



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 12:07 PM UTC

PDB ID : 8UGI / pdb_00008ugi
EMDB ID : EMD-42226
Title : High resolution in-situ structure of typeA supercomplex in respiratory chain (I1III2IV1,composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

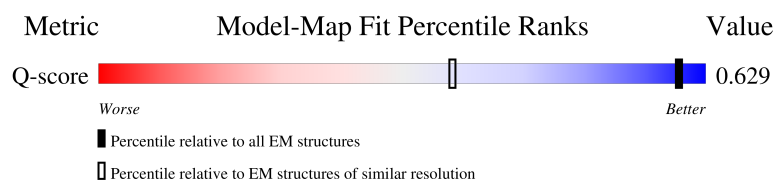
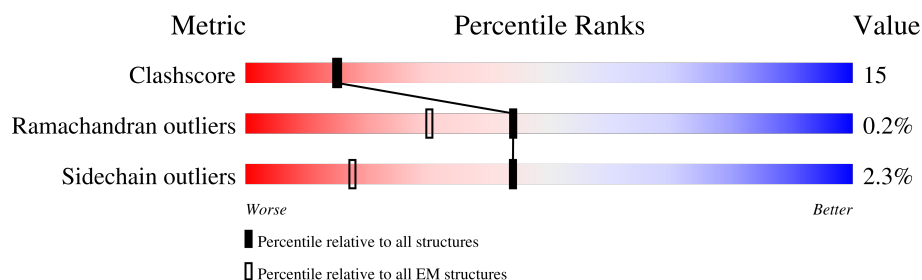
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	37% 63% 35% .
2	1B	258	36% 22% 40% .
3	1C	264	59% 20% 21%
4	1D	476	9% 63% 27% 10%

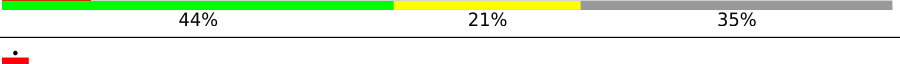
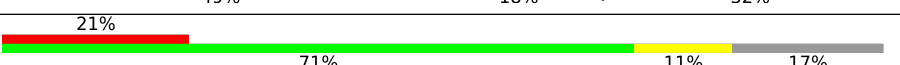
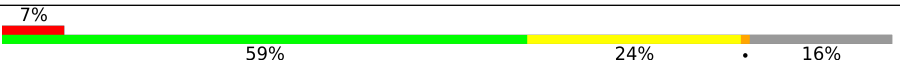
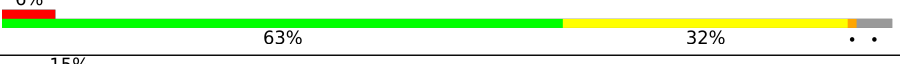
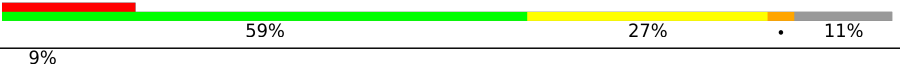
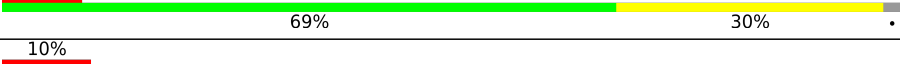
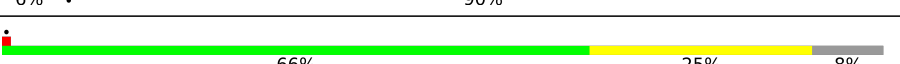
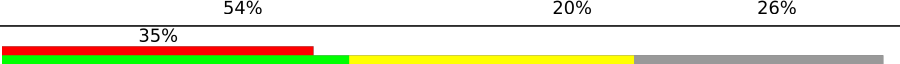
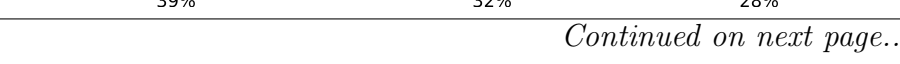
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24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

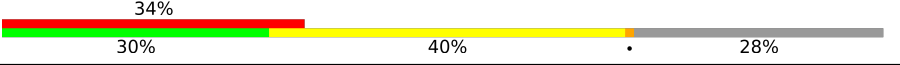
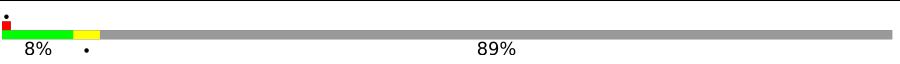
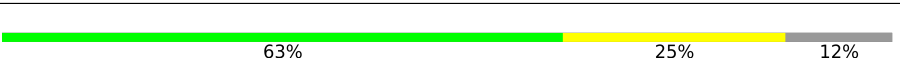
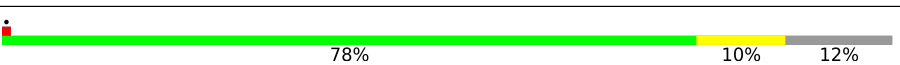
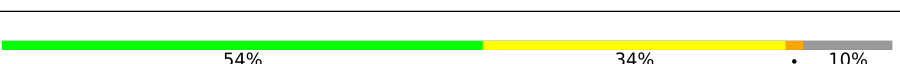
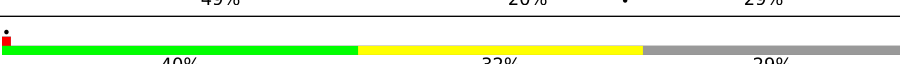
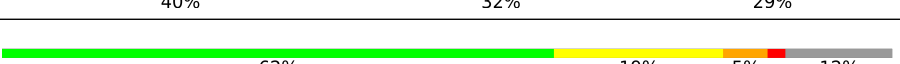
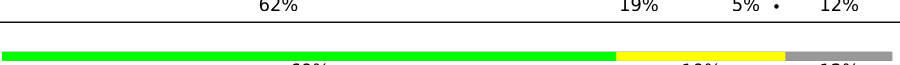
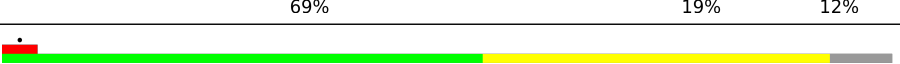
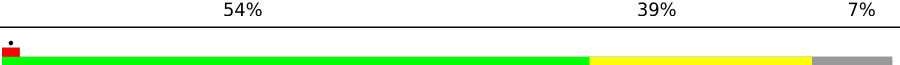
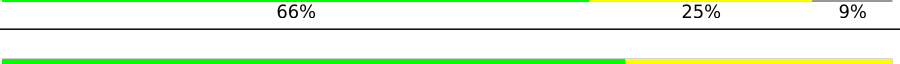
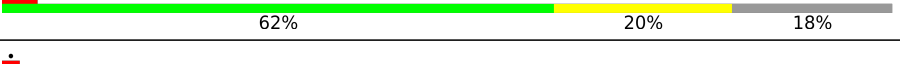
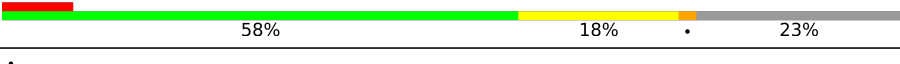
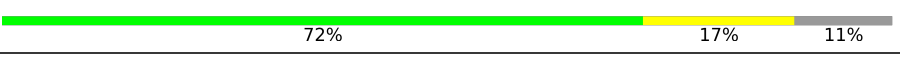
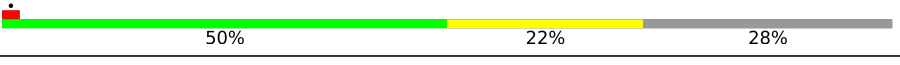
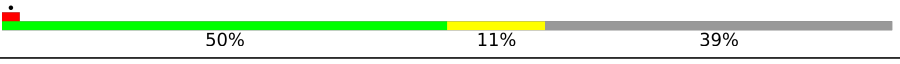
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Mol	Chain	Length	Quality of chain
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	325	
48	3Q	325	
49	3E	274	

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Mol	Chain	Length	Quality of chain
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	64	
53	3W	64	
54	3X	56	
54	3Y	56	
55	4A	514	
56	4B	227	
57	4C	261	
58	4D	169	
59	4E	152	
60	4F	129	
61	4G	97	
62	4H	86	
63	4I	75	
64	4J	80	
65	4K	80	
66	4L	63	

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Mol	Chain	Length	Quality of chain
67	4M	70	
68	4N	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
71	SF4	1B	201	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	3R	301	-	-	X	-
89	CUA	4B	303	-	-	X	-

2 Entry composition

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

1 [Sus scrofa].

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

4.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

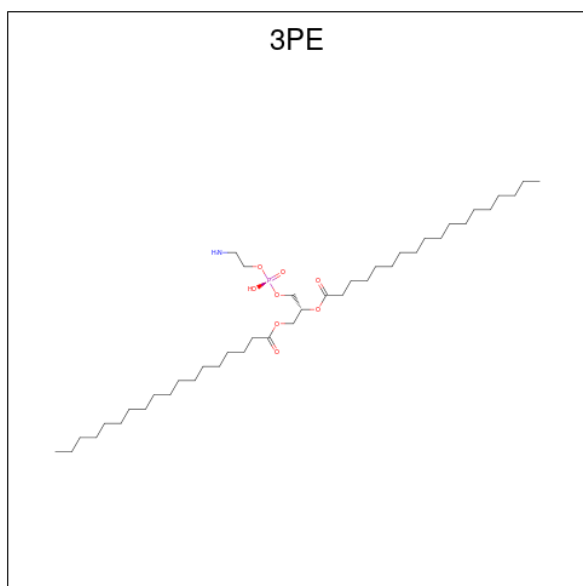
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

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

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

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

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



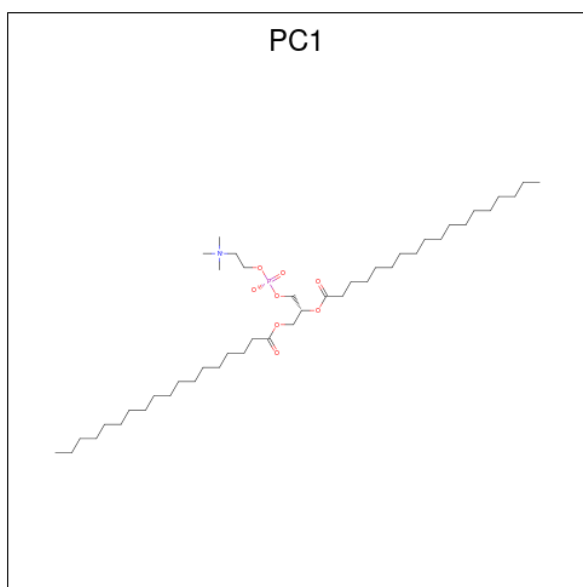
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0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

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

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



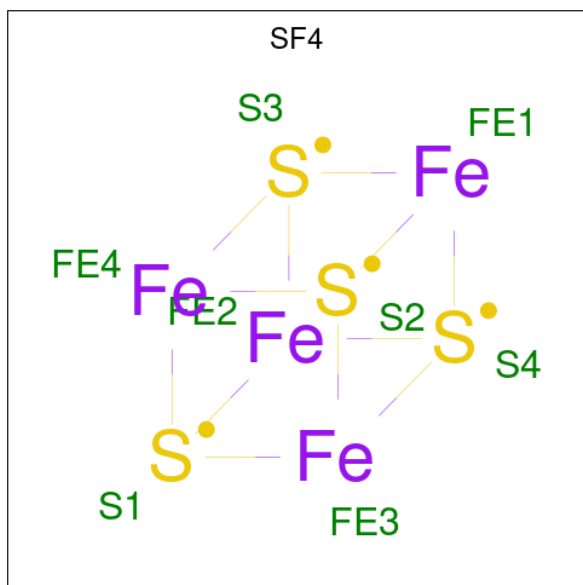
Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1P	1	Total	C	N	O	P	0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

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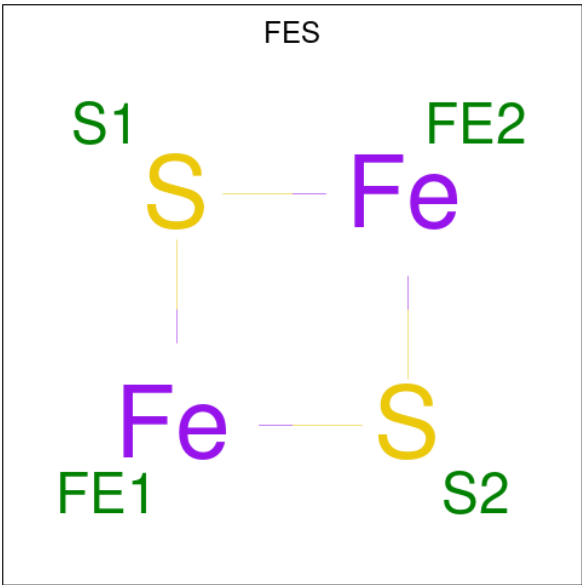
Mol	Chain	Residues	Atoms					AltConf
70	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

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



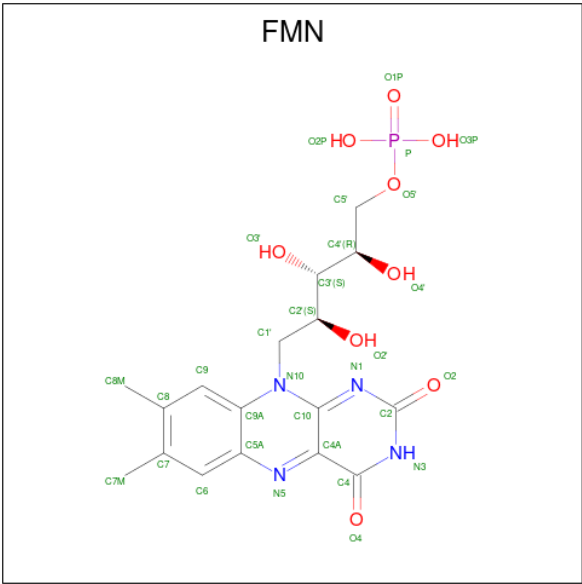
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

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



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

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

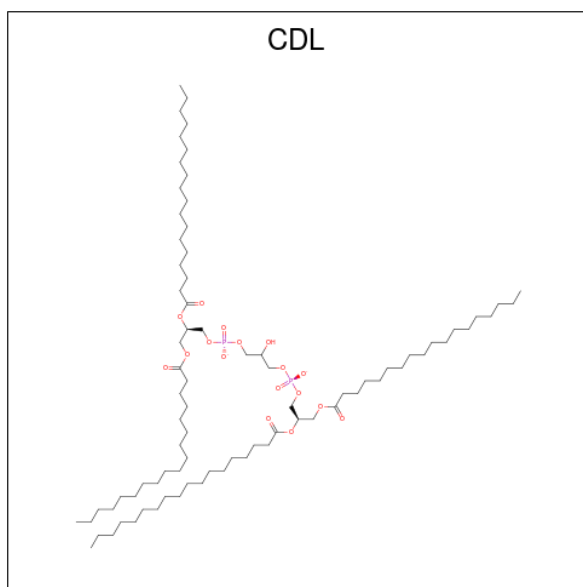


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

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



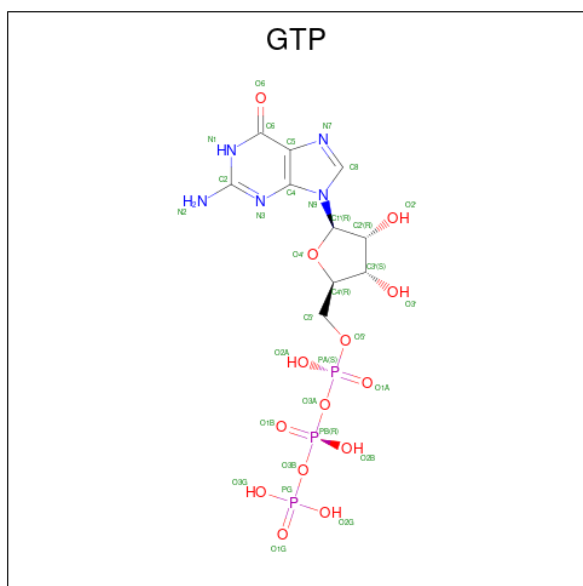
Mol	Chain	Residues	Atoms				AltConf
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1h	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	3A	1	Total	C	O	P	0
			58	39	17	2	
75	3G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

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

- Molecule 76 is GUANOSINE-5'-TRIPHOSPHATE (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	

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

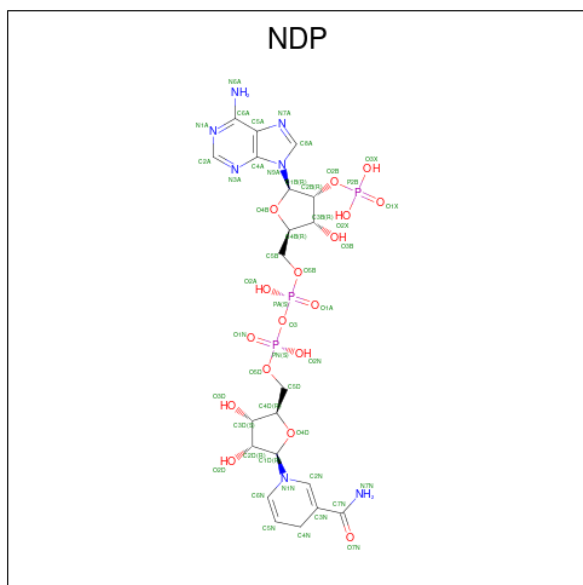
Mol	Chain	Residues	Atoms		AltConf
77	1O	1	Total	Mg	0
			1	1	

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

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

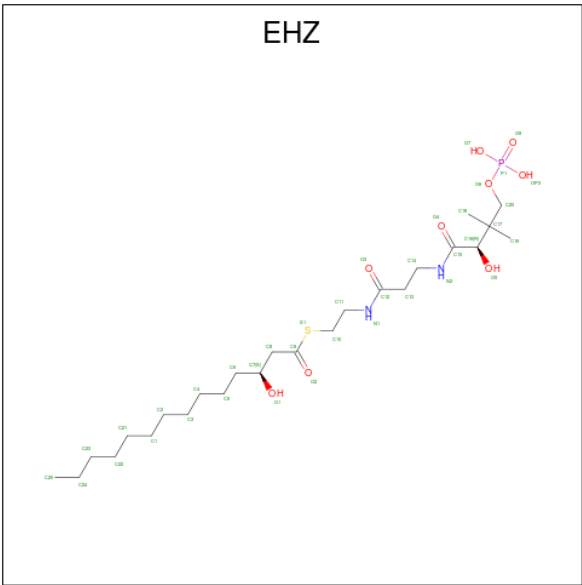


Mol	Chain	Residues	Atoms					AltConf
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

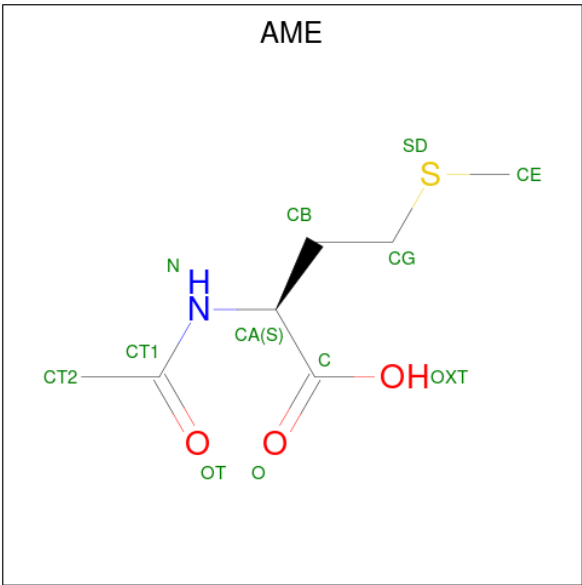
Mol	Chain	Residues	Atoms		AltConf
79	1R	1	Total	Zn	0
			1	1	
79	4F	1	Total	Zn	0
			1	1	

- 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: $C_{25}H_{49}N_2O_9PS$).



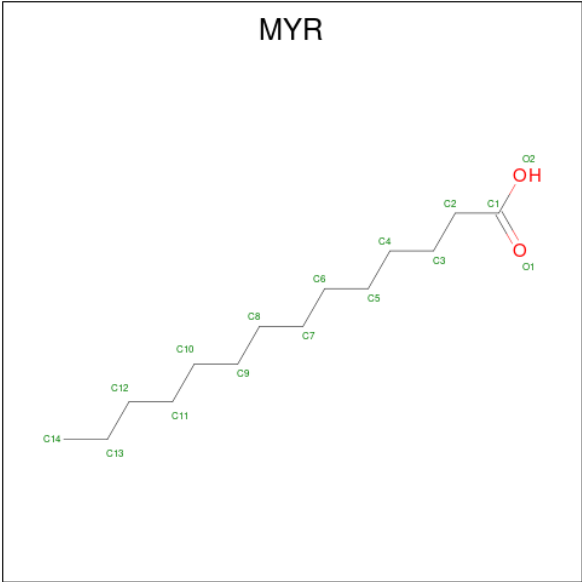
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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



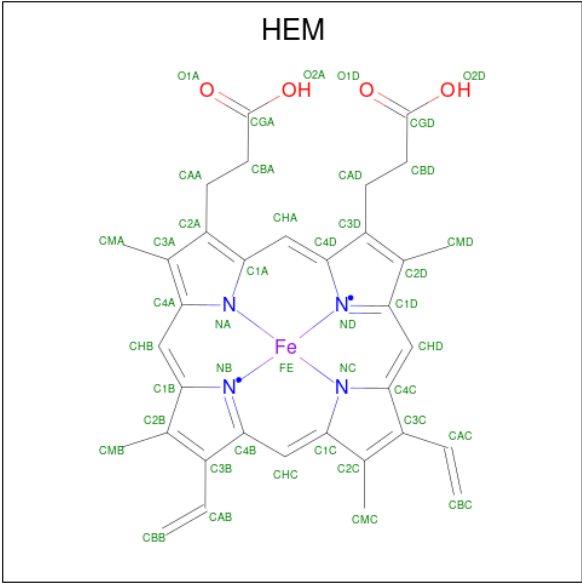
Mol	Chain	Residues	Atoms					AltConf
81	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 82 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms				AltConf
82	1l	1	Total	C	O		0
			15	14	1		

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



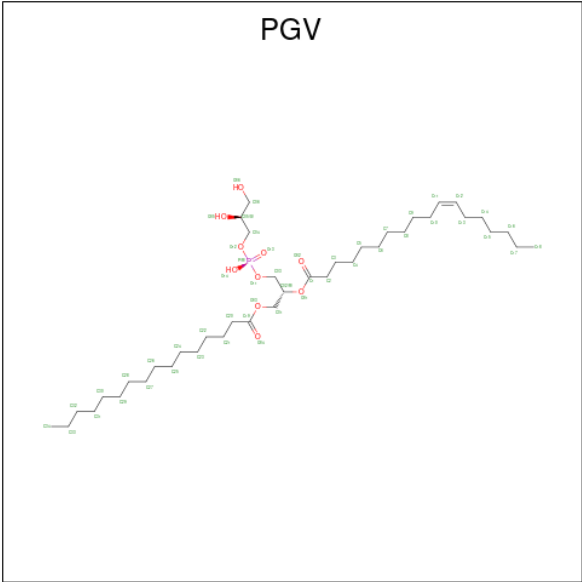
Mol	Chain	Residues	Atoms					AltConf
83	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
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

-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydroxyl group (OH). The atoms are labeled with their respective identifiers: O1A, O2A, O1D, O2D, CGA, CGD, CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CBB, C1A, C1B, C2A, C2B, C3C, C4C, C1C, C2C, C3D, C4D, C1D, C2D, C3E, C4E, C1F, C2F, C3G, C4G, C1H, C2H, C3I, C4I, C1J, C2J, C3K, C4K, C1L, C2L, C3M, C4M, C1N, C2N, C3O, C4O, C1P, C2P, C3Q, C4Q, C1R, C2R, C3S, C4S, C1T, C2T, C3U, C4U, C1V, C2V, C3W, C4W, C1X, C2X, C3Y, C4Y, C1Z, C2Z, C3AA, C4AA, C1AB, C2AB, C3AC, C4AC, C1AD, C2AD, C3AE, C4AE, C1AF, C2AF, C3AG, C4AG, C1AH, C2AH, C3AI, C4AI, C1AJ, C2AJ, C3AK, C4AK, C1AL, C2AL, C3AM, C4AM, C1AN, C2AN, C3AO, C4AO, C1AP, C2AP, C3AQ, C4AQ, C1AR, C2AR, C3AS, C4AS, C1AT, C2AT, C3AU, C4AU, C1AV, C2AV, C3AW, C4AW, C1AX, C2AX, C3AY, C4AY, C1AZ, C2AZ, C3BA, C4BA, C1BB, C2BB, C1BC, C2BC, C1BD, C2BD, C1BE, C2BE, C1BF, C2BF, C1BG, C2BG, C1BH, C2BH, C1BI, C2BI, C1BJ, C2BJ, C1BK, C2BK, C1BL, C2BL, C1BM, C2BM, C1BN, C2BN, C1BO, C2BO, C1BP, C2BP, C1BQ, C2BQ, C1BR, C2BR, C1BS, C2BS, C1BT, C2BT, C1BU, C2BU, C1BV, C2BV, C1BW, C2BW, C1BX, C2BX, C1BY, C2BY, C1BZ, C2BZ, C1CA, C2CA, C1CB, C2CB, C1CC, C2CC, C1CD, C2CD, C1CE, C2CE, C1CF, C2CF, C1CG, C2CG, C1CH, C2CH, C1CI, C2CI, C1CJ, C2CJ, C1CK, C2CK, C1CL, C2CL, C1CM, C2CM, C1CN, C2CN, C1CO, C2CO, C1CP, C2CP, C1CQ, C2CQ, C1CR, C2CR, C1CS, C2CS, C1CT, C2CT, C1CU, C2CU, C1CV, C2CV, C1CW, C2CW, C1CX, C2CX, C1CY, C2CY, C1CZ, C2CZ, C1DA, C2DA, C1DB, C2DB, C1DC, C2DC, C1DD, C2DD, C1DE, C2DE, C1DF, C2DF, C1DG, C2DG, C1DH, C2DH, C1DI, C2DI, C1DJ, C2DJ, C1DK, C2DK, C1DL, C2DL, C1DM, C2DM, C1DN, C2DN, C1DO, C2DO, C1DP, C2DP, C1DQ, C2DQ, C1DR, C2DR, C1DS, C2DS, C1DT, C2DT, C1DU, C2DU, C1DV, C2DV, C1DW, C2DW, C1DX, C2DX, C1DY, C2DY, C1DZ, C2DZ, C1EA, C2EA, C1EB, C2EB, C1EC, C2EC, C1ED, C2ED, C1EE, C2EE, C1EF, C2EF, C1EG, C2EG, C1EH, C2EH, C1EI, C2EI, C1EJ, C2EJ, C1EK, C2EK, C1EL, C2EL, C1EM, C2EM, C1EN, C2EN, C1EO, C2EO, C1EP, C2EP, C1EQ, C2EQ, C1ER, C2ER, C1ES, C2ES, C1ET, C2ET, C1EU, C2EU, C1EV, C2EV, C1EW, C2EW, C1EX, C2EX, C1EY, C2EY, C1EZ, C2EZ, C1FA, C2FA, 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C1OS, C2OS, C1OT, C2OT, C1OU, C2OU, C1OV, C2OV, C1OW, C2OW, C1OX, C2OX, C1OY, C2OY, C1OZ, C2OZ, C1PA, C2PA, C1PB, C2PB, C1PC, C2PC, C1PD, C2PD, C1PE, C2PE, C1PF, C2PF, C1PG, C2PG, C1PH, C2PH, C1PI, C2PI, C1PJ, C2PJ, C1PK, C2PK, C1PL, C2PL, C1PM, C2PM, C1PN, C2PN, C1PO, C2PO, C1PP, C2PP, C1PQ, C2PQ, C1PR, C2PR, C1PS, C2PS, C1PT, C2PT, C1PU, C2PU, C1PV, C2PV, C1PW, C2PW, C1PX, C2PX, C1PY, C2PY, C1PZ, C2PZ, C1QA, C2QA, C1QB, C2QB, C1QC, C2QC, C1QD, C2QD, C1QE, C2QE, C1QF, C2QF, C1QG, C2QG, C1QH, C2QH, C1QI, C2QI, C1QJ, C2QJ, C1QK, C2QK, C1QL, C2QL, C1QM, C2QM, C1QN, C2QN, C1QO, C2QO, C1QP, C2QP, C1QQ, C2QQ, C1QR, C2QR, C1QS, C2QS, C1QT, C2QT, C1QU, C2QU, C1QV, C2QV, C1QW, C2QW, C1QX, C2QX, C1QY, C2QY, C1QZ, C2QZ, C1RA, C2RA, C1RB, C2RB, C1RC, C2RC, C1RD, C2RD, C1RE, C2RE, C1RF, C2RF, C1RG, C2RG, C1RH, C2RH,

- Molecule 85 is (1R)-2-[[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



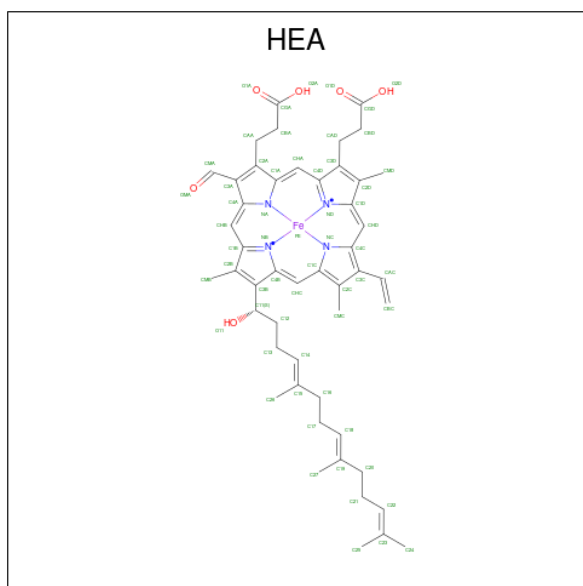
Mol	Chain	Residues	Atoms				AltConf
85	4A	1	Total	C	O	P	0
			51	40	10	1	
85	4A	1	Total	C	O	P	0
			51	40	10	1	
85	4A	1	Total	C	O	P	0
			51	40	10	1	
85	4B	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C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

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

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



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

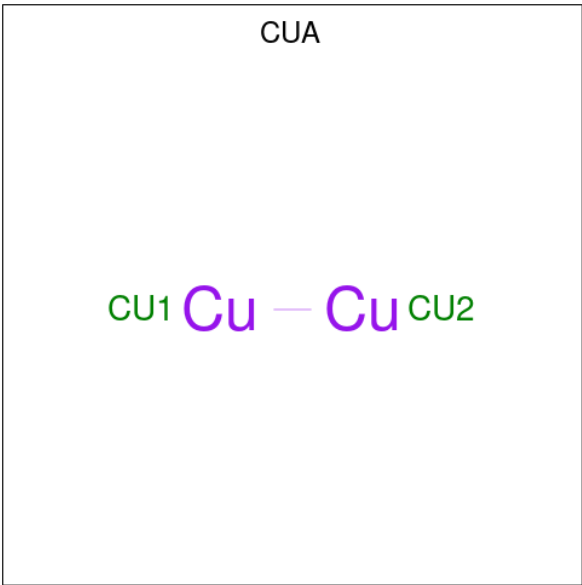
- Molecule 87 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 88 is SODIUM ION (CCD ID: NA) (formula: Na).

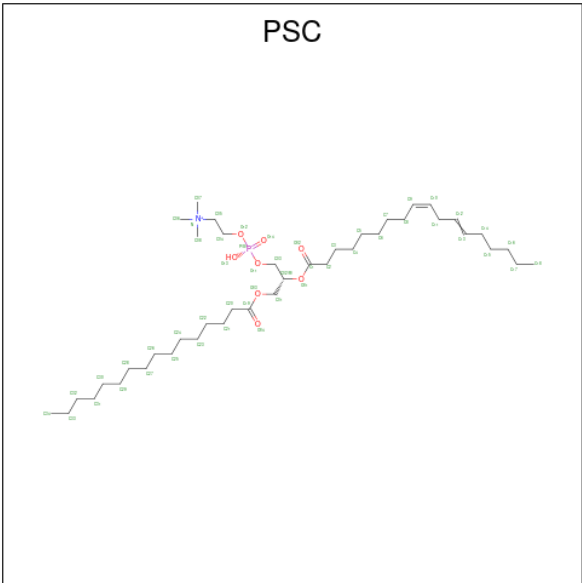
Mol	Chain	Residues	Atoms		AltConf
88	4A	1	Total	Na	0
			1	1	

- Molecule 89 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

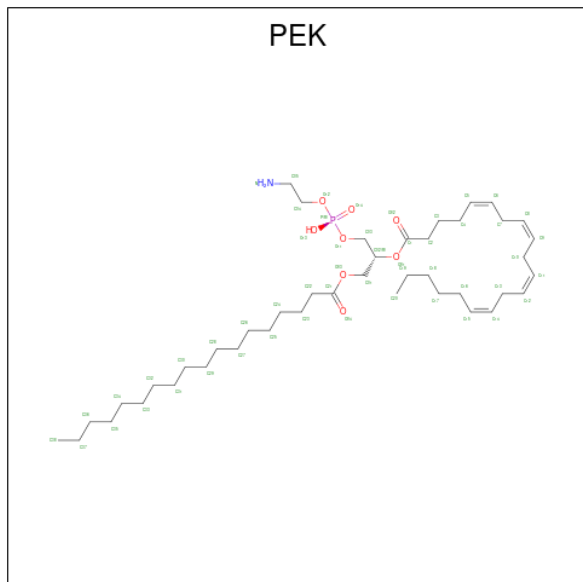
- Molecule 90 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

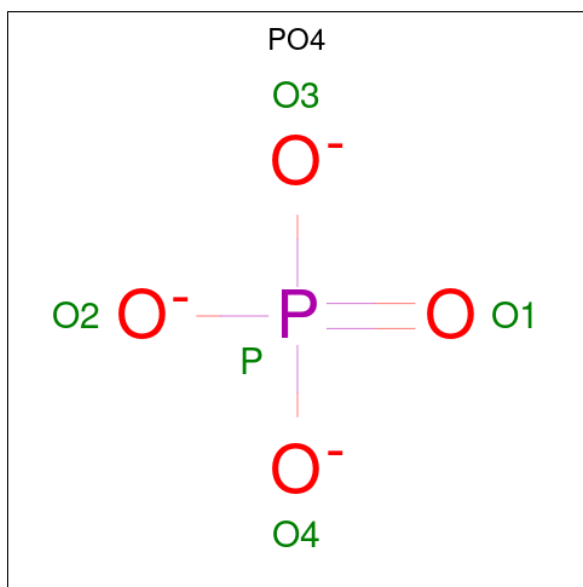
- Molecule 91 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(ST

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



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

- Molecule 92 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 93 is water.

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

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

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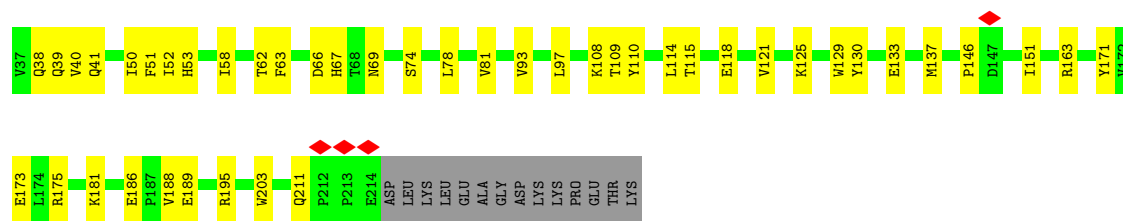
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Mol	Chain	Residues	Atoms		AltConf
93	1o	101	Total 101	O 101	0
93	1p	141	Total 141	O 141	0
93	1q	47	Total 47	O 47	0
93	1r	25	Total 25	O 25	0
93	1s	15	Total 15	O 15	0
93	3A	184	Total 184	O 184	0
93	3B	110	Total 110	O 110	0
93	3C	222	Total 222	O 222	0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

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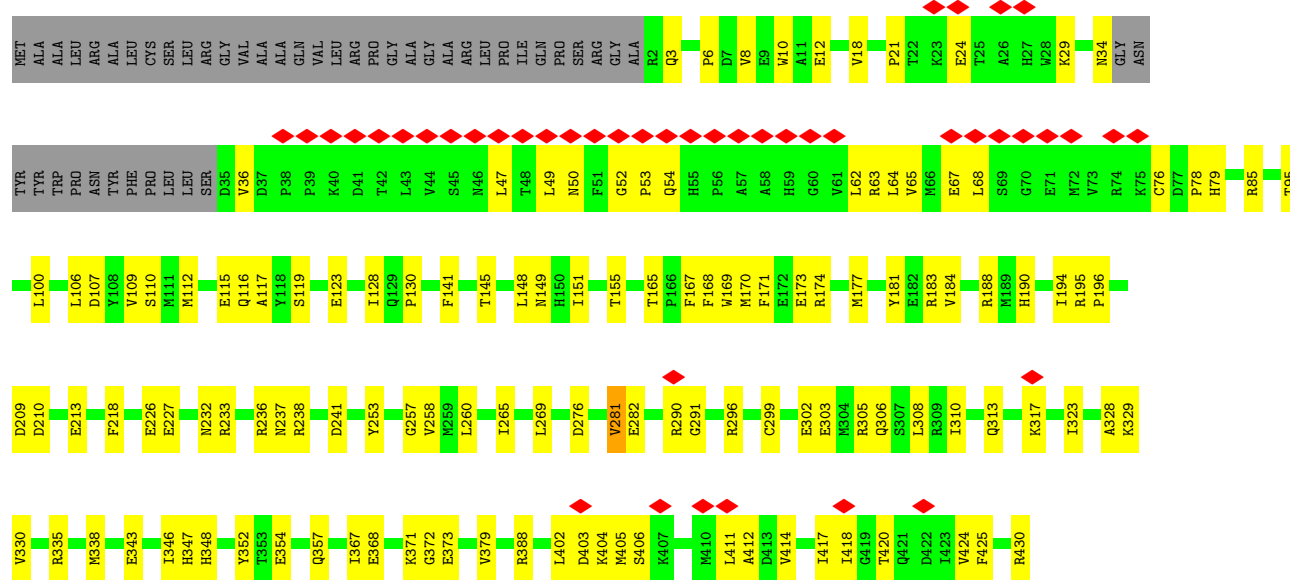
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Mol	Chain	Residues	Atoms		AltConf
93	3T	40	Total 40	O 40	0
93	3U	110	Total 110	O 110	0
93	3V	7	Total 7	O 7	0
93	3W	31	Total 31	O 31	0
93	3X	25	Total 25	O 25	0
93	3Y	16	Total 16	O 16	0
93	4A	110	Total 110	O 110	0
93	4B	115	Total 115	O 115	0
93	4C	103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



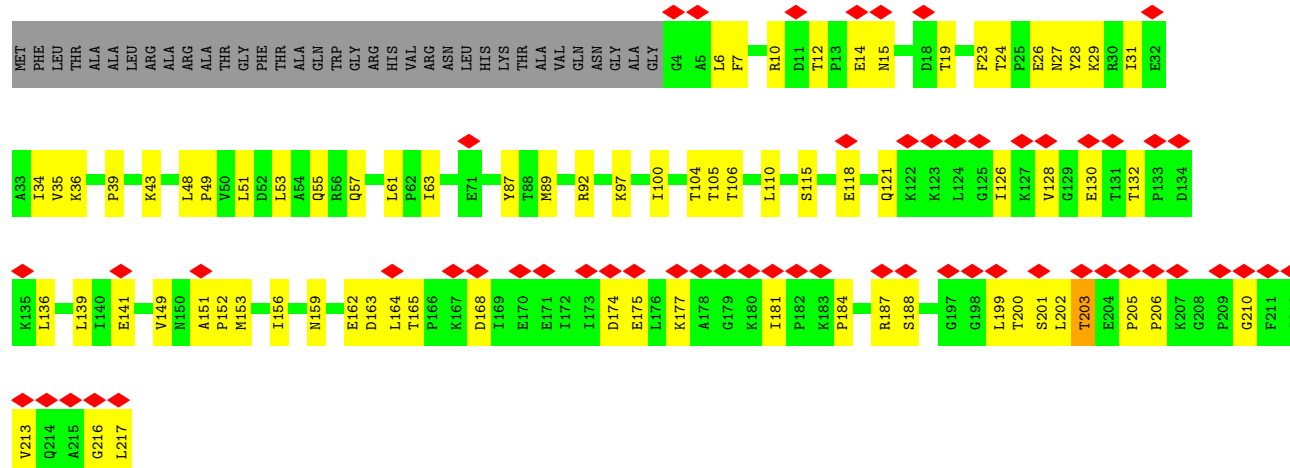
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D: 9% 63% 27% 10%

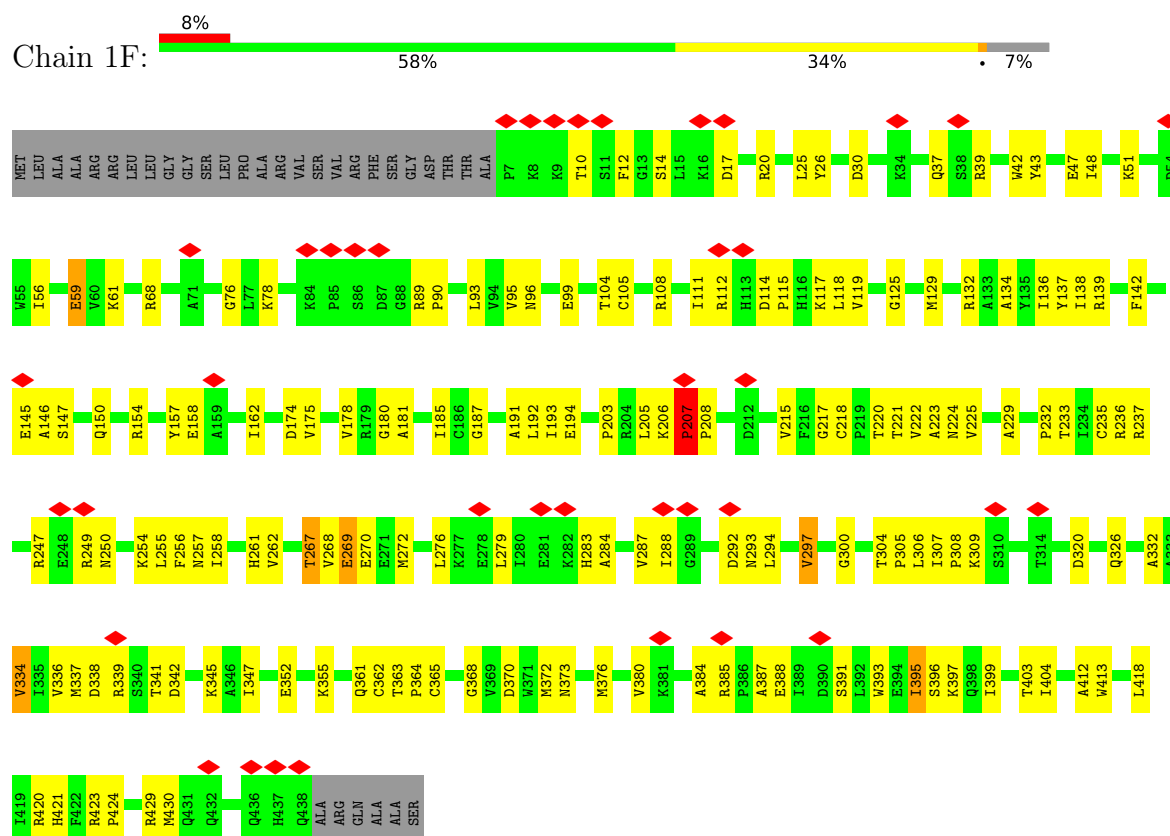


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

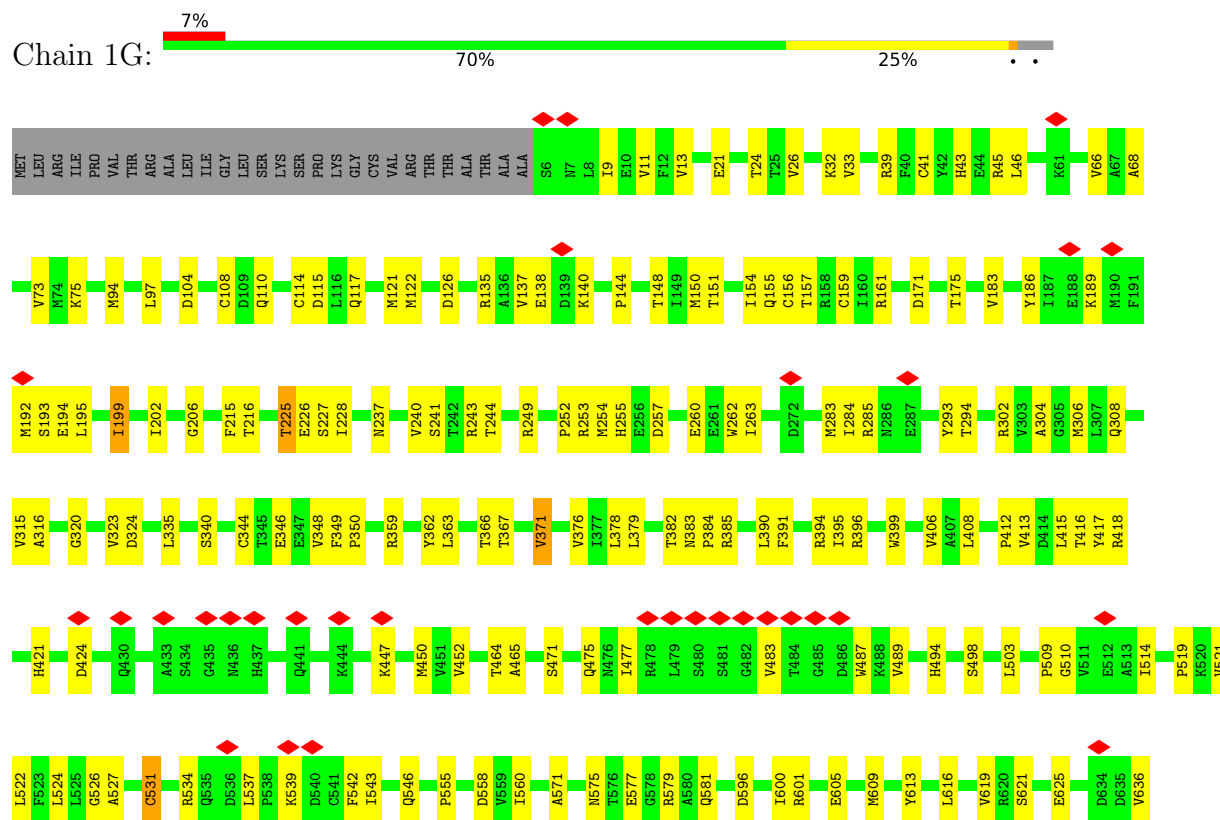
Chain 1E: 23% 56% 30% 14%



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

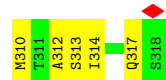
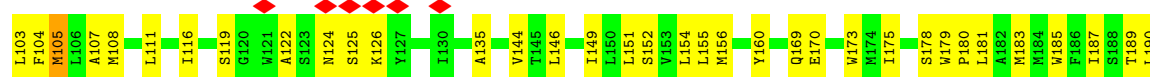


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

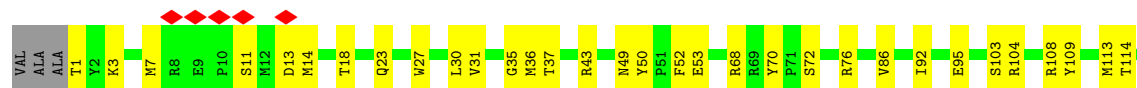




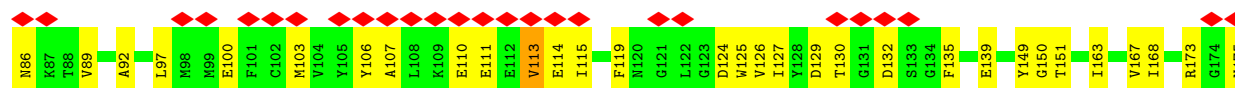
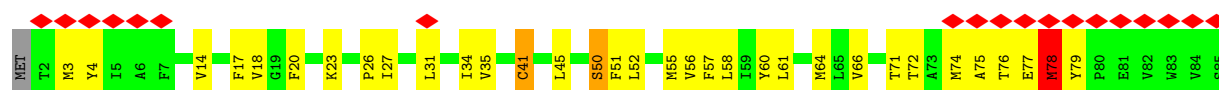
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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

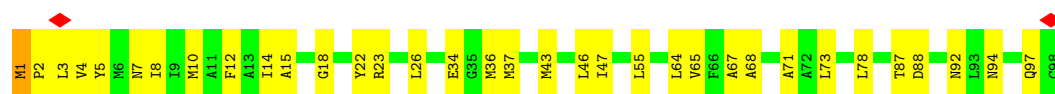


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

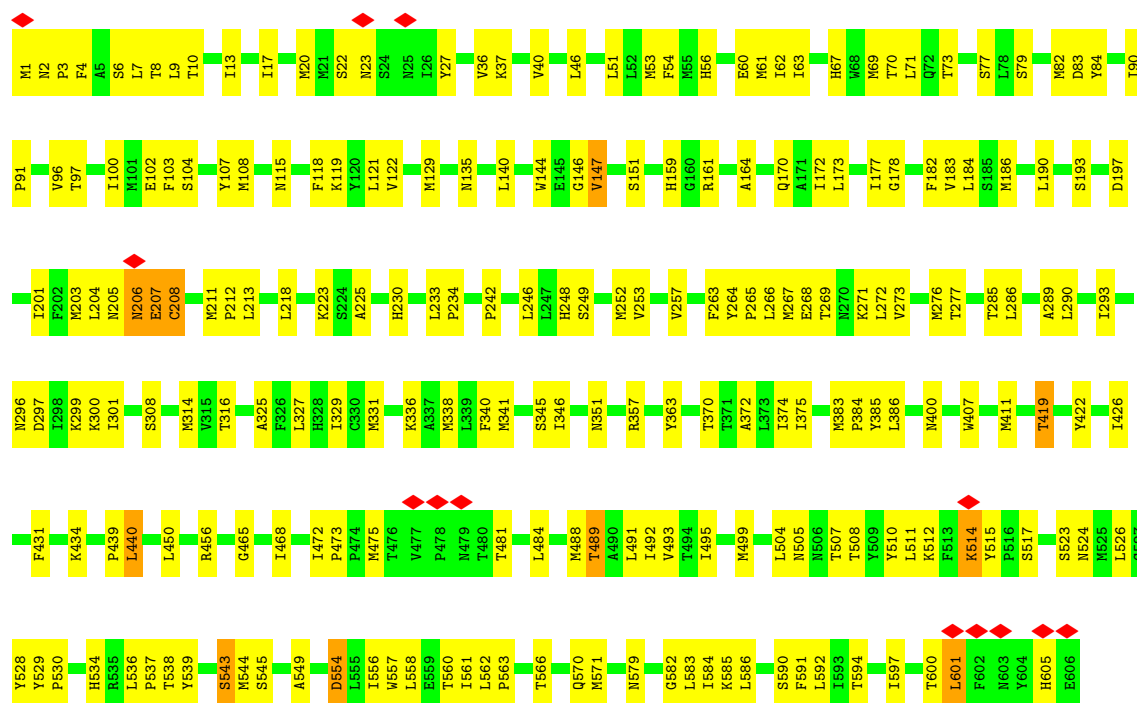


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

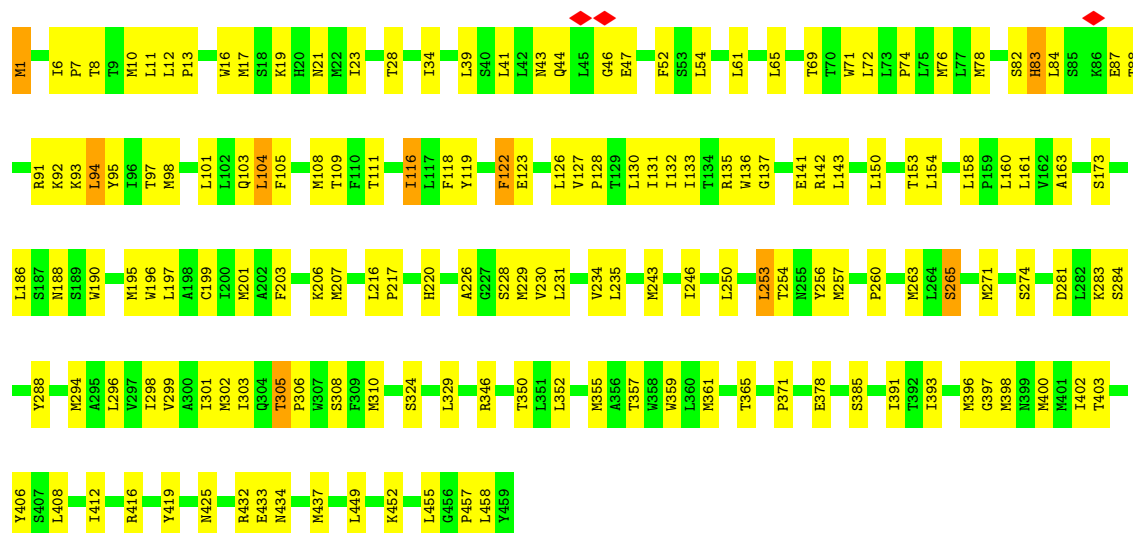




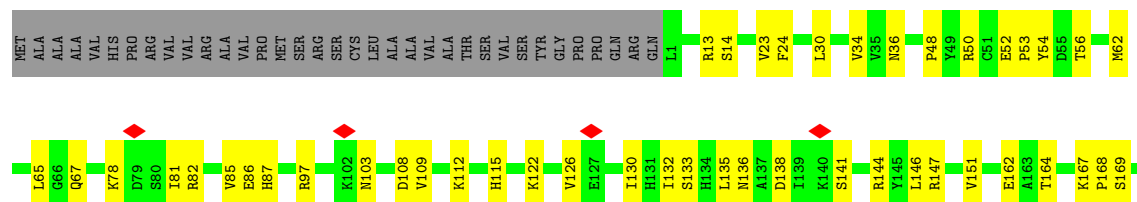
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

