



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 11:04 am BST

PDB ID : 9F5X / pdb_00009f5x
EMDB ID : EMD-50202
Title : Structure of the Chlamydomonas reinhardtii respiratory supercomplex I1 III2 IV2
Authors : Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on : 2024-04-30
Resolution : 2.82 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:

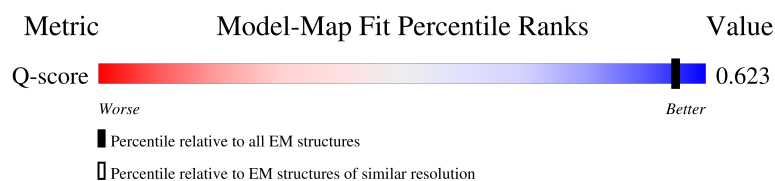
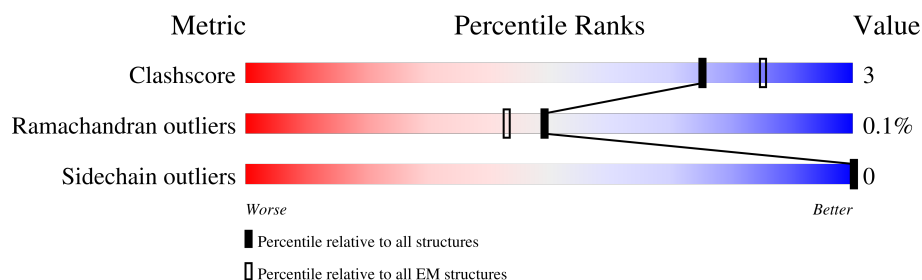
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.82 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	11795 (2.32 - 3.32)

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	381	
1	1B	381	
2	1C	262	
2	1D	262	

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Mol	Chain	Length	Quality of chain
3	1E	314	
3	1F	314	
4	1G	60	
4	1H	60	
5	1I	69	
5	1J	69	
6	1K	73	
6	1L	73	
7	1M	495	
7	1N	495	
8	1O	59	
8	1P	59	
9	1Q	485	
9	1S	485	
10	1R	123	
10	1T	123	
11	2A	504	
11	3A	504	
12	2B	284	
12	3B	284	
13	2C	153	
13	3C	153	
14	2D	382	
14	3D	382	
15	2E	175	

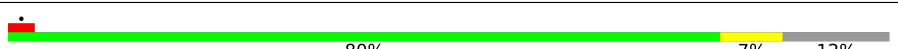
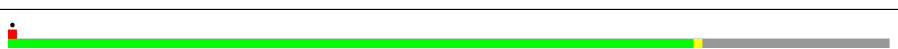
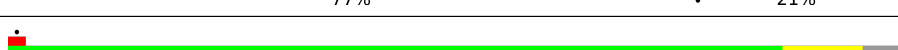
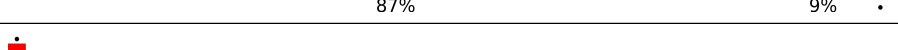
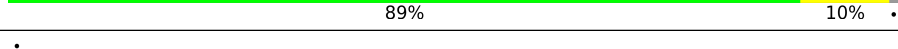
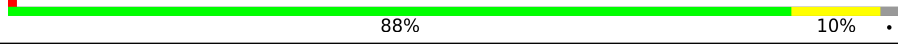
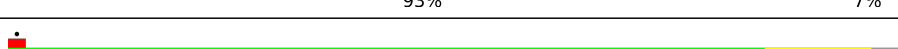
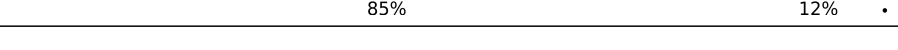
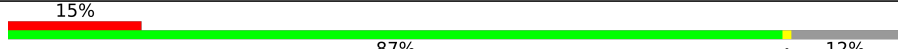
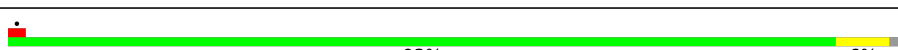
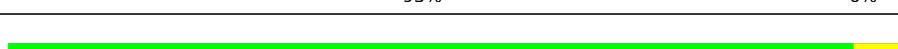
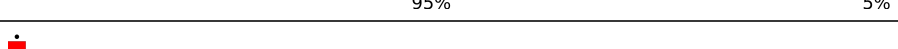
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Mol	Chain	Length	Quality of chain
15	3E	175	
16	2F	96	
16	3F	96	
17	2G	125	
17	3G	125	
18	2H	148	
18	3H	148	
19	2I	101	
19	3I	101	
20	2J	105	
20	3J	105	
21	2K	58	
21	3K	58	
22	2L	87	
22	3L	87	
23	A	282	
24	B	484	
25	C	733	
26	D	282	
27	E	467	
28	F	164	
29	G	231	
30	H	118	
31	I	165	
32	J	128	

