5C	191/228 (84%)	187 (98%)	4 (2%)	47	65
4	1D	371/396 (94%)	362 (98%)	9 (2%)	43	64
4	5D	371/396 (94%)	362 (98%)	9 (2%)	43	64
5	1E	183/207 (88%)	176 (96%)	7 (4%)	29	50
5	5E	183/207 (88%)	176 (96%)	7 (4%)	29	50
6	1F	346/368 (94%)	335 (97%)	11 (3%)	34	56
6	5F	346/368 (94%)	335 (97%)	11 (3%)	34	56
7	1G	588/610 (96%)	570 (97%)	18 (3%)	35	56
7	5G	588/610 (96%)	568 (97%)	20 (3%)	32	54
8	1H	274/274 (100%)	264 (96%)	10 (4%)	31	52
8	5H	274/274 (100%)	264 (96%)	10 (4%)	31	52
9	1I	151/201 (75%)	147 (97%)	4 (3%)	40	62
9	5I	151/201 (75%)	147 (97%)	4 (3%)	40	62
10	1J	140/141 (99%)	132 (94%)	8 (6%)	18	40
10	5J	140/141 (99%)	132 (94%)	8 (6%)	18	40
11	1K	84/84 (100%)	84 (100%)	0	100	100
11	5K	84/84 (100%)	83 (99%)	1 (1%)	63	75
12	1L	539/539 (100%)	526 (98%)	13 (2%)	43	64
12	5L	539/539 (100%)	527 (98%)	12 (2%)	45	64
13	1M	408/408 (100%)	397 (97%)	11 (3%)	39	61
13	5M	408/408 (100%)	397 (97%)	11 (3%)	39	61
14	1N	310/310 (100%)	305 (98%)	5 (2%)	55	70
14	5N	310/310 (100%)	305 (98%)	5 (2%)	55	70
15	1O	283/307 (92%)	268 (95%)	15 (5%)	20	41
15	5O	283/307 (92%)	269 (95%)	14 (5%)	22	43
16	1P	296/323 (92%)	289 (98%)	7 (2%)	43	64
16	5P	296/323 (92%)	289 (98%)	7 (2%)	43	64
17	1Q	117/152 (77%)	110 (94%)	7 (6%)	17	39
17	5Q	117/152 (77%)	110 (94%)	7 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1R	79/97 (81%)	78 (99%)	1 (1%)	61	74
18	5R	79/97 (81%)	78 (99%)	1 (1%)	61	74
19	1S	77/82 (94%)	74 (96%)	3 (4%)	28	49
19	5S	77/82 (94%)	74 (96%)	3 (4%)	28	49
20	1T	79/133 (59%)	78 (99%)	1 (1%)	61	74
20	1U	79/133 (59%)	73 (92%)	6 (8%)	12	33
20	5T	79/133 (59%)	78 (99%)	1 (1%)	61	74
20	5U	79/133 (59%)	73 (92%)	6 (8%)	12	33
21	1V	100/101 (99%)	97 (97%)	3 (3%)	36	57
21	5V	100/101 (99%)	97 (97%)	3 (3%)	36	57
22	1W	107/112 (96%)	105 (98%)	2 (2%)	50	67
22	5W	107/112 (96%)	105 (98%)	2 (2%)	50	67
23	1X	153/154 (99%)	148 (97%)	5 (3%)	33	55
23	5X	153/154 (99%)	147 (96%)	6 (4%)	28	49
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	28	49
24	5Y	101/102 (99%)	97 (96%)	4 (4%)	28	49
25	1Z	123/124 (99%)	121 (98%)	2 (2%)	55	70
25	5Z	123/124 (99%)	121 (98%)	2 (2%)	55	70
26	1a	58/58 (100%)	57 (98%)	1 (2%)	53	69
26	5a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	35
27	5b	69/70 (99%)	64 (93%)	5 (7%)	13	35
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	36
28	5c	45/66 (68%)	42 (93%)	3 (7%)	15	36
29	1d	106/109 (97%)	101 (95%)	5 (5%)	23	45
29	5d	106/109 (97%)	101 (95%)	5 (5%)	23	45
30	1e	87/94 (93%)	84 (97%)	3 (3%)	32	54
30	5e	87/94 (93%)	84 (97%)	3 (3%)	32	54
31	1f	54/55 (98%)	53 (98%)	1 (2%)	50	67
31	5f	54/55 (98%)	53 (98%)	1 (2%)	50	67
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	5g	92/129 (71%)	91 (99%)	1 (1%)	65	76
33	1h	121/158 (77%)	117 (97%)	4 (3%)	33	55
33	5h	121/158 (77%)	117 (97%)	4 (3%)	33	55
34	1i	120/120 (100%)	118 (98%)	2 (2%)	53	69
34	5i	120/120 (100%)	118 (98%)	2 (2%)	53	69
35	1j	62/84 (74%)	61 (98%)	1 (2%)	55	70
35	5j	62/84 (74%)	60 (97%)	2 (3%)	34	56
36	1k	63/76 (83%)	62 (98%)	1 (2%)	55	70
36	5k	63/76 (83%)	59 (94%)	4 (6%)	16	37
37	1l	141/161 (88%)	139 (99%)	2 (1%)	59	72
37	5l	141/161 (88%)	139 (99%)	2 (1%)	59	72
38	1m	113/114 (99%)	109 (96%)	4 (4%)	32	53
38	5m	113/114 (99%)	109 (96%)	4 (4%)	32	53
39	1n	156/160 (98%)	153 (98%)	3 (2%)	50	67
39	5n	156/160 (98%)	153 (98%)	3 (2%)	50	67
40	1o	110/119 (92%)	104 (94%)	6 (6%)	19	41
40	5o	110/119 (92%)	104 (94%)	6 (6%)	19	41
41	1p	154/156 (99%)	150 (97%)	4 (3%)	40	62
41	5p	154/156 (99%)	150 (97%)	4 (3%)	40	62
42	1q	131/131 (100%)	129 (98%)	2 (2%)	57	72
42	5q	131/131 (100%)	129 (98%)	2 (2%)	57	72
43	1r	85/98 (87%)	83 (98%)	2 (2%)	43	64
43	5r	85/98 (87%)	83 (98%)	2 (2%)	43	64
44	1s	44/351 (12%)	39 (89%)	5 (11%)	5	18
44	5s	44/351 (12%)	39 (89%)	5 (11%)	5	18
45	3A	367/397 (92%)	360 (98%)	7 (2%)	50	67
45	3N	371/397 (94%)	353 (95%)	18 (5%)	22	43
45	6A	367/397 (92%)	234 (64%)	133 (36%)	0	1
45	6N	371/397 (94%)	295 (80%)	76 (20%)	1	7
46	3B	329/355 (93%)	322 (98%)	7 (2%)	47	65
46	3O	328/355 (92%)	298 (91%)	30 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	6B	329/355 (93%)	195 (59%)	134 (41%)	0	0
46	6O	328/355 (92%)	202 (62%)	126 (38%)	0	1
47	3C	332/332 (100%)	300 (90%)	32 (10%)	8	25
47	3P	332/332 (100%)	330 (99%)	2 (1%)	78	83
47	6C	332/332 (100%)	212 (64%)	120 (36%)	0	1
47	6P	332/332 (100%)	331 (100%)	1 (0%)	86	86
48	3D	202/259 (78%)	198 (98%)	4 (2%)	48	66
48	3Q	204/259 (79%)	202 (99%)	2 (1%)	68	78
48	6D	202/259 (78%)	123 (61%)	79 (39%)	0	1
48	6Q	204/259 (79%)	201 (98%)	3 (2%)	57	72
49	3E	166/225 (74%)	164 (99%)	2 (1%)	63	75
49	3I	36/225 (16%)	30 (83%)	6 (17%)	2	10
49	3R	166/225 (74%)	158 (95%)	8 (5%)	23	44
49	3V	24/225 (11%)	22 (92%)	2 (8%)	10	30
49	6E	166/225 (74%)	164 (99%)	2 (1%)	63	75
49	6I	36/225 (16%)	31 (86%)	5 (14%)	3	14
49	6R	166/225 (74%)	158 (95%)	8 (5%)	23	44
49	6V	24/225 (11%)	22 (92%)	2 (8%)	10	30
50	3F	90/99 (91%)	90 (100%)	0	100	100
50	3S	90/99 (91%)	90 (100%)	0	100	100
50	6F	90/99 (91%)	90 (100%)	0	100	100
50	6S	90/99 (91%)	90 (100%)	0	100	100
51	3G	66/73 (90%)	60 (91%)	6 (9%)	9	27
51	3T	67/73 (92%)	67 (100%)	0	100	100
51	6G	66/73 (90%)	66 (100%)	0	100	100
51	6T	67/73 (92%)	67 (100%)	0	100	100
52	3H	62/85 (73%)	57 (92%)	5 (8%)	11	31
52	3U	62/85 (73%)	57 (92%)	5 (8%)	11	31
52	6H	62/85 (73%)	59 (95%)	3 (5%)	23	44
52	6U	62/85 (73%)	57 (92%)	5 (8%)	11	31
53	3J	46/52 (88%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	3W	46/52 (88%)	46 (100%)	0	100	100
53	6J	46/52 (88%)	25 (54%)	21 (46%)	0	0
53	6W	46/52 (88%)	46 (100%)	0	100	100
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	40 (98%)	1 (2%)	43	64
54	6X	42/46 (91%)	42 (100%)	0	100	100
54	6Y	41/46 (89%)	23 (56%)	18 (44%)	0	0
55	4A	424/424 (100%)	417 (98%)	7 (2%)	53	69
55	8A	424/424 (100%)	296 (70%)	128 (30%)	0	2
56	4B	210/211 (100%)	198 (94%)	12 (6%)	18	40
56	8B	210/211 (100%)	200 (95%)	10 (5%)	23	44
57	4C	223/225 (99%)	215 (96%)	8 (4%)	31	52
57	8C	223/225 (99%)	215 (96%)	8 (4%)	31	52
58	4D	124/149 (83%)	121 (98%)	3 (2%)	43	64
58	8D	124/149 (83%)	121 (98%)	3 (2%)	43	64
59	4E	92/124 (74%)	87 (95%)	5 (5%)	20	41
59	8E	92/124 (74%)	87 (95%)	5 (5%)	20	41
60	4F	80/101 (79%)	74 (92%)	6 (8%)	12	33
60	8F	80/101 (79%)	74 (92%)	6 (8%)	12	33
61	4G	65/80 (81%)	60 (92%)	5 (8%)	12	32
61	8G	65/80 (81%)	60 (92%)	5 (8%)	12	32
62	4H	73/76 (96%)	70 (96%)	3 (4%)	27	49
62	8H	73/76 (96%)	70 (96%)	3 (4%)	27	49
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	49
64	8J	49/68 (72%)	47 (96%)	2 (4%)	27	49
65	4K	38/66 (58%)	35 (92%)	3 (8%)	11	32
65	8K	38/66 (58%)	36 (95%)	2 (5%)	20	41
66	4L	39/55 (71%)	38 (97%)	1 (3%)	40	62
66	8L	39/55 (71%)	38 (97%)	1 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	4M	37/57 (65%)	36 (97%)	1 (3%)	39	61
67	8M	37/57 (65%)	36 (97%)	1 (3%)	39	61
68	4N	70/70 (100%)	67 (96%)	3 (4%)	26	47
68	8N	70/70 (100%)	67 (96%)	3 (4%)	26	47
All	All	24534/28538 (86%)	22927 (93%)	1607 (7%)	17	37

5 of 1607 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	6B	335	ASP
48	6D	303	LEU
64	8J	10	LYS
46	6B	421	ARG
46	6B	329	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 378 such sidechains are listed below:

Mol	Chain	Res	Type
25	5Z	76	GLN
47	6C	263	ASN
29	5d	88	HIS
44	5s	43	HIS
49	6E	257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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
8	FME	5H	1	8	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
56	FME	8B	1	56	8,9,10	0.53	0	8,9,11	1.02	1 (12%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	1.07	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	0.92	1 (12%)
1	FME	5A	1	1	8,9,10	0.59	0	8,9,11	1.00	1 (12%)
11	FME	5K	1	11	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
56	FME	4B	1	56	8,9,10	0.54	0	8,9,11	1.02	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	0.97	1 (12%)
1	FME	1A	1	-	8,9,10	0.54	0	8,9,11	1.09	1 (12%)
12	FME	5L	1	12	8,9,10	0.53	0	8,9,11	0.90	1 (12%)
13	FME	5M	1	13	8,9,10	0.54	0	8,9,11	1.08	1 (12%)
14	FME	5N	1	14	8,9,10	0.59	0	8,9,11	0.98	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
8	FME	5H	1	8	-	1/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
56	FME	8B	1	56	-	4/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
1	FME	5A	1	1	-	0/7/9/11	-
11	FME	5K	1	11	-	1/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
56	FME	4B	1	56	-	4/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
1	FME	1A	1	-	-	5/7/9/11	-
12	FME	5L	1	12	-	0/7/9/11	-
13	FME	5M	1	13	-	1/7/9/11	-
14	FME	5N	1	14	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1	FME	O-C-CA	-2.87	117.40	124.77
11	5K	1	FME	O-C-CA	-2.68	117.89	124.77
14	5N	1	FME	O-C-CA	-2.66	117.92	124.77
11	1K	1	FME	O-C-CA	-2.65	117.95	124.77
13	5M	1	FME	O-C-CA	-2.65	117.96	124.77

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O1-CN-N-CA
1	1A	1	FME	C-CA-CB-CG
1	1A	1	FME	O-C-CA-CB
8	1H	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	8B	1	FME	1	0
13	1M	1	FME	2	0
1	5A	1	FME	3	0
11	5K	1	FME	1	0
11	1K	1	FME	2	0
56	4B	1	FME	1	0
14	1N	1	FME	3	0
13	5M	1	FME	2	0
14	5N	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 169 ligands modelled in this entry, 14 are monoatomic - leaving 155 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
84	HEC	3Q	501	48	46,50,50	2.60	25 (54%)	58,82,82	2.05	18 (31%)
82	PGV	8J	101	-	50,50,50	0.29	0	53,56,56	0.34	0
81	AME	1h	201	-	9,10,11	0.52	0	9,11,13	1.08	1 (11%)
72	FES	6R	301	49	0,4,4	-	-	-	-	-
85	HEA	8A	605	55	67,67,67	2.39	23 (34%)	81,103,103	2.51	32 (39%)
71	PC1	5M	502	-	43,43,53	0.32	0	49,51,61	0.37	0
72	FES	6E	301	49	0,4,4	-	-	-	-	-
71	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.32	0
75	CDL	8A	610	-	99,99,99	0.28	0	105,111,111	0.42	1 (0%)
91	PO4	8H	101	-	4,4,4	1.01	0	6,6,6	0.44	0
83	HEM	6P	501	47	50,50,50	1.58	8 (16%)	67,82,82	1.56	11 (16%)
82	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.32	0
90	PEK	4C	307	-	51,51,52	0.27	0	54,56,57	0.39	0
82	PGV	8K	101	-	50,50,50	0.30	0	53,56,56	0.32	0
75	CDL	5L	702	-	75,75,99	0.30	0	81,87,111	0.39	0
75	CDL	4C	308	-	99,99,99	0.28	0	105,111,111	0.42	1 (0%)
70	SF4	1F	502	6	0,12,12	-	-	-	-	-
70	SF4	1I	203	9	0,12,12	-	-	-	-	-
83	HEM	3C	501	47	50,50,50	1.61	9 (18%)	67,82,82	1.75	14 (20%)
75	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.39	0
71	PC1	5B	202	-	45,45,53	0.28	0	51,53,61	0.33	0
75	CDL	1L	702	-	75,75,99	0.30	0	81,87,111	0.39	0
71	PC1	1P	401	-	32,32,53	0.35	0	38,40,61	0.40	0
69	3PE	5Y	204	-	32,32,50	0.33	0	35,37,55	0.45	0
75	CDL	1i	201	-	79,79,99	0.30	0	85,91,111	0.44	0
81	AME	5h	201	-	9,10,11	0.52	0	9,11,13	1.07	1 (11%)
69	3PE	1J	202	-	43,43,50	0.29	0	46,48,55	0.39	0
83	HEM	6C	502	47	50,50,50	1.63	8 (16%)	67,82,82	1.58	14 (20%)
71	PC1	1Y	201	-	34,34,53	0.32	0	40,42,61	0.42	0
69	3PE	5M	501	-	44,44,50	0.29	0	47,49,55	0.37	0
80	EHZ	5n	201	-	31,36,37	0.18	0	36,44,47	1.14	1 (2%)
75	CDL	5N	903	-	61,61,99	0.31	0	67,73,111	0.57	1 (1%)
71	PC1	5m	201	-	45,45,53	0.30	0	51,53,61	1.06	3 (5%)
88	CUA	4B	302	56	0,1,1	-	-	-	-	-
82	PGV	8G	101	-	50,50,50	0.29	0	53,56,56	0.39	0
88	CUA	8B	303	56	0,1,1	-	-	-	-	-
82	PGV	4A	604	-	50,50,50	0.31	0	53,56,56	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.32	0
75	CDL	5q	201	-	60,60,99	0.34	0	66,72,111	0.41	0
76	GTP	1O	401	77	33,34,34	0.59	0	50,54,54	0.65	0
69	3PE	1N	901	-	48,48,50	0.33	0	51,53,55	0.39	0
70	SF4	5G	801	7	0,12,12	-	-	-		
71	PC1	1H	401	-	47,47,53	0.28	0	53,55,61	0.37	0
69	3PE	1Y	203	-	29,29,50	0.34	0	32,34,55	0.69	1 (3%)
72	FES	3R	301	49	0,4,4	-	-	-		
70	SF4	1G	801	7	0,12,12	-	-	-		
90	PEK	8C	306	-	52,52,52	0.26	0	55,57,57	0.47	0
82	PGV	4C	303	-	50,50,50	0.31	0	53,56,56	0.42	0
83	HEM	6C	501	47	50,50,50	1.64	9 (18%)	67,82,82	1.79	17 (25%)
69	3PE	5L	701	-	45,45,50	0.29	0	48,50,55	0.42	0
69	3PE	5d	201	-	47,47,50	0.29	0	50,52,55	0.42	0
71	PC1	1M	502	-	43,43,53	0.31	0	49,51,61	0.37	0
71	PC1	5I	201	-	53,53,53	0.27	0	59,61,61	0.35	0
75	CDL	1q	201	-	60,60,99	0.34	0	66,72,111	0.41	0
69	3PE	1j	101	-	43,43,50	0.28	0	46,48,55	0.48	0
69	3PE	5N	902	-	50,50,50	0.28	0	53,55,55	0.41	0
83	HEM	6P	502	47	50,50,50	1.59	9 (18%)	67,82,82	1.59	14 (20%)
84	HEC	6Q	501	48	46,50,50	2.60	25 (54%)	58,82,82	2.05	18 (31%)
70	SF4	1G	802	7	0,12,12	-	-	-		
82	PGV	4C	302	-	50,50,50	0.30	0	53,56,56	0.34	0
82	PGV	8L	101	-	50,50,50	0.31	0	53,56,56	0.40	0
69	3PE	1Y	206	-	40,40,50	0.30	0	43,45,55	0.68	1 (2%)
82	PGV	8A	602	-	50,50,50	0.29	0	53,56,56	0.44	0
82	PGV	8C	301	-	50,50,50	0.29	0	53,56,56	0.39	0
72	FES	1G	803	7	0,4,4	-	-	-		
80	EHZ	1T	101	-	31,36,37	0.20	0	36,44,47	1.14	1 (2%)
69	3PE	1M	501	-	44,44,50	0.30	0	47,49,55	0.37	0
78	NDP	5P	402	-	51,52,52	0.51	0	71,80,80	0.81	2 (2%)
71	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.39	0
91	PO4	4H	101	-	4,4,4	1.00	0	6,6,6	0.44	0
69	3PE	5j	101	-	43,43,50	0.28	0	46,48,55	0.48	0
89	PSC	4B	303	-	51,51,51	0.30	0	57,59,59	0.43	0
69	3PE	5Y	202	-	39,39,50	0.29	0	42,44,55	0.39	0
75	CDL	5i	201	-	79,79,99	0.30	0	85,91,111	0.44	0
69	3PE	5L	703	-	44,44,50	0.28	0	47,49,55	0.42	0
78	NDP	1P	402	-	51,52,52	0.51	0	71,80,80	0.81	2 (2%)
90	PEK	8C	307	-	51,51,52	0.27	0	54,56,57	0.39	0
69	3PE	5N	901	-	48,48,50	0.32	0	51,53,55	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	SF4	5I	203	9	0,12,12	-	-	-		
70	SF4	5I	202	9	0,12,12	-	-	-		
71	PC1	1J	201	-	34,34,53	0.33	0	40,42,61	0.35	0
85	HEA	8A	606	55	67,67,67	2.44	24 (35%)	81,103,103	2.46	32 (39%)
82	PGV	4K	101	-	50,50,50	0.29	0	53,56,56	0.35	0
69	3PE	5Y	206	-	40,40,50	0.30	0	43,45,55	0.68	1 (2%)
75	CDL	5X	201	-	85,85,99	0.28	0	91,97,111	0.39	0
72	FES	5G	803	7	0,4,4	-	-	-		
69	3PE	5J	201	-	43,43,50	0.29	0	46,48,55	0.38	0
71	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.33	0
82	PGV	8A	603	-	50,50,50	0.33	0	53,56,56	0.36	0
73	FMN	1F	501	-	33,33,33	0.61	0	48,50,50	0.66	1 (2%)
69	3PE	1Y	202	-	39,39,50	0.29	0	42,44,55	0.39	0
75	CDL	4B	301	-	99,99,99	0.27	0	105,111,111	0.32	0
69	3PE	1N	902	-	50,50,50	0.28	0	53,55,55	0.41	0
84	HEC	6D	501	-	44,49,50	2.82	27 (61%)	56,80,82	1.90	18 (32%)
75	CDL	8B	302	-	99,99,99	0.27	0	105,111,111	0.31	0
82	PGV	4J	101	-	50,50,50	0.32	0	53,56,56	0.38	0
70	SF4	5B	201	2	0,12,12	-	-	-		
69	3PE	5Y	203	-	29,29,50	0.34	0	32,34,55	0.68	1 (3%)
75	CDL	5d	202	-	64,64,99	0.33	0	70,76,111	0.41	0
69	3PE	1M	503	-	49,49,50	0.27	0	52,54,55	0.36	0
75	CDL	8D	201	-	99,99,99	0.28	0	105,111,111	0.33	0
71	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
71	PC1	5I	204	-	43,43,53	0.29	0	49,51,61	0.33	0
82	PGV	4C	304	-	50,50,50	0.30	0	53,56,56	0.61	1 (1%)
69	3PE	1Y	205	-	26,26,50	0.35	0	29,31,55	0.43	0
82	PGV	4A	603	-	50,50,50	0.29	0	53,56,56	0.37	0
83	HEM	3P	502	47	50,50,50	1.58	9 (18%)	67,82,82	1.60	14 (20%)
82	PGV	8C	304	-	50,50,50	0.29	0	53,56,56	0.33	0
72	FES	3E	301	49	0,4,4	-	-	-		
82	PGV	8A	601	-	50,50,50	0.30	0	53,56,56	0.31	0
73	FMN	5F	501	-	33,33,33	0.61	0	48,50,50	0.66	1 (2%)
69	3PE	5A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
84	HEC	3D	501	48	44,49,50	2.63	24 (54%)	56,80,82	2.06	17 (30%)
80	EHZ	5T	101	-	31,36,37	0.19	0	36,44,47	1.14	1 (2%)
75	CDL	1d	202	-	64,64,99	0.33	0	70,76,111	0.41	0
76	GTP	5O	401	77	33,34,34	0.58	0	50,54,54	0.64	0
69	3PE	5M	503	-	49,49,50	0.27	0	52,54,55	0.36	0
82	PGV	8C	305	-	50,50,50	0.31	0	53,56,56	0.38	0
89	PSC	8A	611	-	51,51,51	0.29	0	57,59,59	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	HEM	3P	501	47	50,50,50	1.58	9 (18%)	67,82,82	1.57	10 (14%)
82	PGV	4L	101	-	50,50,50	0.31	0	53,56,56	0.40	0
71	PC1	5Y	201	-	34,34,53	0.33	0	40,42,61	0.42	0
80	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.14	1 (2%)
82	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.33	0
69	3PE	1L	704	-	30,30,50	0.34	0	33,35,55	0.68	1 (3%)
69	3PE	1d	201	-	47,47,50	0.29	0	50,52,55	0.43	0
85	HEA	4A	605	55	67,67,67	2.40	24 (35%)	81,103,103	2.51	33 (40%)
71	PC1	1m	201	-	45,45,53	0.31	0	51,53,61	1.07	3 (5%)
70	SF4	5G	802	7	0,12,12	-	-	-		
72	FES	5E	301	5	0,4,4	-	-	-		
71	PC1	5H	401	-	47,47,53	0.28	0	53,55,61	0.37	0
71	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.43	0
82	PGV	8B	301	-	50,50,50	0.31	0	53,56,56	0.31	0
82	PGV	8C	303	-	50,50,50	0.31	0	53,56,56	0.33	0
71	PC1	5h	202	-	46,46,53	0.27	0	52,54,61	0.31	0
72	FES	1E	301	5	0,4,4	-	-	-		
82	PGV	1p	201	-	50,50,50	0.29	0	53,56,56	0.33	0
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.42	0
82	PGV	4A	601	-	50,50,50	0.27	0	53,56,56	0.33	0
82	PGV	4C	305	-	50,50,50	0.31	0	53,56,56	0.38	0
70	SF4	1B	201	2	0,12,12	-	-	-		
70	SF4	5F	502	6	0,12,12	-	-	-		
85	HEA	4A	606	55	67,67,67	2.43	24 (35%)	81,103,103	2.46	33 (40%)
69	3PE	5Y	205	-	26,26,50	0.36	0	29,31,55	0.43	0
90	PEK	4C	306	-	52,52,52	0.26	0	55,57,57	0.47	0
69	3PE	1Y	204	-	32,32,50	0.33	0	35,37,55	0.45	0
70	SF4	1I	202	9	0,12,12	-	-	-		
71	PC1	1h	202	-	46,46,53	0.28	0	52,54,61	0.31	0
82	PGV	8A	604	-	50,50,50	0.31	0	53,56,56	0.35	0
75	CDL	1N	903	-	61,61,99	0.31	0	67,73,111	0.57	1 (1%)
83	HEM	3C	502	47	50,50,50	1.59	9 (18%)	67,82,82	1.65	14 (20%)
82	PGV	4C	301	-	50,50,50	0.30	0	53,56,56	0.72	1 (1%)
69	3PE	1L	701	-	45,45,50	0.30	0	48,50,55	0.42	0
82	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.44	1 (1%)
69	3PE	5L	704	-	30,30,50	0.34	0	33,35,55	0.69	1 (3%)

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
84	HEC	3Q	501	48	-	3/14/54/54	-
82	PGV	8J	101	-	-	29/55/55/55	-
81	AME	1h	201	-	-	2/9/10/12	-
72	FES	6R	301	49	-	-	0/1/1/1
85	HEA	8A	605	55	-	11/36/76/76	-
71	PC1	5M	502	-	-	7/47/47/57	-
72	FES	6E	301	49	-	-	0/1/1/1
71	PC1	1I	204	-	-	1/47/47/57	-
75	CDL	8A	610	-	-	28/110/110/110	-
83	HEM	6P	501	47	-	8/14/54/54	-
82	PGV	8C	302	-	-	31/55/55/55	-
90	PEK	4C	307	-	-	6/55/55/56	-
82	PGV	8K	101	-	-	29/55/55/55	-
75	CDL	5L	702	-	-	9/86/86/110	-
75	CDL	4C	308	-	-	27/110/110/110	-
70	SF4	1F	502	6	-	-	0/6/5/5
70	SF4	1I	203	9	-	-	0/6/5/5
83	HEM	3C	501	47	-	7/14/54/54	-
75	CDL	1X	201	-	-	18/96/96/110	-
71	PC1	5B	202	-	-	8/49/49/57	-
75	CDL	1L	702	-	-	9/86/86/110	-
71	PC1	1P	401	-	-	19/36/36/57	-
69	3PE	5Y	204	-	-	3/36/36/54	-
75	CDL	1i	201	-	-	9/90/90/110	-
81	AME	5h	201	-	-	2/9/10/12	-
69	3PE	1J	202	-	-	10/47/47/54	-
83	HEM	6C	502	47	-	5/14/54/54	-
71	PC1	1Y	201	-	-	8/38/38/57	-
69	3PE	5M	501	-	-	7/48/48/54	-
80	EHZ	5n	201	-	-	3/42/44/45	-
75	CDL	5N	903	-	-	8/71/71/110	-
71	PC1	5m	201	-	-	12/49/49/57	-
82	PGV	8G	101	-	-	29/55/55/55	-
82	PGV	4A	604	-	-	10/55/55/55	-
69	3PE	1A	201	-	-	26/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	5q	201	-	-	7/71/71/110	-
76	GTP	1O	401	77	-	4/22/38/38	0/3/3/3
69	3PE	1N	901	-	-	11/52/52/54	-
70	SF4	5G	801	7	-	-	0/6/5/5
71	PC1	1H	401	-	-	11/51/51/57	-
69	3PE	1Y	203	-	-	14/33/33/54	-
72	FES	3R	301	49	-	-	0/1/1/1
90	PEK	8C	306	-	-	10/56/56/56	-
70	SF4	1G	801	7	-	-	0/6/5/5
82	PGV	4C	303	-	-	16/55/55/55	-
83	HEM	6C	501	47	-	6/14/54/54	-
69	3PE	5L	701	-	-	5/49/49/54	-
69	3PE	5d	201	-	-	15/51/51/54	-
71	PC1	1M	502	-	-	7/47/47/57	-
71	PC1	5I	201	-	-	10/57/57/57	-
75	CDL	1q	201	-	-	7/71/71/110	-
69	3PE	1j	101	-	-	5/47/47/54	-
69	3PE	5N	902	-	-	8/54/54/54	-
83	HEM	6P	502	47	-	8/14/54/54	-
84	HEC	6Q	501	48	-	3/14/54/54	-
70	SF4	1G	802	7	-	-	0/6/5/5
82	PGV	4C	302	-	-	11/55/55/55	-
82	PGV	8L	101	-	-	7/55/55/55	-
69	3PE	1Y	206	-	-	12/44/44/54	-
82	PGV	8A	602	-	-	30/55/55/55	-
82	PGV	8C	301	-	-	34/55/55/55	-
72	FES	1G	803	7	-	-	0/1/1/1
80	EHZ	1T	101	-	-	15/42/44/45	-
69	3PE	1M	501	-	-	7/48/48/54	-
78	NDP	5P	402	-	-	3/34/77/77	0/5/5/5
71	PC1	5A	202	-	-	3/38/38/57	-
69	3PE	5j	101	-	-	5/47/47/54	-
89	PSC	4B	303	-	-	13/55/55/55	-
69	3PE	5Y	202	-	-	9/43/43/54	-
75	CDL	5i	201	-	-	9/90/90/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	5L	703	-	-	9/48/48/54	-
78	NDP	1P	402	-	-	3/34/77/77	0/5/5/5
90	PEK	8C	307	-	-	6/55/55/56	-
69	3PE	5N	901	-	-	11/52/52/54	-
70	SF4	5I	203	9	-	-	0/6/5/5
70	SF4	5I	202	9	-	-	0/6/5/5
71	PC1	1J	201	-	-	27/38/38/57	-
85	HEA	8A	606	55	-	5/36/76/76	-
82	PGV	4K	101	-	-	14/55/55/55	-
69	3PE	5Y	206	-	-	12/44/44/54	-
75	CDL	5X	201	-	-	18/96/96/110	-
72	FES	5G	803	7	-	-	0/1/1/1
69	3PE	5J	201	-	-	10/47/47/54	-
71	PC1	1B	202	-	-	8/49/49/57	-
82	PGV	8A	603	-	-	28/55/55/55	-
73	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
69	3PE	1Y	202	-	-	9/43/43/54	-
75	CDL	4B	301	-	-	21/110/110/110	-
69	3PE	1N	902	-	-	8/54/54/54	-
84	HEC	6D	501	-	-	4/13/53/54	-
75	CDL	8B	302	-	-	21/110/110/110	-
82	PGV	4J	101	-	-	11/55/55/55	-
70	SF4	5B	201	2	-	-	0/6/5/5
69	3PE	5Y	203	-	-	14/33/33/54	-
75	CDL	5d	202	-	-	22/75/75/110	-
69	3PE	1M	503	-	-	5/53/53/54	-
75	CDL	8D	201	-	-	66/110/110/110	-
71	PC1	1I	201	-	-	10/57/57/57	-
71	PC1	5I	204	-	-	1/47/47/57	-
82	PGV	4C	304	-	-	16/55/55/55	-
69	3PE	1Y	205	-	-	5/30/30/54	-
82	PGV	4A	603	-	-	7/55/55/55	-
83	HEM	3P	502	47	-	8/14/54/54	-
82	PGV	8C	304	-	-	35/55/55/55	-
72	FES	3E	301	49	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PGV	8A	601	-	-	32/55/55/55	-
73	FMN	5F	501	-	-	1/18/18/18	0/3/3/3
69	3PE	5A	201	-	-	9/50/50/54	-
84	HEC	3D	501	48	-	3/13/53/54	-
80	EHZ	5T	101	-	-	15/42/44/45	-
75	CDL	1d	202	-	-	22/75/75/110	-
76	GTP	5O	401	77	-	4/22/38/38	0/3/3/3
69	3PE	5M	503	-	-	5/53/53/54	-
82	PGV	8C	305	-	-	5/55/55/55	-
89	PSC	8A	611	-	-	13/55/55/55	-
83	HEM	3P	501	47	-	8/14/54/54	-
82	PGV	4L	101	-	-	7/55/55/55	-
71	PC1	5Y	201	-	-	8/38/38/57	-
80	EHZ	1n	201	-	-	3/42/44/45	-
82	PGV	4A	602	-	-	2/55/55/55	-
69	3PE	1L	704	-	-	7/34/34/54	-
69	3PE	1d	201	-	-	15/51/51/54	-
85	HEA	4A	605	55	-	11/36/76/76	-
71	PC1	1m	201	-	-	12/49/49/57	-
70	SF4	5G	802	7	-	-	0/6/5/5
72	FES	5E	301	5	-	-	0/1/1/1
71	PC1	5H	401	-	-	11/51/51/57	-
71	PC1	5P	401	-	-	9/36/36/57	-
82	PGV	8B	301	-	-	40/55/55/55	-
82	PGV	8C	303	-	-	32/55/55/55	-
71	PC1	5h	202	-	-	12/50/50/57	-
72	FES	1E	301	5	-	-	0/1/1/1
82	PGV	1p	201	-	-	40/55/55/55	-
69	3PE	1L	703	-	-	9/48/48/54	-
82	PGV	4A	601	-	-	13/55/55/55	-
82	PGV	4C	305	-	-	5/55/55/55	-
85	HEA	4A	606	55	-	5/36/76/76	-
70	SF4	1B	201	2	-	-	0/6/5/5
70	SF4	5F	502	6	-	-	0/6/5/5
69	3PE	5Y	205	-	-	5/30/30/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	PEK	4C	306	-	-	10/56/56/56	-
69	3PE	1Y	204	-	-	3/36/36/54	-
70	SF4	1I	202	9	-	-	0/6/5/5
71	PC1	1h	202	-	-	12/50/50/57	-
82	PGV	8A	604	-	-	35/55/55/55	-
75	CDL	1N	903	-	-	8/71/71/110	-
83	HEM	3C	502	47	-	6/14/54/54	-
82	PGV	4C	301	-	-	7/55/55/55	-
69	3PE	1L	701	-	-	5/49/49/54	-
82	PGV	4G	101	-	-	11/55/55/55	-
69	3PE	5L	704	-	-	7/34/34/54	-

The worst 5 of 266 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	4A	605	HEA	FE-NB	5.65	2.12	1.94
85	8A	605	HEA	FE-ND	5.63	2.12	1.94
85	4A	606	HEA	FE-NB	5.61	2.12	1.94
85	4A	605	HEA	FE-ND	5.60	2.12	1.94
85	8A	606	HEA	FE-NB	5.59	2.12	1.94

The worst 5 of 340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	4A	606	HEA	C3D-C4D-ND	6.93	117.05	110.35
85	8A	606	HEA	C3D-C4D-ND	6.90	117.02	110.35
85	8A	605	HEA	C3D-C4D-ND	6.45	116.58	110.35
80	5n	201	EHZ	C10-S1-C9	6.37	120.68	101.84
80	1n	201	EHZ	C10-S1-C9	6.37	120.67	101.84

There are no chirality outliers.

5 of 1571 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C1-O11-P-O14
69	1A	201	3PE	O13-C11-C12-N
69	1A	201	3PE	O32-C31-O31-C3
69	1A	201	3PE	C32-C31-O31-C3
69	1J	202	3PE	C1-O11-P-O13

There are no ring outliers.

144 monomers are involved in 752 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	3Q	501	HEC	2	0
82	8J	101	PGV	11	0
81	1h	201	AME	3	0
72	6R	301	FES	1	0
85	8A	605	HEA	10	0
71	5M	502	PC1	8	0
72	6E	301	FES	4	0
71	1I	204	PC1	5	0
75	8A	610	CDL	28	0
83	6P	501	HEM	1	0
82	8C	302	PGV	6	0
90	4C	307	PEK	4	0
82	8K	101	PGV	9	0
75	5L	702	CDL	2	0
75	4C	308	CDL	18	0
70	1F	502	SF4	2	0
83	3C	501	HEM	5	0
75	1X	201	CDL	12	0
71	5B	202	PC1	2	0
75	1L	702	CDL	3	0
71	1P	401	PC1	5	0
69	5Y	204	3PE	2	0
75	1i	201	CDL	8	0
81	5h	201	AME	3	0
69	1J	202	3PE	5	0
83	6C	502	HEM	6	0
71	1Y	201	PC1	3	0
69	5M	501	3PE	5	0
80	5n	201	EHZ	1	0
75	5N	903	CDL	4	0
71	5m	201	PC1	5	0
88	4B	302	CUA	3	0
82	8G	101	PGV	12	0
82	4A	604	PGV	7	0
69	1A	201	3PE	4	0
75	5q	201	CDL	5	0
76	1O	401	GTP	4	0
69	1N	901	3PE	4	0
71	1H	401	PC1	7	0
69	1Y	203	3PE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	3R	301	FES	1	0
90	8C	306	PEK	4	0
82	4C	303	PGV	8	0
83	6C	501	HEM	10	0
69	5L	701	3PE	2	0
69	5d	201	3PE	12	0
71	1M	502	PC1	8	0
71	5I	201	PC1	7	0
75	1q	201	CDL	5	0
69	5N	902	3PE	15	0
83	6P	502	HEM	5	0
84	6Q	501	HEC	2	0
70	1G	802	SF4	1	0
82	4C	302	PGV	9	0
82	8L	101	PGV	7	0
69	1Y	206	3PE	5	0
82	8A	602	PGV	13	0
82	8C	301	PGV	2	0
72	1G	803	FES	1	0
80	1T	101	EHZ	1	0
69	1M	501	3PE	5	0
78	5P	402	NDP	1	0
71	5A	202	PC1	1	0
89	4B	303	PSC	7	0
69	5Y	202	3PE	1	0
75	5i	201	CDL	9	0
69	5L	703	3PE	4	0
78	1P	402	NDP	1	0
90	8C	307	PEK	5	0
69	5N	901	3PE	5	0
71	1J	201	PC1	4	0
85	8A	606	HEA	6	0
82	4K	101	PGV	7	0
69	5Y	206	3PE	5	0
75	5X	201	CDL	13	0
72	5G	803	FES	1	0
69	5J	201	3PE	5	0
71	1B	202	PC1	3	0
82	8A	603	PGV	19	0
73	1F	501	FMN	2	0
69	1Y	202	3PE	1	0
75	4B	301	CDL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	1N	902	3PE	15	0
84	6D	501	HEC	5	0
75	8B	302	CDL	7	0
82	4J	101	PGV	11	0
70	5B	201	SF4	2	0
69	5Y	203	3PE	5	0
75	5d	202	CDL	7	0
69	1M	503	3PE	7	0
75	8D	201	CDL	19	0
71	1I	201	PC1	6	0
71	5I	204	PC1	4	0
82	4C	304	PGV	6	0
69	1Y	205	3PE	4	0
82	4A	603	PGV	10	0
83	3P	502	HEM	5	0
82	8C	304	PGV	10	0
72	3E	301	FES	4	0
82	8A	601	PGV	7	0
73	5F	501	FMN	1	0
69	5A	201	3PE	2	0
84	3D	501	HEC	2	0
80	5T	101	EHZ	1	0
75	1d	202	CDL	7	0
76	5O	401	GTP	5	0
69	5M	503	3PE	8	0
82	8C	305	PGV	12	0
89	8A	611	PSC	7	0
83	3P	501	HEM	1	0
82	4L	101	PGV	12	0
71	5Y	201	PC1	3	0
80	1n	201	EHZ	1	0
82	4A	602	PGV	3	0
69	1L	704	3PE	1	0
69	1d	201	3PE	11	0
85	4A	605	HEA	5	0
71	1m	201	PC1	5	0
70	5G	802	SF4	1	0
72	5E	301	FES	1	0
71	5H	401	PC1	5	0
71	5P	401	PC1	2	0
82	8B	301	PGV	10	0
82	8C	303	PGV	11	0

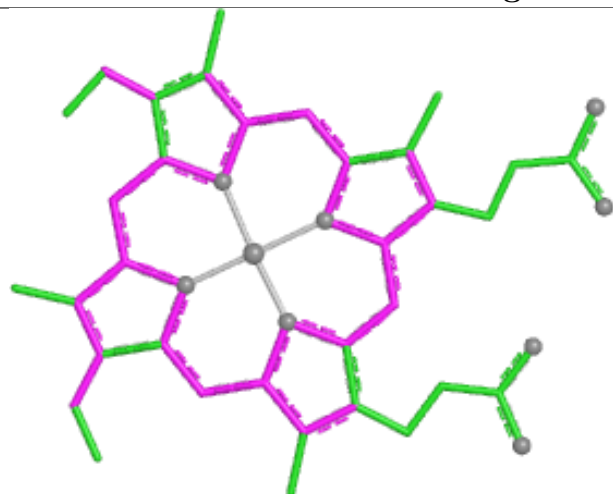
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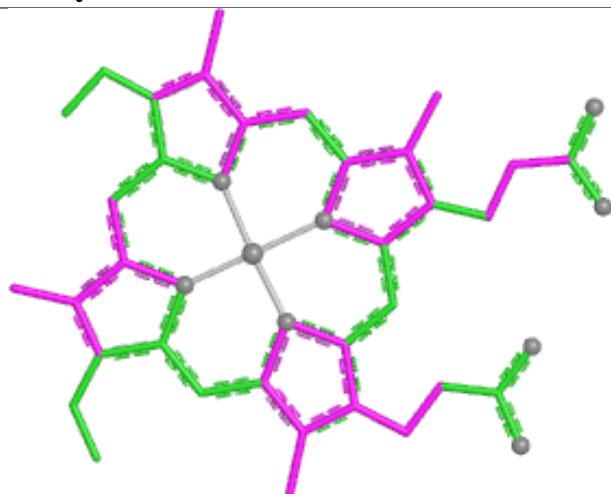
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	5h	202	PC1	3	0
72	1E	301	FES	1	0
82	1p	201	PGV	4	0
69	1L	703	3PE	4	0
82	4A	601	PGV	10	0
82	4C	305	PGV	7	0
70	1B	201	SF4	5	0
70	5F	502	SF4	2	0
85	4A	606	HEA	3	0
69	5Y	205	3PE	4	0
90	4C	306	PEK	3	0
69	1Y	204	3PE	2	0
71	1h	202	PC1	3	0
82	8A	604	PGV	7	0
75	1N	903	CDL	4	0
83	3C	502	HEM	6	0
82	4C	301	PGV	4	0
69	1L	701	3PE	3	0
82	4G	101	PGV	8	0
69	5L	704	3PE	1	0