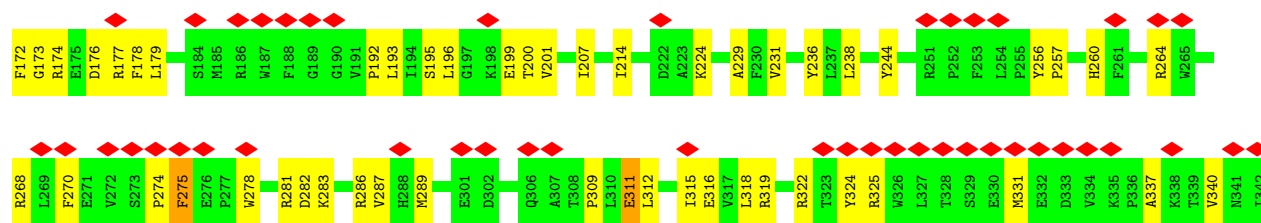


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

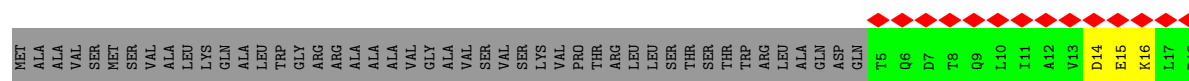


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

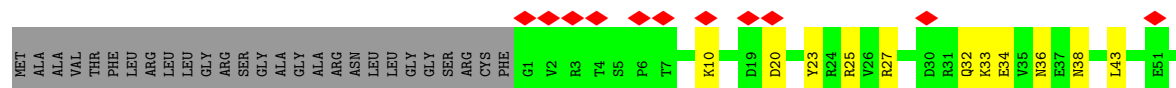




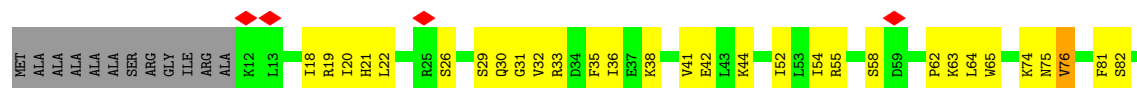
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



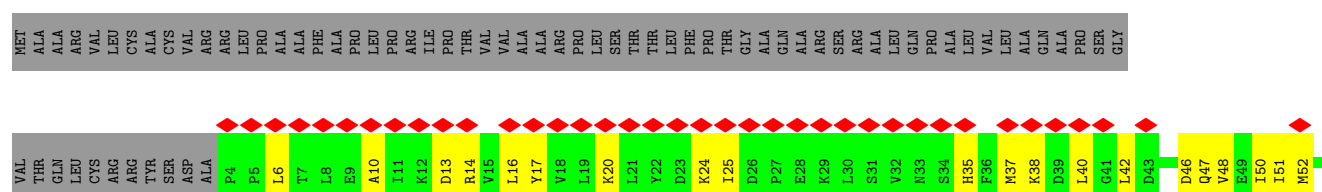
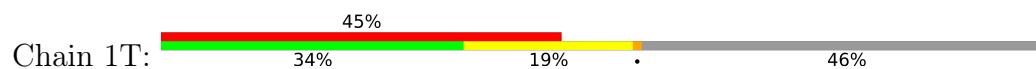
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

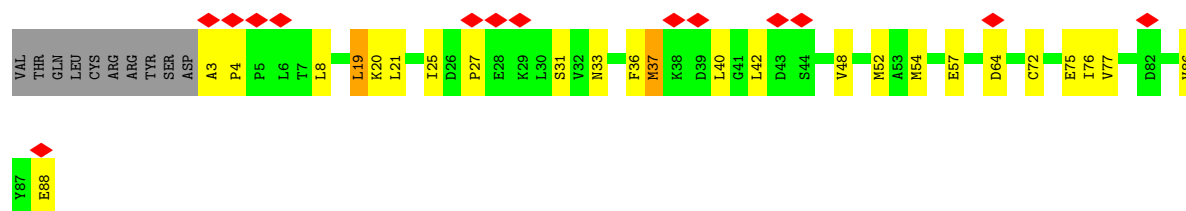
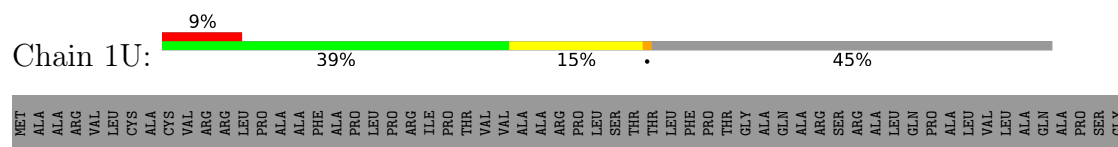


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

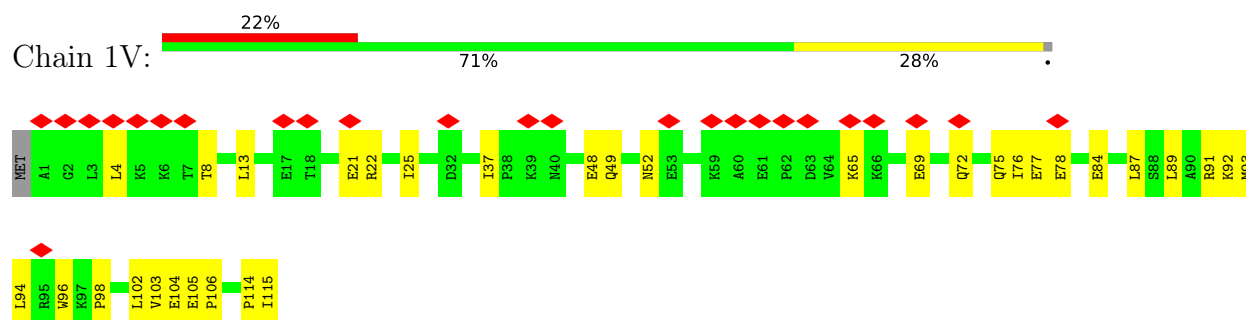




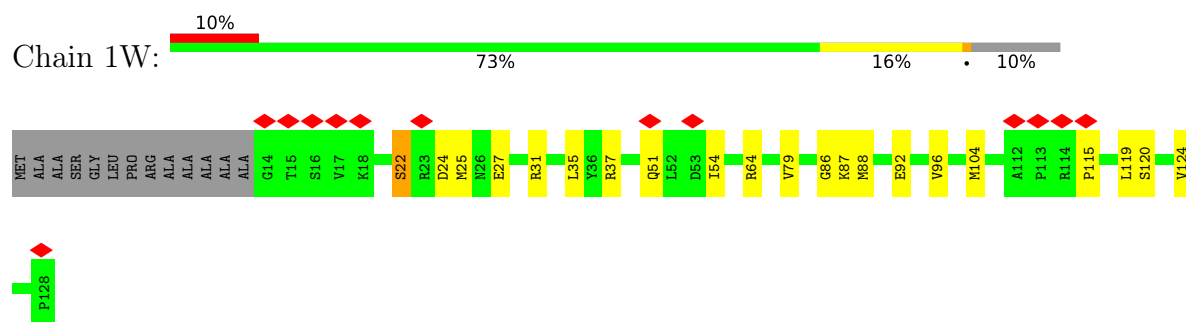
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



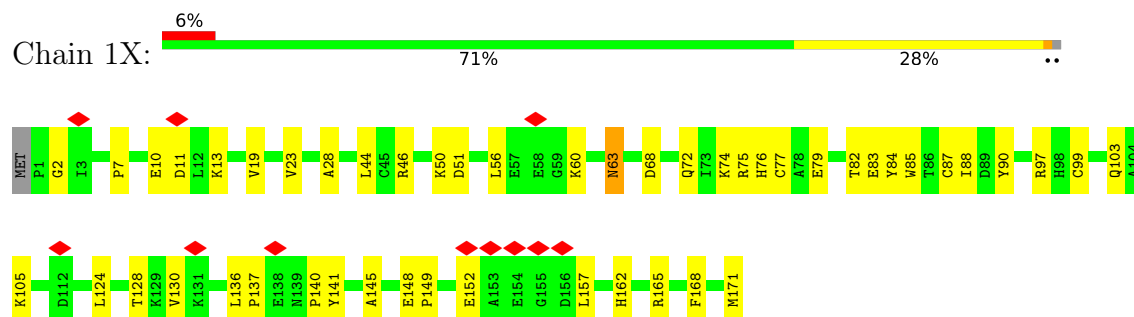
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



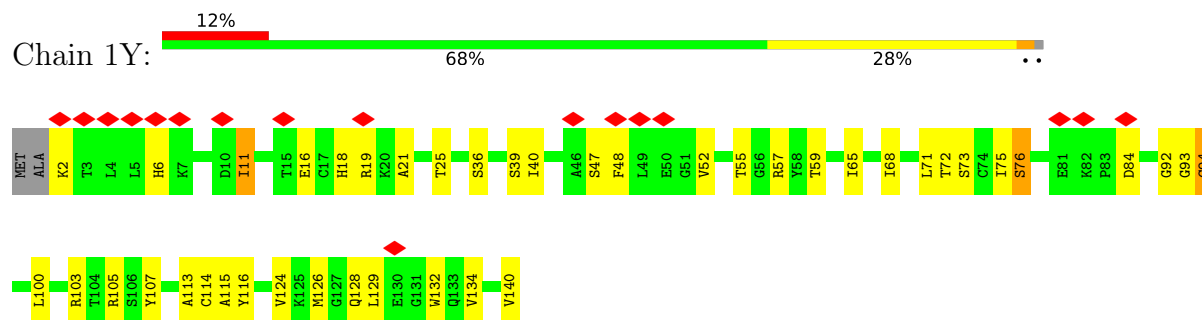
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



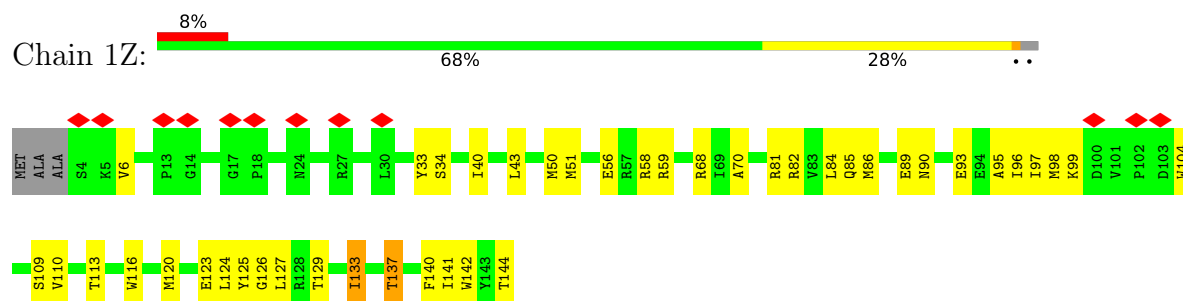
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



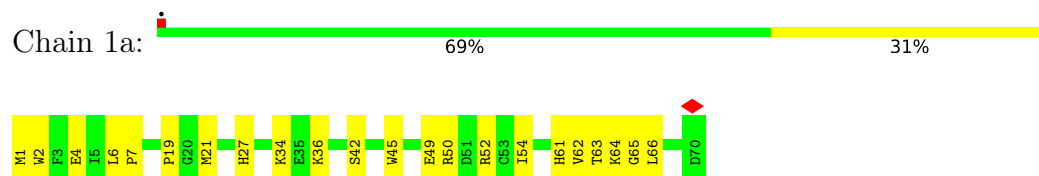
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



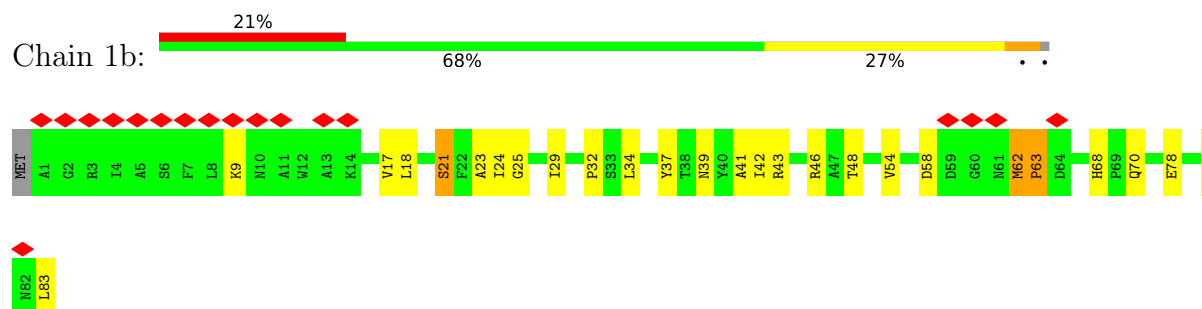
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



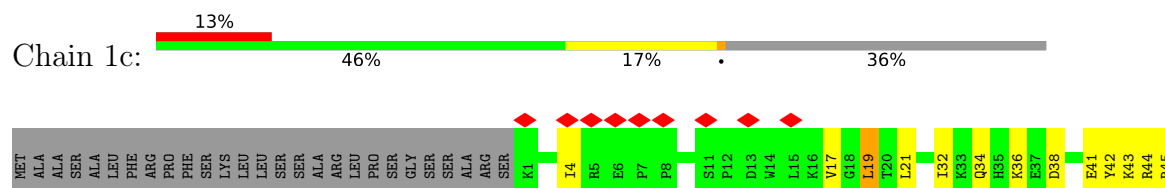
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

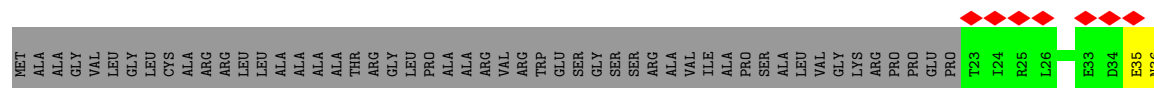


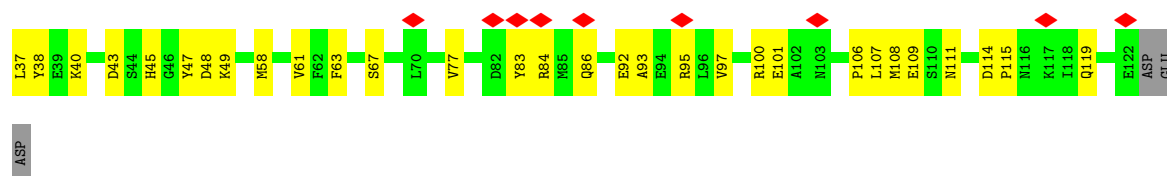
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



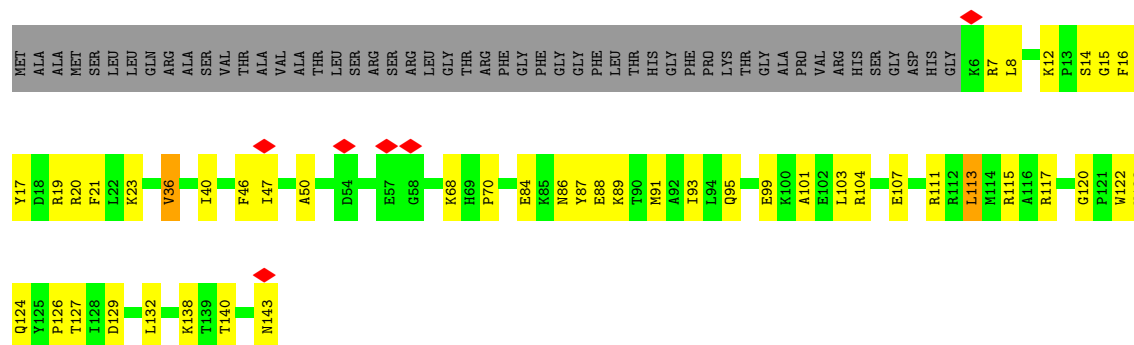
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



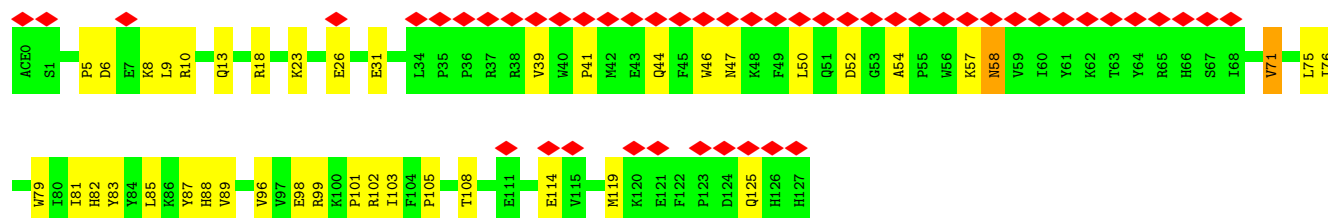
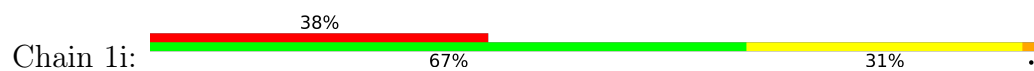




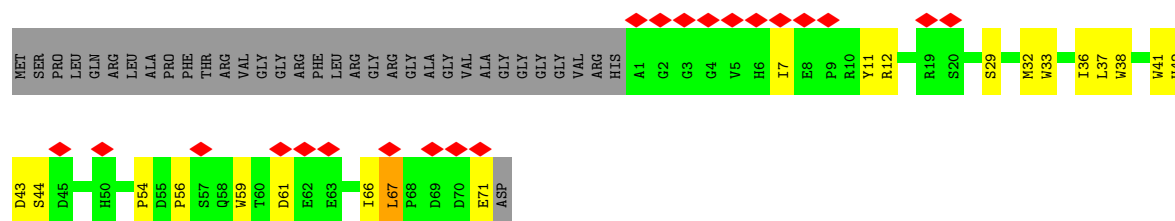
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

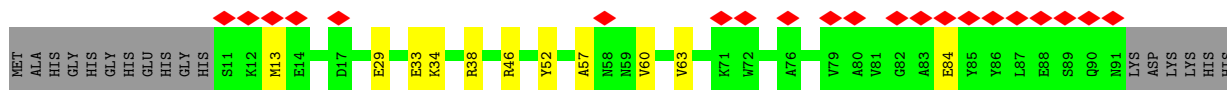


- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

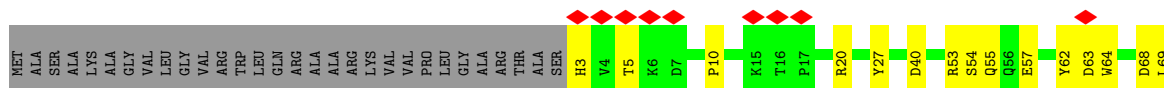


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

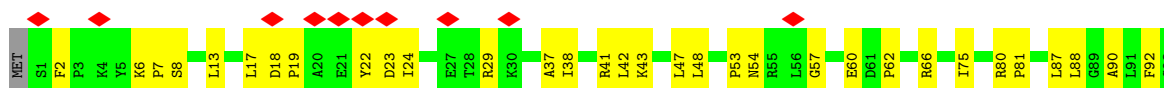




- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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



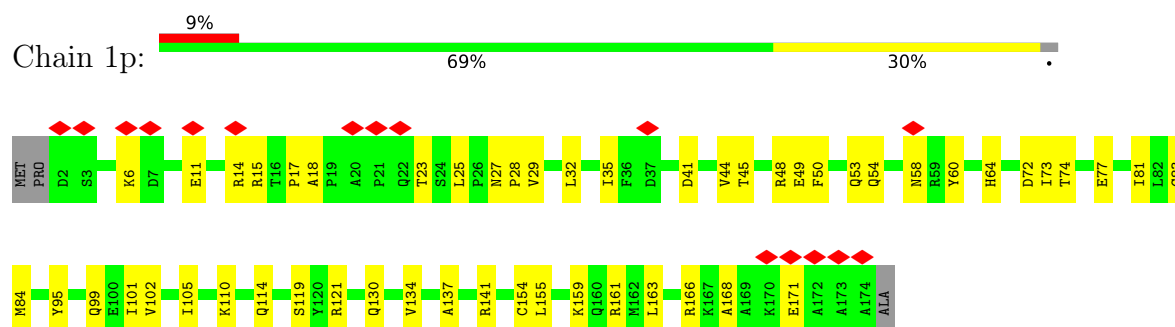
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



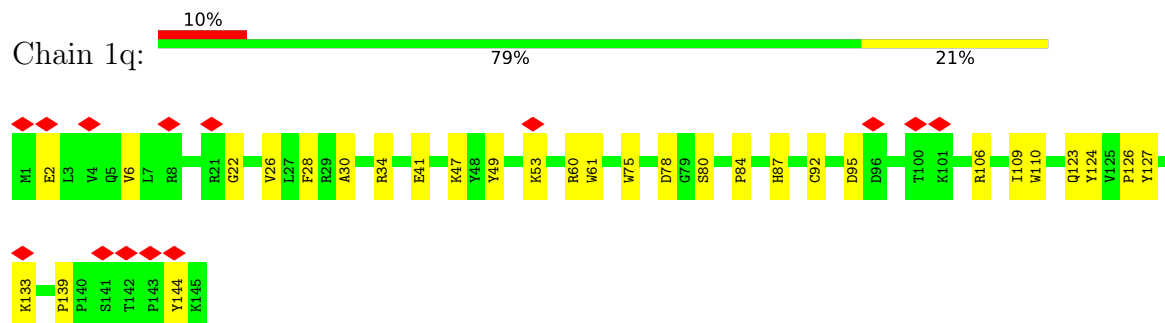
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



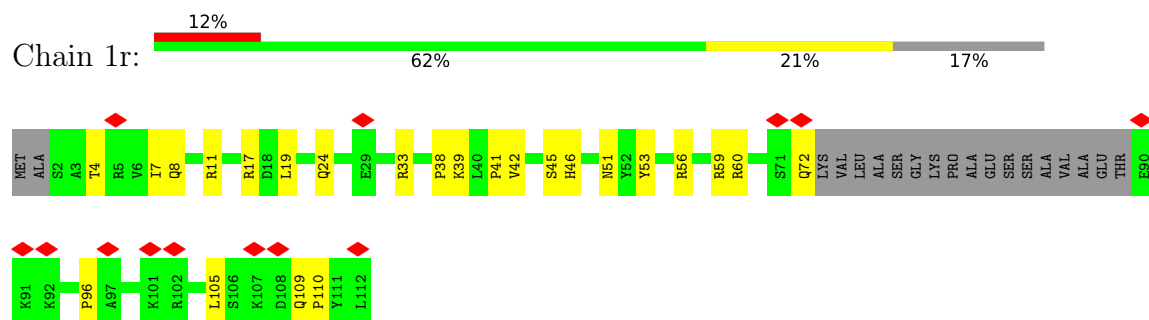
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



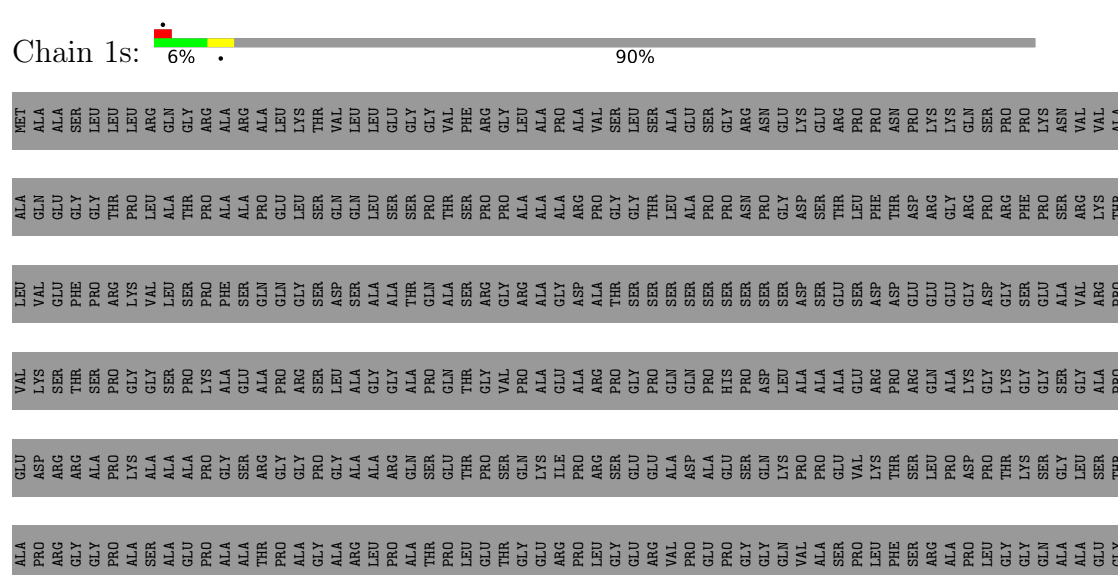
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

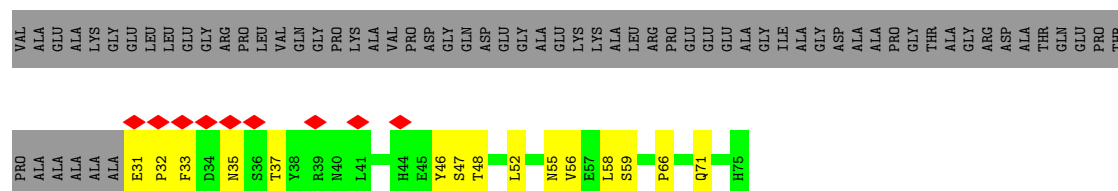


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



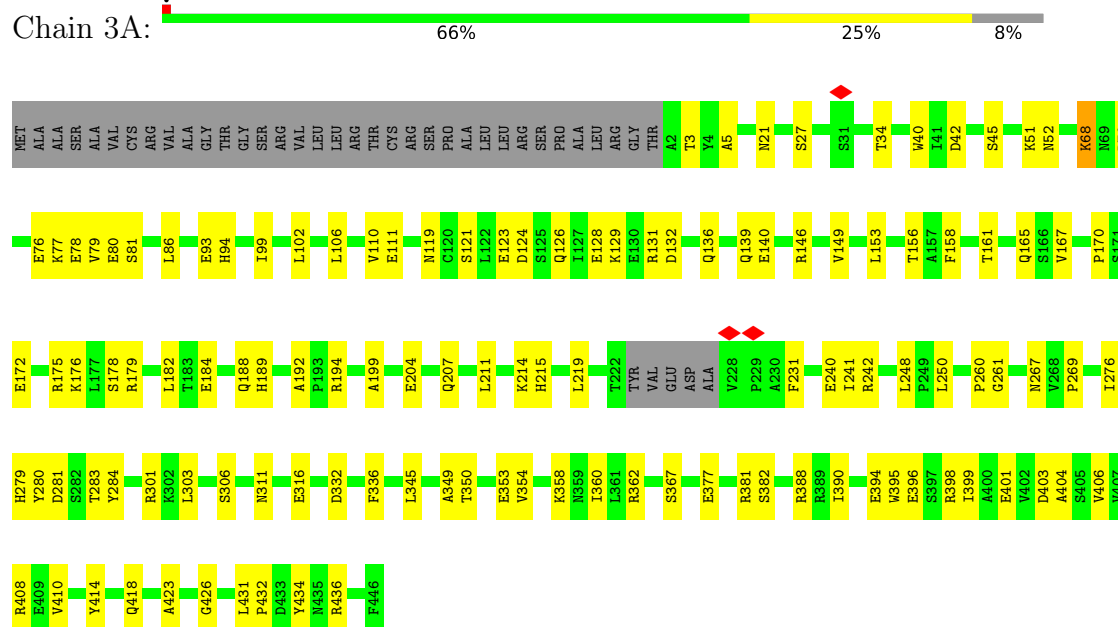
- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial





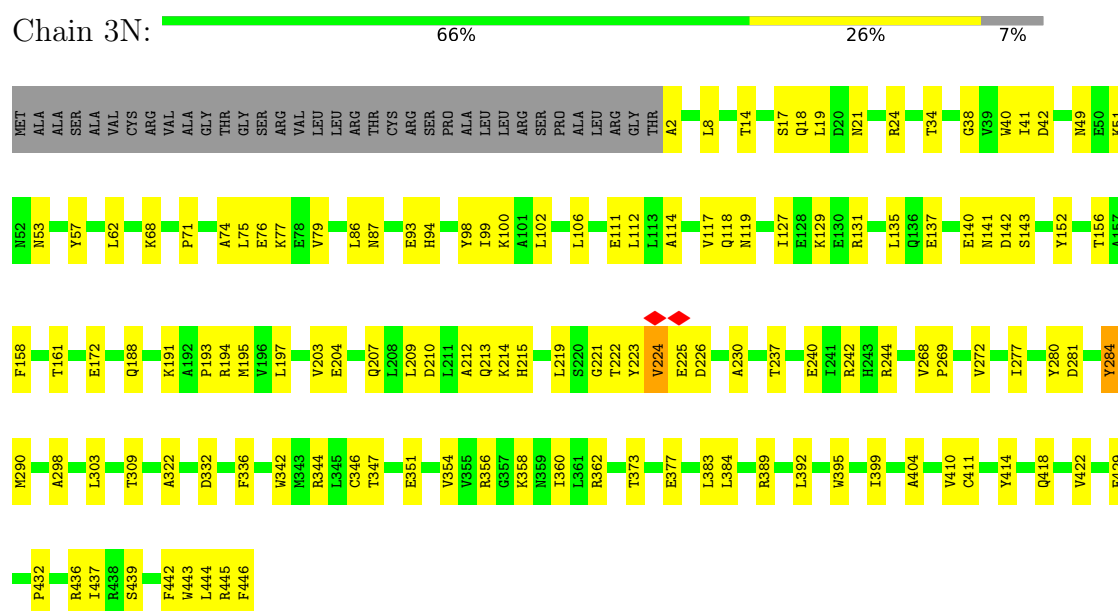
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 3A:



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

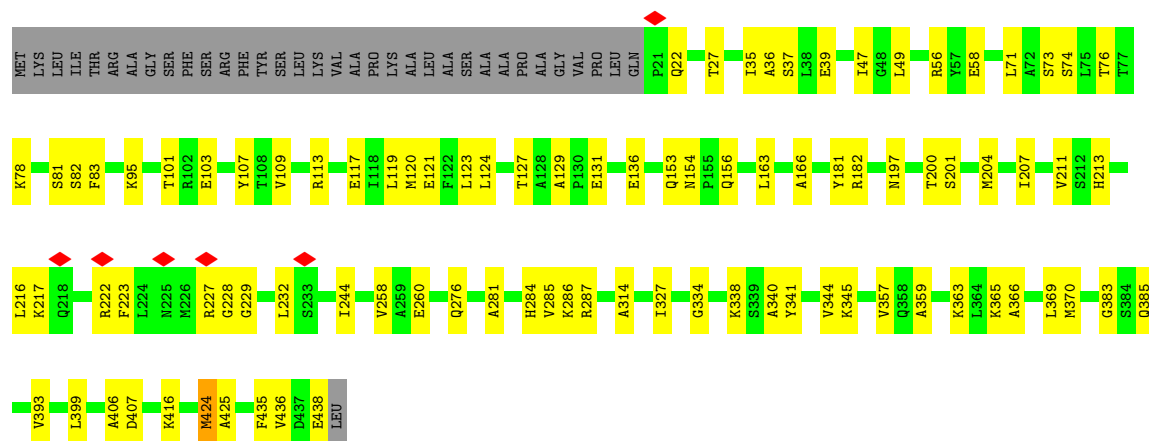
Chain 3N:



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

Chain 3B:





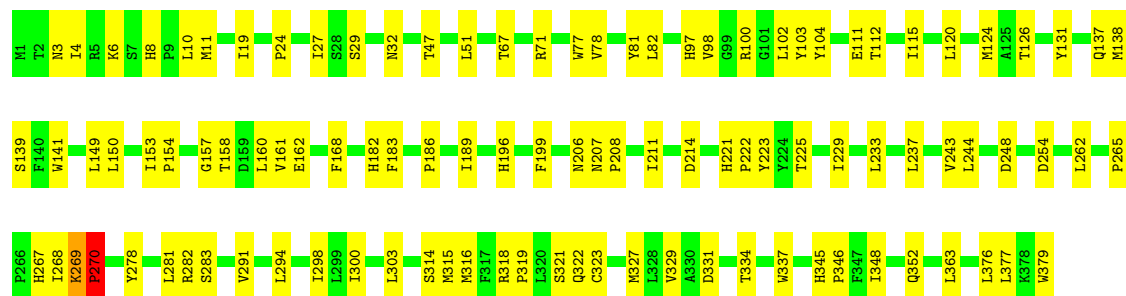
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 30: 73% 19% 8%



- Molecule 47: Cytochrome b

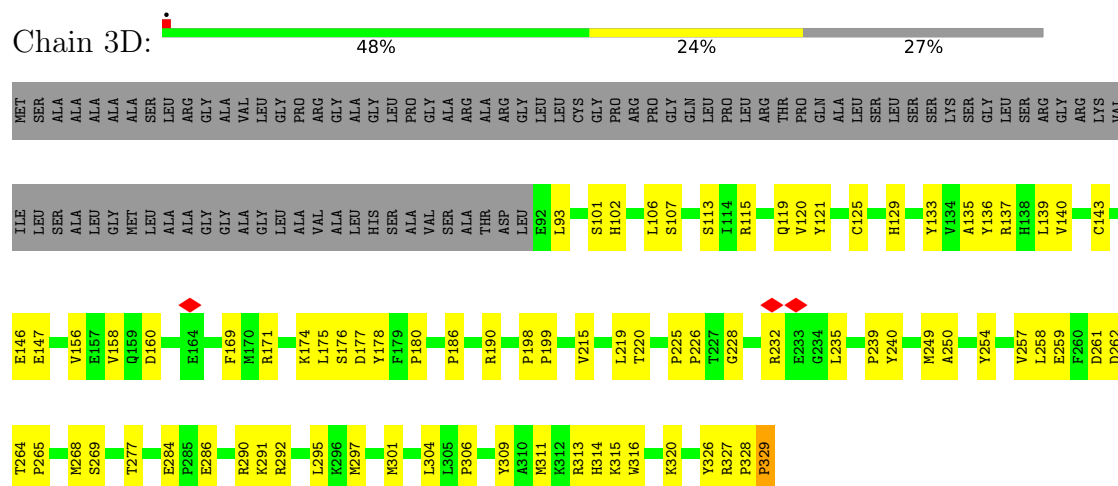
Chain 3C: 73% 27%



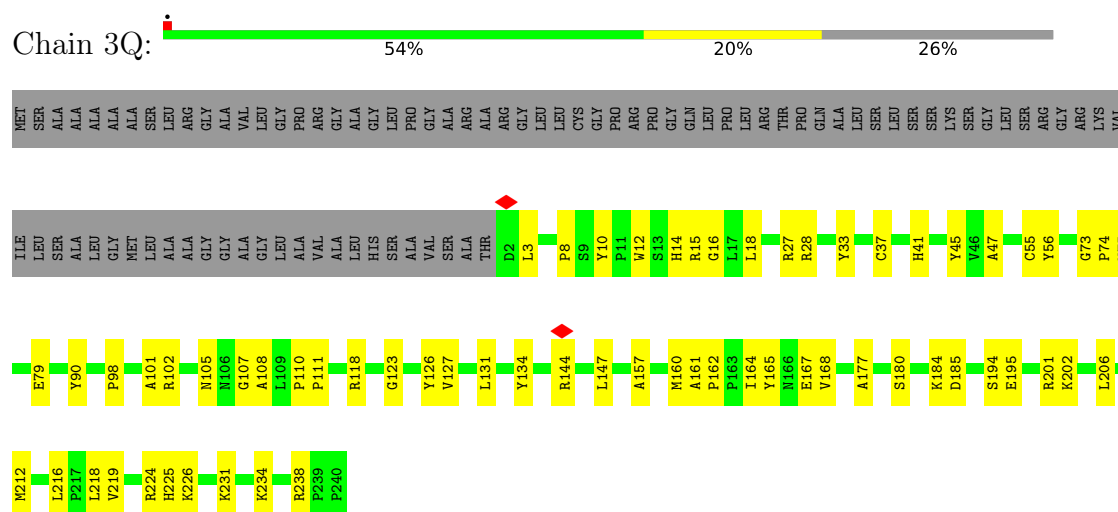
- Molecule 47: Cytochrome b

Chain 3P: 75% 25%

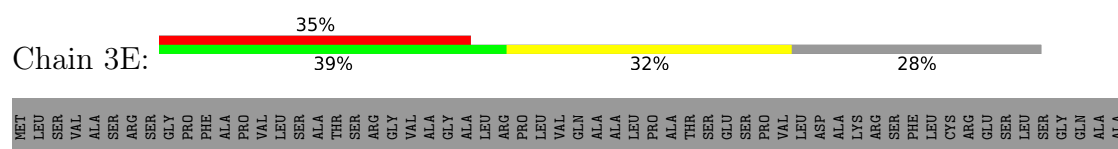
- Molecule 48: Cytochrome c1, heme protein, mitochondrial

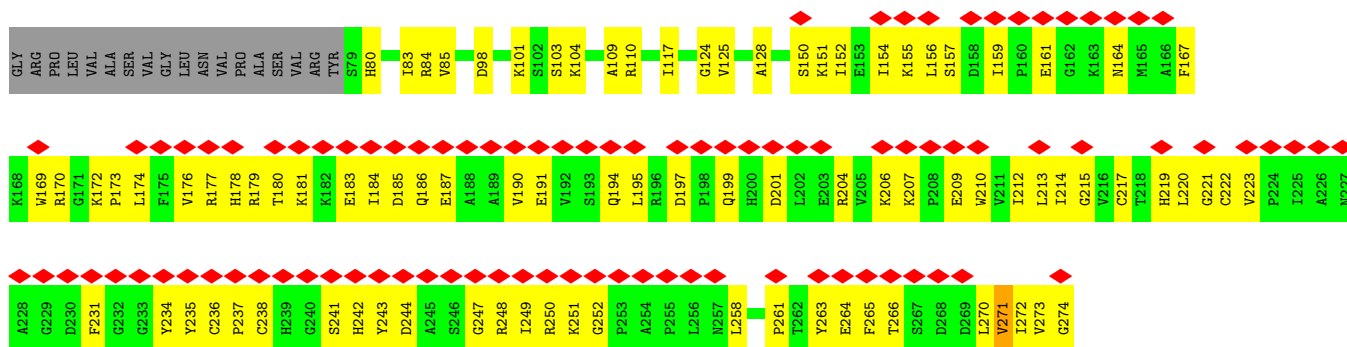


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

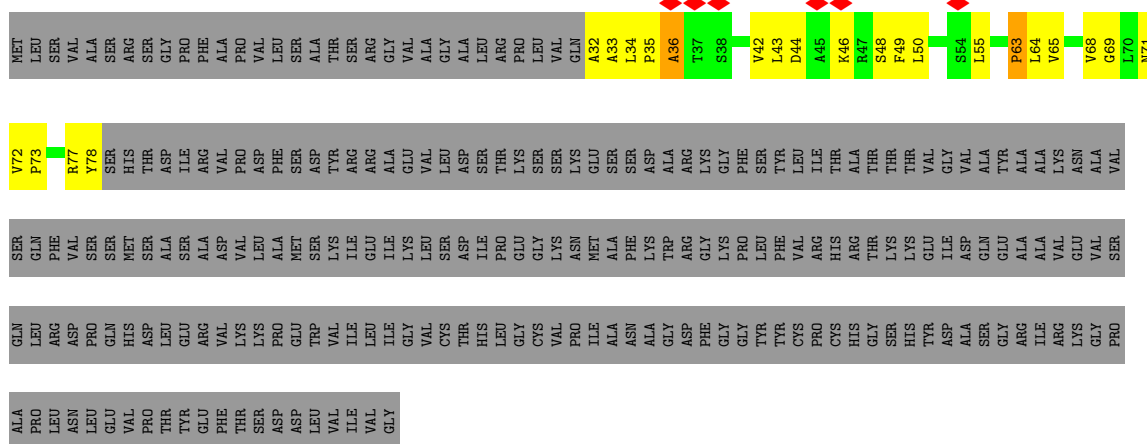


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

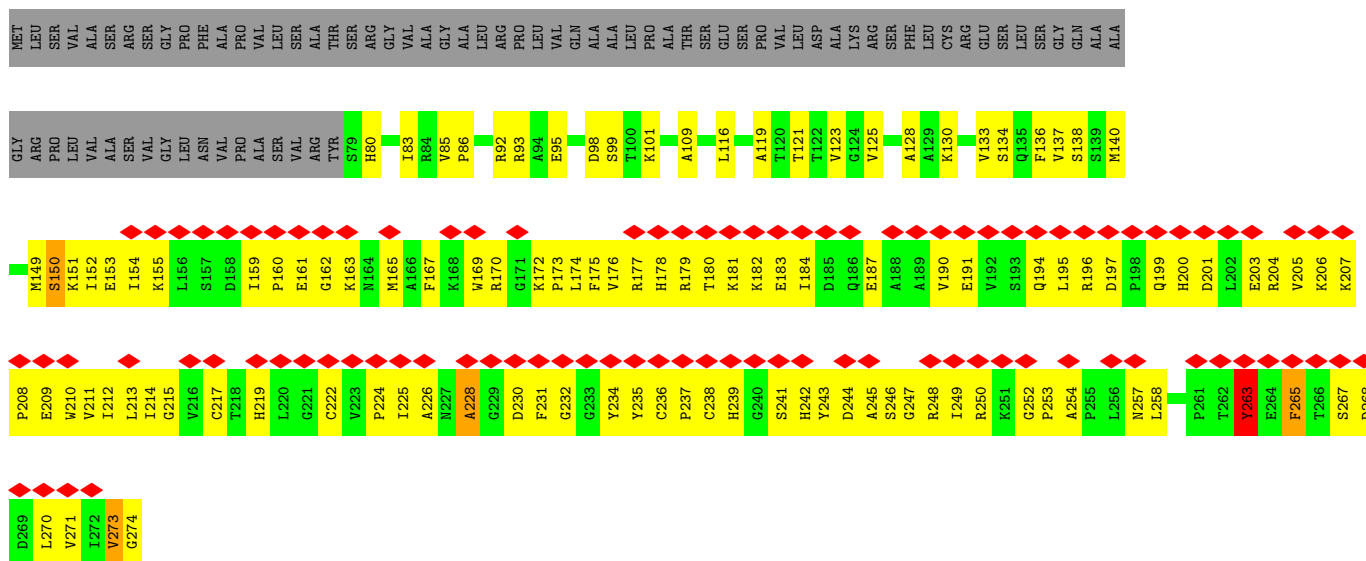




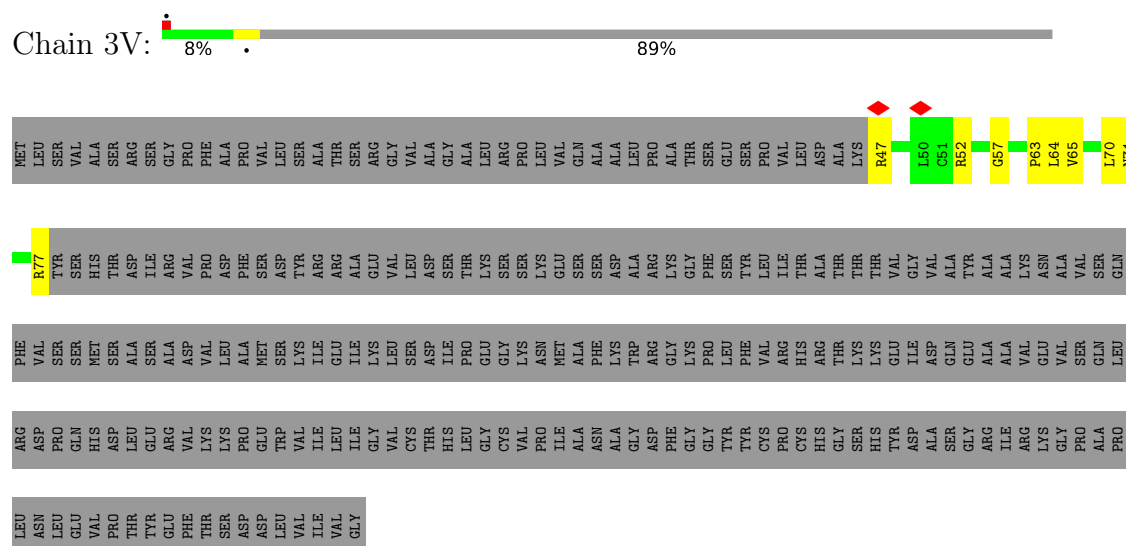
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



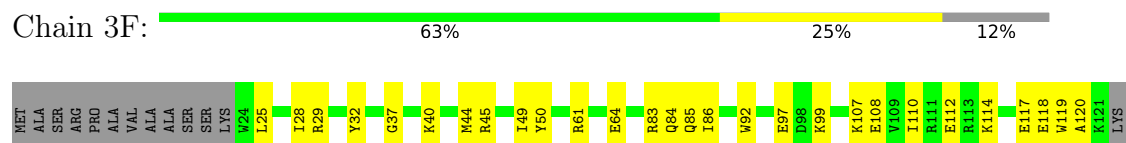
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



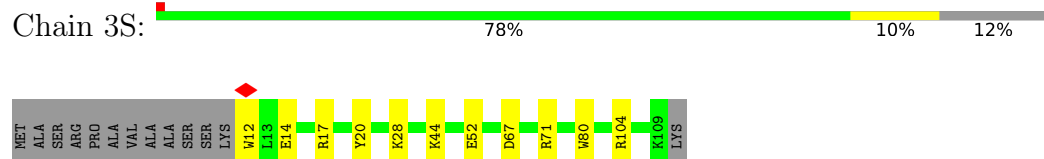
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



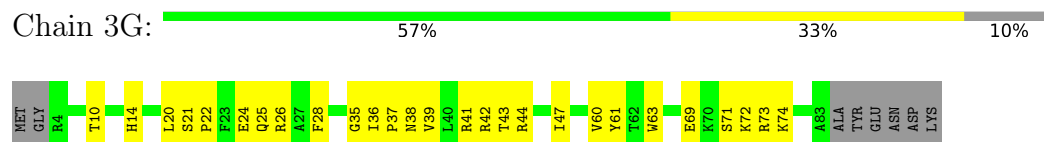
- Molecule 50: Cytochrome b-c1 complex subunit 7



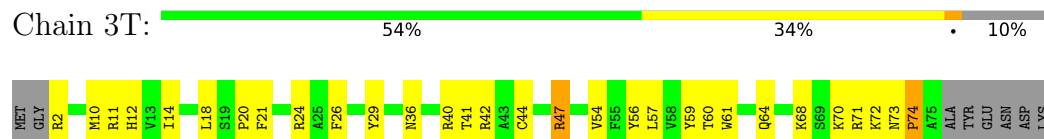
- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 51: Cytochrome b-c1 complex subunit 8

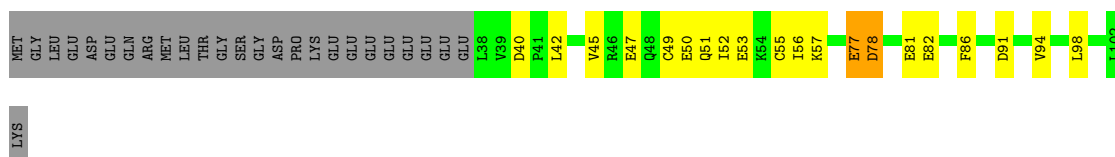


- Molecule 51: Cytochrome b-c1 complex subunit 8



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





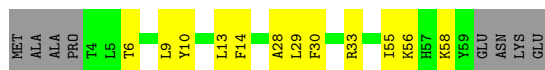
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



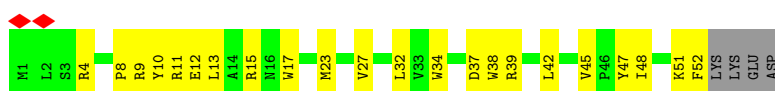
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



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



- Molecule 54: Cytochrome b-c1 complex subunit 10

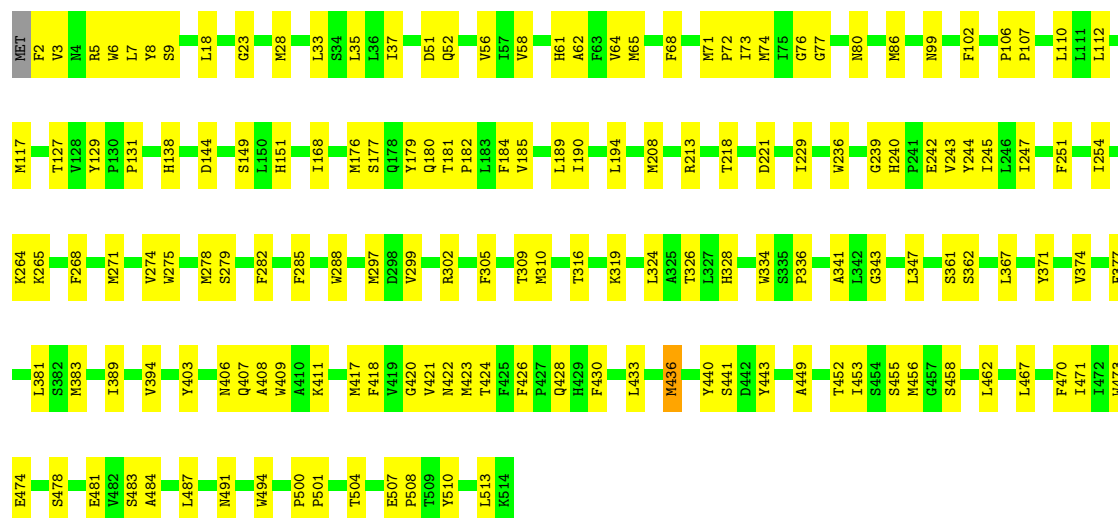


- Molecule 54: Cytochrome b-c1 complex subunit 10

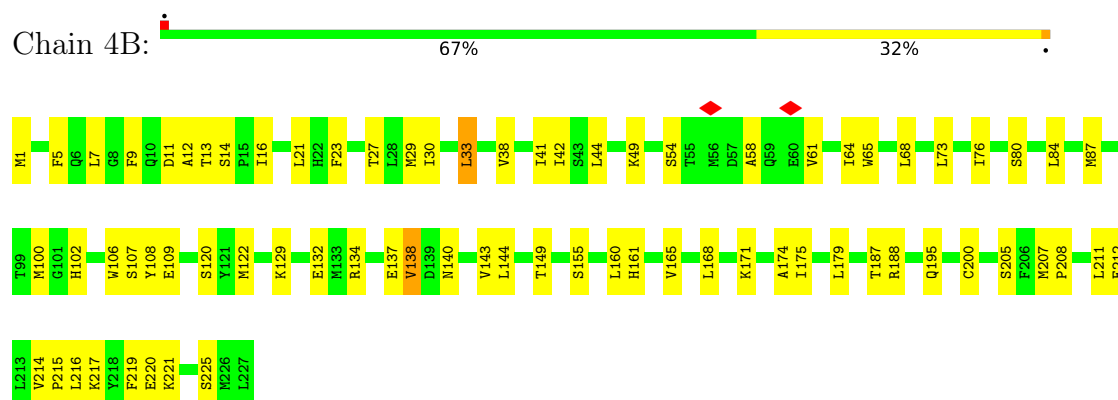


- Molecule 55: Cytochrome c oxidase subunit 1

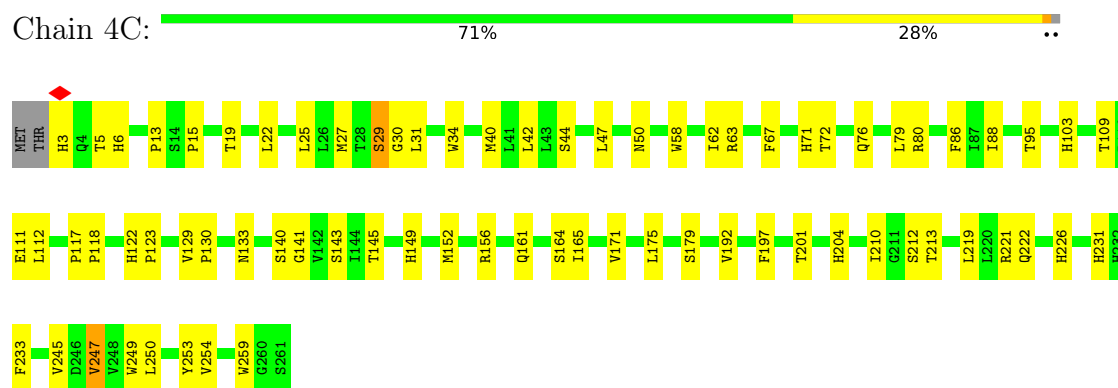




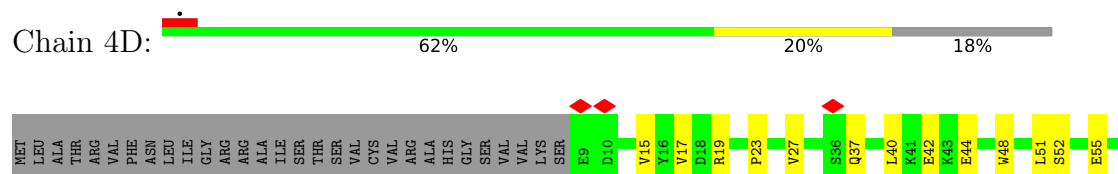
• Molecule 56: Cytochrome c oxidase subunit 2