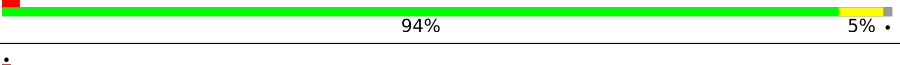
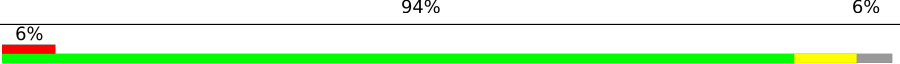
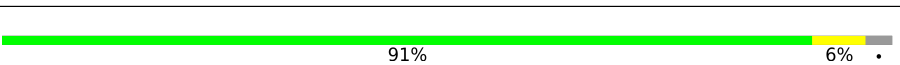
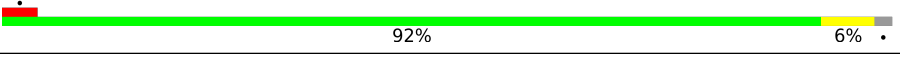
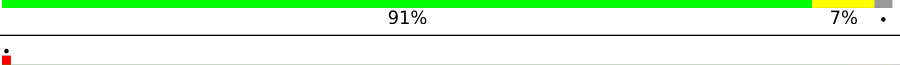
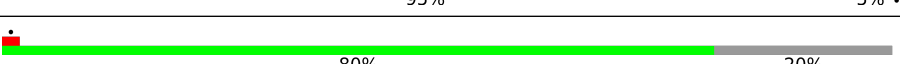
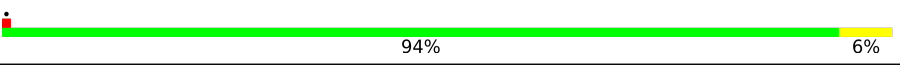
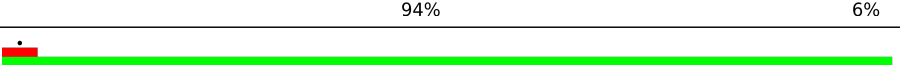
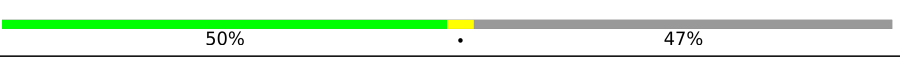
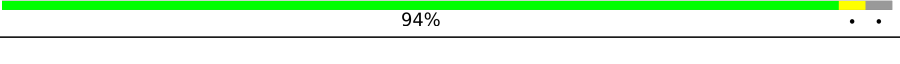
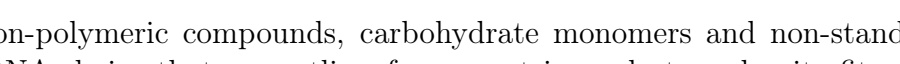
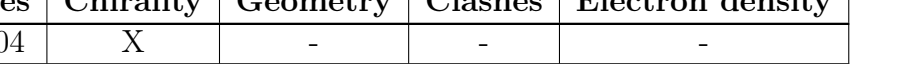
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Mol	Chain	Length	Quality of chain
32	r	128	
33	K	138	
34	L	187	
35	M	154	
36	N	156	
37	O	101	
38	P	397	
39	Q	292	
40	R	387	
41	S	279	
42	T	443	
43	U	227	
44	V	546	
45	W	162	
46	X	149	
47	Y	64	
48	Z	124	
49	a	129	
50	b	172	
51	c	67	
52	d	86	
53	e	219	
54	f	65	
55	g	55	
56	h	142	