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

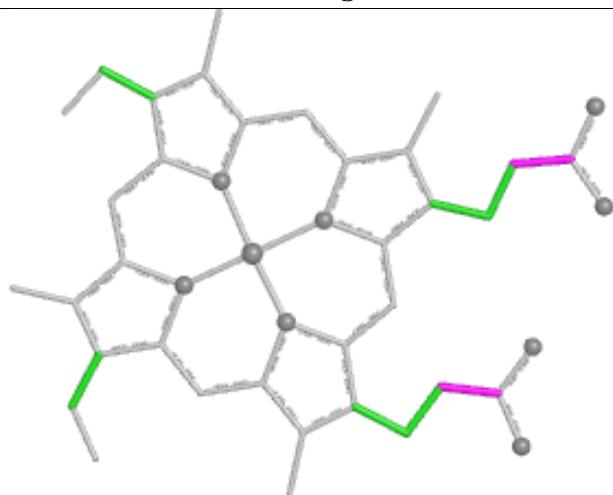
Ligand HEC 3Q 501



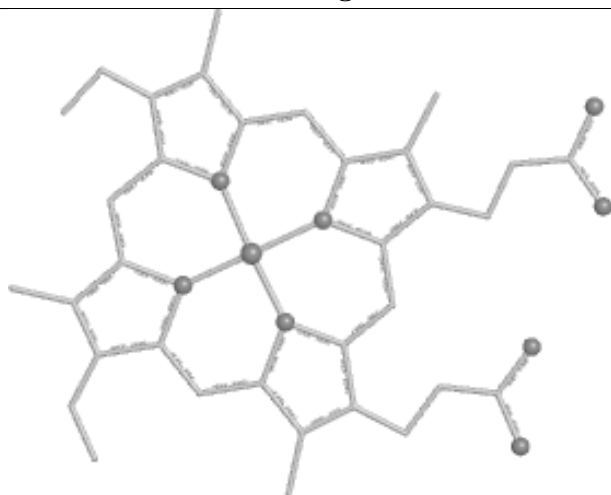
Bond lengths



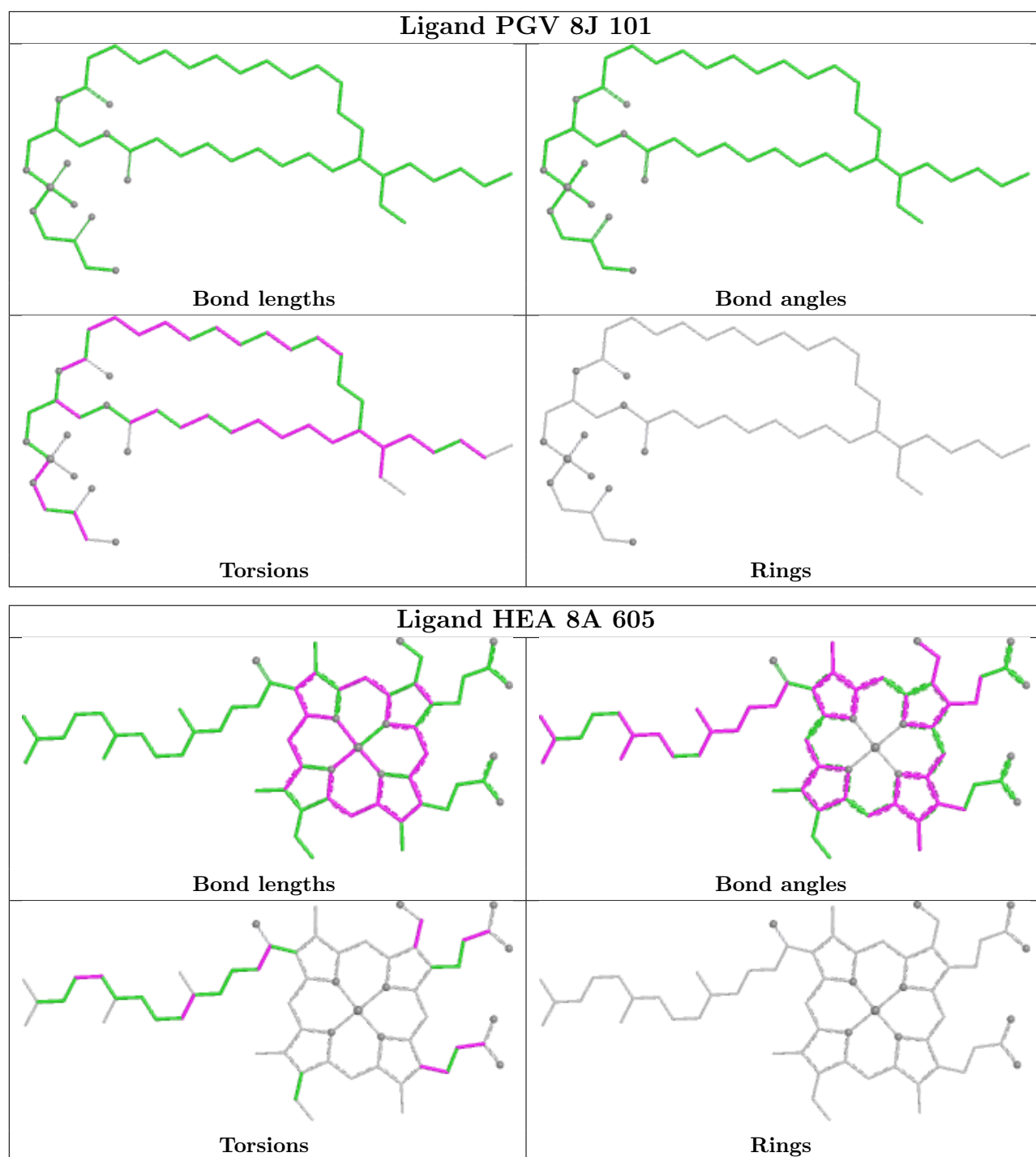
Bond angles

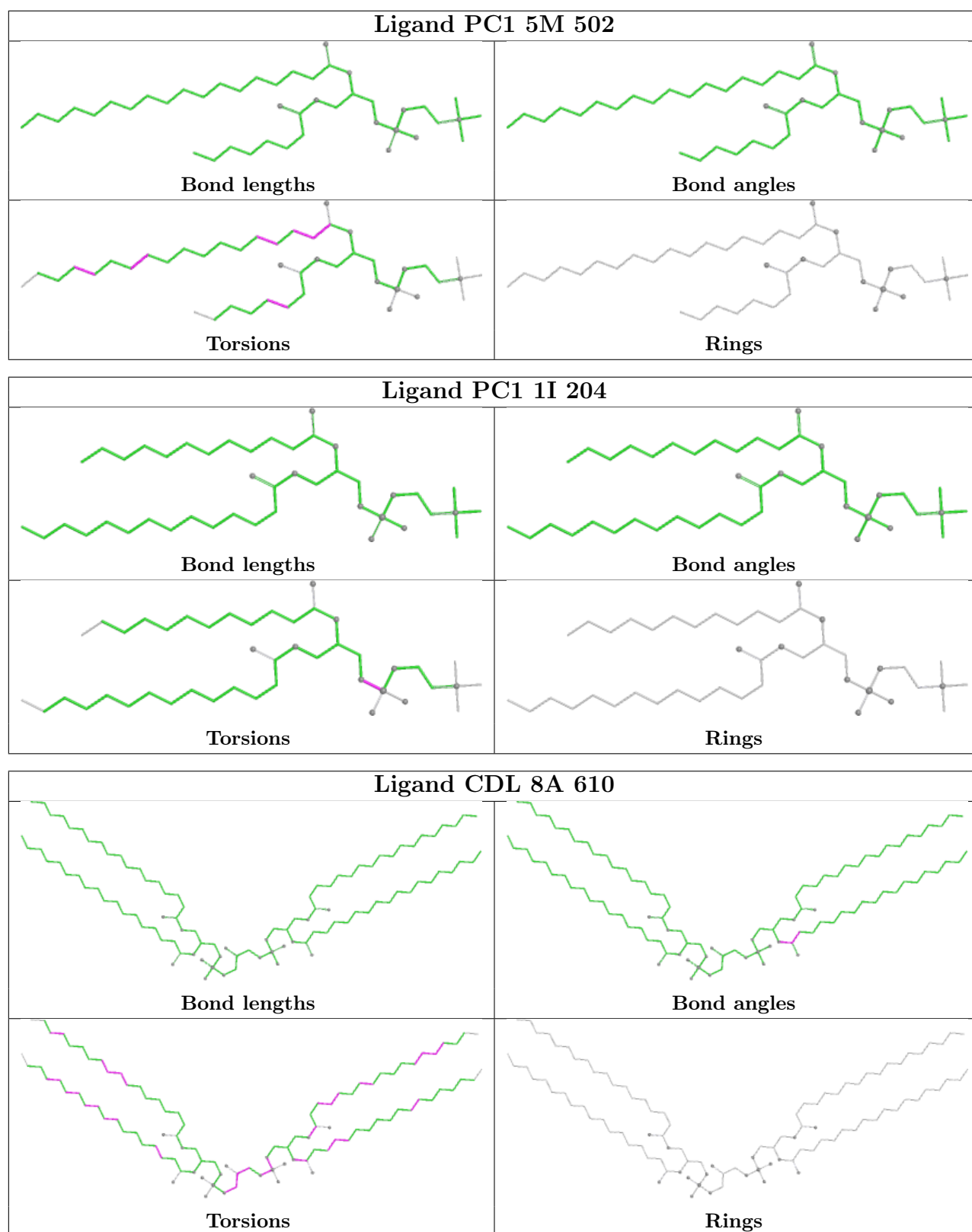


Torsions

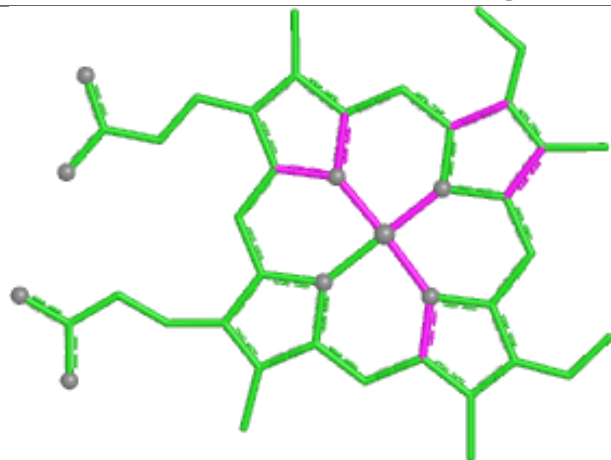


Rings

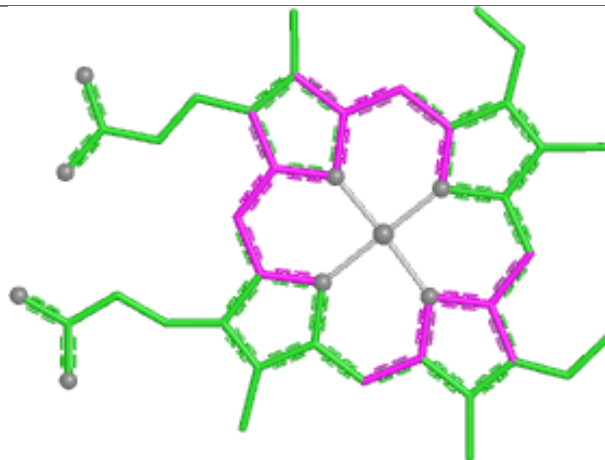




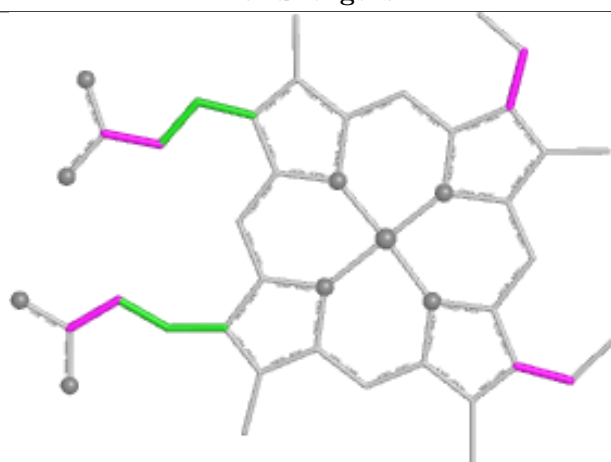
Ligand HEM 6P 501



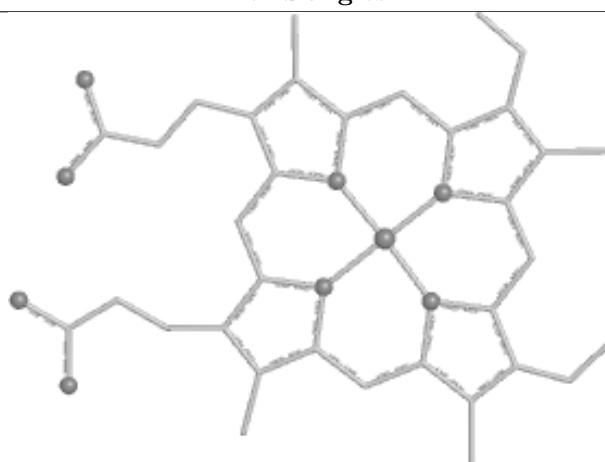
Bond lengths



Bond angles

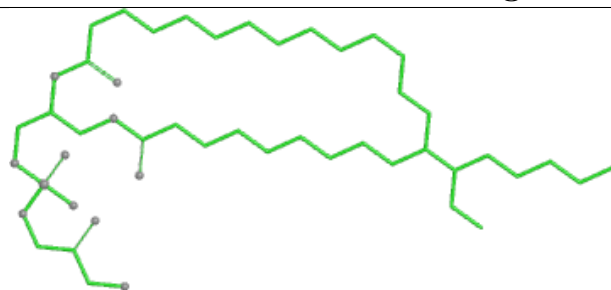


Torsions

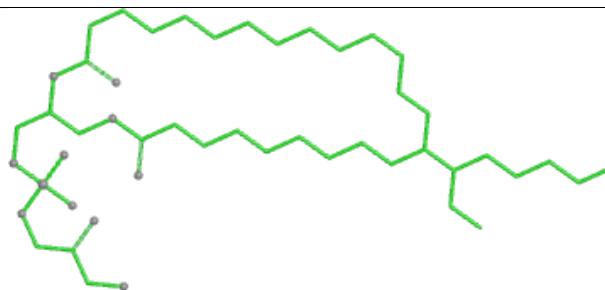


Rings

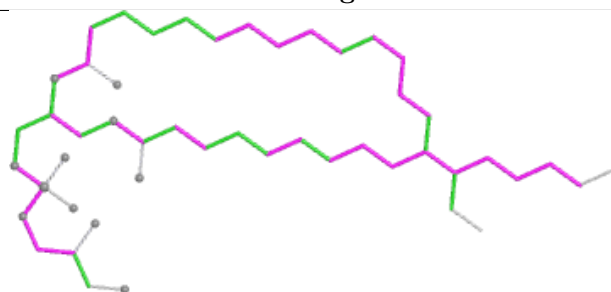
Ligand PGV 8C 302



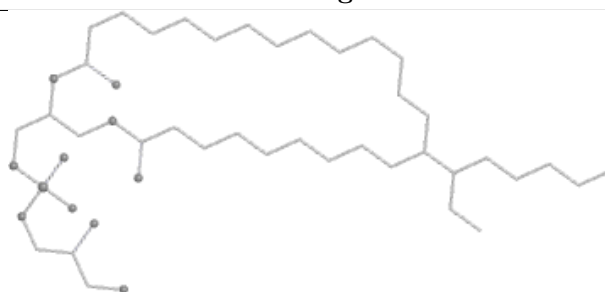
Bond lengths



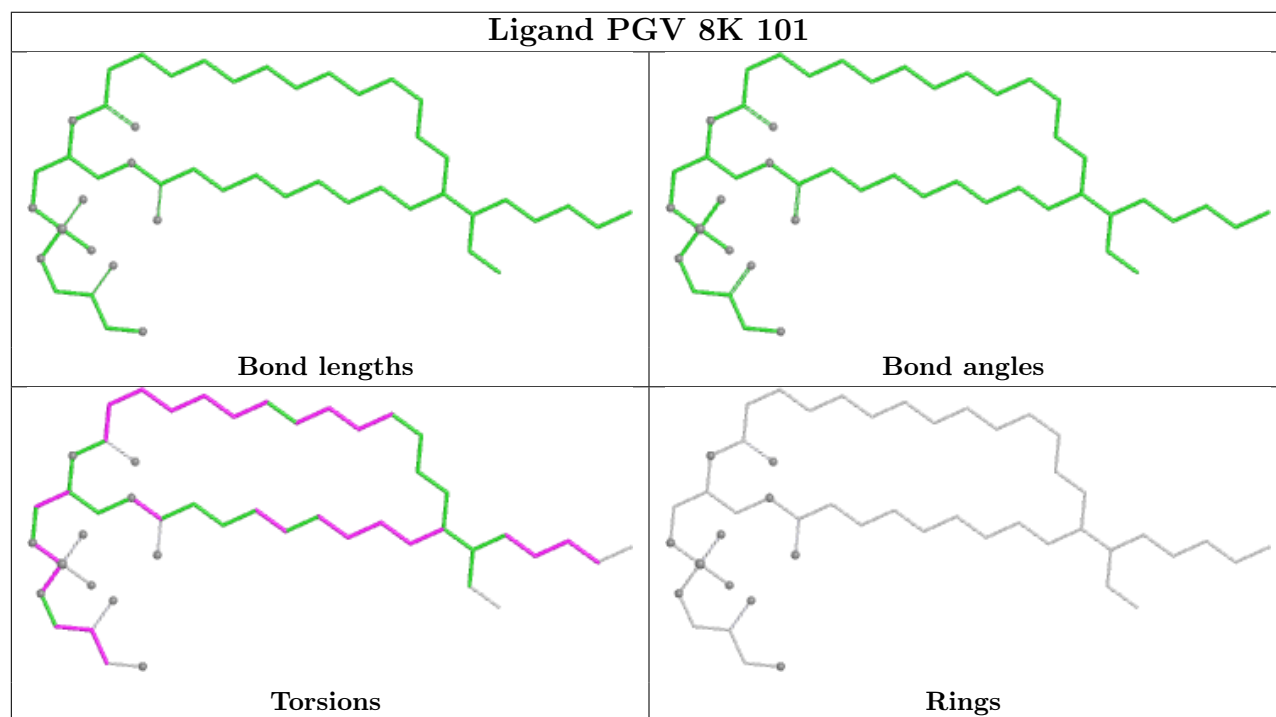
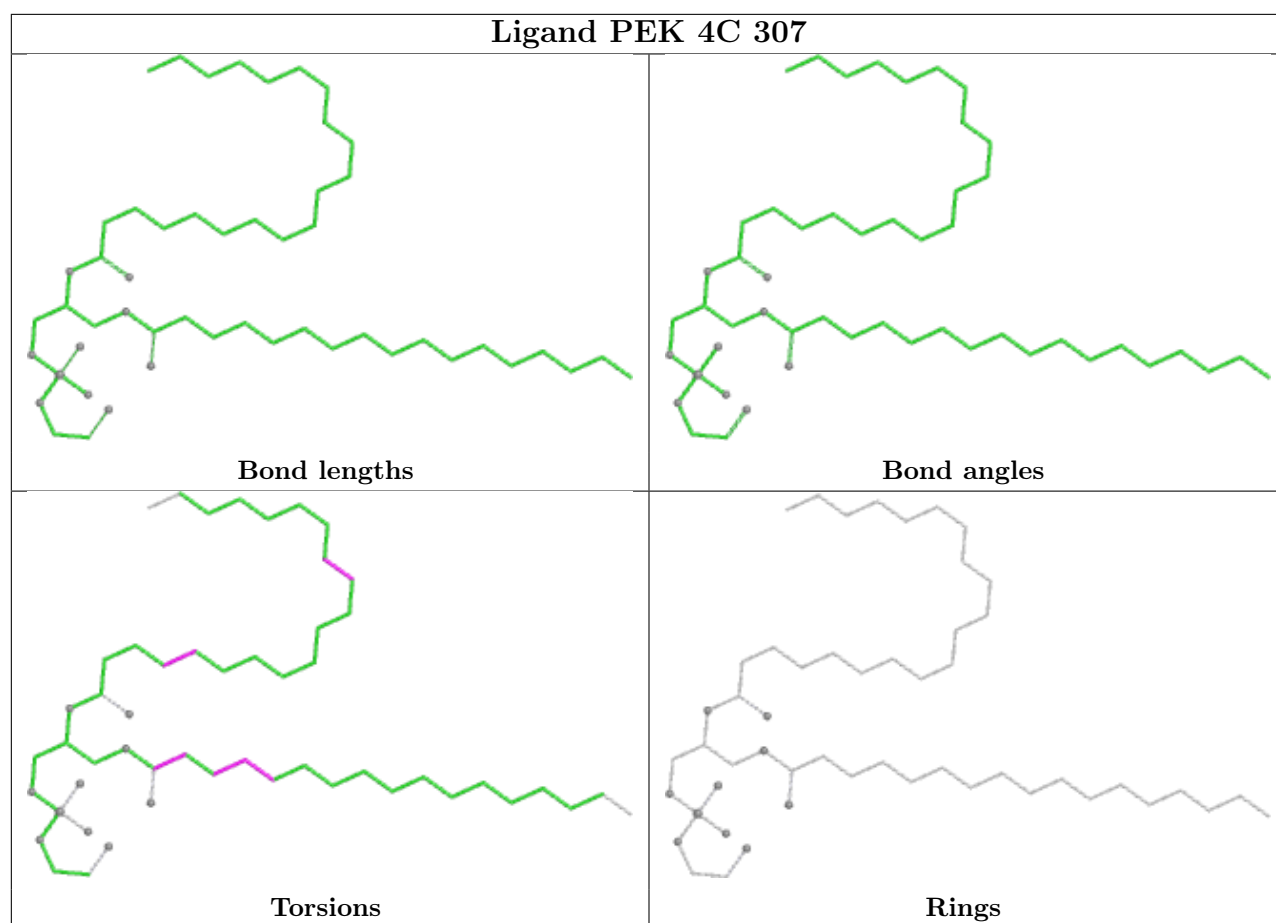
Bond angles

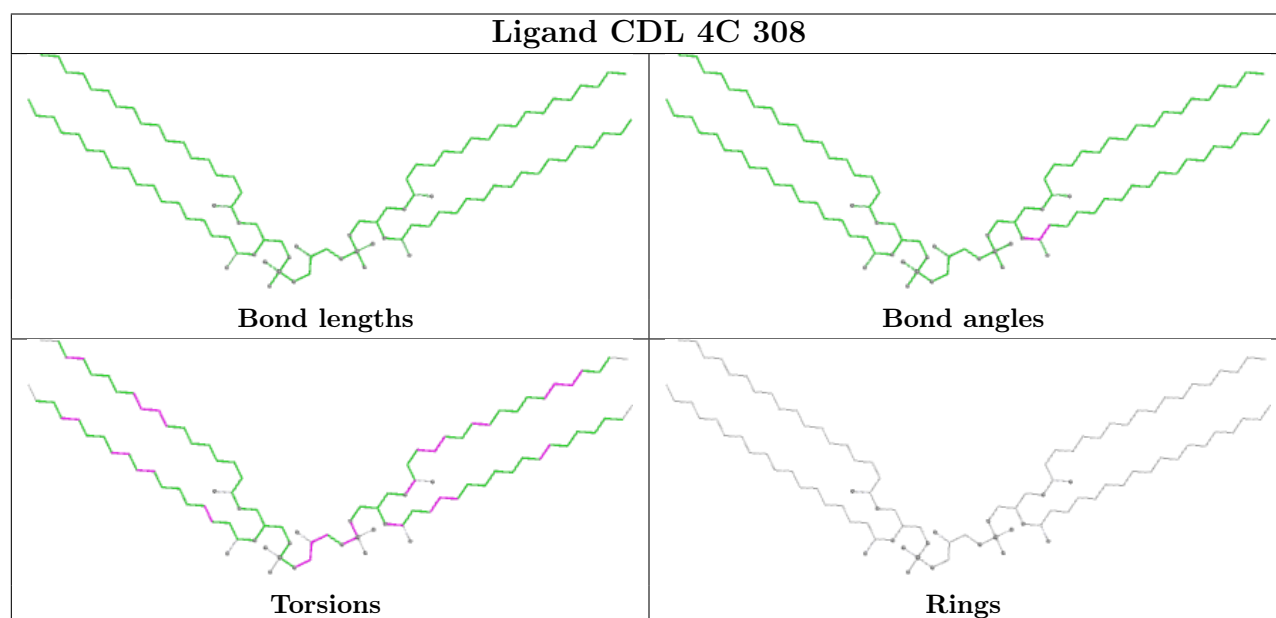
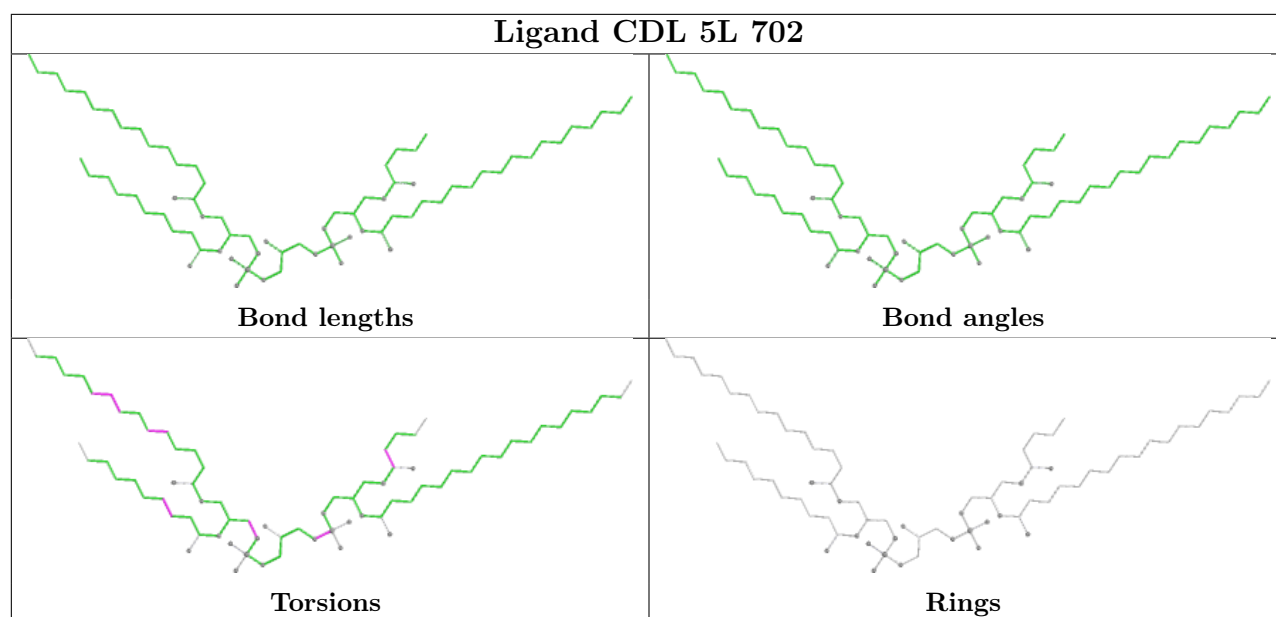


Torsions

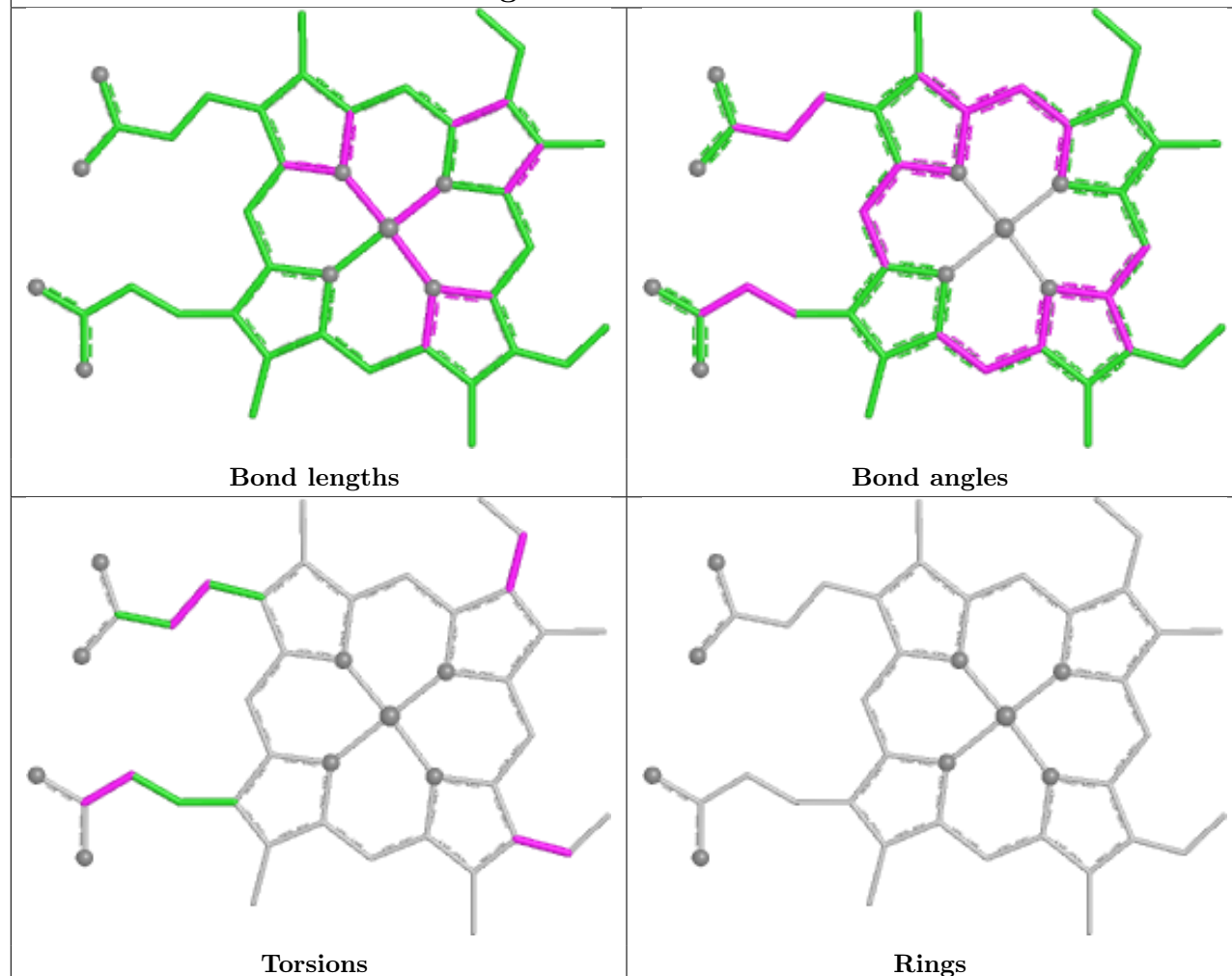


Rings

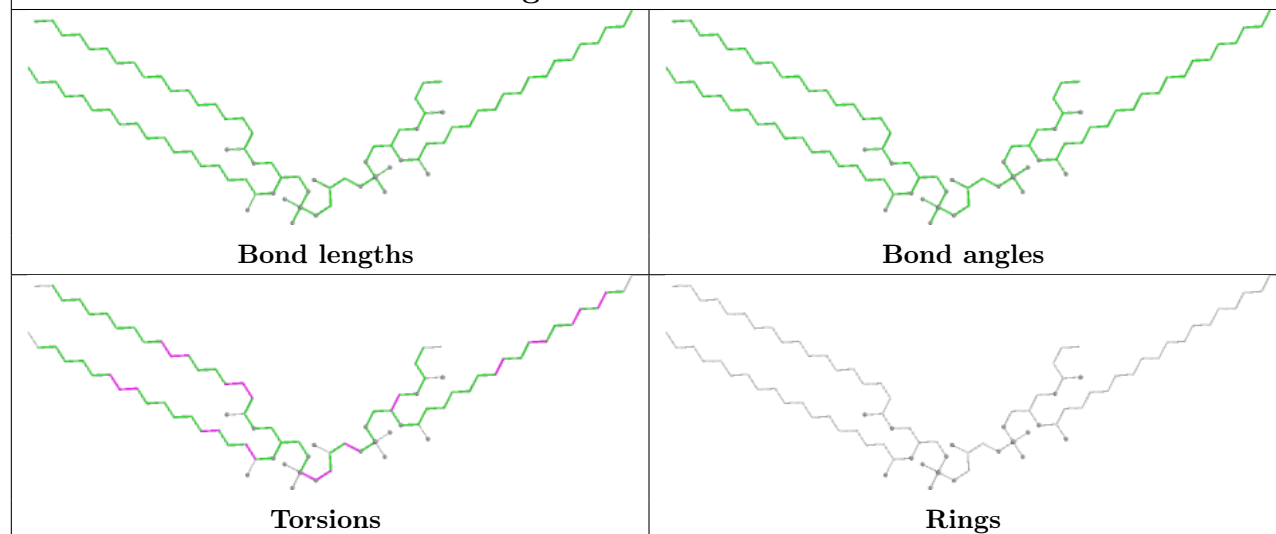


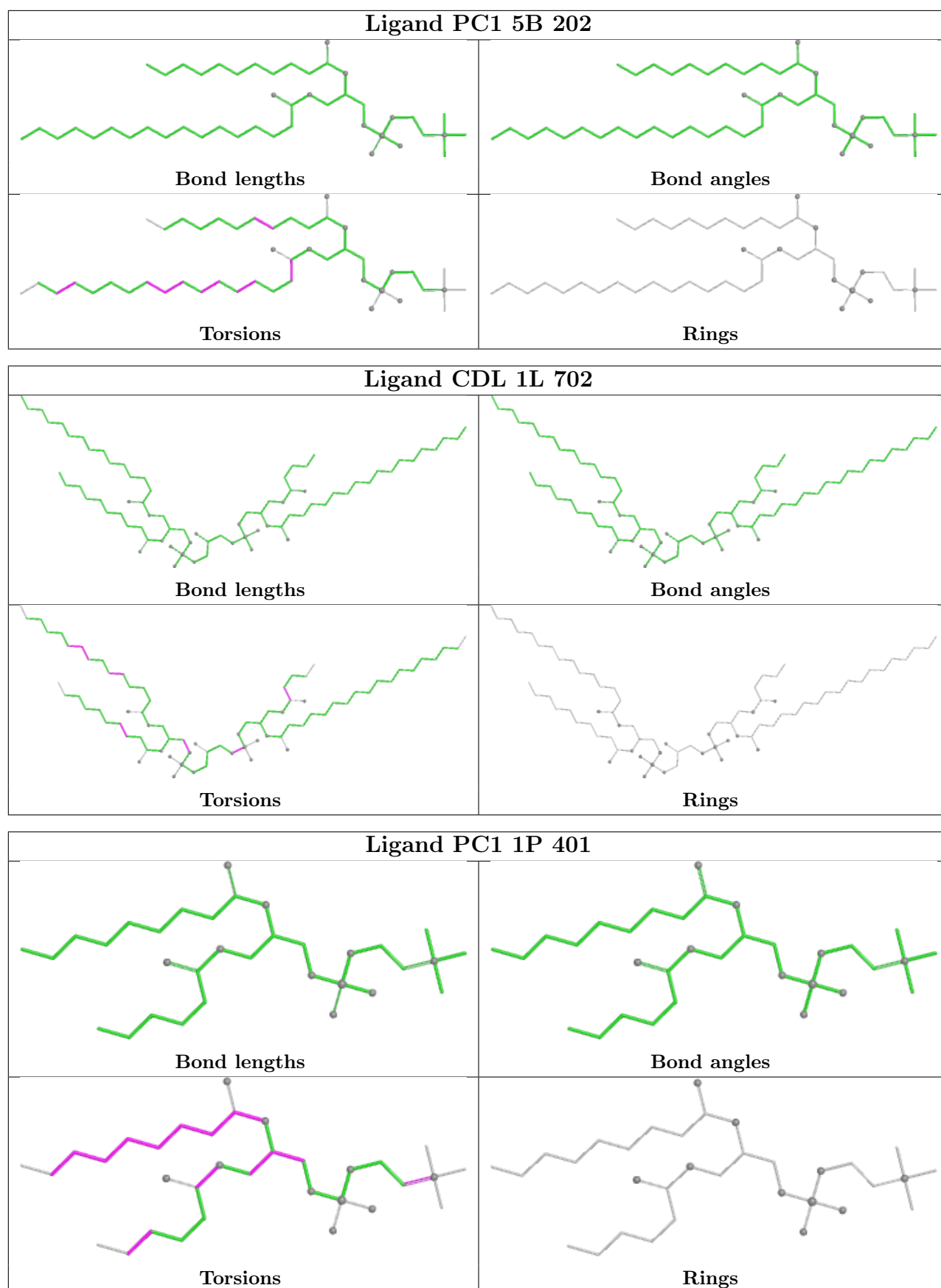


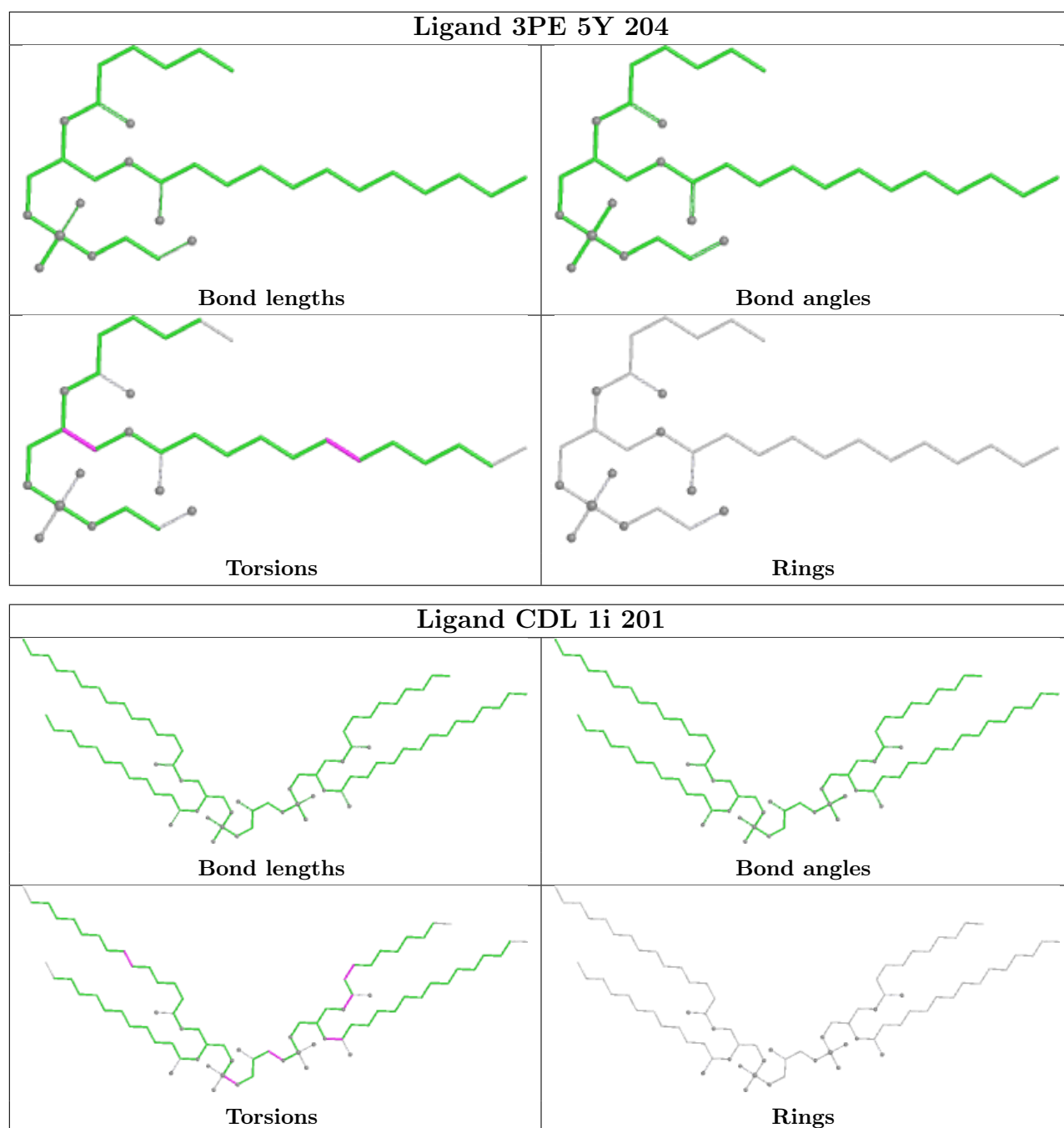
Ligand HEM 3C 501

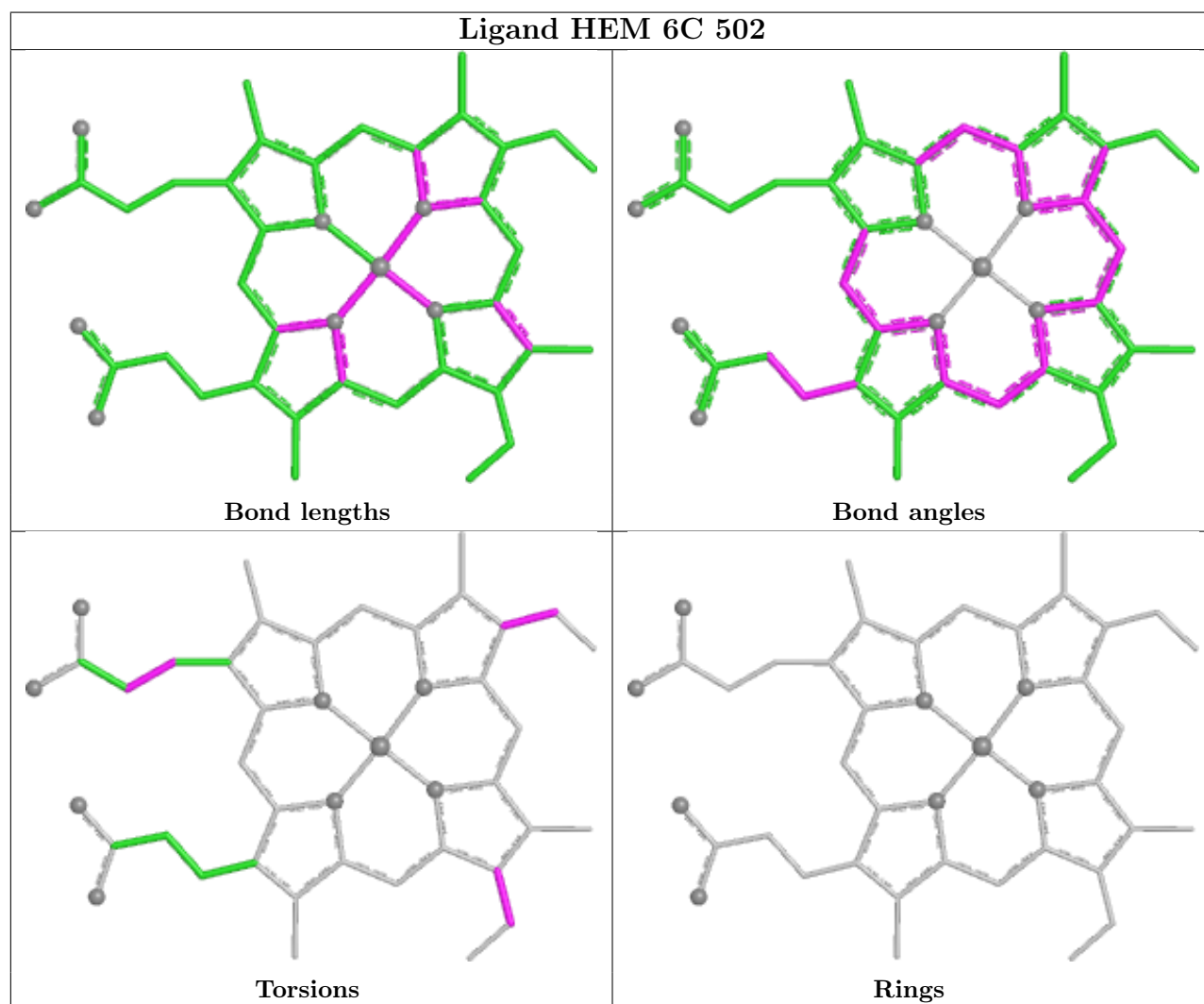
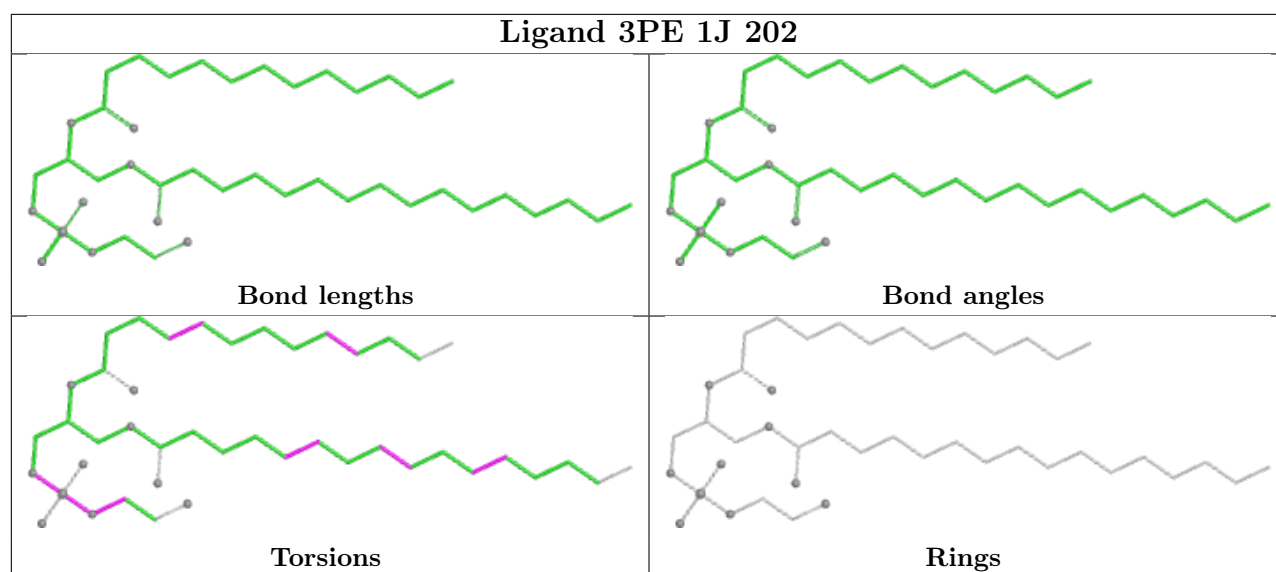


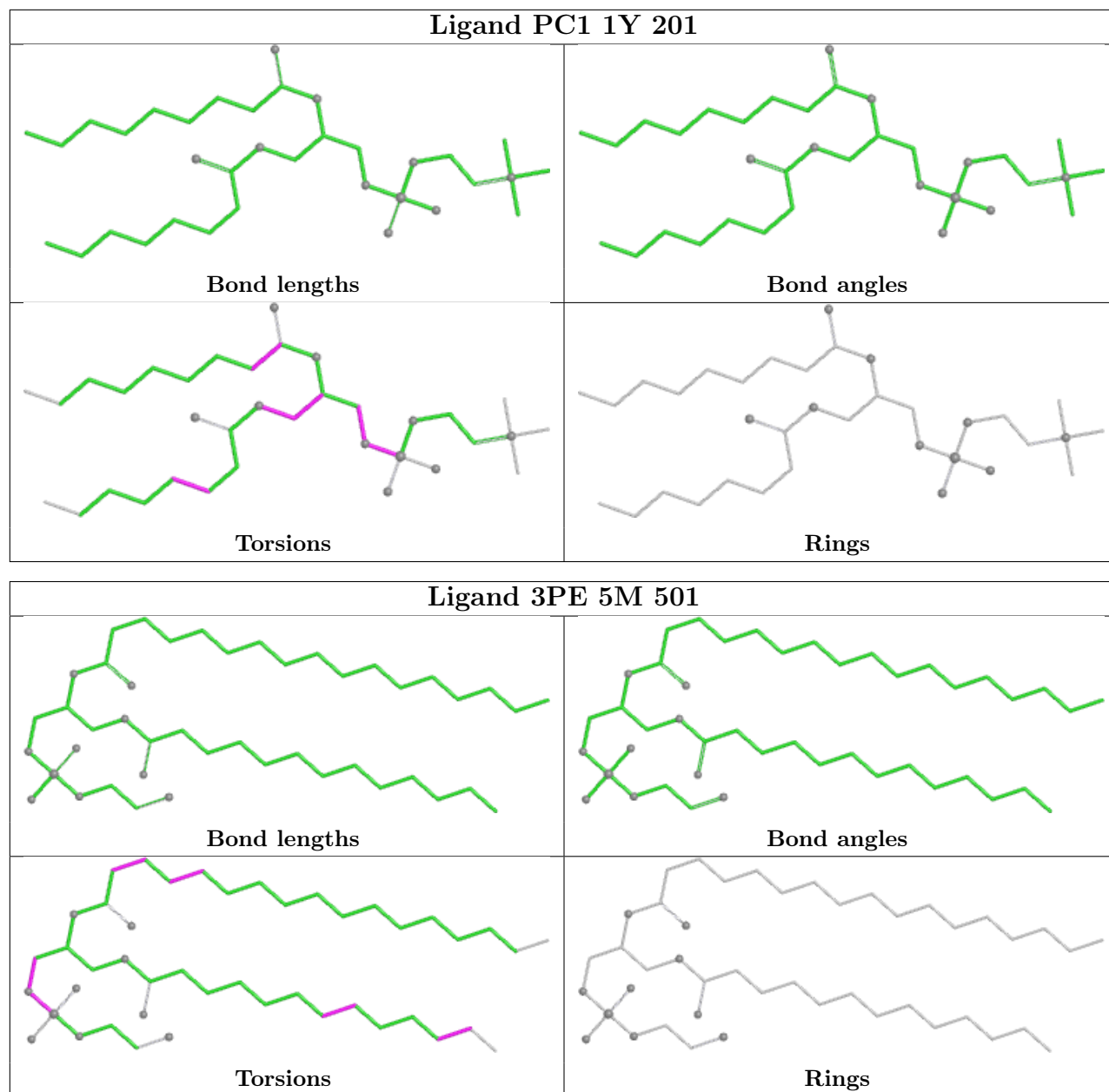
Ligand CDL 1X 201

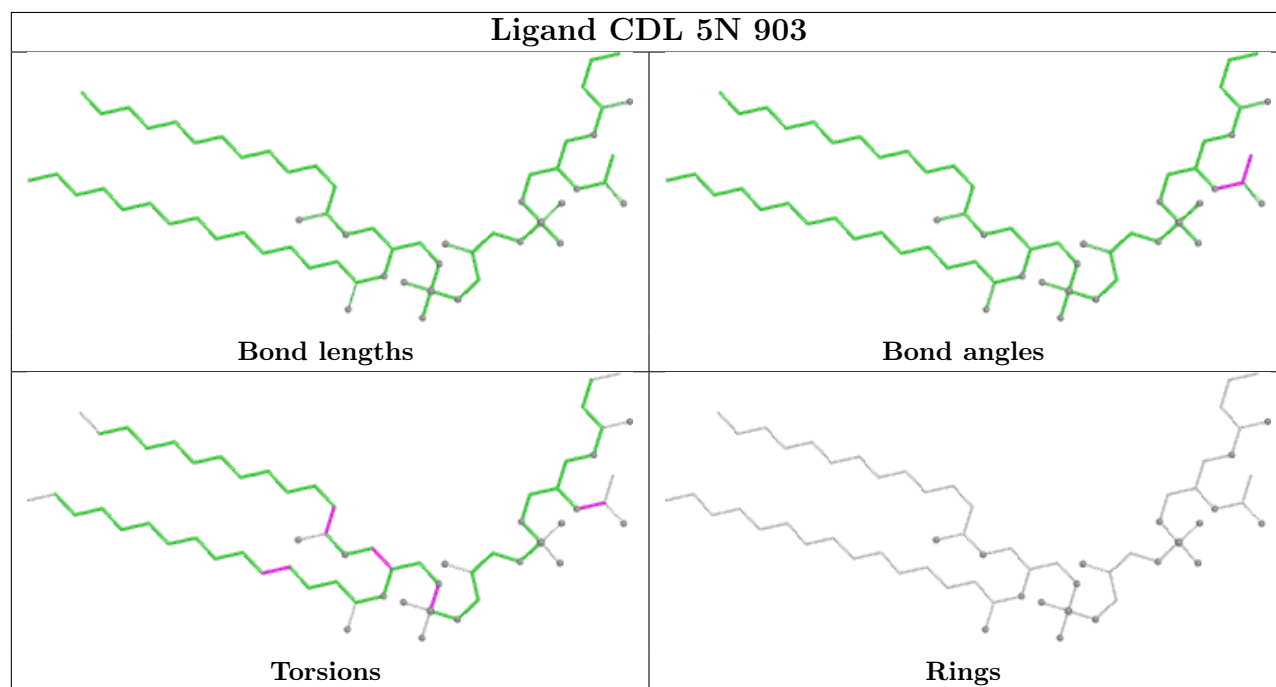
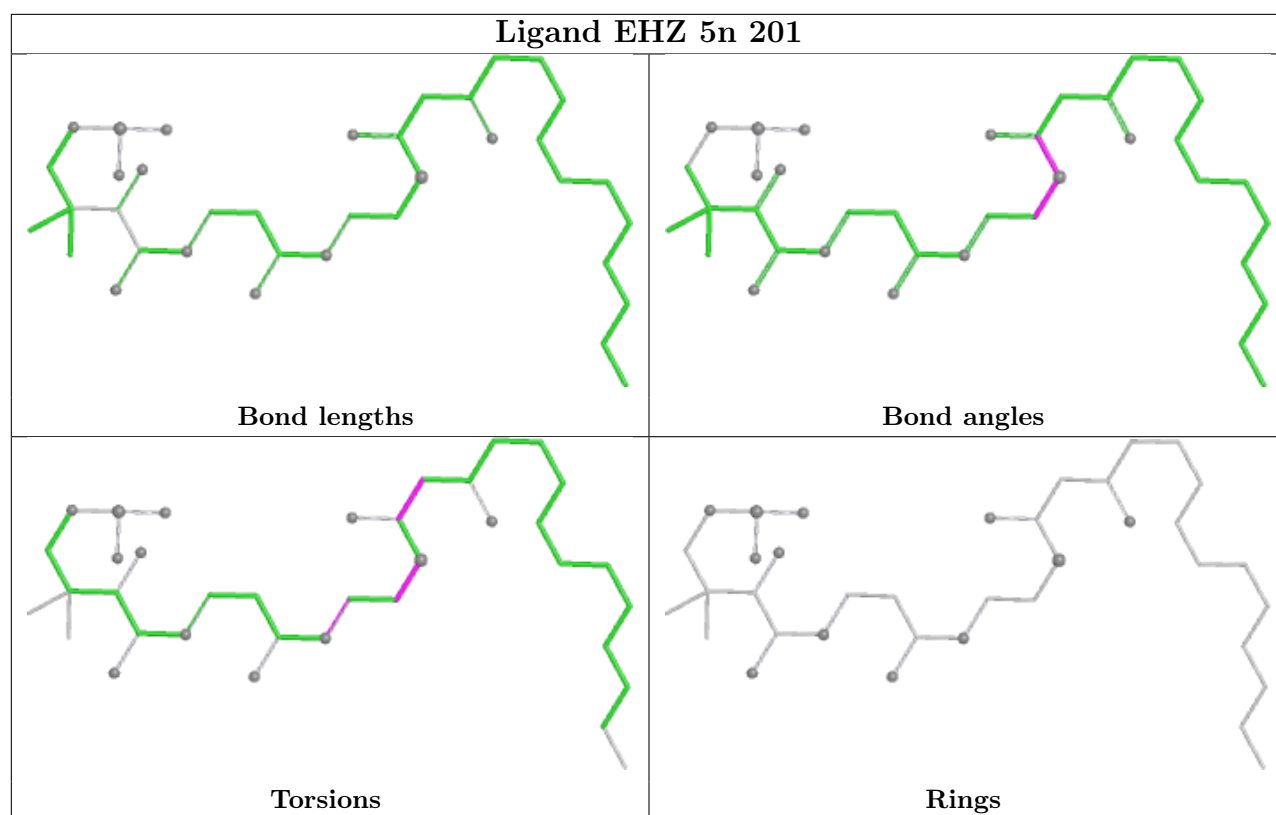