• Molecule 57: Cytochrome c oxidase subunit 3

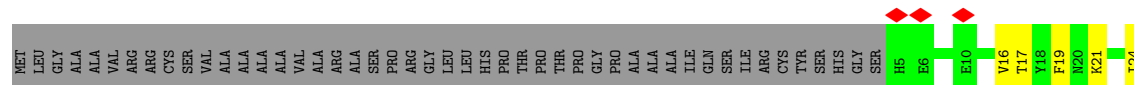


• Molecule 58: Cytochrome c oxidase subunit 4

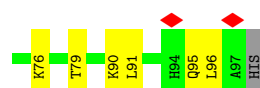
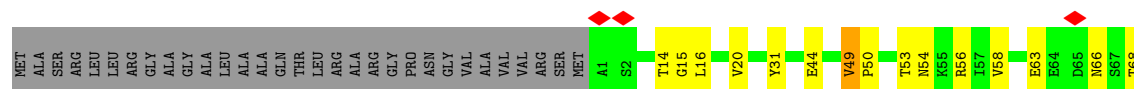




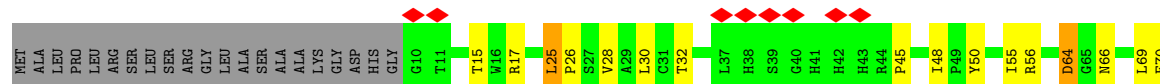
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



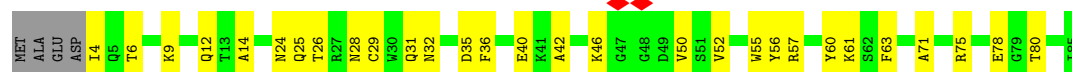
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 61: Cytochrome c oxidase subunit 6A2



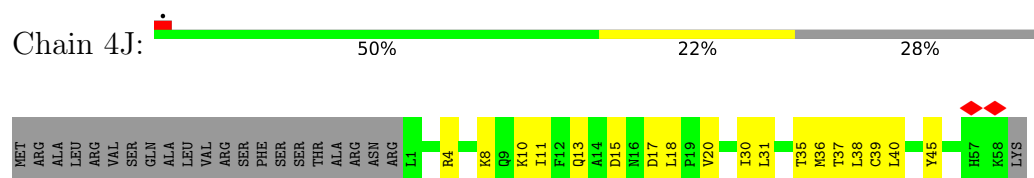
- Molecule 62: Cytochrome c oxidase subunit 6B1



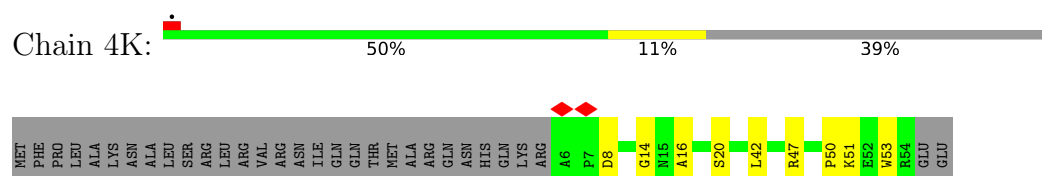
- Molecule 63: Cytochrome c oxidase subunit 6C



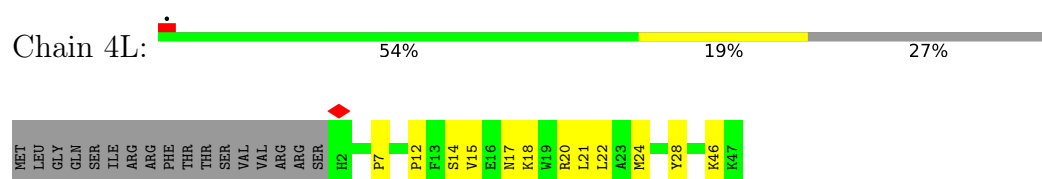
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



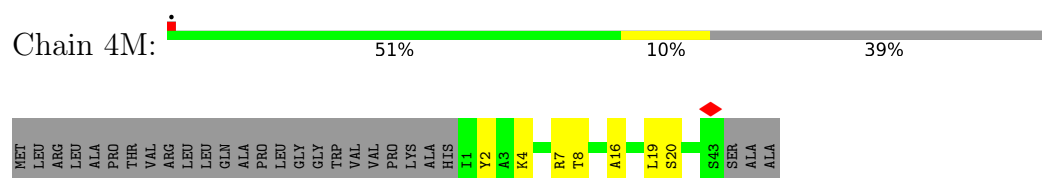
- Molecule 65: Cytochrome c oxidase subunit 7B



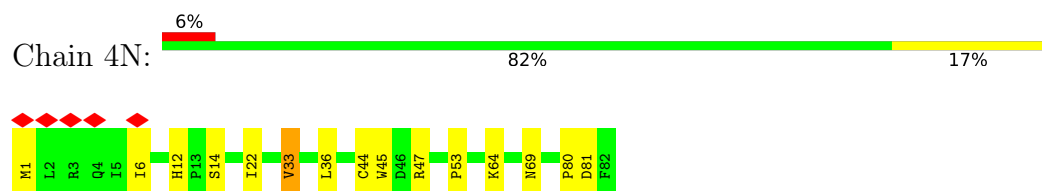
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.632	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	370.296, 370.296, 370.296	wwPDB
Map dimensions	888, 888, 888	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.417, 0.417, 0.417	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.16	0/930	0.47	0/1271
2	1B	0.15	0/1273	0.39	0/1722
3	1C	0.14	0/1791	0.36	0/2439
4	1D	0.29	2/3545 (0.1%)	0.57	5/4806 (0.1%)
5	1E	0.17	0/1698	0.41	0/2311
6	1F	0.29	1/3401 (0.0%)	0.55	7/4595 (0.2%)
7	1G	0.14	0/5451	0.38	1/7387 (0.0%)
8	1H	0.18	0/2566	0.50	4/3509 (0.1%)
9	1I	0.14	0/1443	0.35	0/1952
10	1J	0.19	0/1364	0.56	1/1850 (0.1%)
11	1K	0.17	0/751	0.45	0/1018
12	1L	0.16	0/4939	0.40	0/6718
13	1M	0.16	0/3713	0.40	0/5063
14	1N	0.17	0/2765	0.40	0/3758
15	1O	0.16	0/2650	0.43	0/3588
16	1P	0.16	0/2828	0.37	0/3834
17	1Q	0.14	0/1070	0.35	0/1446
18	1R	0.12	0/755	0.32	0/1018
19	1S	0.18	0/711	0.40	0/956
20	1T	0.14	0/701	0.36	0/946
20	1U	0.13	0/706	0.33	0/954
21	1V	0.14	0/946	0.34	0/1281
22	1W	0.14	0/995	0.34	0/1340
23	1X	0.15	0/1436	0.39	0/1938
24	1Y	0.23	0/1037	0.47	3/1404 (0.2%)
25	1Z	0.17	0/1199	0.37	0/1617
26	1a	0.15	0/577	0.34	0/777
27	1b	1.10	3/664 (0.5%)	1.34	6/912 (0.7%)
28	1c	0.13	0/430	0.35	0/581
29	1d	0.15	0/1016	0.34	0/1374
30	1e	0.17	0/836	0.40	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	1f	0.16	0/499	0.42	0/673
32	1g	0.16	0/858	0.45	0/1165
33	1h	0.16	0/1184	0.43	0/1603
34	1i	0.14	0/1138	0.36	0/1551
35	1j	0.14	0/627	0.46	2/858 (0.2%)
36	1k	0.13	0/668	0.32	0/903
37	1l	0.35	1/1365 (0.1%)	0.67	4/1867 (0.2%)
38	1m	0.15	0/1092	0.39	0/1481
39	1n	0.15	0/1549	0.36	0/2098
40	1o	0.15	0/1069	0.38	0/1430
41	1p	0.14	0/1481	0.36	0/1997
42	1q	0.13	0/1253	0.36	1/1704 (0.1%)
43	1r	0.14	0/777	0.37	0/1051
44	1s	0.15	0/394	0.37	0/533
45	3A	0.20	0/3481	0.45	0/4722
45	3N	0.21	0/3496	0.44	1/4723 (0.0%)
46	3B	0.20	0/3190	0.44	0/4317
46	3O	0.21	0/3175	0.46	0/4292
47	3C	0.57	4/3123 (0.1%)	0.77	7/4269 (0.2%)
47	3P	0.20	0/3122	0.42	0/4269
48	3D	0.83	8/1946 (0.4%)	1.03	13/2641 (0.5%)
48	3Q	0.57	4/1962 (0.2%)	0.78	8/2663 (0.3%)
49	3E	0.23	0/1551	0.52	0/2098
49	3I	1.13	2/342 (0.6%)	1.71	7/465 (1.5%)
49	3R	0.35	0/1551	0.55	0/2098
49	3V	0.18	0/225	0.37	0/303
50	3F	0.21	0/888	0.43	0/1193
50	3S	0.19	0/888	0.36	0/1193
51	3G	0.23	0/649	0.49	0/878
51	3T	1.14	5/649 (0.8%)	1.38	7/878 (0.8%)
52	3H	0.26	0/539	0.84	2/724 (0.3%)
52	3U	0.31	0/539	0.57	0/724
53	3J	0.65	0/476	0.69	1/641 (0.2%)
53	3W	0.21	0/476	0.42	0/641
54	3X	0.20	0/445	0.43	0/608
54	3Y	0.20	0/437	0.44	0/598
55	4A	0.25	2/4165 (0.0%)	0.53	4/5691 (0.1%)
56	4B	0.13	0/1866	0.33	0/2544
57	4C	0.11	0/2179	0.26	0/2981
58	4D	0.10	0/1197	0.27	0/1617
59	4E	0.12	0/871	0.33	0/1182
60	4F	0.12	0/749	0.32	0/1016
61	4G	0.10	0/644	0.28	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
62	4H	0.12	0/708	0.34	0/956
63	4I	0.10	0/563	0.24	0/748
64	4J	0.10	0/466	0.23	0/631
65	4K	0.11	0/396	0.30	0/543
66	4L	0.11	0/394	0.28	0/528
67	4M	0.10	0/349	0.24	0/477
68	4N	0.12	0/680	0.39	0/921
All	All	0.28	32/116518 (0.0%)	0.49	84/158051 (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
6	1F	0	2
8	1H	0	1
49	3R	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	3D	265	PRO	CG-CD	-22.21	0.75	1.50
51	3T	74	PRO	CG-CD	-20.96	0.79	1.50
27	1b	63	PRO	CB-CG	20.95	2.54	1.49
47	3C	270	PRO	CB-CG	19.89	2.49	1.49
48	3Q	74	PRO	CG-CD	-18.99	0.86	1.50

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3C	270	PRO	CB-CG-CD	-31.05	6.74	106.10
27	1b	63	PRO	CB-CG-CD	-30.88	7.28	106.10
48	3Q	74	PRO	N-CD-CG	-23.27	68.30	103.20
48	3D	329	PRO	CB-CG-CD	23.08	179.96	106.10
51	3T	74	PRO	N-CD-CG	-22.38	69.62	103.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	41	0
2	1B	1242	0	1249	53	0
3	1C	1740	0	1691	42	0
4	1D	3452	0	3389	89	0
5	1E	1658	0	1662	56	0
6	1F	3325	0	3288	125	0
7	1G	5362	0	5388	125	0
8	1H	2504	0	2602	96	0
9	1I	1412	0	1366	47	0
10	1J	1329	0	1326	54	0
11	1K	750	0	798	35	0
12	1L	4818	0	4956	189	0
13	1M	3632	0	3836	150	0
14	1N	2712	0	2871	95	0
15	1O	2590	0	2556	99	0
16	1P	2751	0	2776	77	0
17	1Q	1047	0	1042	26	0
18	1R	741	0	704	11	0
19	1S	700	0	719	26	0
20	1T	689	0	687	22	0
20	1U	694	0	691	15	0
21	1V	927	0	972	26	0
22	1W	971	0	975	15	0
23	1X	1398	0	1378	46	0
24	1Y	1016	0	1020	36	0
25	1Z	1168	0	1161	45	0
26	1a	562	0	557	19	0
27	1b	643	0	645	25	0
28	1c	417	0	425	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1d	985	0	978	41	0
30	1e	816	0	823	39	0
31	1f	487	0	498	14	0
32	1g	835	0	795	33	0
33	1h	1151	0	1164	46	0
34	1i	1100	0	1107	41	0
35	1j	601	0	546	17	0
36	1k	649	0	626	14	0
37	1l	1310	0	1204	46	0
38	1m	1062	0	1075	44	0
39	1n	1495	0	1432	67	0
40	1o	1045	0	1016	39	0
41	1p	1449	0	1416	47	0
42	1q	1212	0	1174	28	0
43	1r	759	0	783	21	0
44	1s	382	0	351	13	0
45	3A	3411	0	3308	86	0
45	3N	3424	0	3350	131	0
46	3B	3138	0	3116	78	0
46	3O	3124	0	3108	74	0
47	3C	3025	0	3090	124	0
47	3P	3024	0	3090	85	0
48	3D	1888	0	1834	71	0
48	3Q	1904	0	1849	58	0
49	3E	1518	0	1498	87	0
49	3I	337	0	345	29	0
49	3R	1518	0	1498	160	0
49	3V	223	0	233	11	0
50	3F	868	0	857	28	0
50	3S	868	0	857	9	0
51	3G	628	0	634	26	0
51	3T	628	0	634	37	0
52	3H	533	0	513	17	0
52	3U	533	0	513	26	0
53	3J	464	0	467	14	0
53	3W	464	0	467	10	0
54	3X	429	0	430	25	0
54	3Y	421	0	418	13	0
55	4A	4025	0	3999	126	0
56	4B	1829	0	1837	65	0
57	4C	2096	0	2027	60	0
58	4D	1163	0	1143	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	4E	852	0	845	19	0
60	4F	734	0	718	14	0
61	4G	617	0	585	16	0
62	4H	687	0	645	20	0
63	4I	550	0	560	9	0
64	4J	456	0	455	34	0
65	4K	383	0	366	9	0
66	4L	381	0	380	10	0
67	4M	338	0	345	9	0
68	4N	660	0	664	13	0
69	1A	47	0	71	3	0
69	1J	44	0	62	6	0
69	1L	122	0	172	9	0
69	1M	146	0	223	27	0
69	1N	82	0	115	6	0
69	1Y	138	0	178	15	0
69	1d	48	0	73	12	0
69	1j	44	0	65	1	0
69	3A	59	0	66	13	0
69	3C	69	0	86	13	0
69	3D	33	0	40	5	0
69	3G	29	0	32	3	0
69	3N	58	0	62	12	0
69	3P	33	0	40	5	0
69	3R	47	0	71	8	0
69	3Y	30	0	34	1	0
70	1A	35	0	44	1	0
70	1B	94	0	136	11	0
70	1H	48	0	73	6	0
70	1I	54	0	88	4	0
70	1M	44	0	65	8	0
70	1P	33	0	40	0	0
70	1Y	35	0	44	4	0
70	1Z	44	0	62	5	0
70	1h	47	0	71	2	0
70	1m	46	0	66	9	0
70	1q	49	0	75	10	0
70	3E	47	0	68	7	0
70	3R	45	0	64	10	0
70	3X	29	0	32	4	0
71	1B	8	0	0	2	0
71	1F	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	1G	16	0	0	1	0
71	1I	16	0	0	0	0
72	1E	4	0	0	1	0
72	1G	4	0	0	1	0
72	3E	4	0	0	2	0
72	3R	4	0	0	5	0
73	1F	31	0	19	2	0
74	1G	1	0	0	0	0
75	1L	76	0	99	4	0
75	1N	62	0	68	4	0
75	1X	86	0	125	13	0
75	1d	65	0	77	9	0
75	1h	80	0	104	10	0
75	1q	61	0	66	6	0
75	3A	58	0	60	13	0
75	3G	108	0	104	8	0
75	3N	43	0	30	8	0
75	3P	56	0	56	6	0
75	3T	57	0	58	6	0
75	4B	100	0	156	9	0
75	4C	100	0	156	14	0
75	4D	100	0	156	20	0
76	1O	32	0	12	2	0
77	1O	1	0	0	0	0
77	4A	1	0	0	0	0
78	1P	48	0	26	1	0
79	1R	1	0	0	0	0
79	4F	1	0	0	0	0
80	1T	37	0	0	1	0
80	1n	37	0	0	1	0
81	1h	11	0	12	4	0
82	1l	15	0	27	0	0
83	3C	86	0	60	7	0
83	3P	86	0	60	4	0
84	3D	42	0	32	2	0
84	3Q	43	0	32	2	0
85	4A	153	0	228	22	0
85	4B	51	0	76	13	0
85	4C	306	0	456	39	0
85	4G	51	0	76	5	0
85	4J	51	0	76	7	0
85	4K	51	0	76	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	4L	51	0	76	10	0
85	4M	51	0	76	5	0
86	4A	120	0	108	7	0
87	4A	1	0	0	0	0
88	4A	1	0	0	0	0
89	4B	2	0	0	2	0
90	4B	52	0	80	7	0
91	4G	105	0	149	9	0
92	4H	5	0	0	0	0
93	1A	21	0	0	6	0
93	1B	53	0	0	4	0
93	1C	96	0	0	7	0
93	1D	138	0	0	3	0
93	1E	55	0	0	7	0
93	1F	113	0	0	17	0
93	1G	255	0	0	8	0
93	1H	80	0	0	8	0
93	1I	75	0	0	3	0
93	1J	56	0	0	2	0
93	1K	38	0	0	7	0
93	1L	228	0	0	23	0
93	1M	201	0	0	14	0
93	1N	154	0	0	10	0
93	1O	150	0	0	21	0
93	1P	118	0	0	14	0
93	1Q	63	0	0	2	0
93	1R	41	0	0	2	0
93	1S	56	0	0	6	0
93	1T	12	0	0	1	0
93	1U	26	0	0	2	0
93	1V	20	0	0	2	0
93	1W	37	0	0	1	0
93	1X	106	0	0	8	0
93	1Y	39	0	0	1	0
93	1Z	83	0	0	6	0
93	1a	30	0	0	3	0
93	1b	35	0	0	3	0
93	1c	23	0	0	4	0
93	1d	95	0	0	2	0
93	1e	91	0	0	17	0
93	1f	43	0	0	1	0
93	1g	76	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	1h	116	0	0	13	0
93	1i	48	0	0	6	0
93	1j	37	0	0	3	0
93	1k	35	0	0	4	0
93	1l	97	0	0	9	0
93	1m	78	0	0	3	0
93	1n	122	0	0	7	0
93	1o	101	0	0	13	0
93	1p	141	0	0	15	0
93	1q	47	0	0	1	0
93	1r	25	0	0	0	0
93	1s	15	0	0	0	0
93	3A	184	0	0	14	0
93	3B	110	0	0	5	0
93	3C	222	0	0	28	0
93	3D	131	0	0	7	0
93	3E	45	0	0	1	0
93	3F	115	0	0	7	0
93	3G	78	0	0	7	0
93	3H	26	0	0	0	0
93	3I	5	0	0	0	0
93	3J	27	0	0	4	0
93	3N	231	0	0	26	0
93	3O	184	0	0	16	0
93	3P	152	0	0	20	0
93	3Q	98	0	0	5	0
93	3R	47	0	0	6	0
93	3S	71	0	0	3	0
93	3T	40	0	0	9	0
93	3U	110	0	0	10	0
93	3V	7	0	0	2	0
93	3W	31	0	0	2	0
93	3X	25	0	0	3	0
93	3Y	16	0	0	0	0
93	4A	110	0	0	6	0
93	4B	115	0	0	8	0
93	4C	103	0	0	3	0
93	4D	81	0	0	4	0
93	4E	55	0	0	1	0
93	4F	67	0	0	1	0
93	4G	39	0	0	1	0
93	4H	43	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	4I	25	0	0	0	0
93	4J	34	0	0	1	0
93	4K	27	0	0	0	0
93	4L	23	0	0	2	0
93	4M	28	0	0	0	0
93	4N	53	0	0	0	0
All	All	124291	0	118736	3520	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 15.

The worst 5 of 3520 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)
12:1L:504:LEU:CD1	64:4J:30:ILE:HD11	1.26	1.58
47:3C:270:PRO:CG	47:3C:270:PRO:N	1.82	1.40
27:1b:63:PRO:N	27:1b:63:PRO:CG	1.85	1.39
93:1n:353:HOH:O	64:4J:15:ASP:HB3	1.26	1.29
51:3T:59:TYR:HE2	93:3T:226:HOH:O	0.98	1.28

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	105 (93%)	6 (5%)	2 (2%)	6	3
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	204 (99%)	3 (1%)	0	100	100
4	1D	427/476 (90%)	408 (96%)	19 (4%)	0	100	100
5	1E	212/249 (85%)	198 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	1F	430/464 (93%)	410 (95%)	18 (4%)	2 (0%)	24	22
7	1G	697/727 (96%)	672 (96%)	22 (3%)	3 (0%)	30	28
8	1H	316/318 (99%)	297 (94%)	18 (6%)	1 (0%)	36	36
9	1I	174/239 (73%)	169 (97%)	5 (3%)	0	100	100
10	1J	172/175 (98%)	157 (91%)	13 (8%)	2 (1%)	10	7
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	1L	604/606 (100%)	572 (95%)	30 (5%)	2 (0%)	36	36
13	1M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	43	44
14	1N	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	36	36
15	1O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
17	1Q	127/175 (73%)	120 (94%)	7 (6%)	0	100	100
18	1R	94/123 (76%)	88 (94%)	6 (6%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	83 (100%)	0	0	100	100
20	1U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
22	1W	113/128 (88%)	109 (96%)	4 (4%)	0	100	100
23	1X	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	21	18
24	1Y	137/141 (97%)	136 (99%)	1 (1%)	0	100	100
25	1Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	47 (100%)	0	0	100	100
29	1d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	87 (89%)	11 (11%)	0	100	100
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	1i	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	1m	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	7 (4%)	0	100	100
40	1o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	1r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
45	3A	436/480 (91%)	423 (97%)	12 (3%)	1 (0%)	43	44
45	3N	444/480 (92%)	424 (96%)	18 (4%)	2 (0%)	24	22
46	3B	414/453 (91%)	397 (96%)	17 (4%)	0	100	100
46	3O	413/453 (91%)	402 (97%)	10 (2%)	1 (0%)	43	44
47	3C	377/379 (100%)	370 (98%)	6 (2%)	1 (0%)	36	36
47	3P	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
48	3D	235/325 (72%)	232 (99%)	3 (1%)	0	100	100
48	3Q	237/325 (73%)	228 (96%)	9 (4%)	0	100	100
49	3E	194/274 (71%)	169 (87%)	24 (12%)	1 (0%)	24	22
49	3I	45/274 (16%)	40 (89%)	4 (9%)	1 (2%)	5	2
49	3R	194/274 (71%)	167 (86%)	23 (12%)	4 (2%)	5	2
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	72/82 (88%)	70 (97%)	2 (3%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	0	1 (1%)	9	5
52	3H	63/91 (69%)	61 (97%)	1 (2%)	1 (2%)	7	4
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/64 (84%)	51 (94%)	1 (2%)	2 (4%)	2	1
53	3W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
54	3X	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	4A	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
56	4B	225/227 (99%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
58	4D	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
60	4F	95/129 (74%)	94 (99%)	1 (1%)	0	100	100
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
65	4K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
66	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	6
All	All	14074/17005 (83%)	13535 (96%)	508 (4%)	31 (0%)	44	44

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1J	66	VAL
13	1M	82	SER
23	1X	28	ALA
47	3C	270	PRO
49	3E	271	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	93 (94%)	6 (6%)	17	15
2	1B	131/212 (62%)	122 (93%)	9 (7%)	14	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1C	190/227 (84%)	187 (98%)	3 (2%)	55	64
4	1D	371/405 (92%)	363 (98%)	8 (2%)	45	53
5	1E	183/207 (88%)	176 (96%)	7 (4%)	29	32
6	1F	346/368 (94%)	334 (96%)	12 (4%)	32	35
7	1G	588/610 (96%)	571 (97%)	17 (3%)	37	42
8	1H	274/274 (100%)	265 (97%)	9 (3%)	33	37
9	1I	151/201 (75%)	147 (97%)	4 (3%)	40	46
10	1J	140/141 (99%)	131 (94%)	9 (6%)	16	14
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	521 (97%)	18 (3%)	33	37
13	1M	408/408 (100%)	395 (97%)	13 (3%)	34	38
14	1N	310/310 (100%)	303 (98%)	7 (2%)	44	51
15	1O	283/307 (92%)	270 (95%)	13 (5%)	24	25
16	1P	296/323 (92%)	290 (98%)	6 (2%)	48	56
17	1Q	117/152 (77%)	110 (94%)	7 (6%)	17	15
18	1R	79/97 (81%)	77 (98%)	2 (2%)	42	48
19	1S	77/82 (94%)	73 (95%)	4 (5%)	21	20
20	1T	79/133 (59%)	77 (98%)	2 (2%)	42	48
20	1U	79/133 (59%)	73 (92%)	6 (8%)	12	9
21	1V	100/101 (99%)	99 (99%)	1 (1%)	68	76
22	1W	107/112 (96%)	106 (99%)	1 (1%)	70	78
23	1X	153/154 (99%)	150 (98%)	3 (2%)	48	56
24	1Y	101/102 (99%)	96 (95%)	5 (5%)	22	22
25	1Z	123/124 (99%)	119 (97%)	4 (3%)	33	37
26	1a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	65 (94%)	4 (6%)	18	16
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	12
29	1d	106/109 (97%)	102 (96%)	4 (4%)	29	32
30	1e	87/94 (93%)	85 (98%)	2 (2%)	44	51
31	1f	54/113 (48%)	52 (96%)	2 (4%)	30	33
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	1h	121/158 (77%)	118 (98%)	3 (2%)	42	48
34	1i	120/120 (100%)	118 (98%)	2 (2%)	53	62
35	1j	62/84 (74%)	59 (95%)	3 (5%)	23	23
36	1k	63/76 (83%)	62 (98%)	1 (2%)	55	64
37	1l	141/161 (88%)	138 (98%)	3 (2%)	47	54
38	1m	113/114 (99%)	111 (98%)	2 (2%)	51	60
39	1n	156/160 (98%)	151 (97%)	5 (3%)	34	38
40	1o	110/119 (92%)	104 (94%)	6 (6%)	19	18
41	1p	154/156 (99%)	150 (97%)	4 (3%)	40	46
42	1q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	84 (99%)	1 (1%)	63	72
44	1s	44/351 (12%)	40 (91%)	4 (9%)	9	6
45	3A	367/397 (92%)	365 (100%)	2 (0%)	81	88
45	3N	372/397 (94%)	369 (99%)	3 (1%)	73	81
46	3B	328/355 (92%)	327 (100%)	1 (0%)	86	91
46	3O	327/355 (92%)	326 (100%)	1 (0%)	86	91
47	3C	332/332 (100%)	332 (100%)	0	100	100
47	3P	332/332 (100%)	330 (99%)	2 (1%)	78	86
48	3D	202/258 (78%)	200 (99%)	2 (1%)	68	76
48	3Q	204/258 (79%)	204 (100%)	0	100	100
49	3E	166/225 (74%)	166 (100%)	0	100	100
49	3I	36/225 (16%)	36 (100%)	0	100	100
49	3R	166/225 (74%)	165 (99%)	1 (1%)	78	86
49	3V	24/225 (11%)	24 (100%)	0	100	100
50	3F	90/99 (91%)	90 (100%)	0	100	100
50	3S	90/99 (91%)	90 (100%)	0	100	100
51	3G	67/73 (92%)	67 (100%)	0	100	100
51	3T	67/73 (92%)	66 (98%)	1 (2%)	57	65
52	3H	62/85 (73%)	62 (100%)	0	100	100
52	3U	62/85 (73%)	62 (100%)	0	100	100
53	3J	46/52 (88%)	42 (91%)	4 (9%)	9	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	3W	46/52 (88%)	46 (100%)	0	100	100
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	41 (100%)	0	100	100
55	4A	425/425 (100%)	421 (99%)	4 (1%)	70	78
56	4B	210/210 (100%)	205 (98%)	5 (2%)	43	49
57	4C	223/225 (99%)	217 (97%)	6 (3%)	39	45
58	4D	124/149 (83%)	120 (97%)	4 (3%)	34	38
59	4E	92/124 (74%)	88 (96%)	4 (4%)	26	27
60	4F	80/101 (79%)	78 (98%)	2 (2%)	42	48
61	4G	65/80 (81%)	60 (92%)	5 (8%)	12	9
62	4H	73/76 (96%)	70 (96%)	3 (4%)	27	29
63	4I	54/61 (88%)	54 (100%)	0	100	100
64	4J	49/68 (72%)	48 (98%)	1 (2%)	48	56
65	4K	38/66 (58%)	38 (100%)	0	100	100
66	4L	39/55 (71%)	38 (97%)	1 (3%)	40	46
67	4M	37/57 (65%)	37 (100%)	0	100	100
68	4N	70/70 (100%)	66 (94%)	4 (6%)	18	17
All	All	12267/14333 (86%)	11985 (98%)	282 (2%)	44	51

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	3J	54	LYS
46	3O	211	VAL
58	4D	27	VAL
12	1L	517	SER
12	1L	491	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
33	1h	44	ASN
53	3W	57	HIS
45	3A	21	ASN
51	3T	64	GLN

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Mol	Chain	Res	Type
68	4N	69	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	FME	1K	1	11	8,9,10	0.53	0	8,9,11	0.98	1 (12%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.04	1 (12%)
56	FME	4B	1	56	8,9,10	0.95	0	8,9,11	0.91	0
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	1.08	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	0.91	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	0.96	1 (12%)
1	FME	1A	1	1	8,9,10	0.55	0	8,9,11	1.02	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
11	FME	1K	1	11	-	2/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
56	FME	4B	1	56	-	4/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	1A	1	1	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 7 are monoatomic - leaving 102 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
75	CDL	3T	101	-	56,56,99	0.36	0	62,68,111	0.71	2 (3%)
72	FES	3E	301	49	0,4,4	-	-	-		
70	PC1	1Z	201	-	43,43,53	0.28	0	49,51,61	0.33	0
73	FMN	1F	501	-	33,33,33	0.62	0	48,50,50	0.66	1 (2%)
85	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.36	0
85	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.33	0
69	3PE	3Y	101	-	29,29,50	0.36	0	32,34,55	0.46	0
80	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.12	1 (2%)
75	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.41	1 (0%)
71	SF4	1G	802	7	0,12,12	-	-	-		
85	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.36	0
75	CDL	1q	202	-	60,60,99	0.34	0	66,72,111	0.43	0
72	FES	3R	301	49	0,4,4	-	-	-		
85	PGV	4L	101	-	50,50,50	0.30	0	53,56,56	0.38	0
85	PGV	4A	601	-	50,50,50	0.27	0	53,56,56	0.32	0
83	HEM	3C	502	47	50,50,50	1.59	9 (18%)	67,82,82	1.56	11 (16%)
69	3PE	1N	901	-	48,48,50	0.32	0	51,53,55	0.41	0
69	3PE	1L	704	-	30,30,50	0.34	0	33,35,55	0.69	1 (3%)
69	3PE	1N	903	-	32,32,50	0.33	0	35,37,55	0.44	0
75	CDL	1d	202	-	64,64,99	0.33	0	70,76,111	0.41	0
75	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.55	0
85	PGV	4C	305	-	50,50,50	0.30	0	53,56,56	0.57	1 (1%)
69	3PE	1Y	202	-	39,39,50	0.29	0	42,44,55	0.40	0
86	HEA	4A	605	55	67,67,67	2.46	25 (37%)	81,103,103	2.49	34 (41%)
75	CDL	3N	502	-	42,42,99	0.40	0	48,54,111	0.62	0
71	SF4	1B	201	2	0,12,12	-	-	-		
85	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.31	0
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.39	0
70	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.47	0
85	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.32	0
71	SF4	1G	801	7	0,12,12	-	-	-		
71	SF4	1I	202	9	0,12,12	-	-	-		
75	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	HEA	4A	604	55	67,67,67	2.45	25 (37%)	81,103,103	2.52	33 (40%)
75	CDL	3G	102	-	51,51,99	0.36	0	57,63,111	0.66	1 (1%)
84	HEC	3Q	501	48	46,50,50	2.57	25 (54%)	58,82,82	2.14	18 (31%)
69	3PE	1L	701	-	45,45,50	0.31	0	48,50,55	0.47	0
69	3PE	3A	503	-	31,31,50	0.35	0	34,36,55	0.42	0
70	PC1	3E	302	-	46,46,53	0.28	0	52,54,61	0.39	0
69	3PE	3G	101	-	28,28,50	0.35	0	31,33,55	0.44	0
70	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.38	0
89	CUA	4B	303	56	0,1,1	-	-	-	-	-
70	PC1	1M	503	-	43,43,53	0.32	0	49,51,61	0.37	0
76	GTP	1O	401	77	33,34,34	0.58	0	50,54,54	0.65	0
85	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
75	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.58	1 (1%)
69	3PE	1M	502	-	50,50,50	0.28	0	53,55,55	0.40	0
70	PC1	3X	101	-	28,28,53	0.37	0	34,36,61	0.64	1 (2%)
69	3PE	3N	501	-	31,31,50	0.35	0	34,36,55	0.74	1 (2%)
85	PGV	4J	101	-	50,50,50	0.29	0	53,56,56	0.36	0
69	3PE	3C	504	-	33,33,50	0.36	0	36,38,55	0.53	0
70	PC1	1H	401	-	47,47,53	0.29	0	53,55,61	0.38	0
75	CDL	3G	103	-	55,55,99	0.35	0	61,67,111	0.48	0
69	3PE	1J	201	-	43,43,50	0.29	0	46,48,55	0.39	0
85	PGV	4C	302	-	50,50,50	0.30	0	53,56,56	0.68	1 (1%)
85	PGV	4K	101	-	50,50,50	0.30	0	53,56,56	0.33	0
69	3PE	1L	703	-	44,44,50	0.28	0	47,49,55	0.48	0
75	CDL	1X	201	-	85,85,99	0.28	0	91,97,111	0.40	0
69	3PE	3D	502	-	32,32,50	0.36	0	35,37,55	0.52	0
84	HEC	3D	501	48	44,49,50	2.61	25 (56%)	56,80,82	2.13	17 (30%)
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.31	0
91	PEK	4G	103	-	51,51,52	0.48	0	54,56,57	0.46	0
69	3PE	1Y	203	-	29,29,50	0.34	0	32,34,55	0.71	1 (3%)
70	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.33	0
69	3PE	1Y	205	-	40,40,50	0.30	0	43,45,55	0.68	1 (2%)
70	PC1	3R	303	-	44,44,53	0.30	0	50,52,61	0.42	0
69	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.54	0
69	3PE	1d	201	-	47,47,50	0.29	0	50,52,55	0.44	0
69	3PE	3P	503	-	32,32,50	0.33	0	35,37,55	0.56	0
70	PC1	1A	202	-	34,34,53	0.32	0	40,42,61	0.40	0
69	3PE	3R	302	-	46,46,50	0.29	0	49,51,55	0.34	0
71	SF4	1I	203	9	0,12,12	-	-	-	-	-
71	SF4	1F	502	6	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	1M	504	-	49,49,50	0.27	0	52,54,55	0.36	0
75	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.31	0
85	PGV	4A	603	-	50,50,50	0.30	0	53,56,56	0.35	0
83	HEM	3C	501	47	50,50,50	1.58	8 (16%)	67,82,82	1.62	10 (14%)
92	PO4	4H	101	-	4,4,4	0.97	0	6,6,6	0.44	0
70	PC1	1B	203	-	47,47,53	0.28	0	53,55,61	0.45	0
83	HEM	3P	501	47	50,50,50	1.58	8 (16%)	67,82,82	1.60	12 (17%)
83	HEM	3P	502	47	50,50,50	1.59	8 (16%)	67,82,82	1.60	15 (22%)
70	PC1	1m	201	-	45,45,53	0.30	0	51,53,61	1.10	3 (5%)
82	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.29	0
69	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.37	0
69	3PE	3C	503	-	34,34,50	0.36	0	37,39,55	0.55	0
69	3PE	3A	502	-	26,26,50	0.37	0	29,31,55	0.68	1 (3%)
72	FES	1G	803	7	0,4,4	-	-	-	-	-
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.34	0
80	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.10	1 (2%)
81	AME	1h	201	-	9,10,11	0.52	0	9,11,13	1.10	1 (11%)
70	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.55	1 (1%)
91	PEK	4G	102	-	52,52,52	0.47	0	55,57,57	0.46	0
85	PGV	4B	301	-	50,50,50	0.28	0	53,56,56	0.34	0
70	PC1	1Y	201	-	34,34,53	0.33	0	40,42,61	0.43	0
75	CDL	3P	504	-	55,55,99	0.37	0	61,67,111	0.61	1 (1%)
75	CDL	1h	202	-	79,79,99	0.30	0	85,91,111	0.45	0
90	PSC	4B	304	-	51,51,51	0.48	0	57,59,59	0.44	0
78	NDP	1P	402	-	51,52,52	0.51	0	71,80,80	0.81	2 (2%)
72	FES	1E	301	5	0,4,4	-	-	-	-	-
85	PGV	4C	304	-	50,50,50	0.30	0	53,56,56	0.39	0
69	3PE	1Y	204	-	26,26,50	0.36	0	29,31,55	0.43	0
69	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	3T	101	-	-	13/67/67/110	-
72	FES	3E	301	49	-	-	0/1/1/1
70	PC1	1Z	201	-	-	1/47/47/57	-
73	FMN	1F	501	-	-	1/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	PGV	4A	602	-	-	6/55/55/55	-
85	PGV	4C	303	-	-	10/55/55/55	-
69	3PE	3Y	101	-	-	2/33/33/54	-
80	EHZ	1n	201	-	-	3/42/44/45	-
75	CDL	4C	306	-	-	24/110/110/110	-
71	SF4	1G	802	7	-	-	0/6/5/5
85	PGV	4C	307	-	-	4/55/55/55	-
75	CDL	1q	202	-	-	7/71/71/110	-
72	FES	3R	301	49	-	-	0/1/1/1
85	PGV	4L	101	-	-	7/55/55/55	-
85	PGV	4A	601	-	-	10/55/55/55	-
83	HEM	3C	502	47	-	6/14/54/54	-
69	3PE	1N	901	-	-	13/52/52/54	-
69	3PE	1L	704	-	-	8/34/34/54	-
69	3PE	1N	903	-	-	3/36/36/54	-
75	CDL	1d	202	-	-	22/75/75/110	-
75	CDL	3A	501	-	-	5/68/68/110	-
85	PGV	4C	305	-	-	16/55/55/55	-
69	3PE	1Y	202	-	-	9/43/43/54	-
86	HEA	4A	605	55	-	7/36/76/76	-
75	CDL	3N	502	-	-	8/53/53/110	-
71	SF4	1B	201	2	-	-	0/6/5/5
85	PGV	4M	101	-	-	8/55/55/55	-
75	CDL	1L	702	-	-	11/86/86/110	-
70	PC1	1P	401	-	-	10/36/36/57	-
85	PGV	4C	301	-	-	1/55/55/55	-
71	SF4	1G	801	7	-	-	0/6/5/5
71	SF4	1I	202	9	-	-	0/6/5/5
75	CDL	4D	201	-	-	16/110/110/110	-
86	HEA	4A	604	55	-	8/36/76/76	-
75	CDL	3G	102	-	-	10/62/62/110	-
84	HEC	3Q	501	48	-	4/14/54/54	-
69	3PE	1L	701	-	-	5/49/49/54	-
69	3PE	3A	503	-	-	6/35/35/54	-
70	PC1	3E	302	-	-	2/50/50/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3G	101	-	-	10/32/32/54	-
70	PC1	1I	201	-	-	9/57/57/57	-
70	PC1	1M	503	-	-	8/47/47/57	-
76	GTP	1O	401	77	-	4/22/38/38	0/3/3/3
85	PGV	4G	101	-	-	8/55/55/55	-
75	CDL	1N	902	-	-	10/71/71/110	-
69	3PE	1M	502	-	-	10/54/54/54	-
70	PC1	3X	101	-	-	4/32/32/57	-
69	3PE	3N	501	-	-	10/35/35/54	-
85	PGV	4J	101	-	-	10/55/55/55	-
69	3PE	3C	504	-	-	9/37/37/54	-
70	PC1	1H	401	-	-	13/51/51/57	-
75	CDL	3G	103	-	-	11/66/66/110	-
69	3PE	1J	201	-	-	10/47/47/54	-
85	PGV	4C	302	-	-	6/55/55/55	-
85	PGV	4K	101	-	-	14/55/55/55	-
69	3PE	1L	703	-	-	9/48/48/54	-
75	CDL	1X	201	-	-	18/96/96/110	-
69	3PE	3D	502	-	-	4/36/36/54	-
84	HEC	3D	501	48	-	3/13/53/54	-
70	PC1	1h	203	-	-	12/50/50/57	-
91	PEK	4G	103	-	-	9/55/55/56	-
69	3PE	1Y	203	-	-	13/33/33/54	-
70	PC1	1B	202	-	-	8/49/49/57	-
69	3PE	1Y	205	-	-	15/44/44/54	-
70	PC1	3R	303	-	-	5/48/48/57	-
69	3PE	3N	503	-	-	7/28/28/54	-
69	3PE	1d	201	-	-	16/51/51/54	-
69	3PE	3P	503	-	-	10/36/36/54	-
70	PC1	1A	202	-	-	3/38/38/57	-
69	3PE	3R	302	-	-	9/50/50/54	-
71	SF4	1I	203	9	-	-	0/6/5/5
71	SF4	1F	502	6	-	-	0/6/5/5
69	3PE	1M	504	-	-	5/53/53/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	4B	302	-	-	15/110/110/110	-
85	PGV	4A	603	-	-	11/55/55/55	-
83	HEM	3C	501	47	-	5/14/54/54	-
70	PC1	1B	203	-	-	12/51/51/57	-
83	HEM	3P	501	47	-	7/14/54/54	-
83	HEM	3P	502	47	-	8/14/54/54	-
70	PC1	1m	201	-	-	11/49/49/57	-
82	MYR	1l	201	-	-	2/12/12/13	-
69	3PE	1M	501	-	-	7/48/48/54	-
69	3PE	3C	503	-	-	11/38/38/54	-
69	3PE	3A	502	-	-	7/30/30/54	-
72	FES	1G	803	7	-	-	0/1/1/1
69	3PE	1A	201	-	-	9/50/50/54	-
80	EHZ	1T	101	20	-	14/42/44/45	-
81	AME	1h	201	-	-	2/9/10/12	-
70	PC1	1q	201	-	-	7/52/52/57	-
91	PEK	4G	102	-	-	10/56/56/56	-
85	PGV	4B	301	-	-	11/55/55/55	-
70	PC1	1Y	201	-	-	8/38/38/57	-
75	CDL	3P	504	-	-	13/66/66/110	-
75	CDL	1h	202	-	-	10/90/90/110	-
90	PSC	4B	304	-	-	17/55/55/55	-
78	NDP	1P	402	-	-	2/34/77/77	0/5/5/5
72	FES	1E	301	5	-	-	0/1/1/1
85	PGV	4C	304	-	-	15/55/55/55	-
69	3PE	1Y	204	-	-	5/30/30/54	-
69	3PE	1j	101	-	-	3/47/47/54	-

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	4A	604	HEA	FE-ND	5.69	2.12	1.94
86	4A	605	HEA	FE-NB	5.61	2.12	1.94
86	4A	605	HEA	FE-ND	5.60	2.12	1.94
86	4A	604	HEA	FE-NB	5.56	2.12	1.94
83	3P	501	HEM	FE-NB	5.51	2.11	1.94

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	4A	605	HEA	C3D-C4D-ND	6.71	116.84	110.35
86	4A	604	HEA	C3D-C4D-ND	6.51	116.64	110.35
80	1n	201	EHZ	C10-S1-C9	6.21	120.20	101.84
70	1m	201	PC1	O21-C21-C22	5.92	124.29	111.48
80	1T	101	EHZ	C10-S1-C9	5.91	119.31	101.84

There are no chirality outliers.

5 of 780 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C1-O11-P-O13
69	1A	201	3PE	C1-O11-P-O14
69	1J	201	3PE	C1-O11-P-O13
69	1J	201	3PE	C1-O11-P-O14
69	1J	201	3PE	C11-O13-P-O12

There are no ring outliers.