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Mol	Chain	Length	Quality of chain
57	i	81	
58	j	86	
59	k	117	
60	l	121	
61	m	142	
62	n	106	
63	o	155	
64	p	130	
65	q	197	
66	s	312	
67	t	279	
68	u	229	
69	v	45	
70	w	109	
71	x	157	
72	y	118	

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
78	HEC	1E	404	X	-	-	-
78	HEC	1F	402	X	-	-	-
85	CUA	2C	301	-	-	X	-
85	CUA	3C	301	-	-	X	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 137999 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	1B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	1D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	1F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		

- Molecule 4 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	1H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	1J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	1L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		

- Molecule 7 is a protein called MPP-Beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	1N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	1P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		

- Molecule 9 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	1S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	1T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	3A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	3B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		

- Molecule 13 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	3C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	3D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		

- Molecule 15 is a protein called Cox5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	3E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		

- Molecule 16 is a protein called Cox5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	3F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		

- Molecule 17 is a protein called Cox6a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	3G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		

- Molecule 18 is a protein called Cox6b.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	3H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		

- Molecule 19 is a protein called Cox7c.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	2I	72	Total	C	N	O	0	0
			594	393	98	103		
19	3I	72	Total	C	N	O	0	0
			594	393	98	103		

- Molecule 20 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	3J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		

- Molecule 21 is a protein called Cox7a.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	2K	47	Total	C	N	O	0	0
			382	249	63	70		
21	3K	47	Total	C	N	O	0	0
			382	249	63	70		

- Molecule 22 is a protein called CoxIn.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2L	76	Total	C	N	O	S	0	0
			605	390	100	111	4		
22	3L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase 24 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase 78 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 49 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	383	Total	C	N	O	S	0	0
			3085	1971	537	554	23		

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		

- Molecule 29 is a protein called NADH:ubiquinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		

- Molecule 30 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		

- Molecule 31 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
32	r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase 13 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		

- Molecule 38 is a protein called Putative NADH:ubiquinone oxidoreductase 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		

- Molecule 43 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		

- Molecule 46 is a protein called ASH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		

- Molecule 47 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		

- Molecule 48 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		

- Molecule 49 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		

- Molecule 50 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		

- Molecule 51 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		

- Molecule 52 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		

- Molecule 53 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		

- Molecule 54 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		

- Molecule 55 is a protein called Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5

kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		

- Molecule 56 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		

- Molecule 57 is a protein called NADH:ubiquinone oxidoreductase 15 kDa subunit-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		

- Molecule 60 is a protein called NADH:ubiquinone oxidoreductase 20,9 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		

- Molecule 62 is a protein called Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		

- Molecule 63 is a protein called Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		

- Molecule 64 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		

- Molecule 65 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		

- Molecule 66 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		

- Molecule 67 is a protein called CAG2 - CA-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		

- Molecule 68 is a protein called CAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		

- Molecule 69 is a protein called P10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		

- Molecule 70 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		

- Molecule 71 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		

- Molecule 72 is a protein called NUOP7.

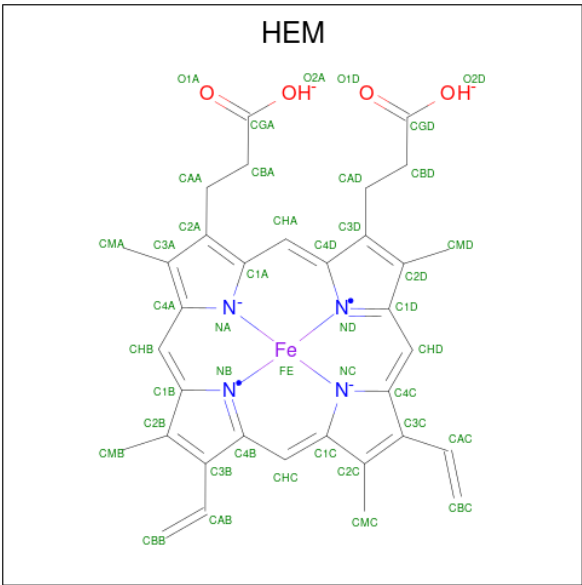
Mol	Chain	Residues	Atoms					AltConf	Trace
72	y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

- Molecule 73 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄).