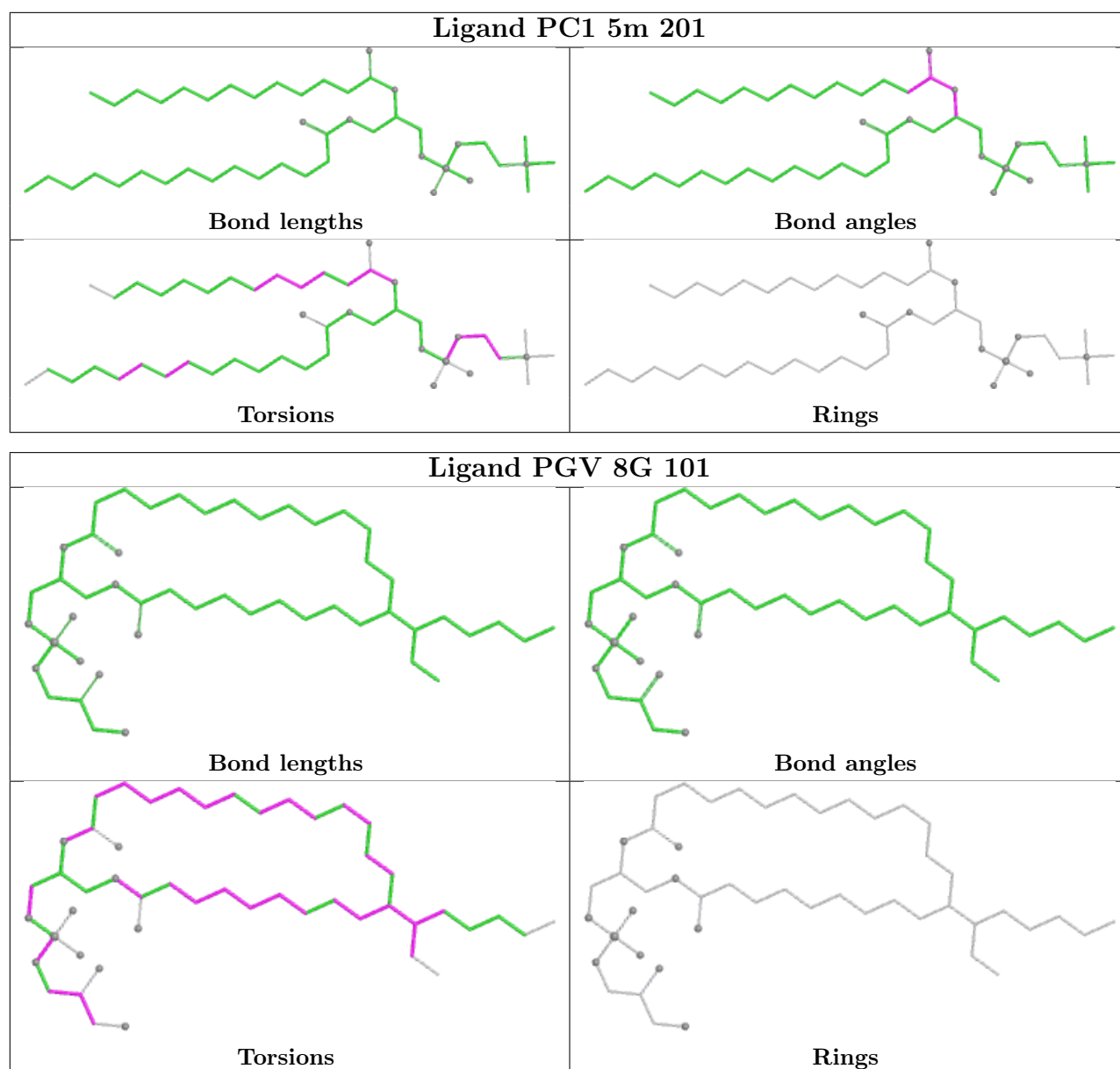


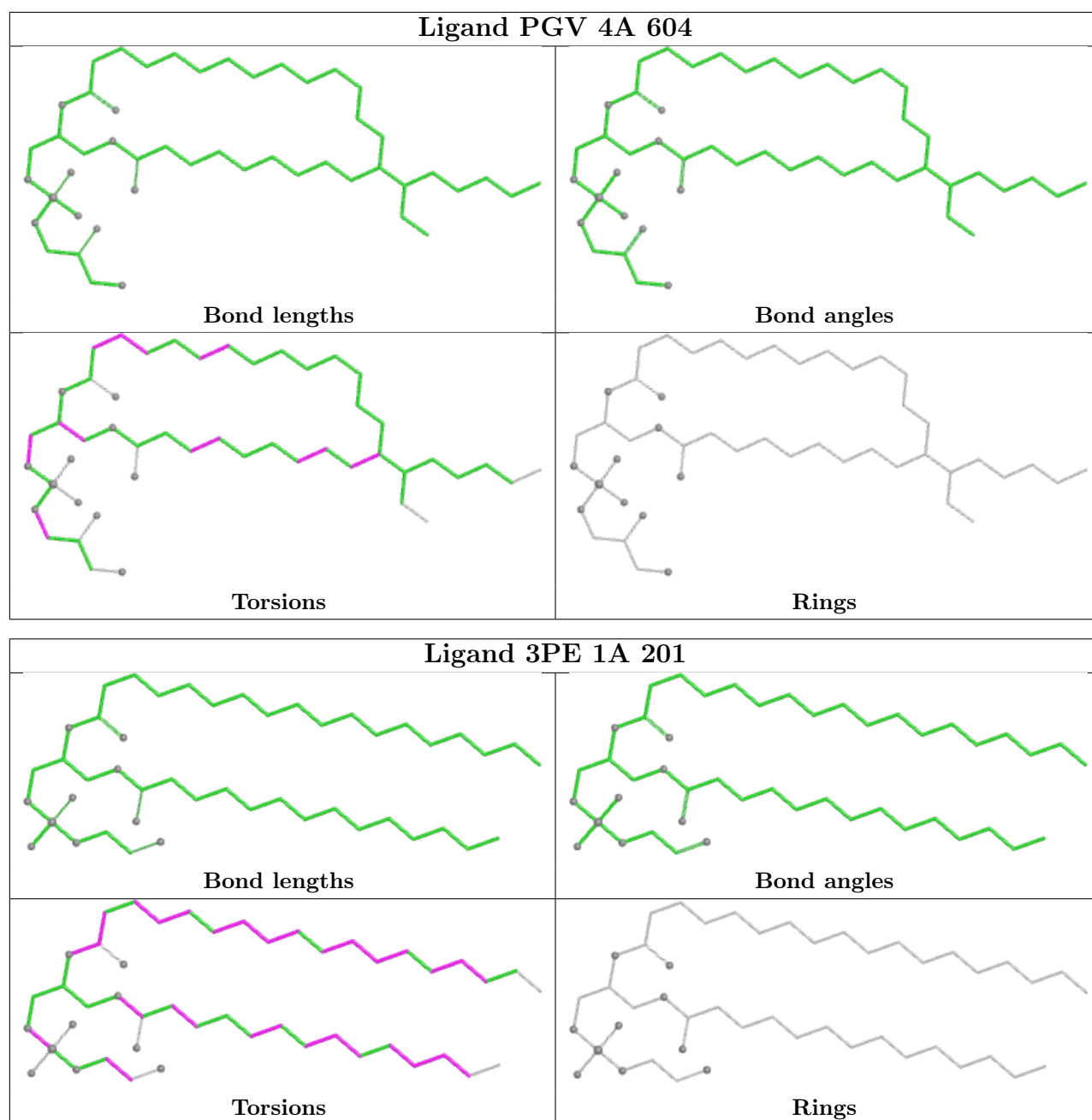


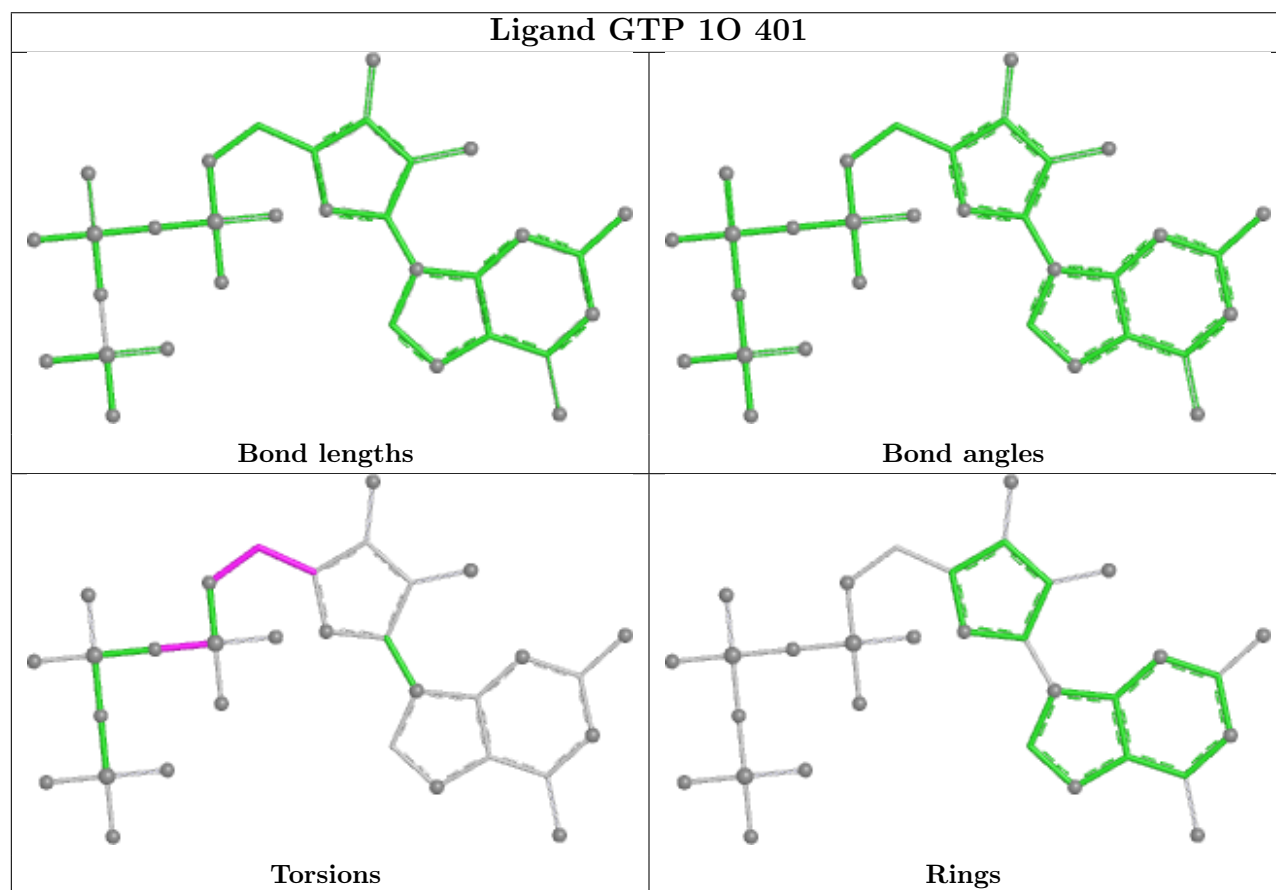
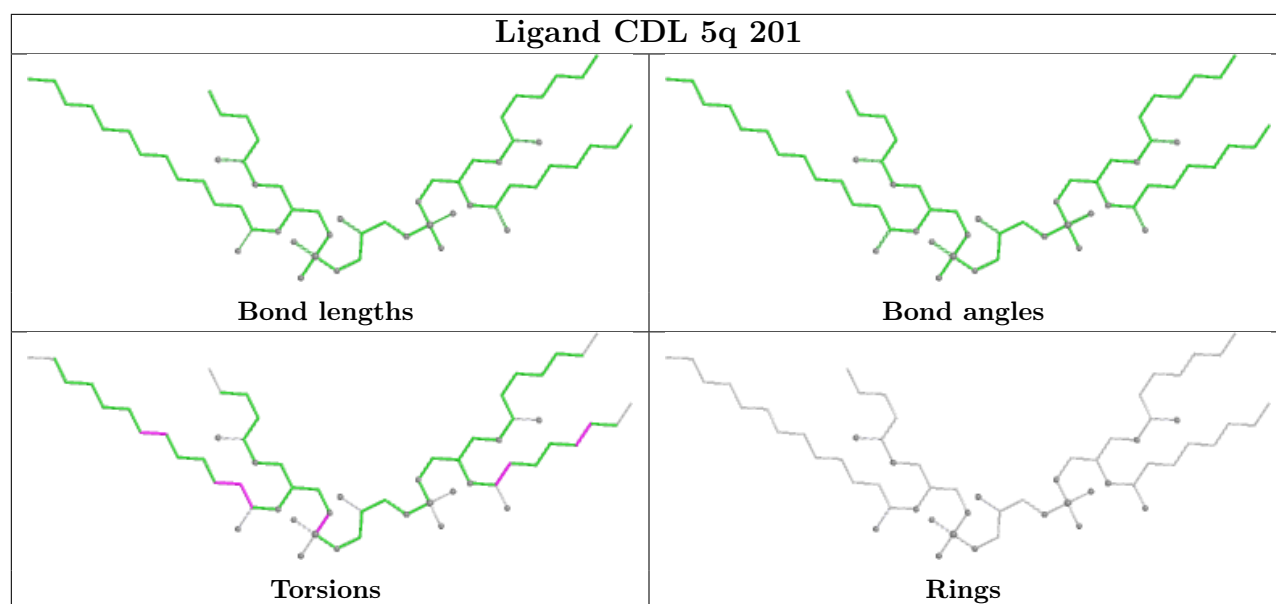


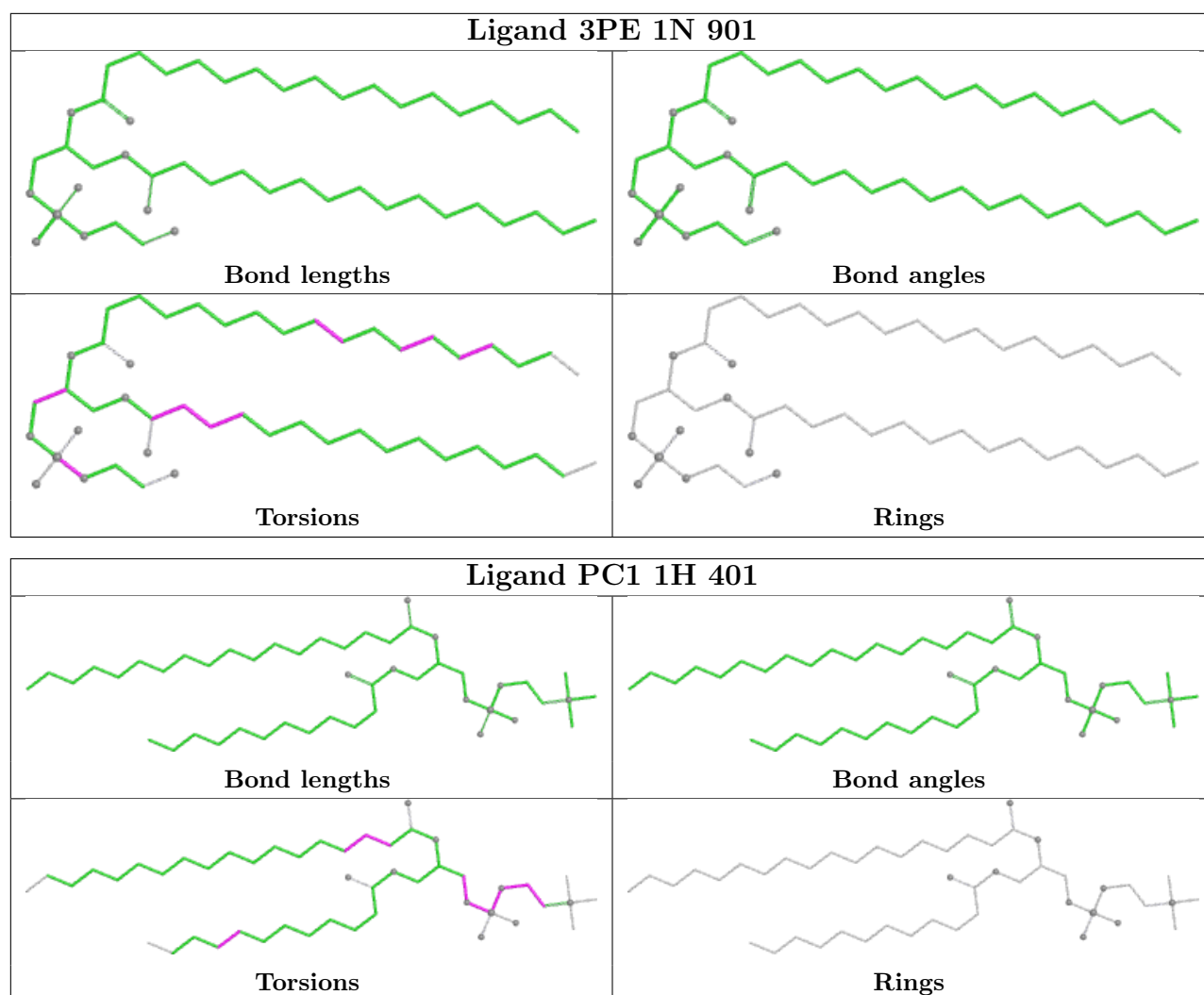


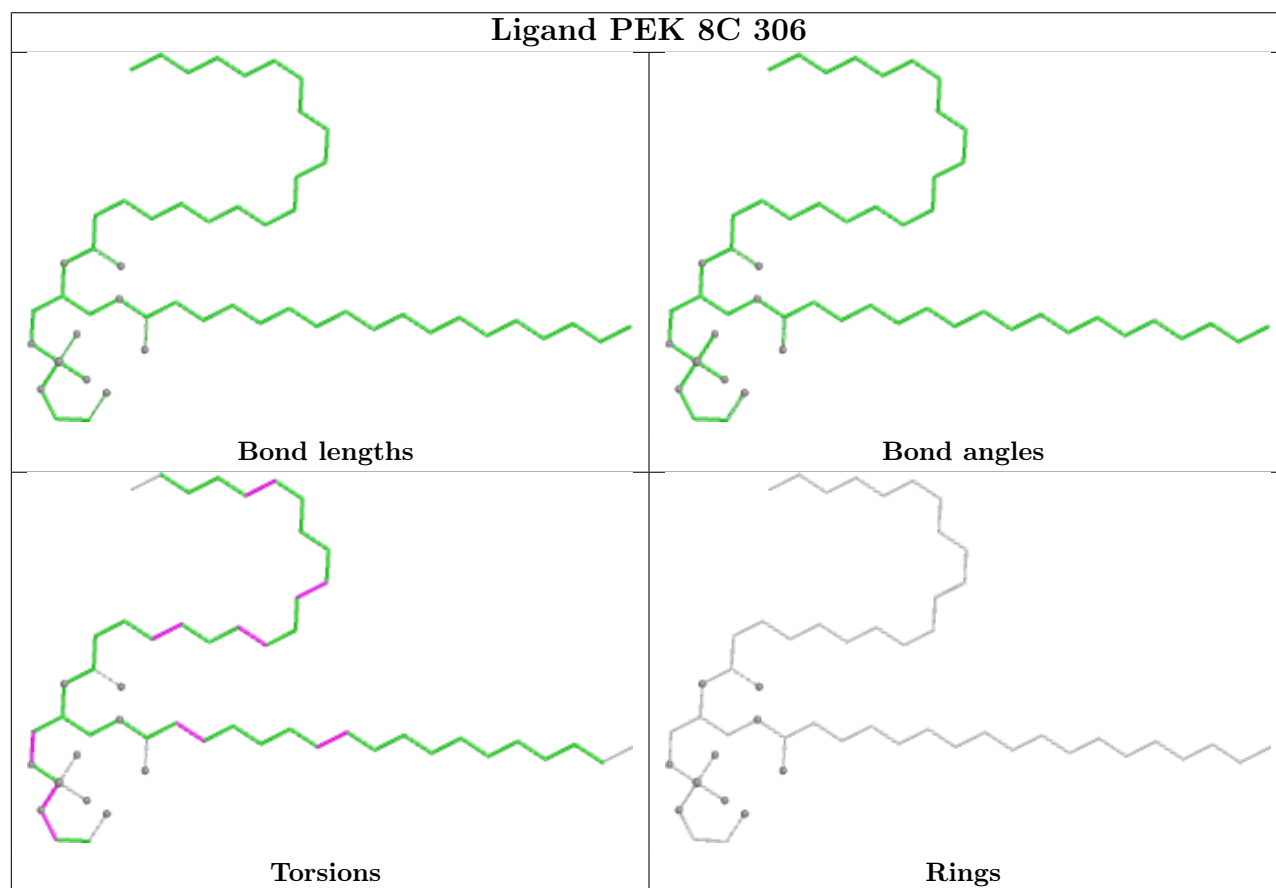
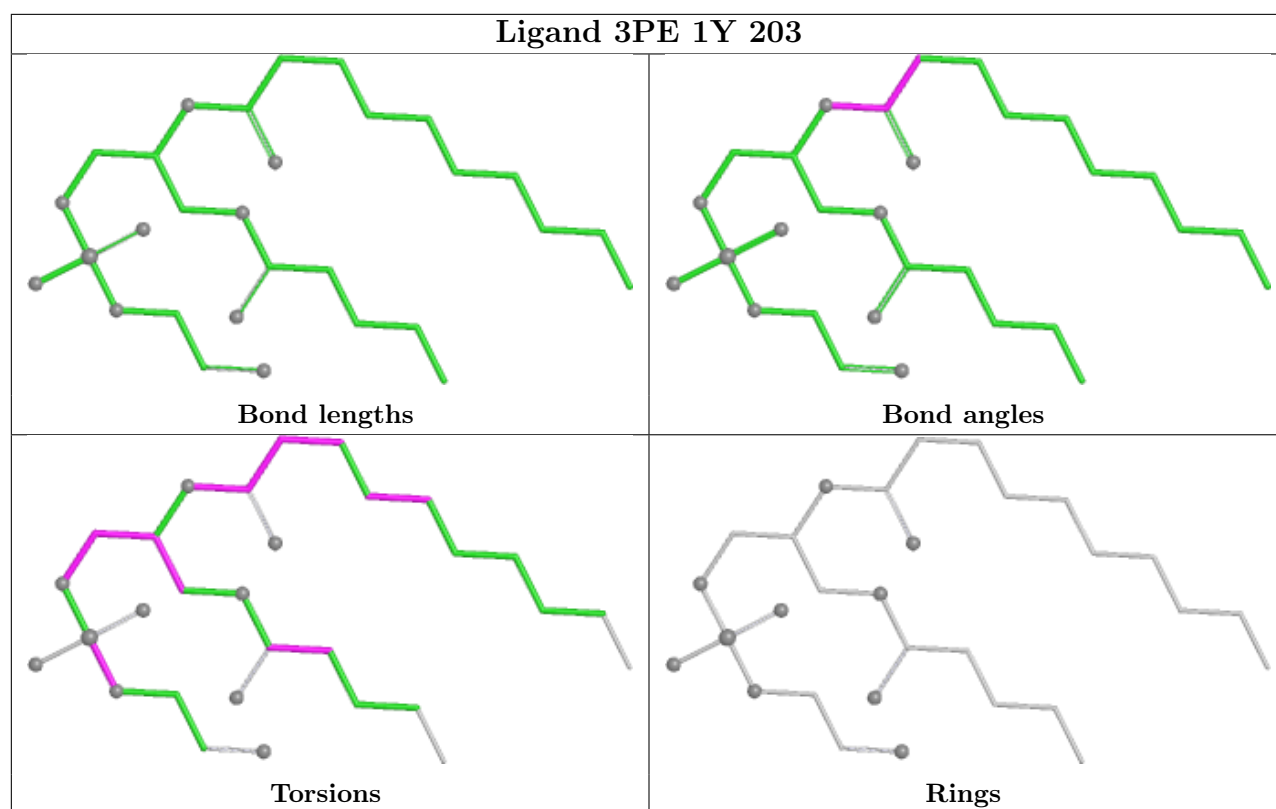




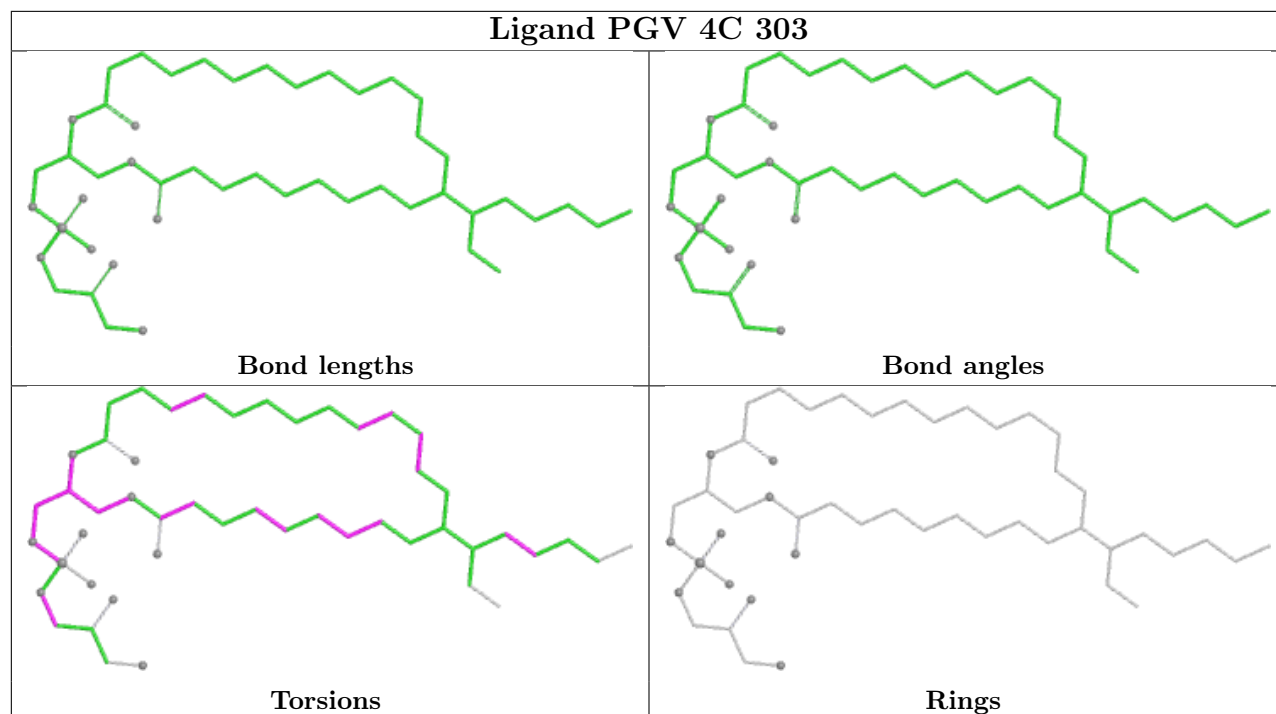




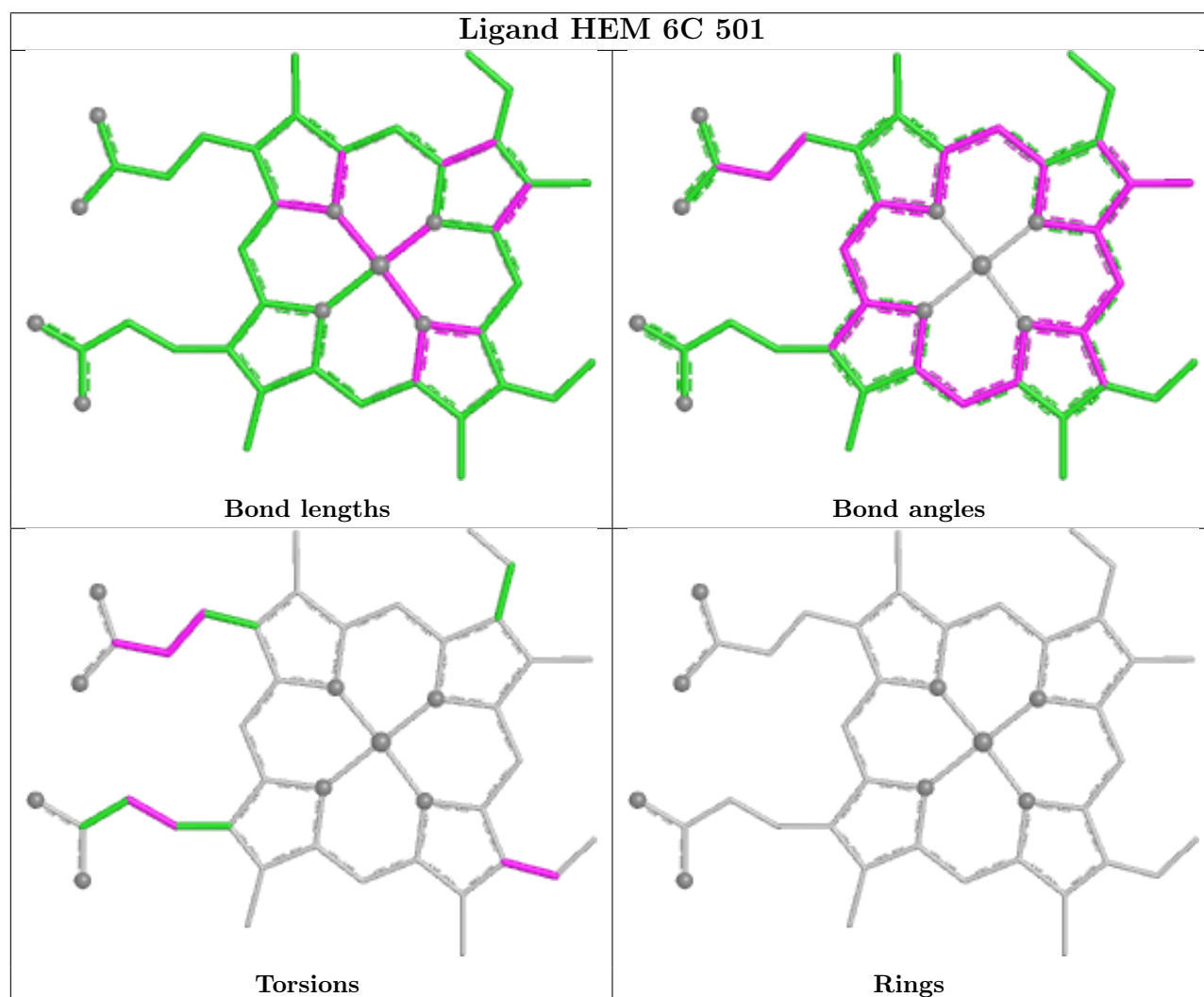


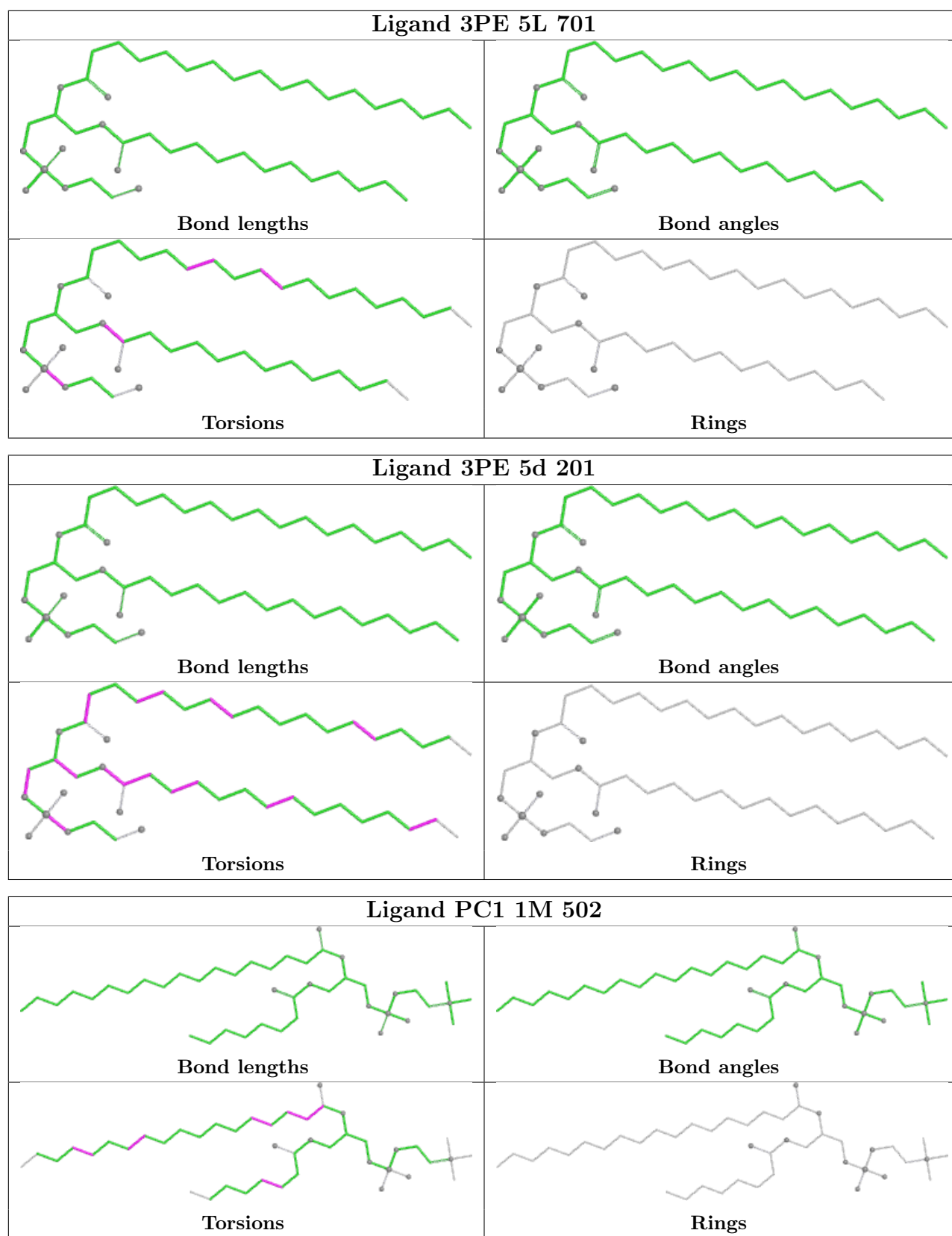


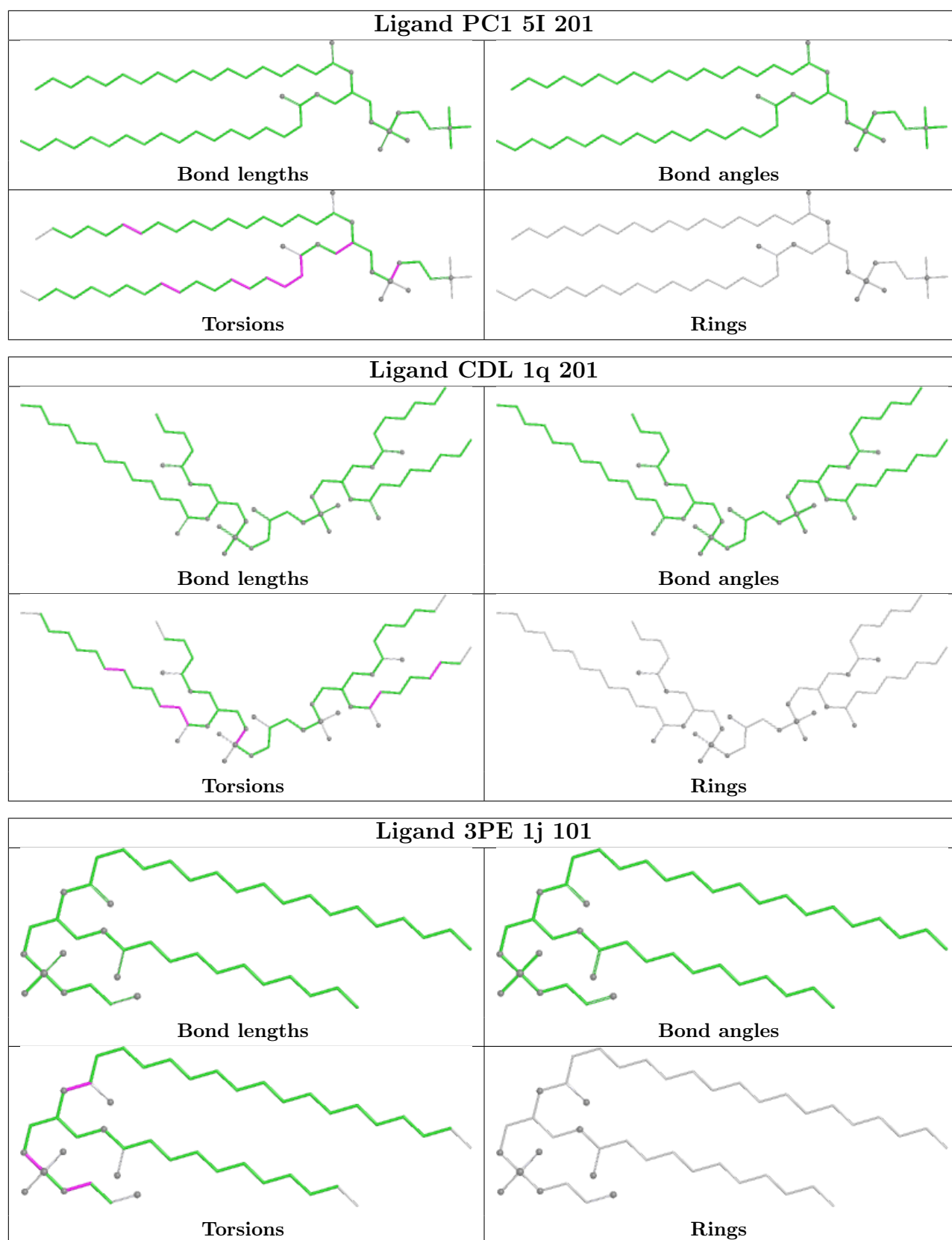
Ligand PGV 4C 303

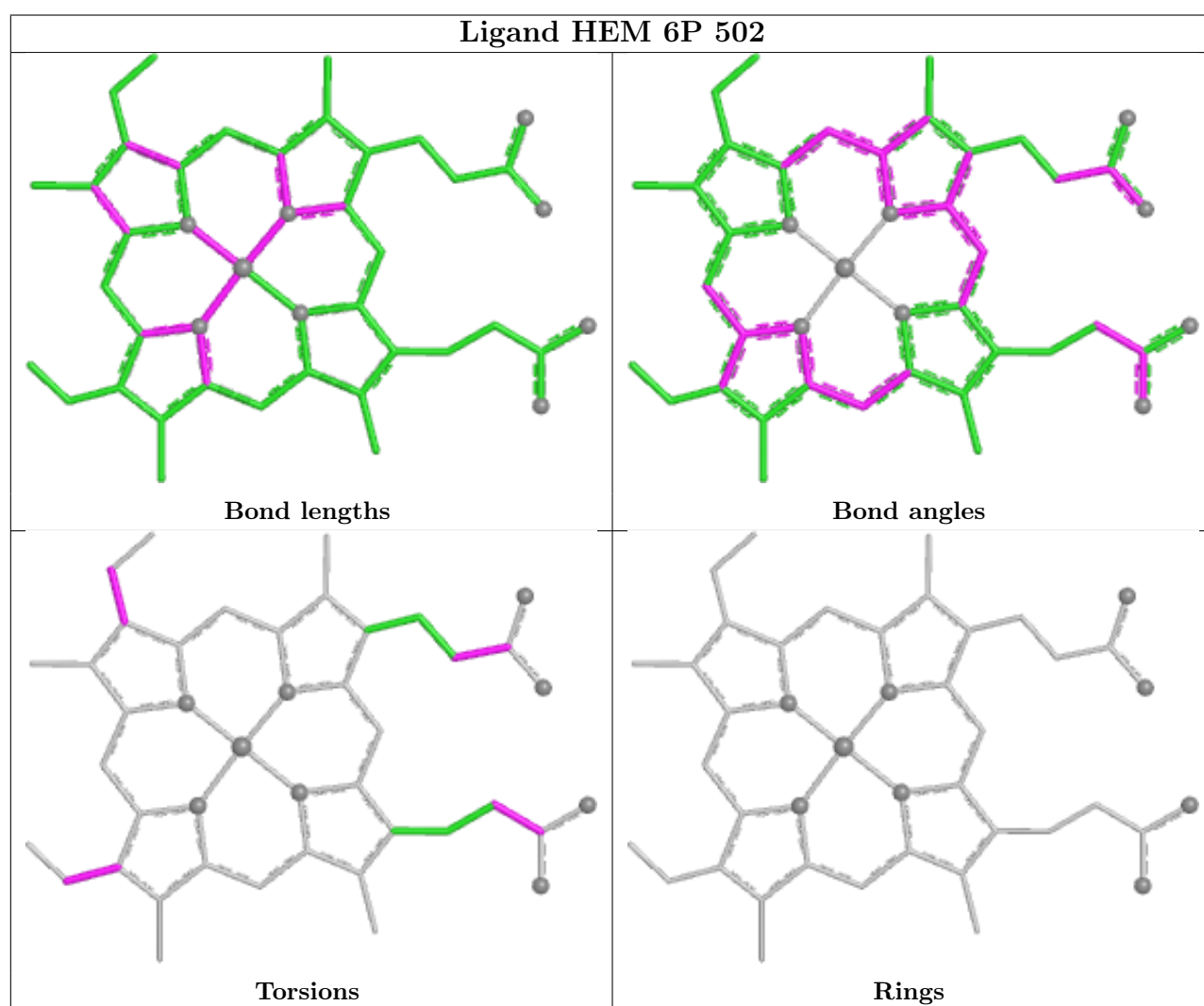
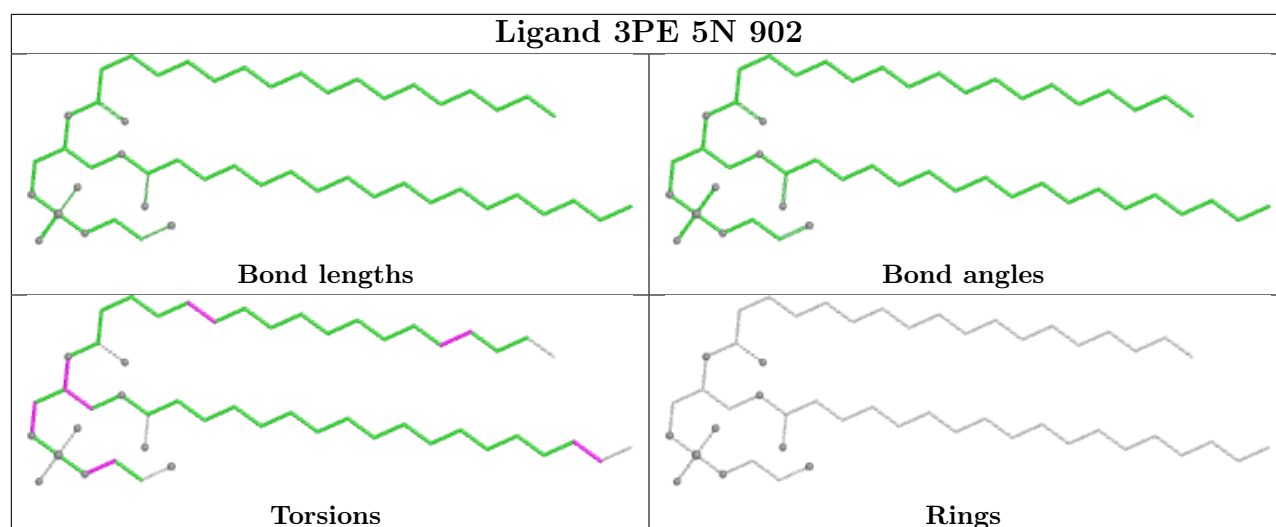


Ligand HEM 6C 501

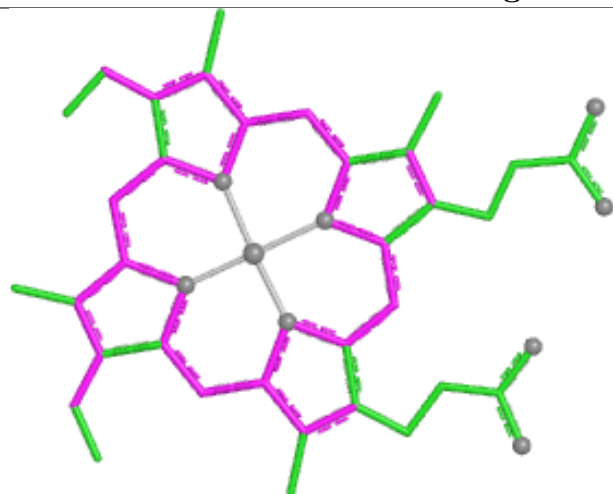




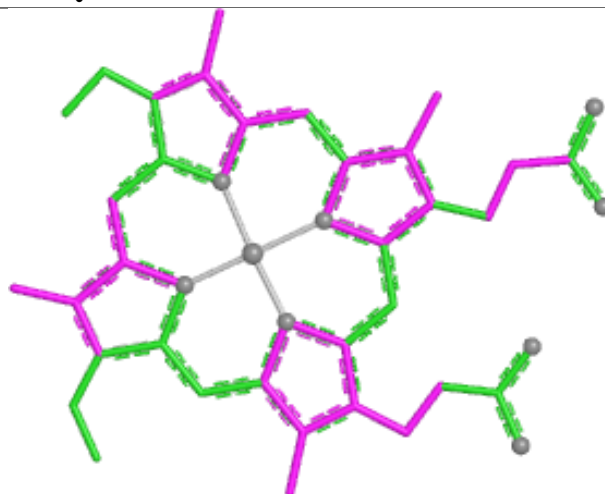




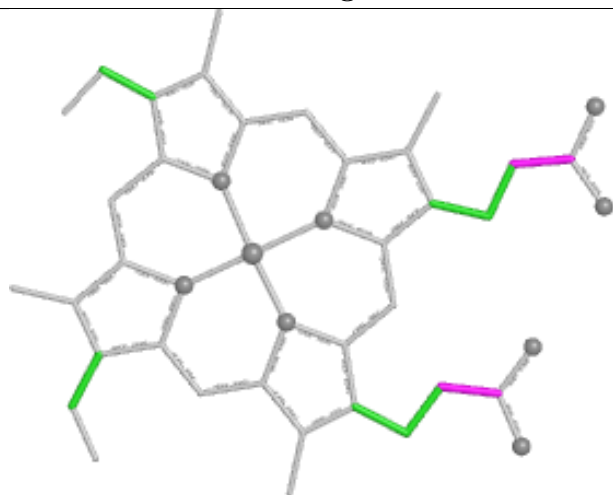
Ligand HEC 6Q 501



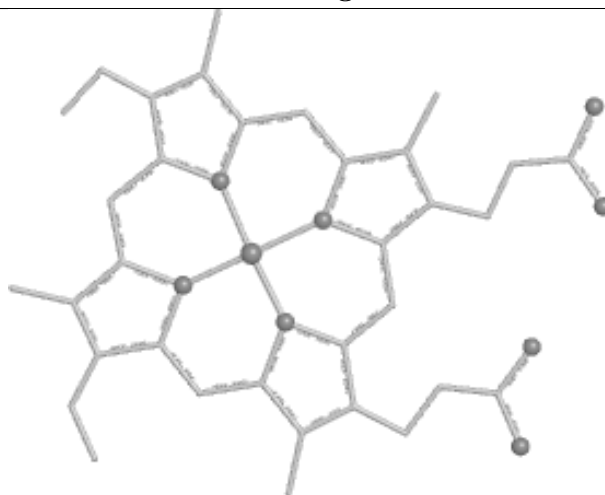
Bond lengths



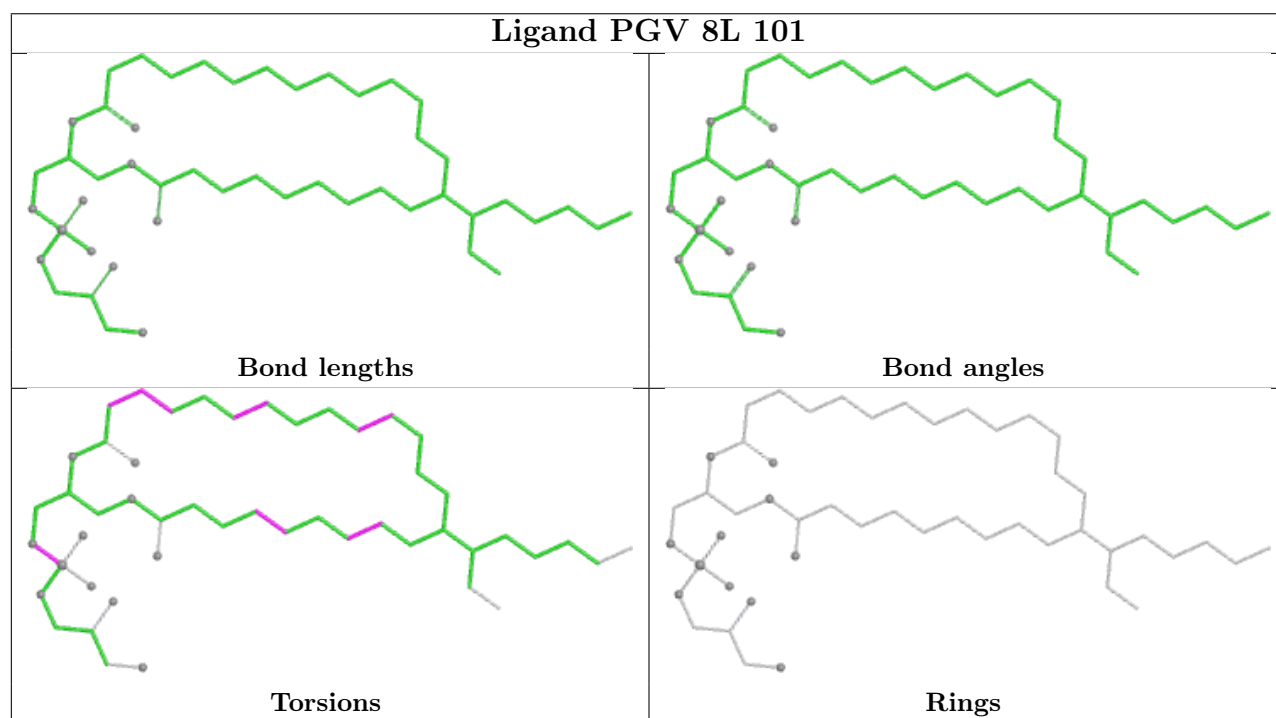
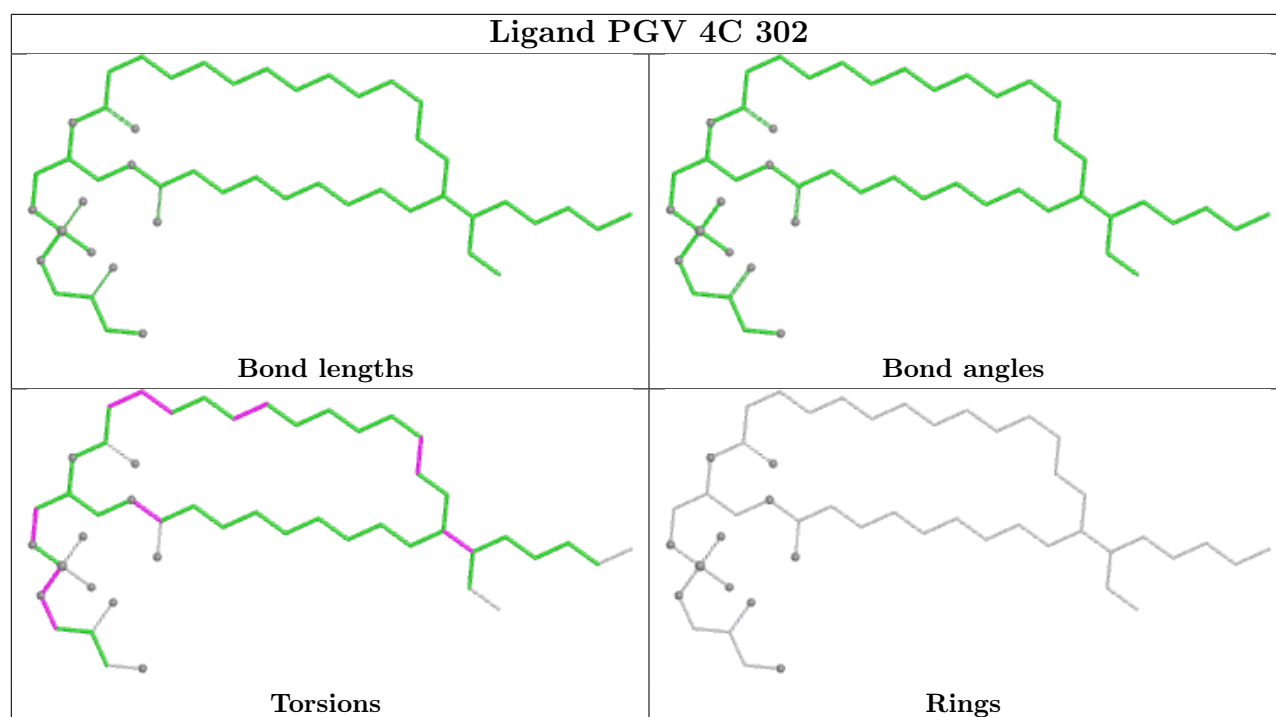
Bond angles