96 monomers are involved in 475 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	3T	101	CDL	6	0
72	3E	301	FES	2	0
70	1Z	201	PC1	5	0
73	1F	501	FMN	2	0
85	4A	602	PGV	7	0
85	4C	303	PGV	7	0
69	3Y	101	3PE	1	0
80	1n	201	EHZ	1	0
75	4C	306	CDL	14	0
71	1G	802	SF4	1	0
85	4C	307	PGV	10	0
75	1q	202	CDL	6	0
72	3R	301	FES	5	0
85	4L	101	PGV	10	0
85	4A	601	PGV	9	0
83	3C	502	HEM	4	0
69	1N	901	3PE	4	0
69	1L	704	3PE	1	0
69	1N	903	3PE	2	0
75	1d	202	CDL	9	0
75	3A	501	CDL	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	4C	305	PGV	4	0
69	1Y	202	3PE	1	0
86	4A	605	HEA	1	0
75	3N	502	CDL	8	0
71	1B	201	SF4	2	0
85	4M	101	PGV	5	0
75	1L	702	CDL	4	0
85	4C	301	PGV	4	0
75	4D	201	CDL	20	0
86	4A	604	HEA	6	0
75	3G	102	CDL	4	0
84	3Q	501	HEC	2	0
69	1L	701	3PE	3	0
69	3A	503	3PE	10	0
70	3E	302	PC1	7	0
69	3G	101	3PE	3	0
70	1I	201	PC1	4	0
89	4B	303	CUA	2	0
70	1M	503	PC1	8	0
76	1O	401	GTP	2	0
85	4G	101	PGV	5	0
75	1N	902	CDL	4	0
69	1M	502	3PE	13	0
70	3X	101	PC1	4	0
69	3N	501	3PE	6	0
85	4J	101	PGV	7	0
69	3C	504	3PE	6	0
70	1H	401	PC1	6	0
75	3G	103	CDL	5	0
69	1J	201	3PE	6	0
85	4C	302	PGV	6	0
85	4K	101	PGV	6	0
69	1L	703	3PE	5	0
75	1X	201	CDL	13	0
69	3D	502	3PE	5	0
84	3D	501	HEC	2	0
70	1h	203	PC1	2	0
91	4G	103	PEK	5	0
69	1Y	203	3PE	5	0
70	1B	202	PC1	4	0
69	1Y	205	3PE	5	0
70	3R	303	PC1	10	0

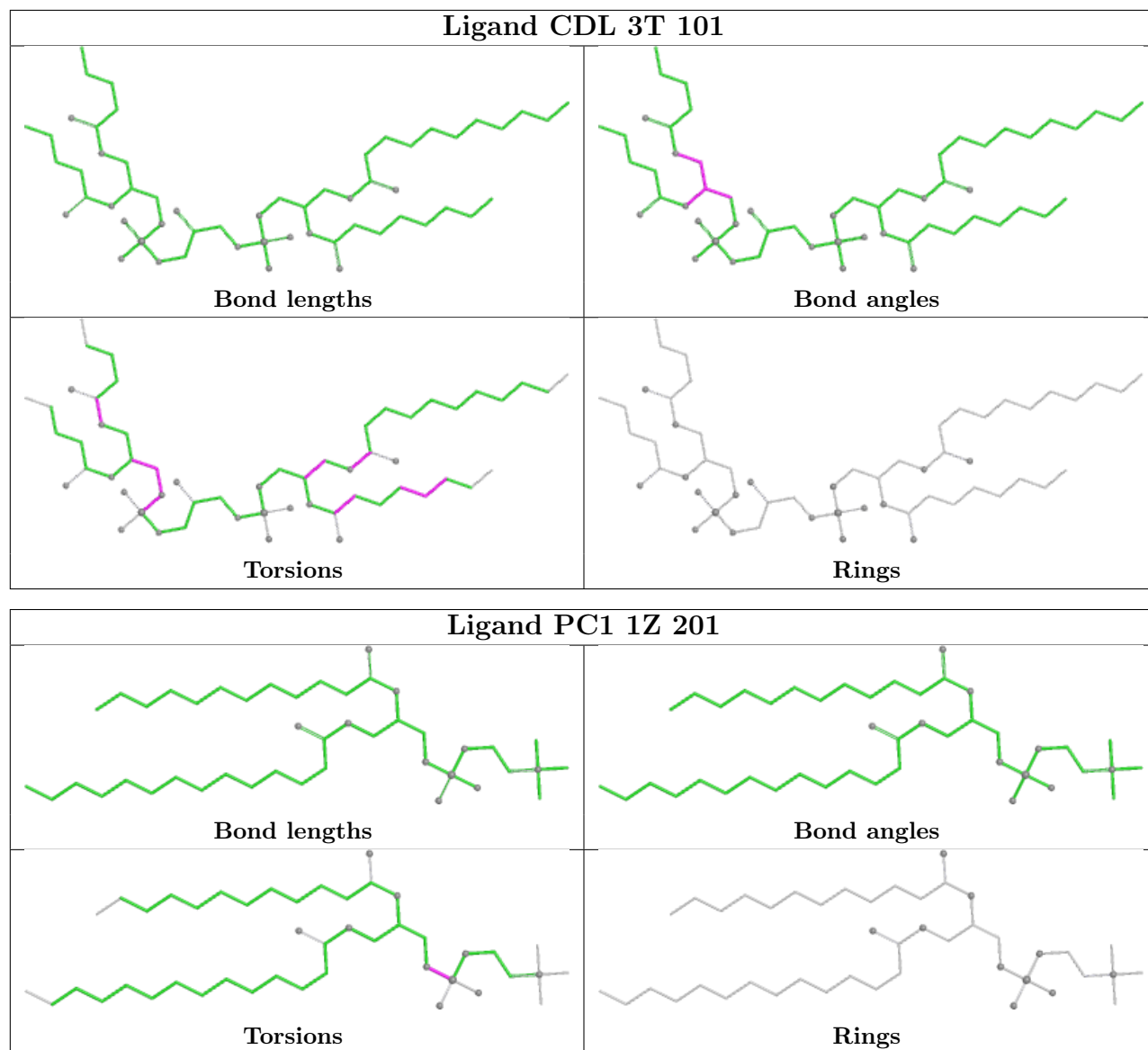
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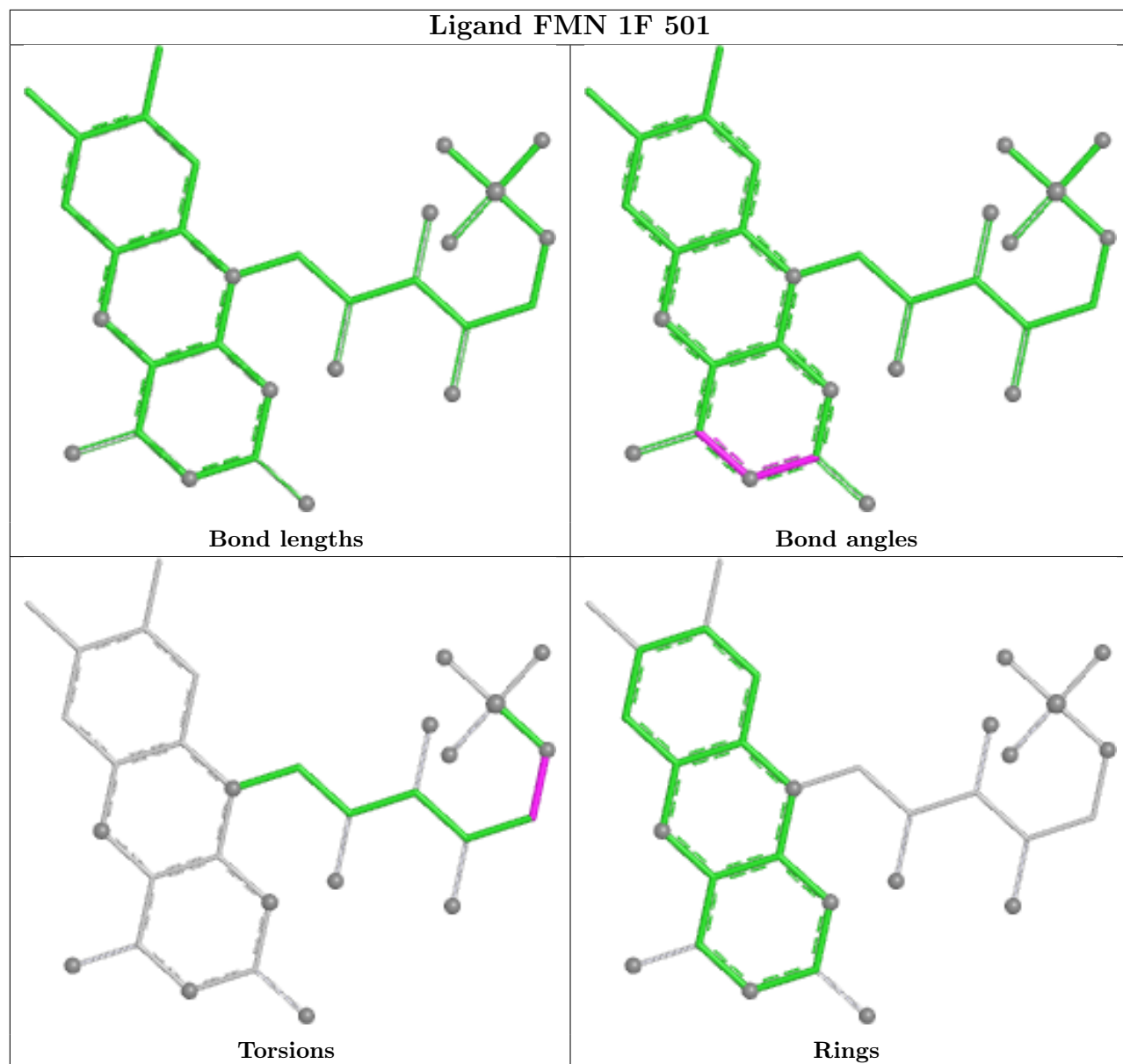
Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	3N	503	3PE	6	0
69	1d	201	3PE	12	0
69	3P	503	3PE	5	0
70	1A	202	PC1	1	0
69	3R	302	3PE	8	0
71	1F	502	SF4	1	0
69	1M	504	3PE	8	0
75	4B	302	CDL	9	0
85	4A	603	PGV	6	0
83	3C	501	HEM	3	0
70	1B	203	PC1	7	0
83	3P	501	HEM	2	0
83	3P	502	HEM	2	0
70	1m	201	PC1	9	0
69	1M	501	3PE	6	0
69	3C	503	3PE	7	0
69	3A	502	3PE	3	0
72	1G	803	FES	1	0
69	1A	201	3PE	3	0
80	1T	101	EHZ	1	0
81	1h	201	AME	4	0
70	1q	201	PC1	10	0
91	4G	102	PEK	4	0
85	4B	301	PGV	13	0
70	1Y	201	PC1	4	0
75	3P	504	CDL	6	0
75	1h	202	CDL	10	0
90	4B	304	PSC	7	0
78	1P	402	NDP	1	0
72	1E	301	FES	1	0
85	4C	304	PGV	10	0
69	1Y	204	3PE	4	0
69	1j	101	3PE	1	0

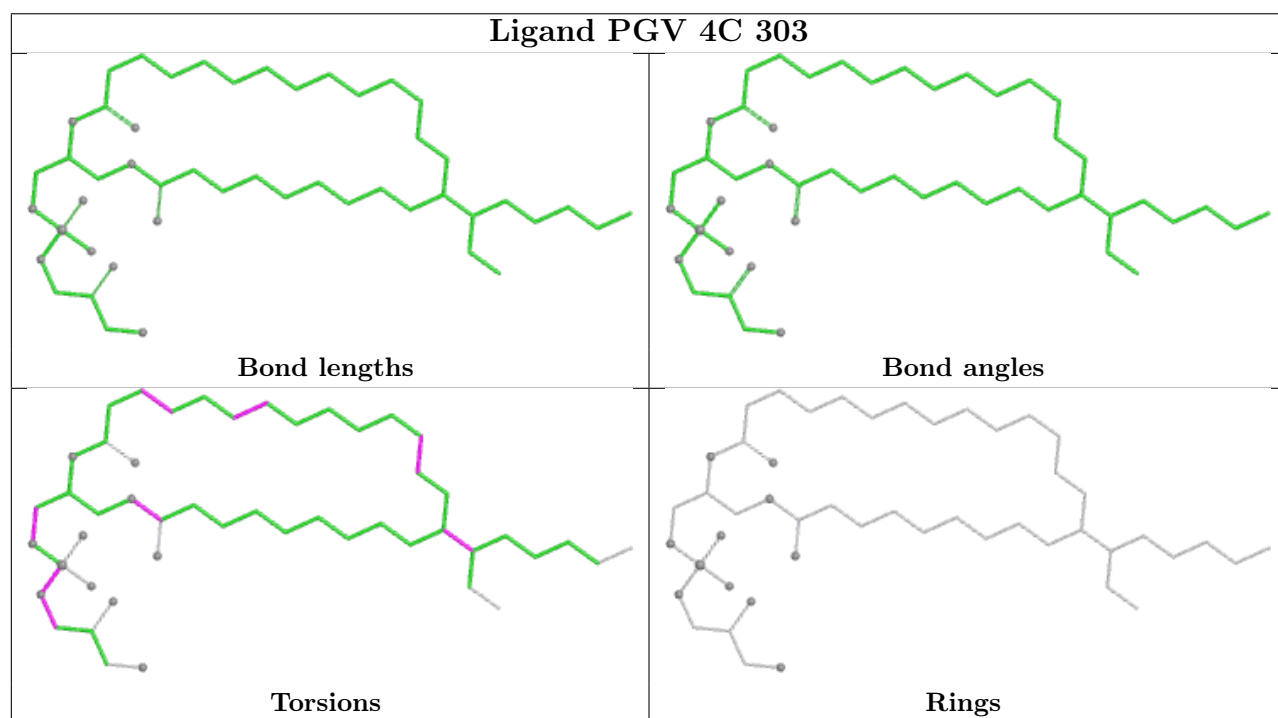
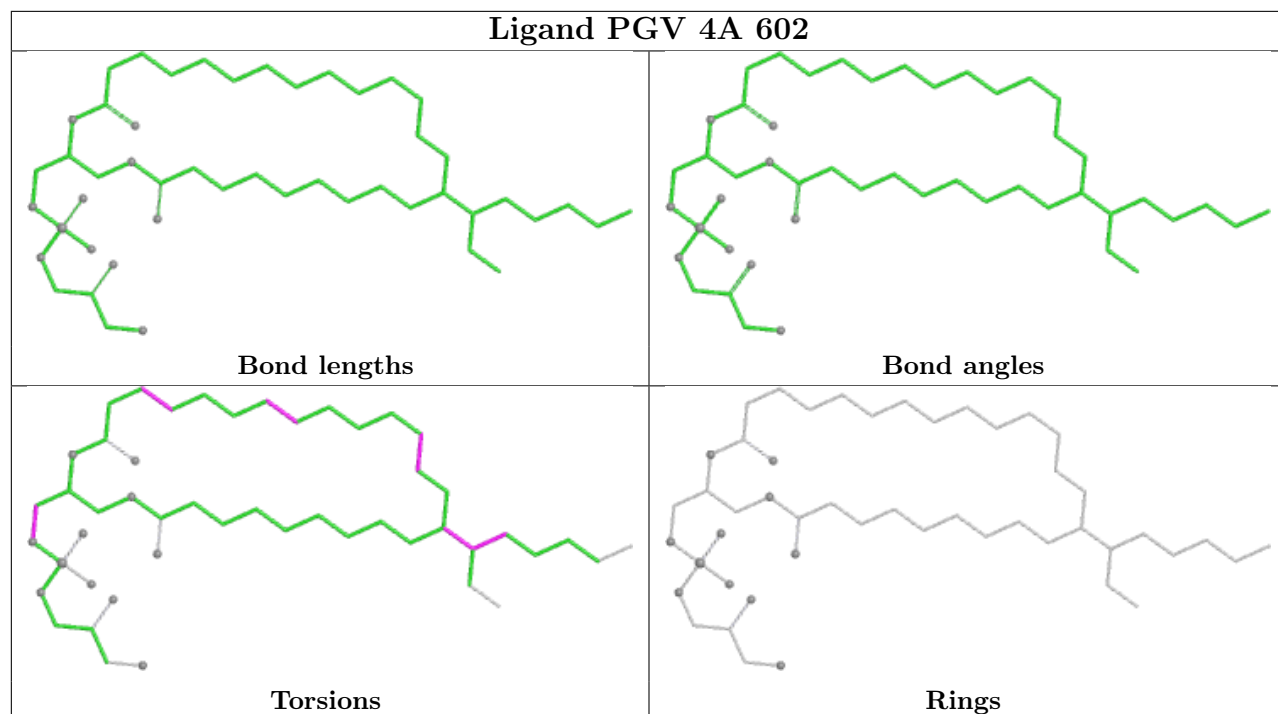
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

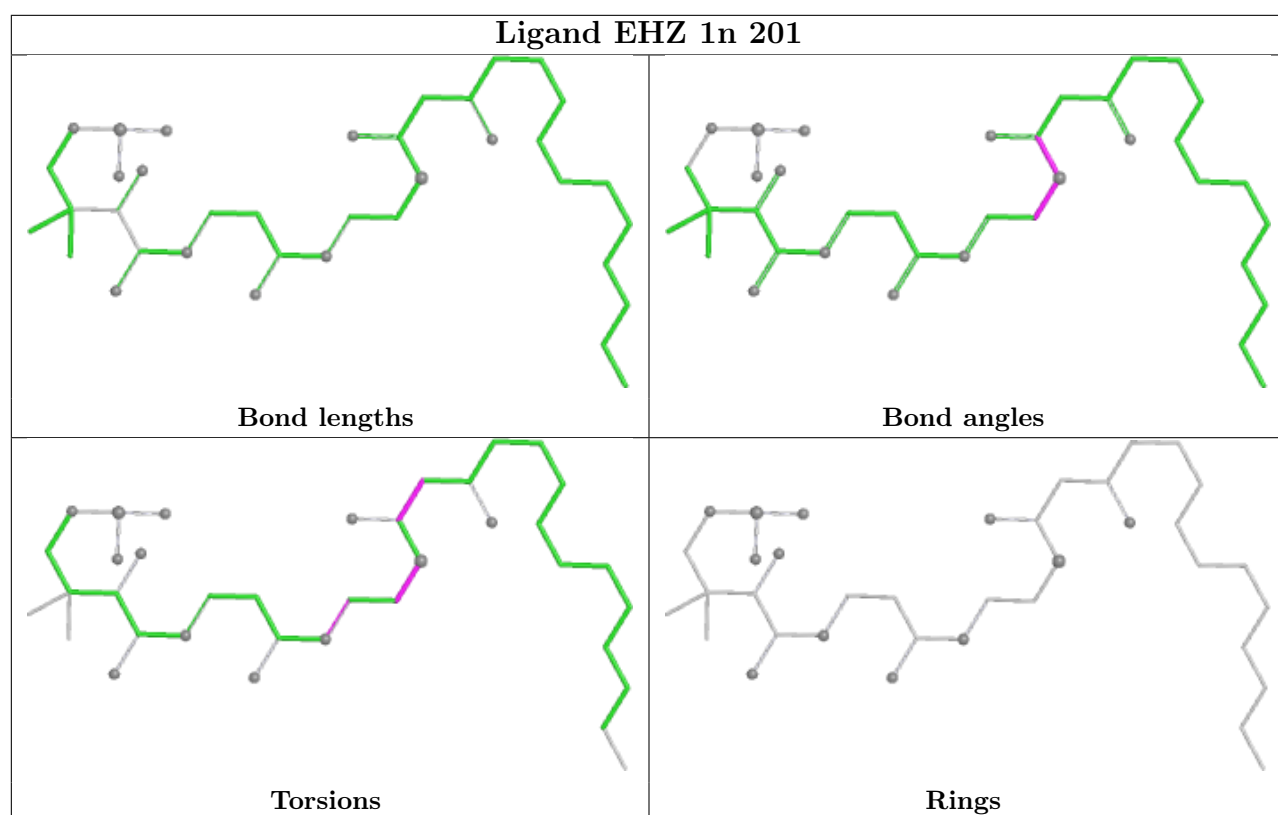
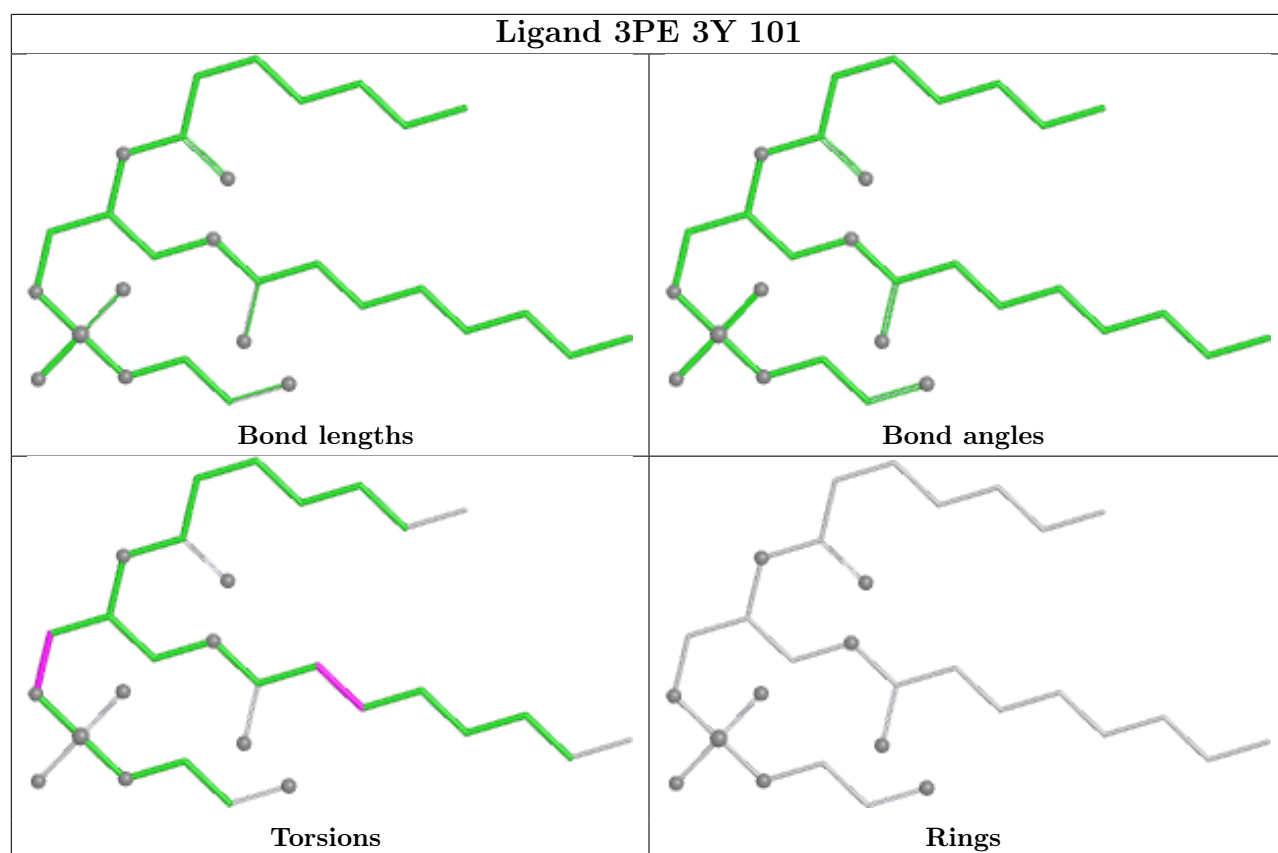
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

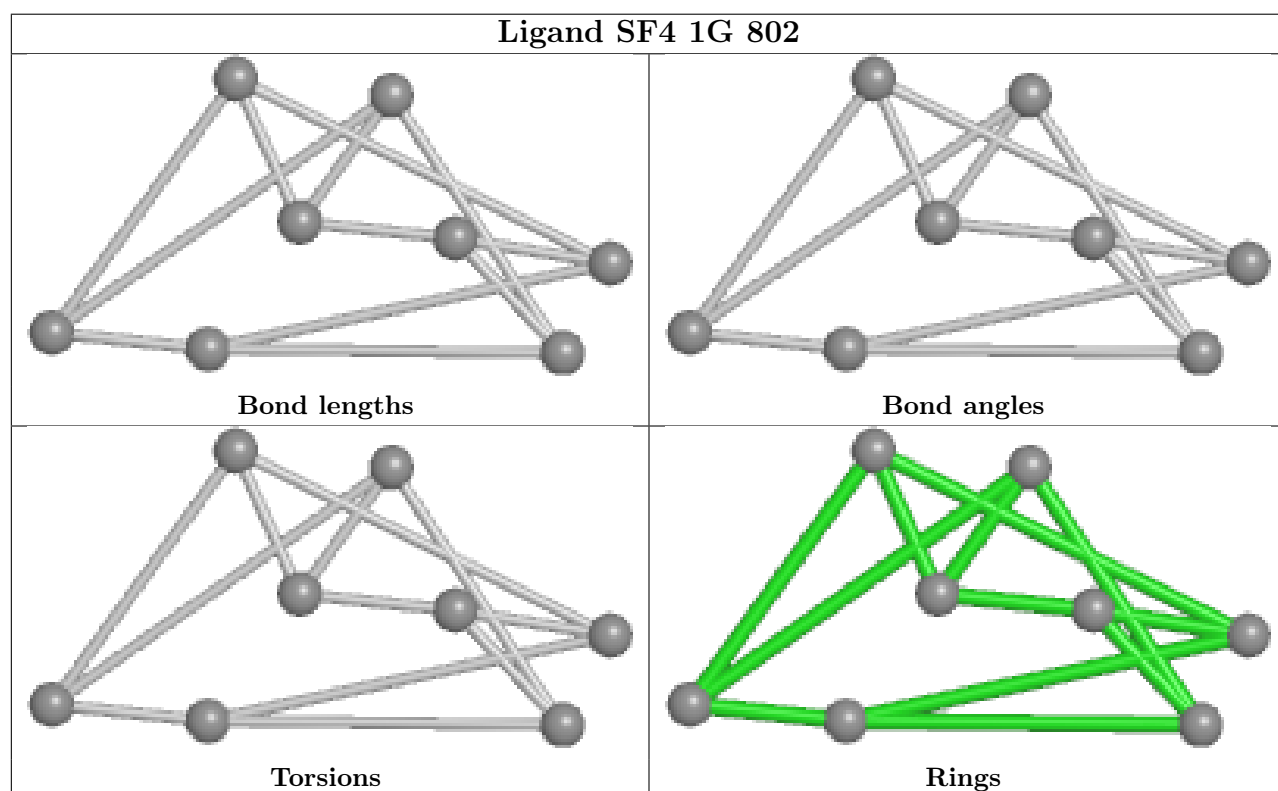
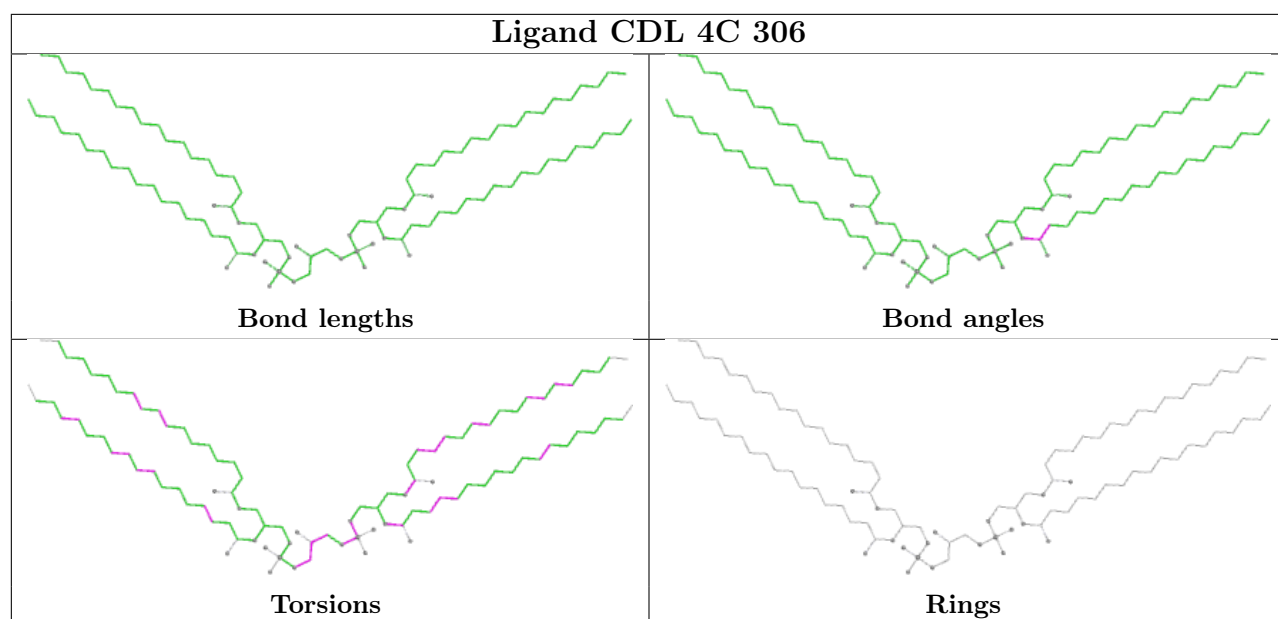


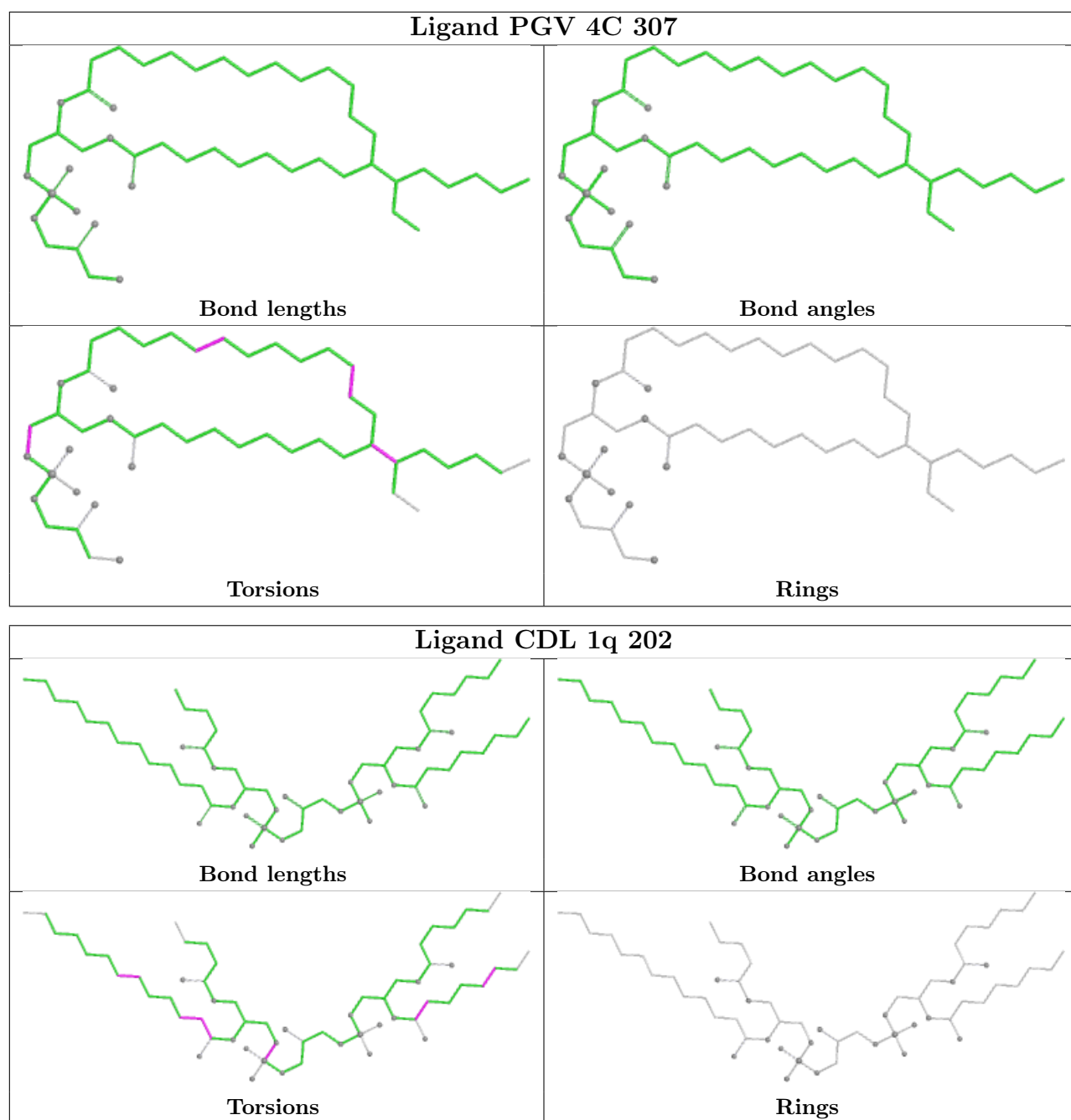
Ligand FMN 1F 501

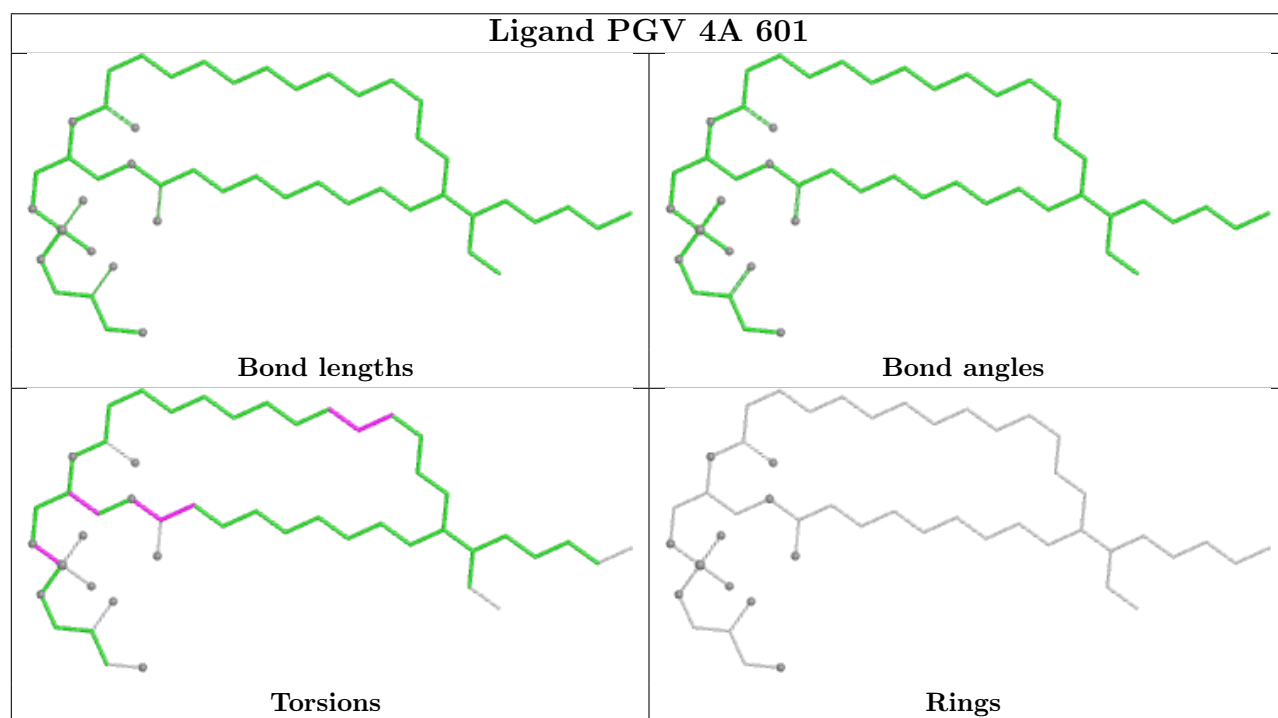
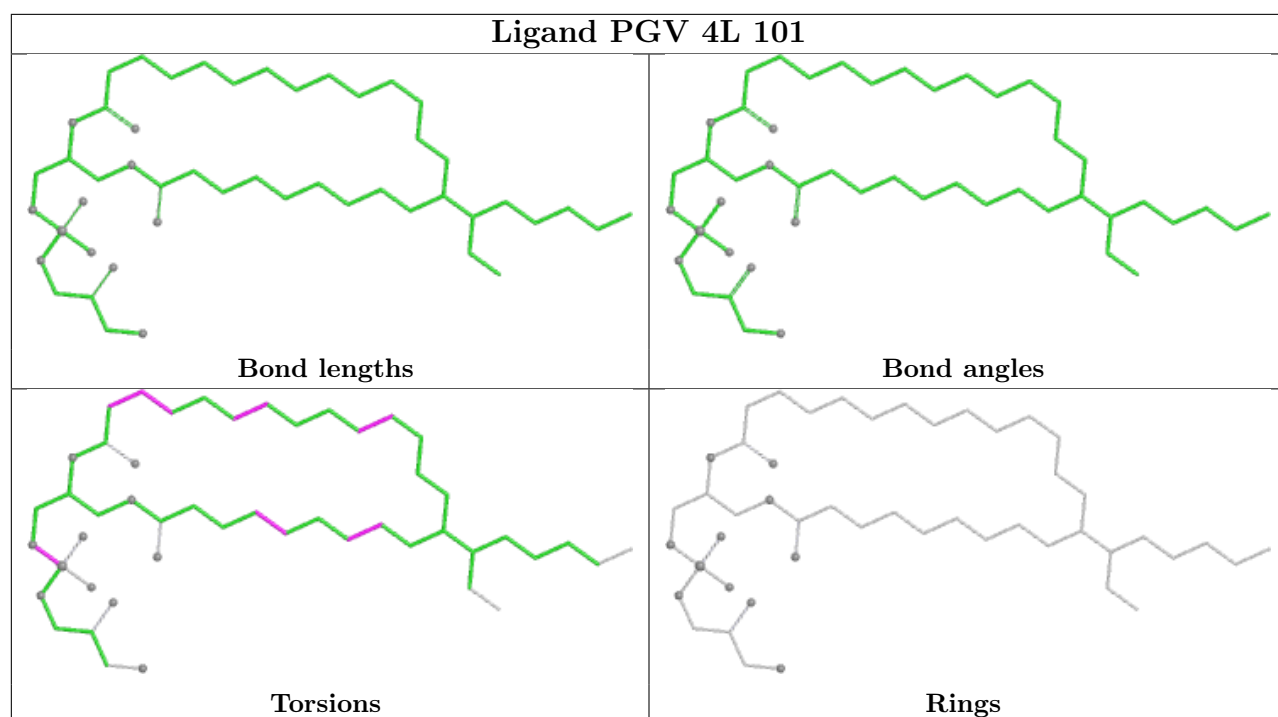




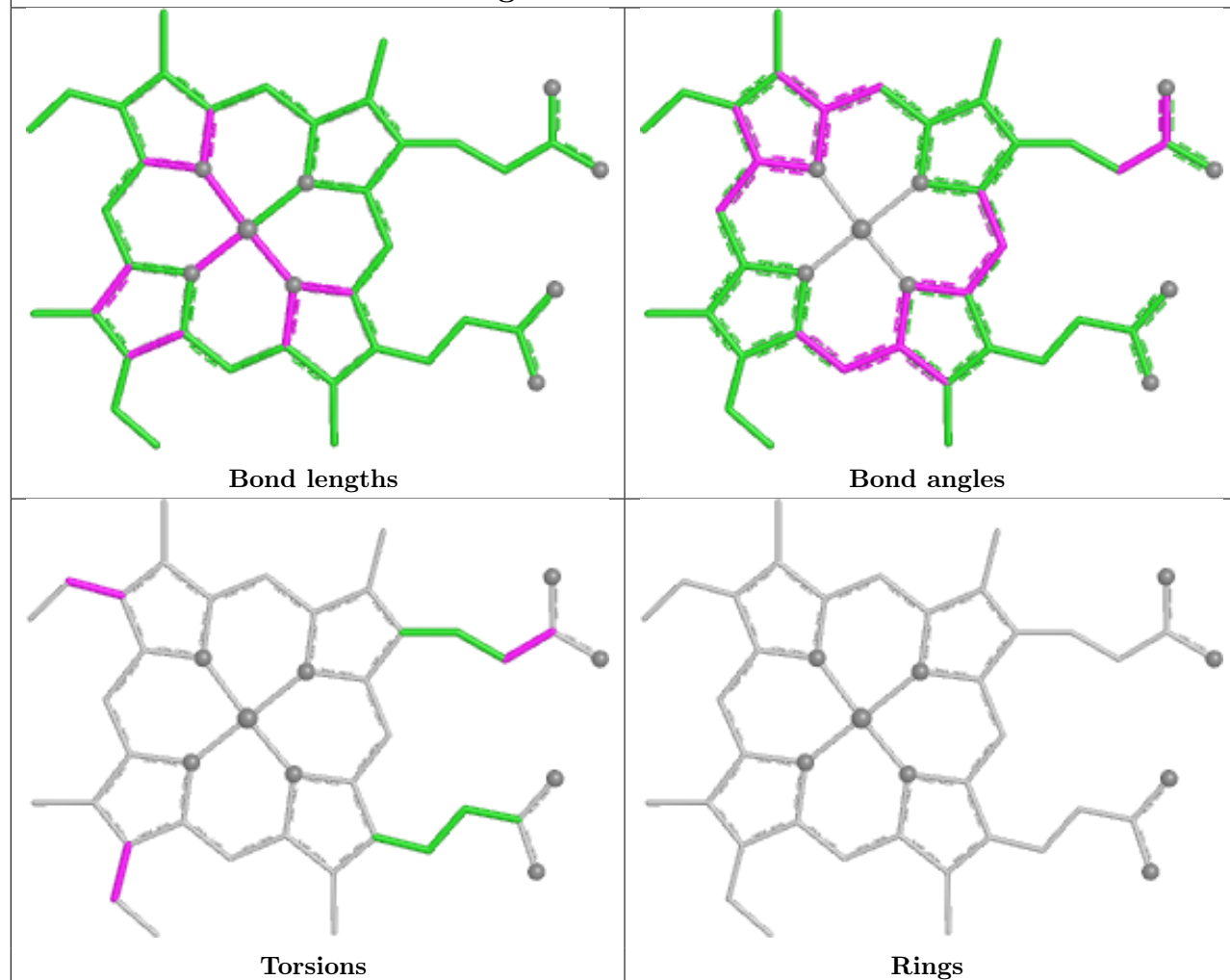




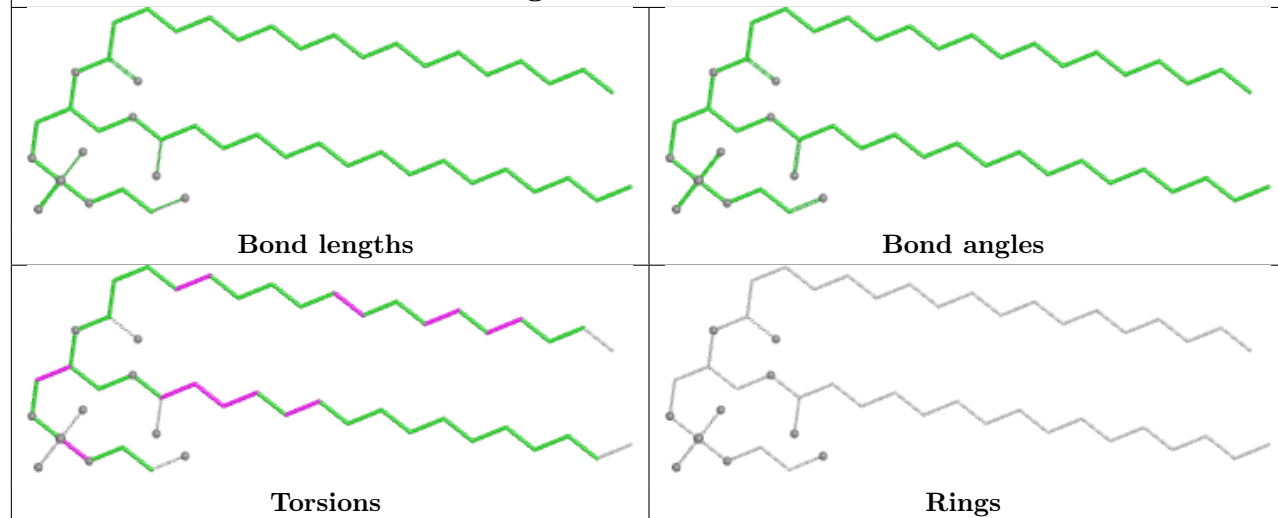


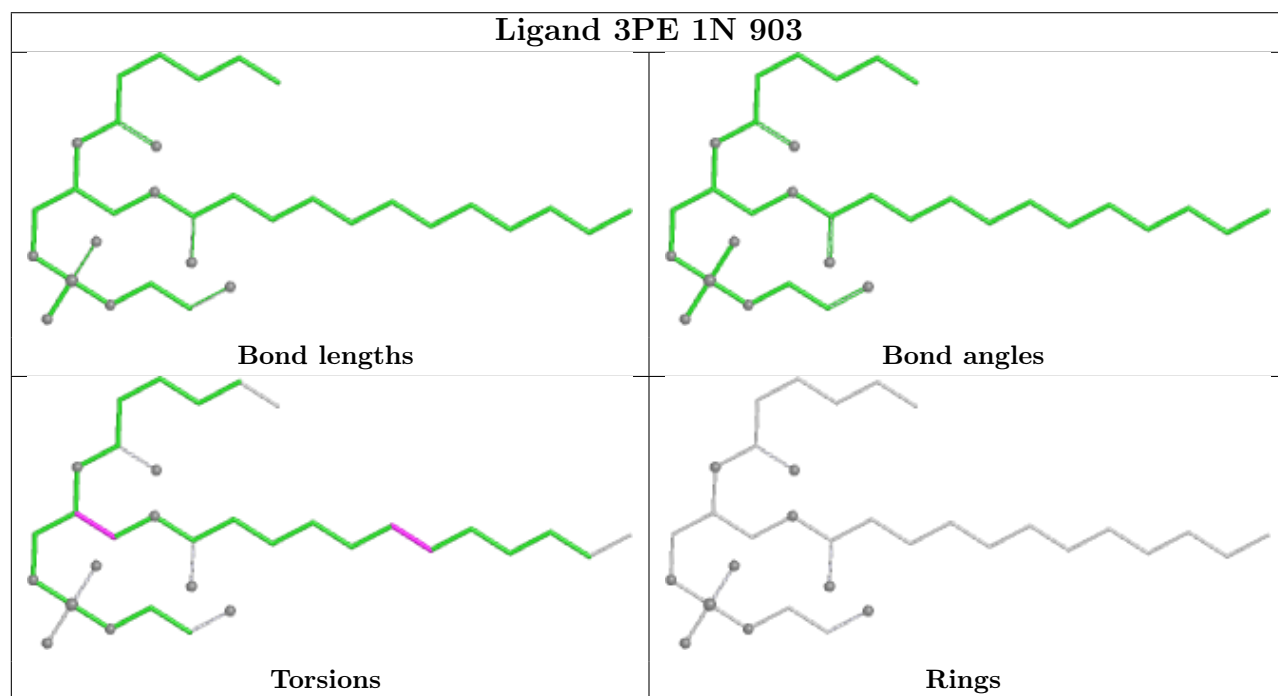
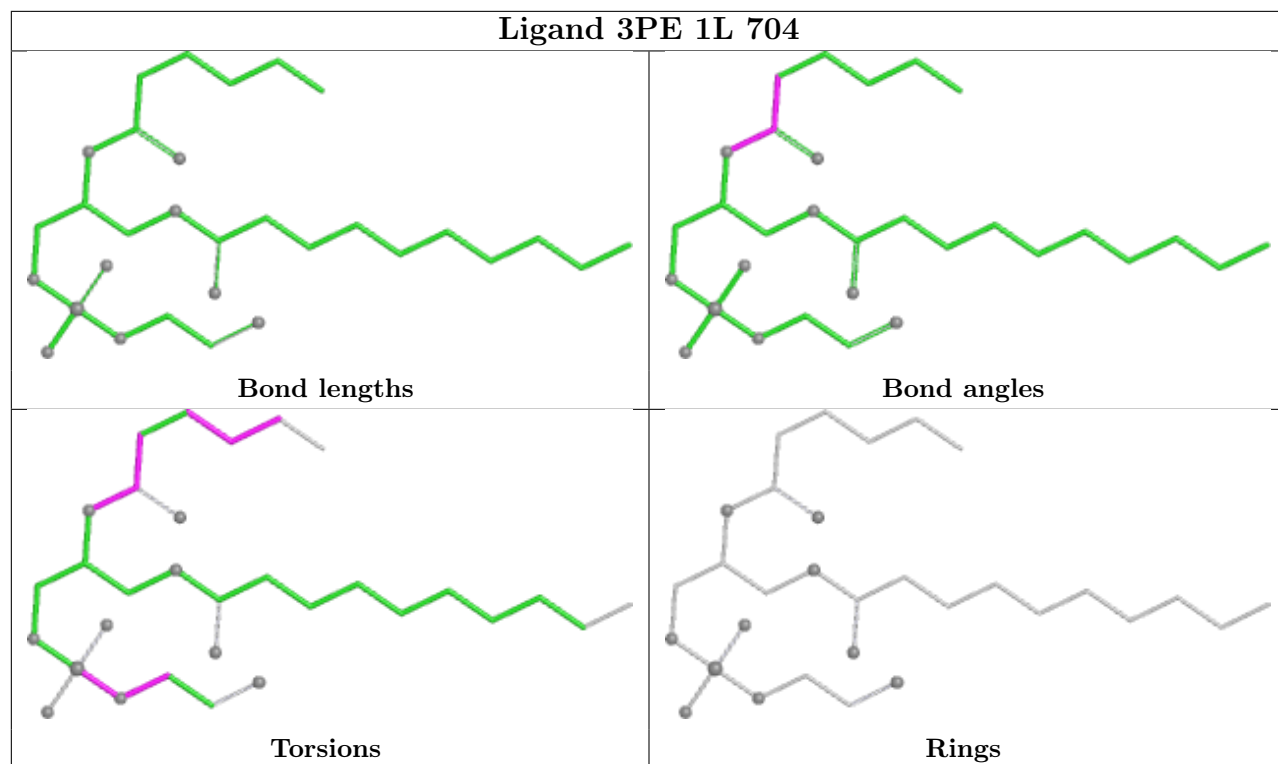


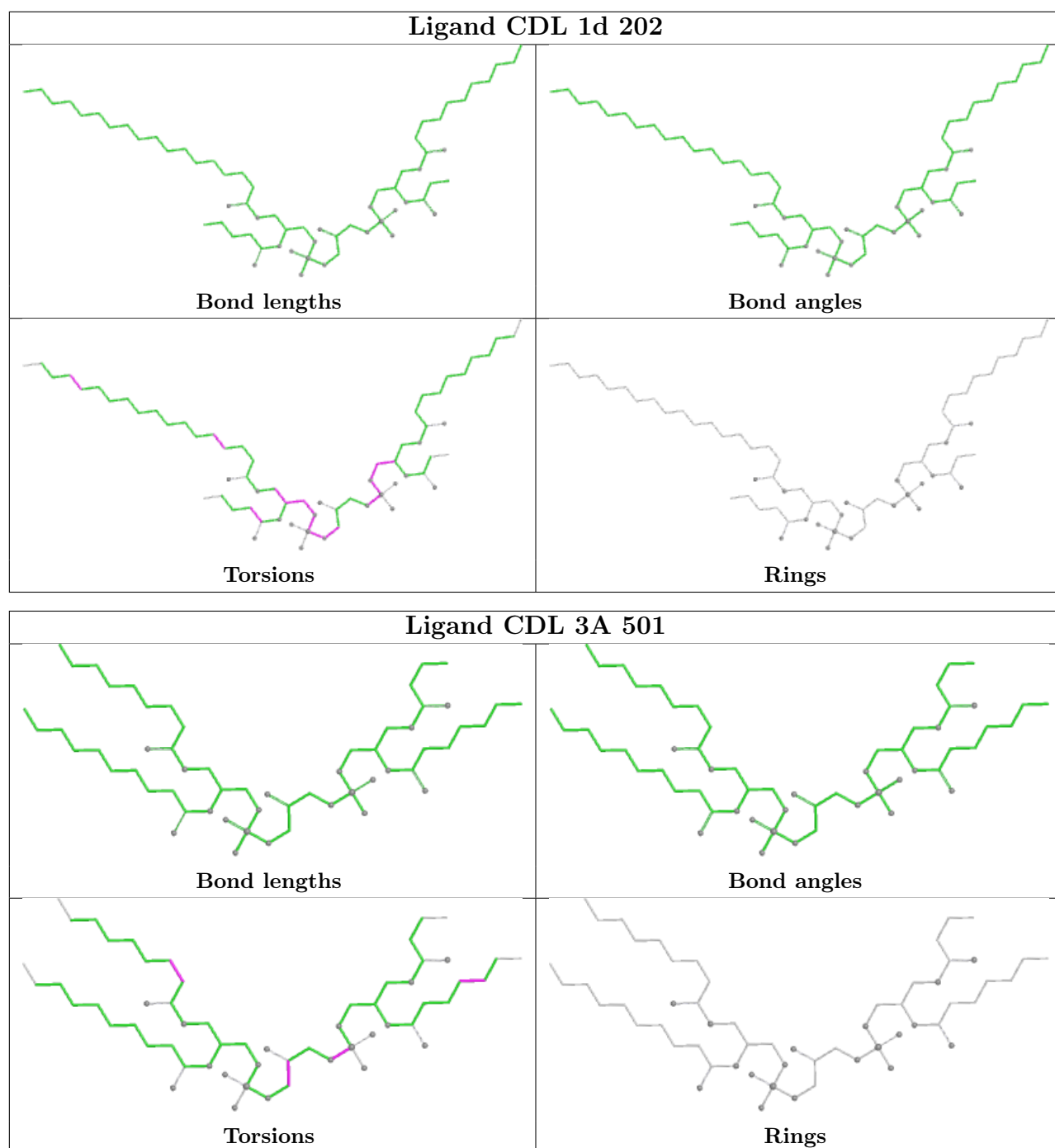
Ligand HEM 3C 502

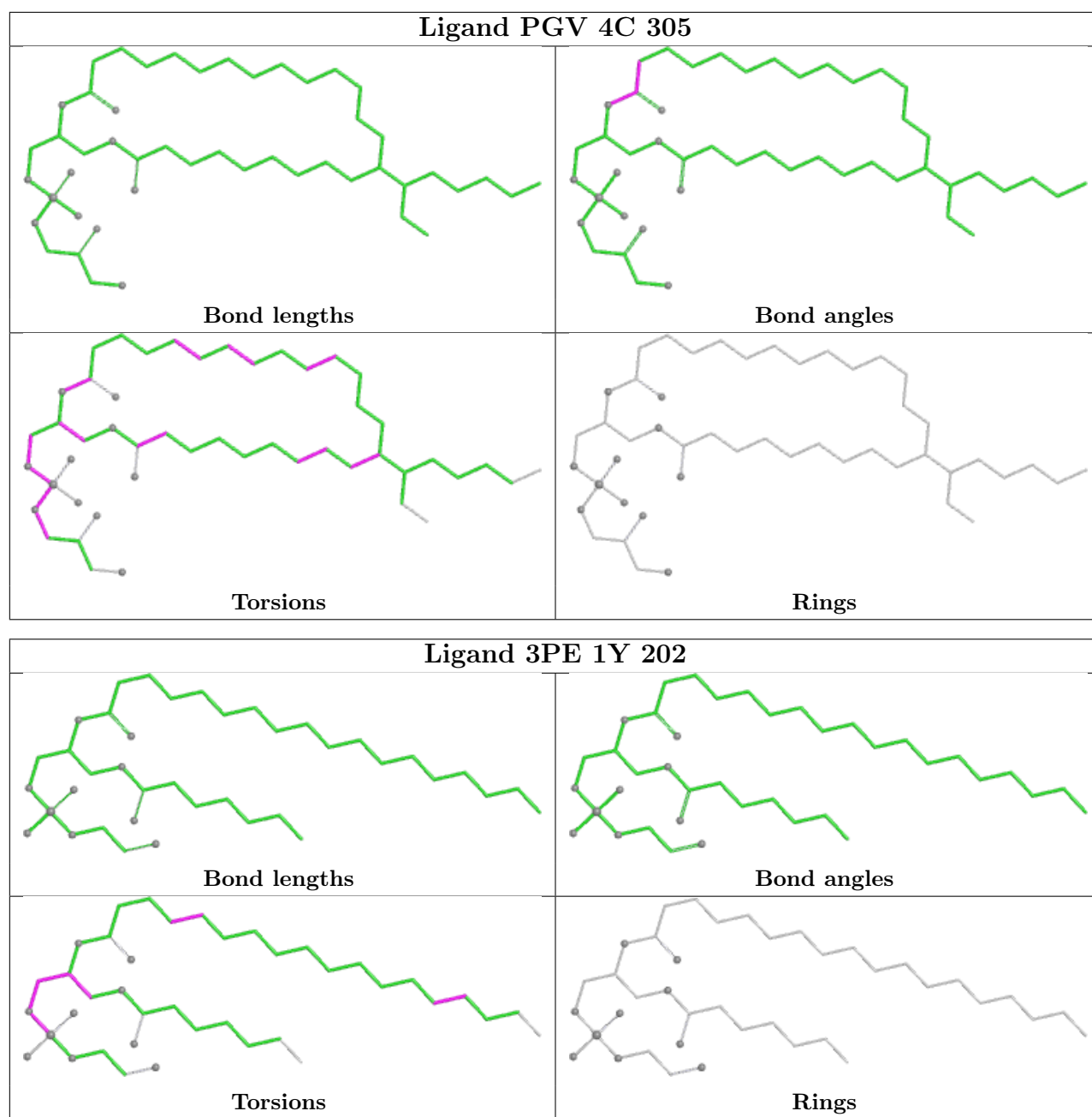


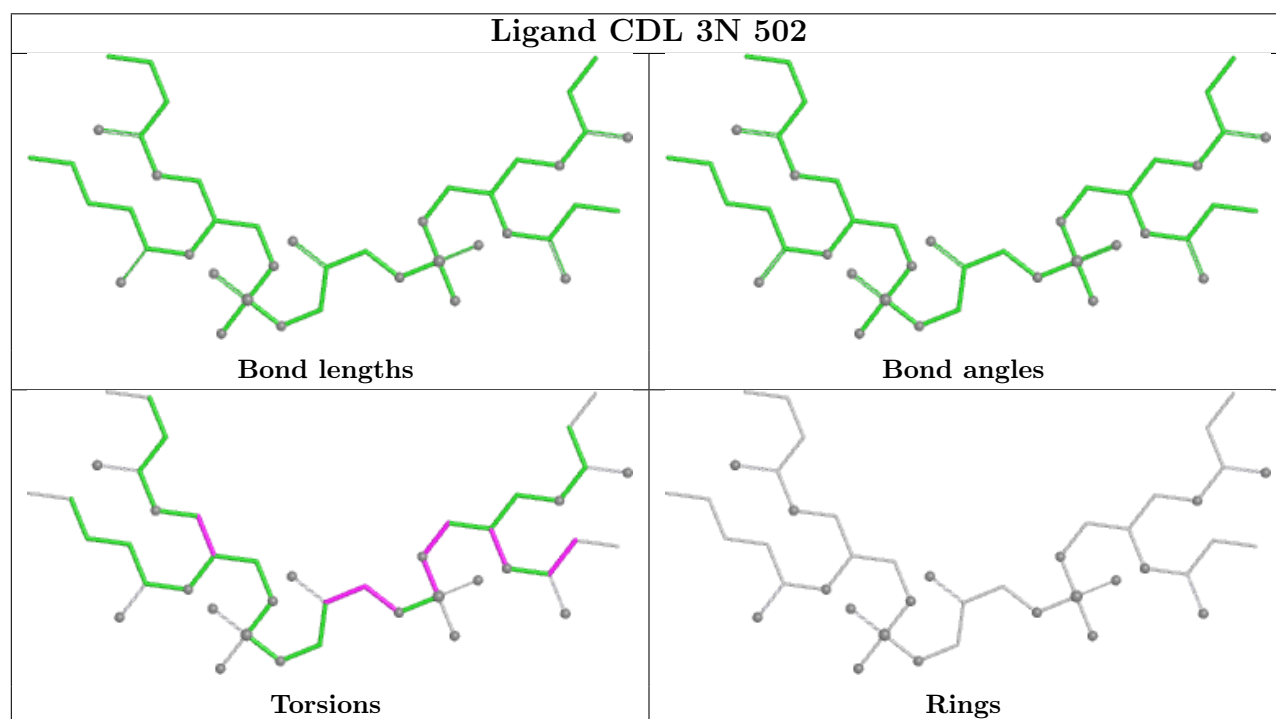
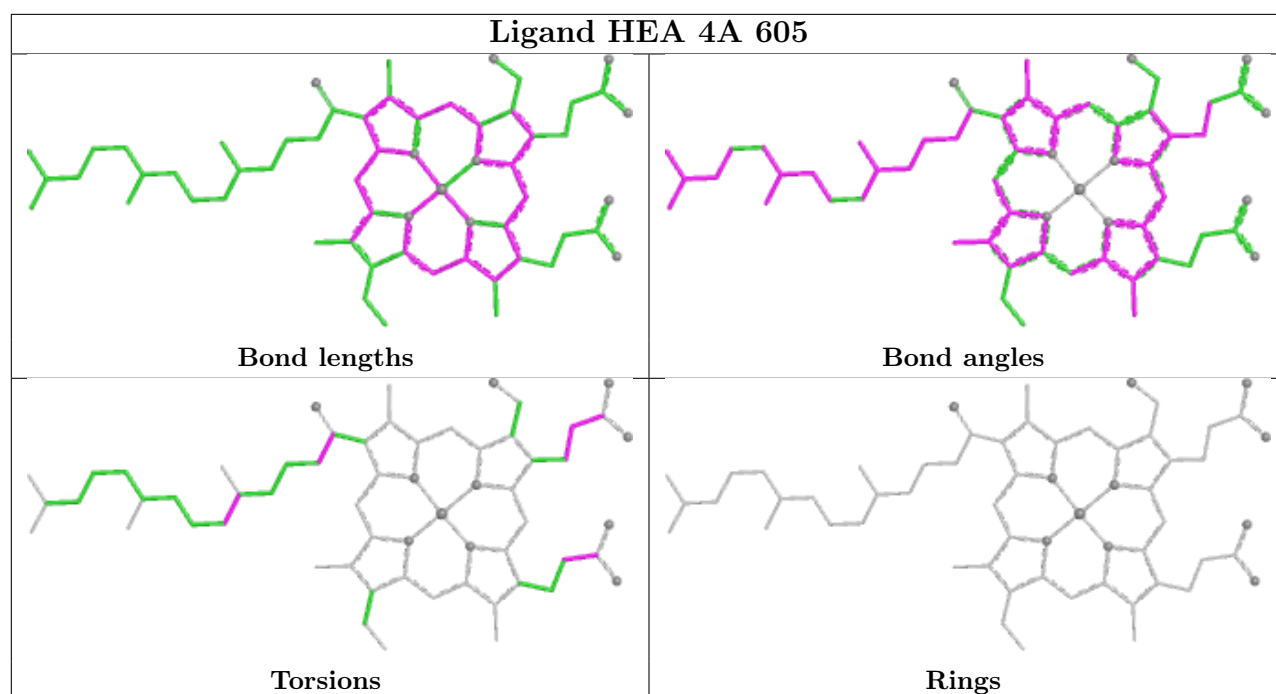
Ligand 3PE 1N 901