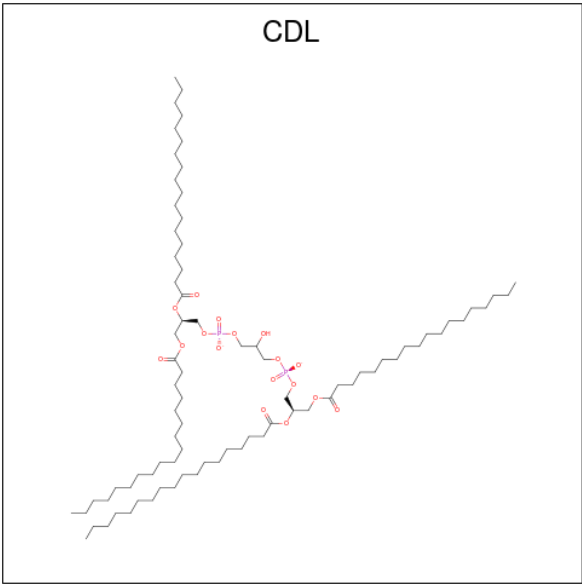
Mol	Chain	Residues	Atoms			AltConf
73	1A	1	Total 38	C 34	O 4	0
73	1A	1	Total 38	C 34	O 4	0
73	1B	1	Total 38	C 34	O 4	0
73	1B	1	Total 38	C 34	O 4	0
73	Q	1	Total 38	C 34	O 4	0

- Molecule 74 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



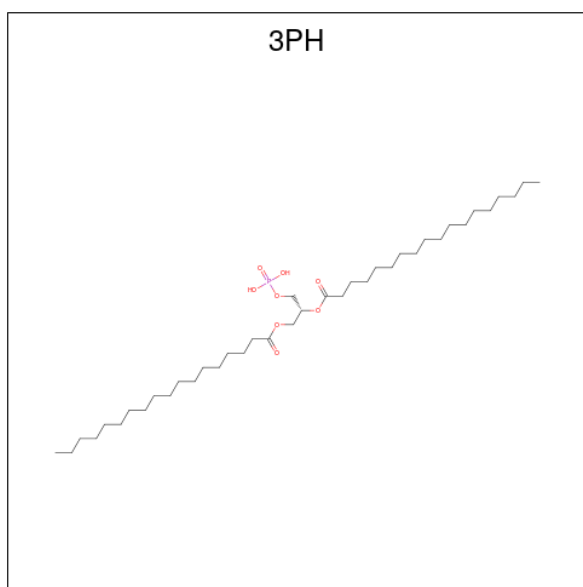
Mol	Chain	Residues	Atoms					AltConf
74	1A	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	1A	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	1B	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	1B	1	Total 43	C 34	Fe 1	N 4	O 4	0

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



Mol	Chain	Residues	Atoms				AltConf
75	1A	1	Total	C	O	P	0
			59	40	17	2	
75	1B	1	Total	C	O	P	0
			64	45	17	2	
75	1B	1	Total	C	O	P	0
			71	52	17	2	
75	1E	1	Total	C	O	P	0
			53	34	17	2	
75	1F	1	Total	C	O	P	0
			56	37	17	2	
75	1K	1	Total	C	O	P	0
			79	60	17	2	
75	1L	1	Total	C	O	P	0
			59	40	17	2	
75	1M	1	Total	C	O	P	0
			54	35	17	2	
75	R	1	Total	C	O	P	0
			63	44	17	2	
75	V	1	Total	C	O	P	0
			64	45	17	2	
75	W	1	Total	C	O	P	0
			95	76	17	2	
75	h	1	Total	C	O	P	0
			77	58	17	2	
75	u	1	Total	C	O	P	0
			83	64	17	2	
75	u	1	Total	C	O	P	0
			71	52	17	2	
75	x	1	Total	C	O	P	0
			92	73	17	2	
75	y	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 76 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