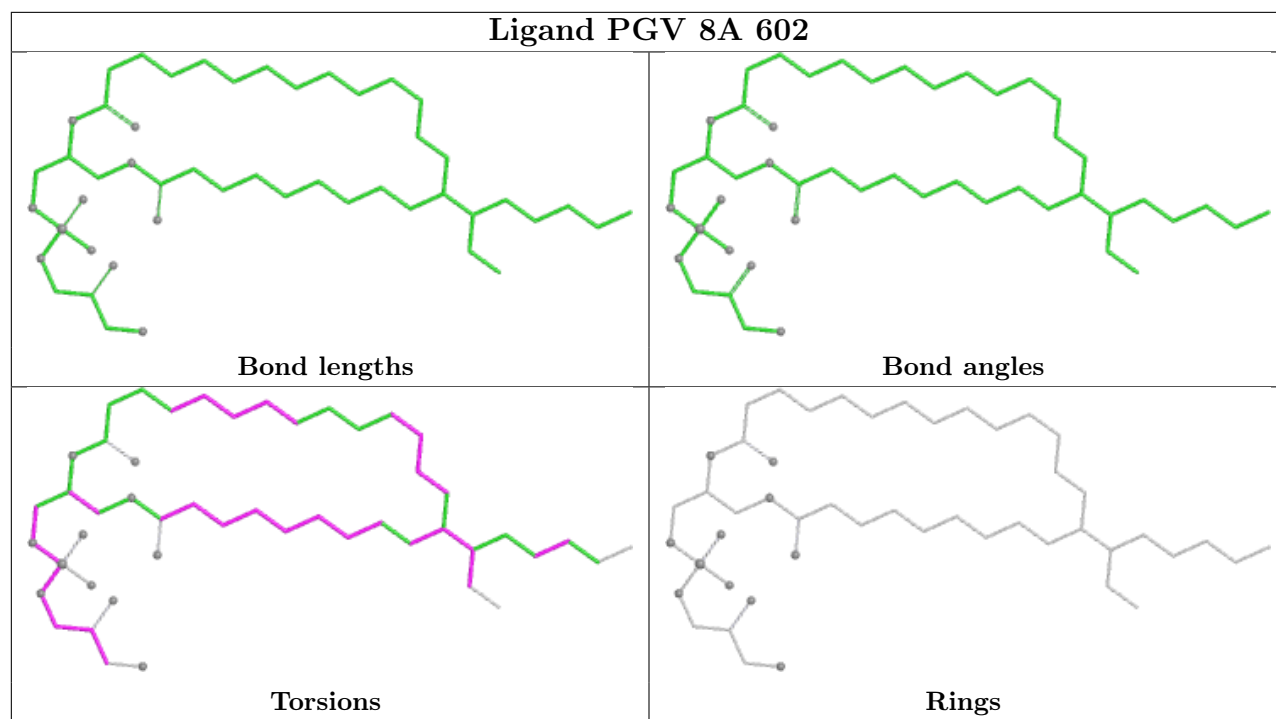
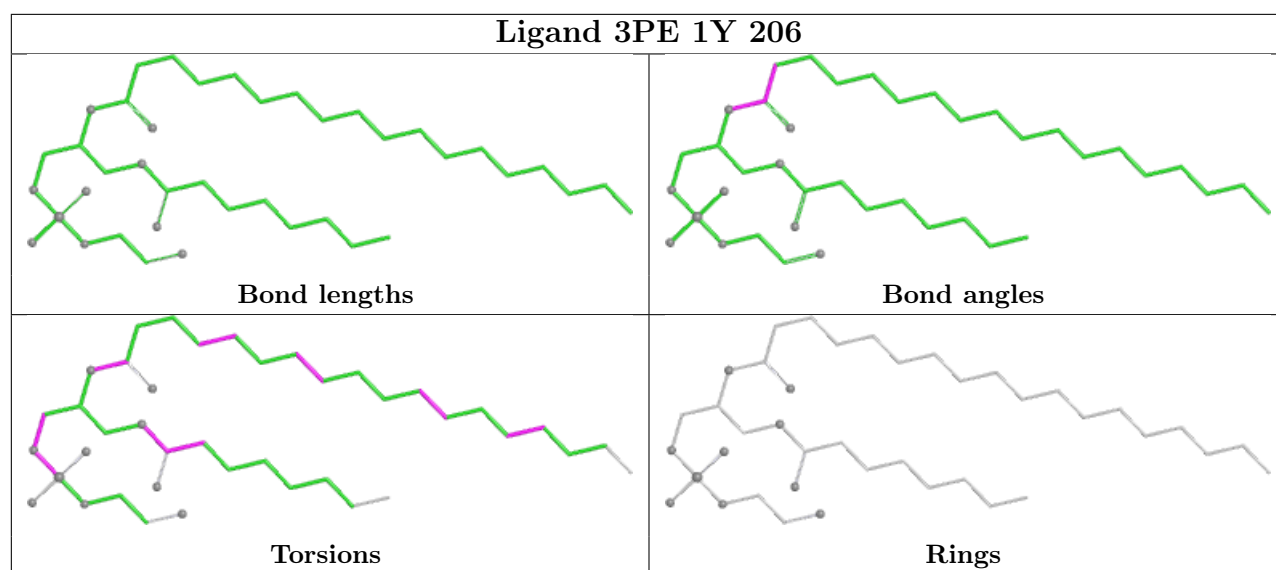


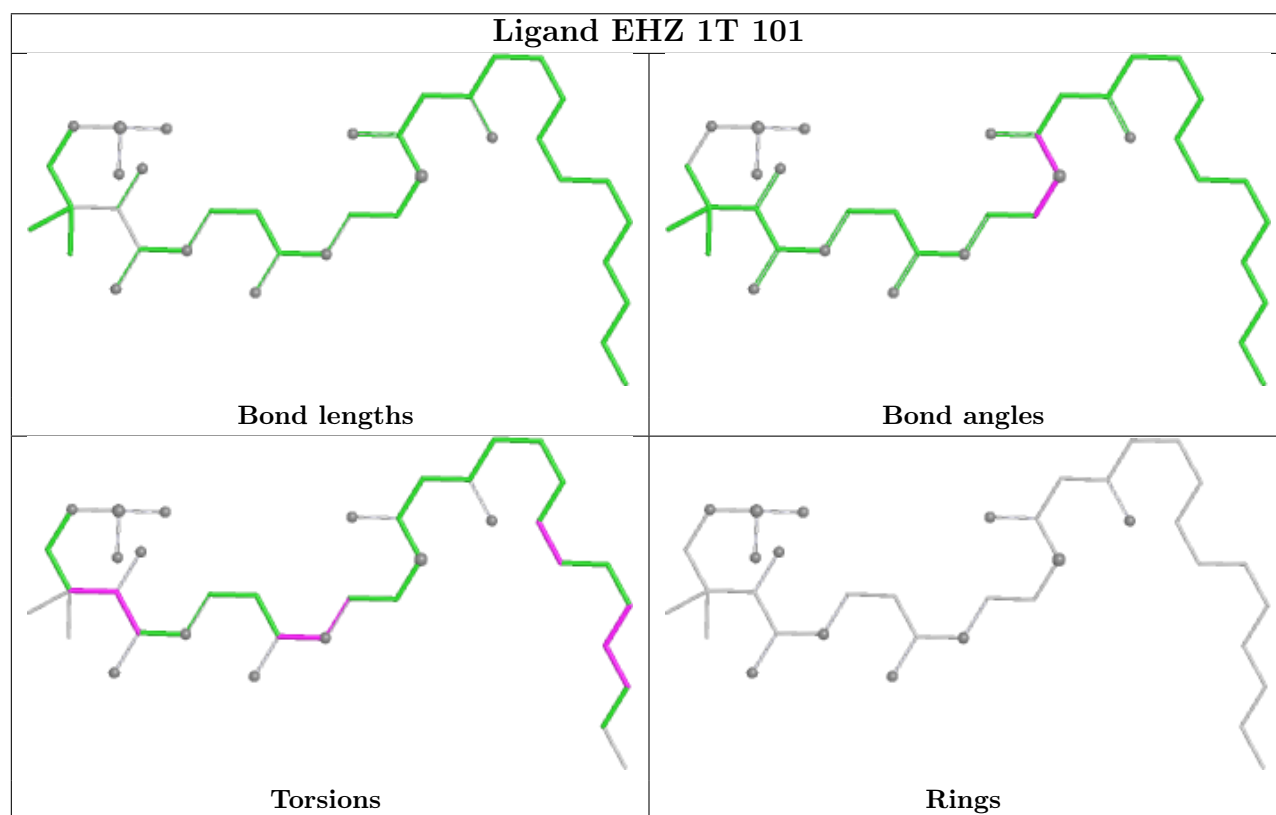
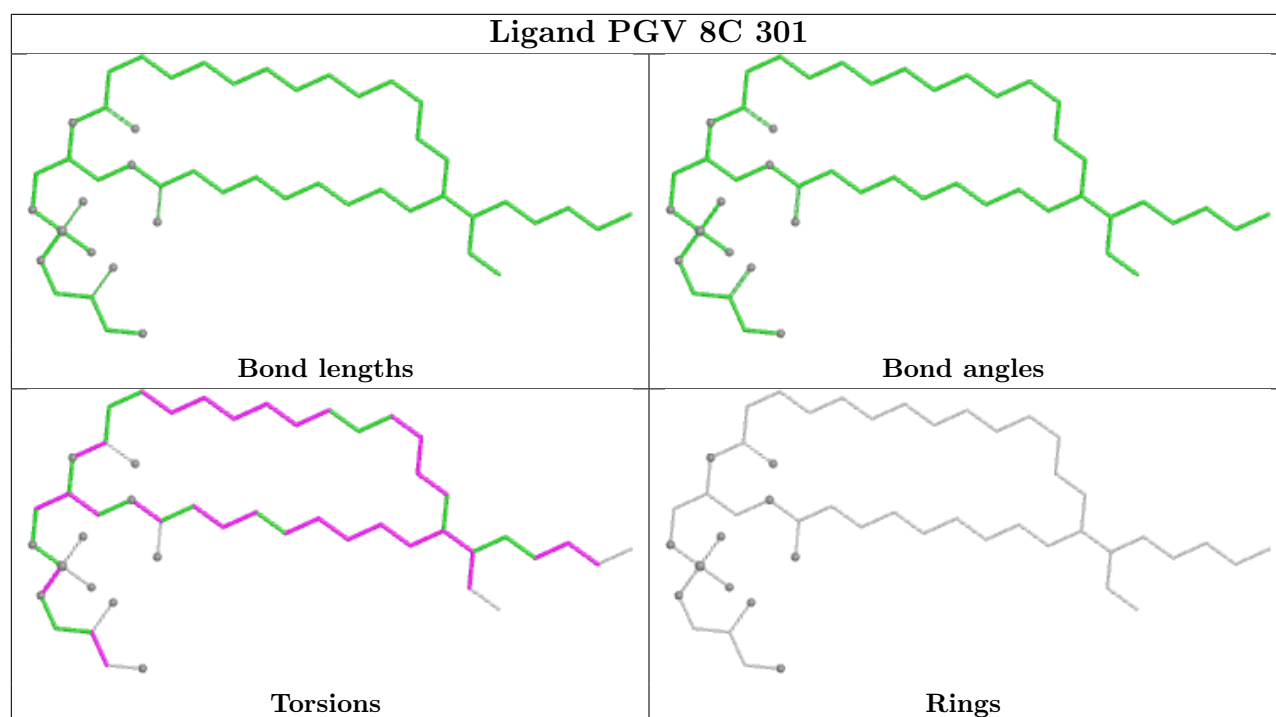
Torsions

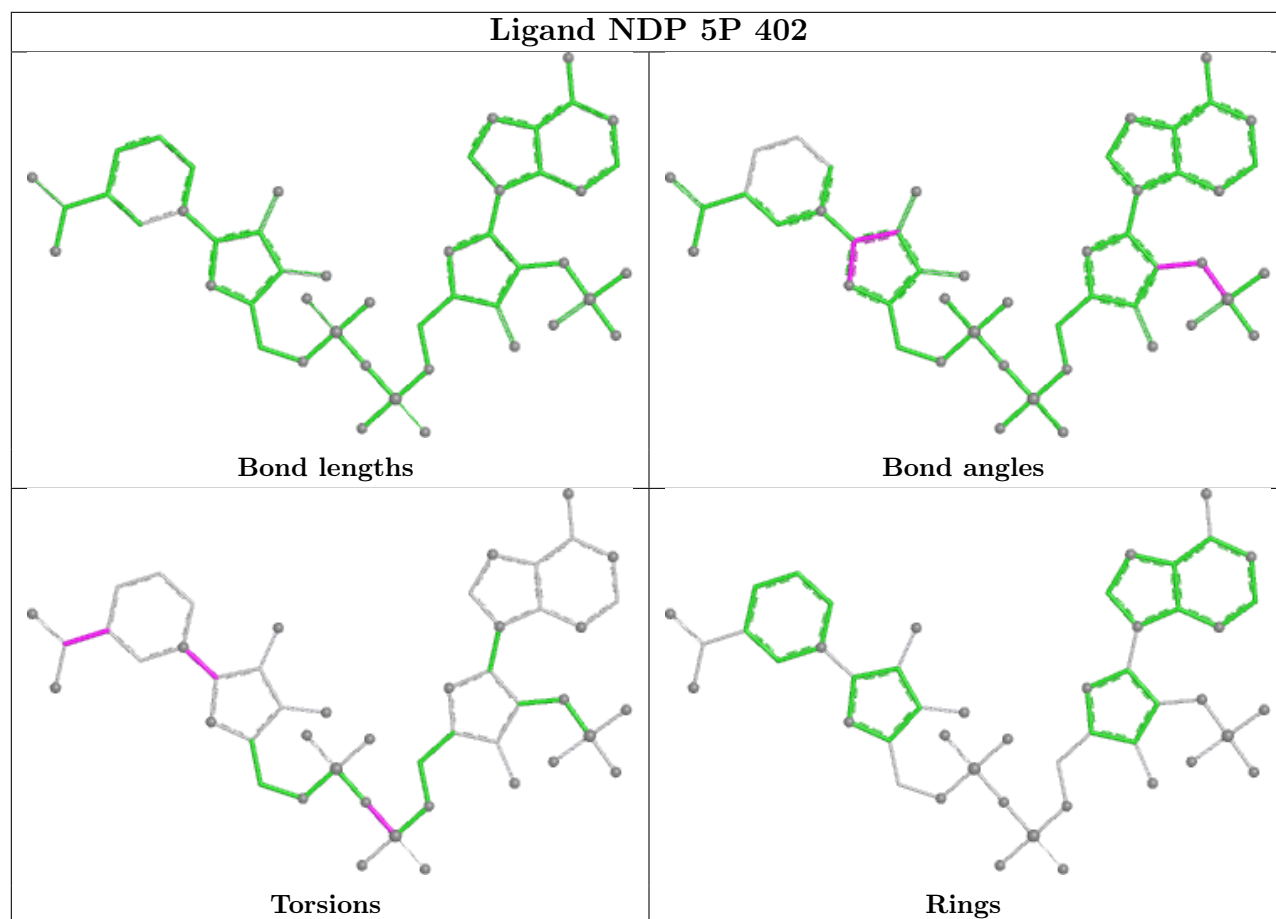
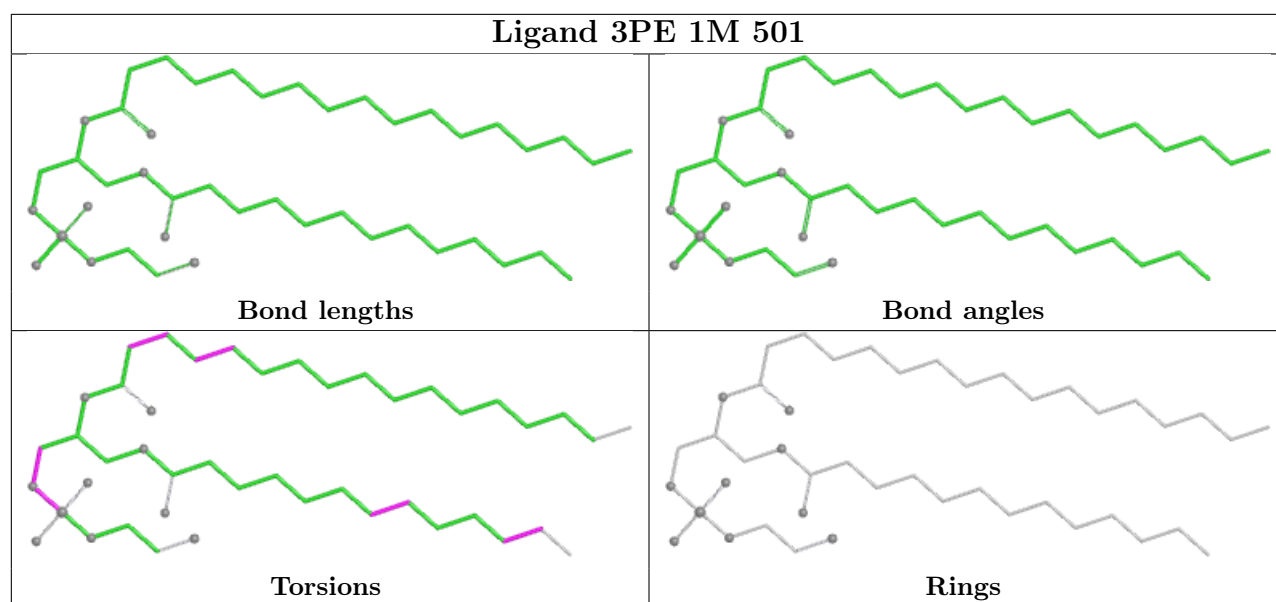


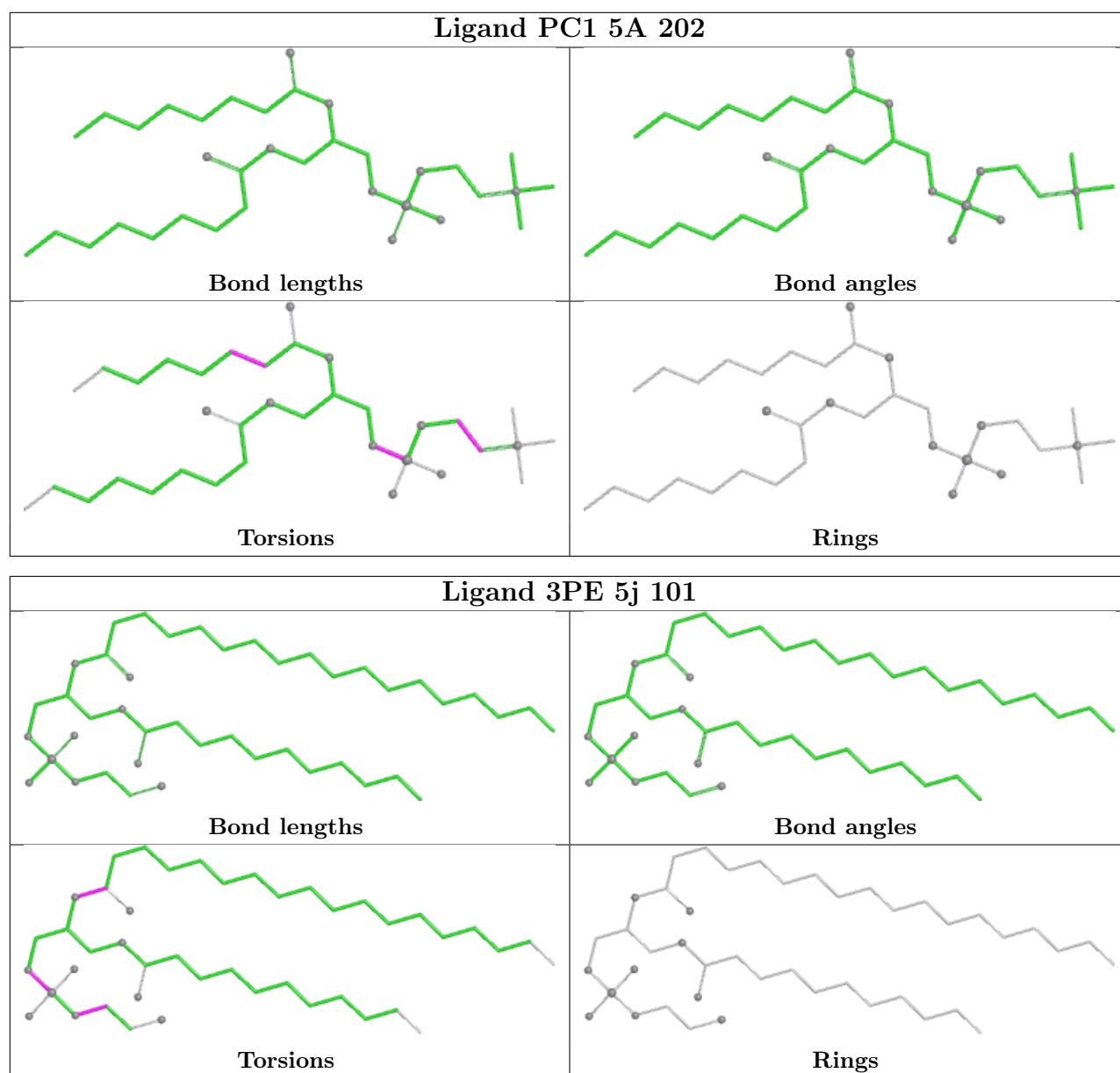
Rings

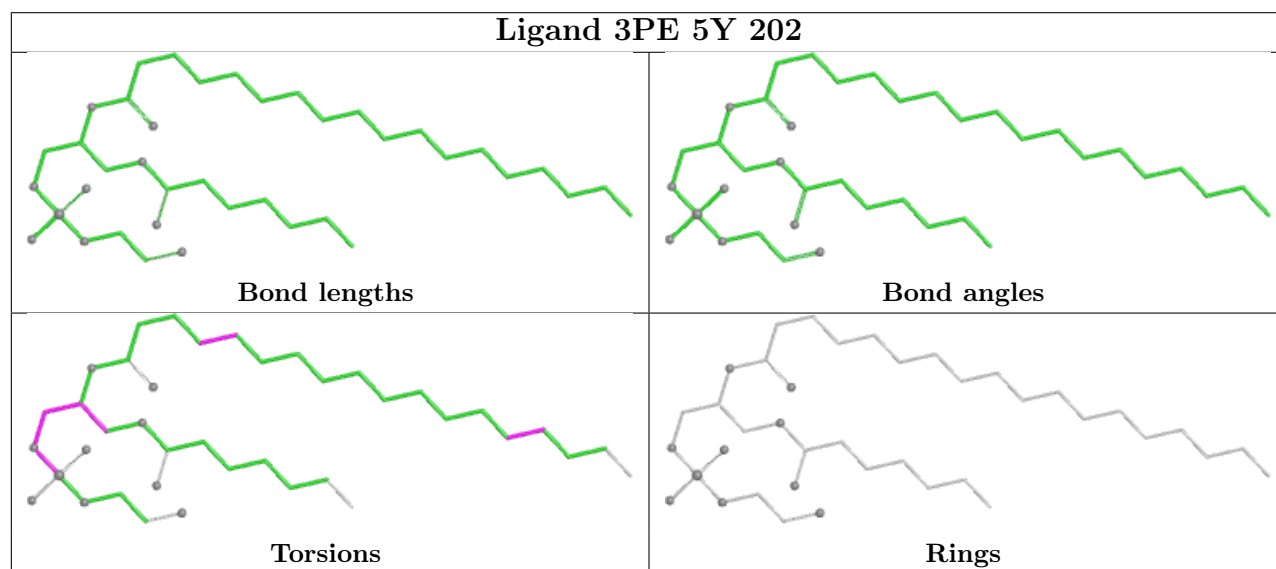
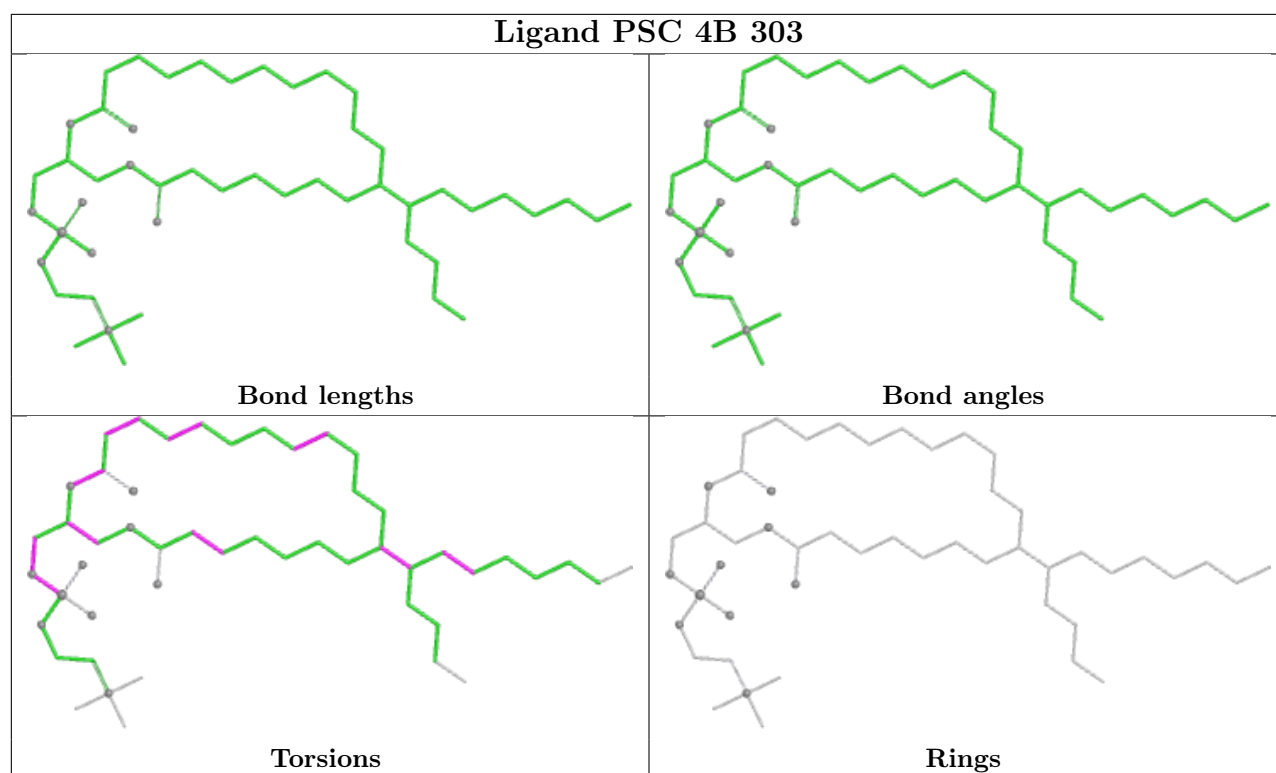


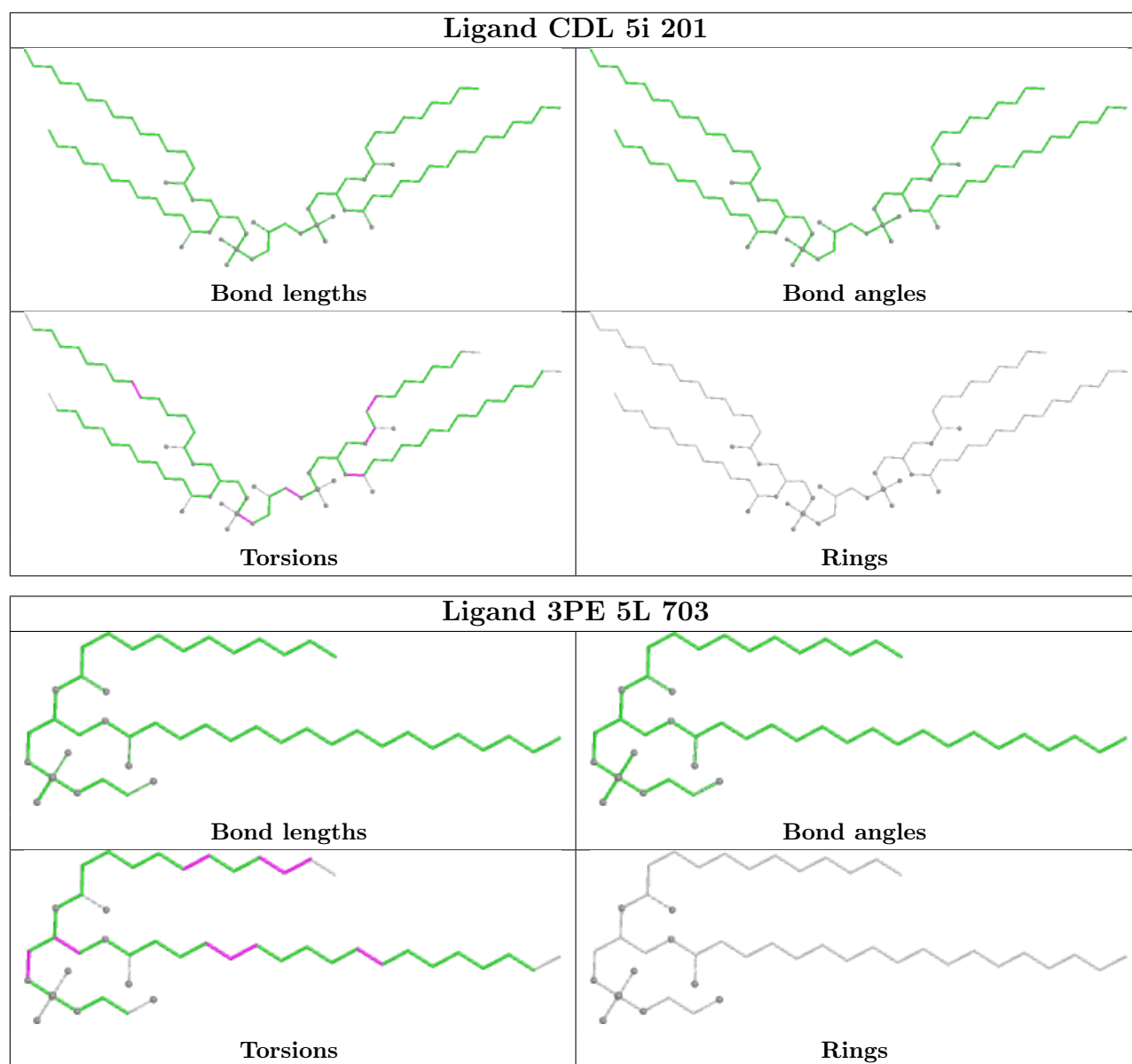


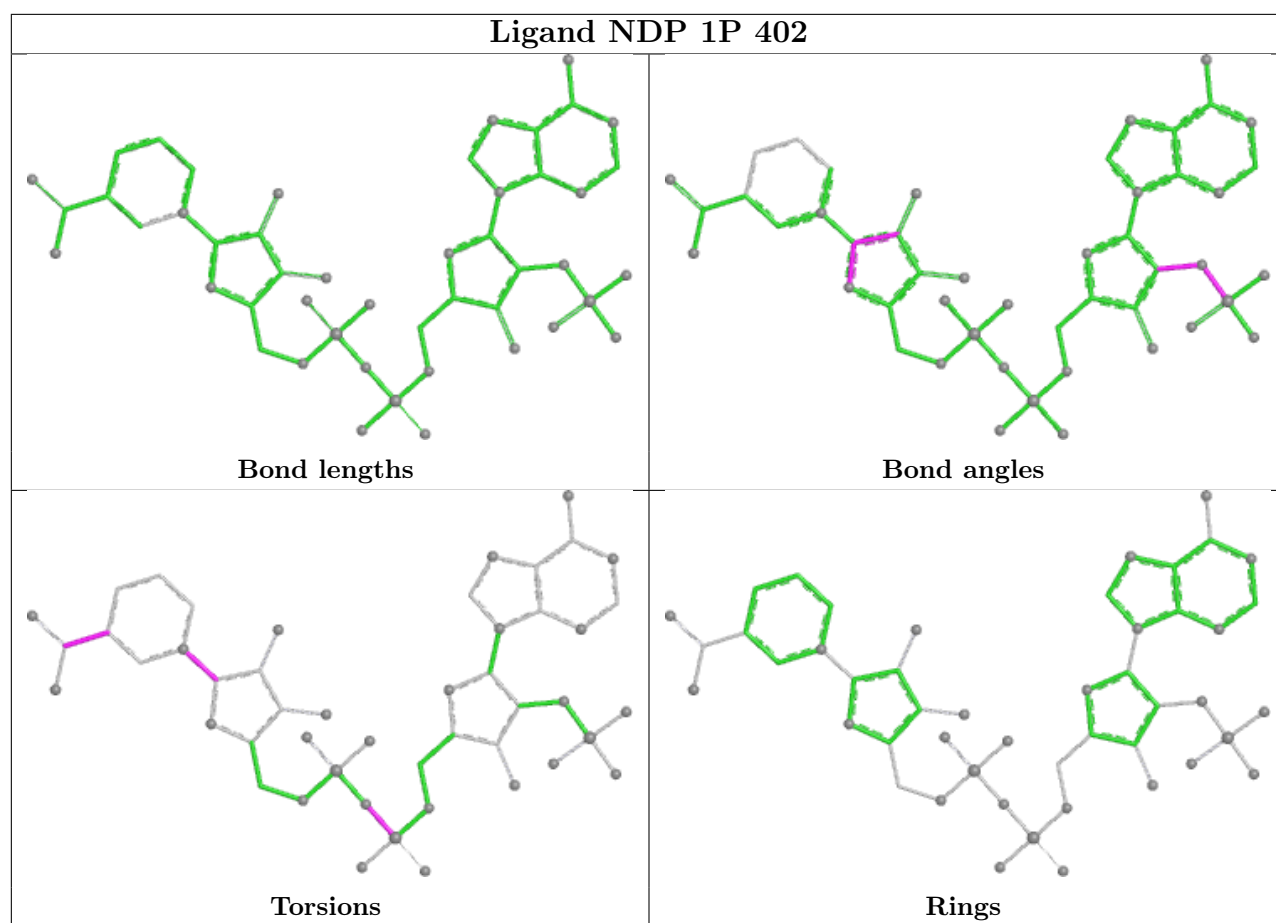


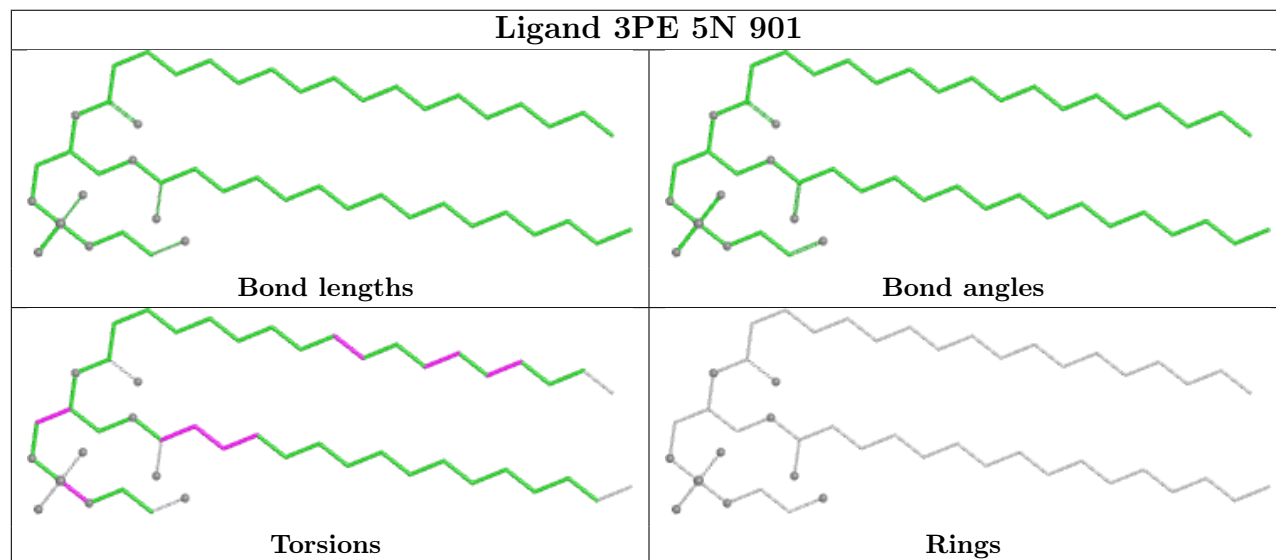
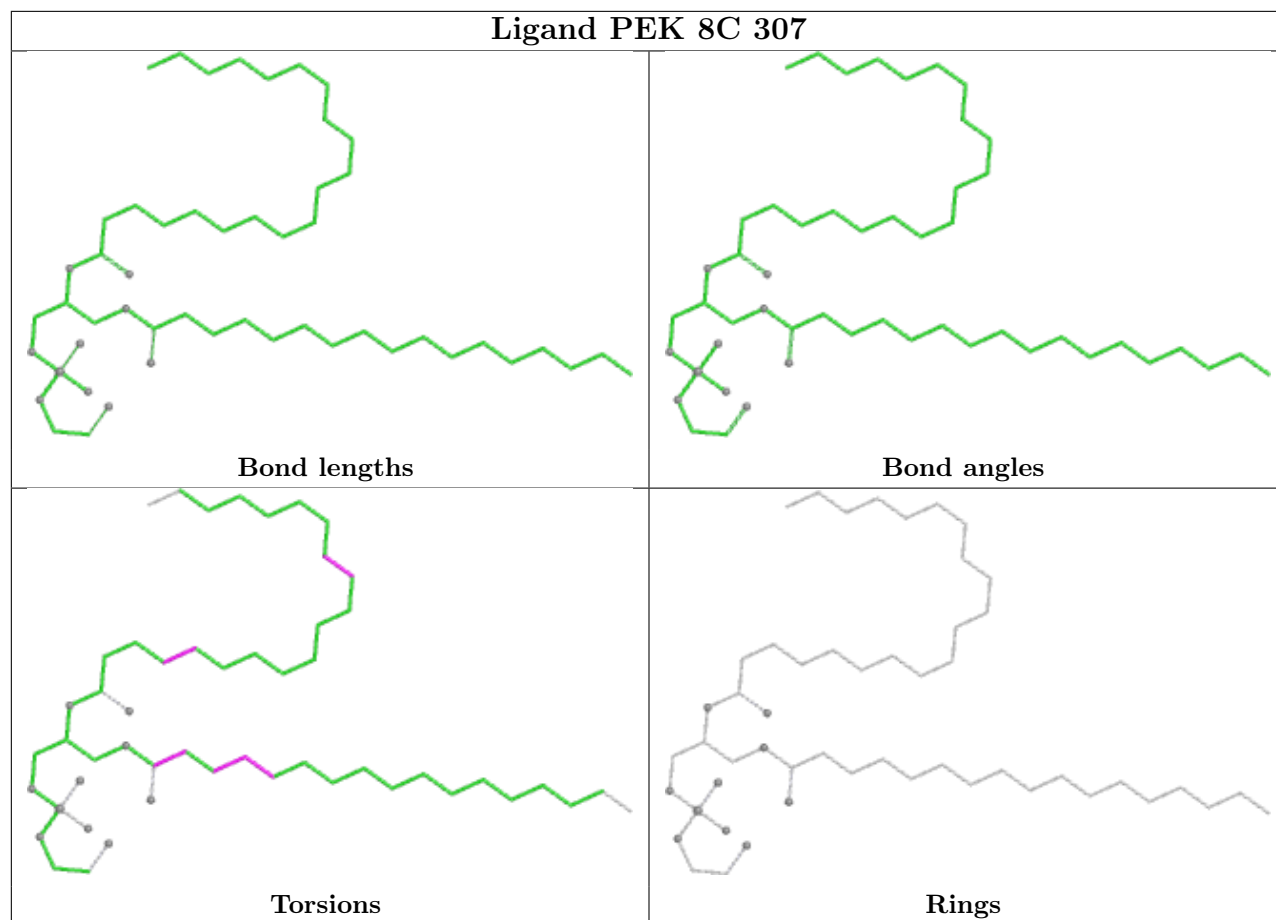