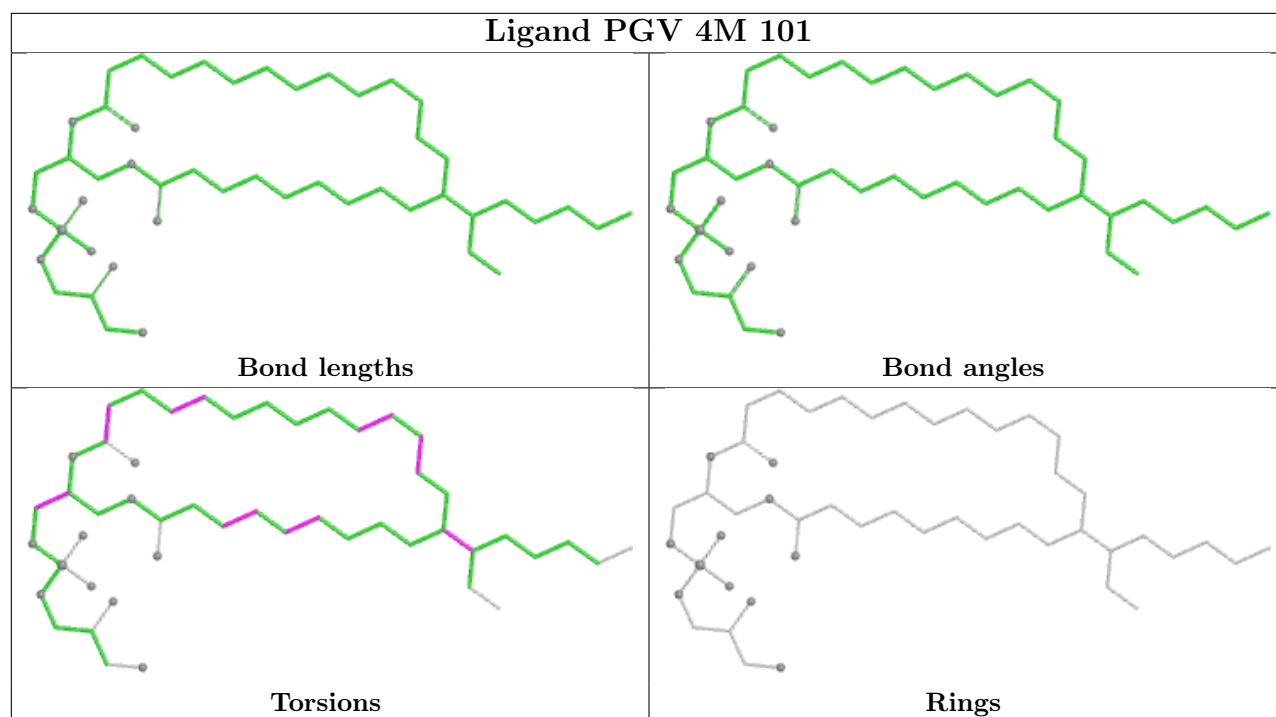
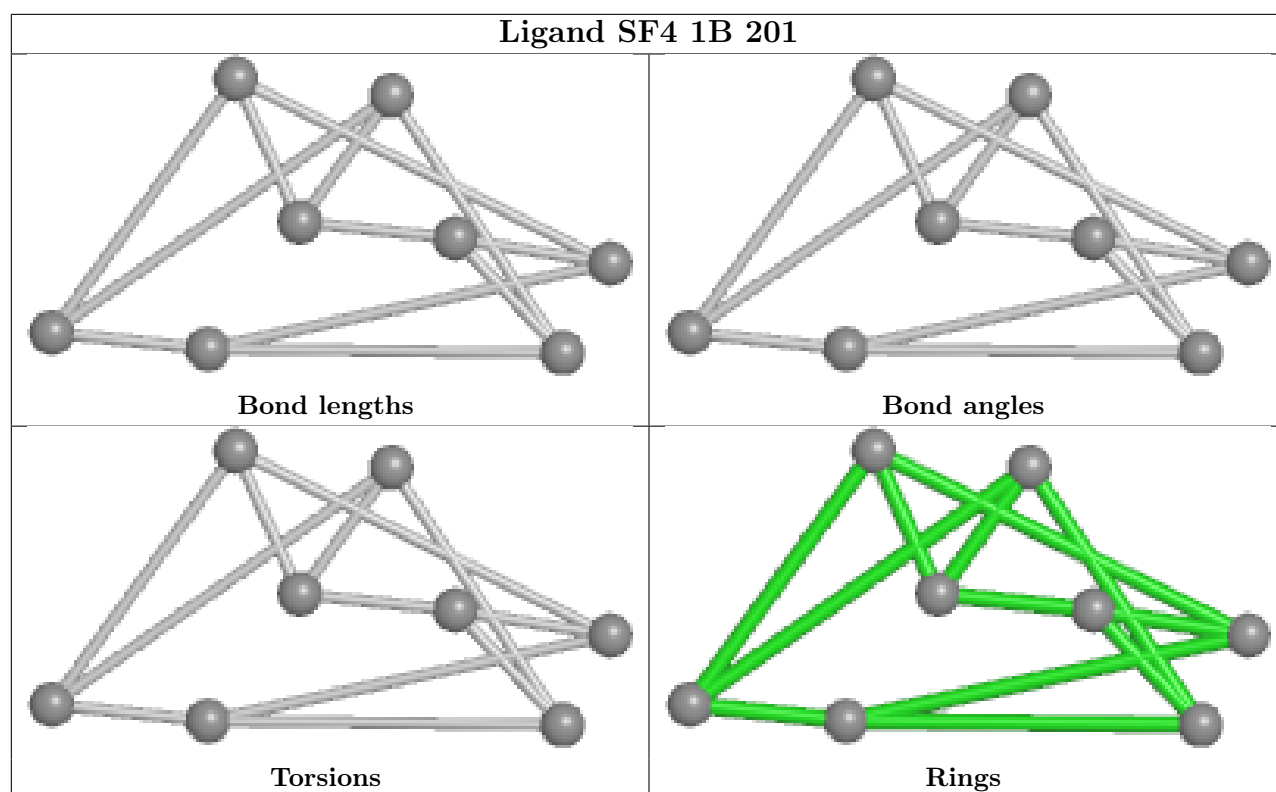


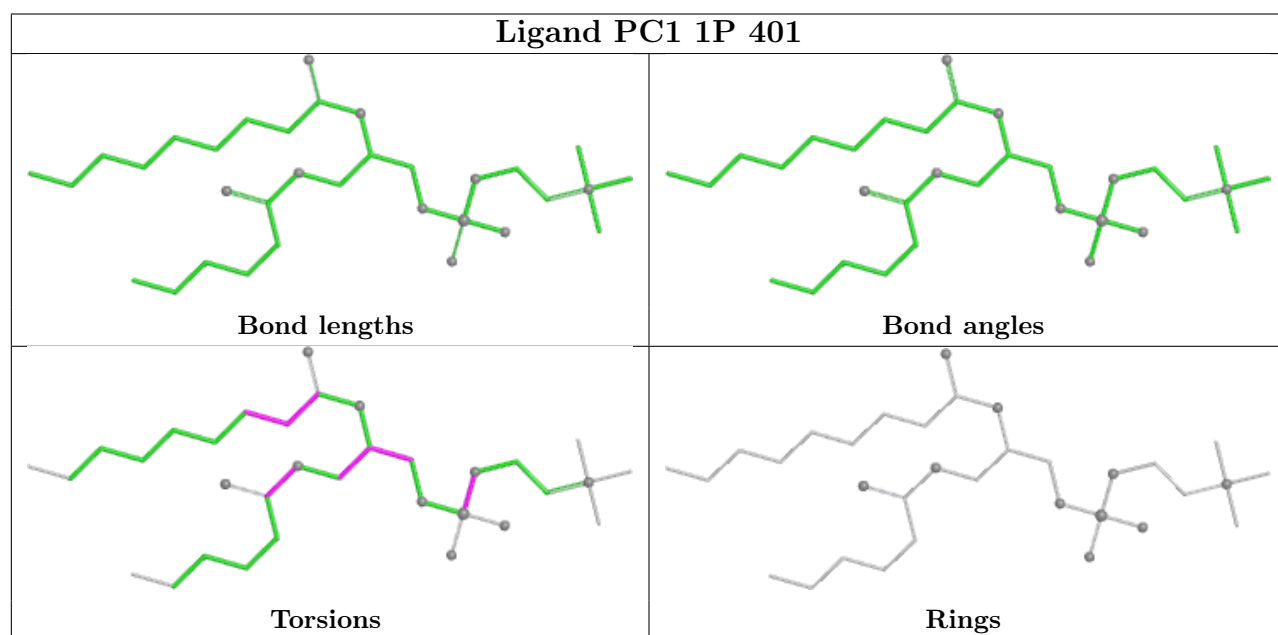
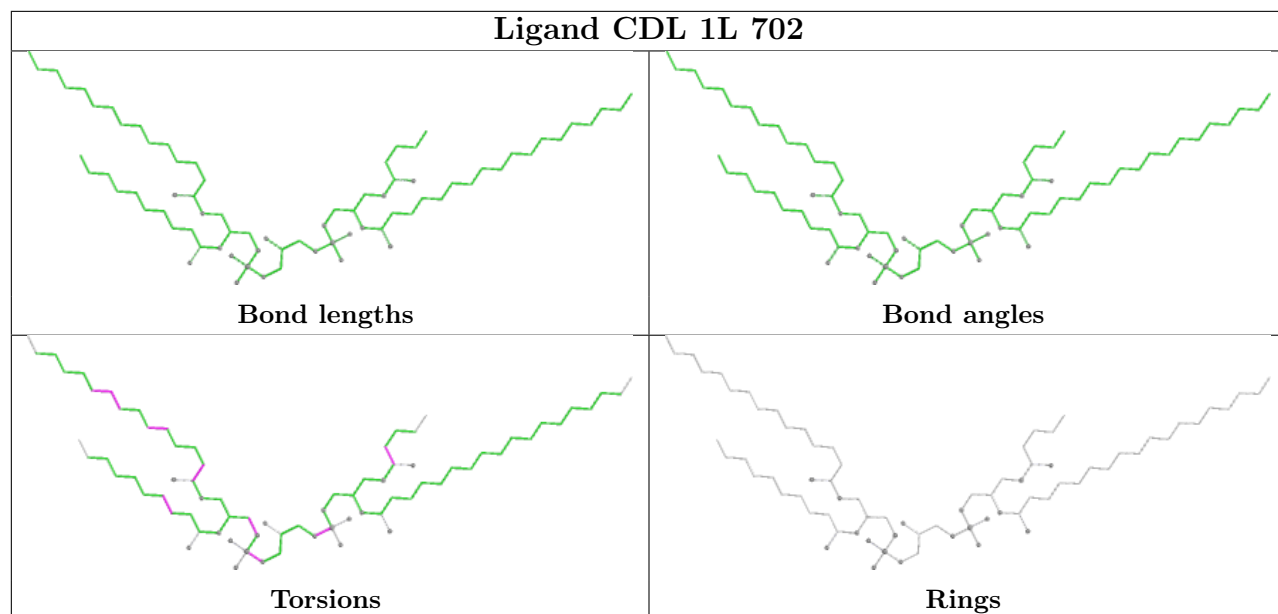


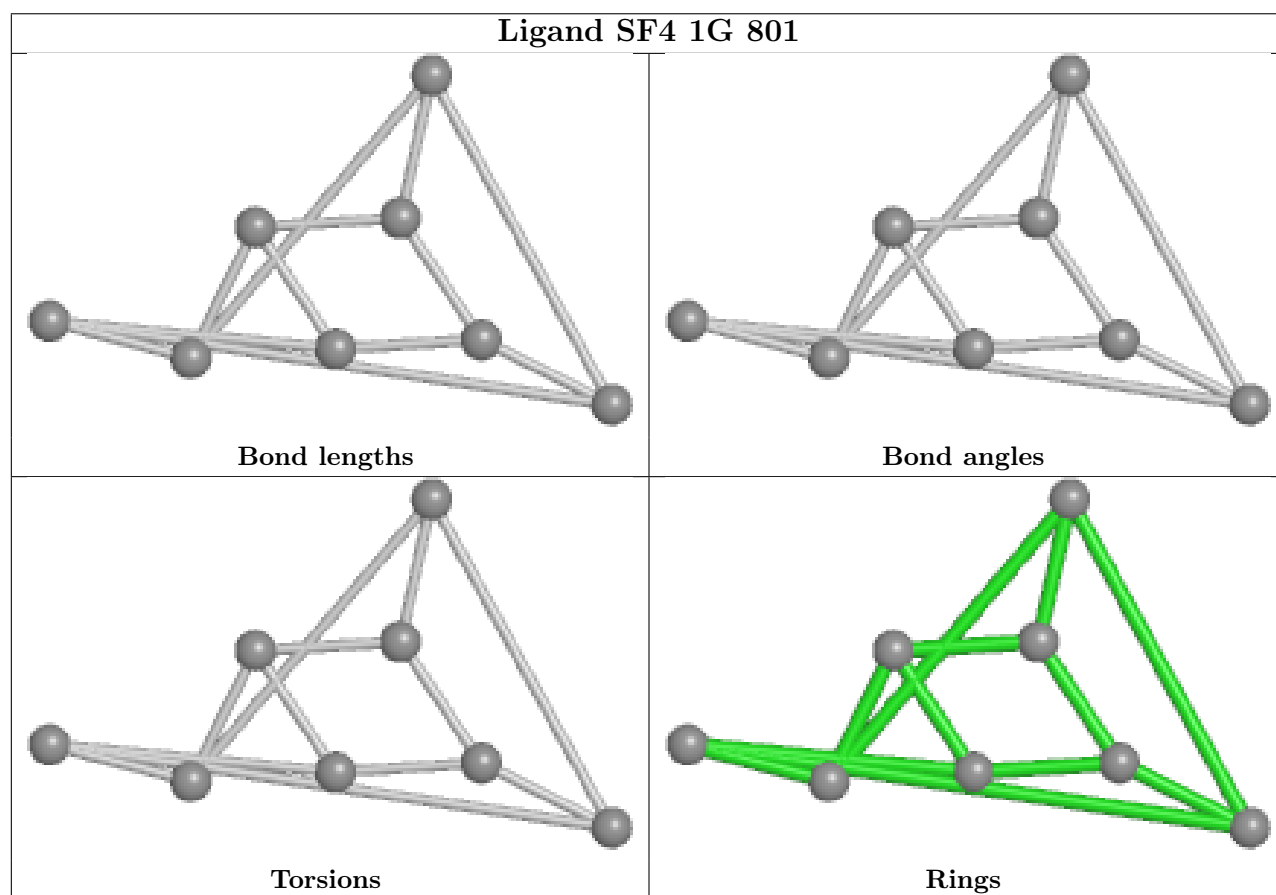
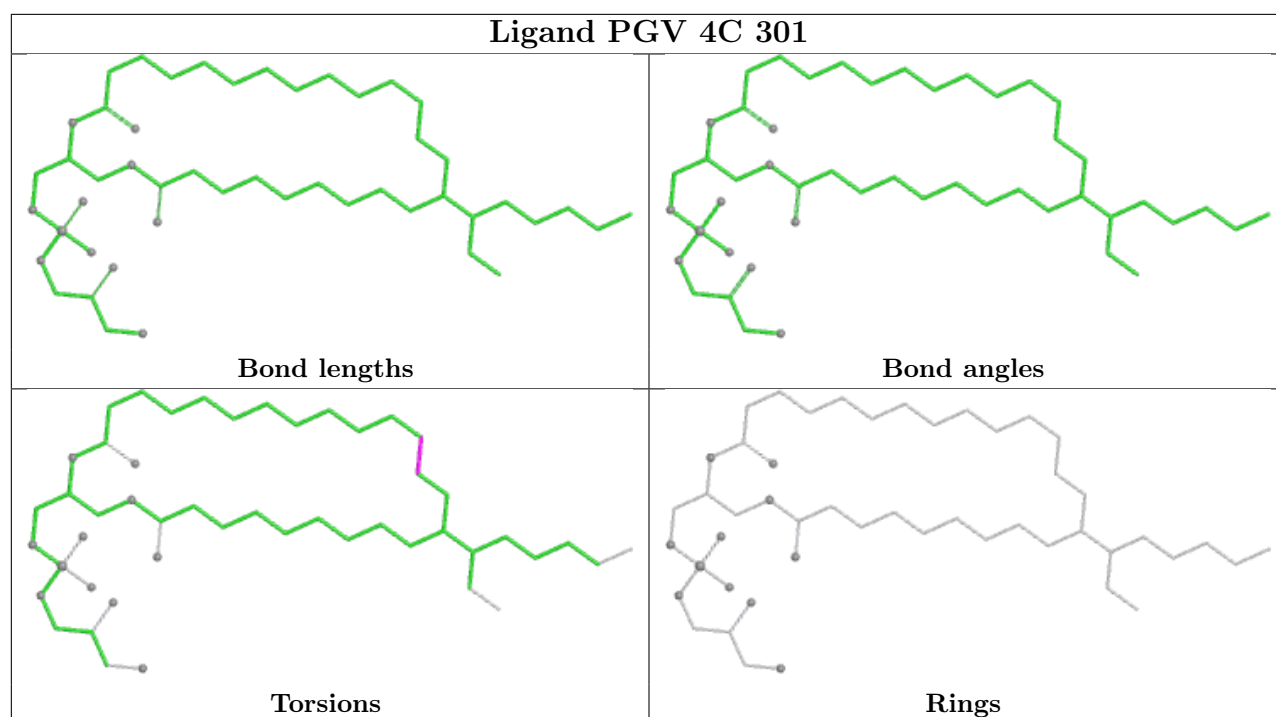


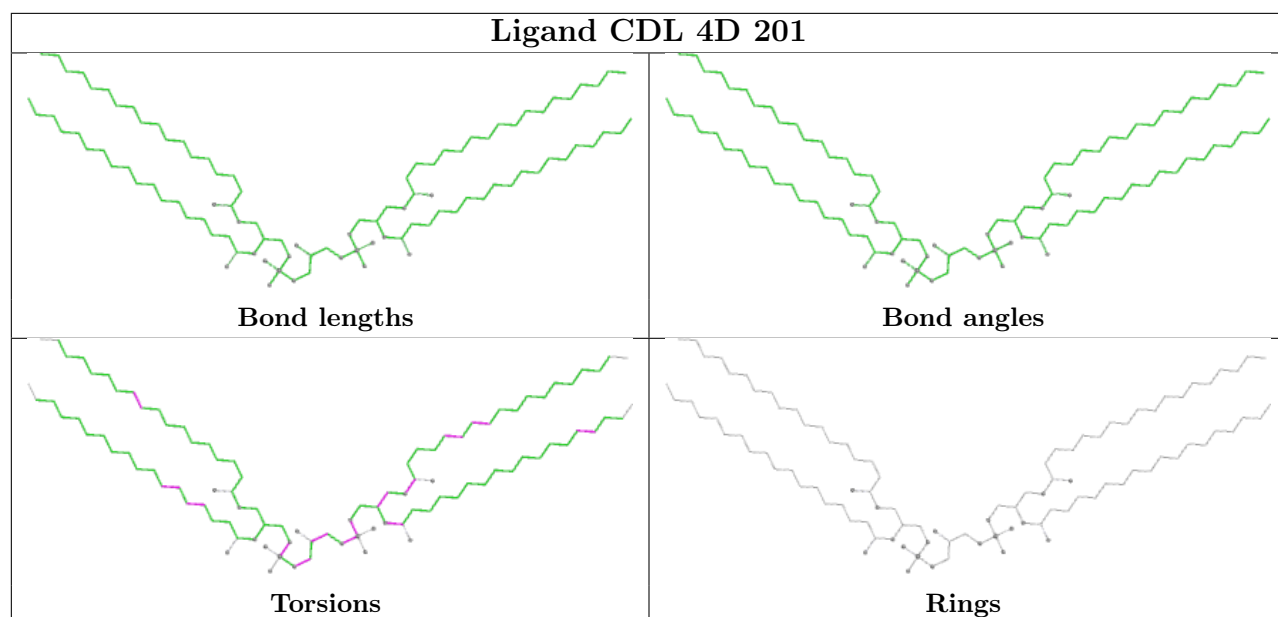
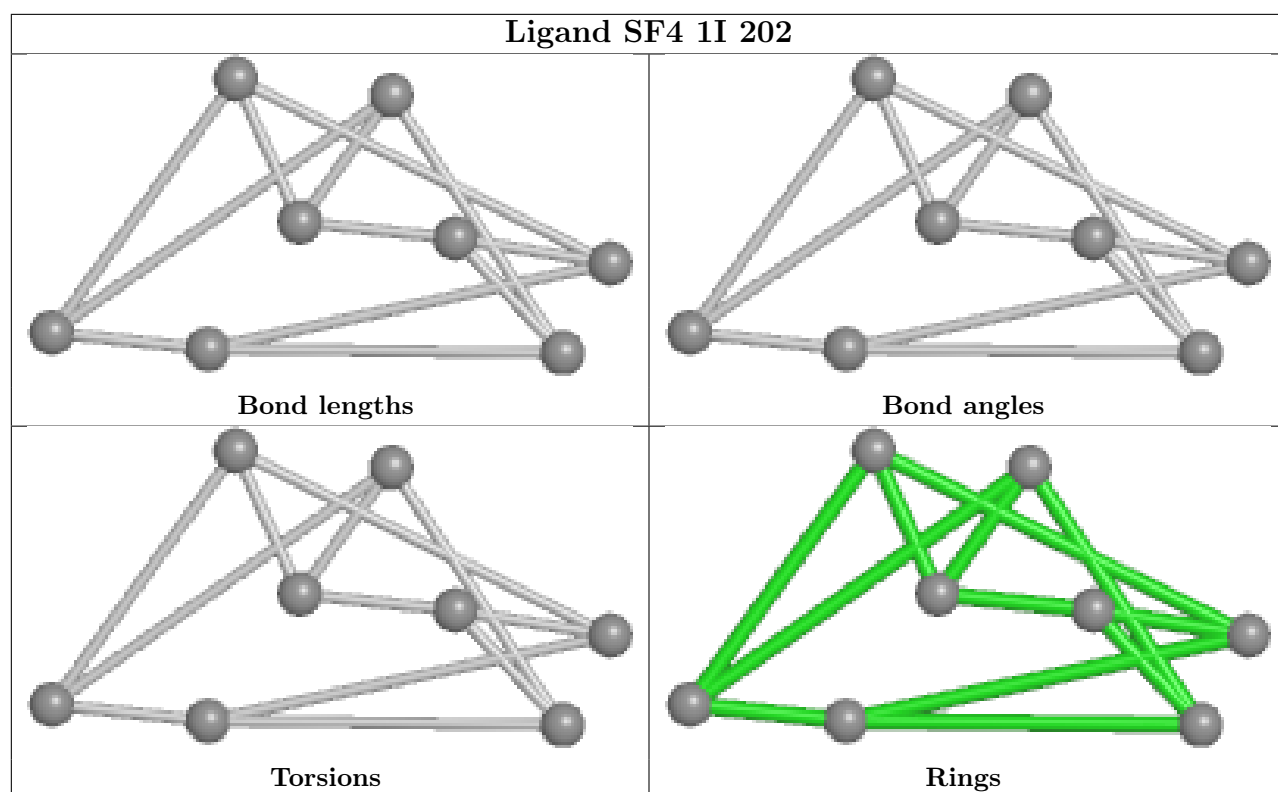


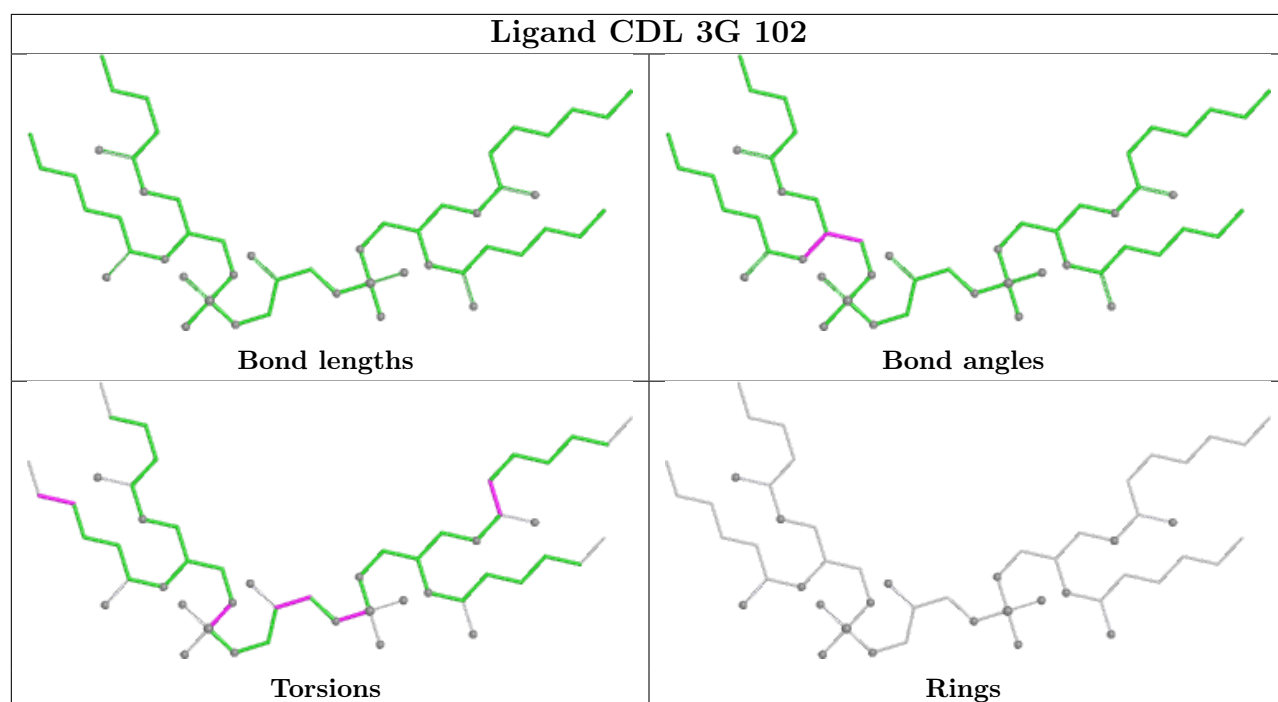
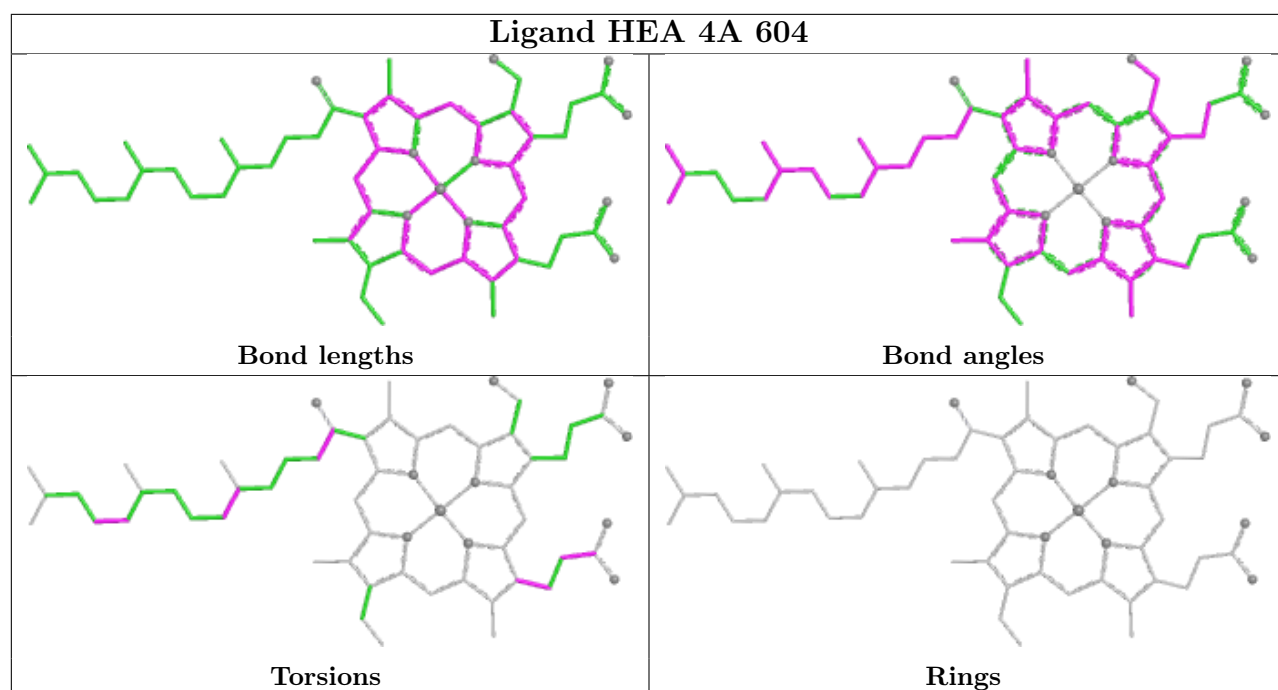




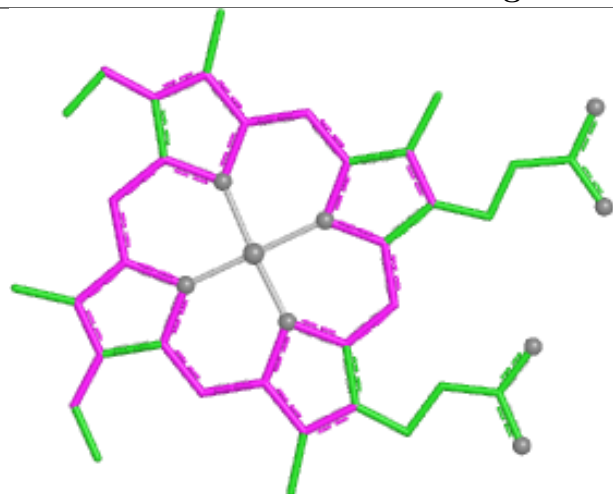




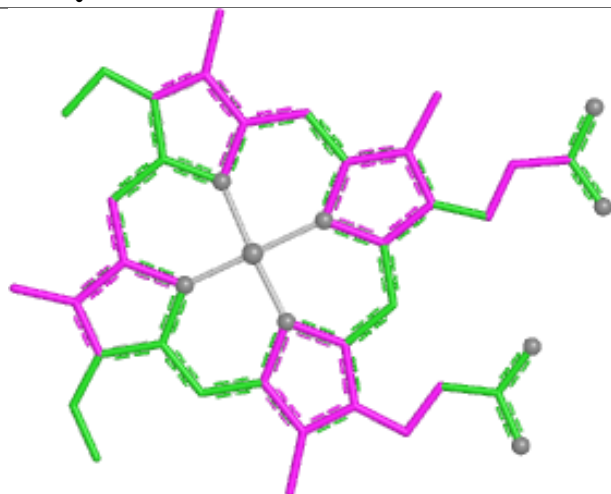




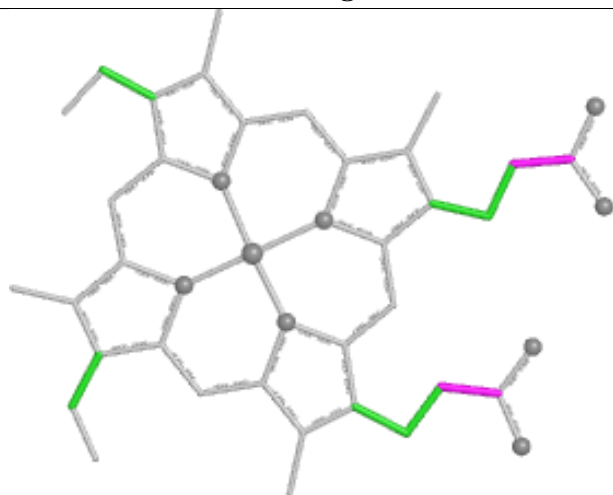
Ligand HEC 3Q 501



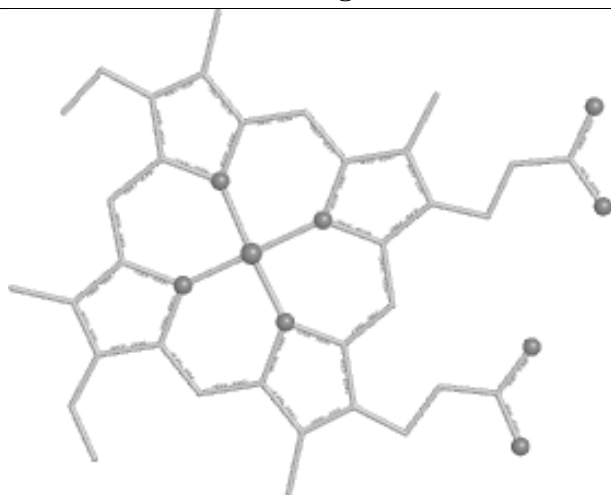
Bond lengths



Bond angles

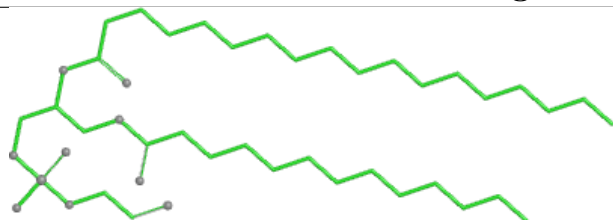


Torsions

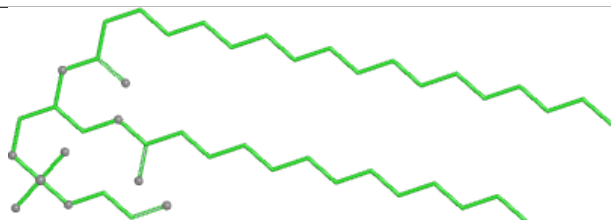


Rings

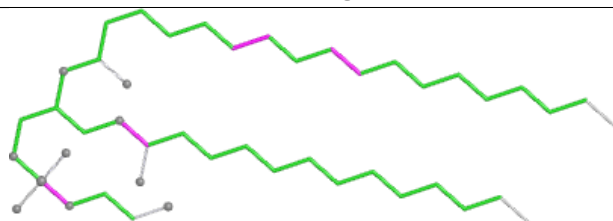
Ligand 3PE 1L 701



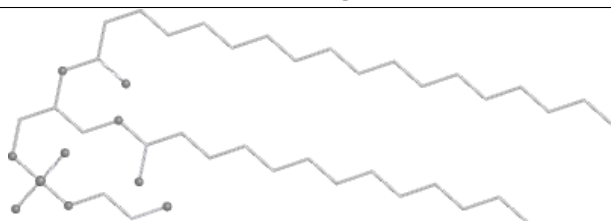
Bond lengths



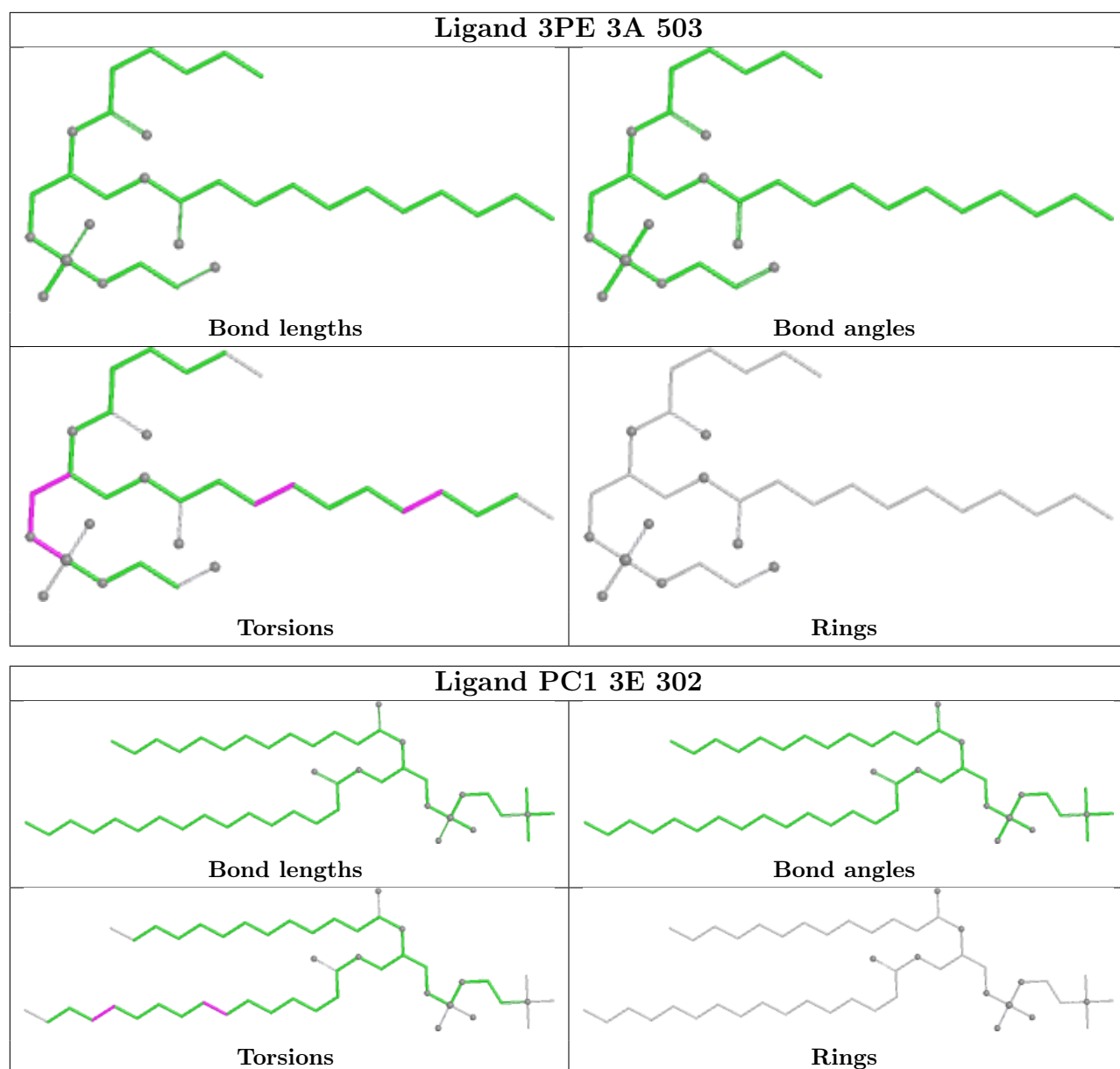
Bond angles

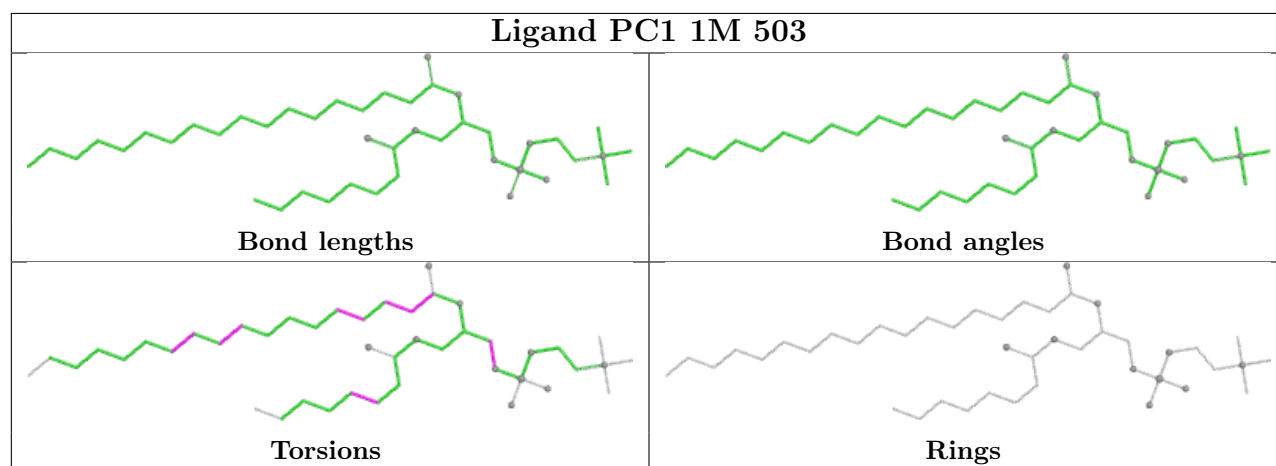
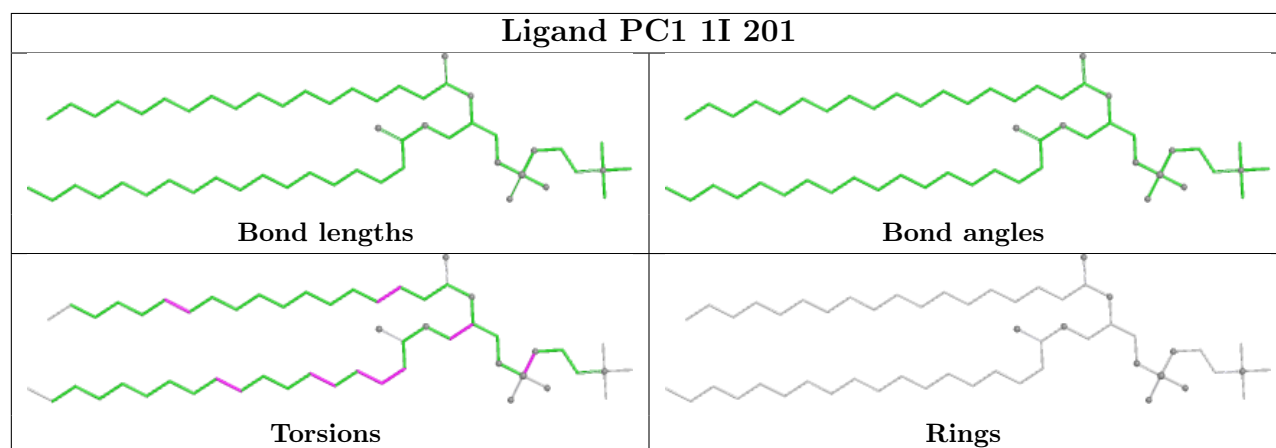
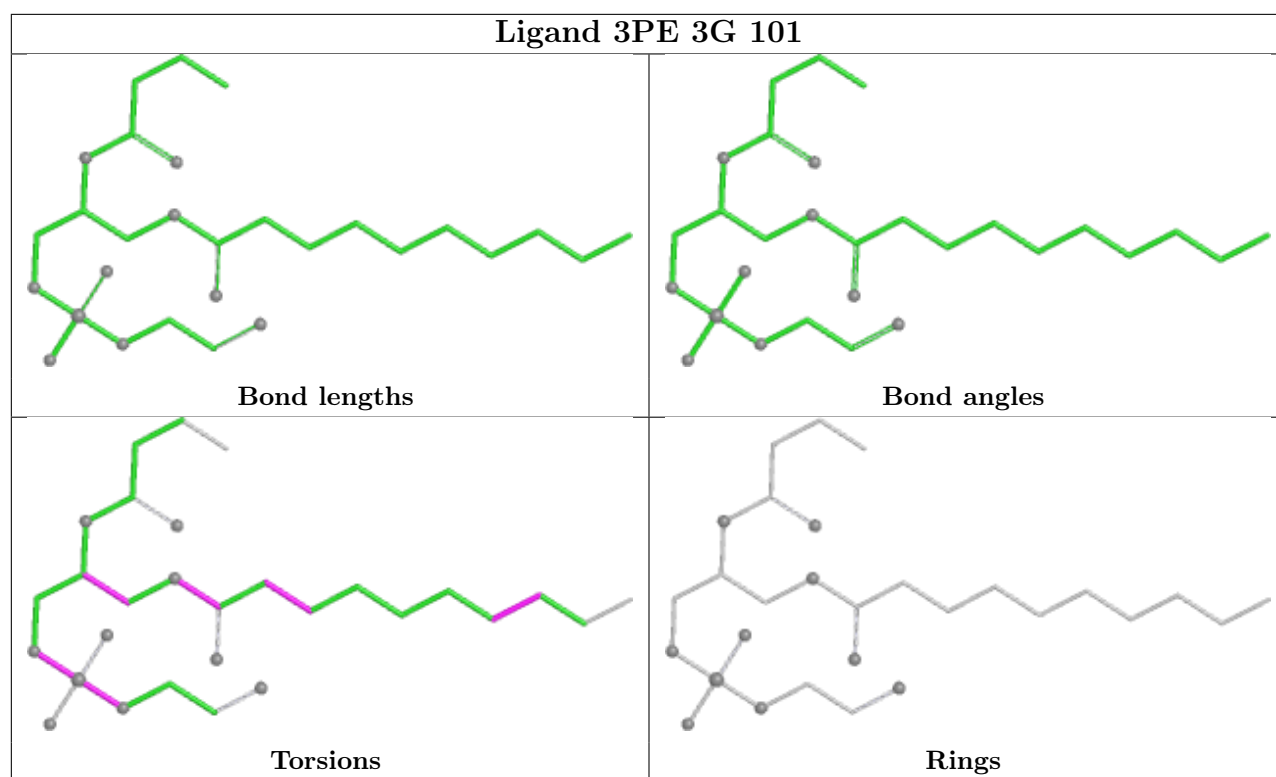


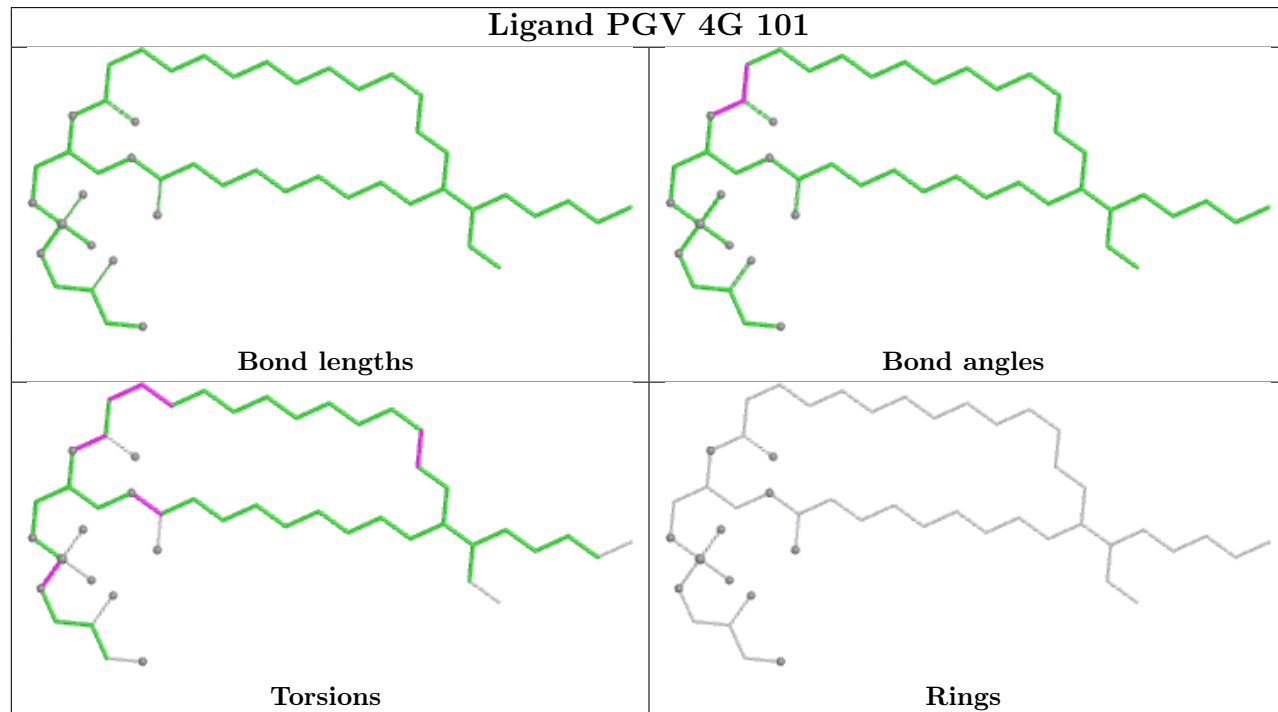
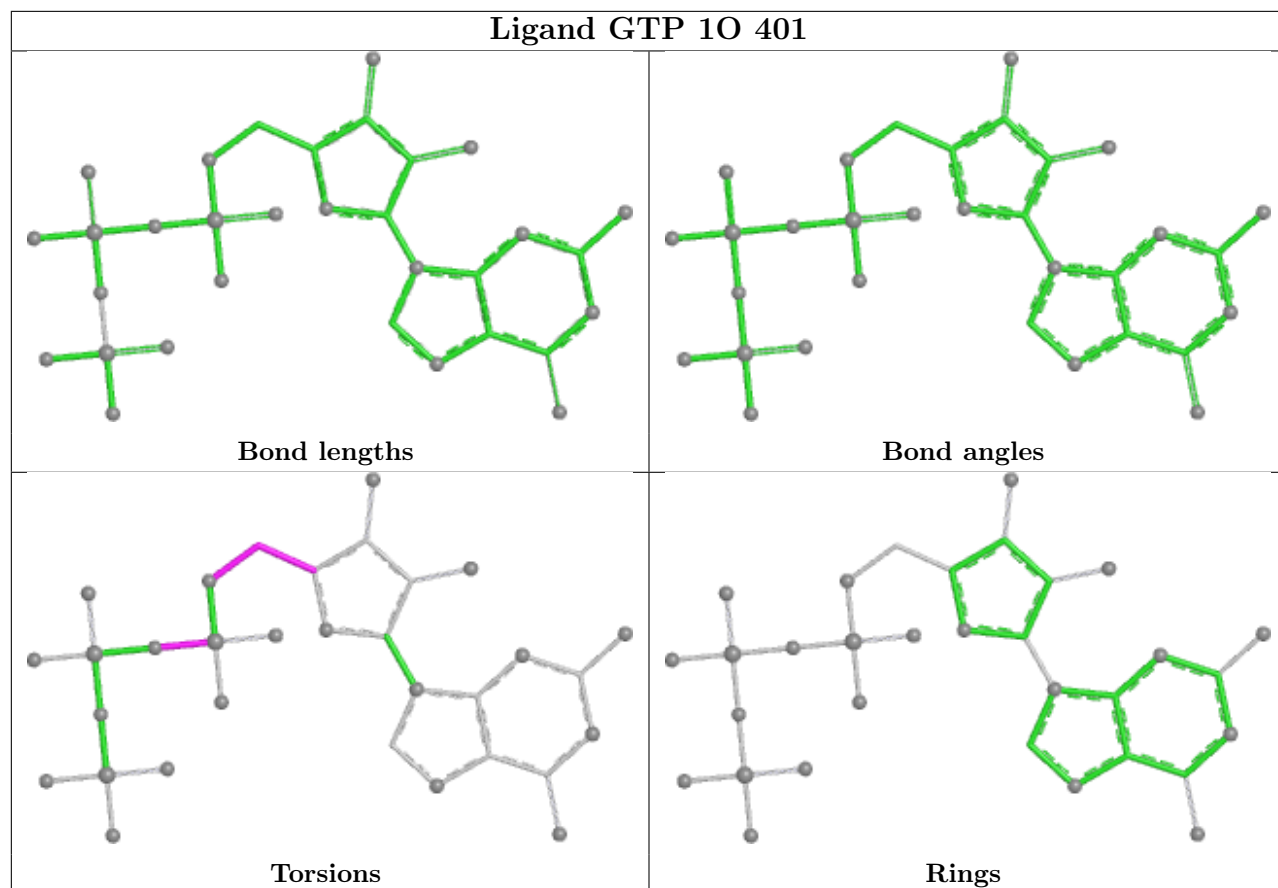
Torsions