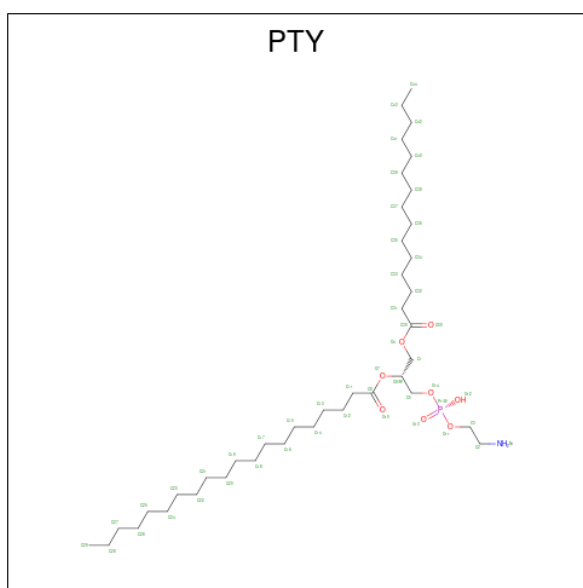
Mol	Chain	Residues	Atoms				AltConf
76	1A	1	Total	C	O	P	0
			31	22	8	1	
76	1B	1	Total	C	O	P	0
			48	39	8	1	
76	1B	1	Total	C	O	P	0
			48	39	8	1	
76	1E	1	Total	C	O	P	0
			40	31	8	1	
76	1K	1	Total	C	O	P	0
			48	39	8	1	
76	1R	1	Total	C	O	P	0
			37	28	8	1	
76	2D	1	Total	C	O	P	0
			32	23	8	1	
76	2I	1	Total	C	O	P	0
			42	33	8	1	
76	3D	1	Total	C	O	P	0
			32	23	8	1	
76	3I	1	Total	C	O	P	0
			42	33	8	1	
76	R	1	Total	C	O	P	0
			32	23	8	1	
76	S	1	Total	C	O	P	0
			37	28	8	1	
76	V	1	Total	C	O	P	0
			42	33	8	1	
76	V	1	Total	C	O	P	0
			41	32	8	1	

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Mol	Chain	Residues	Atoms				AltConf
76	c	1	Total	C	O	P	0
			48	39	8	1	
76	g	1	Total	C	O	P	0
			37	28	8	1	
76	h	1	Total	C	O	P	0
			45	36	8	1	
76	w	1	Total	C	O	P	0
			45	36	8	1	
76	y	1	Total	C	O	P	0
			32	23	8	1	

- Molecule 77 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



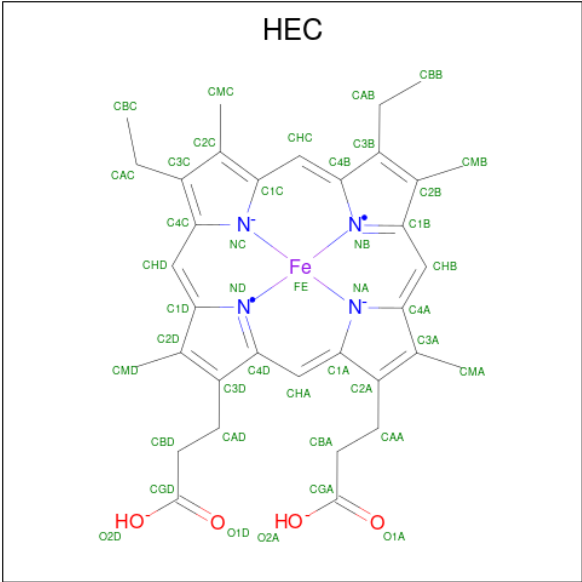
Mol	Chain	Residues	Atoms					AltConf
77	1E	1	Total	C	N	O	P	0
			34	24	1	8	1	
77	1F	1	Total	C	N	O	P	0
			38	28	1	8	1	
77	2D	1	Total	C	N	O	P	0
			35	25	1	8	1	
77	2F	1	Total	C	N	O	P	0
			34	24	1	8	1	
77	3D	1	Total	C	N	O	P	0
			35	25	1	8	1	
77	3F	1	Total	C	N	O	P	0
			34	24	1	8	1	