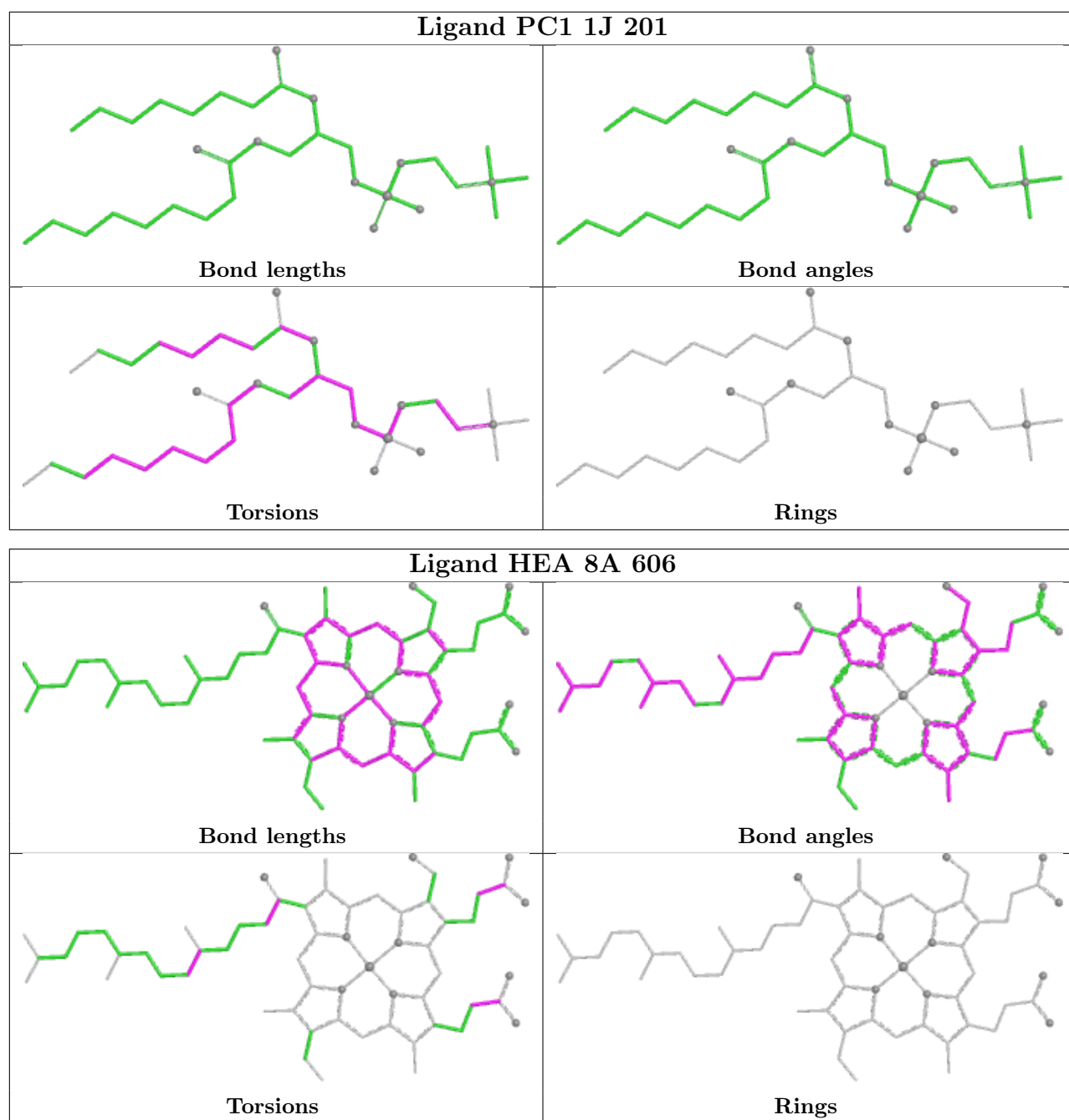


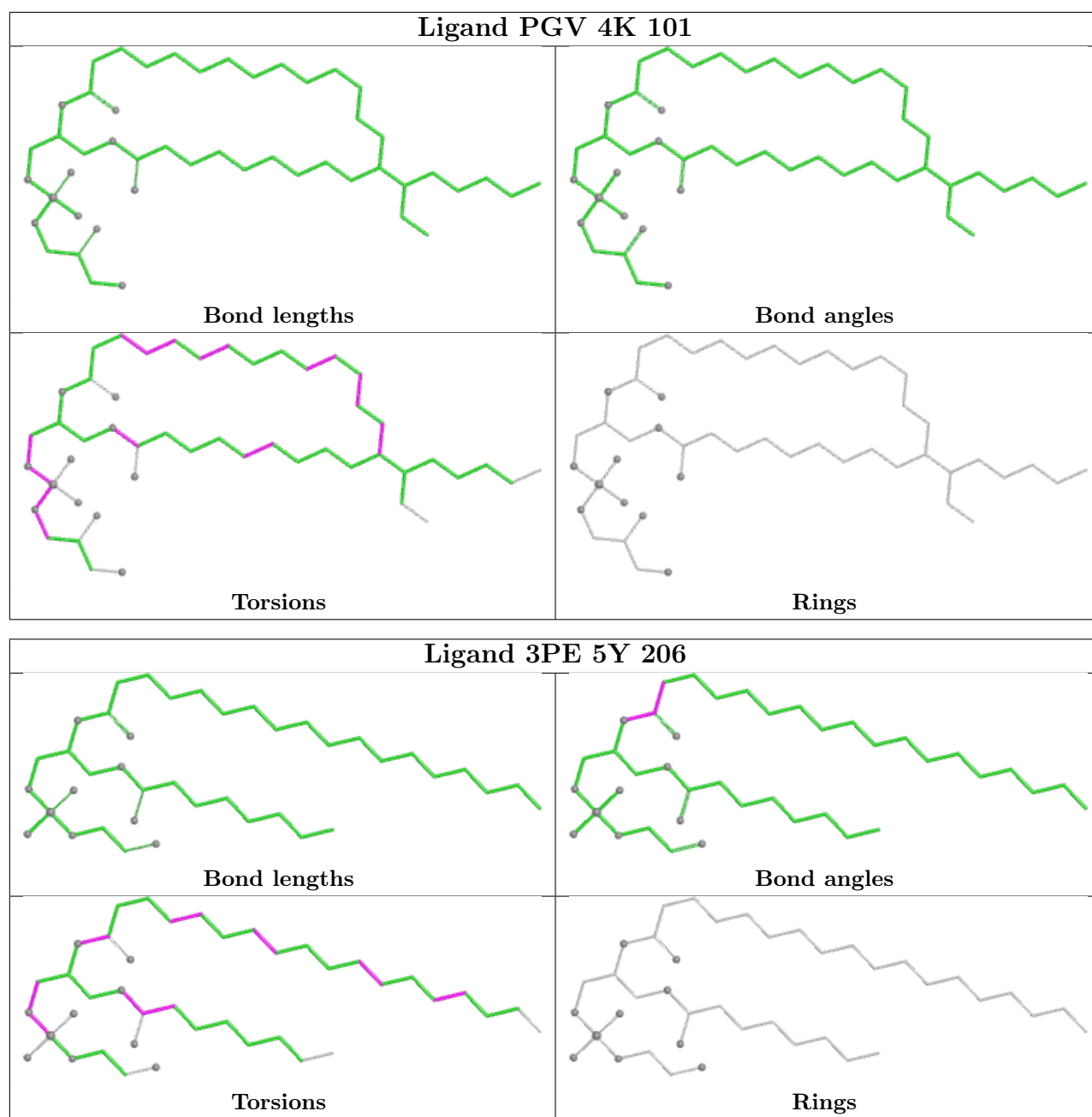


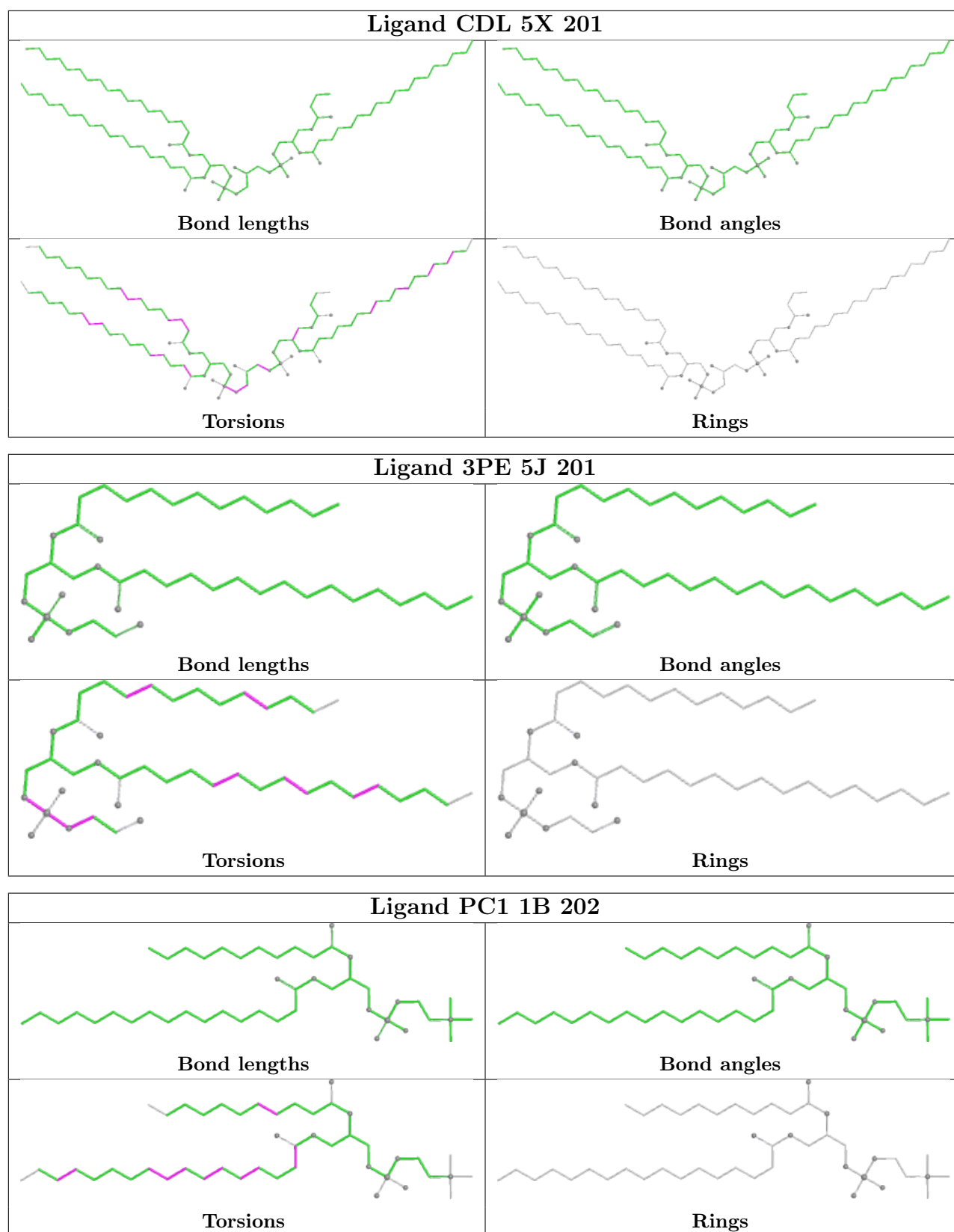


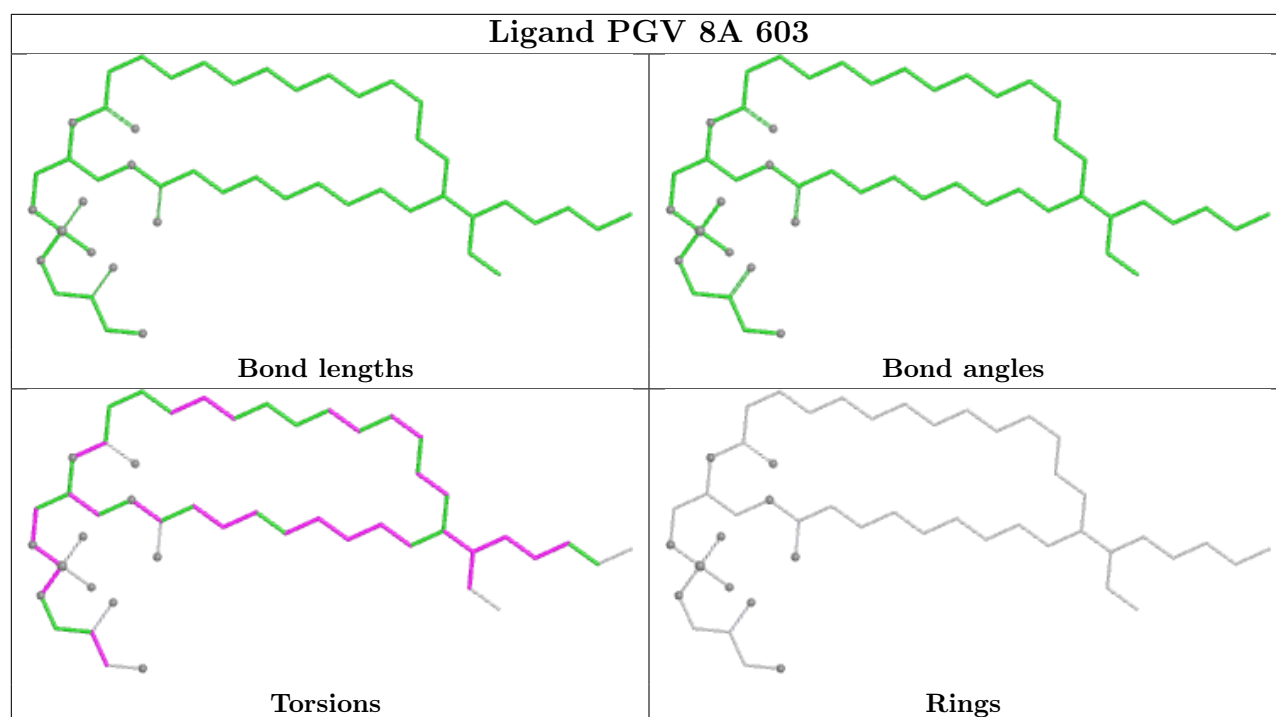


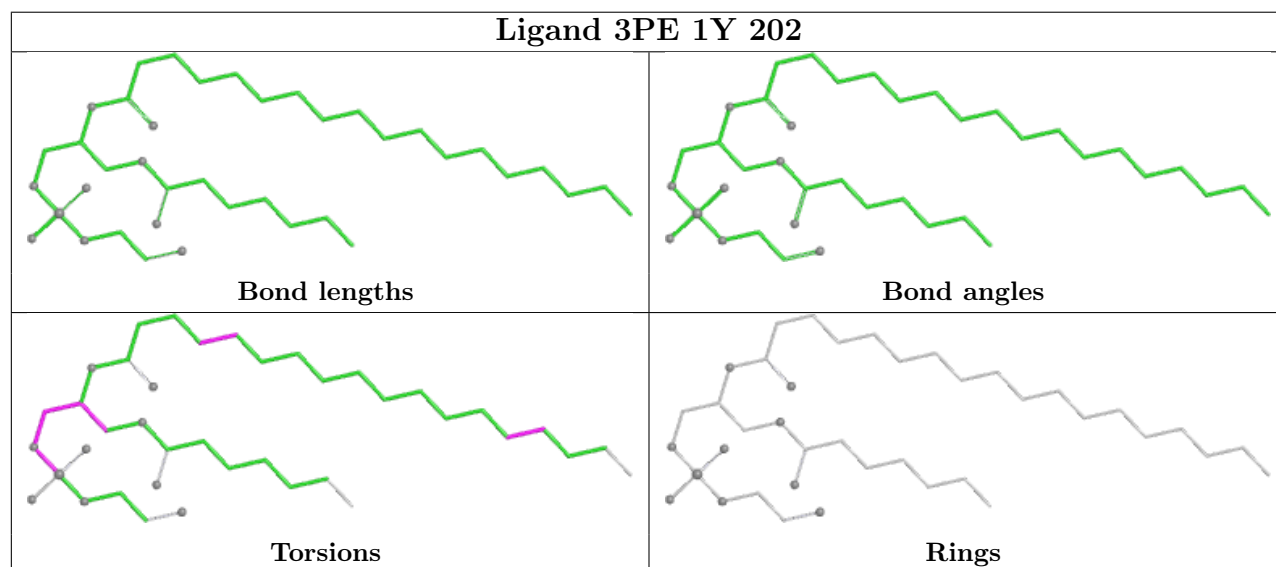
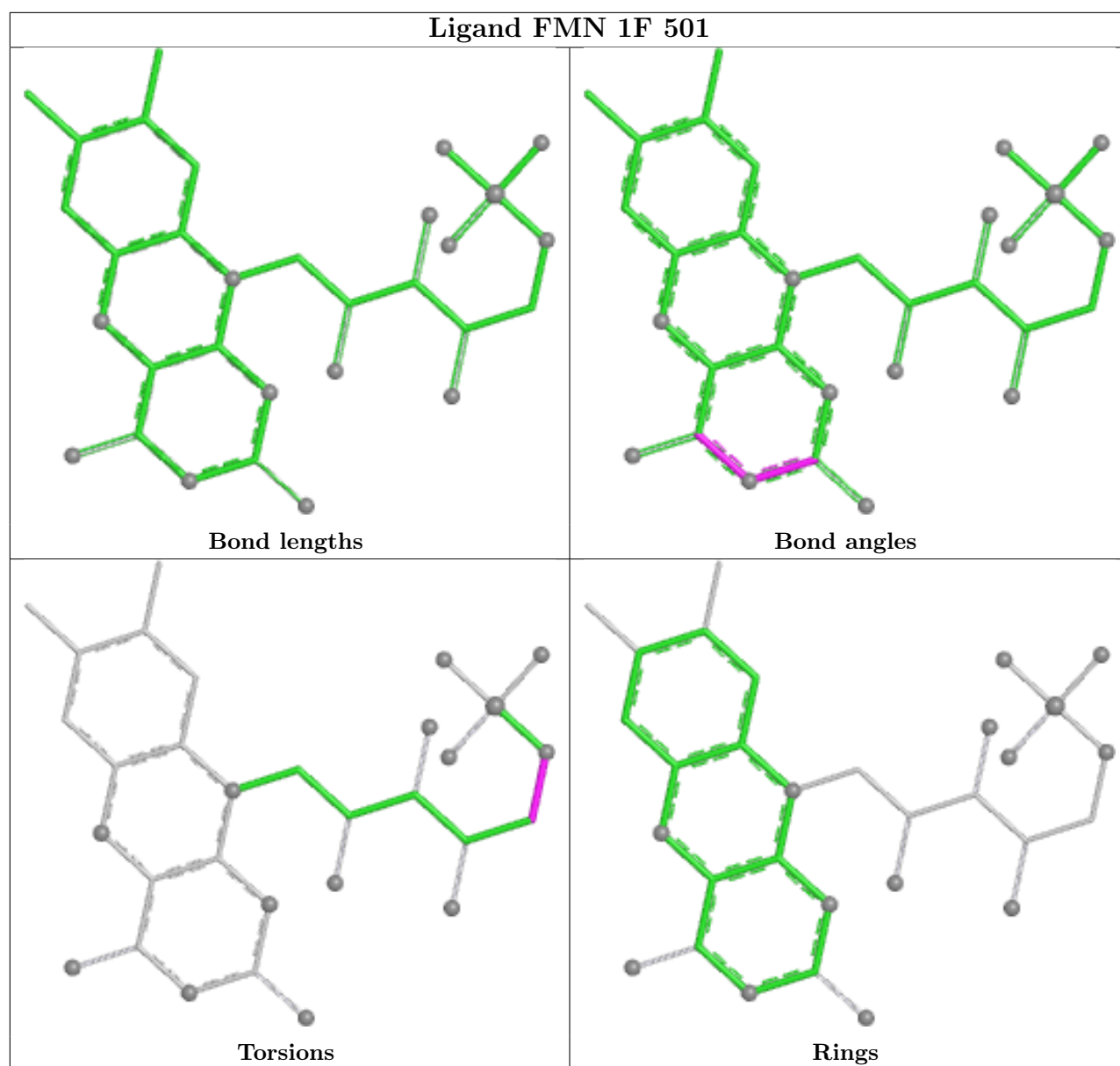


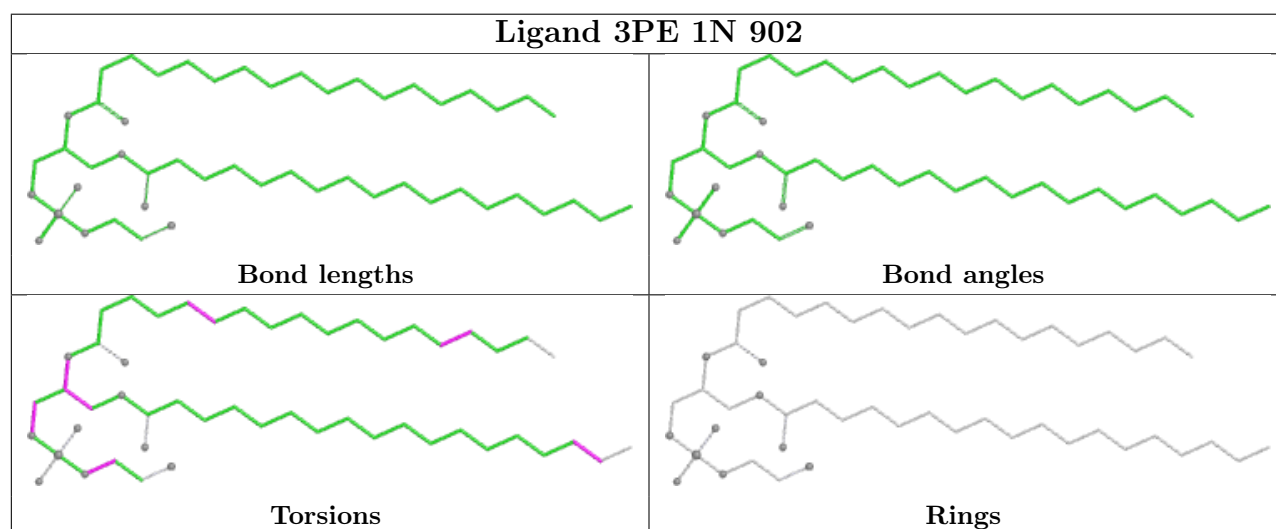
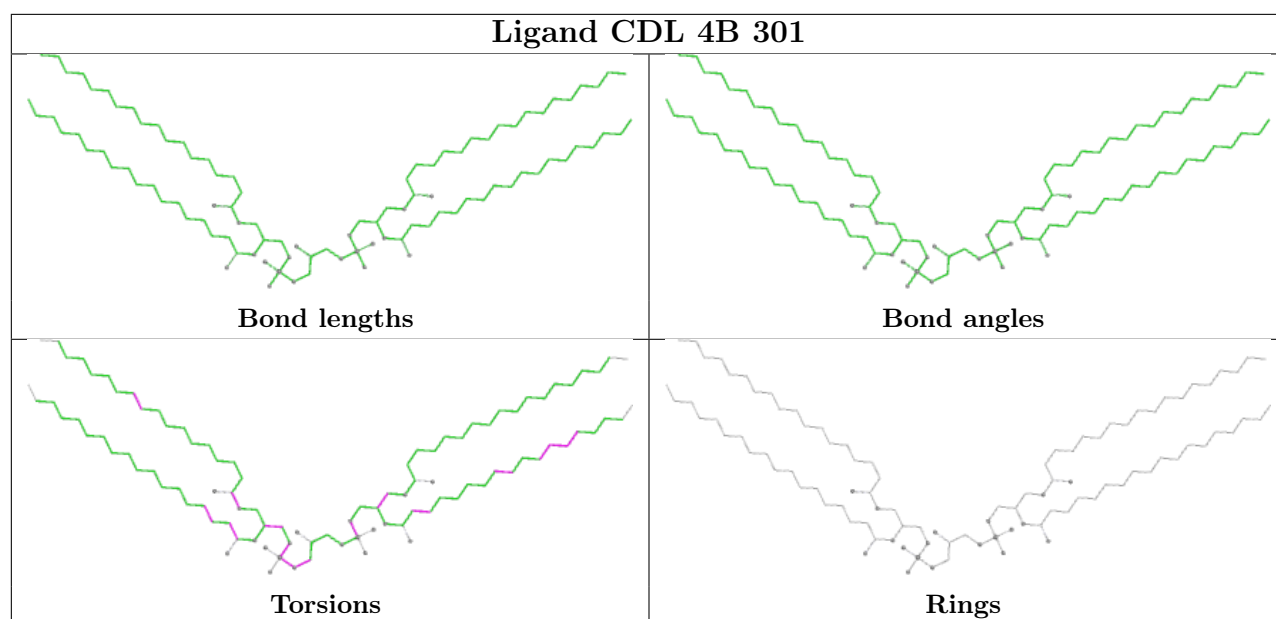




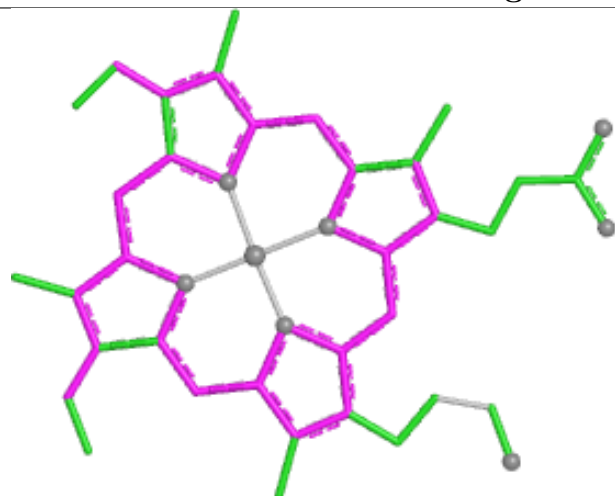




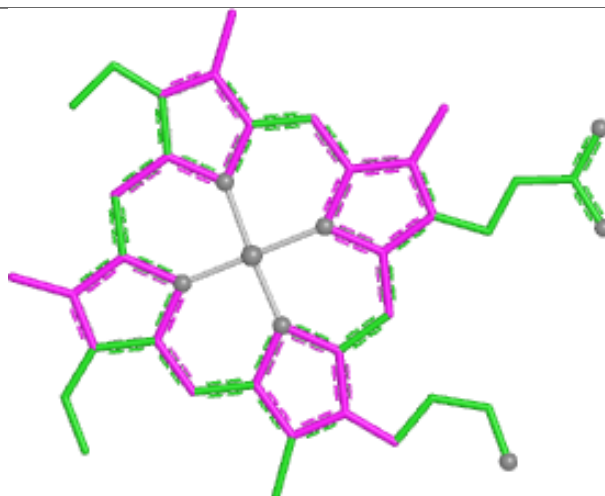




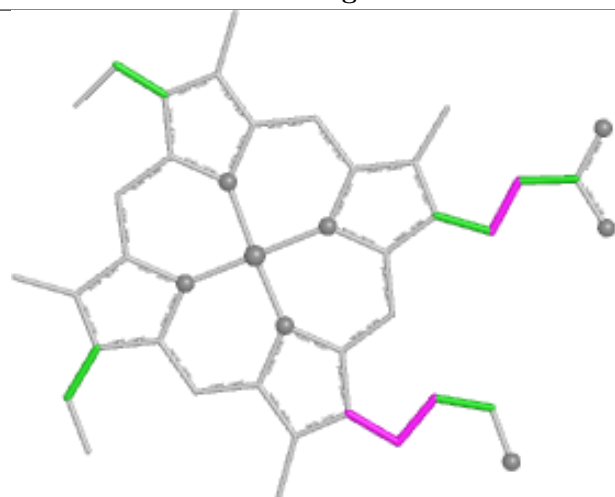
Ligand HEC 6D 501



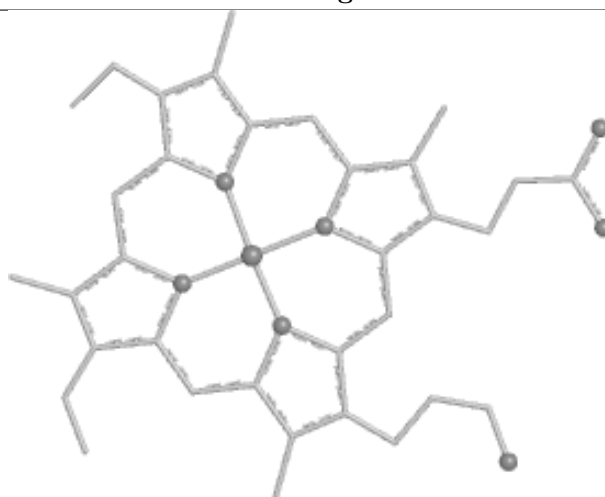
Bond lengths



Bond angles

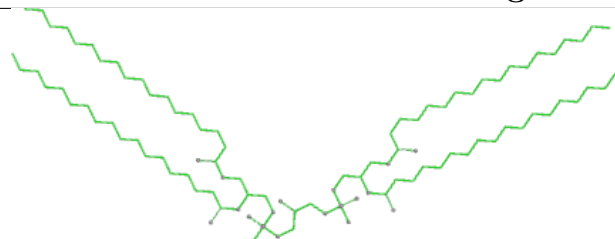


Torsions

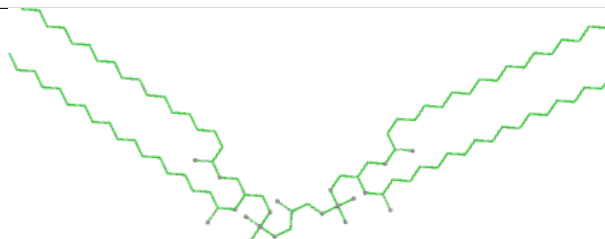


Rings

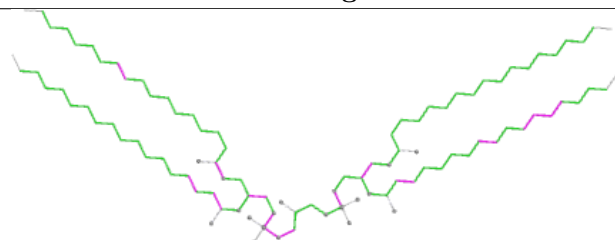
Ligand CDL 8B 302



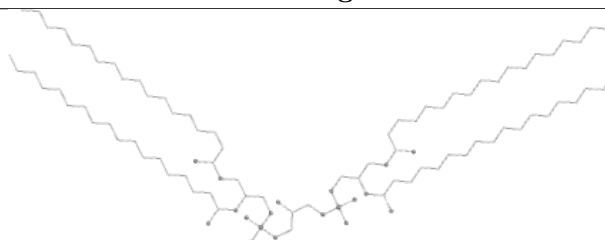
Bond lengths



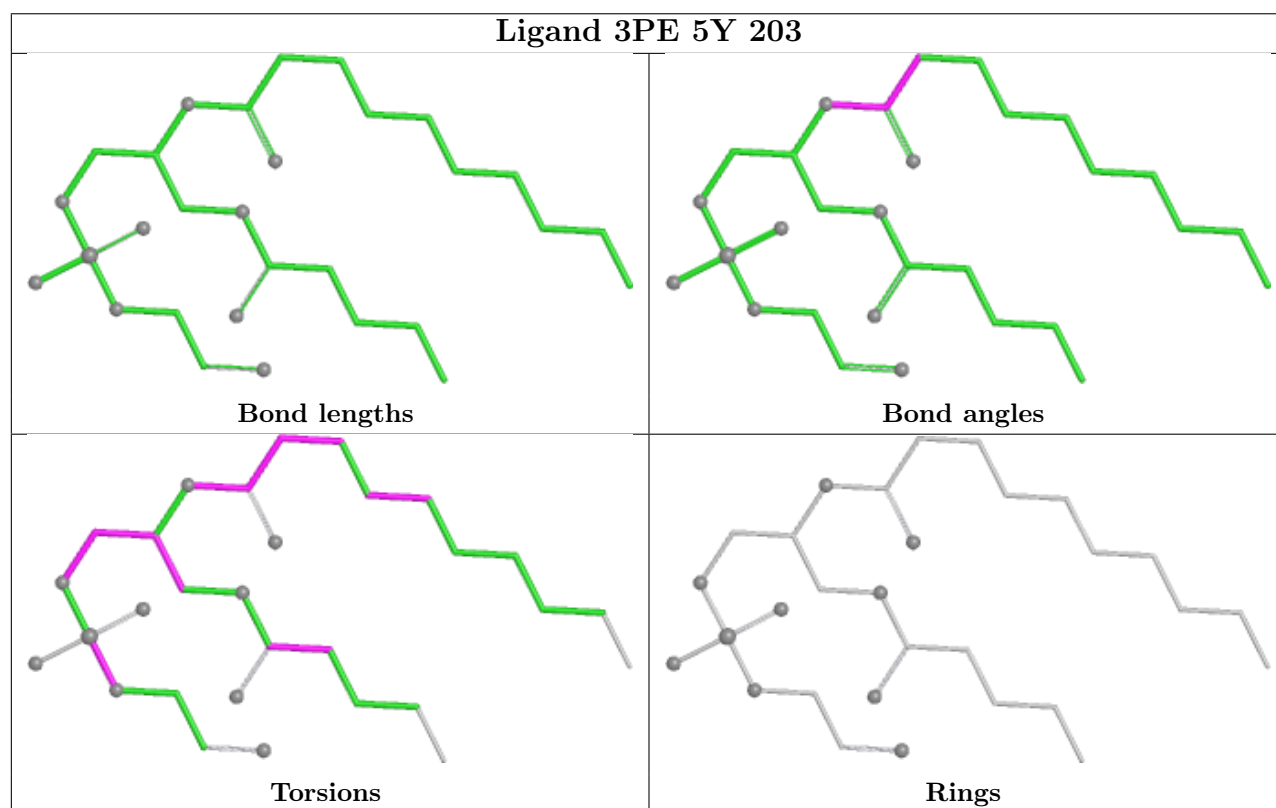
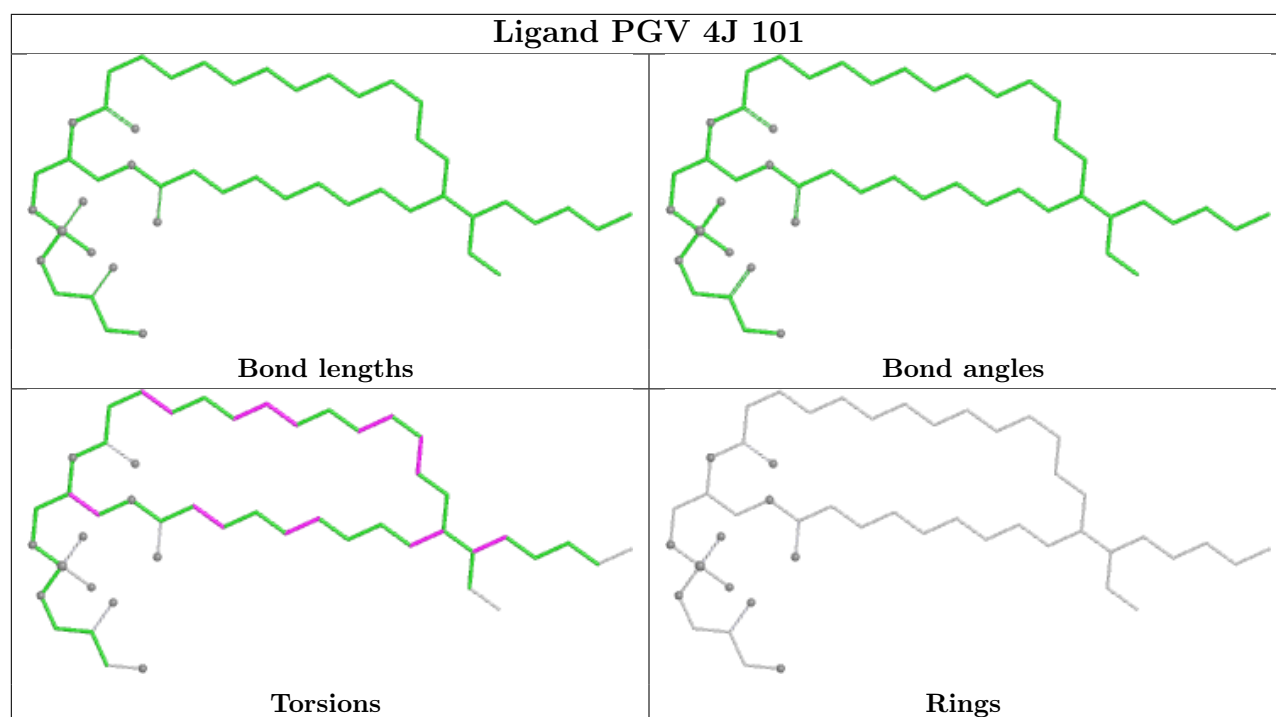
Bond angles

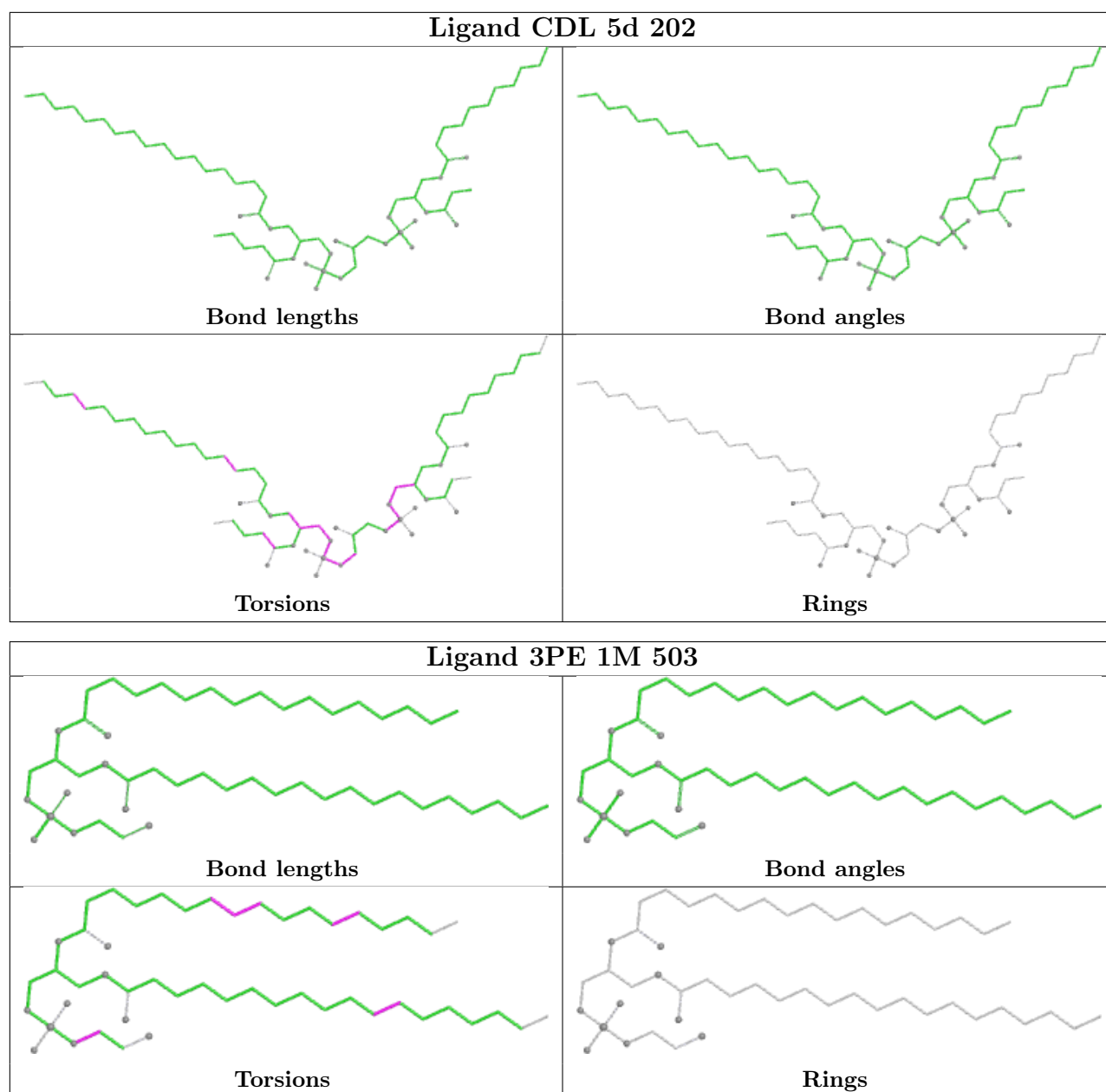


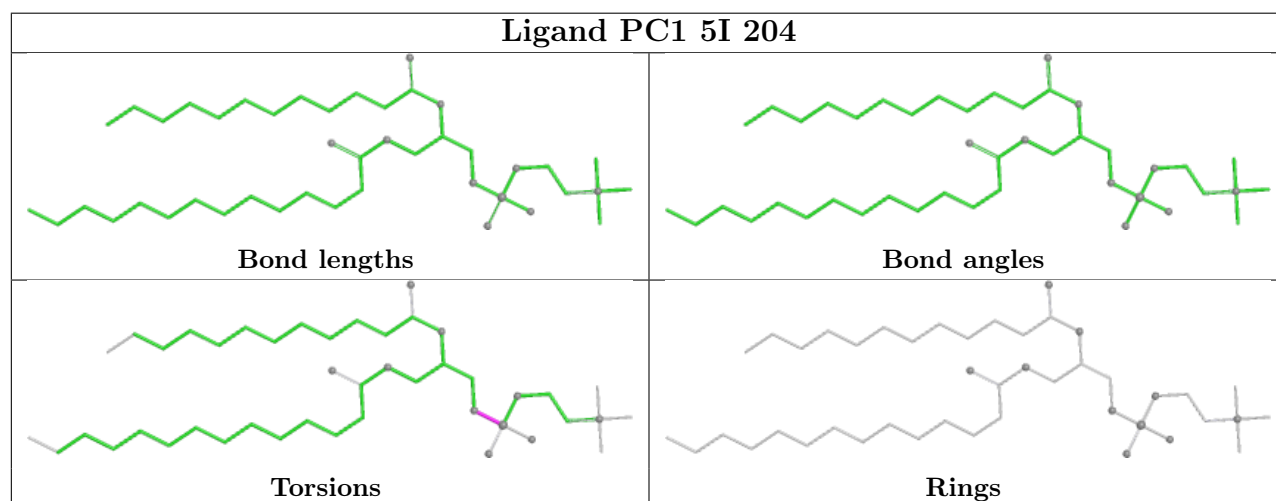
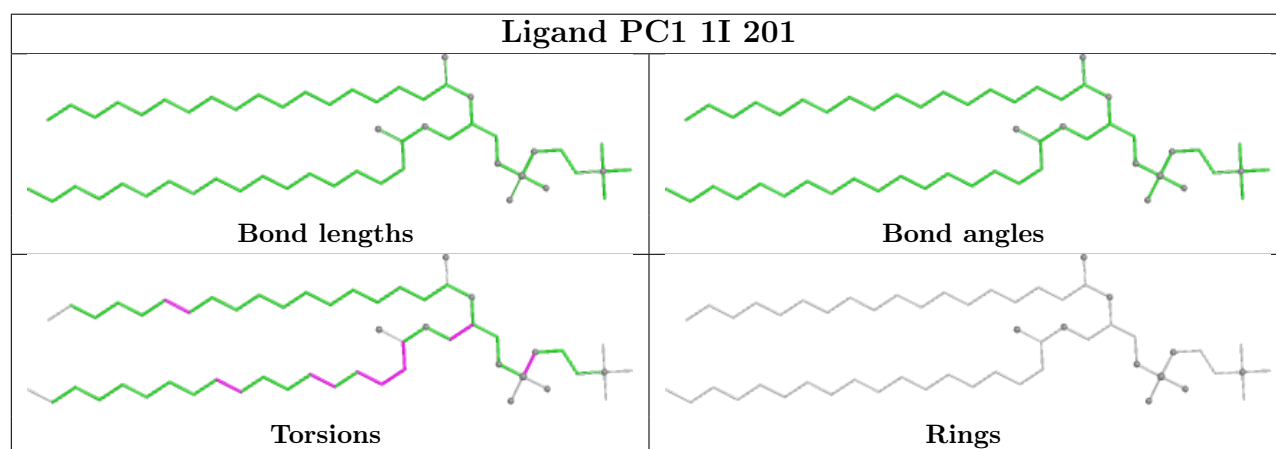
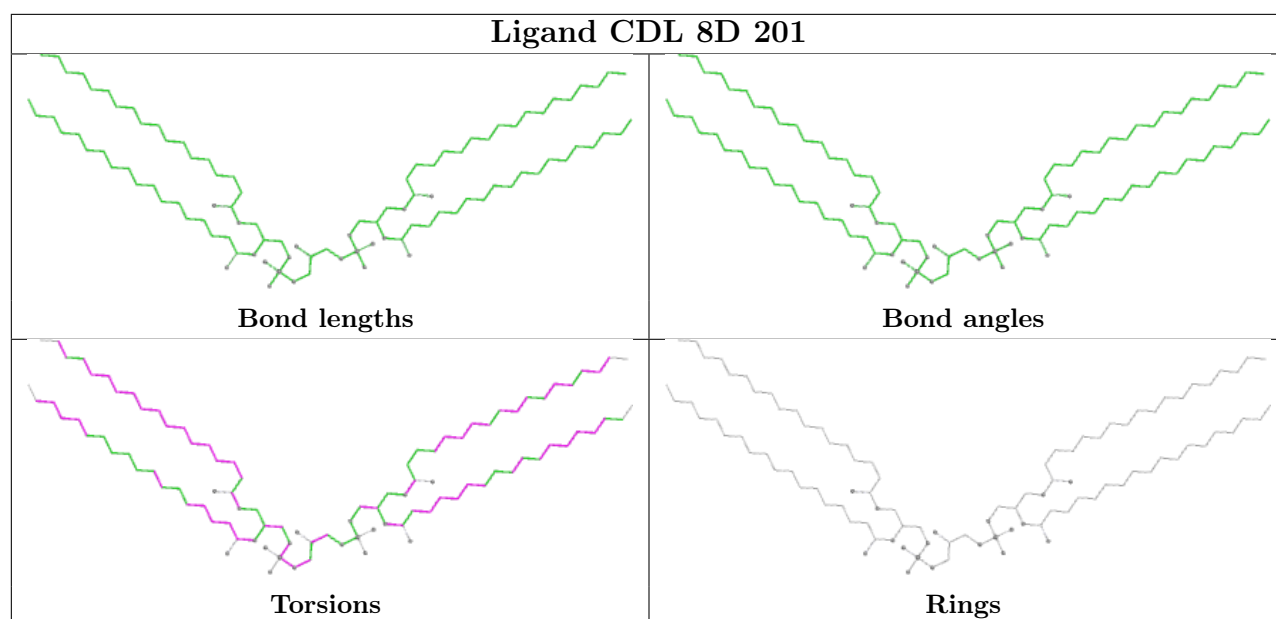
Torsions

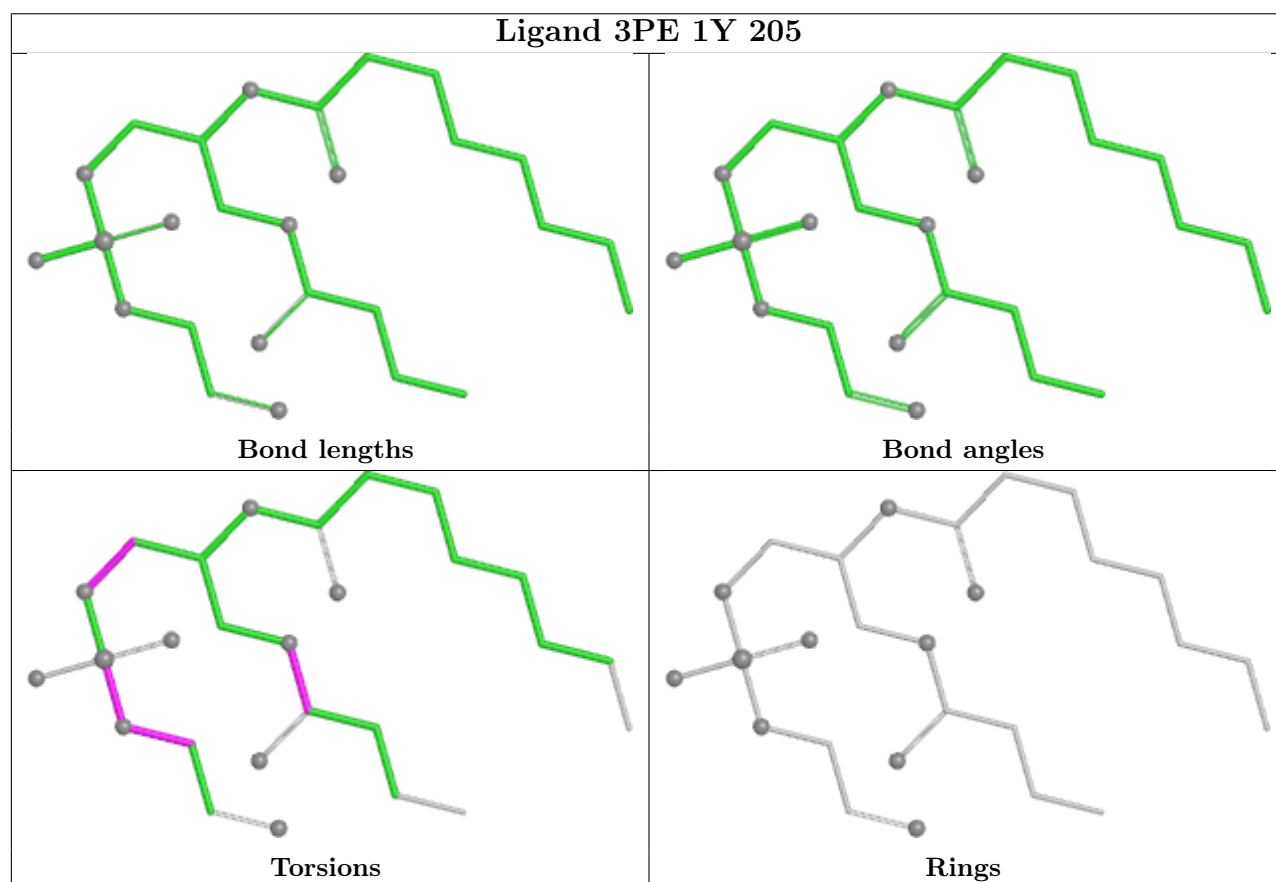
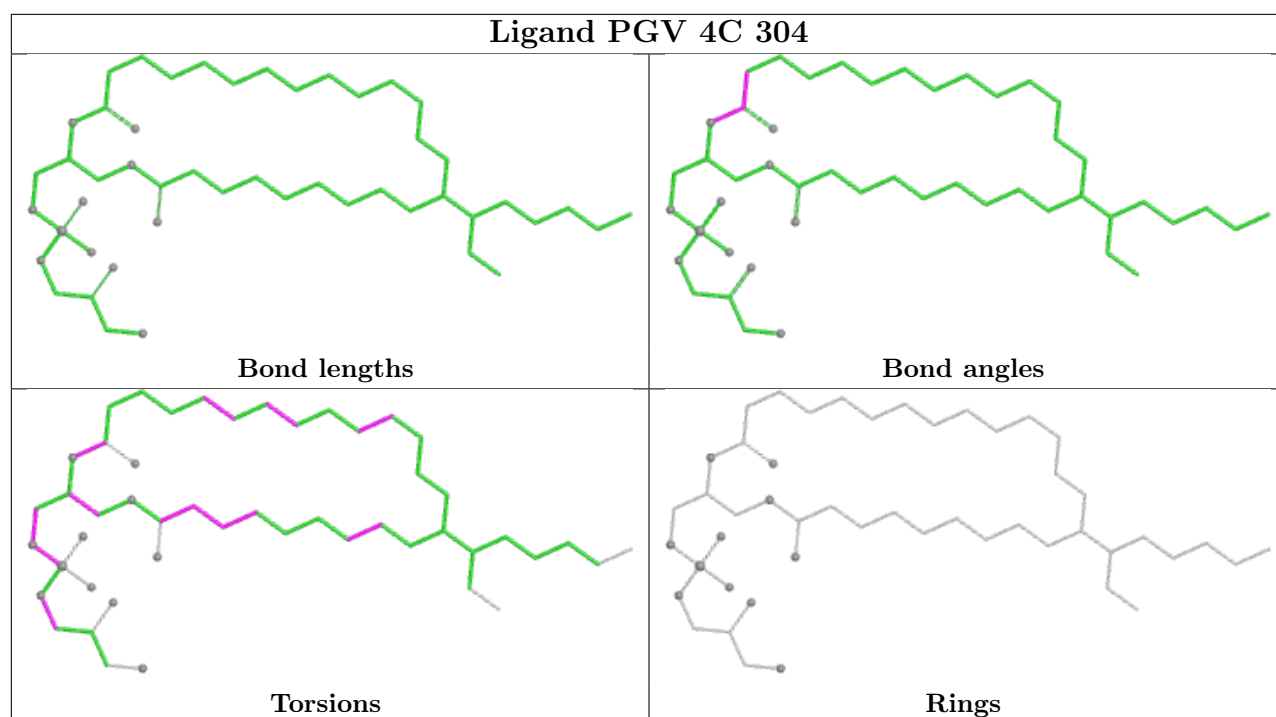