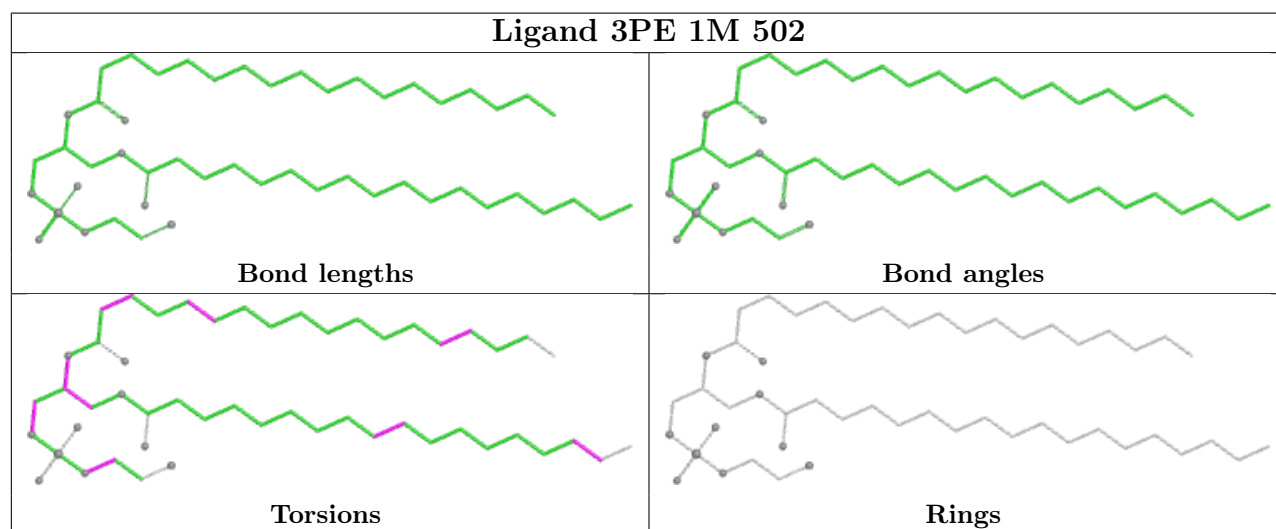
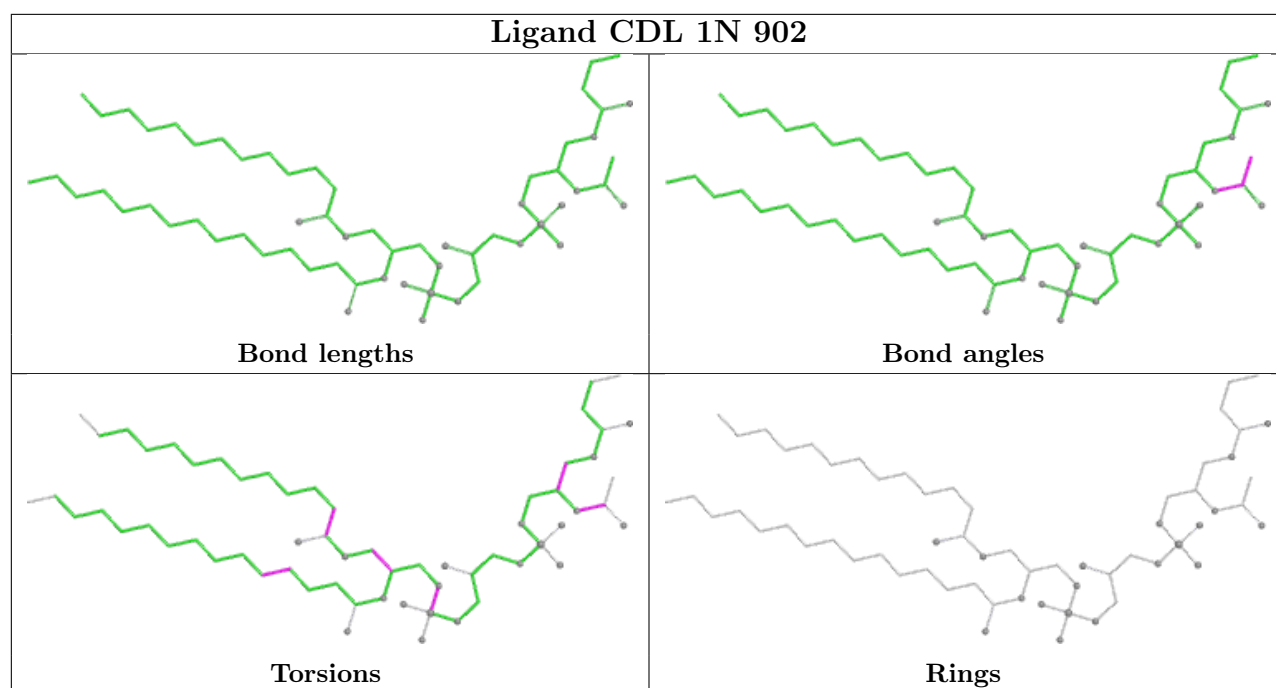


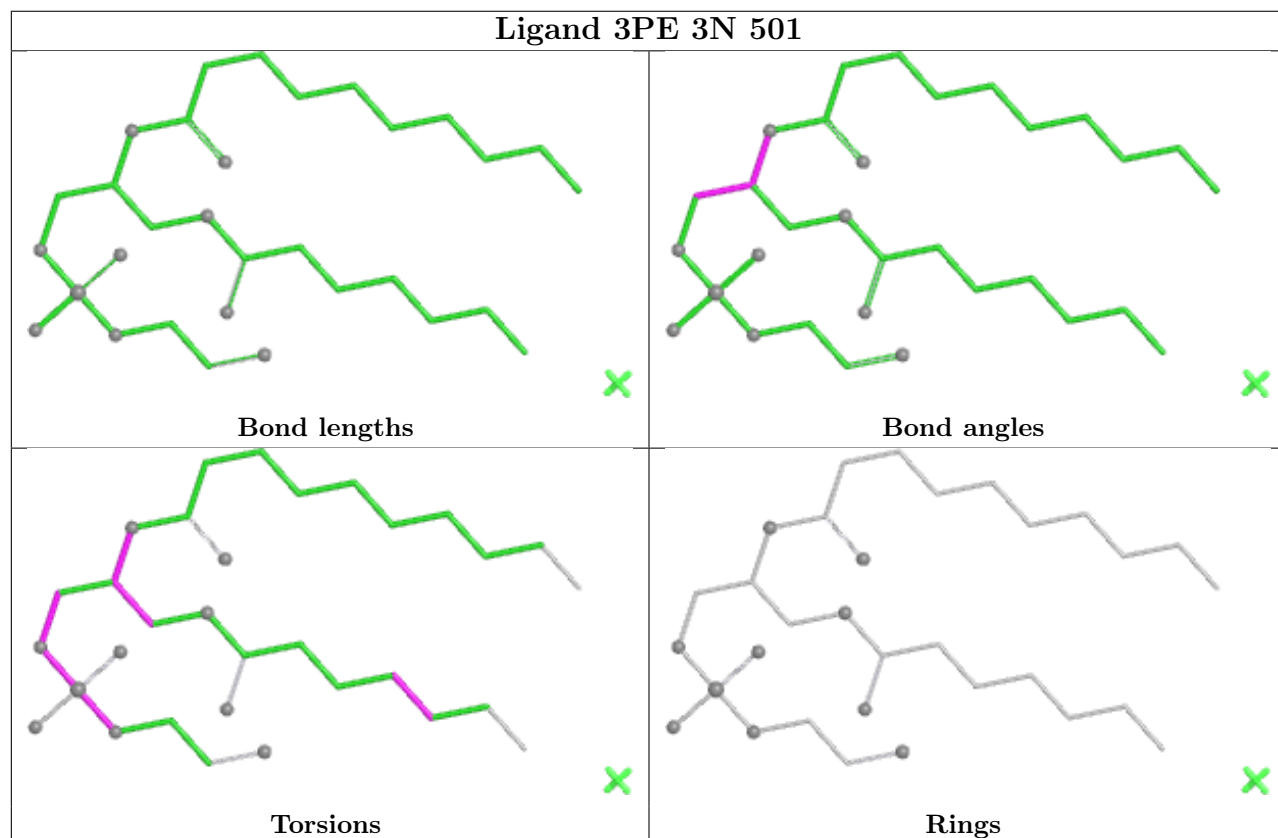
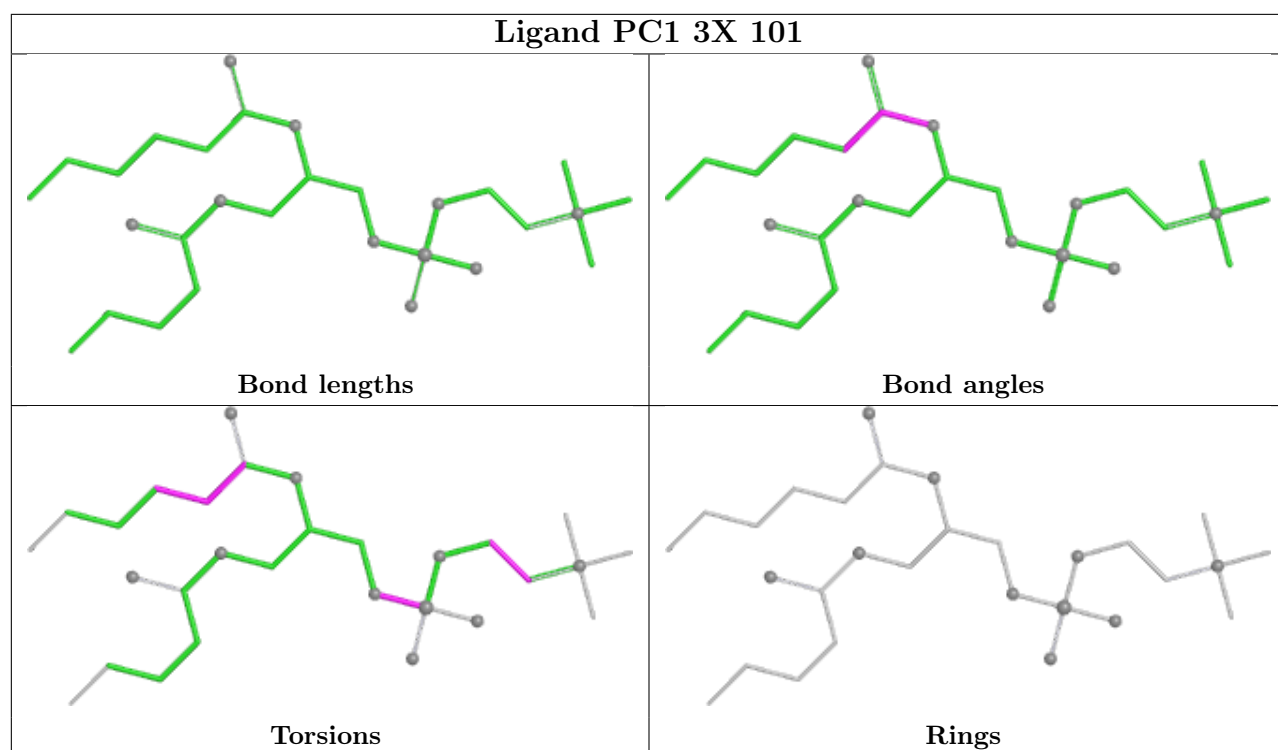
Rings

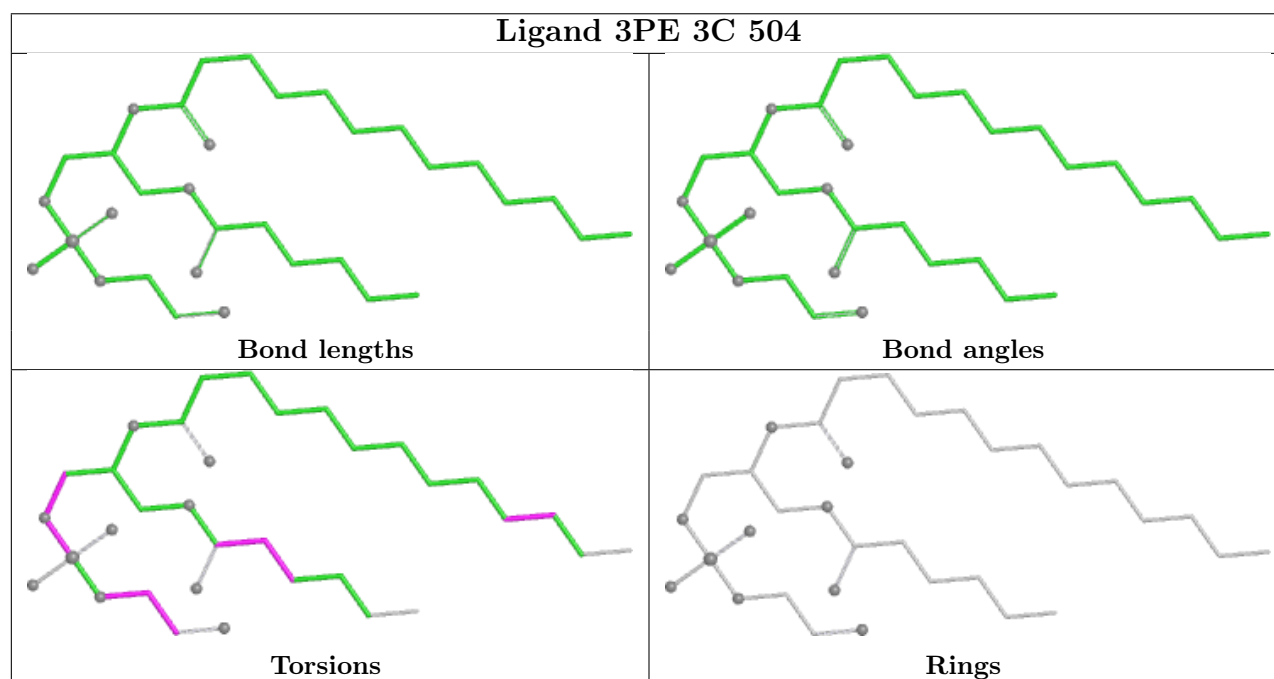
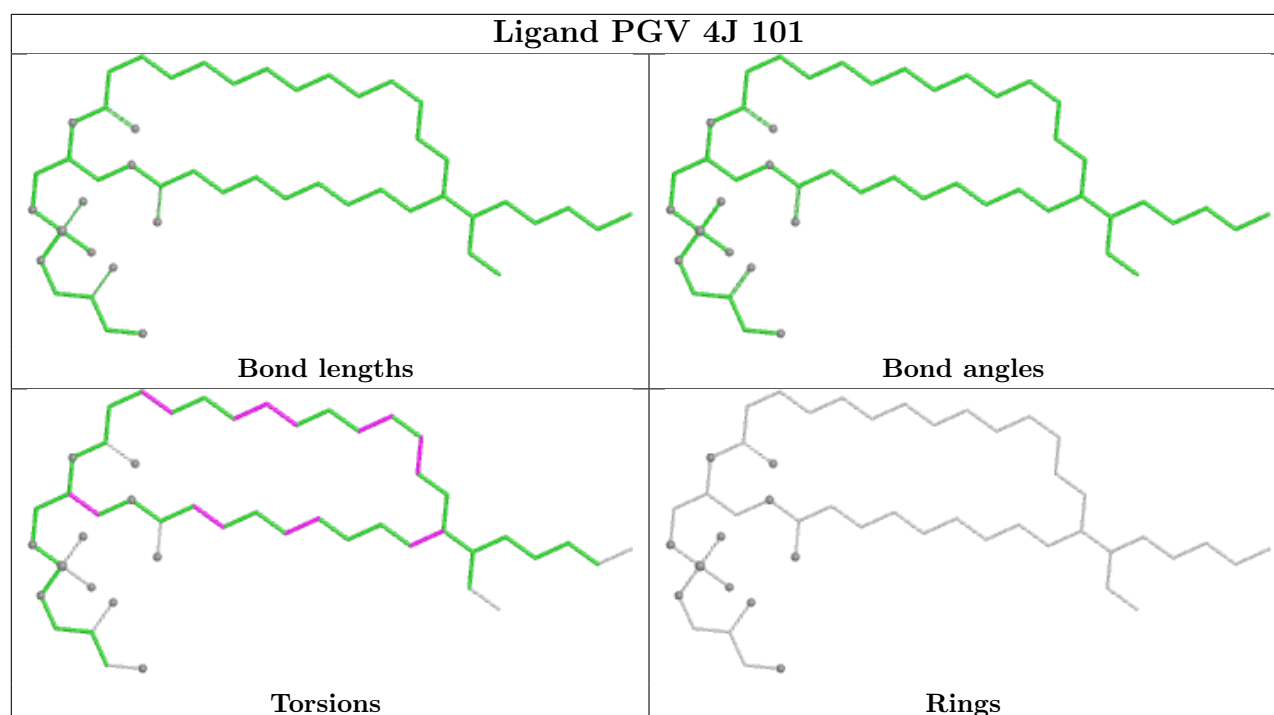


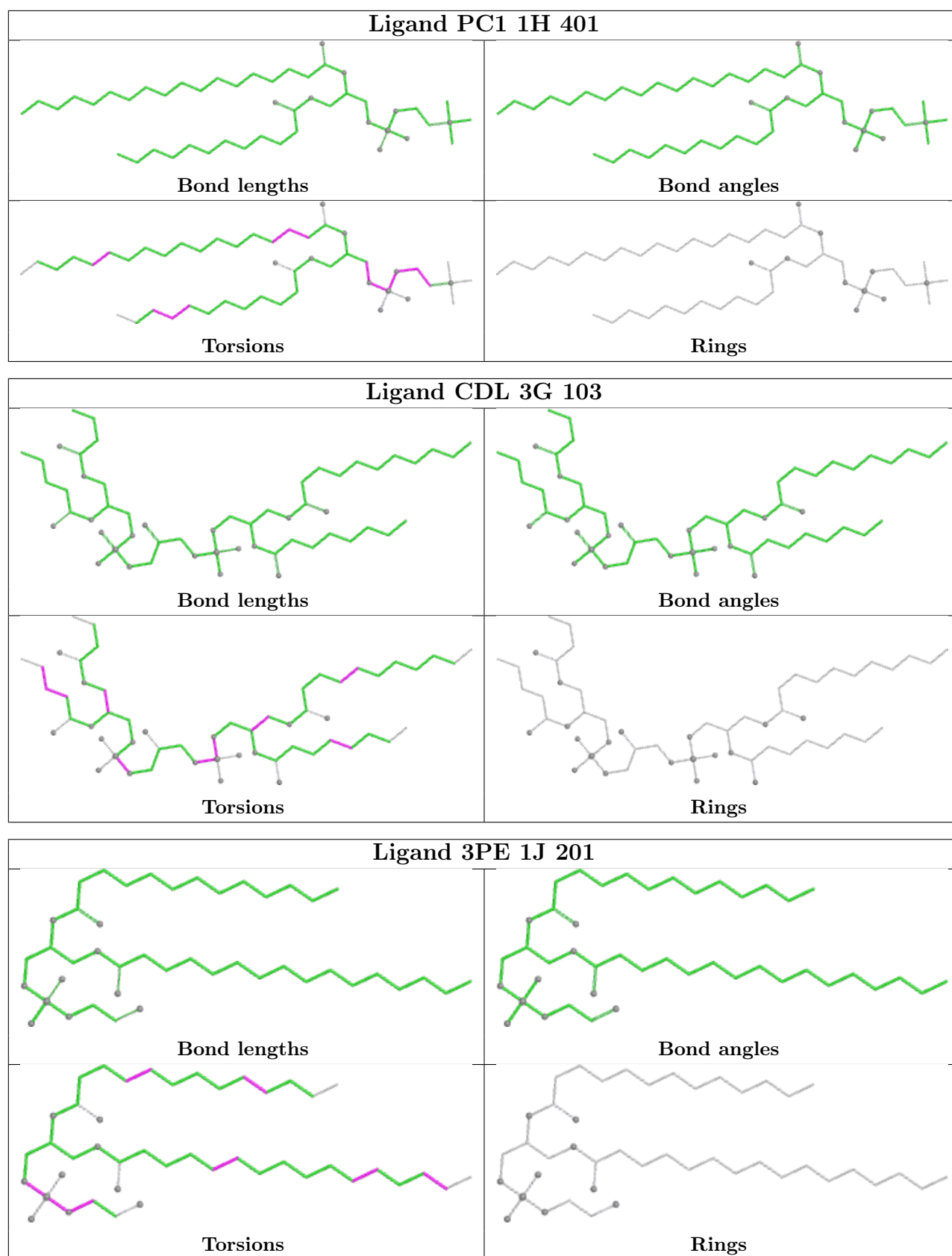


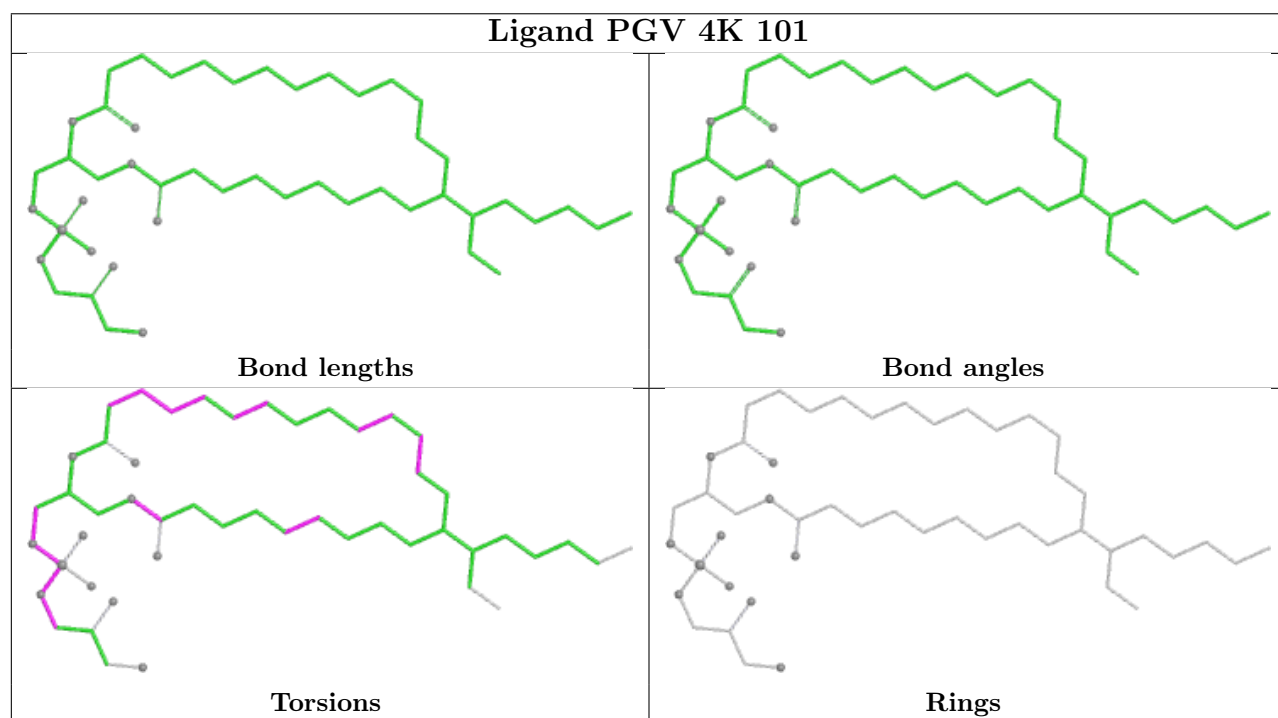
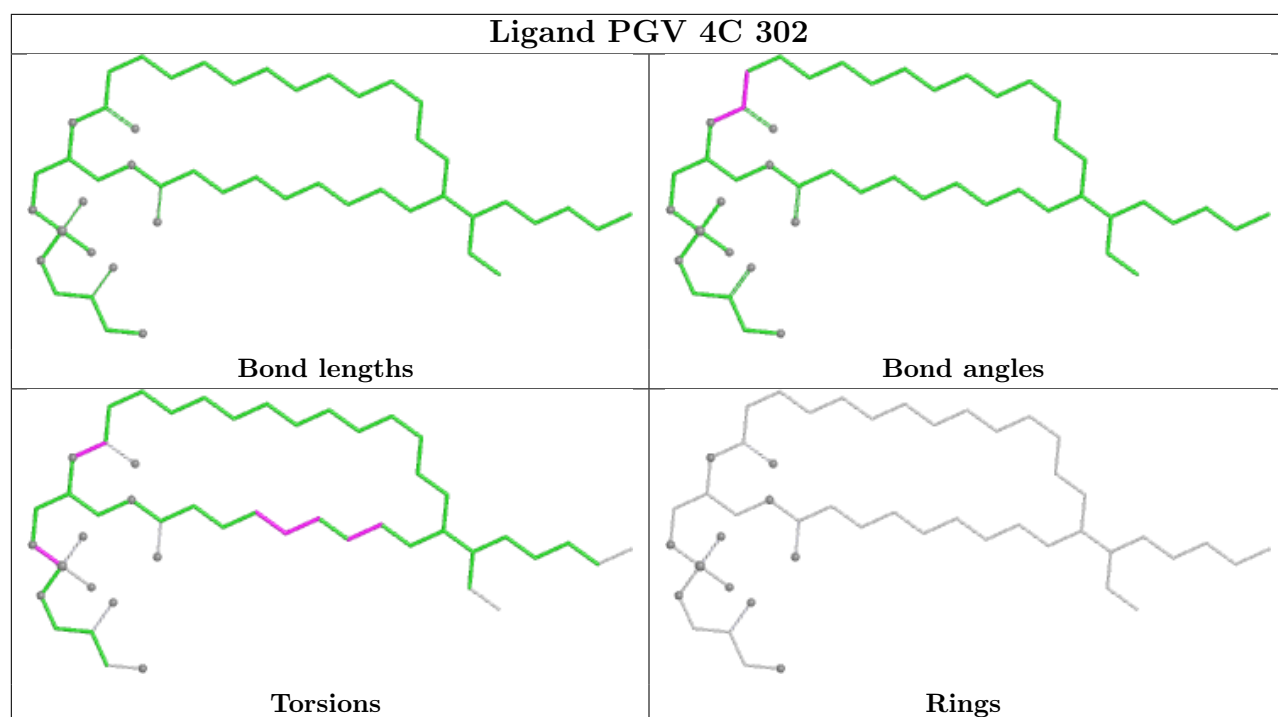


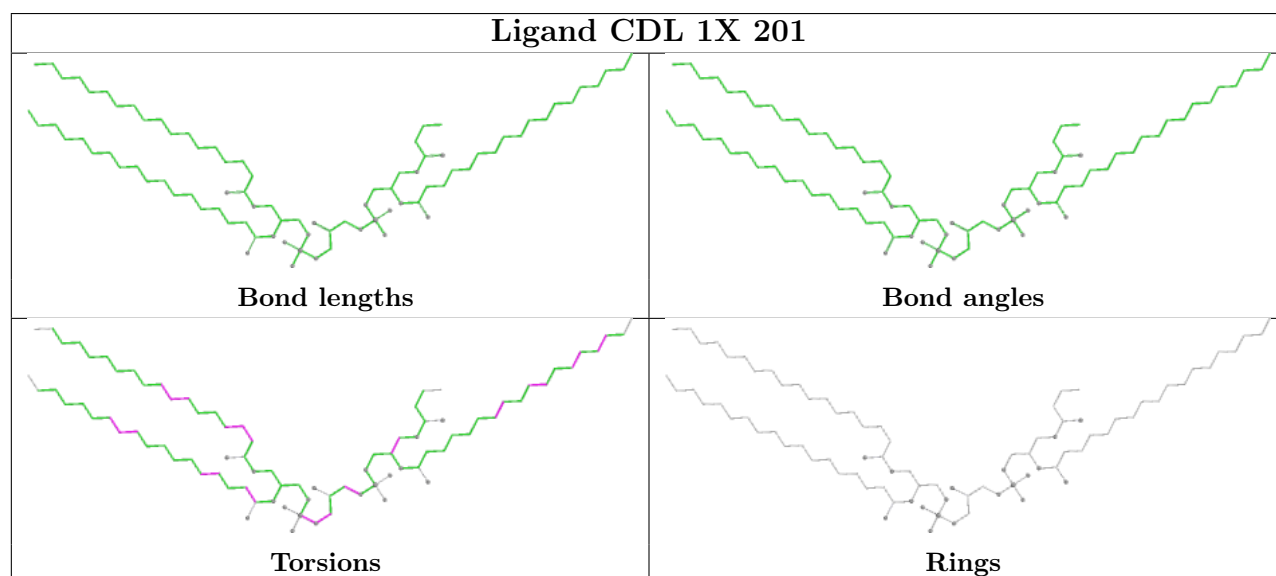
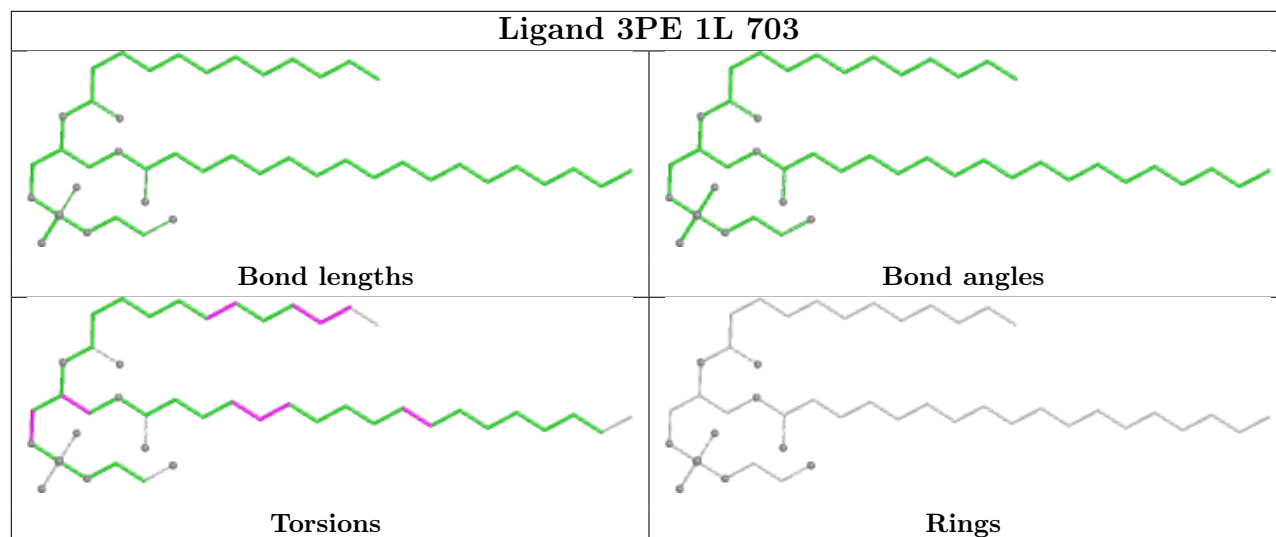


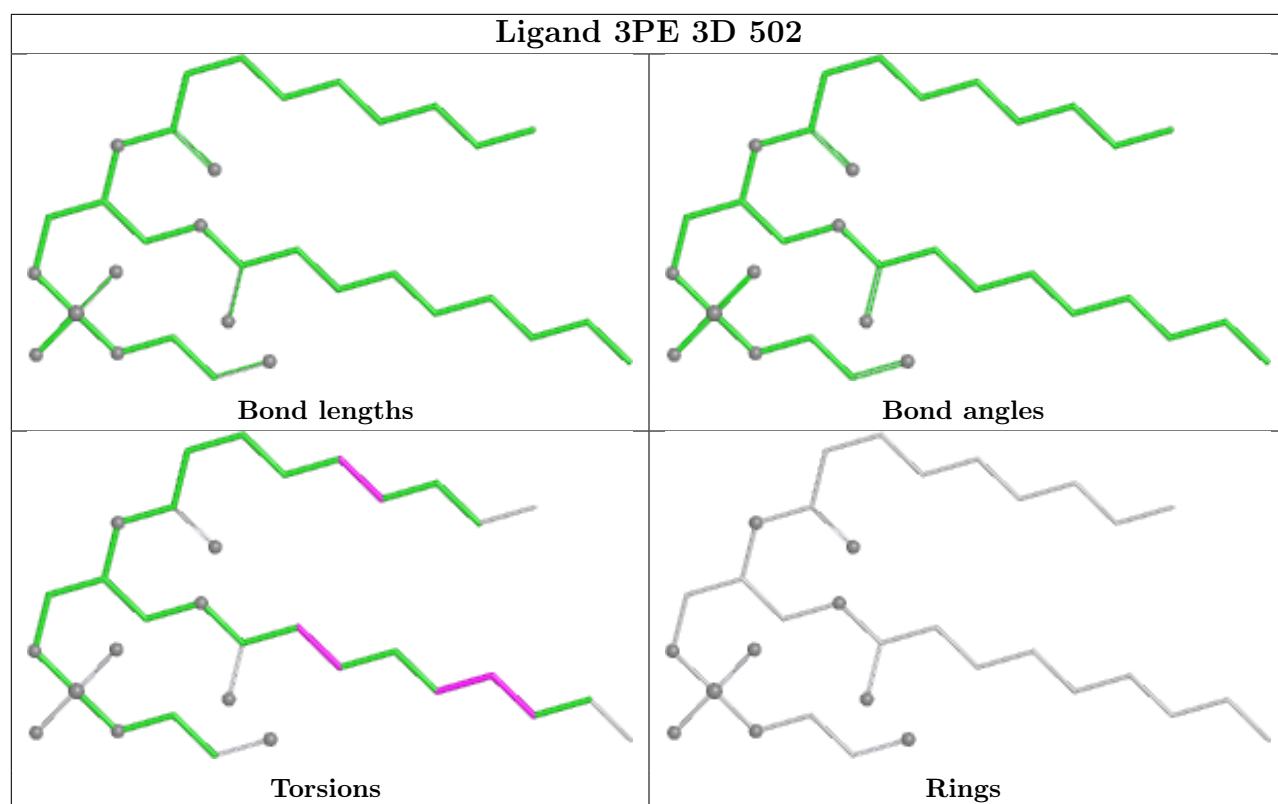




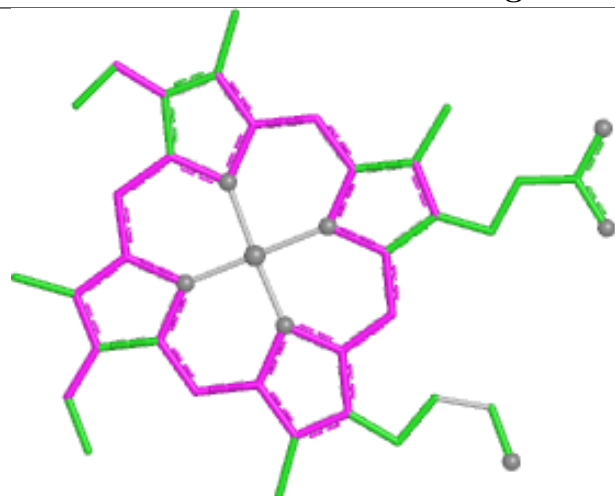




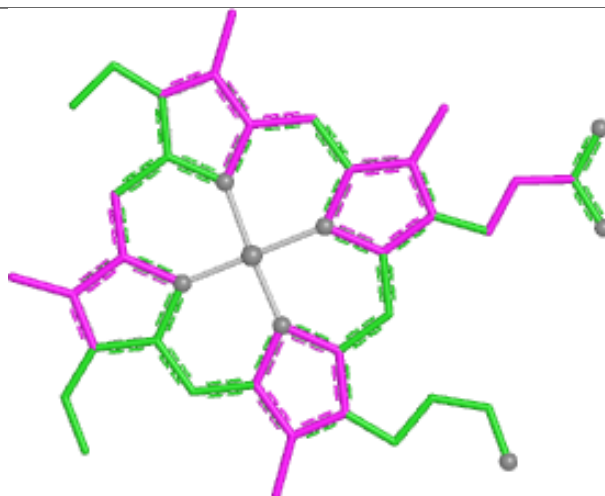




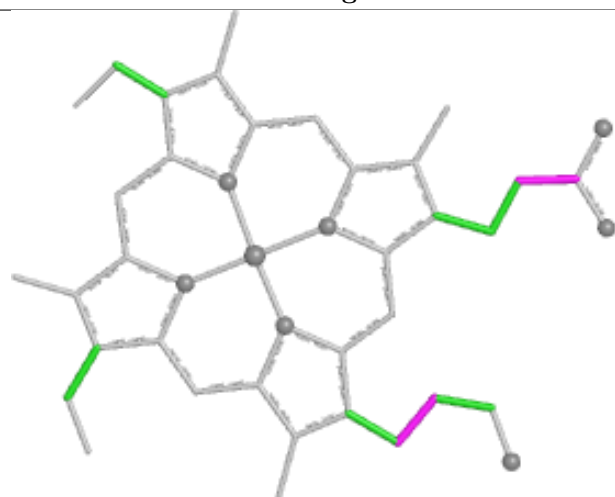
Ligand HEC 3D 501



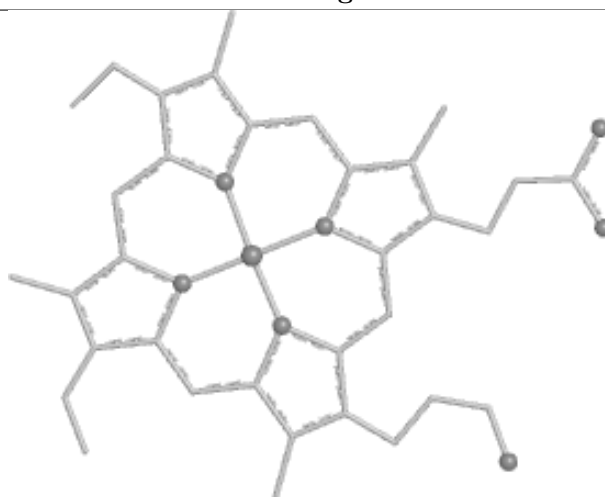
Bond lengths



Bond angles

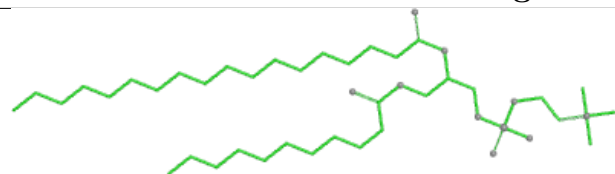


Torsions

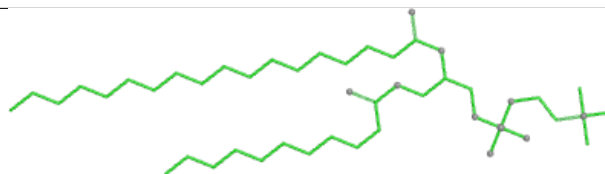


Rings

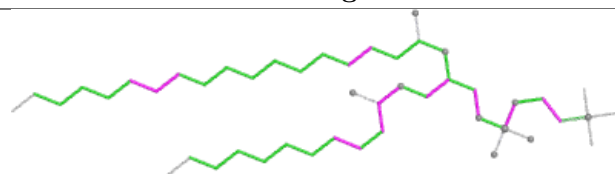
Ligand PC1 1h 203



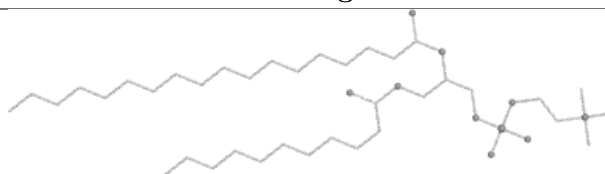
Bond lengths



Bond angles

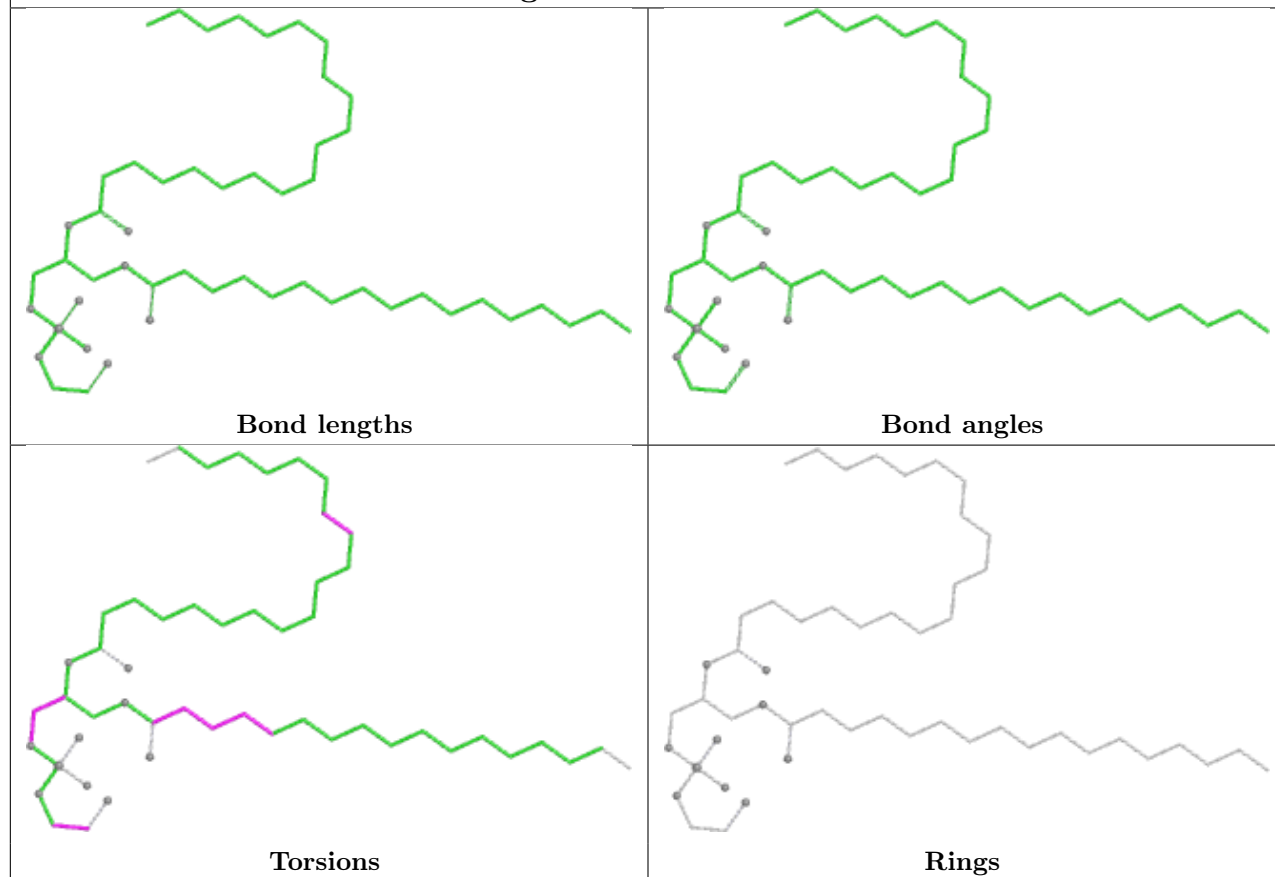


Torsions

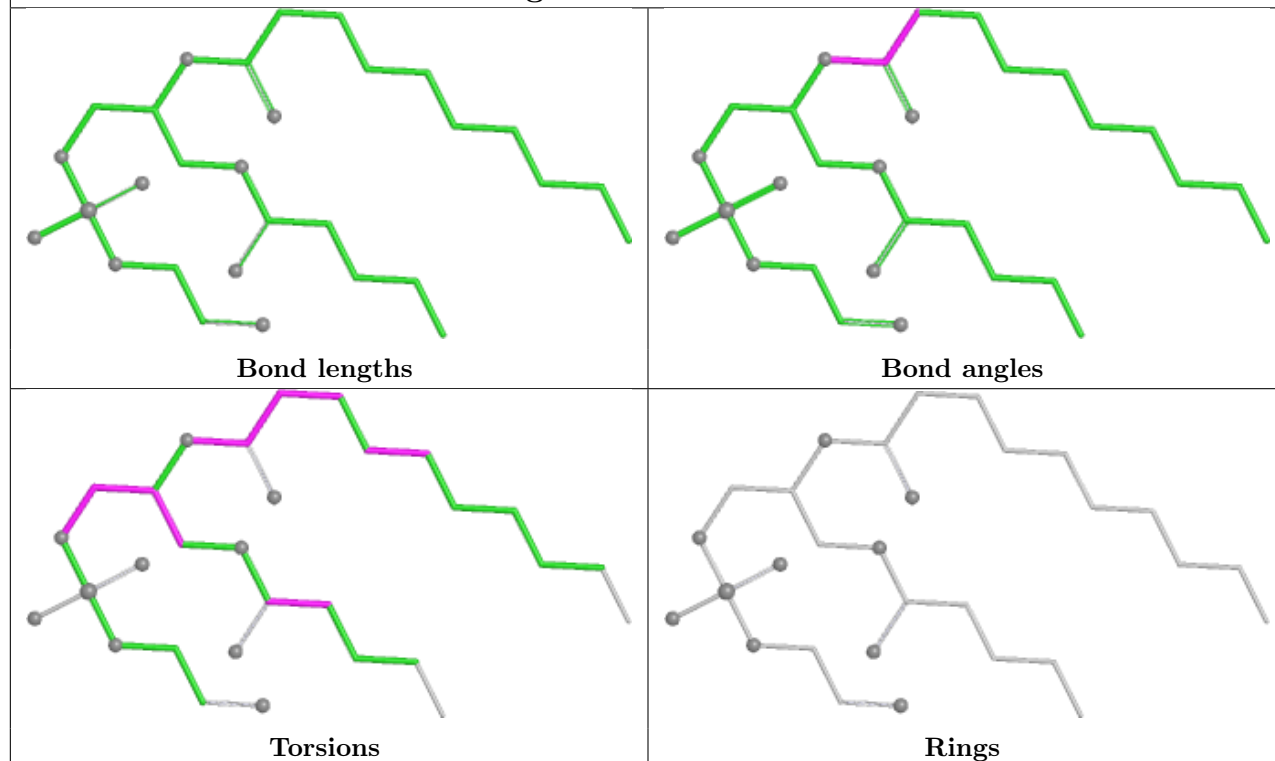


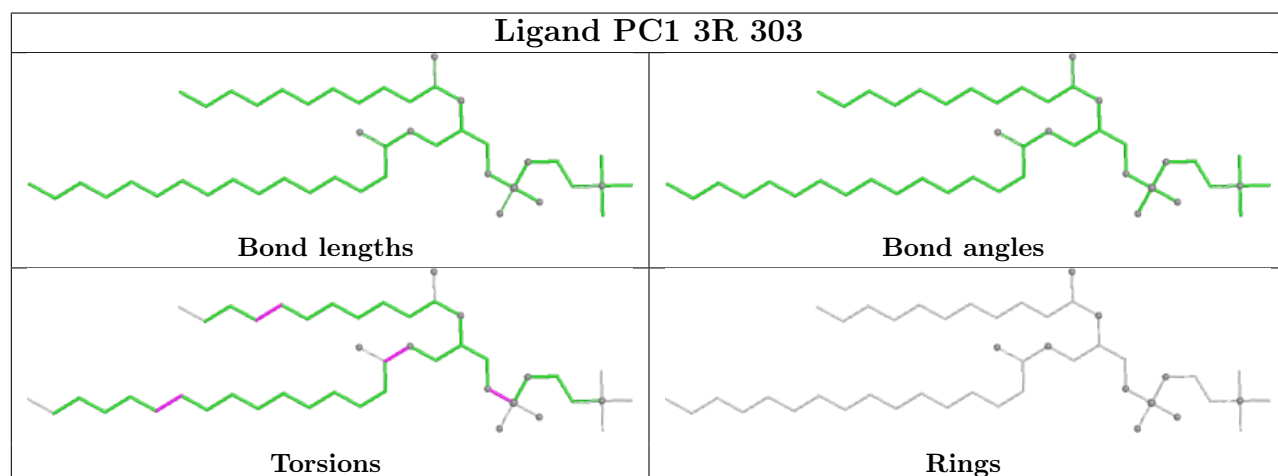
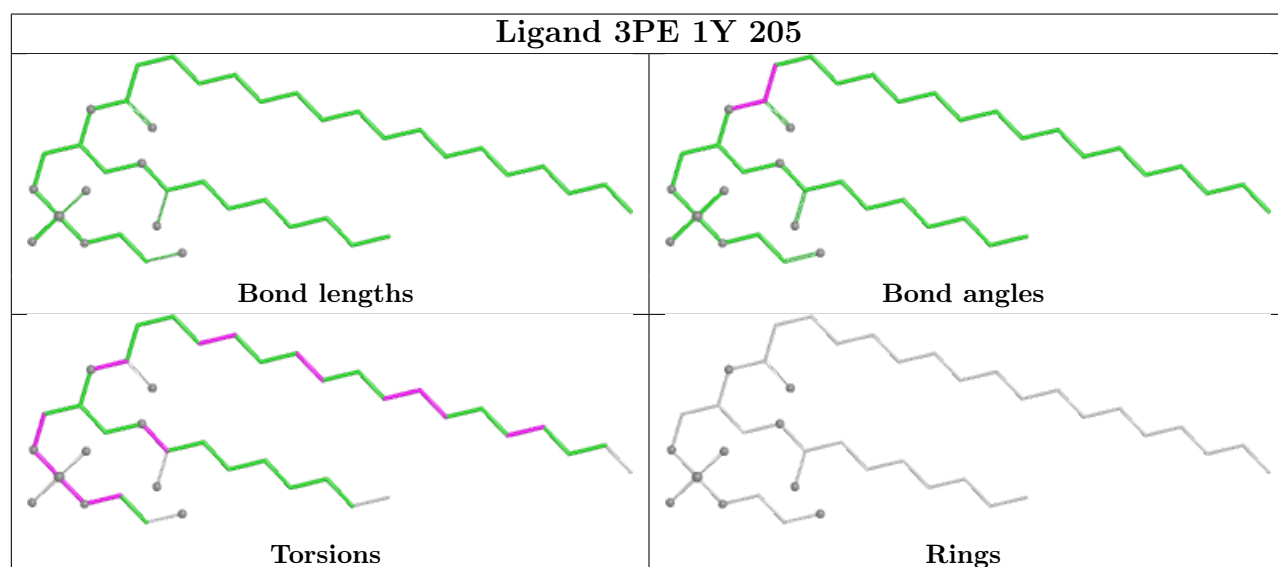
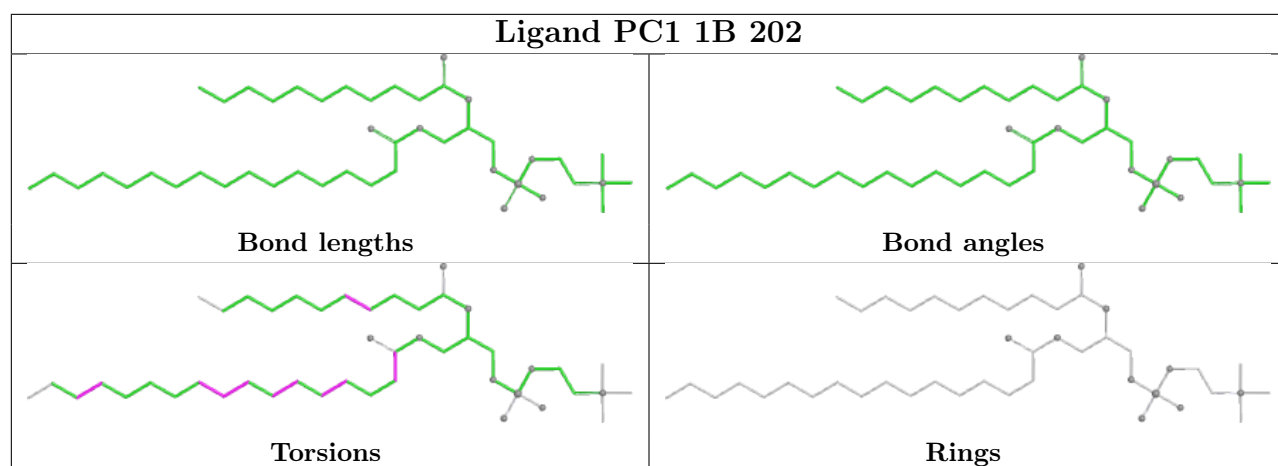
Rings