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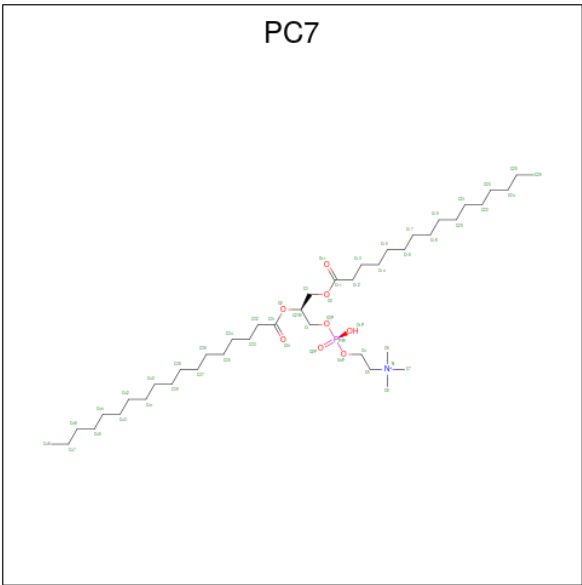
Mol	Chain	Residues	Atoms					AltConf
77	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
77	R	1	Total	C	N	O	P	0
			34	24	1	8	1	
77	R	1	Total	C	N	O	P	0
			44	34	1	8	1	
77	R	1	Total	C	N	O	P	0
			40	30	1	8	1	
77	S	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	T	1	Total	C	N	O	P	0
			50	40	1	8	1	
77	T	1	Total	C	N	O	P	0
			28	18	1	8	1	
77	T	1	Total	C	N	O	P	0
			26	16	1	8	1	
77	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
77	V	1	Total	C	N	O	P	0
			50	40	1	8	1	
77	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
77	e	1	Total	C	N	O	P	0
			25	15	1	8	1	
77	e	1	Total	C	N	O	P	0
			43	33	1	8	1	
77	h	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	x	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 78 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
78	1E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
78	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 79 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
79	1G	1	Total	C	N	O	P	0
			36	26	1	8	1	

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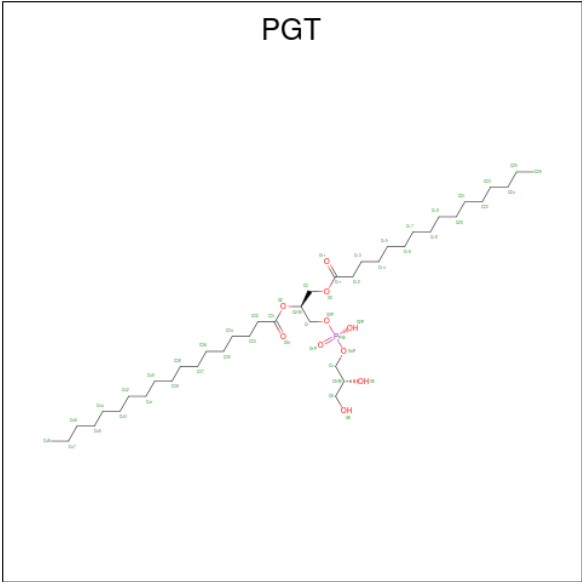
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Mol	Chain	Residues	Atoms					AltConf
79	1H	1	Total	C	N	O	P	0
			39	29	1	8	1	
79	2A	1	Total	C	N	O	P	0
			27	17	1	8	1	
79	3A	1	Total	C	N	O	P	0
			27	17	1	8	1	
79	Q	1	Total	C	N	O	P	0
			33	23	1	8	1	
79	R	1	Total	C	N	O	P	0
			44	34	1	8	1	
79	T	1	Total	C	N	O	P	0
			52	42	1	8	1	
79	u	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