Rings

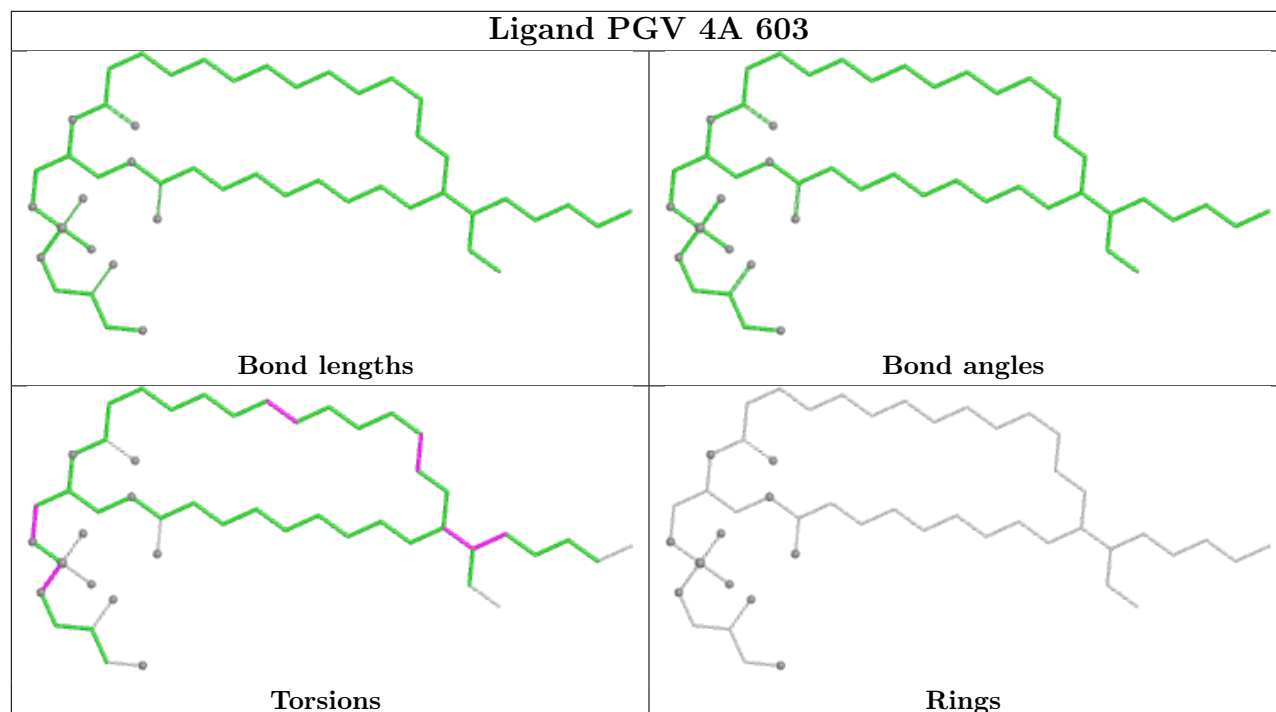




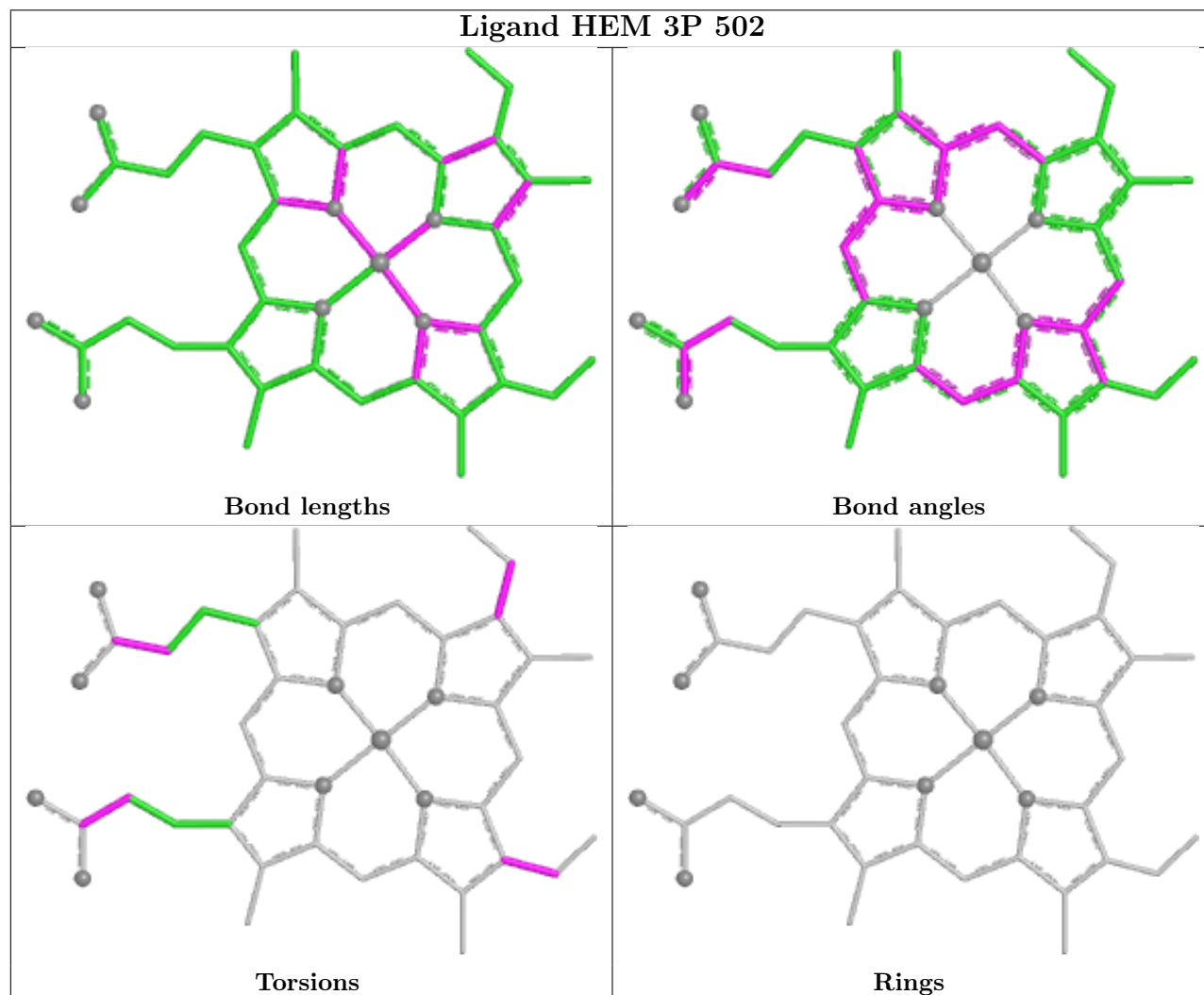


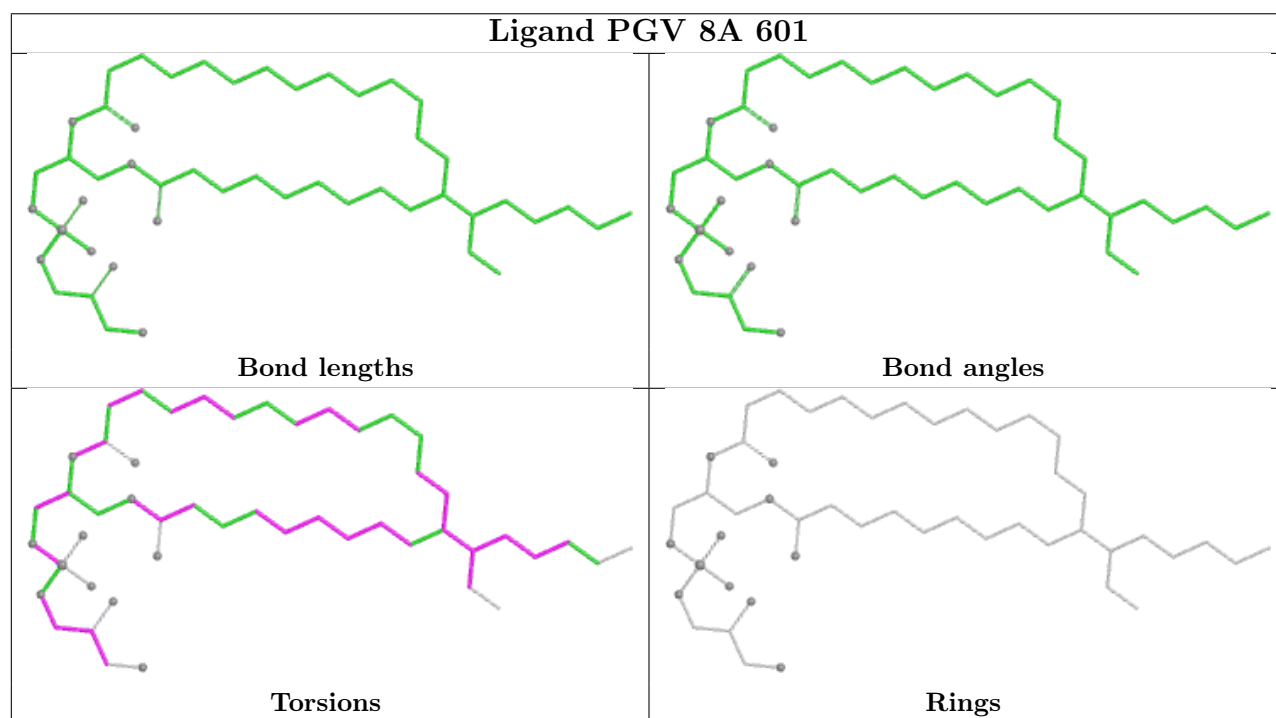
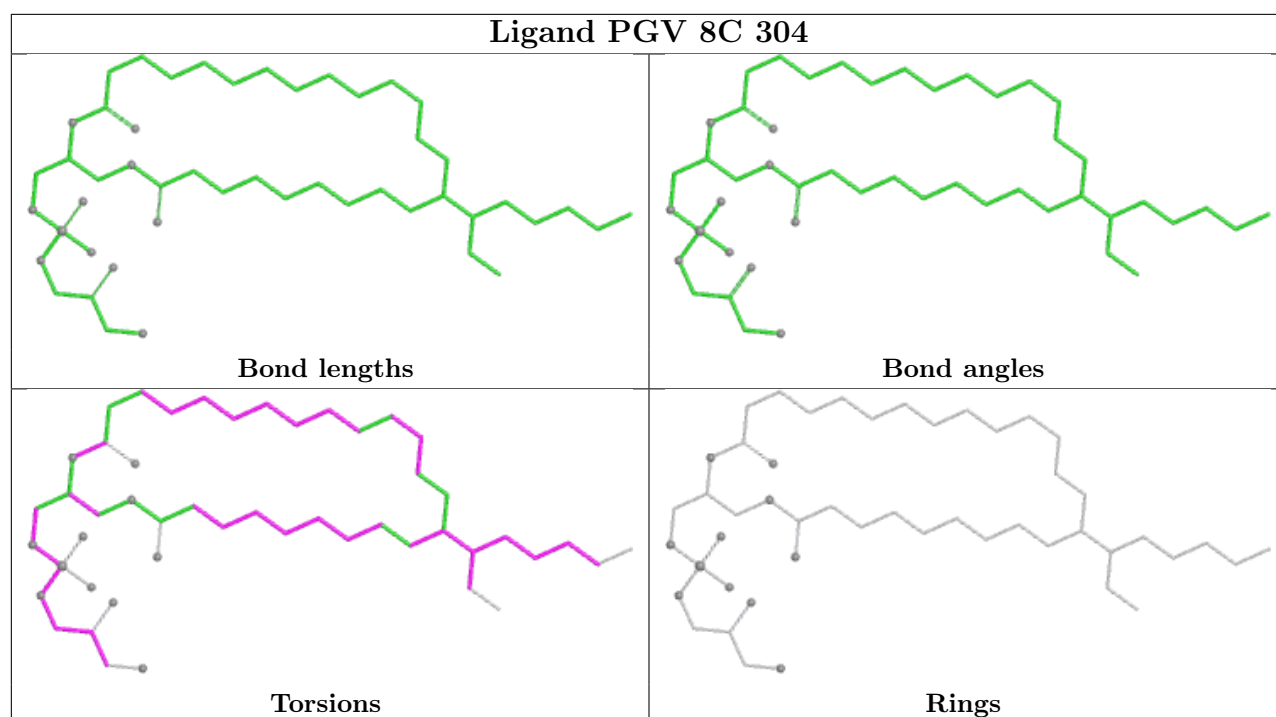


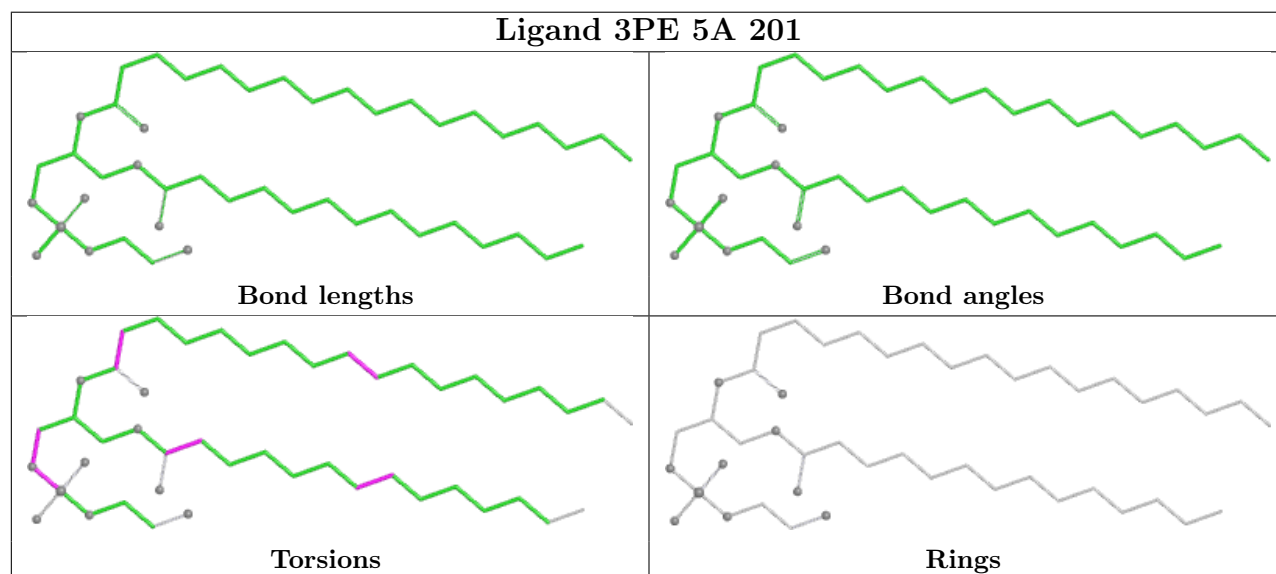
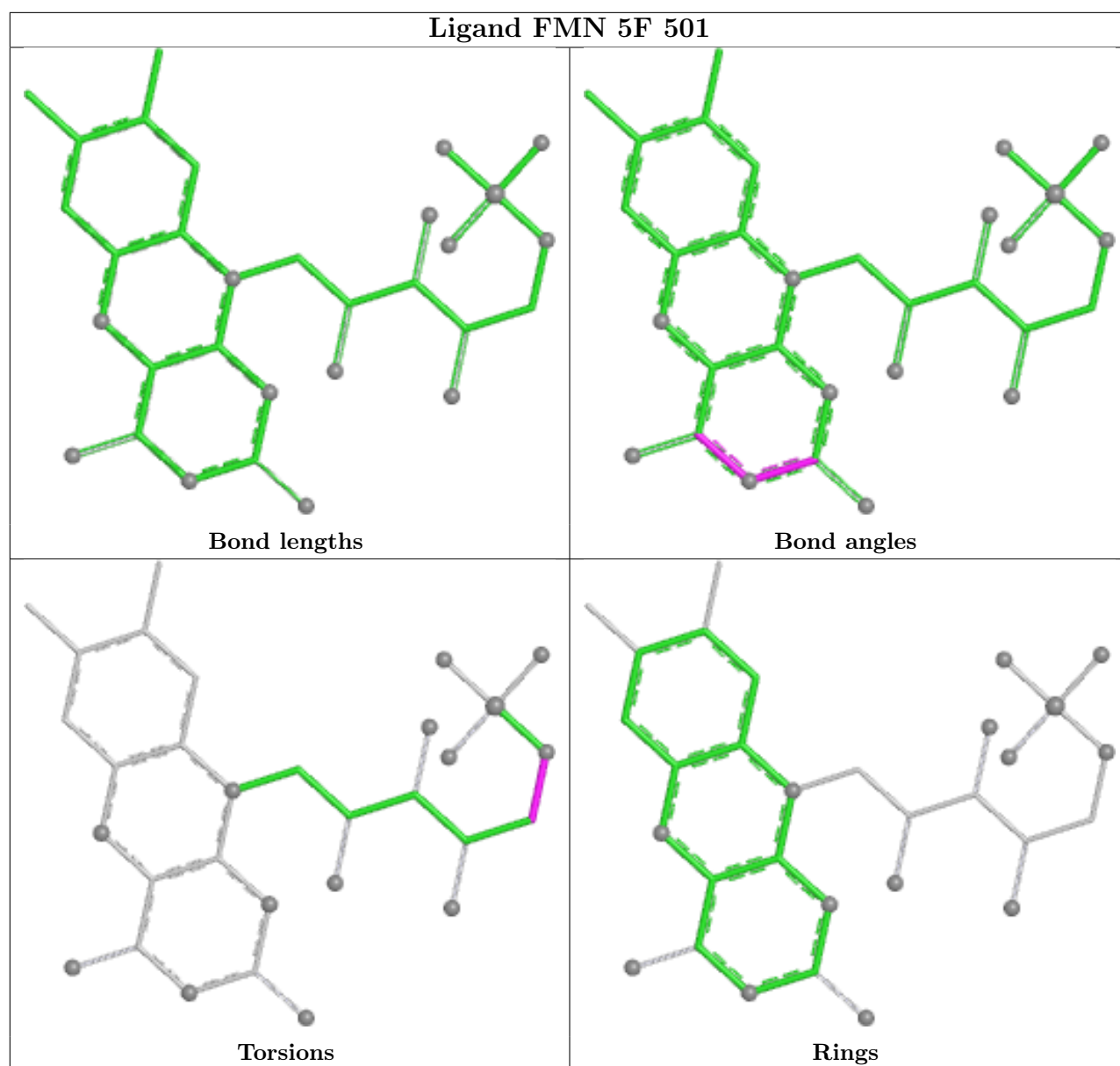
Ligand PGV 4A 603

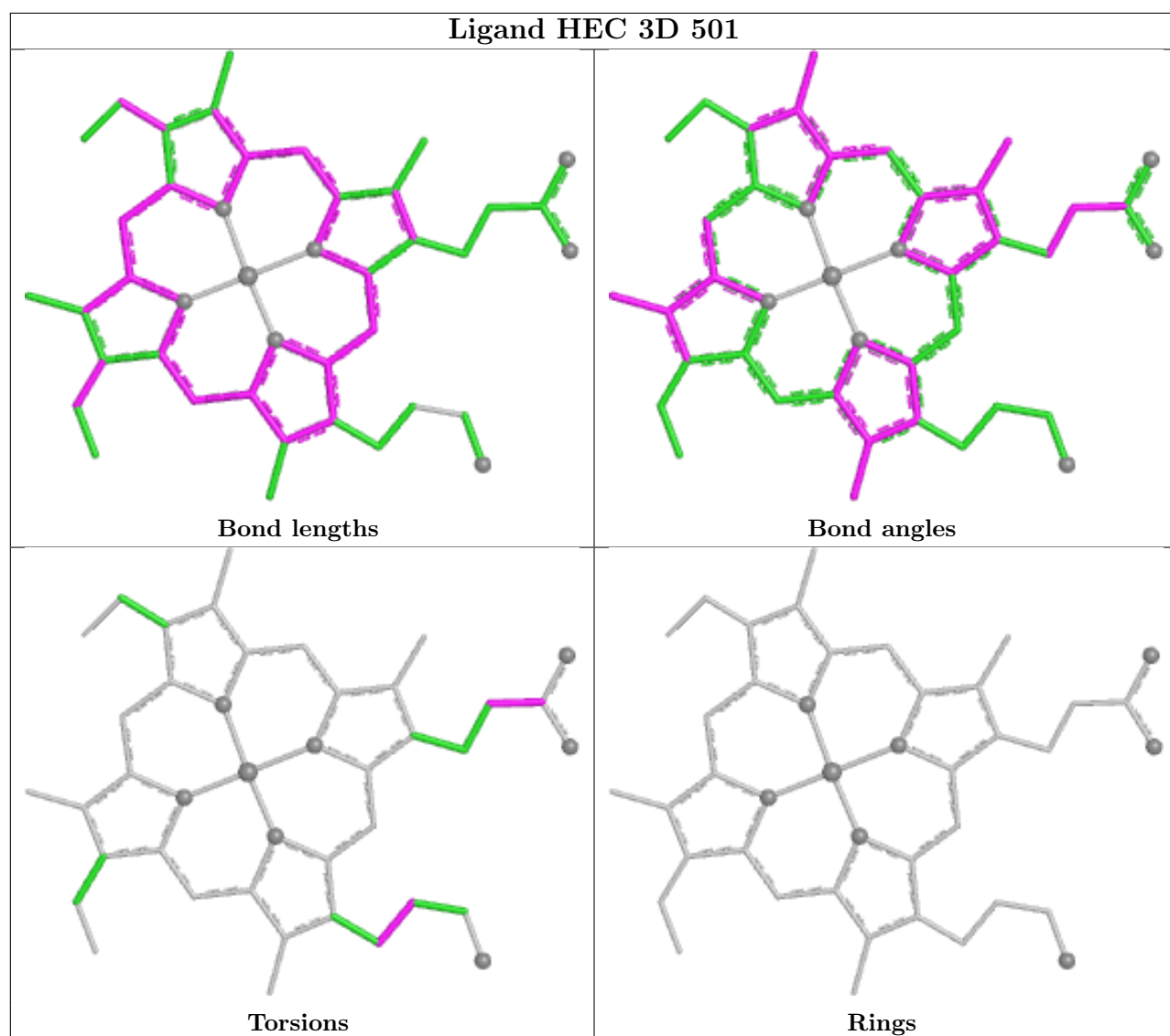


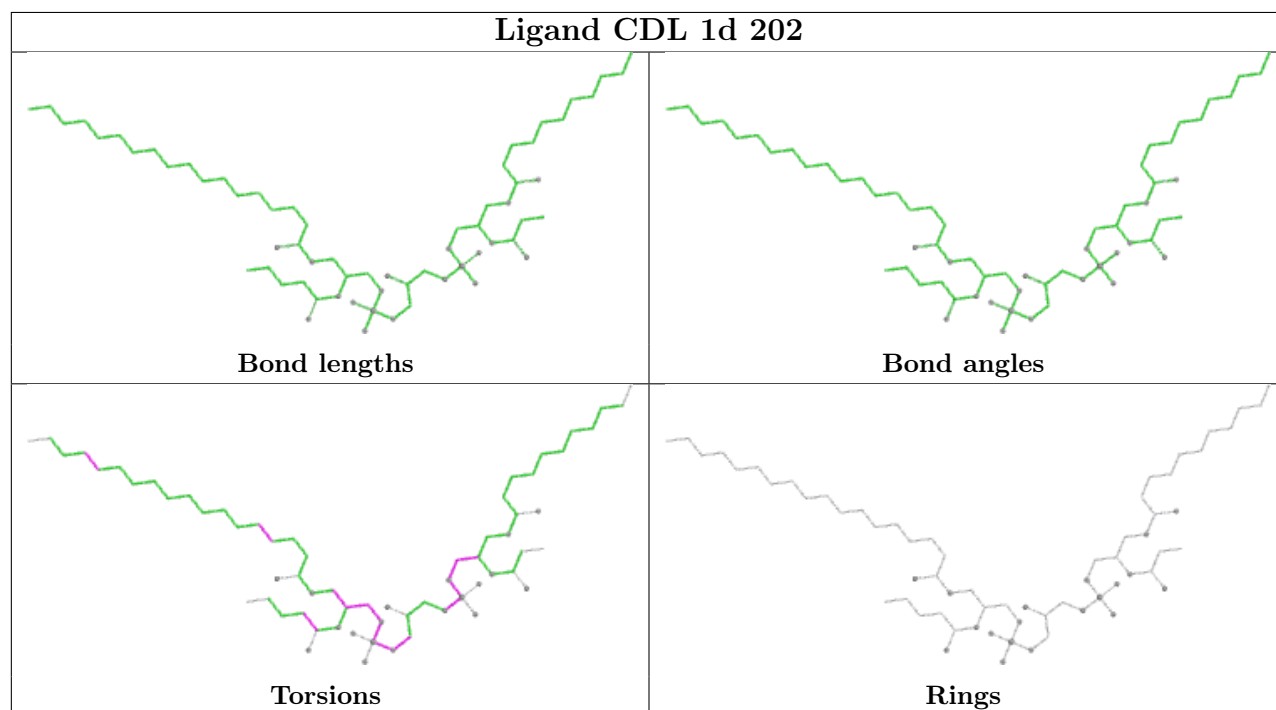
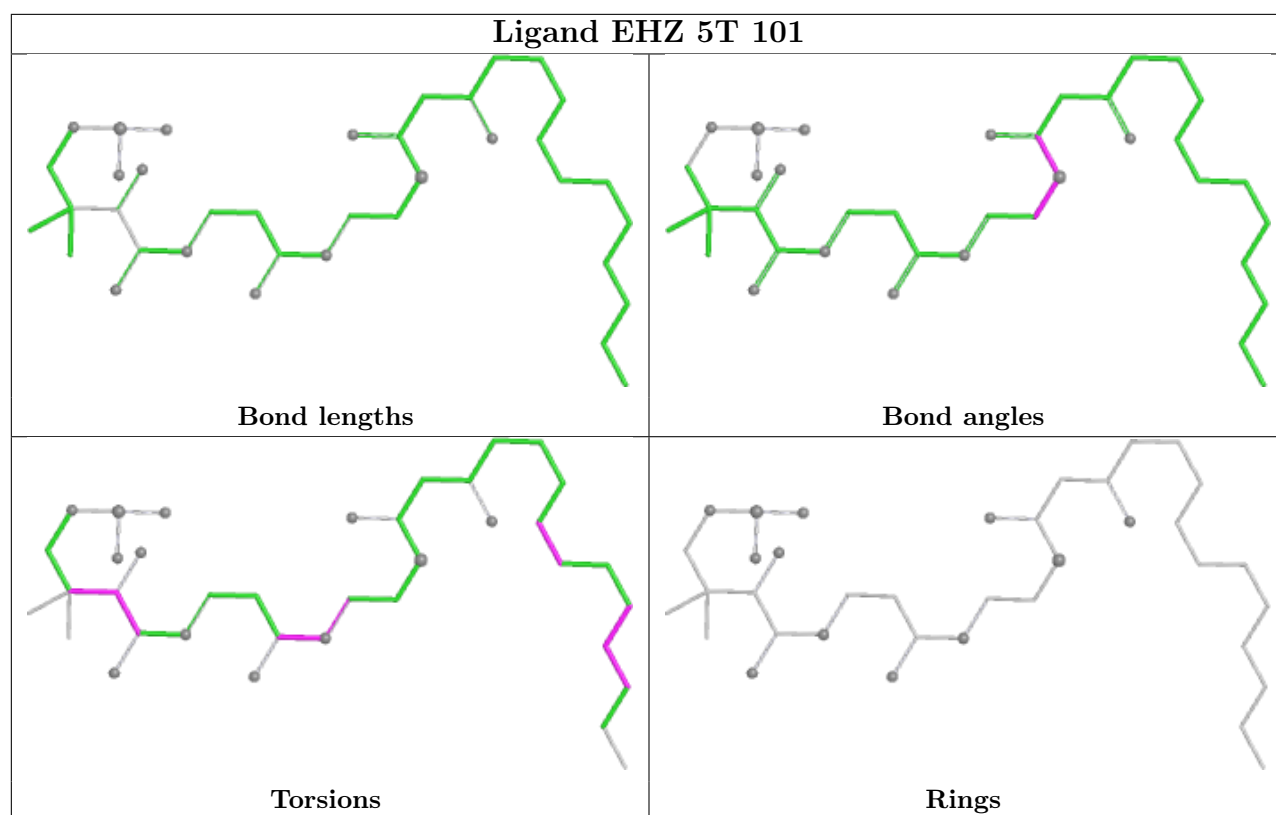
Ligand HEM 3P 502

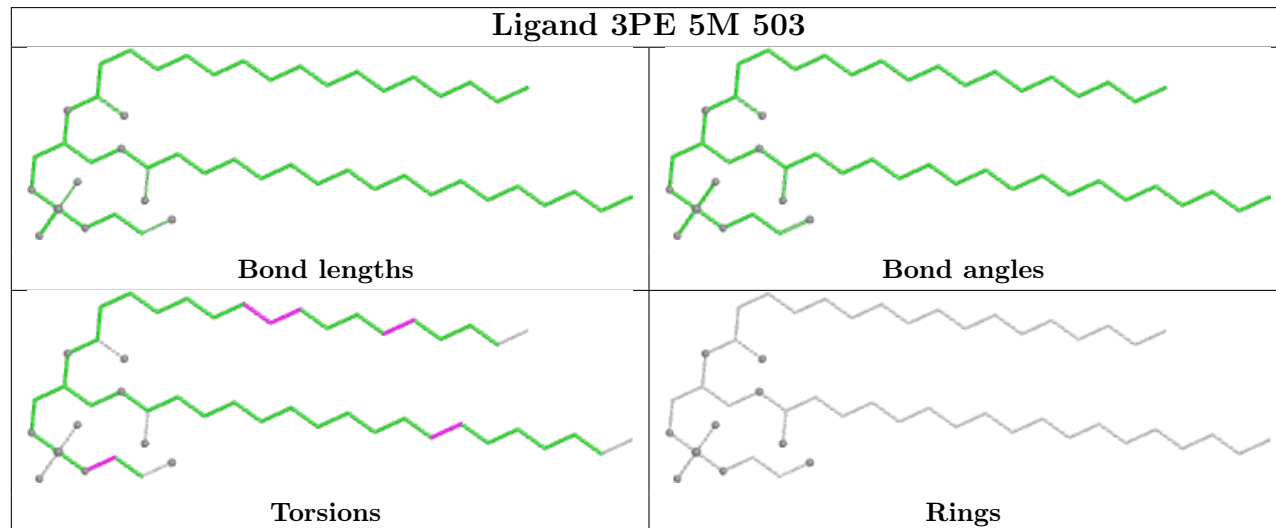
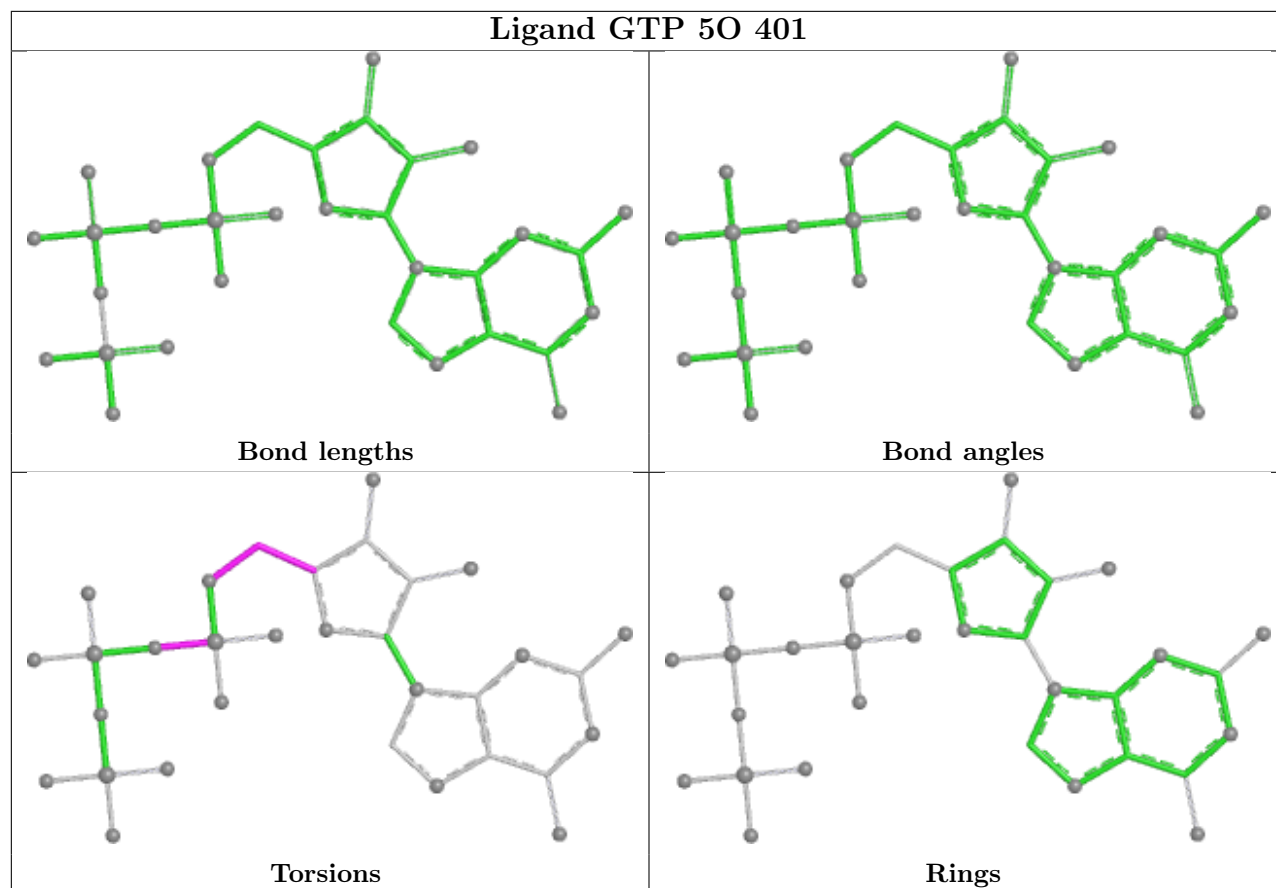


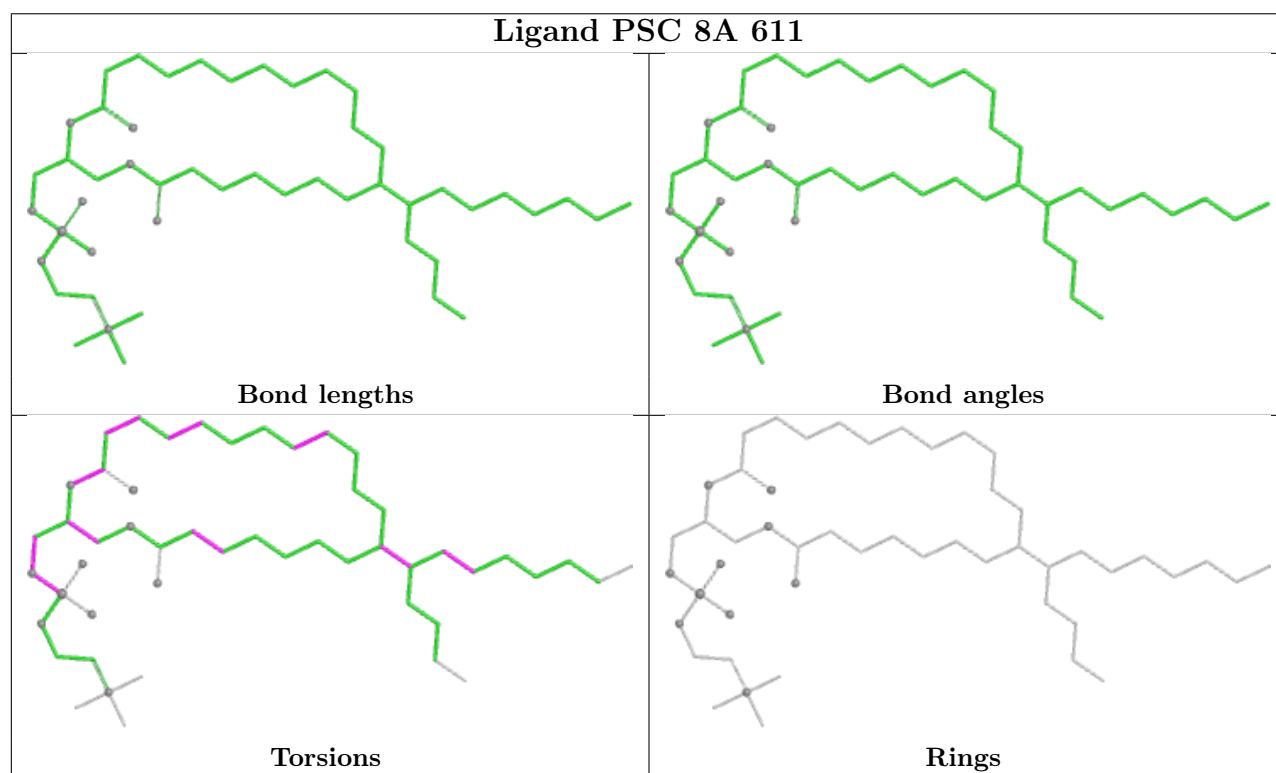
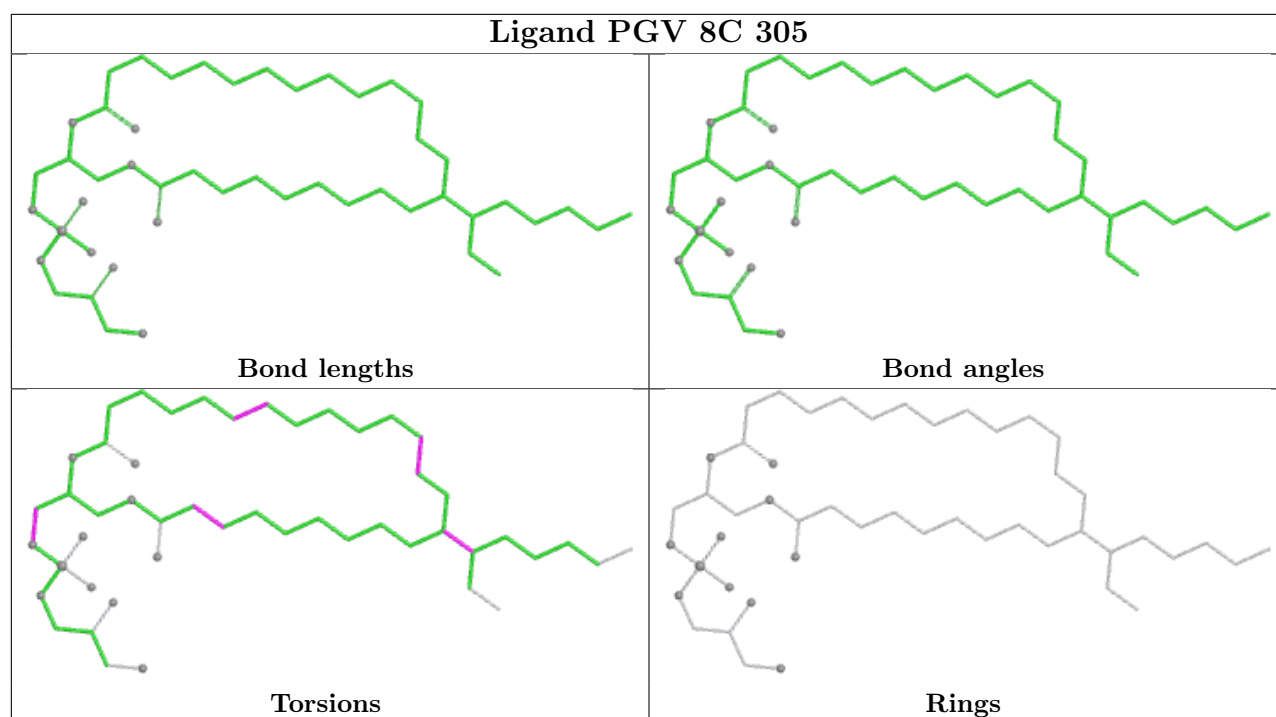




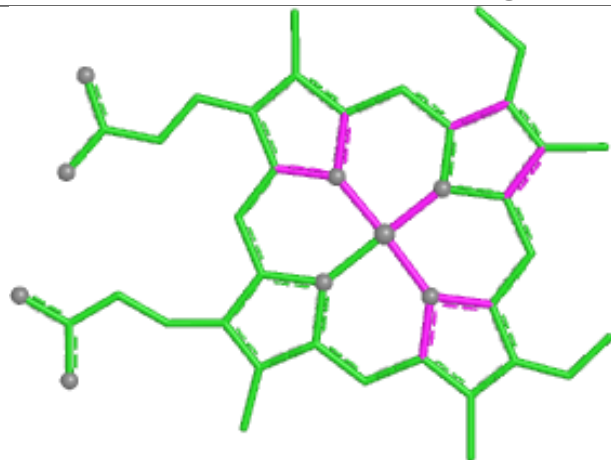




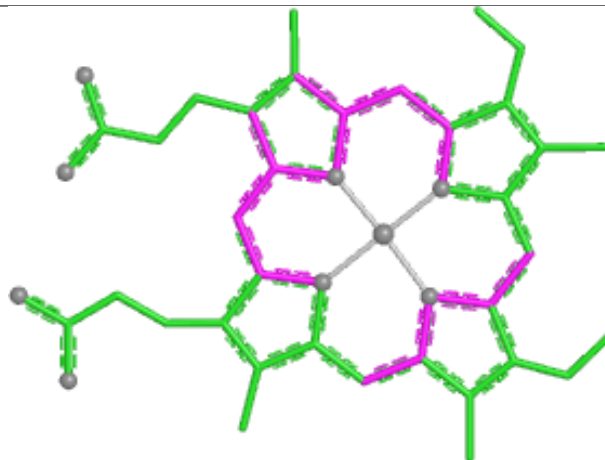




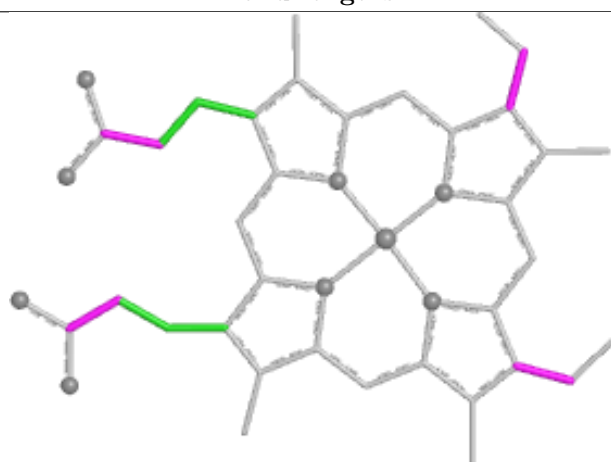
Ligand HEM 3P 501



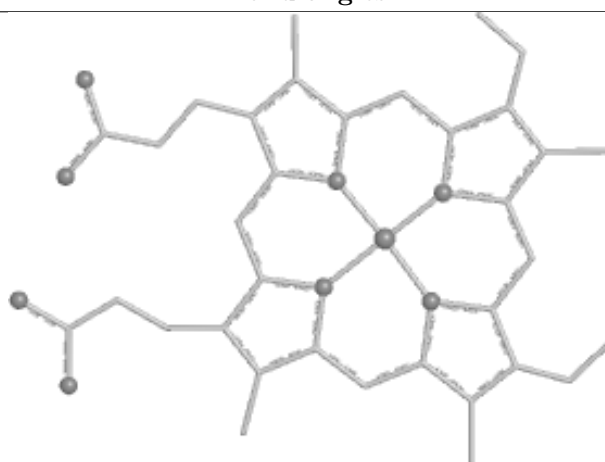
Bond lengths



Bond angles

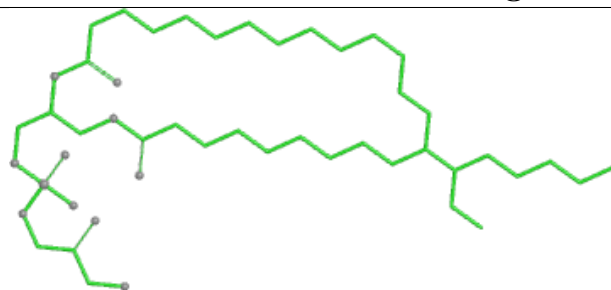


Torsions

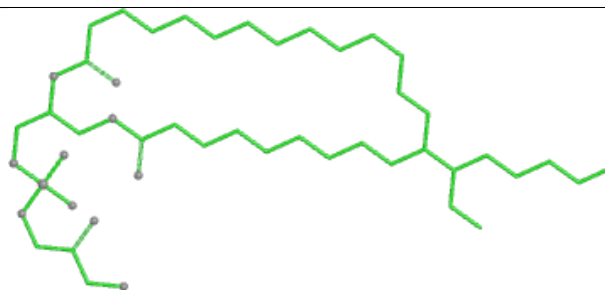


Rings

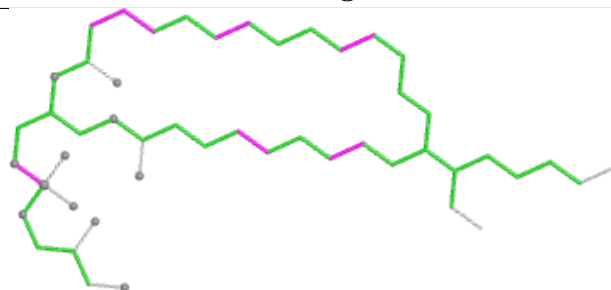
Ligand PGV 4L 101



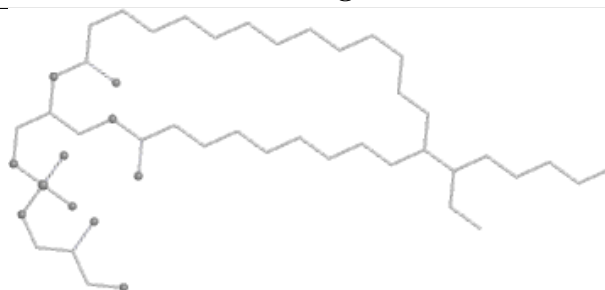
Bond lengths



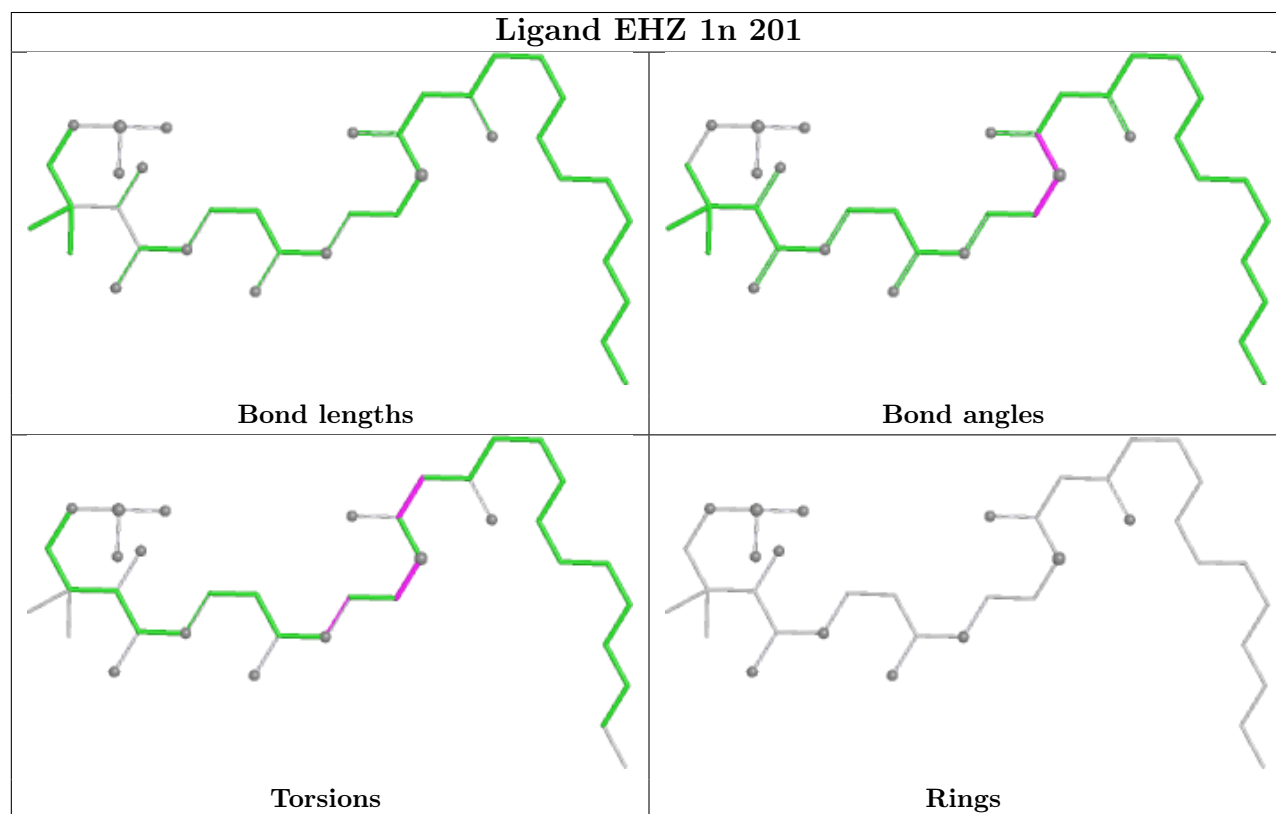
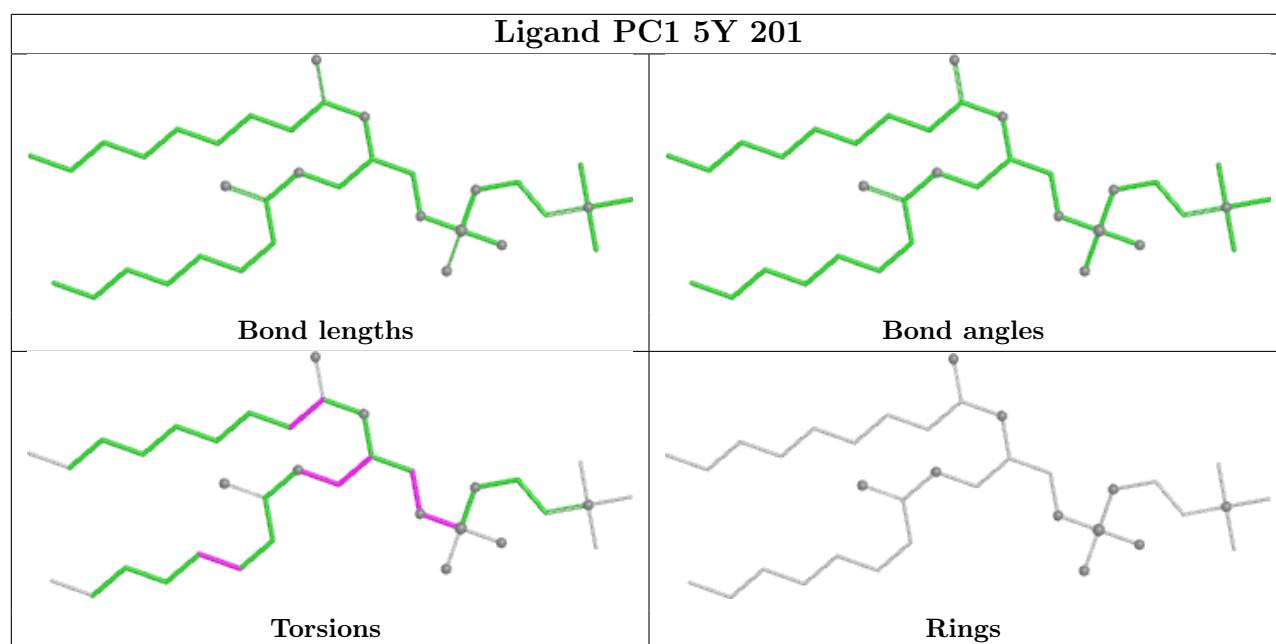
Bond angles