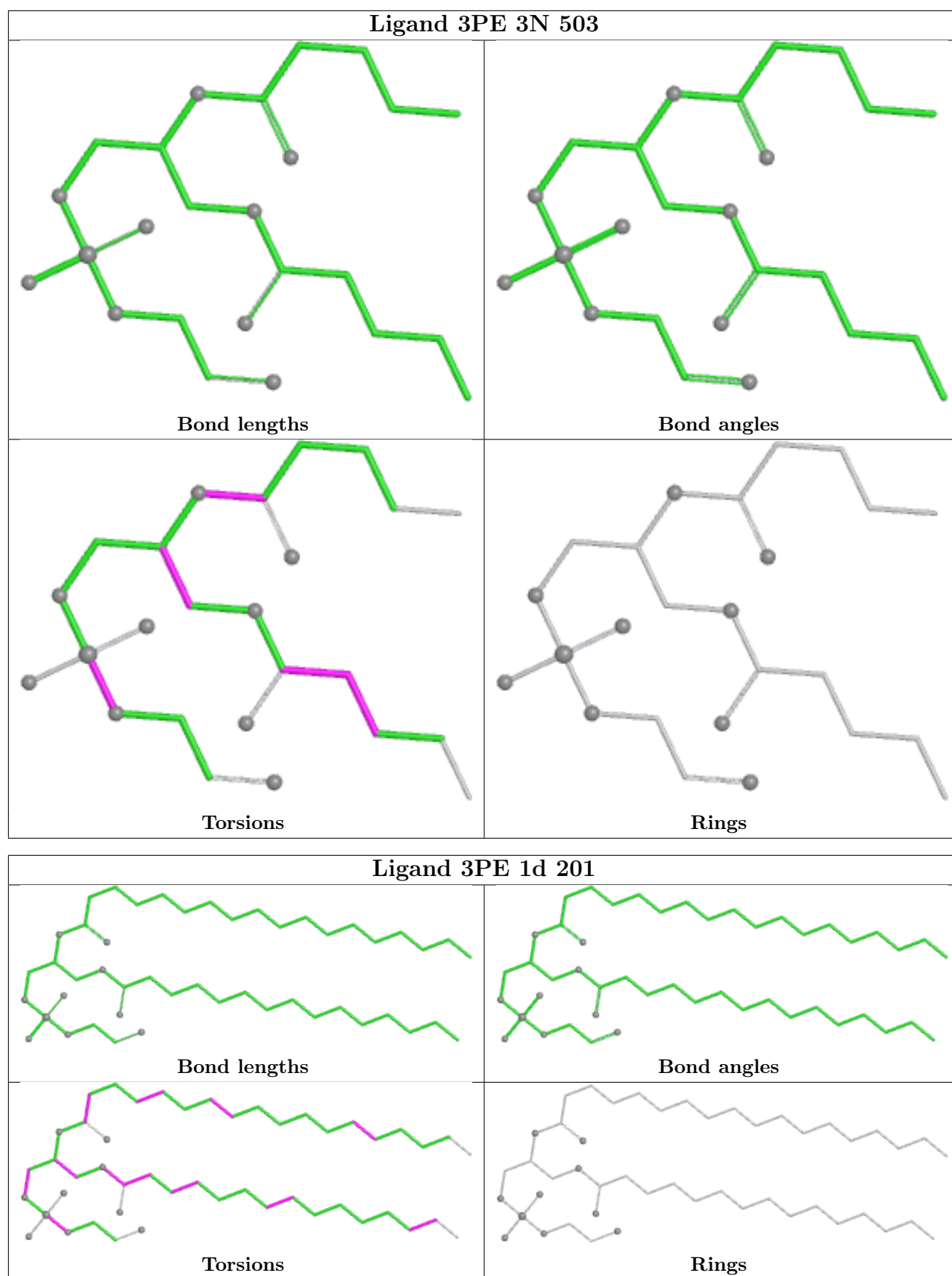
Ligand PEK 4G 103

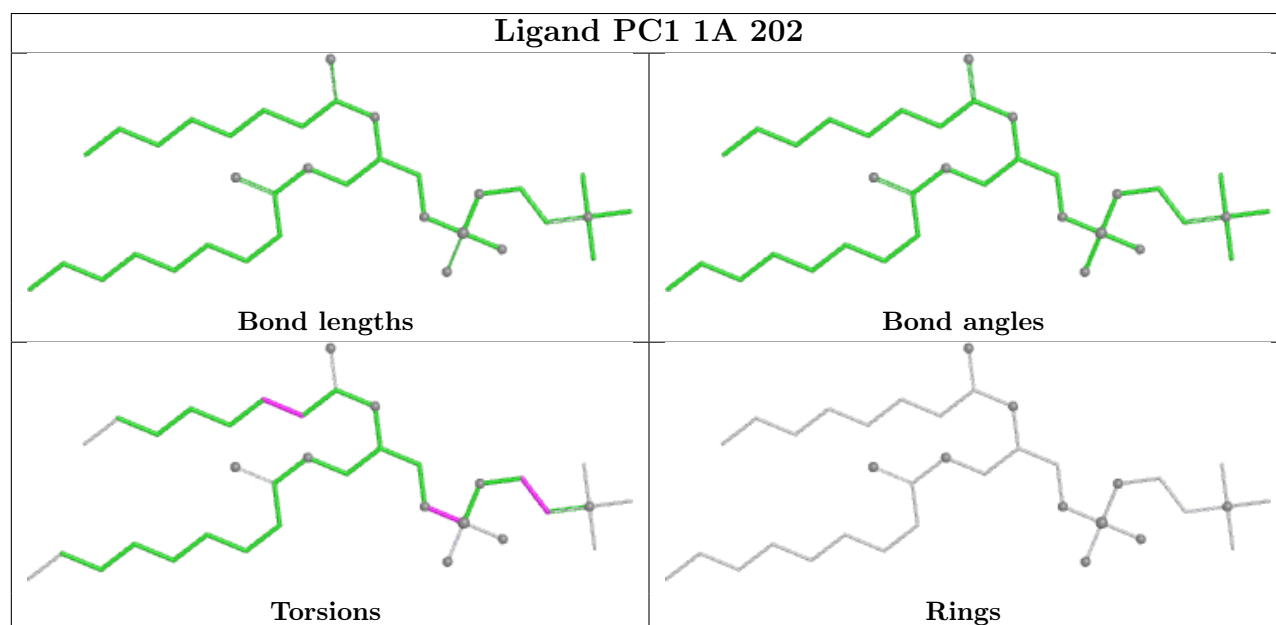
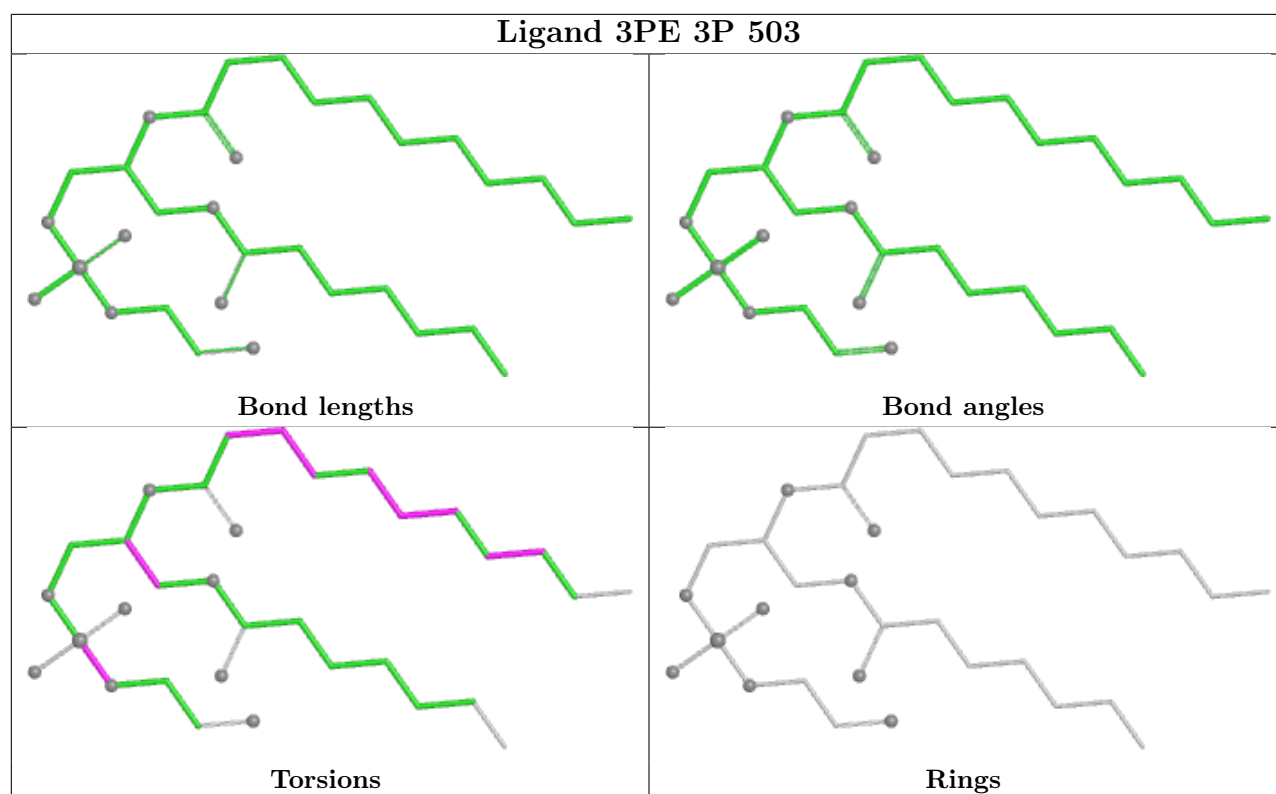


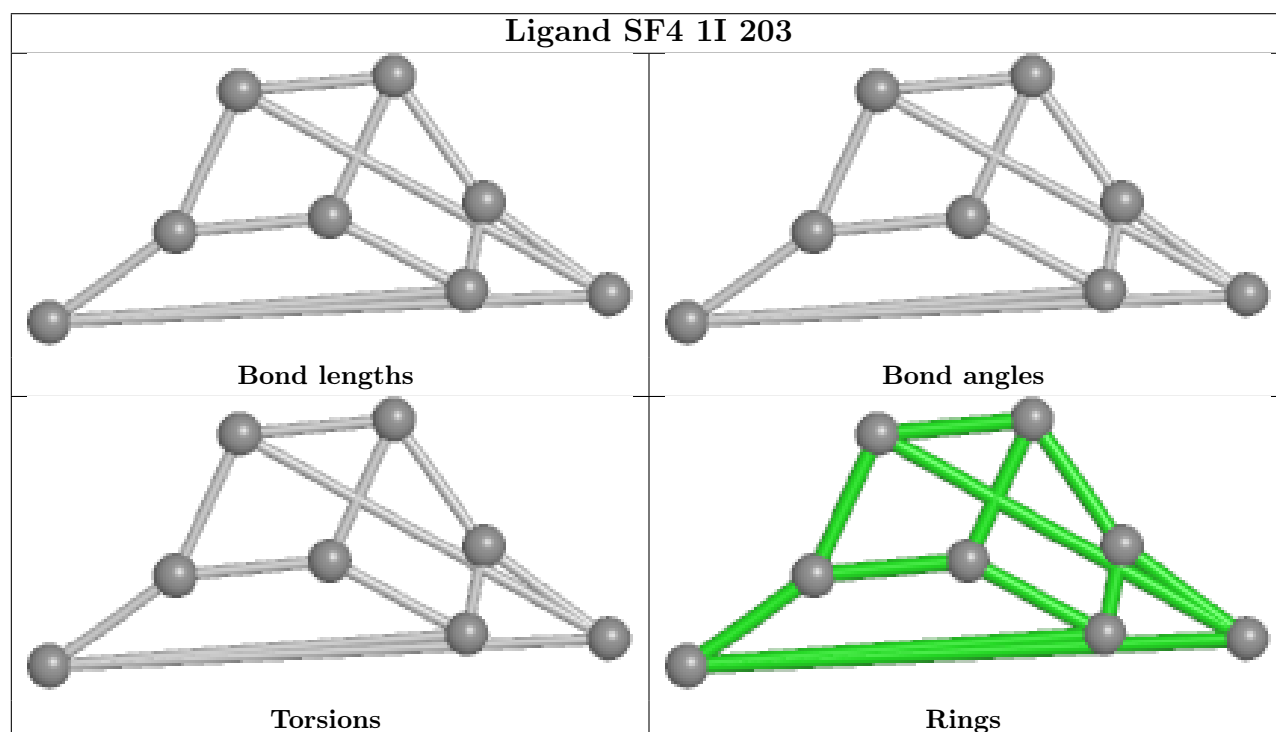
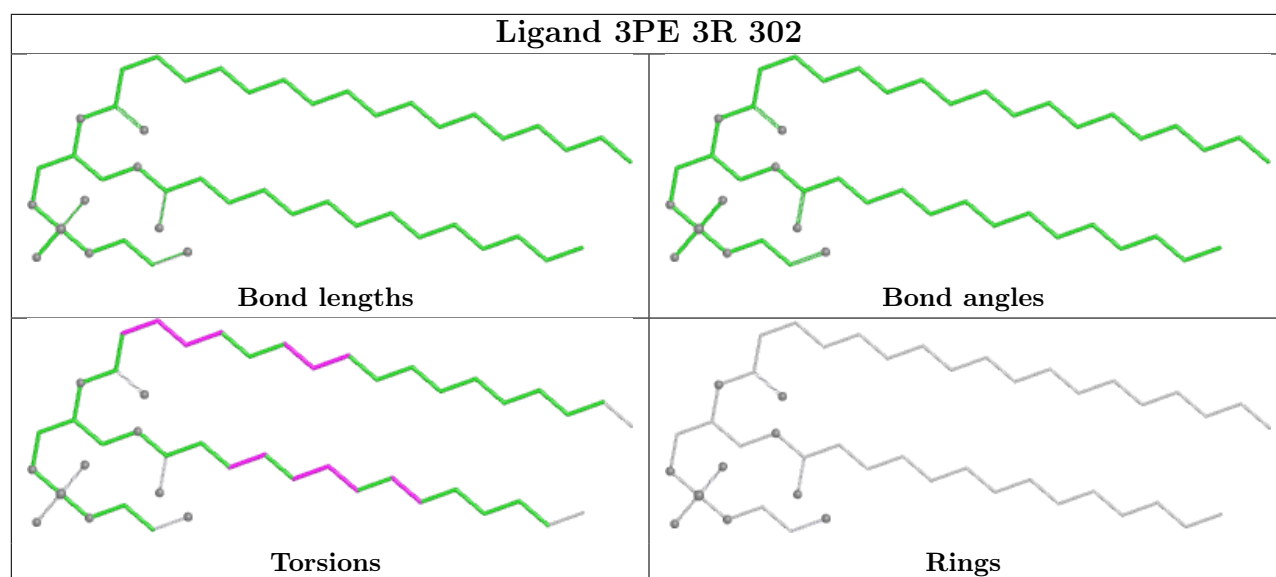
Ligand 3PE 1Y 203

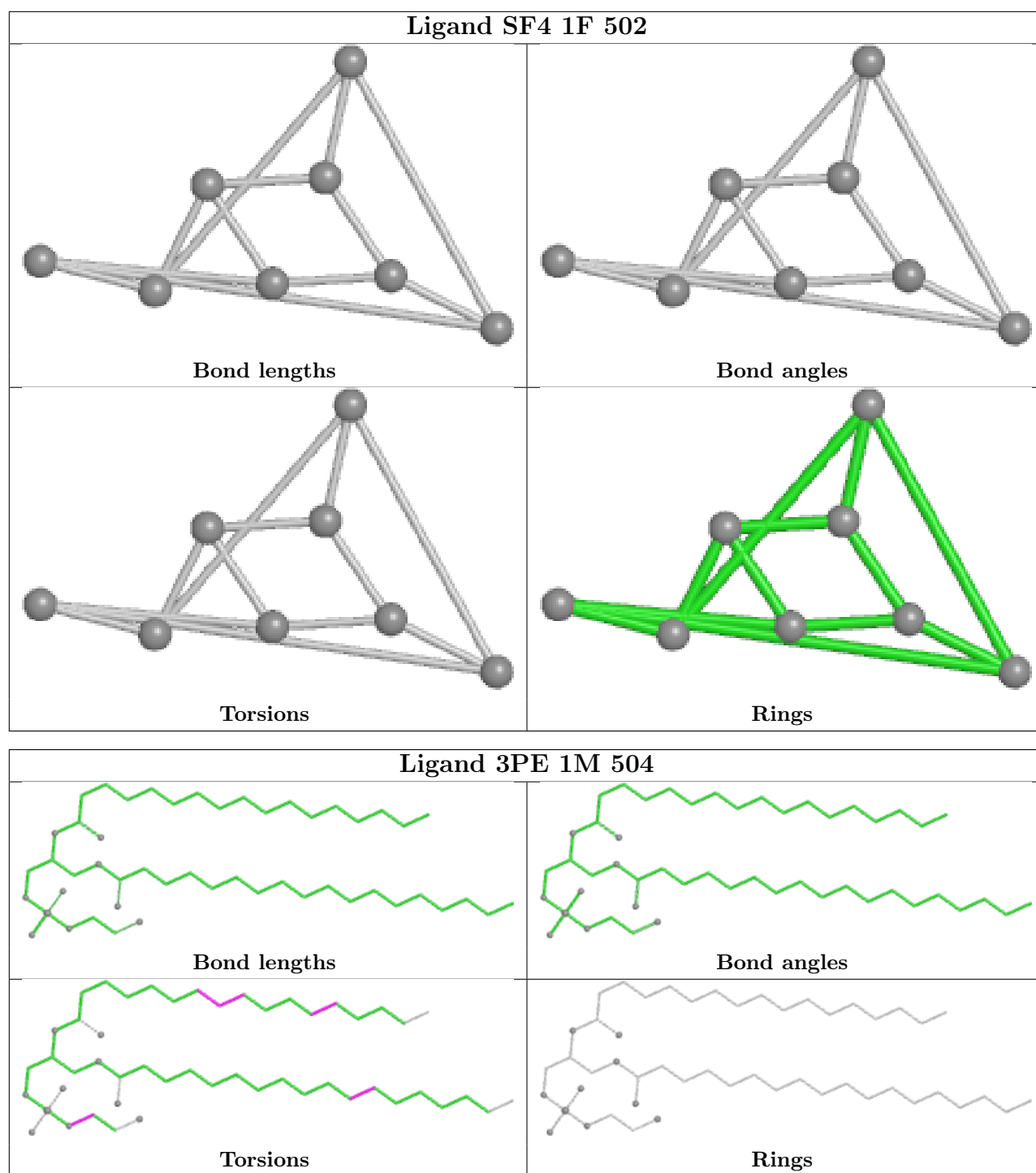


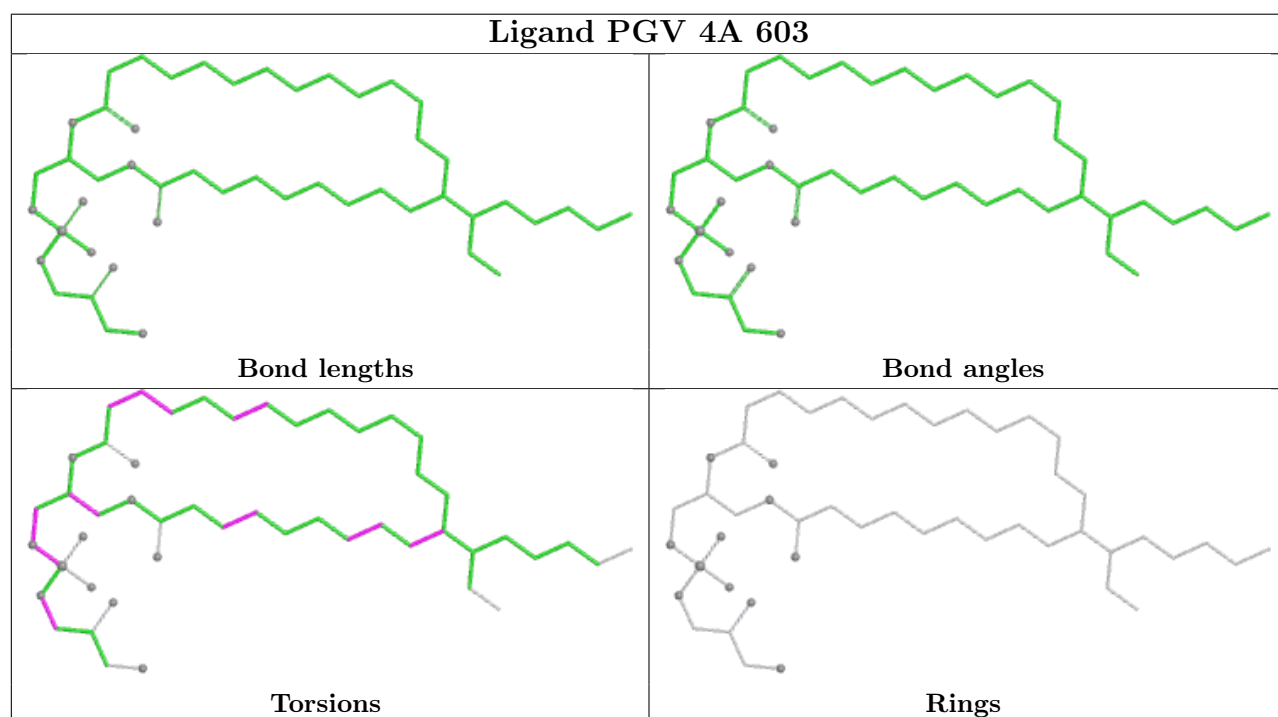
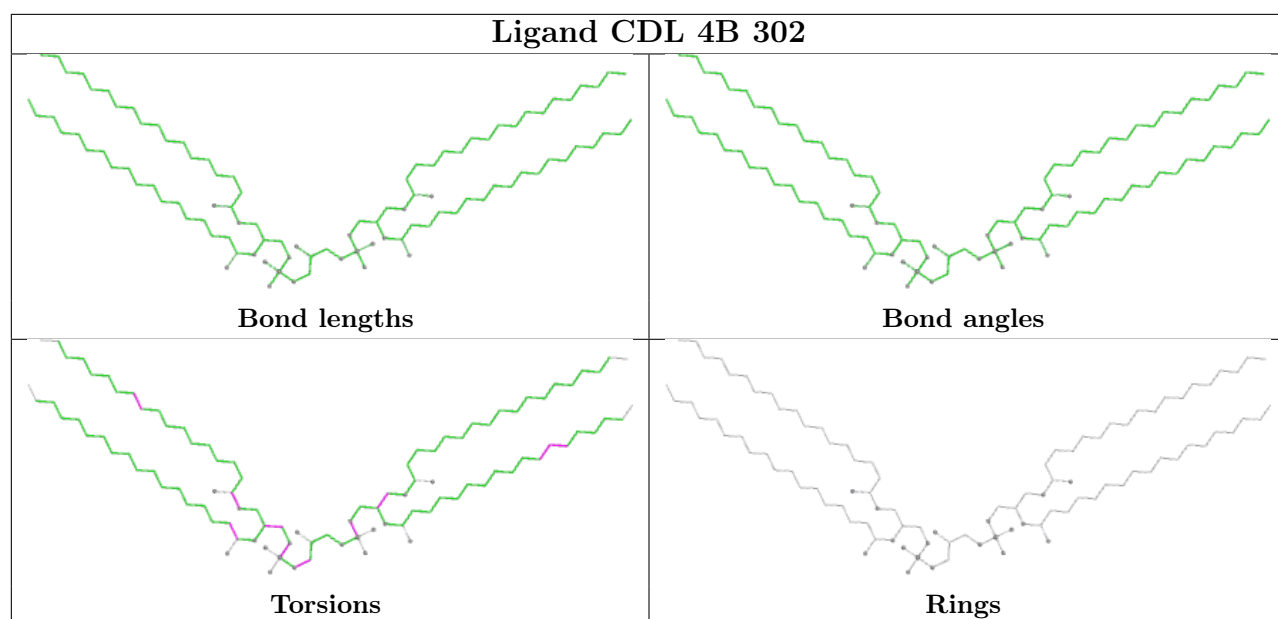




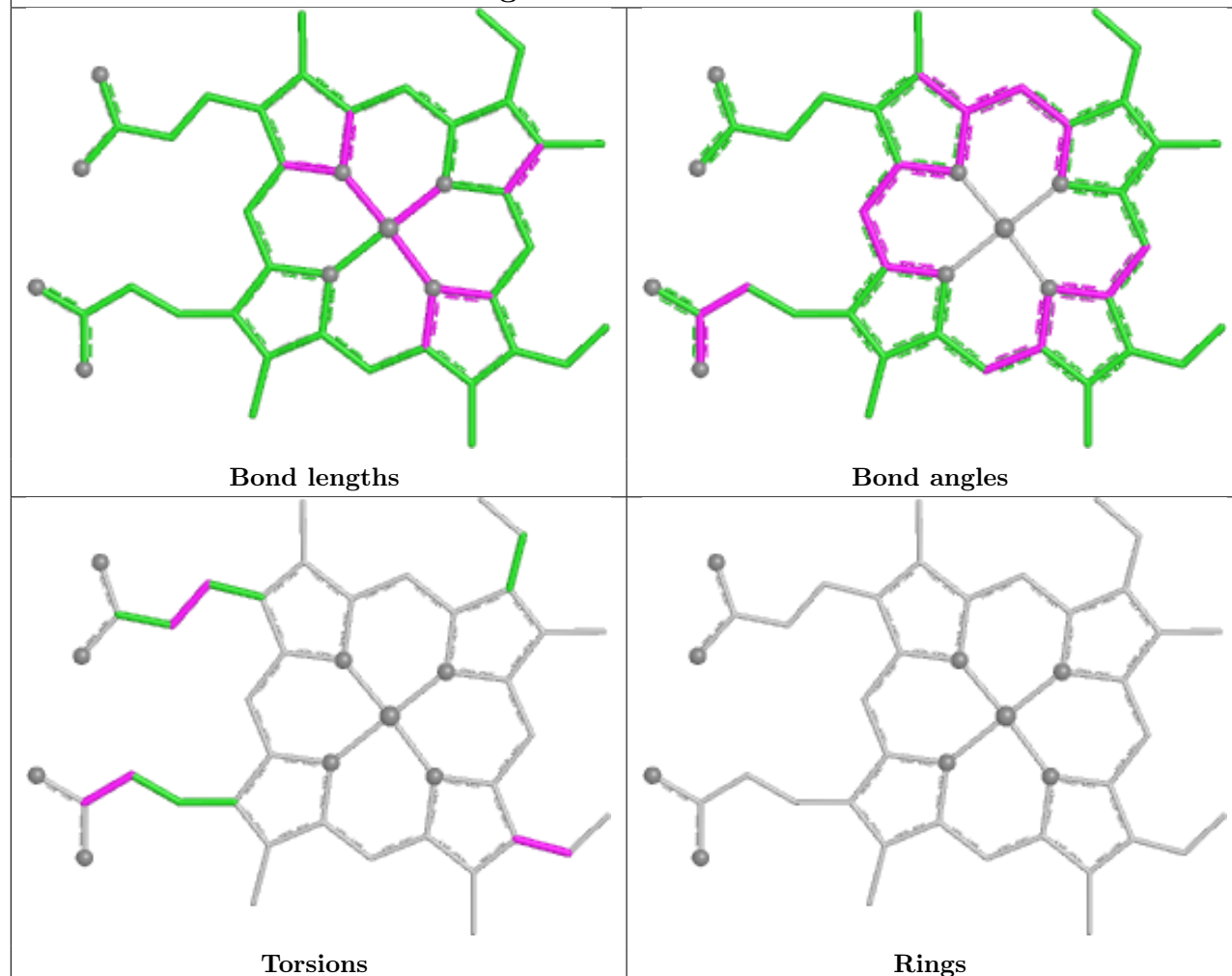




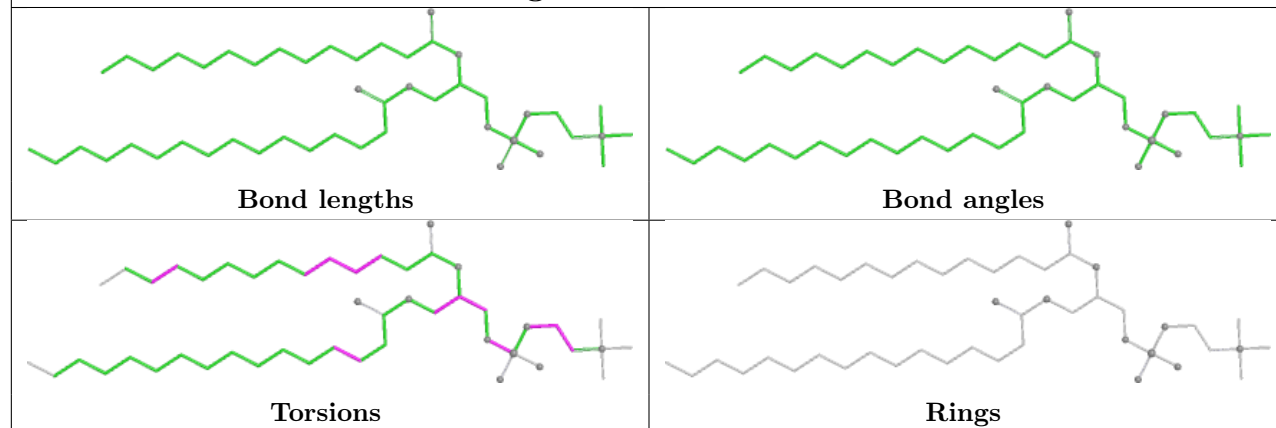




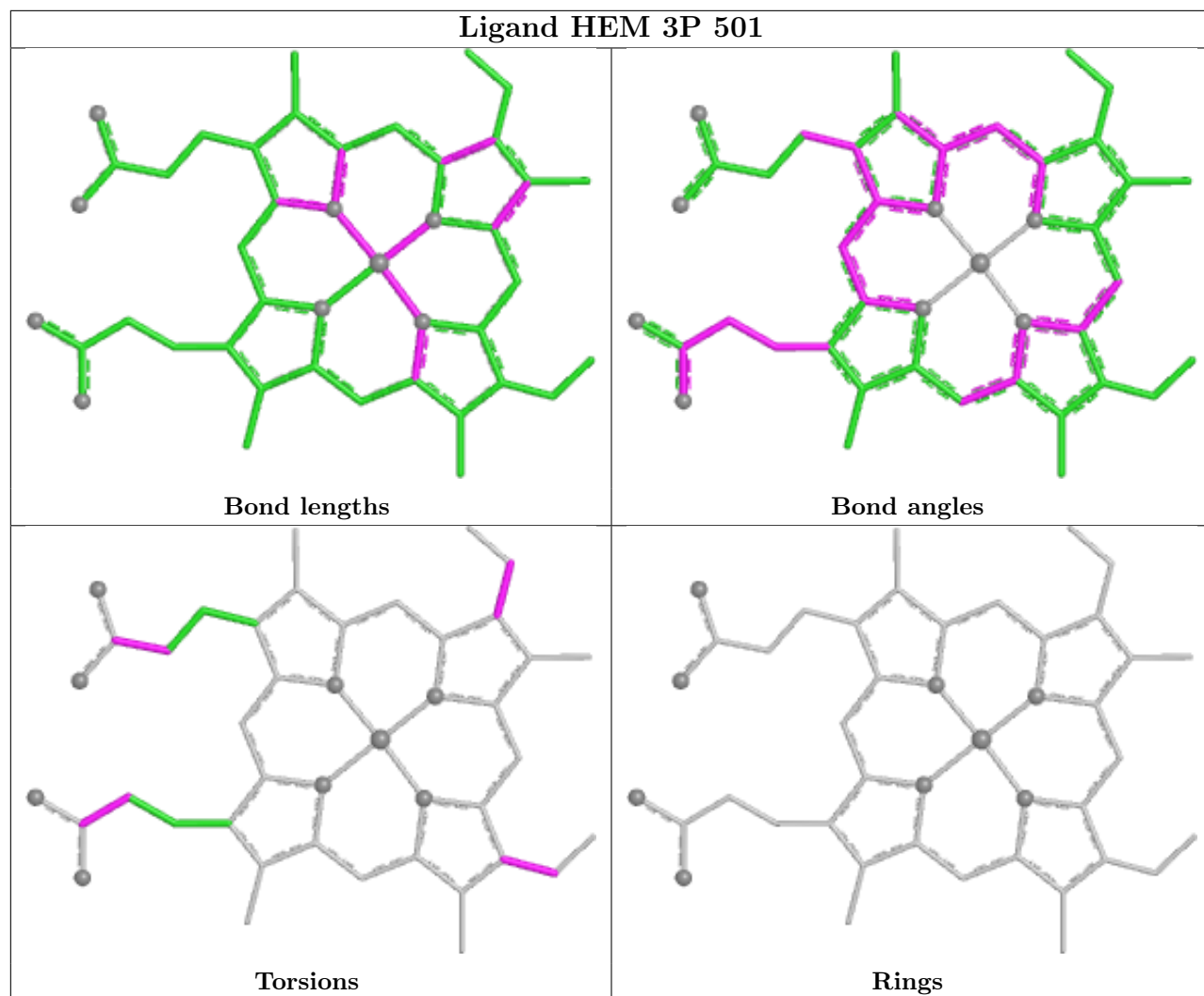
Ligand HEM 3C 501



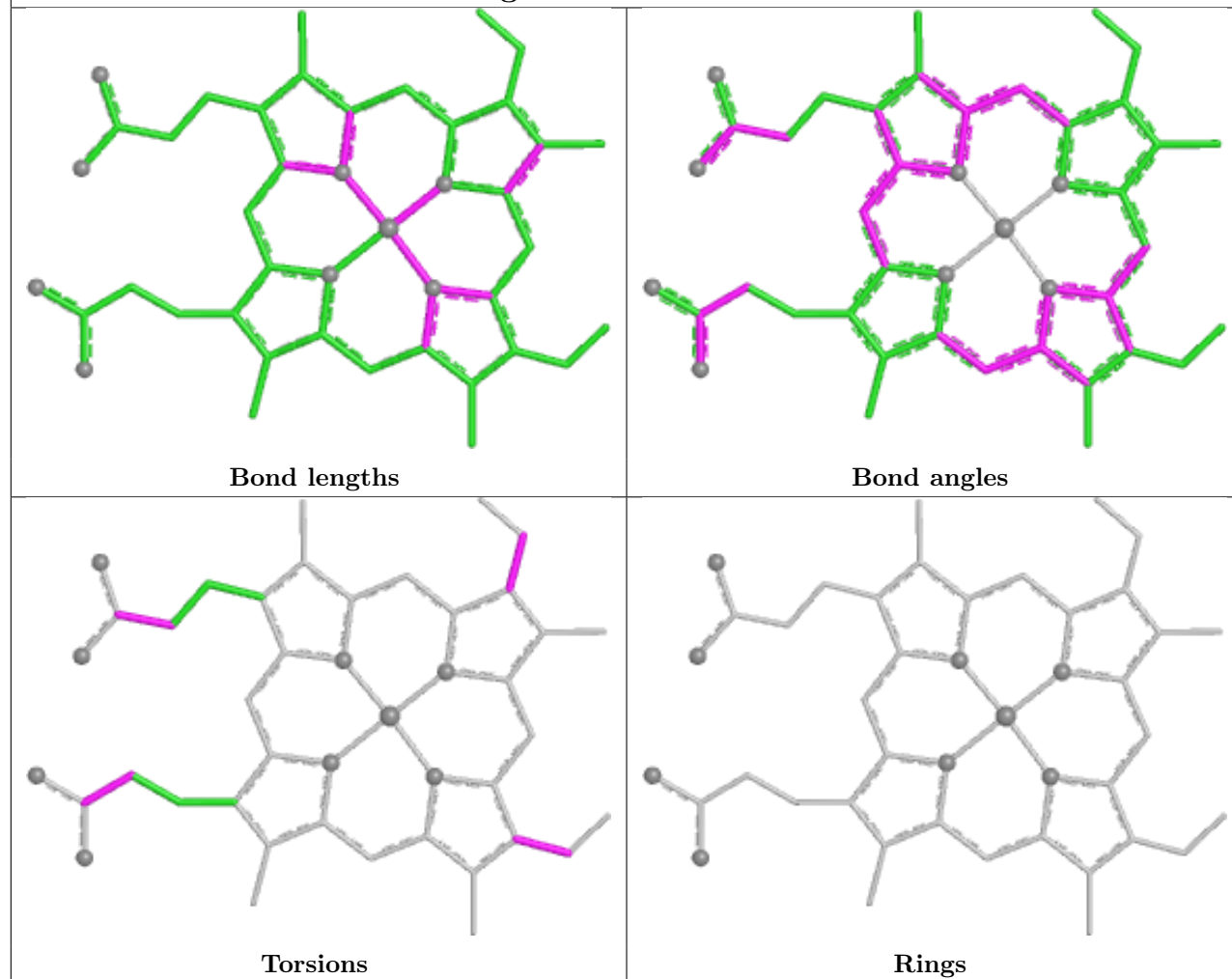
Ligand PC1 1B 203



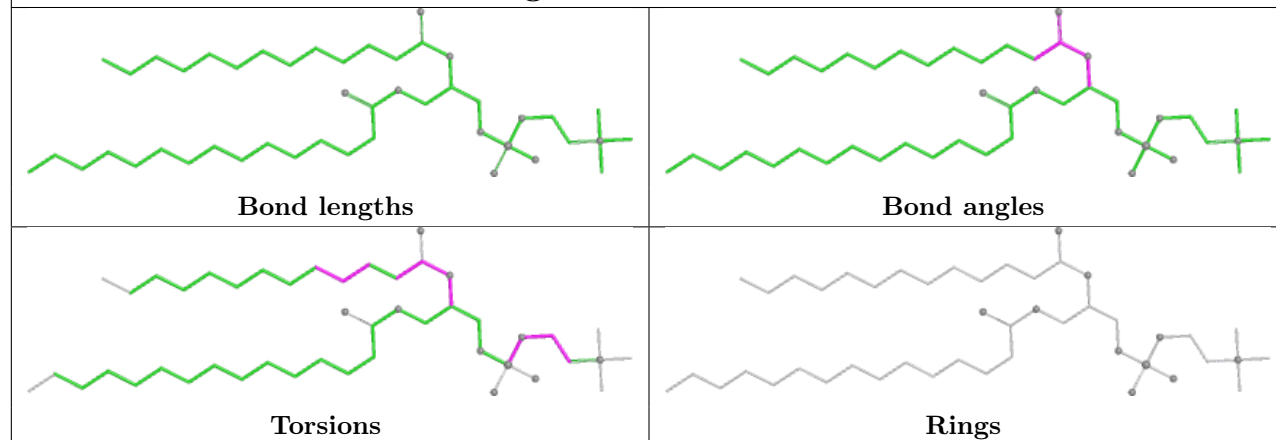
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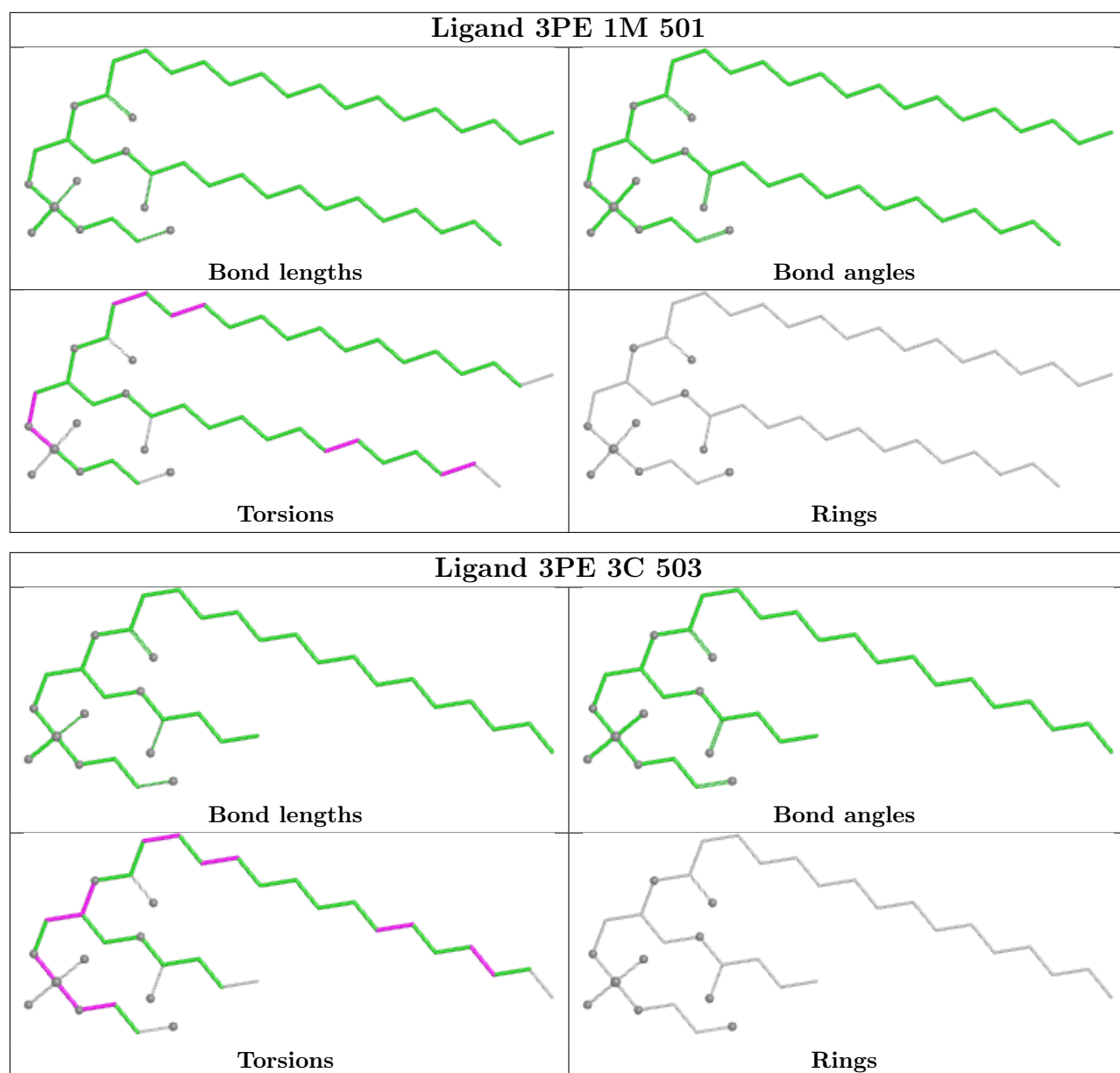


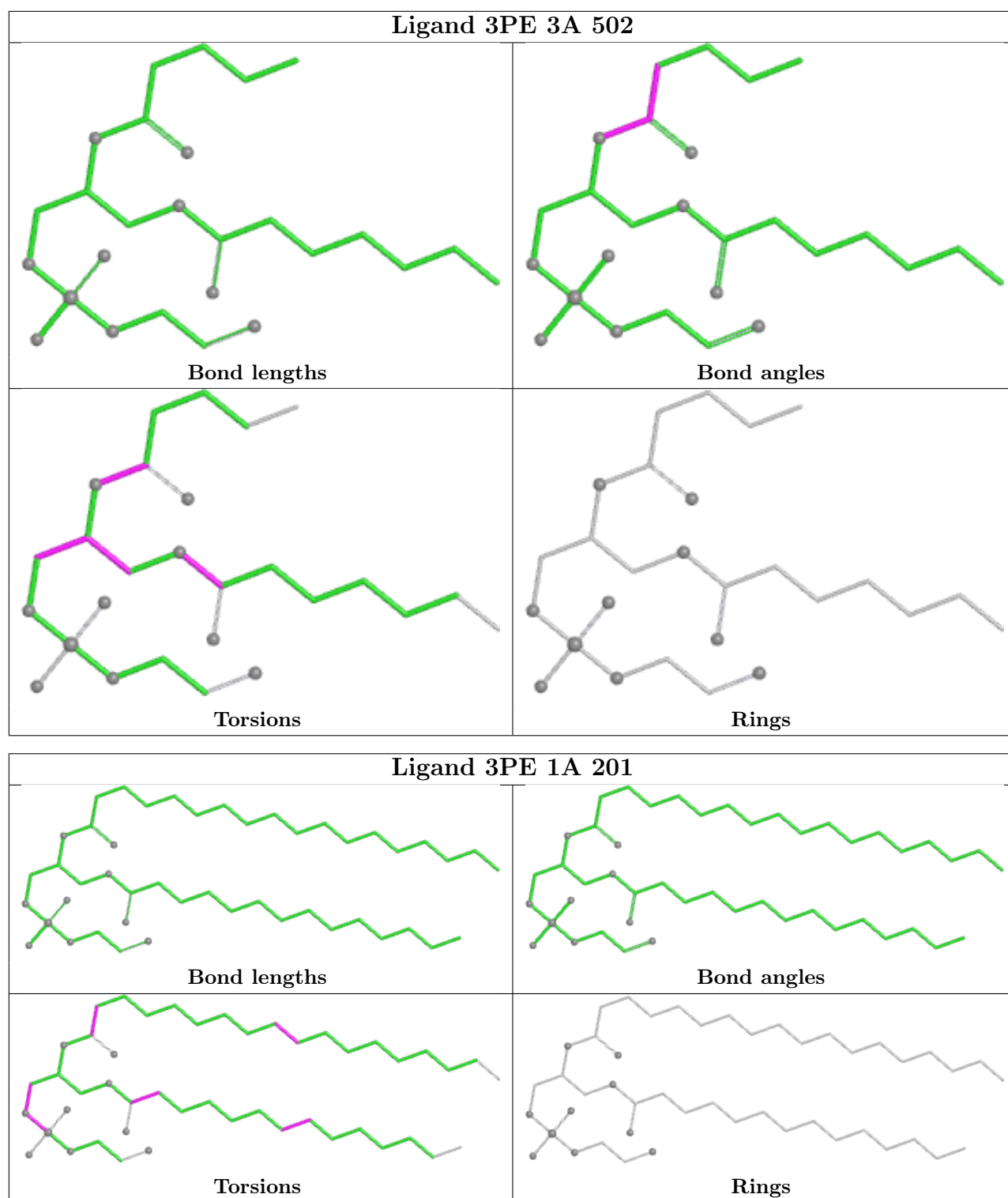
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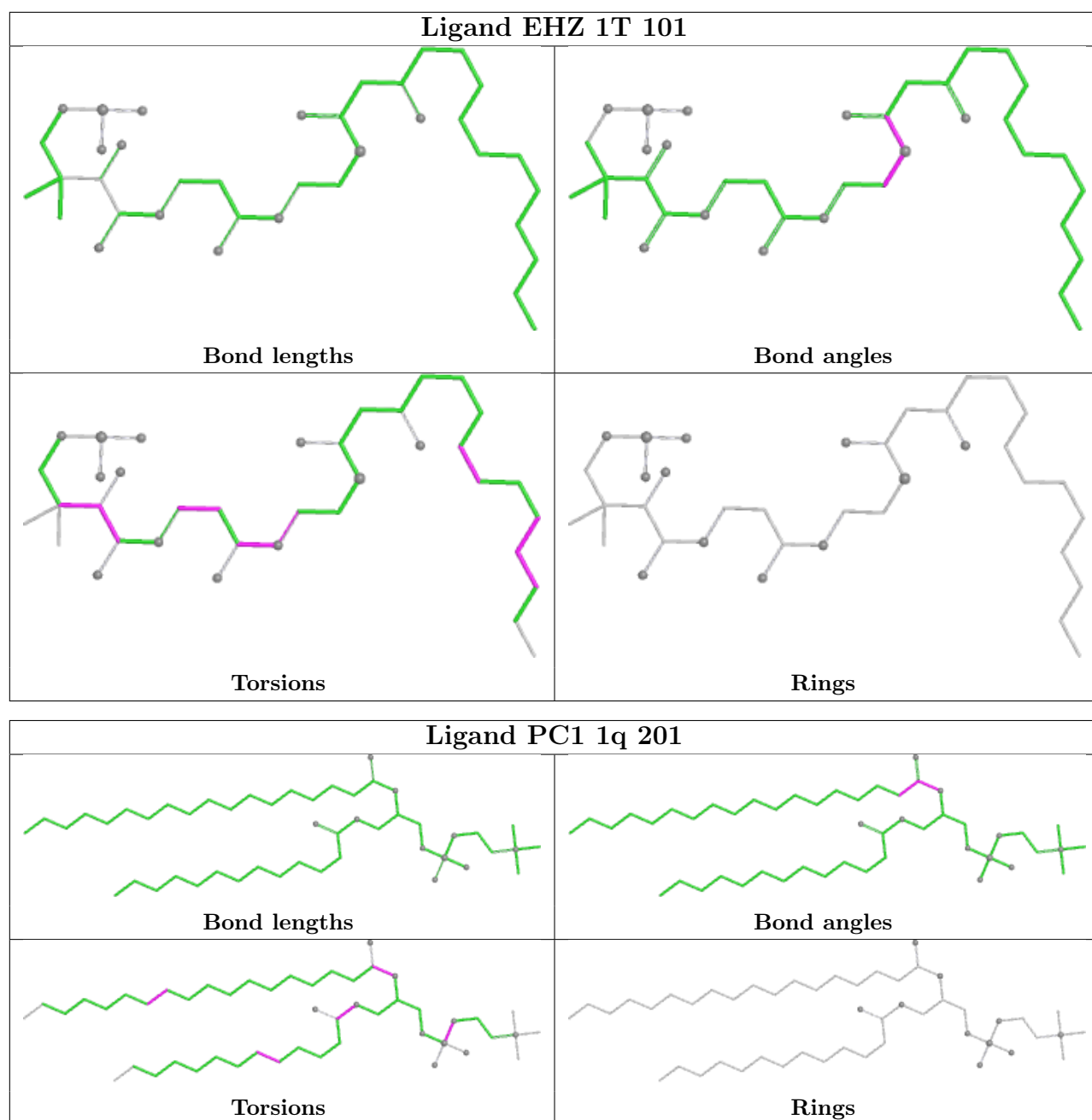


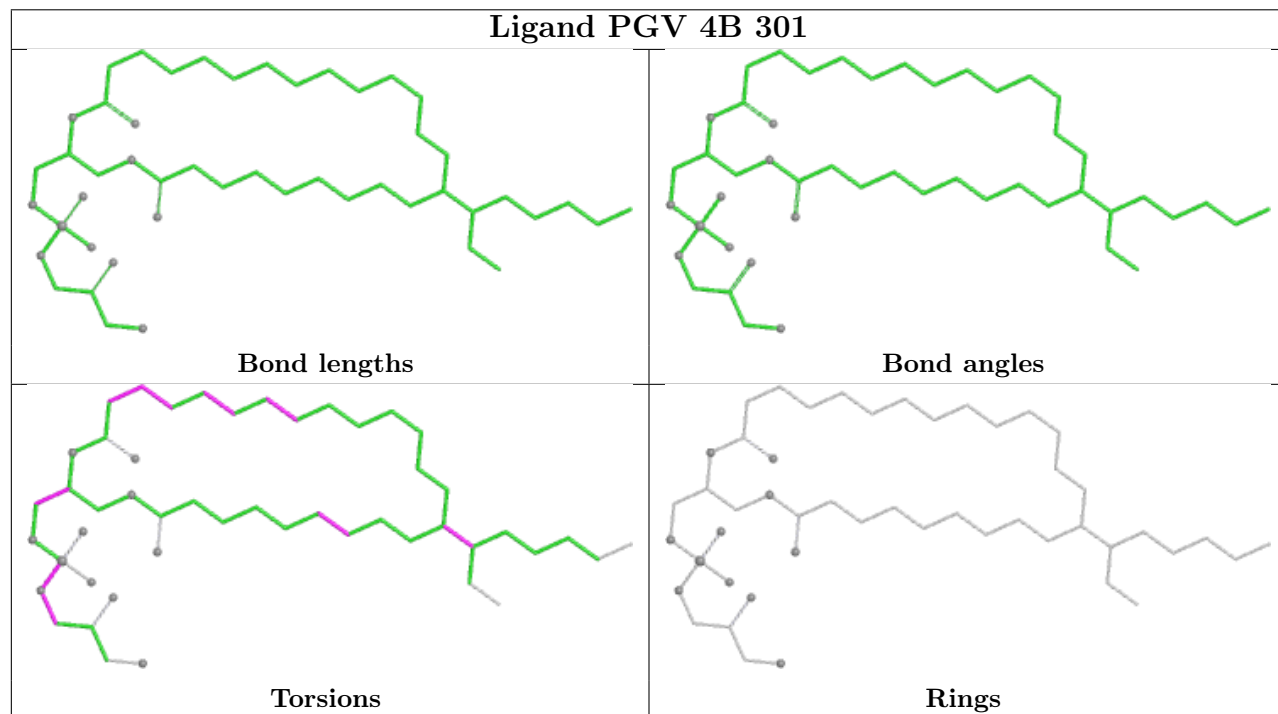
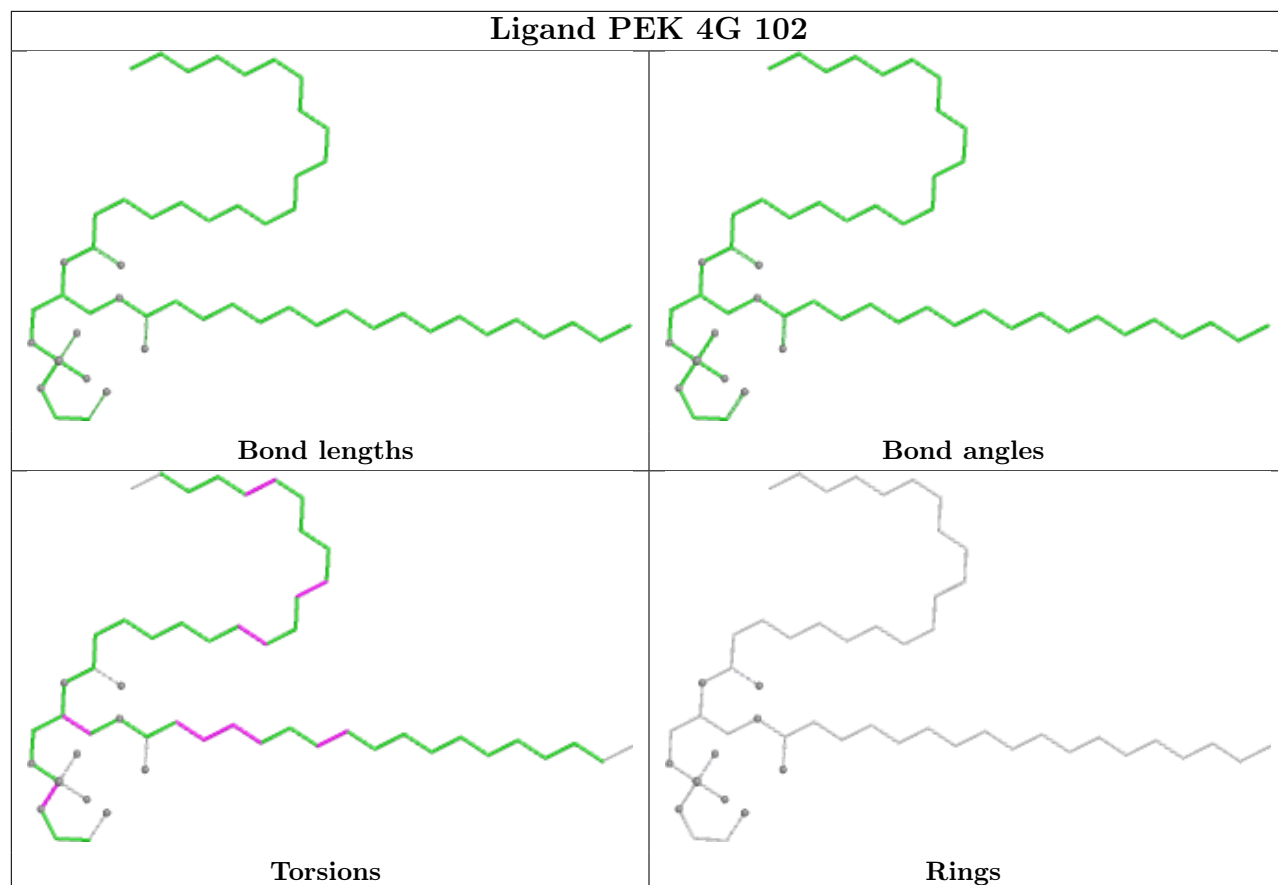
Ligand PC1 1m 201

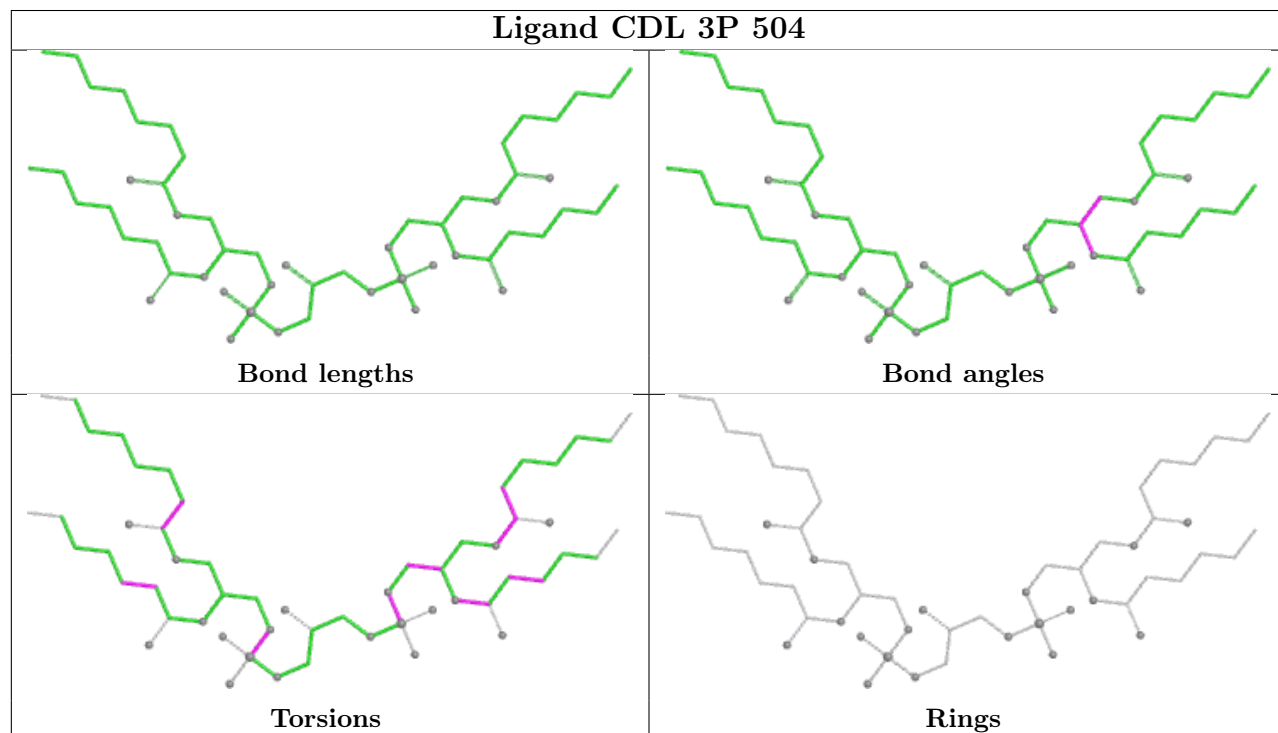
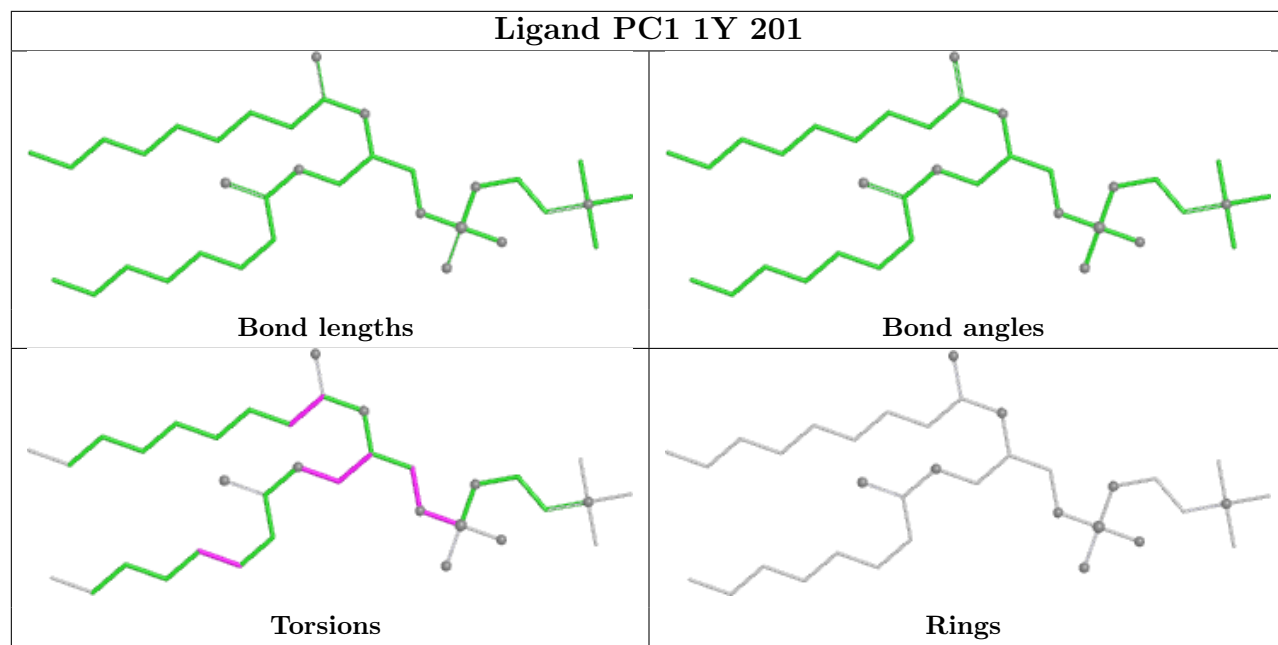


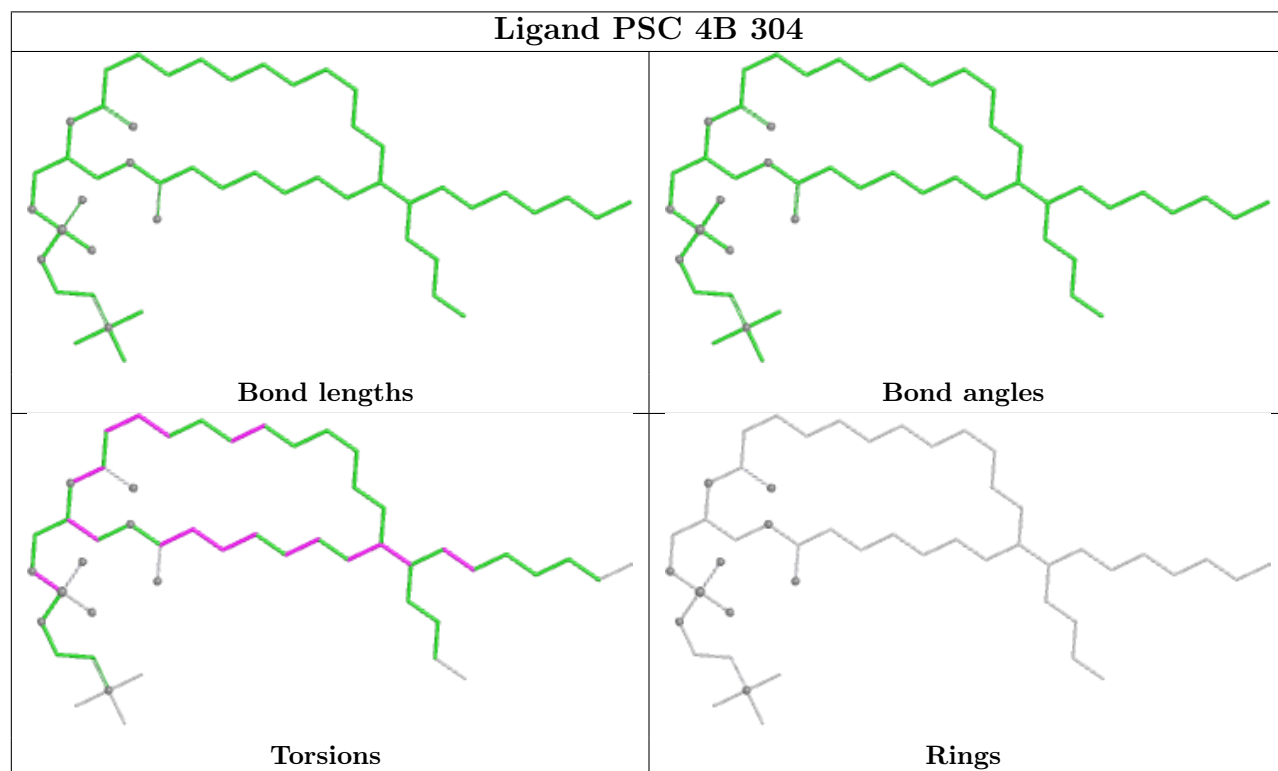
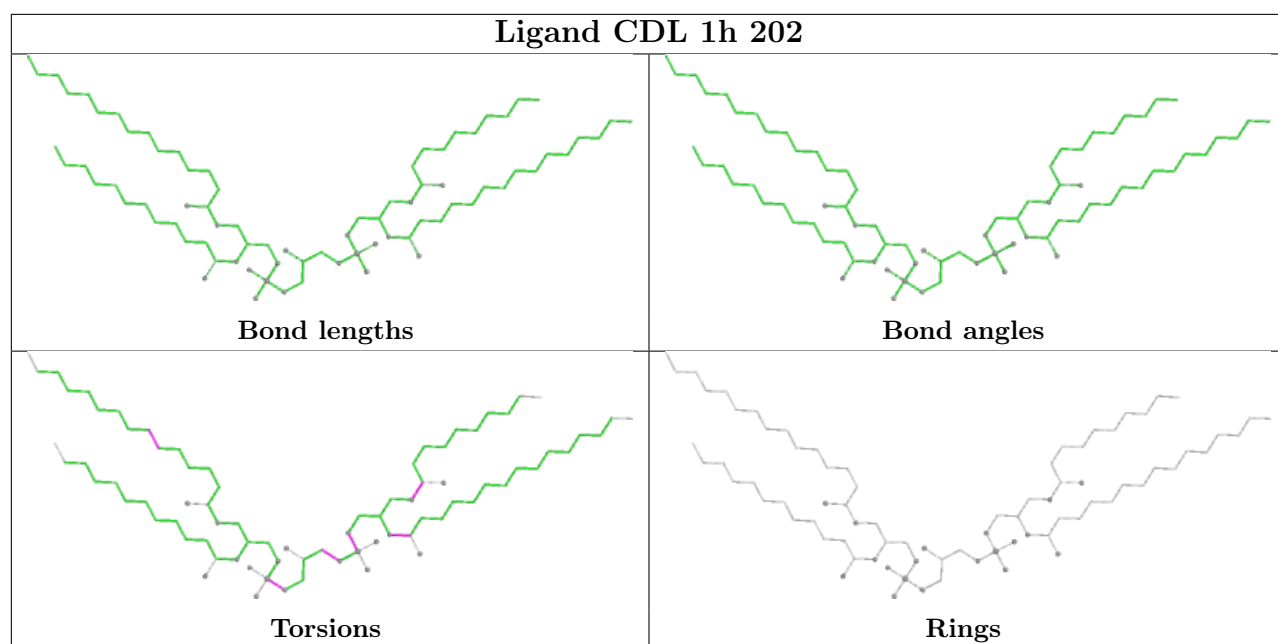


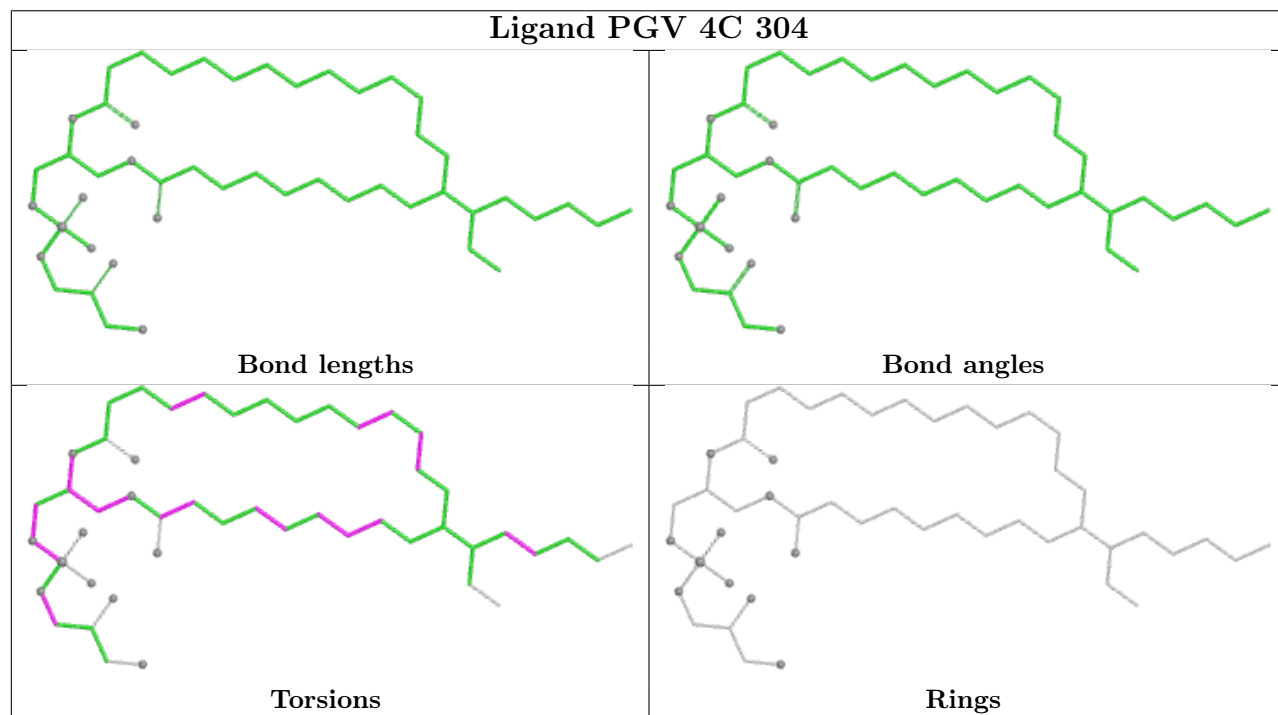
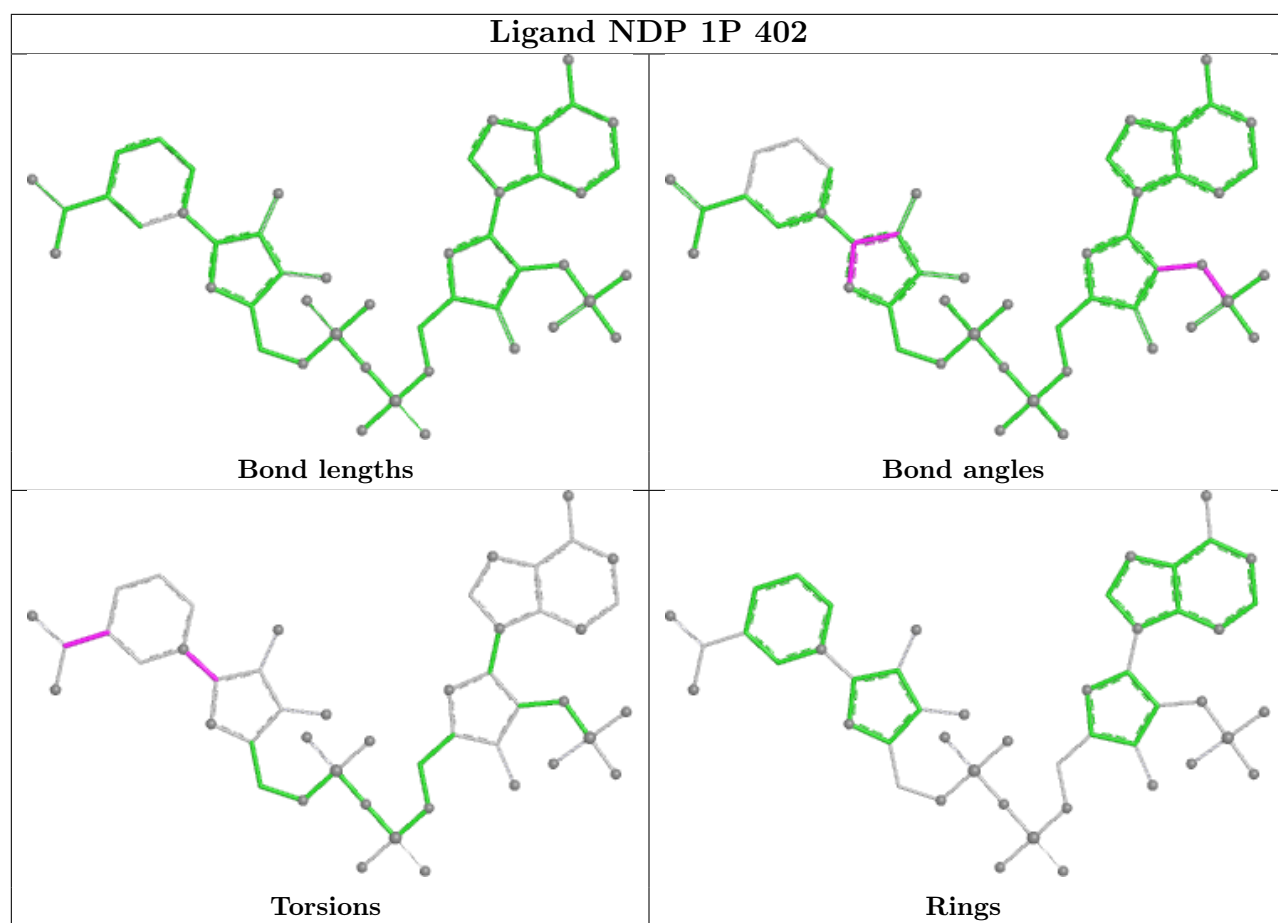


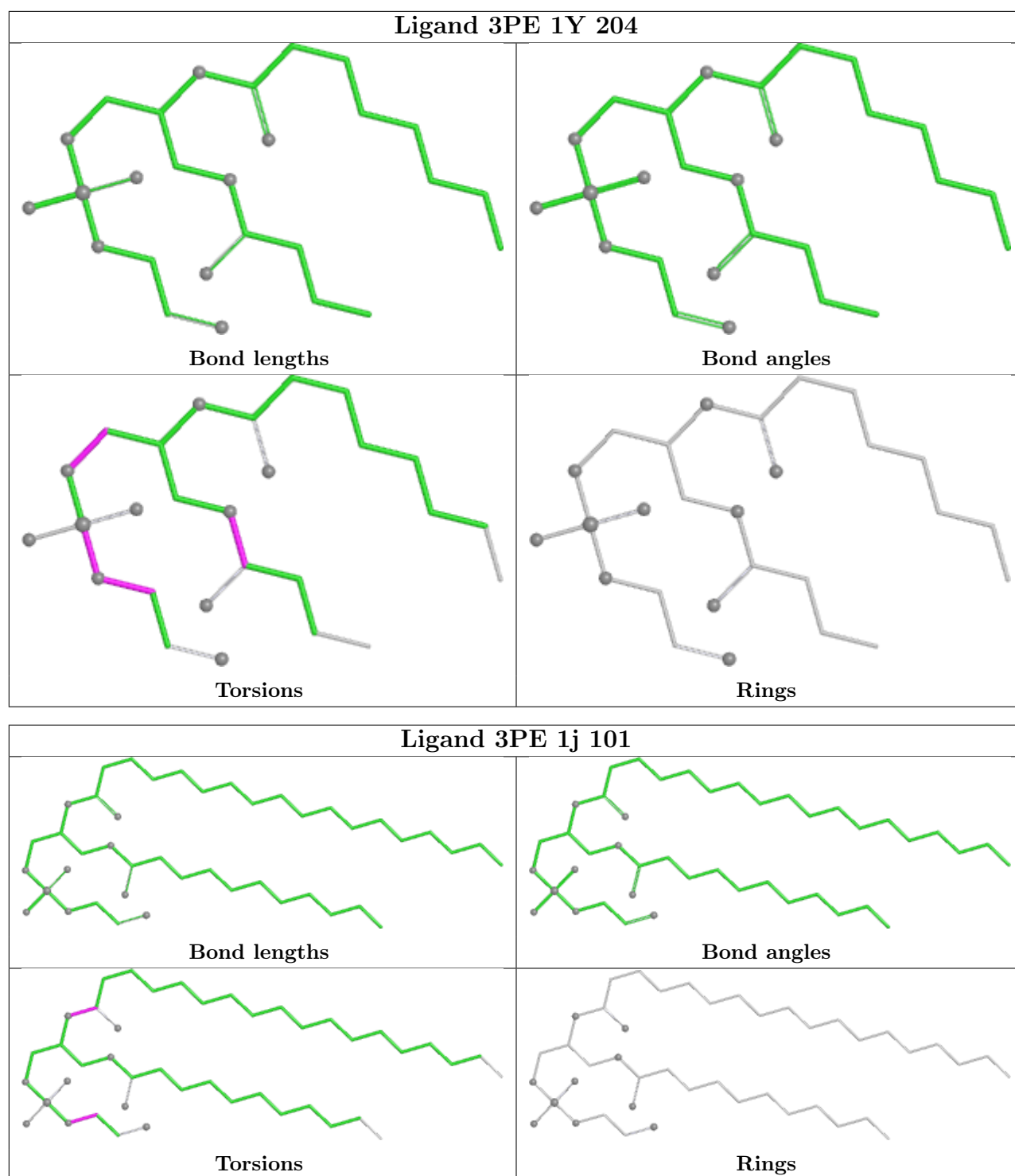












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	3I	1

All chain breaks are listed below:

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

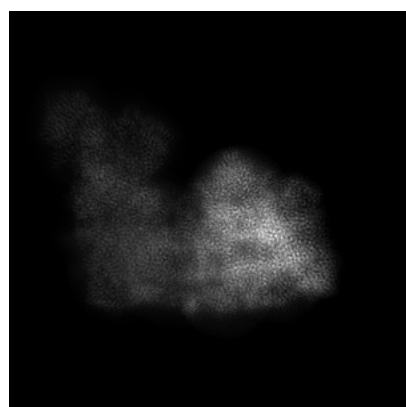
6 Map visualisation [i](#)

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

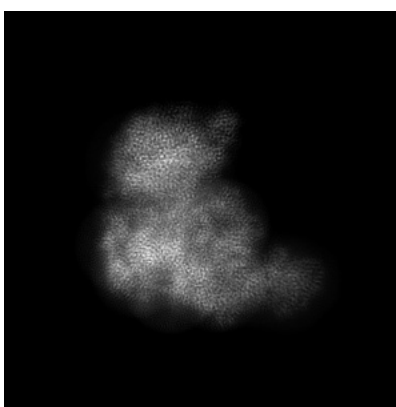
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

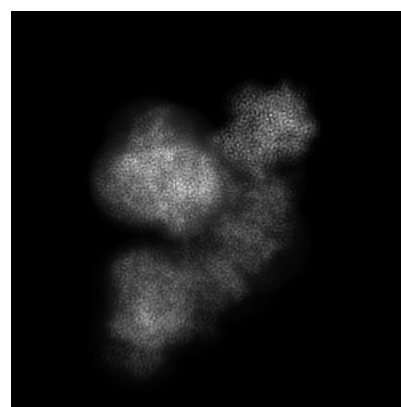
6.1.1 Primary map



X



Y

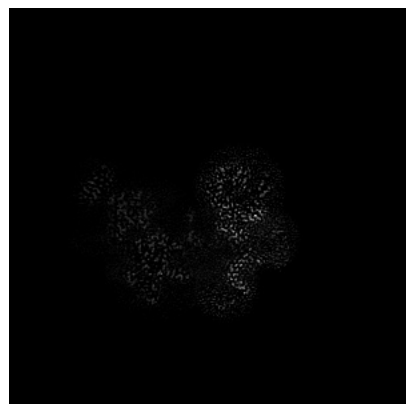


Z

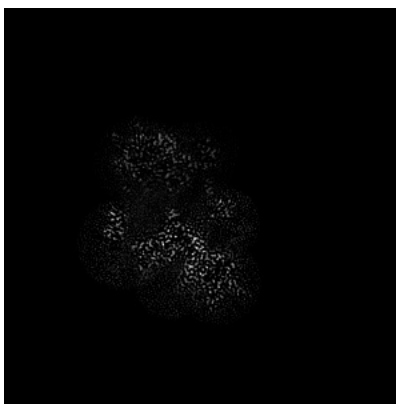
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

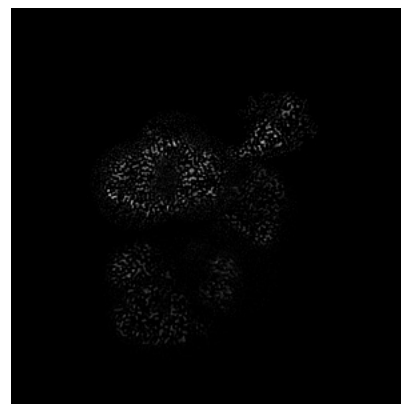
6.2.1 Primary map



X Index: 444



Y Index: 444



Z Index: 444

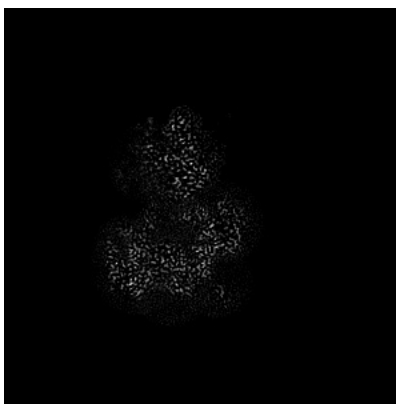
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

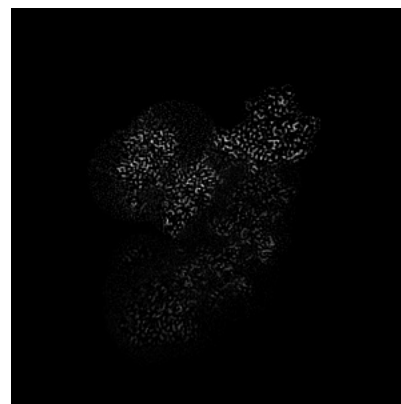
6.3.1 Primary map



X Index: 322



Y Index: 568

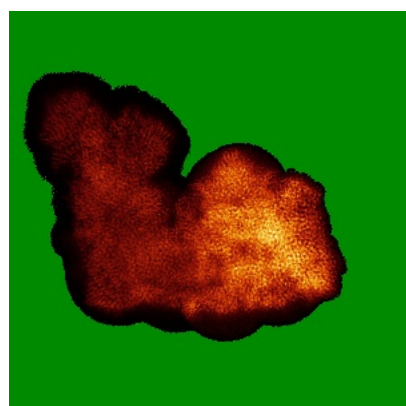


Z Index: 387

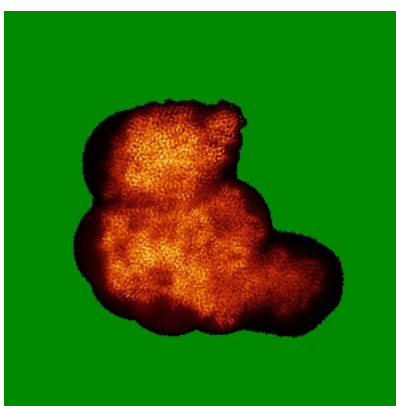
The images above show the largest variance slices of the map in three orthogonal directions.

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

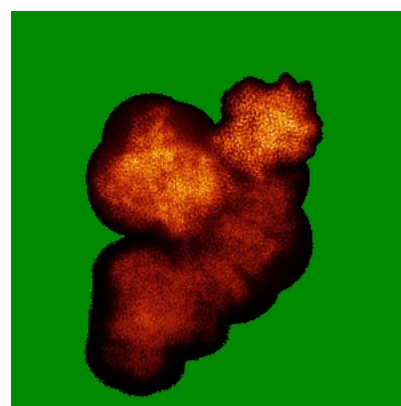
6.4.1 Primary map



X



Y

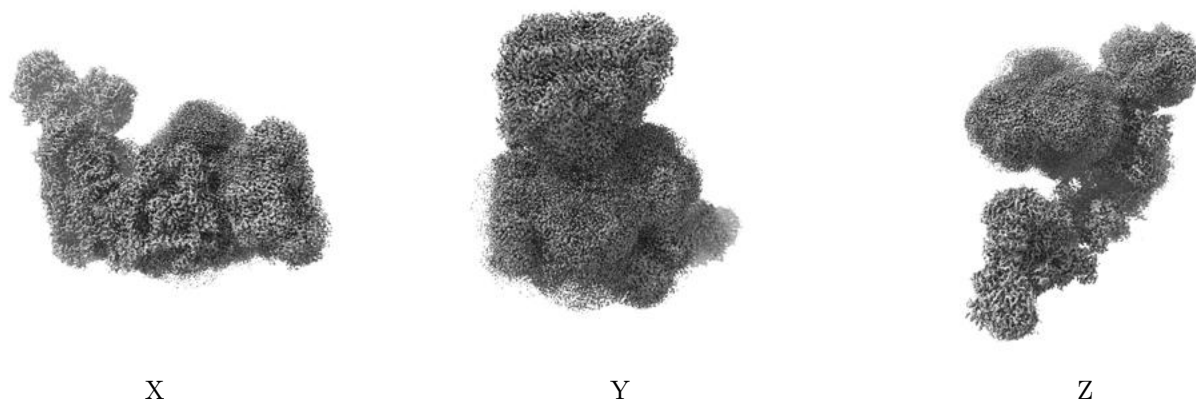


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

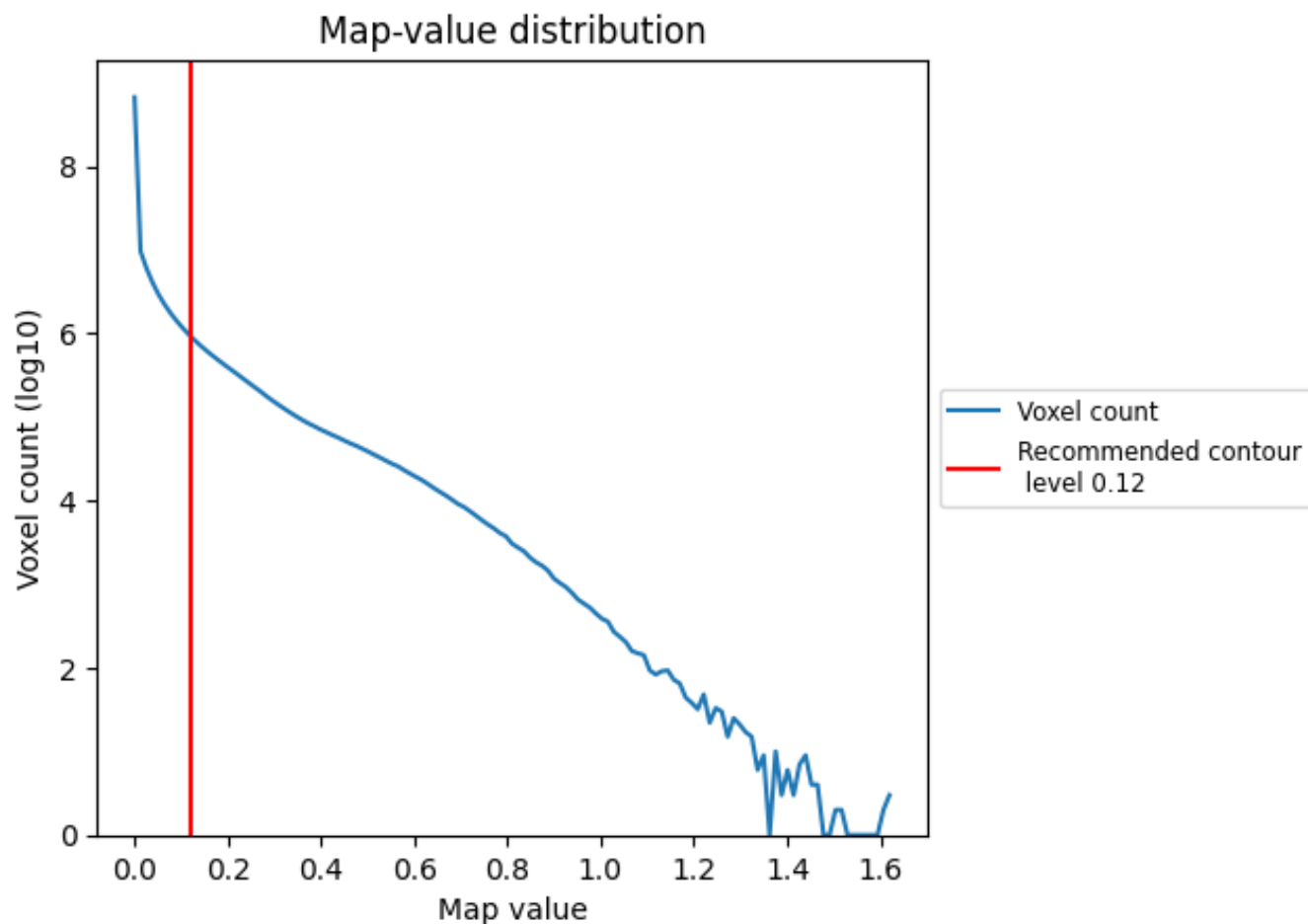
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

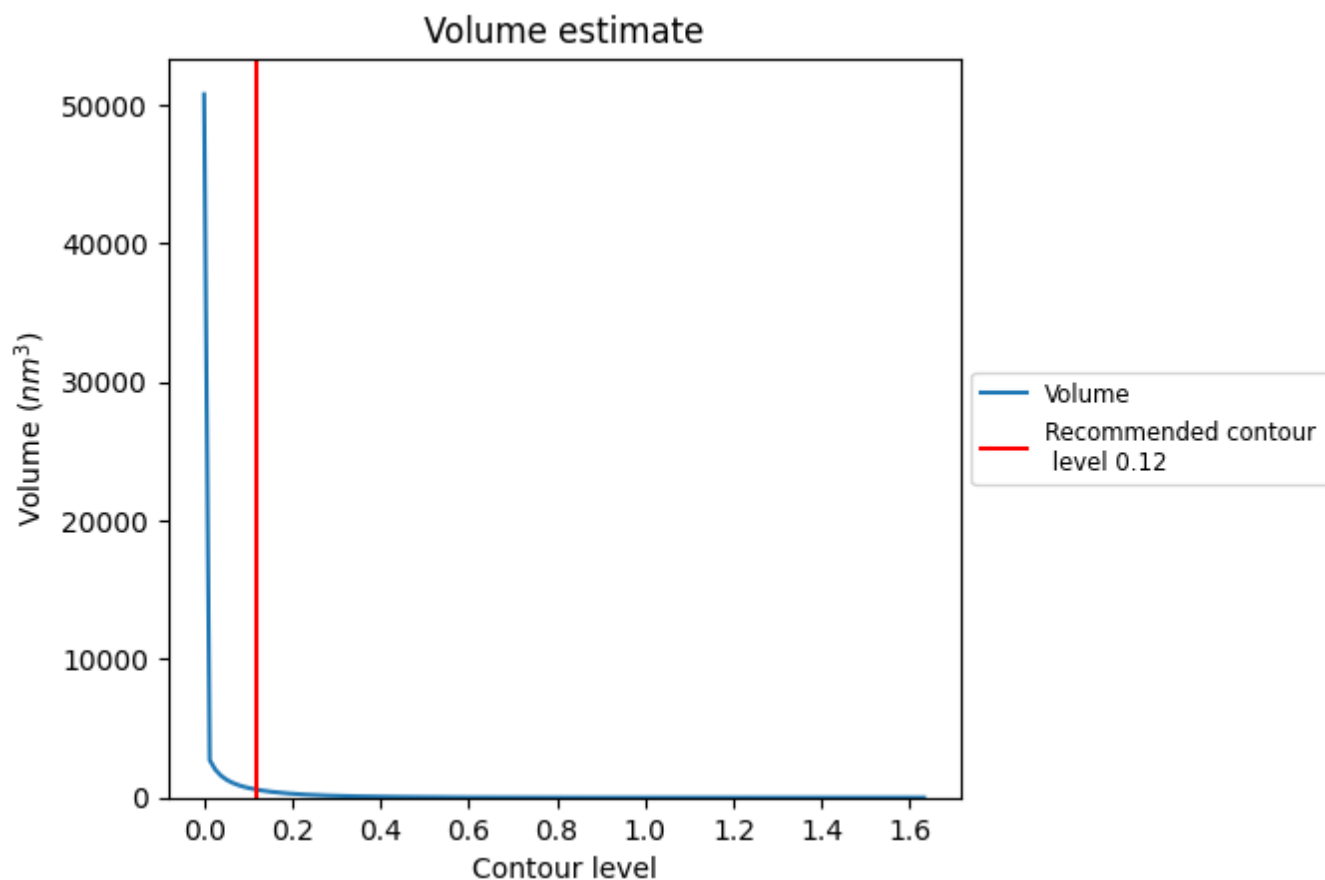
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

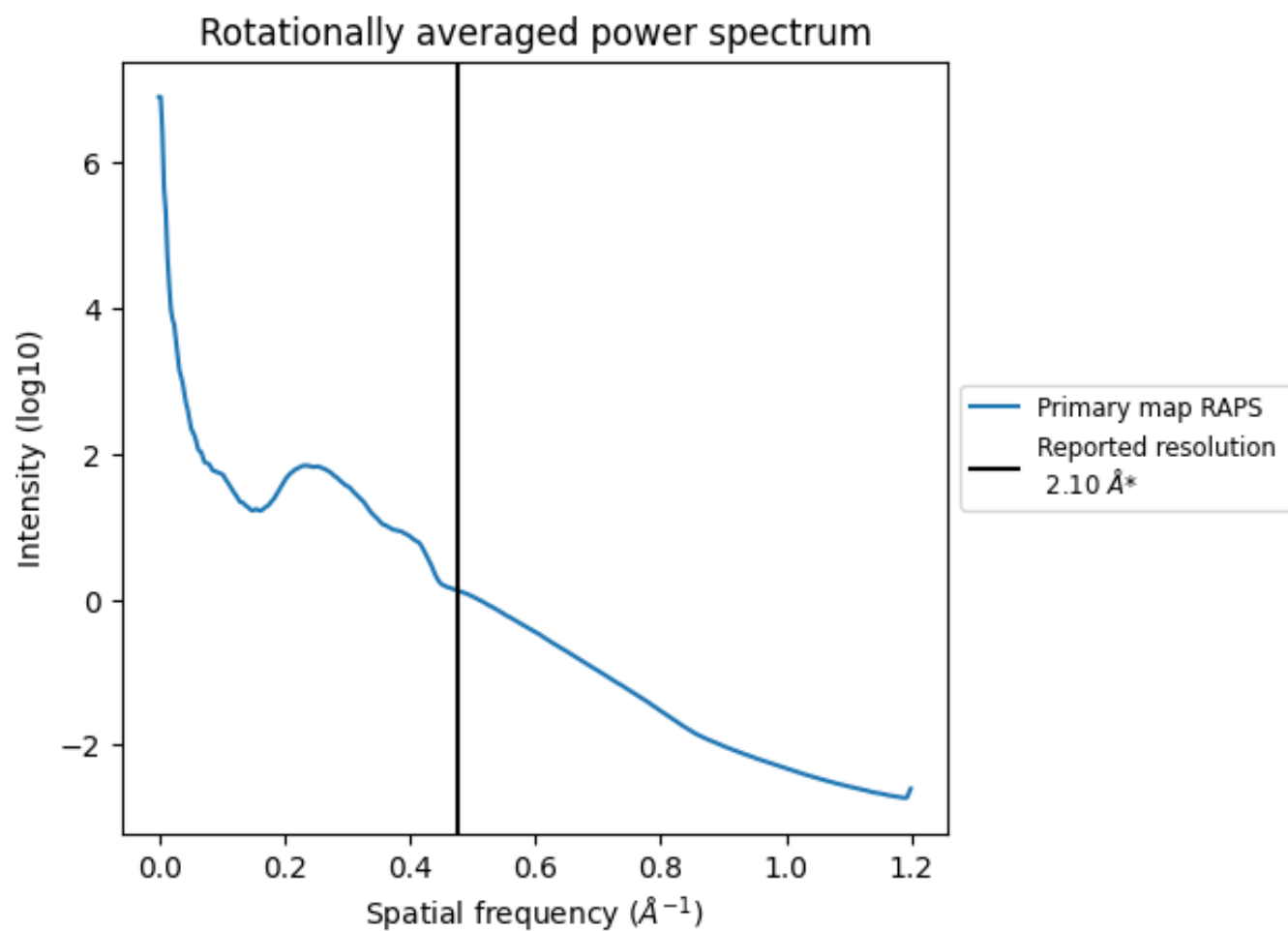
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ



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

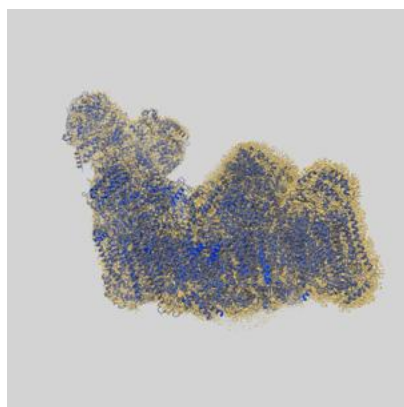
8 Fourier-Shell correlation

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

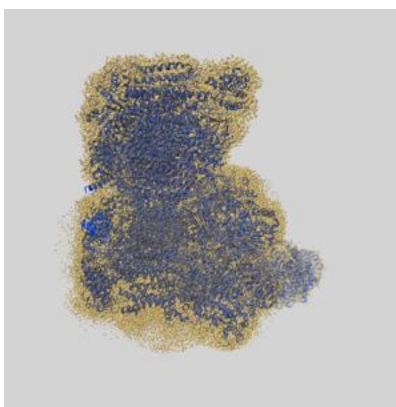
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42226 and PDB model 8UGI. Per-residue inclusion information can be found in section [3](#) on page [38](#).

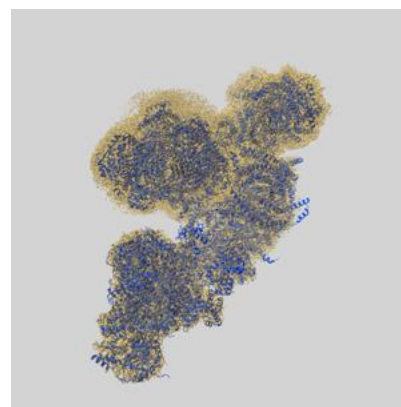
9.1 Map-model overlay [i](#)



X



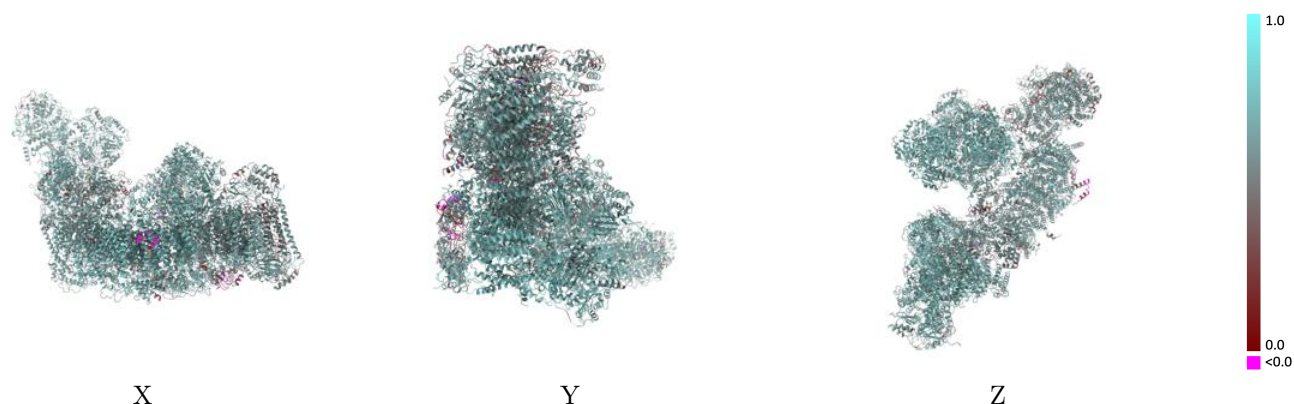
Y



Z

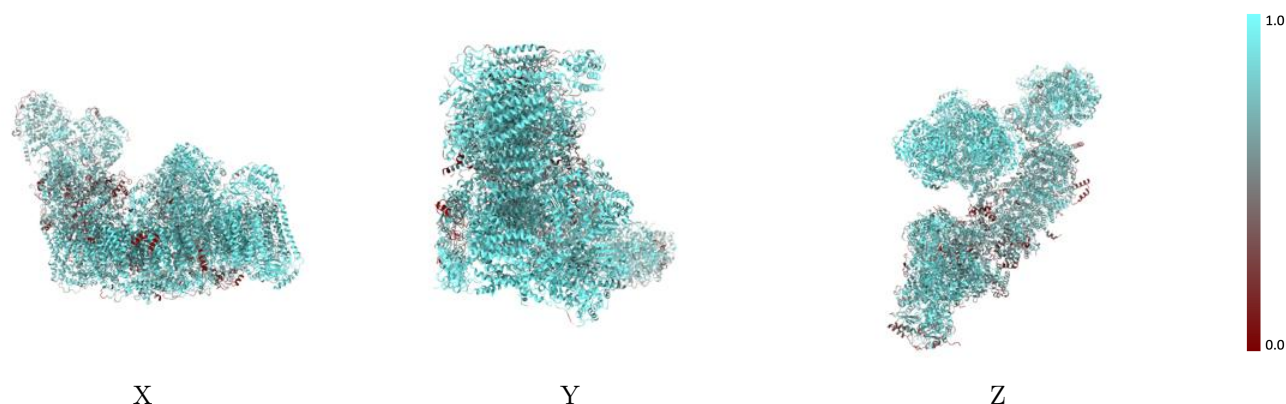
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



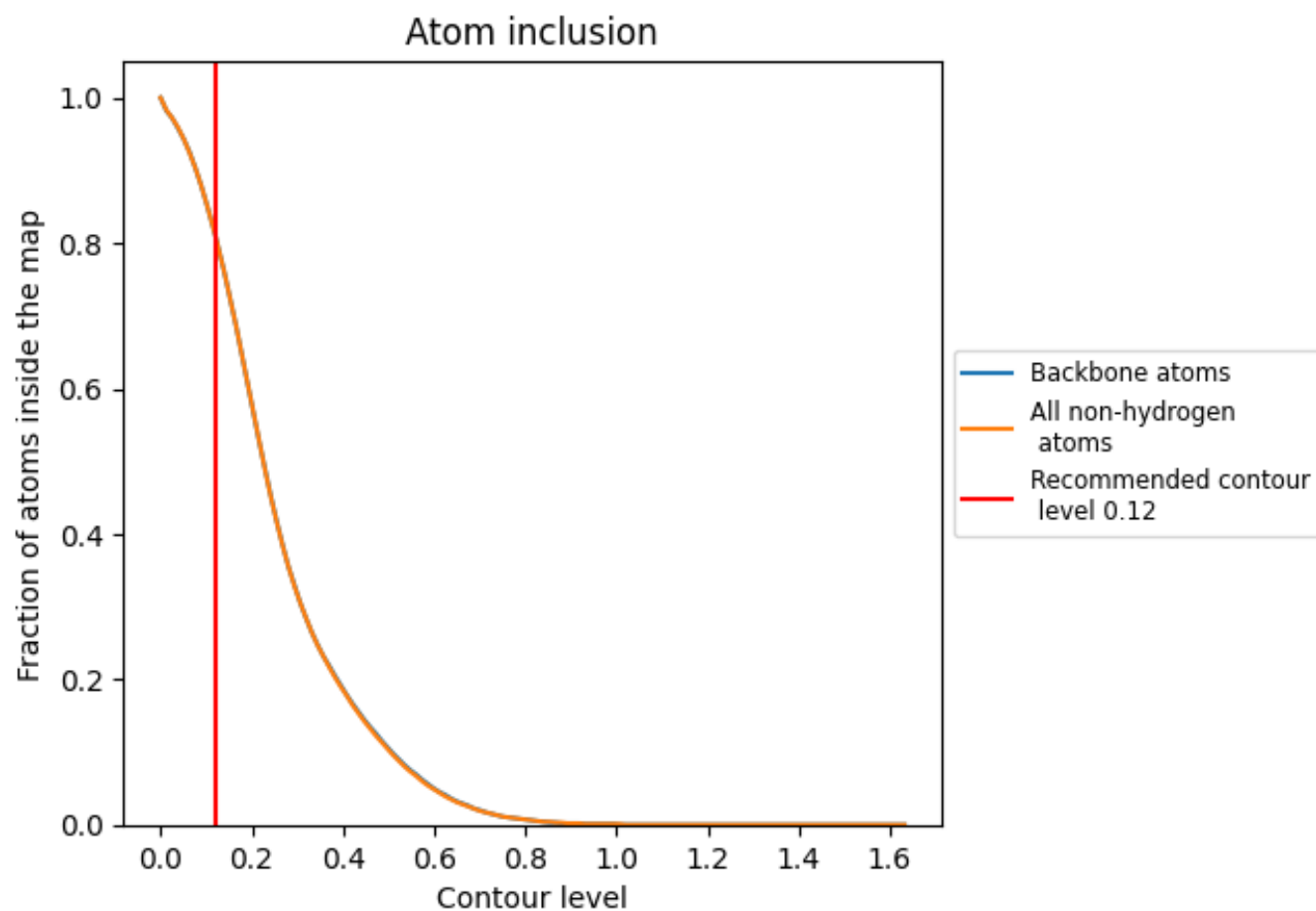
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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



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

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