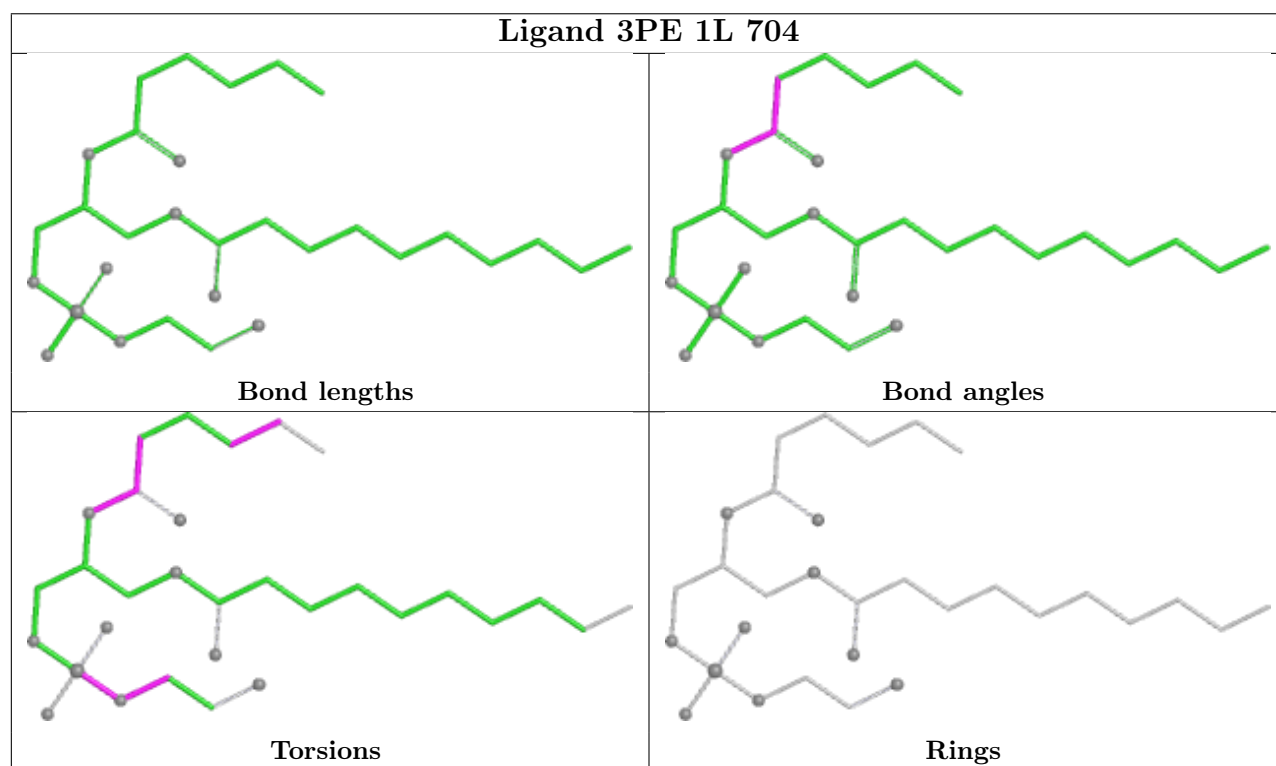
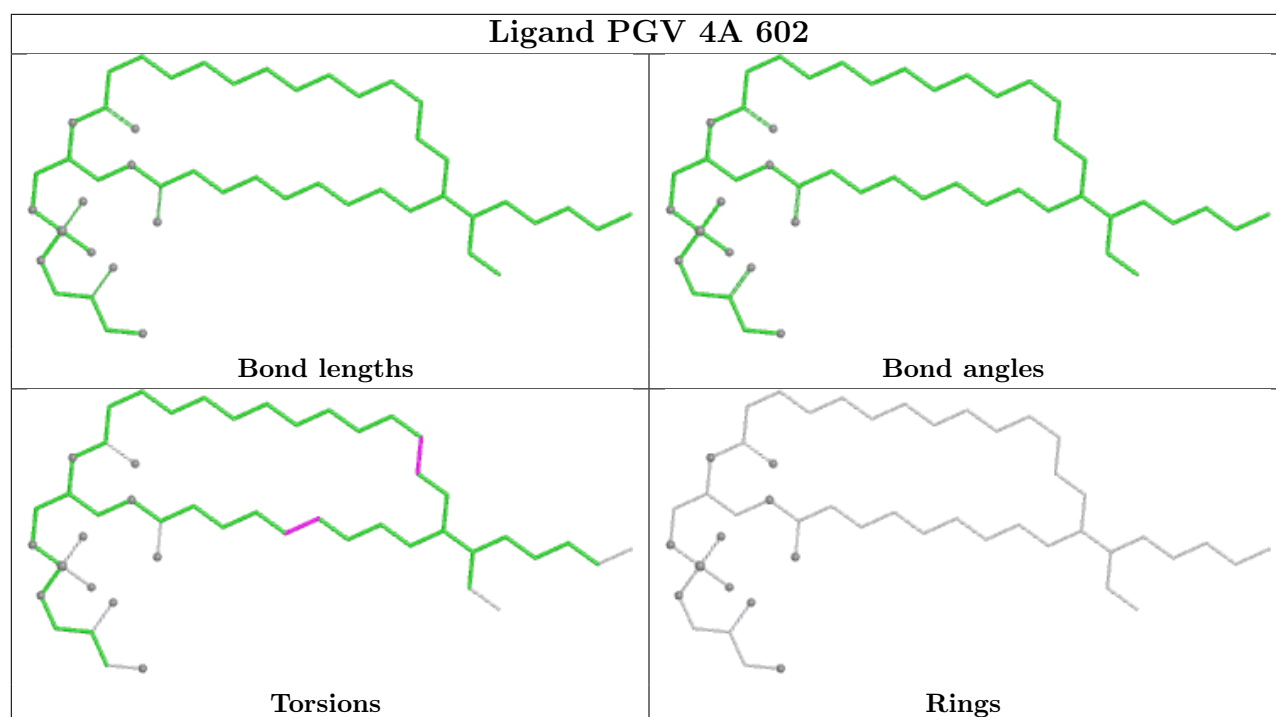


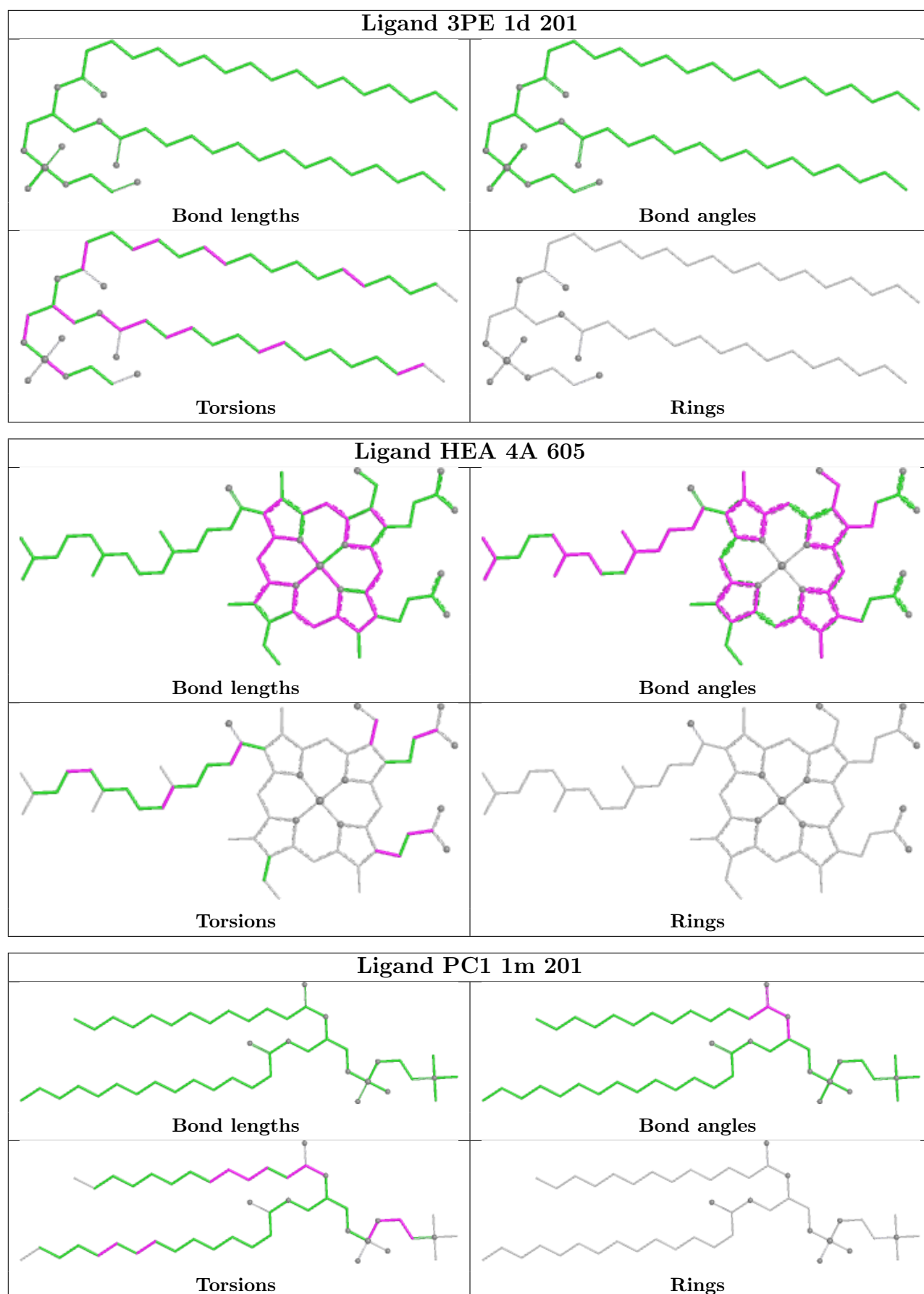
Torsions

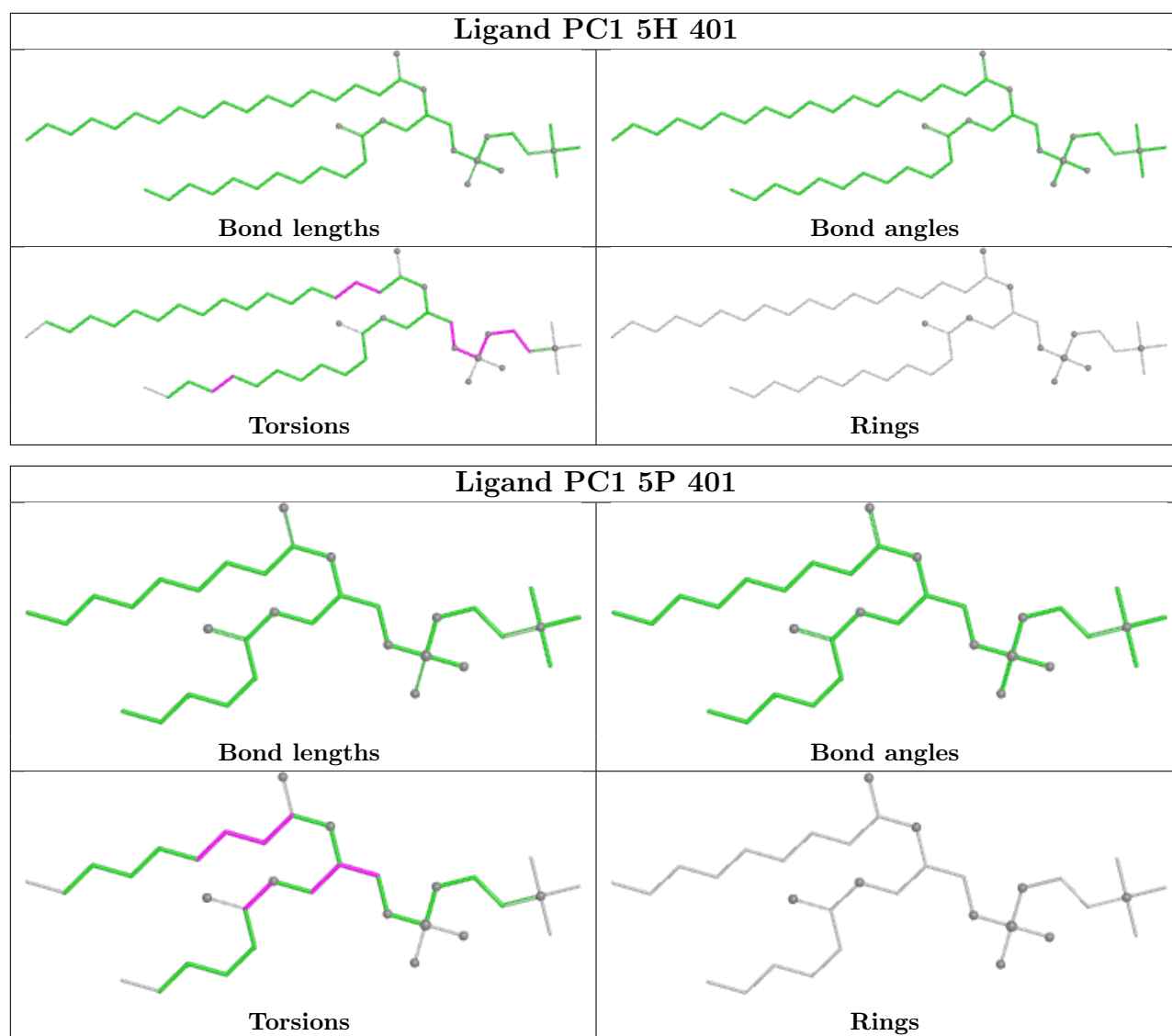


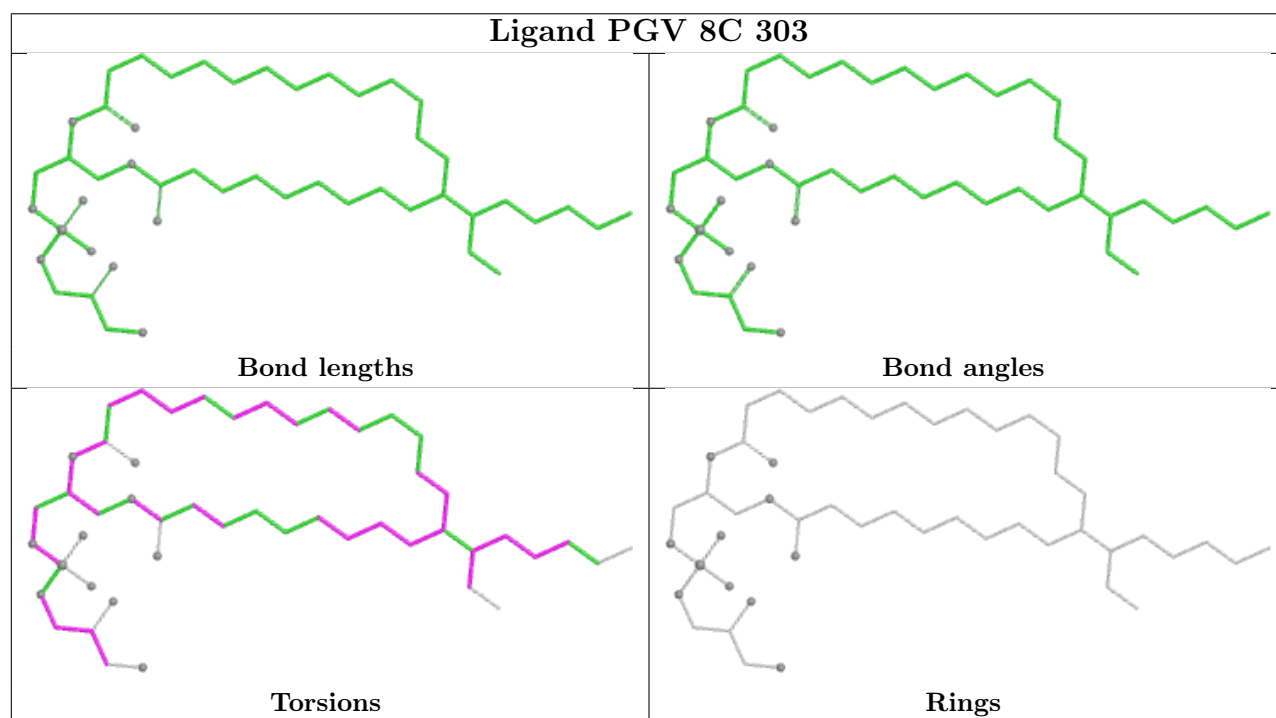
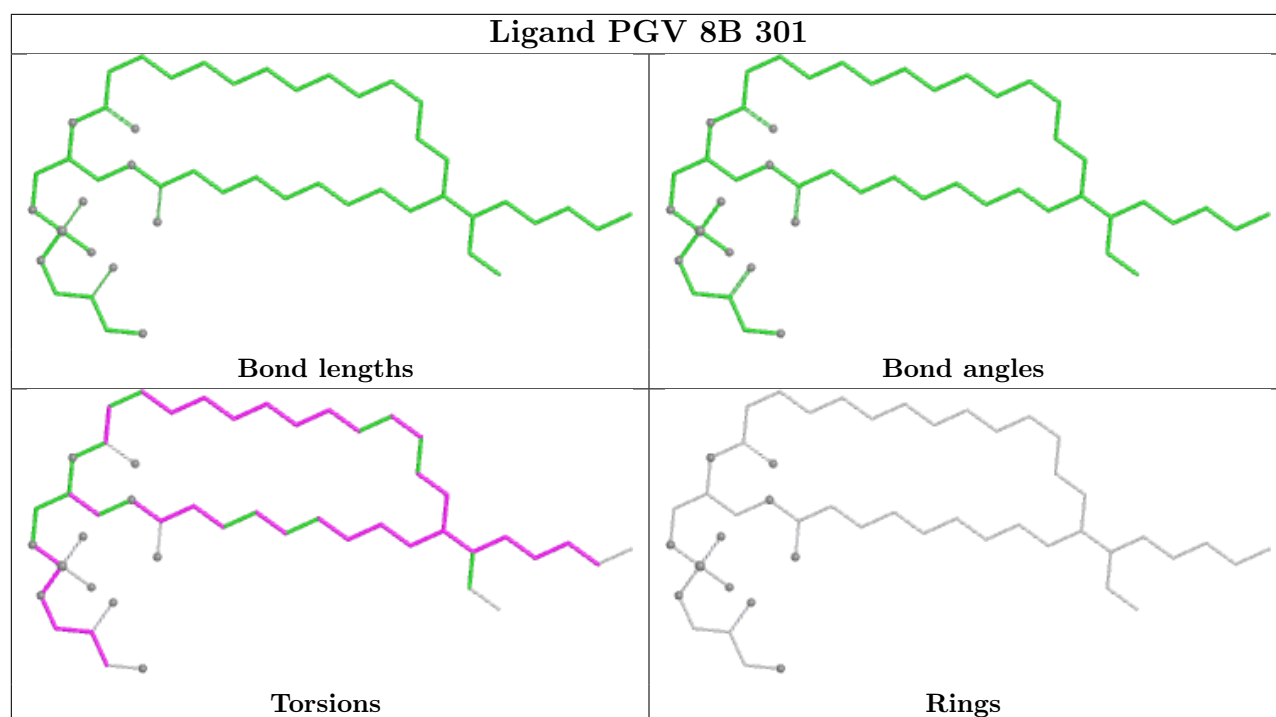
Rings

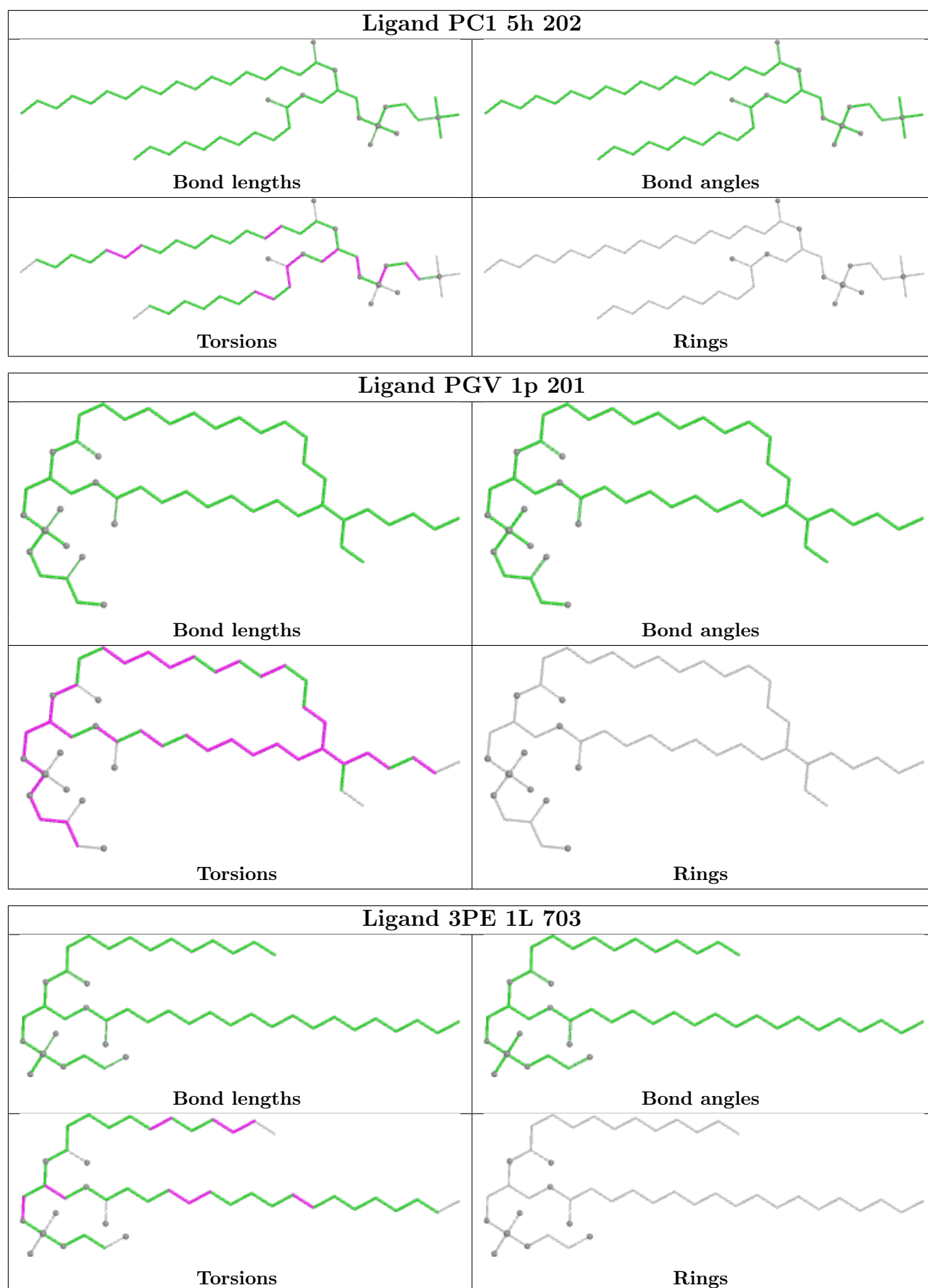


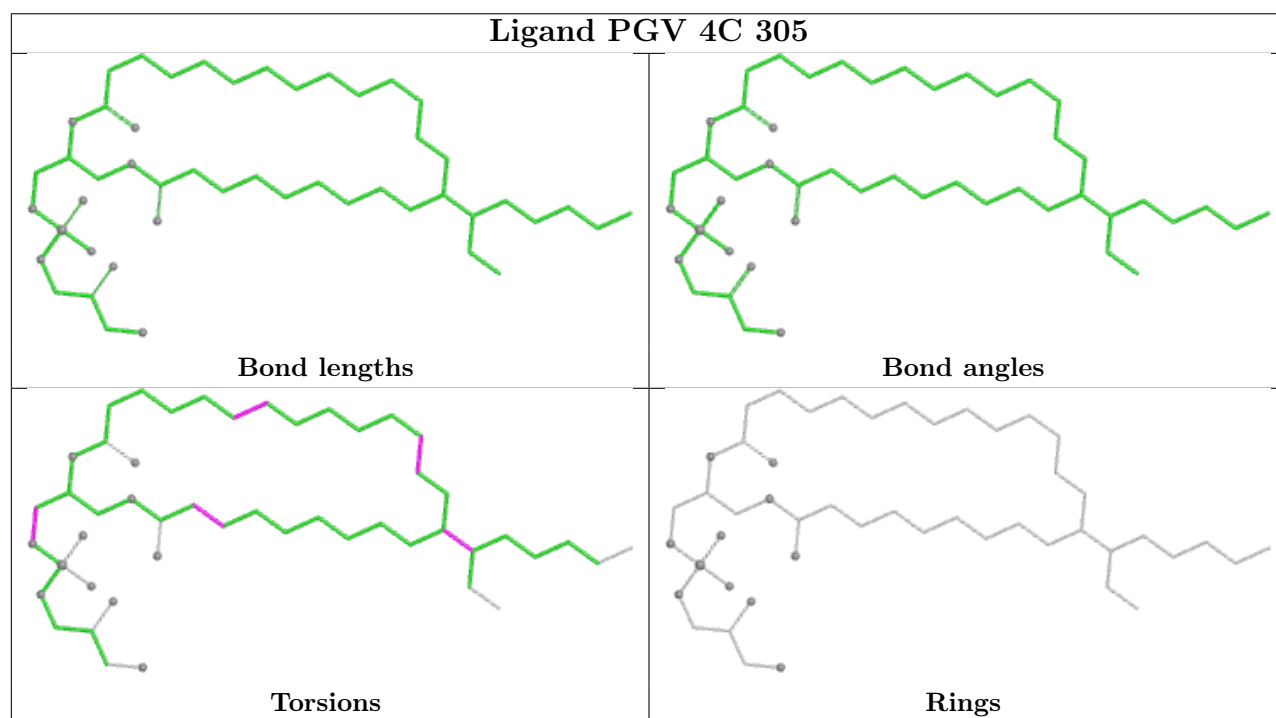
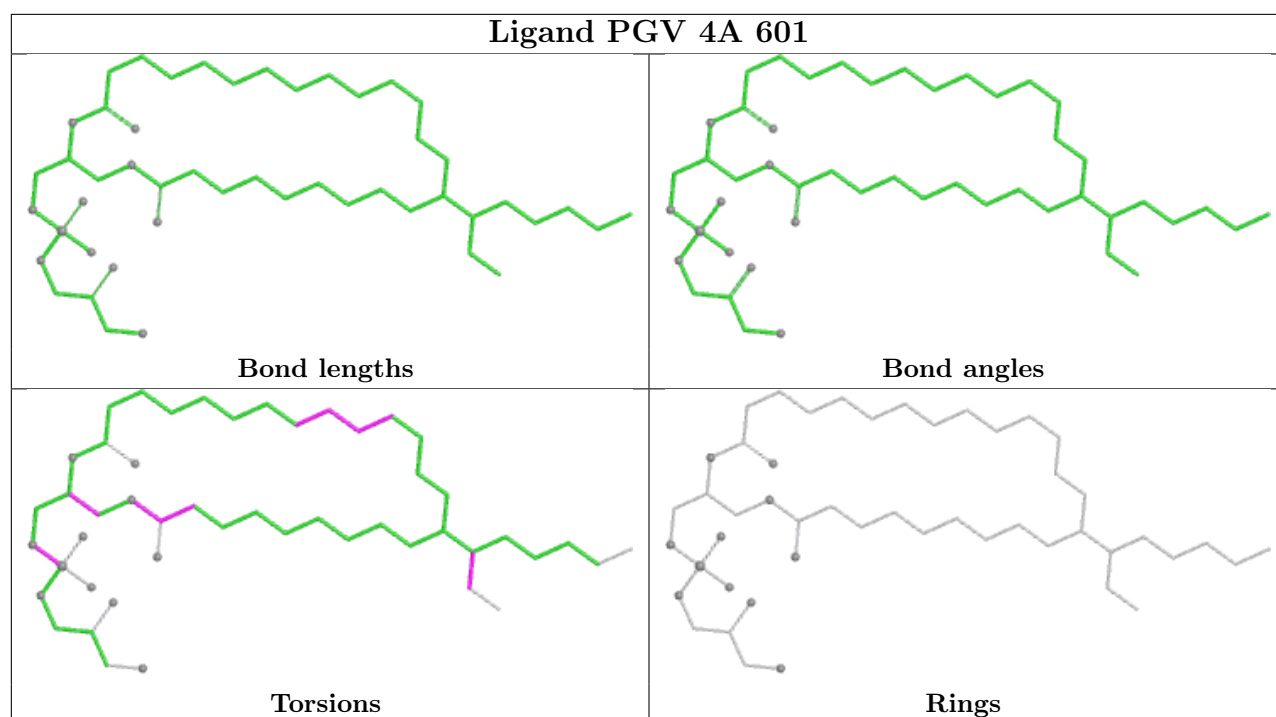


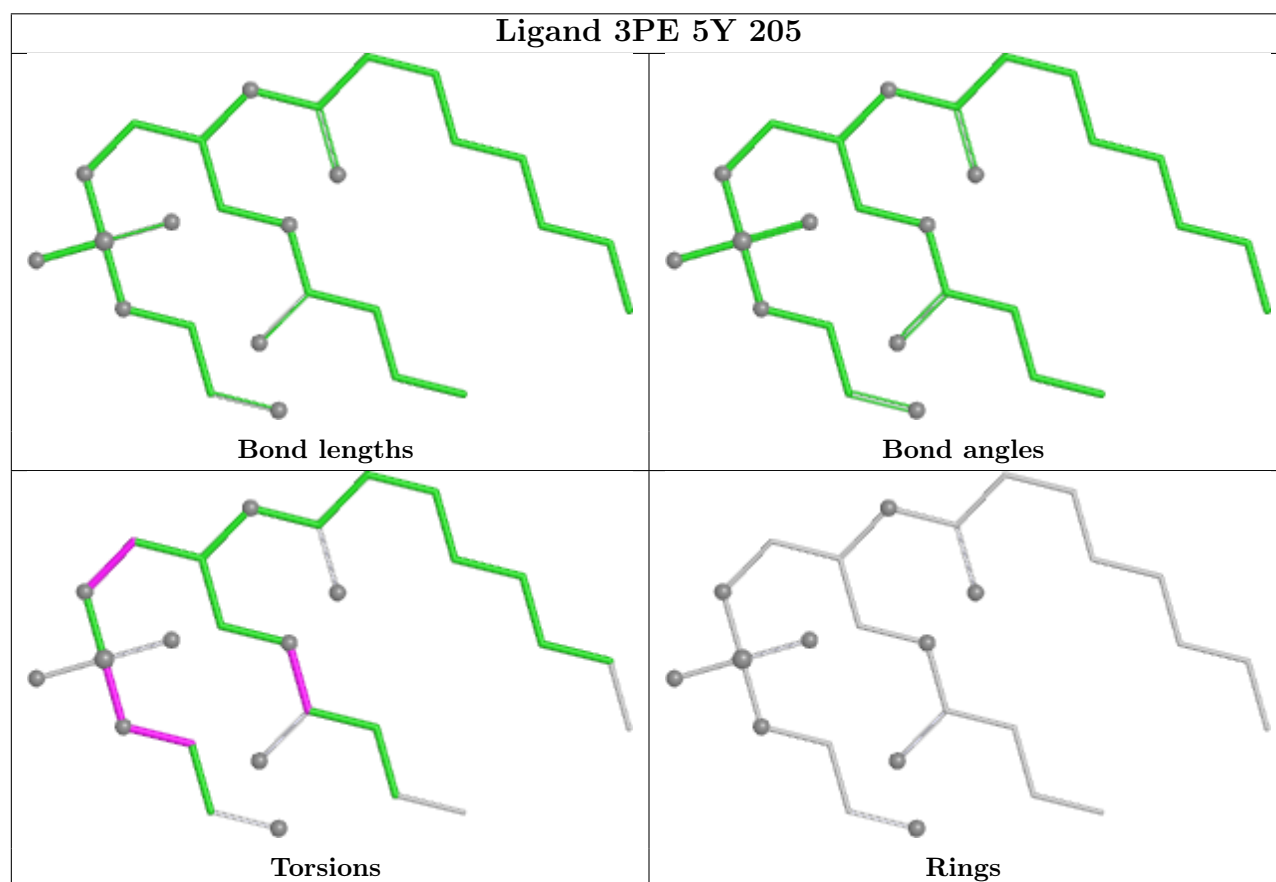
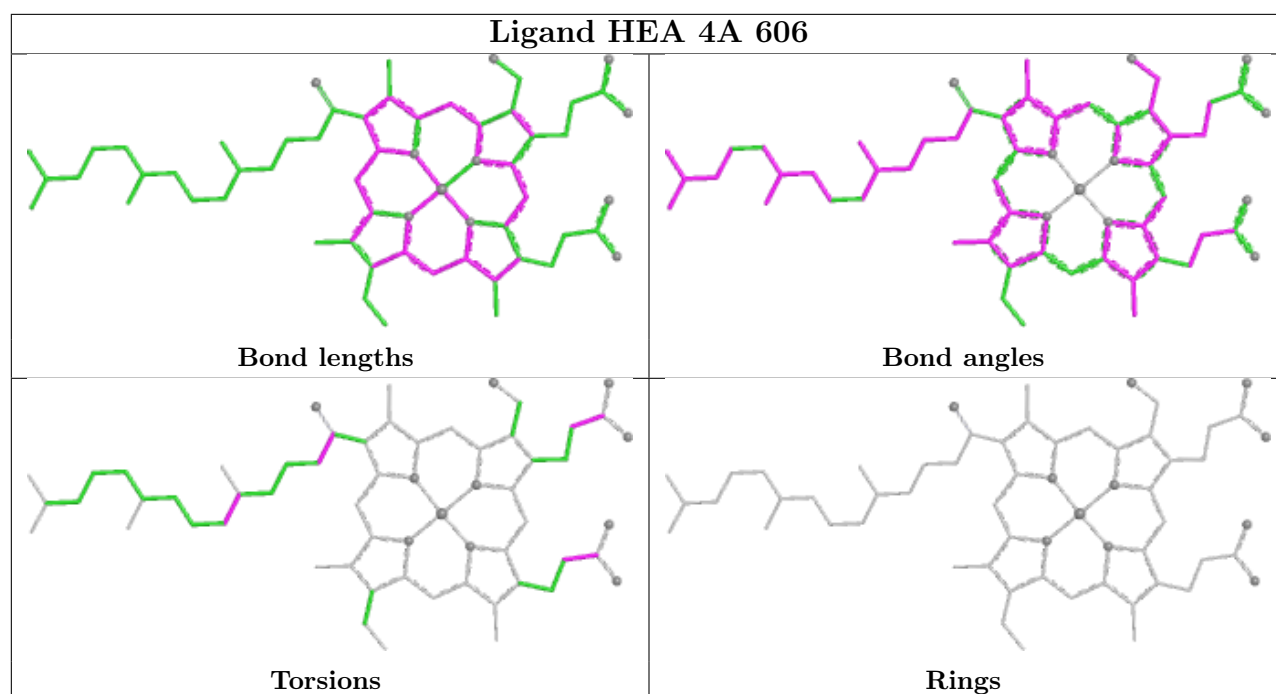


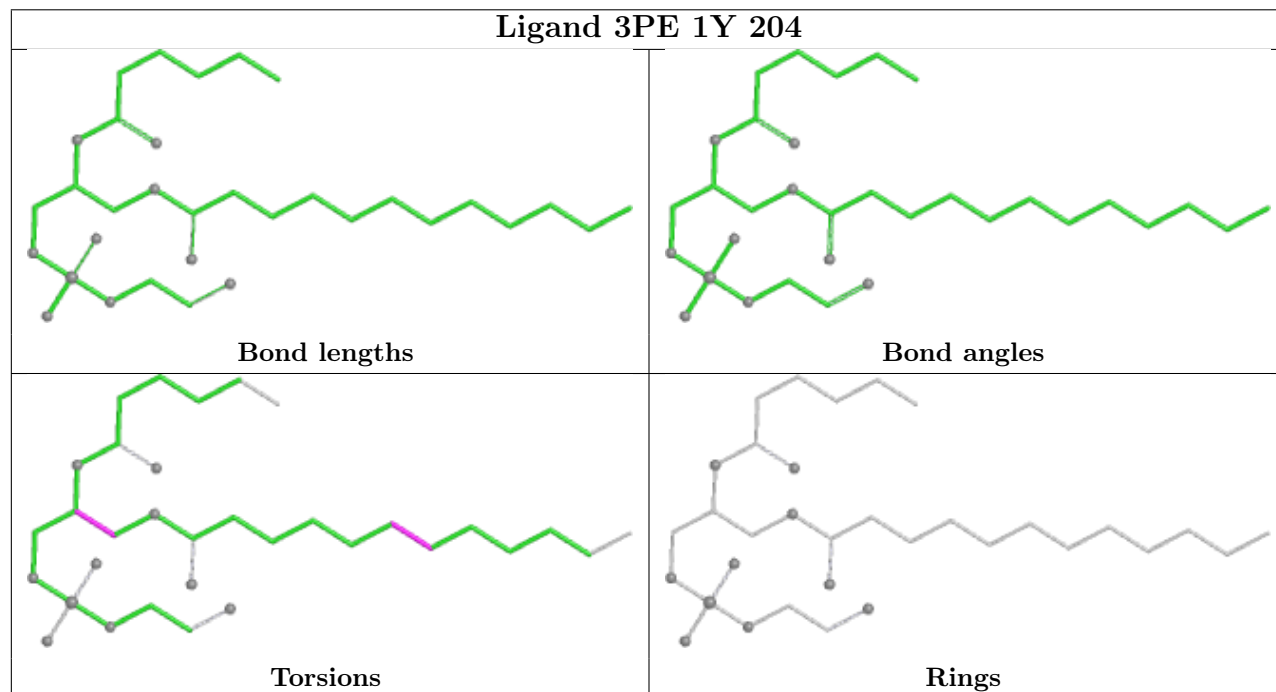
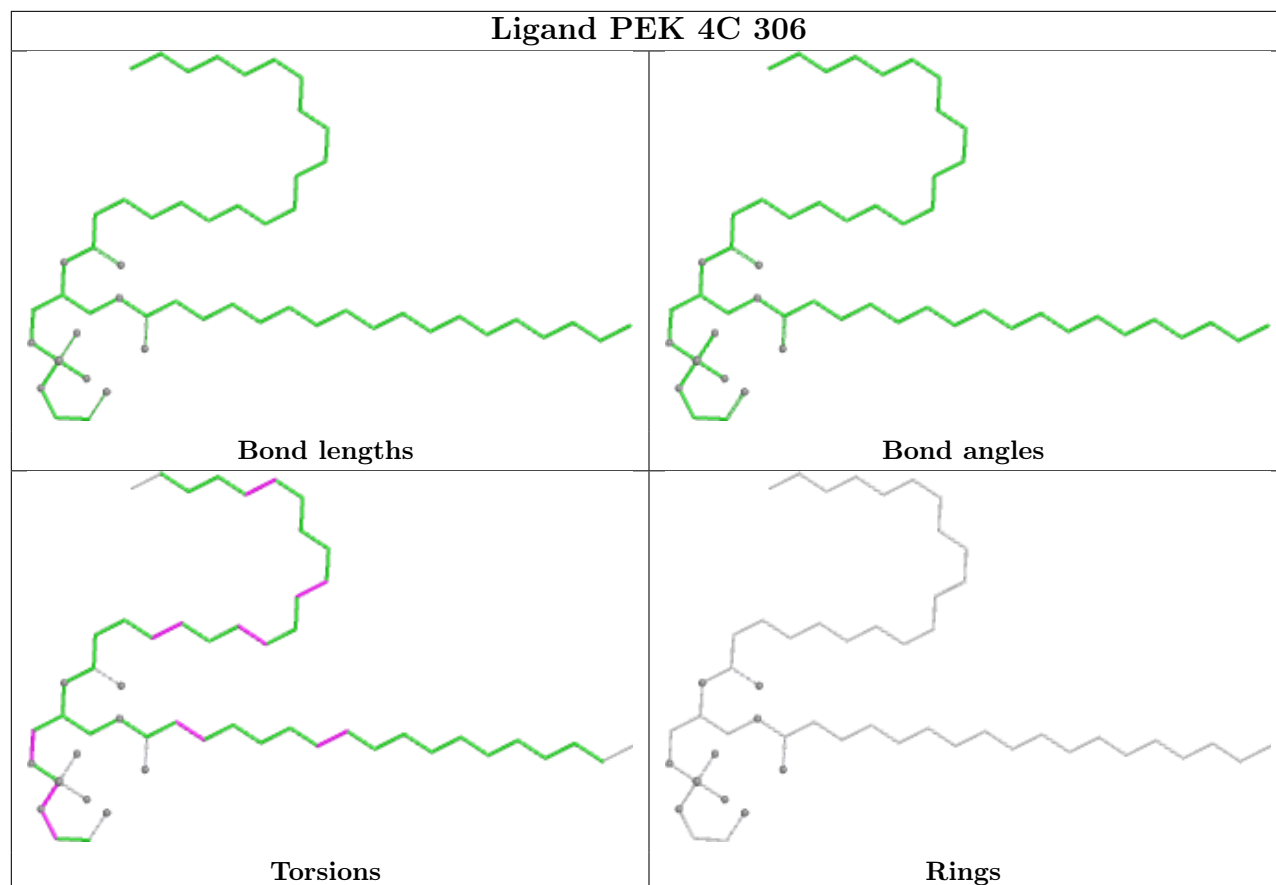


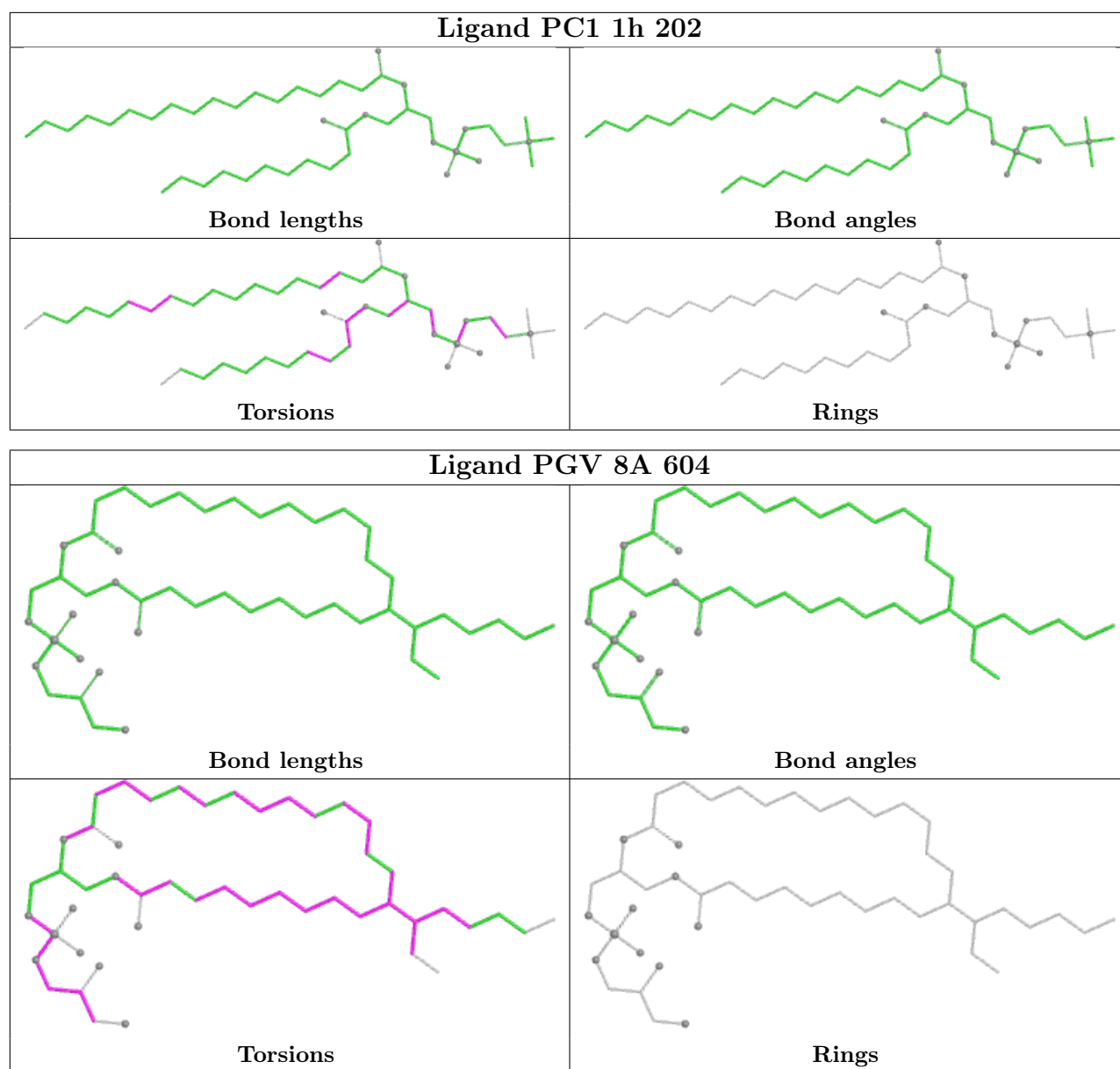


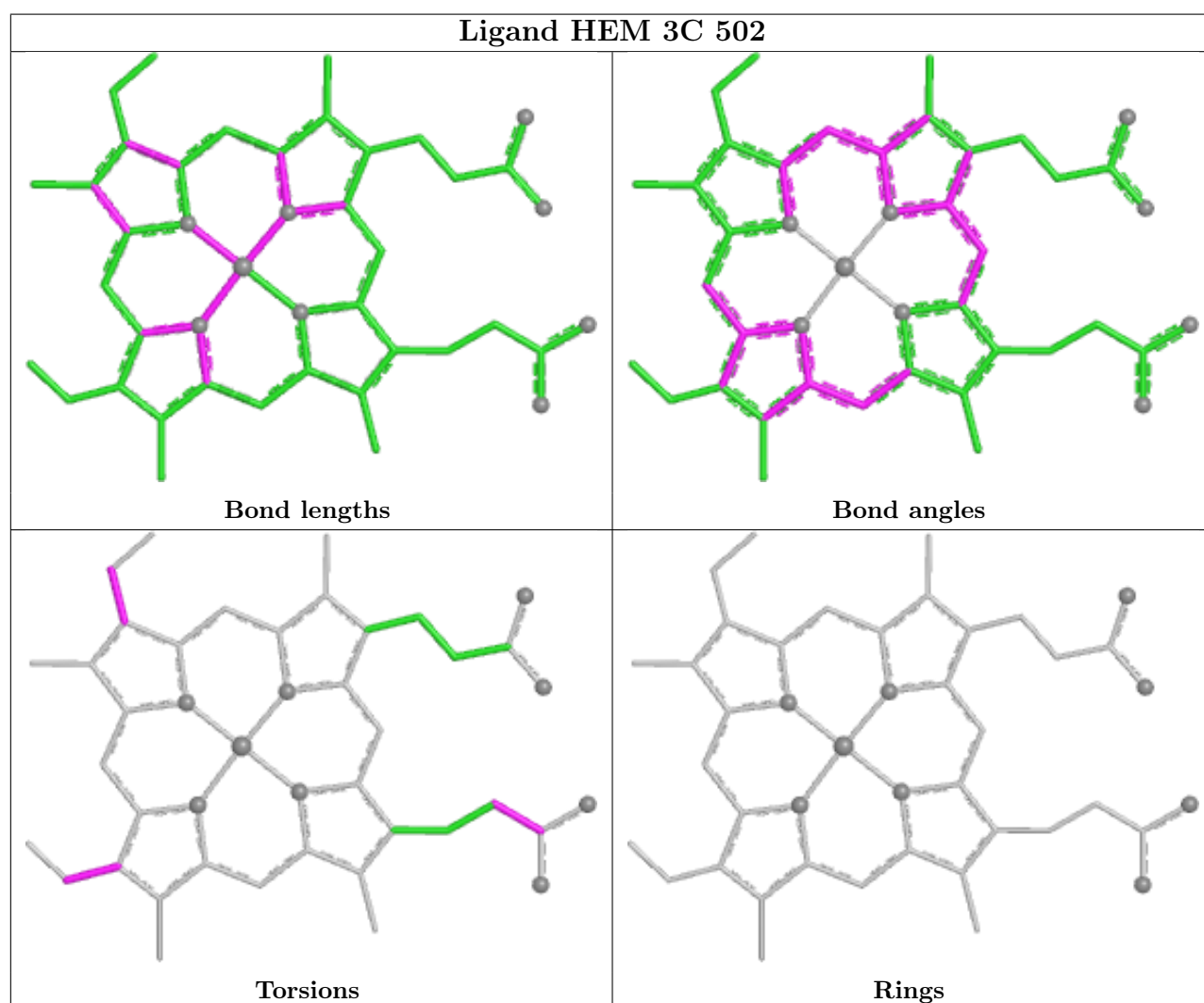
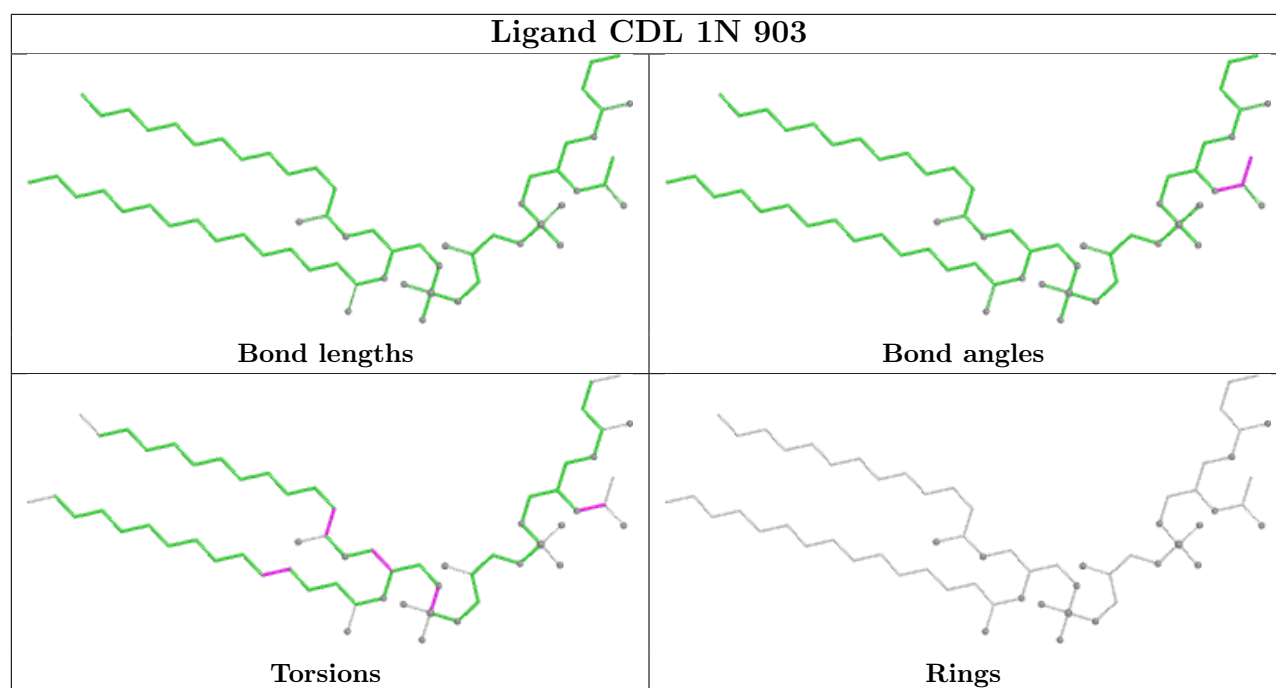


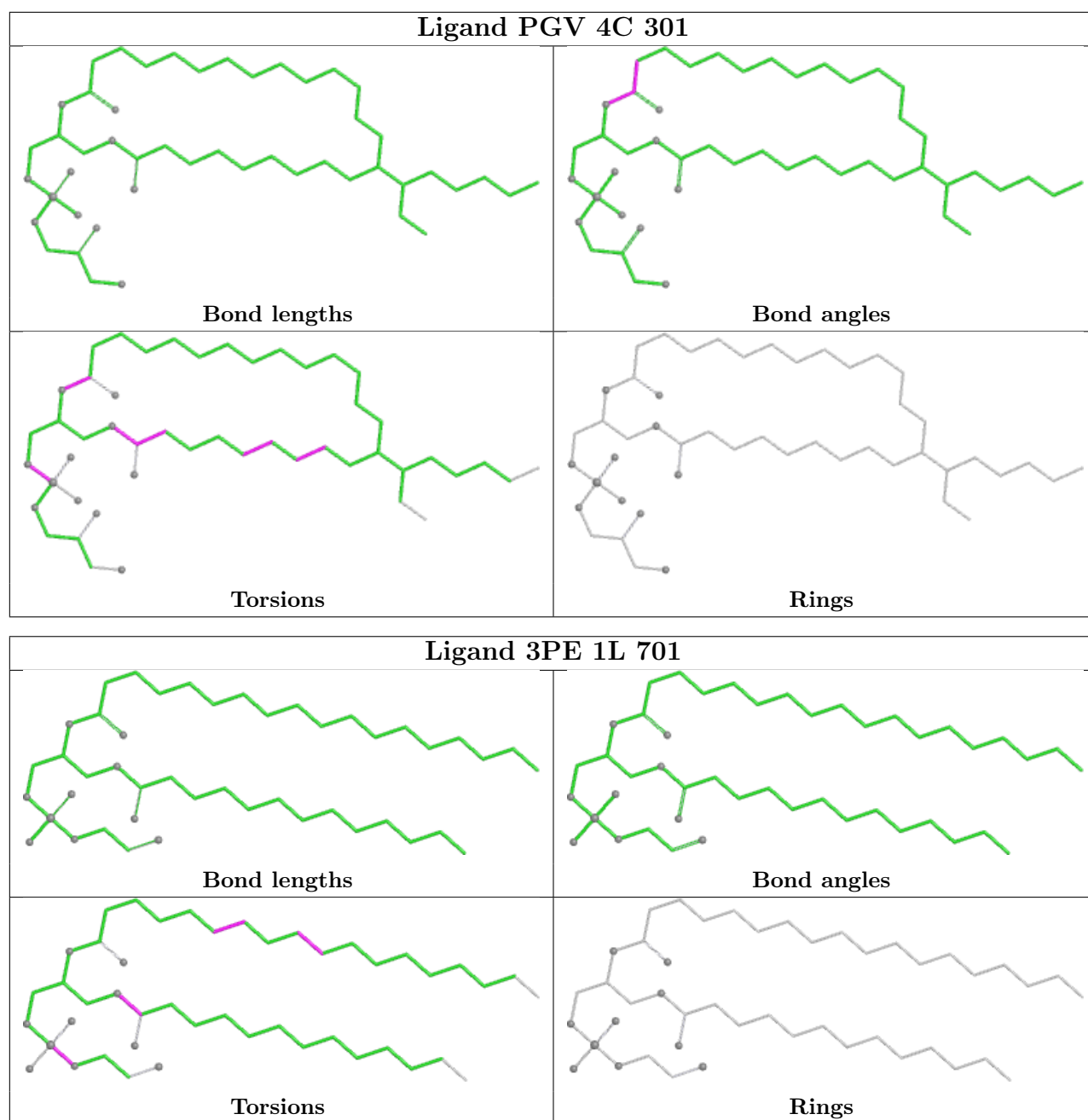


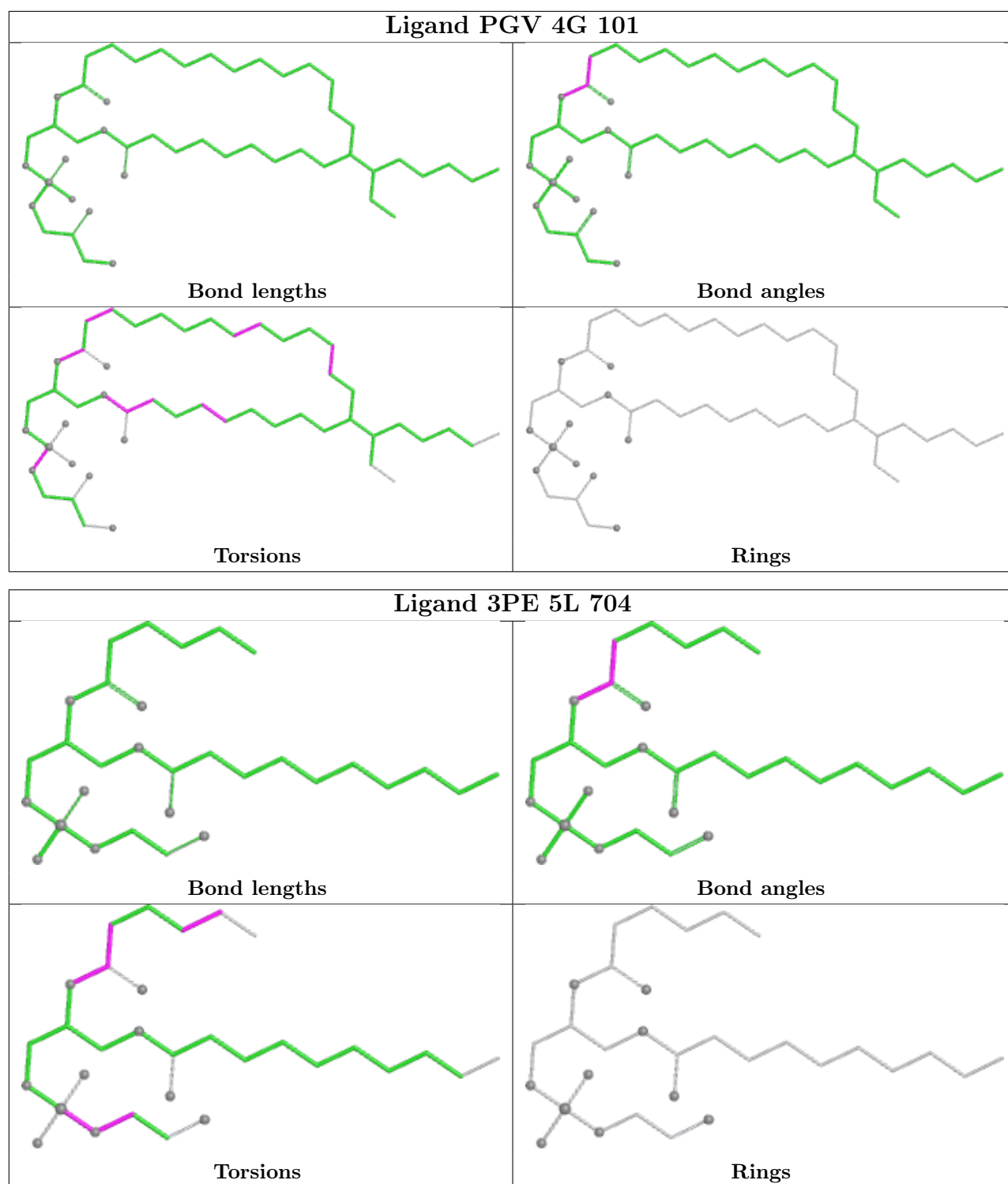












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	1B	6
1	1A	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1A	1:FME	C	2:ASN	N	3.48
1	1B	103:VAL	C	104:TYR	N	2.65
1	1B	60:MET	C	61:HIS	N	2.47
1	1B	100:LEU	C	101:ARG	N	2.08
1	1B	57:VAL	C	58:GLU	N	1.93

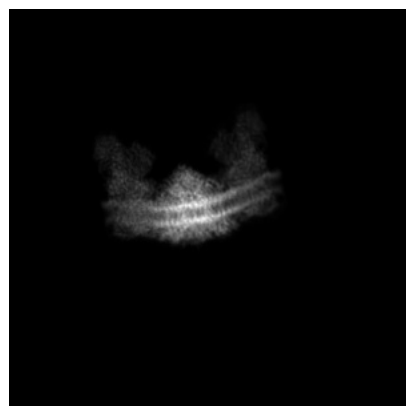
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42233. These allow visual inspection of the internal detail of the map and identification of artifacts.

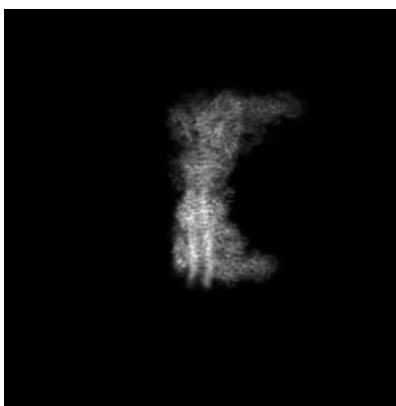
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

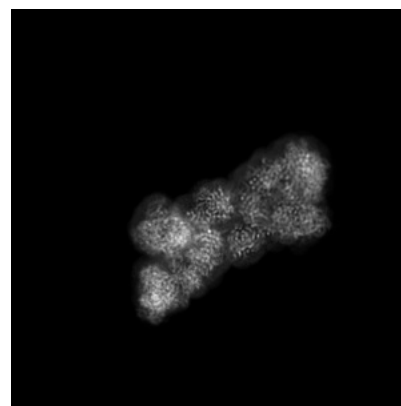
6.1.1 Primary map



X

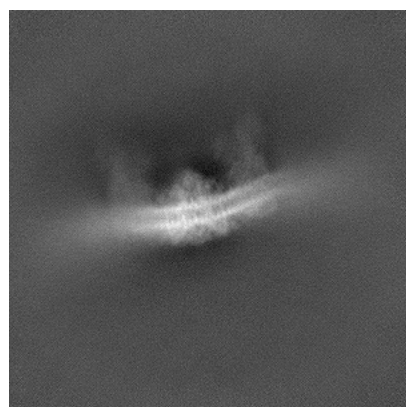


Y

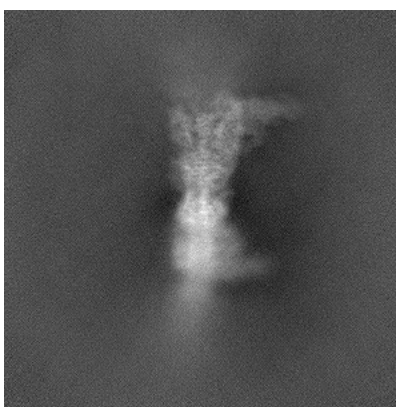


Z

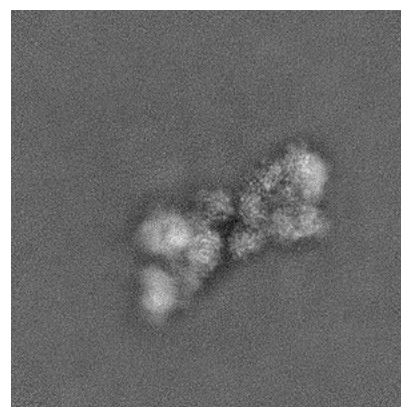
6.1.2 Raw map



X



Y

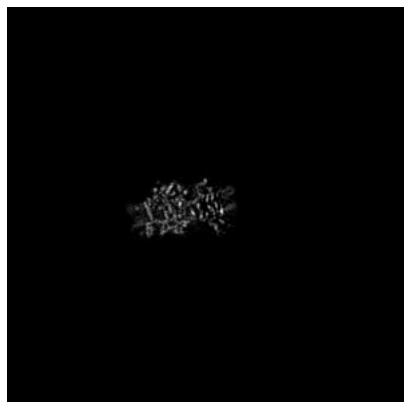


Z

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

6.2 Central slices [i](#)

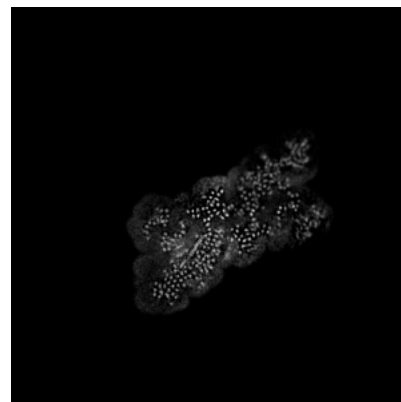
6.2.1 Primary map



X Index: 256

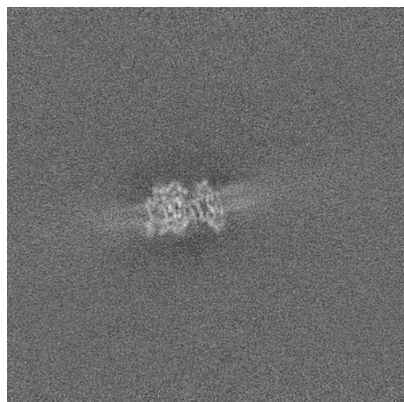


Y Index: 256

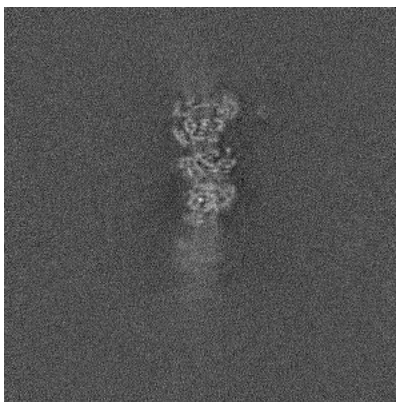


Z Index: 256

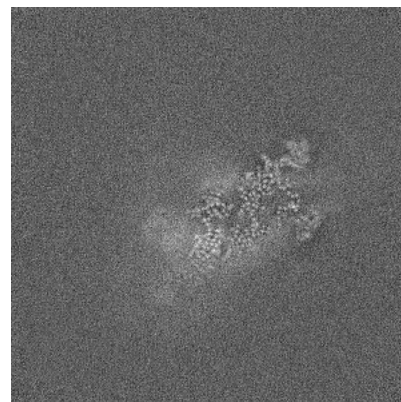
6.2.2 Raw map



X Index: 256



Y Index: 256

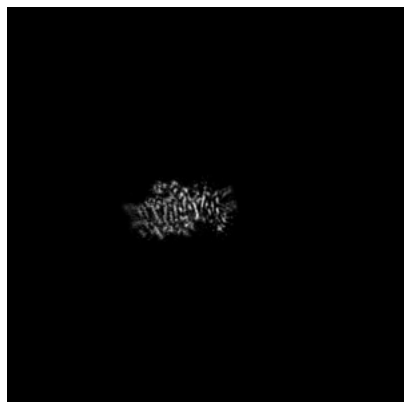


Z Index: 256

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

6.3 Largest variance slices [i](#)

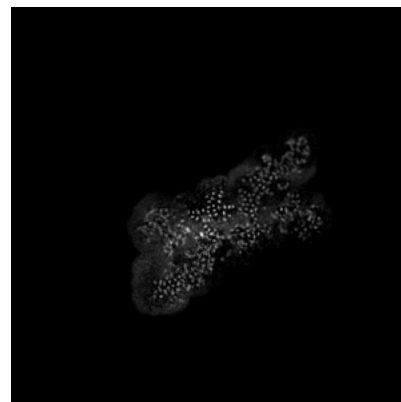
6.3.1 Primary map



X Index: 252

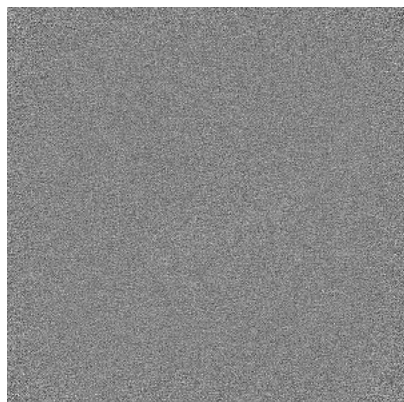


Y Index: 222

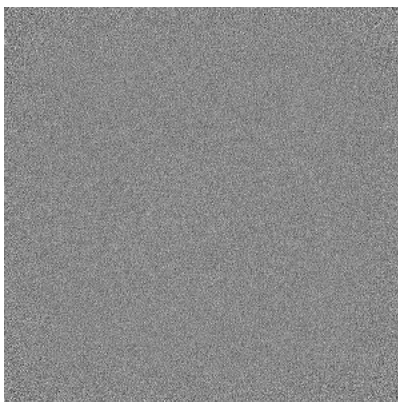


Z Index: 260

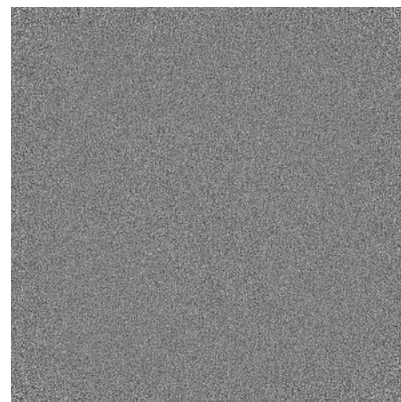
6.3.2 Raw map



X Index: 0



Y Index: 0

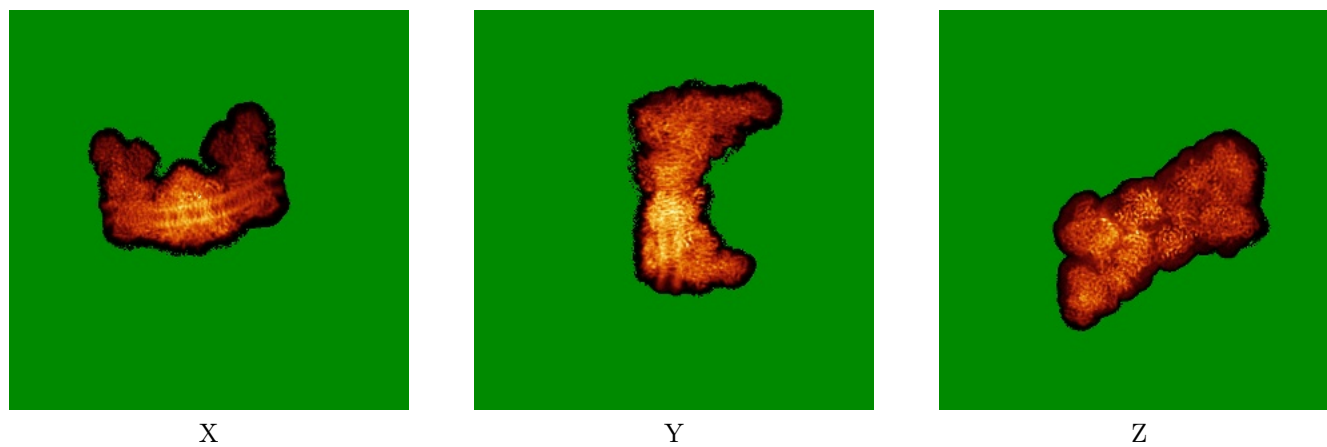


Z Index: 0

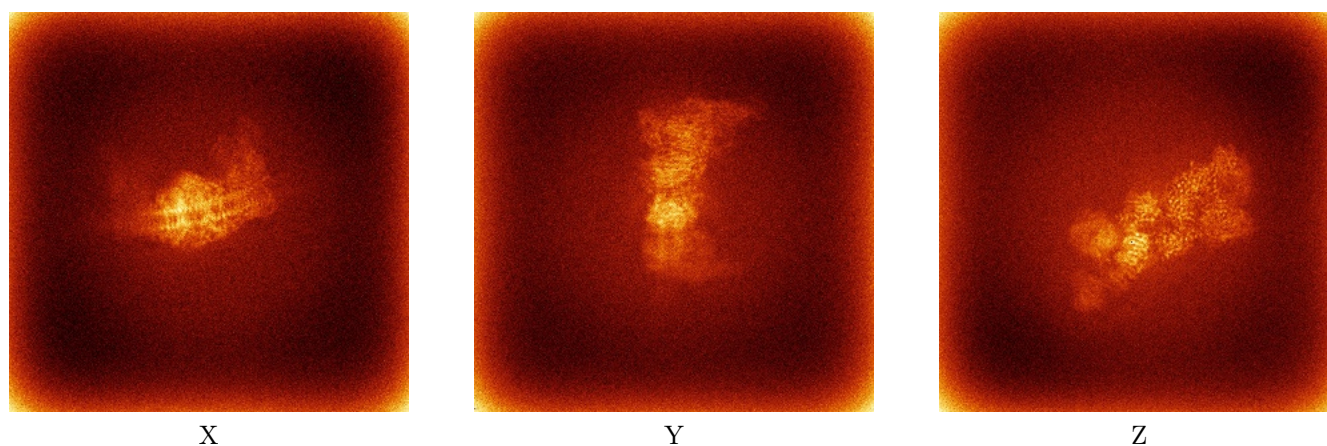
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

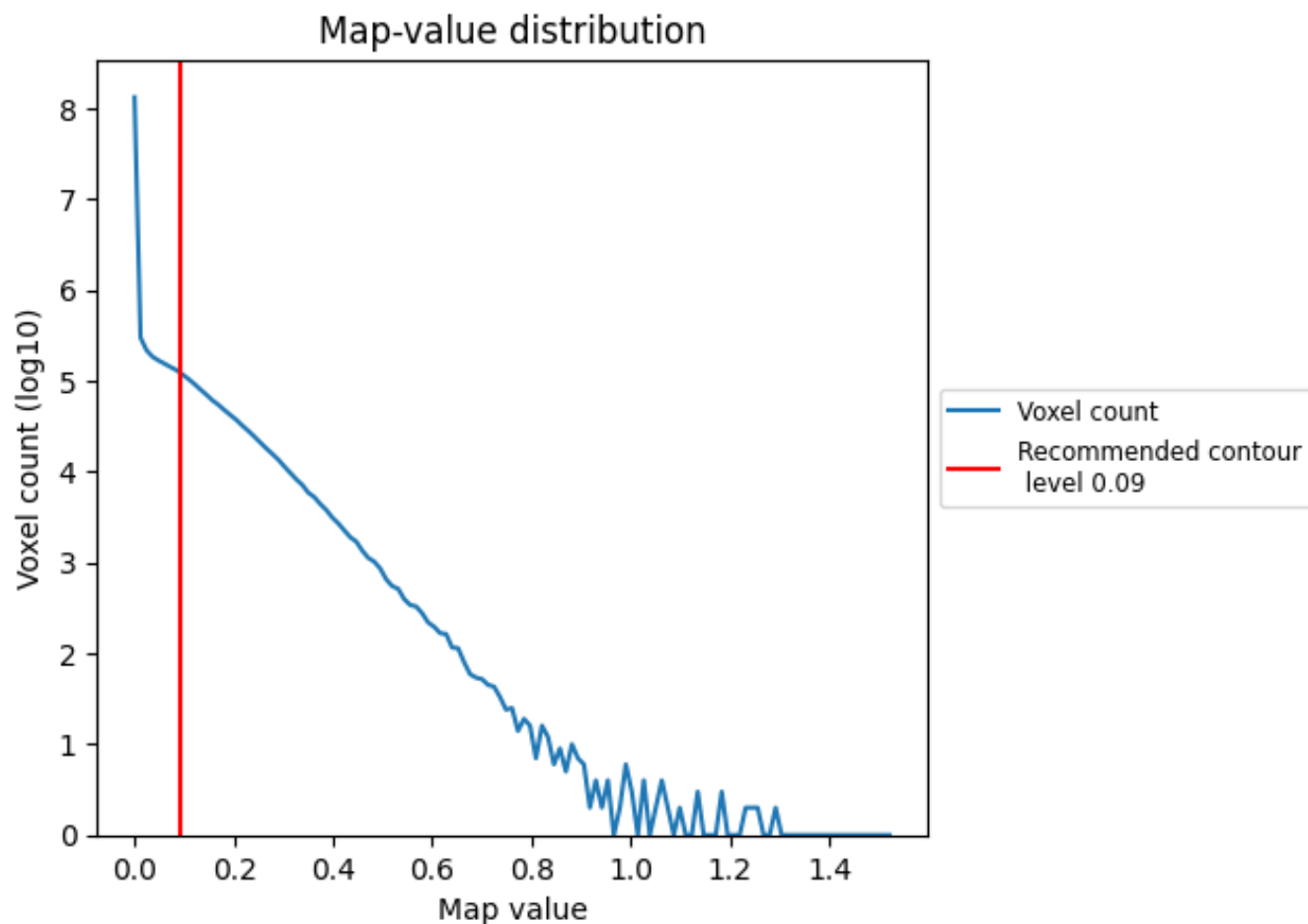
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

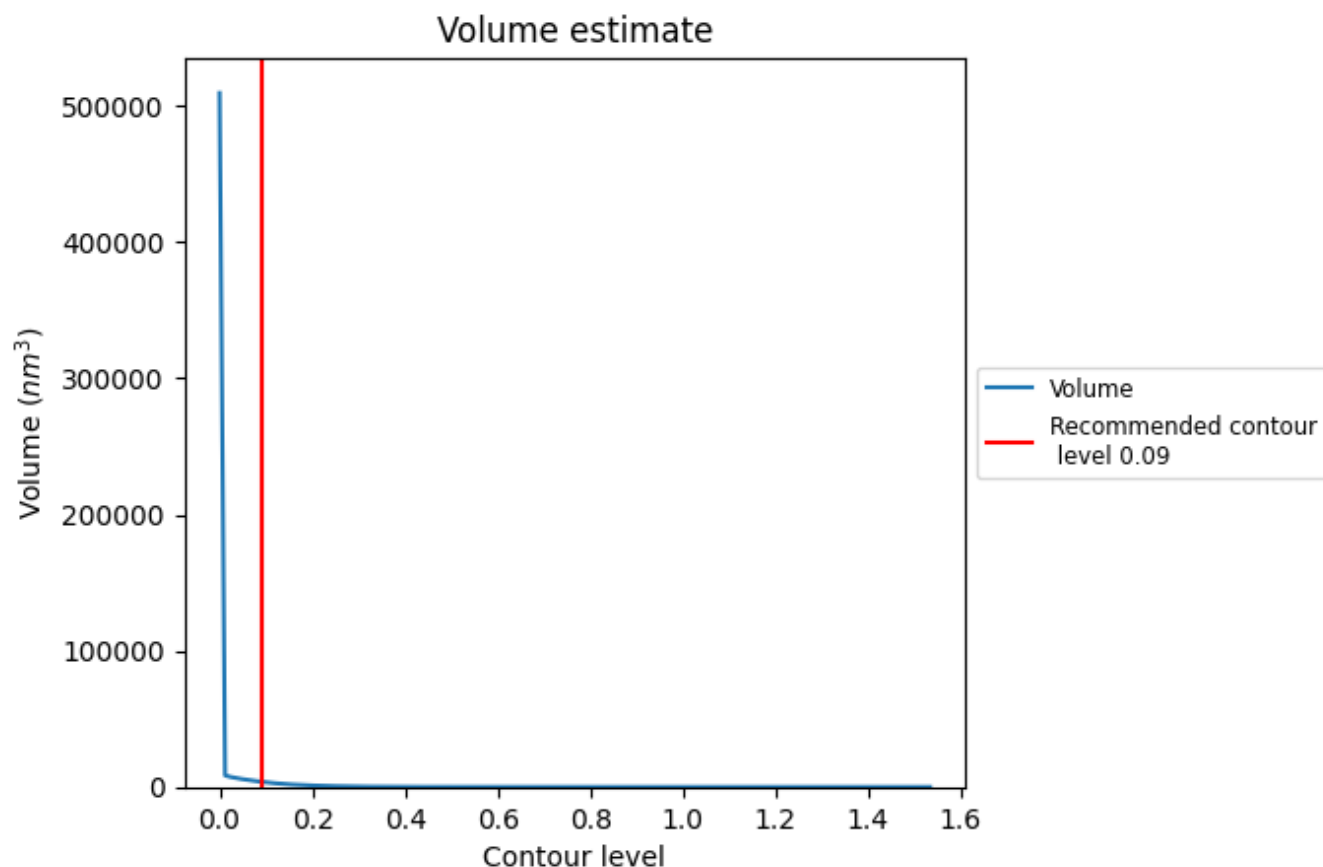
This section contains the results of statistical analysis of the map.

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.

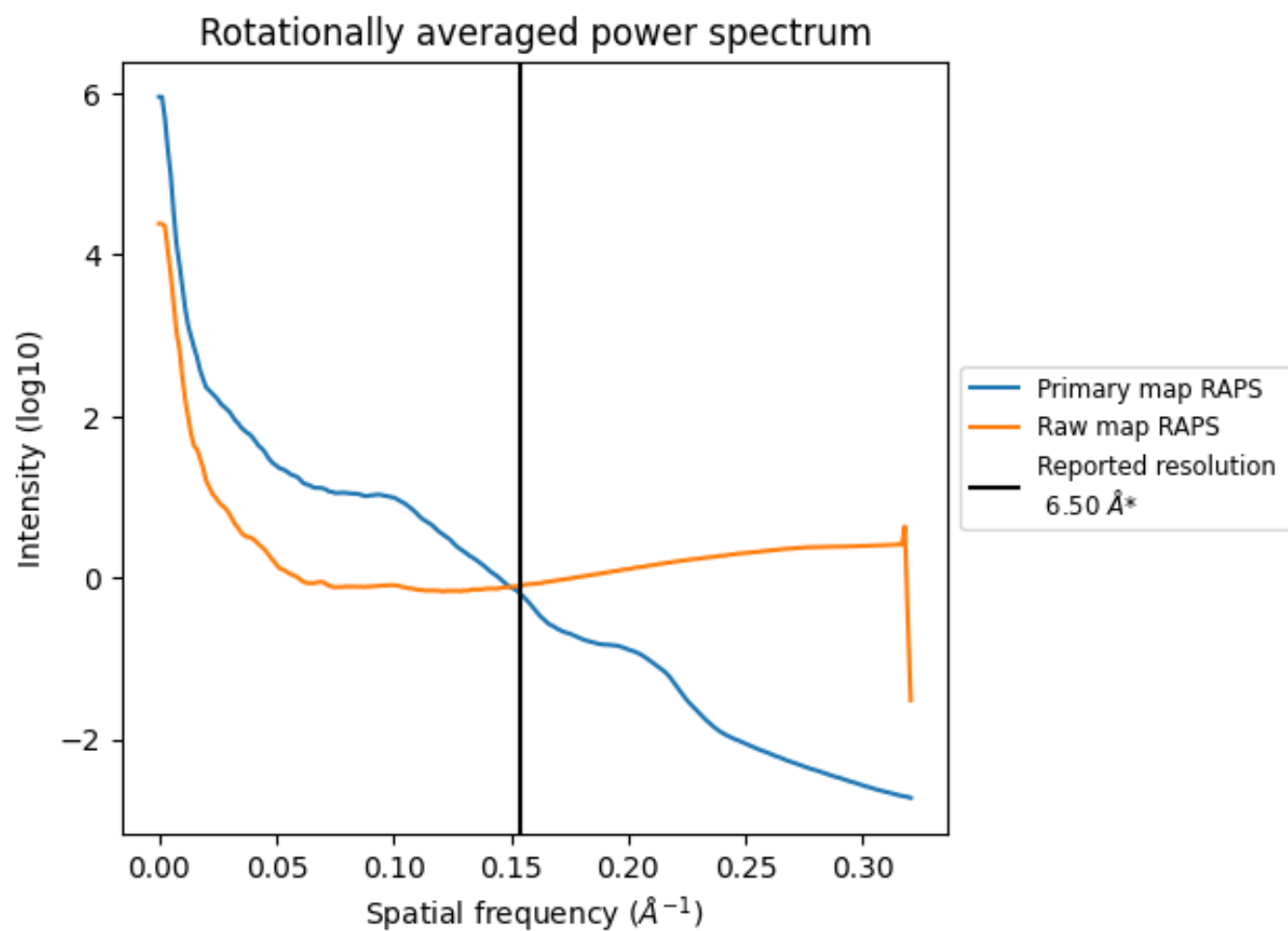
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3822 nm^3 ; this corresponds to an approximate mass of 3453 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 ⓘ

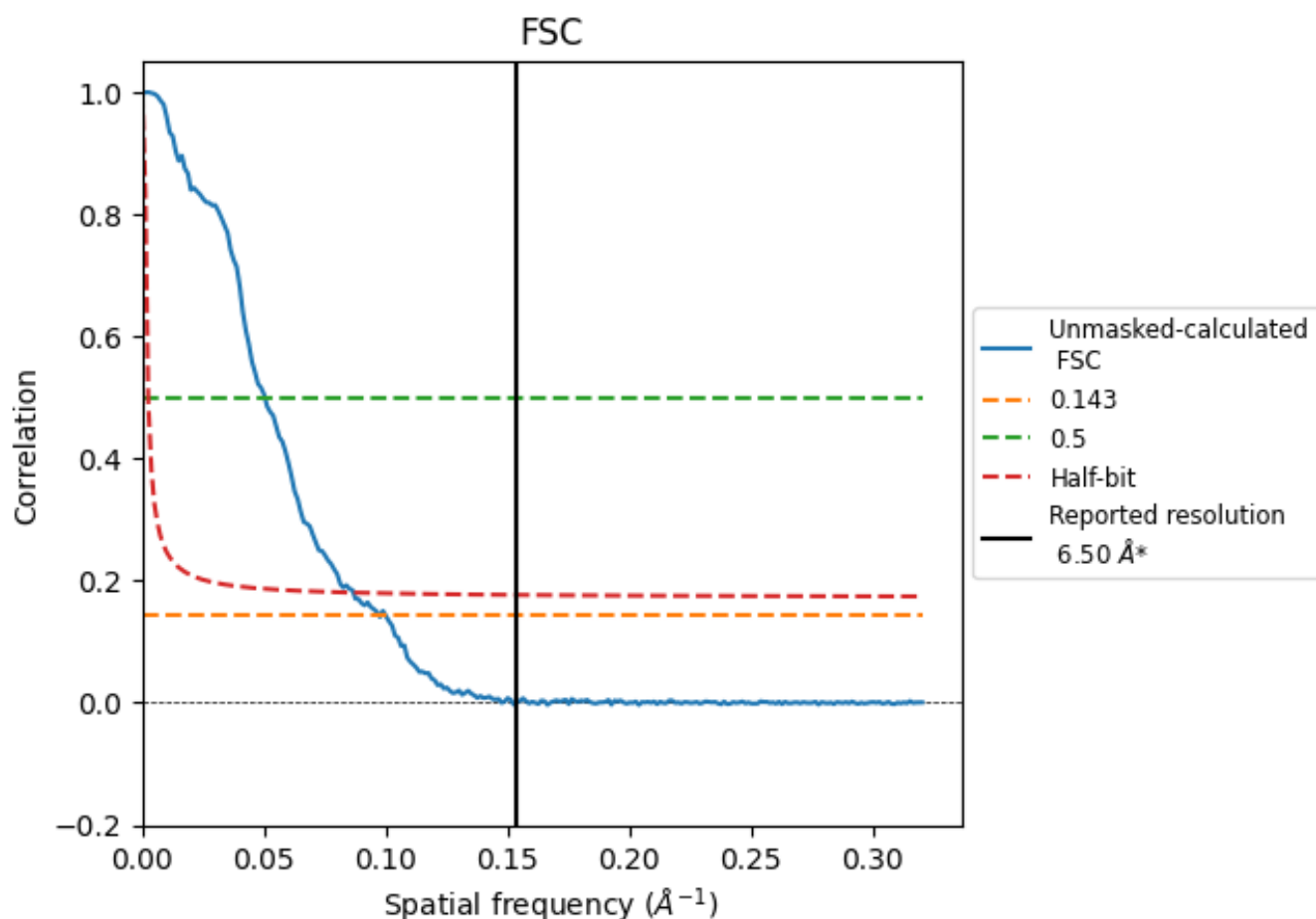


*Reported resolution corresponds to spatial frequency of $0.154 \text{ \AA}^{-1}$

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 0.154 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

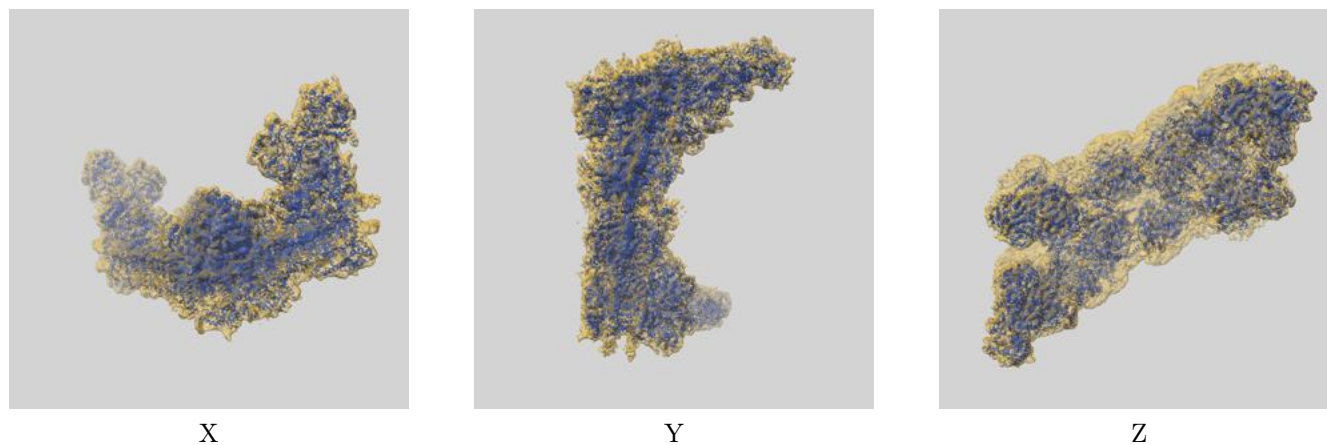
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.28	19.84	11.52

*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 10.28 differs from the reported value 6.5 by more than 10 %

9 Map-model fit [i](#)

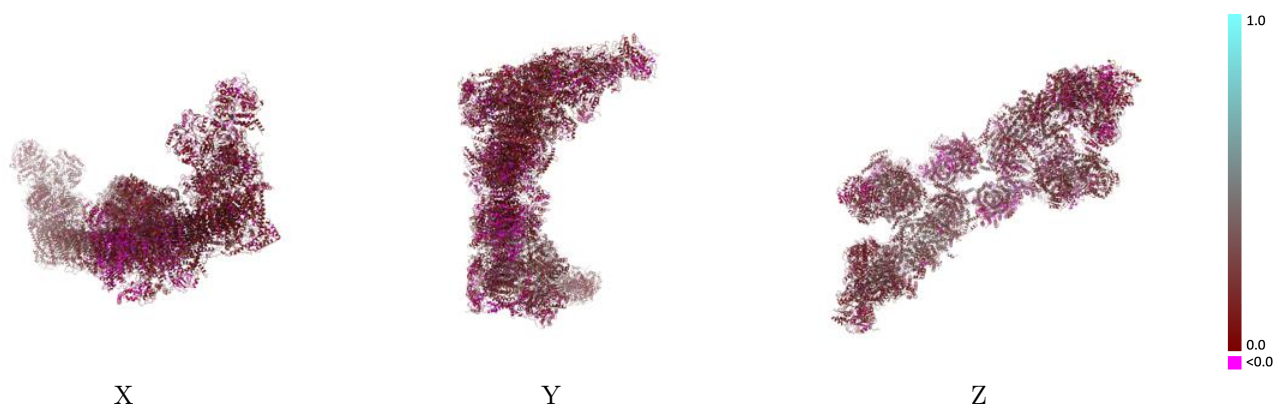
This section contains information regarding the fit between EMDB map EMD-42233 and PDB model 8UGR. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



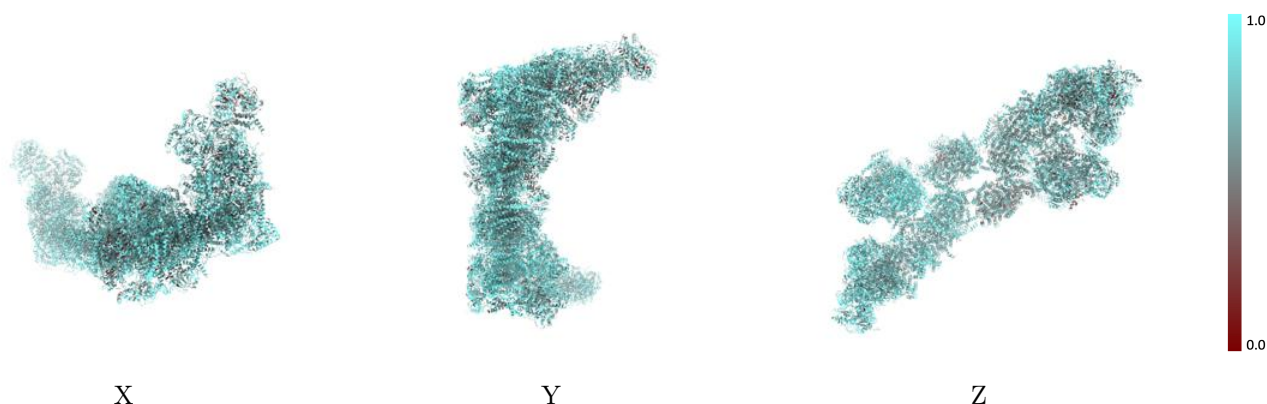
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



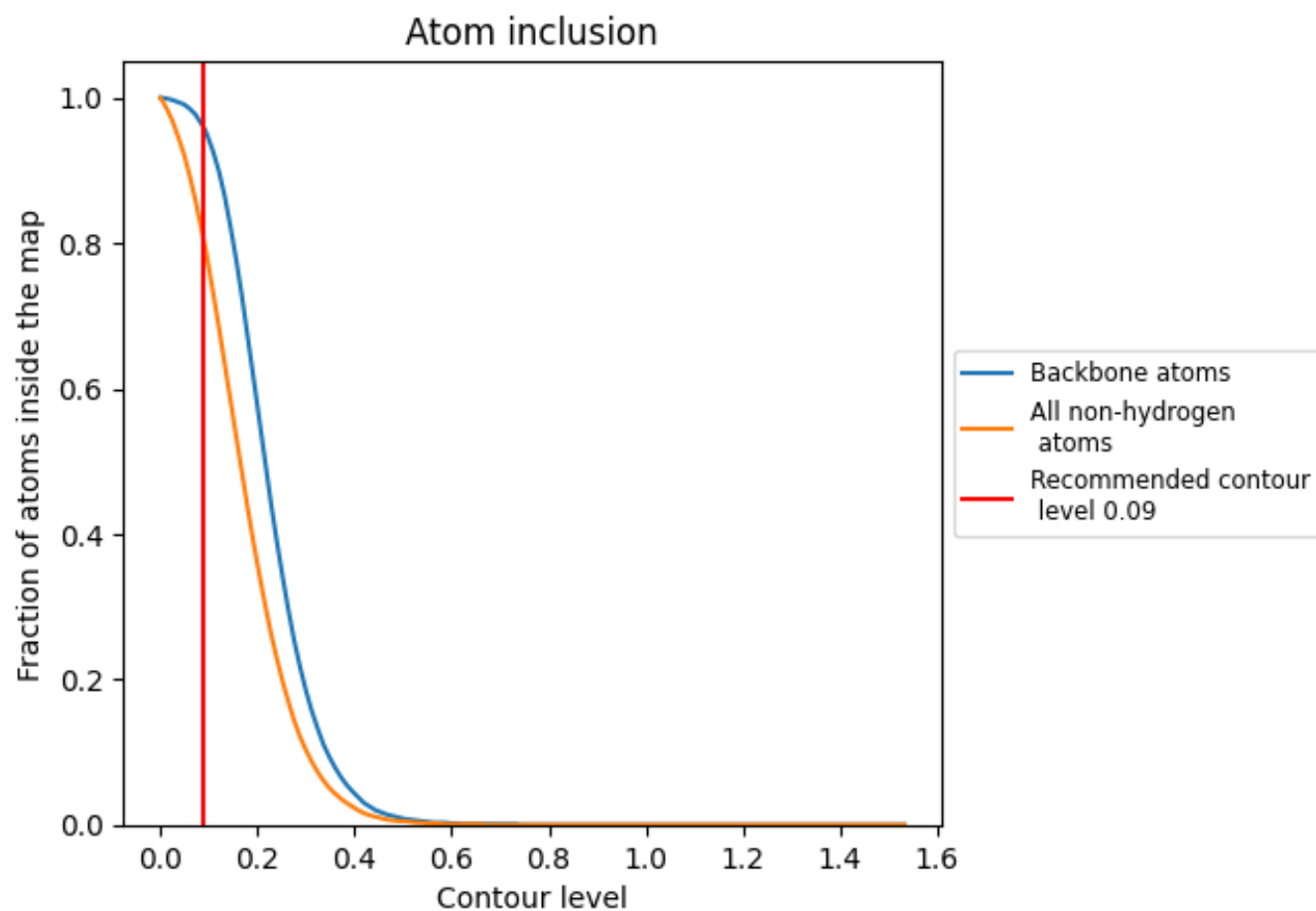
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 80% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8010	 0.1600
1A	 0.7750	 0.1960
1B	 0.8030	 0.2300
1C	 0.7990	 0.2210
1D	 0.7980	 0.2060
1E	 0.8330	 0.2090
1F	 0.8100	 0.1760
1G	 0.8230	 0.2080
1H	 0.8240	 0.1890
1I	 0.8180	 0.2150
1J	 0.8360	 0.1710
1K	 0.8320	 0.1910
1L	 0.9050	 0.1890
1M	 0.8980	 0.2170
1N	 0.8670	 0.2260
1O	 0.8950	 0.1900
1P	 0.8360	 0.1990
1Q	 0.7380	 0.2270
1R	 0.8660	 0.2540
1S	 0.7940	 0.1900
1T	 0.8320	 0.1770
1U	 0.9030	 0.1810
1V	 0.7730	 0.1780
1W	 0.7940	 0.2150
1X	 0.8810	 0.2170
1Y	 0.9370	 0.1820
1Z	 0.8740	 0.2100
1a	 0.9140	 0.2150
1b	 0.9000	 0.2010
1c	 0.8970	 0.2090
1d	 0.8930	 0.2160
1e	 0.8860	 0.2410
1f	 0.9190	 0.2100
1g	 0.9130	 0.2140
1h	 0.9140	 0.2170



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Chain	Atom inclusion	Q-score
1i	 0.9000	 0.1900
1j	 0.9060	 0.1840
1k	 0.9460	 0.1840
1l	 0.9510	 0.2200
1m	 0.9510	 0.2050
1n	 0.9330	 0.1890
1o	 0.9470	 0.1720
1p	 0.9470	 0.2290
1q	 0.8680	 0.2290
1r	 0.8720	 0.2390
1s	 0.8570	 0.1980
3A	 0.7850	 0.1450
3B	 0.8380	 0.1860
3C	 0.8960	 0.2350
3D	 0.7500	 0.0640
3E	 0.8070	 0.0930
3F	 0.7830	 0.0970
3G	 0.9240	 0.2530
3H	 0.9080	 0.2290
3I	 0.5460	 0.0970
3J	 0.8320	 0.0520
3N	 0.9560	 0.2470
3O	 0.9140	 0.2620
3P	 0.9240	 0.1540
3Q	 0.9270	 0.1420
3R	 0.8590	 0.1180
3S	 0.9270	 0.1930
3T	 0.9700	 0.1980
3U	 0.9730	 0.1630
3V	 0.8280	 0.1040
3W	 0.9740	 0.1440
3X	 0.9540	 0.0710
3Y	 0.8370	 0.1400
4A	 0.7520	 0.0940
4B	 0.7360	 0.0870
4C	 0.7760	 0.0760
4D	 0.8200	 0.1170
4E	 0.7670	 0.1020
4F	 0.7570	 0.1150
4G	 0.9230	 0.0980
4H	 0.7550	 0.1060
4I	 0.8330	 0.1040

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Chain	Atom inclusion	Q-score
4J	 0.8820	 0.1400
4K	 0.9410	 0.1290
4L	 0.8350	 0.1060
4M	 0.8940	 0.1470
4N	 0.7210	 0.1040
5A	 0.6350	 0.1250
5B	 0.7630	 0.1540
5C	 0.6670	 0.1480
5D	 0.6810	 0.1290
5E	 0.6880	 0.1480
5F	 0.6680	 0.1040
5G	 0.7200	 0.1450
5H	 0.7410	 0.1400
5I	 0.7430	 0.1400
5J	 0.7850	 0.1320
5K	 0.7740	 0.1440
5L	 0.7720	 0.1170
5M	 0.7660	 0.1390
5N	 0.7650	 0.1480
5O	 0.7860	 0.1540
5P	 0.7960	 0.1530
5Q	 0.6140	 0.1500
5R	 0.8280	 0.1840
5S	 0.7200	 0.1460
5T	 0.6610	 0.1300
5U	 0.6450	 0.1200
5V	 0.6690	 0.1340
5W	 0.7070	 0.1700
5X	 0.8580	 0.1590
5Y	 0.8100	 0.1470
5Z	 0.8100	 0.1520
5a	 0.8800	 0.1540
5b	 0.8470	 0.1620
5c	 0.8370	 0.1710
5d	 0.7980	 0.1620
5e	 0.8850	 0.1810
5f	 0.8620	 0.1810
5g	 0.7860	 0.1680
5h	 0.8290	 0.1570
5i	 0.8060	 0.1430
5j	 0.7770	 0.1340
5k	 0.8330	 0.1680

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Chain	Atom inclusion	Q-score
5l	 0.8180	 0.1470
5m	 0.7910	 0.1490
5n	 0.7600	 0.1410
5o	 0.8730	 0.1290
5p	 0.8710	 0.1700
5q	 0.8340	 0.1840
5r	 0.7520	 0.1750
5s	 0.7280	 0.1300
6A	 0.7950	 0.1940
6B	 0.7630	 0.2100
6C	 0.7630	 0.1870
6D	 0.8430	 0.1830
6E	 0.6680	 0.0550
6F	 0.5410	 0.0580
6G	 0.5580	 0.0190
6H	 0.6470	 0.0480
6I	 0.4020	 0.0390
6J	 0.8980	 0.1760
6N	 0.7960	 0.1940
6O	 0.7720	 0.2160
6P	 0.7230	 0.1030
6Q	 0.7240	 0.1020
6R	 0.6710	 0.0900
6S	 0.7410	 0.1510
6T	 0.8250	 0.1220
6U	 0.7980	 0.1470
6V	 0.4880	 0.0860
6W	 0.7990	 0.1180
6X	 0.7280	 0.0690
6Y	 0.8520	 0.2060
8A	 0.7250	 0.1360
8B	 0.6710	 0.0610
8C	 0.6230	 0.0460
8D	 0.7240	 0.0870
8E	 0.6030	 0.0610
8F	 0.6090	 0.0830
8G	 0.8320	 0.0910
8H	 0.7130	 0.0840
8I	 0.7510	 0.0870
8J	 0.7880	 0.1010
8K	 0.8520	 0.1050
8L	 0.7250	 0.0950

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Chain	Atom inclusion	Q-score
8M	 0.8340	 0.1150
8N	 0.6810	 0.0830