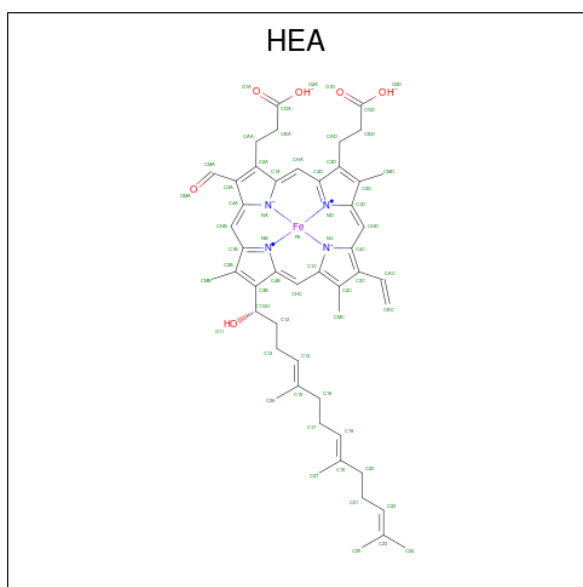
Mol	Chain	Residues	Atoms		AltConf
80	1M	1	Total	Zn	0
			1	1	
80	1N	1	Total	Zn	0
			1	1	
80	s	1	Total	Zn	0
			1	1	

- Molecule 81 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
81	2A	1	Total	C	O	P	0
			33	22	10	1	
81	3A	1	Total	C	O	P	0
			33	22	10	1	
81	T	1	Total	C	O	P	0
			48	37	10	1	
81	T	1	Total	C	O	P	0
			40	29	10	1	
81	b	1	Total	C	O	P	0
			44	33	10	1	
81	l	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 82 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
82	2A	1	Total 60	C 49	Fe 1	N 4	O 6	0
82	2A	1	Total 60	C 49	Fe 1	N 4	O 6	0
82	3A	1	Total 60	C 49	Fe 1	N 4	O 6	0
82	3A	1	Total 60	C 49	Fe 1	N 4	O 6	0

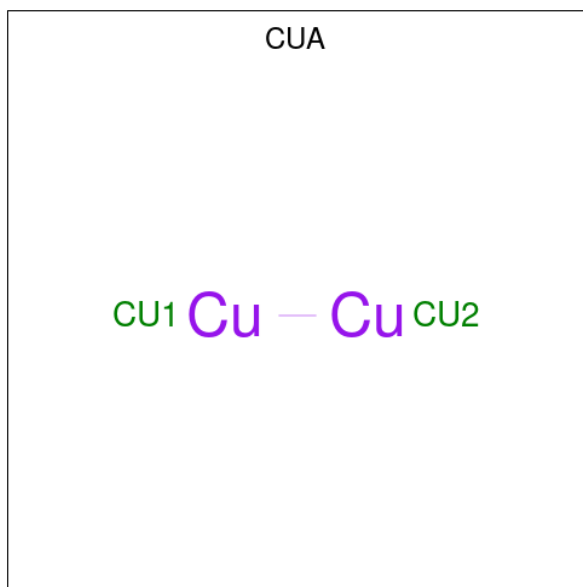
- Molecule 83 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
83	2A	1	Total	Cu	0
			1	1	
83	3A	1	Total	Cu	0
			1	1	

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

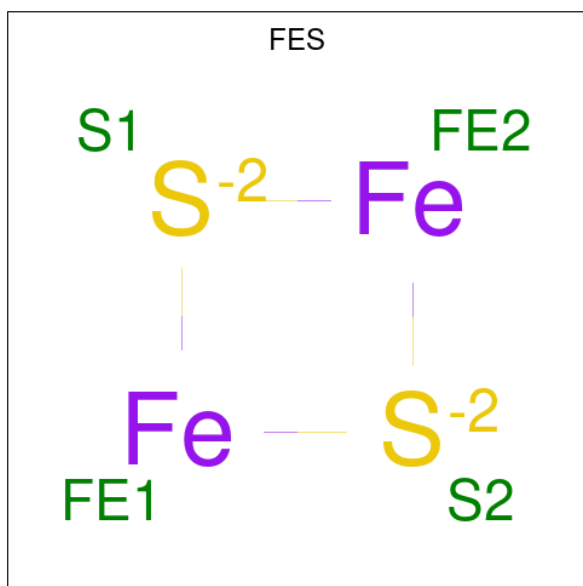
Mol	Chain	Residues	Atoms		AltConf
84	2A	1	Total	Mg	0
			1	1	
84	3A	1	Total	Mg	0
			1	1	

- Molecule 85 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
85	2C	1	Total	Cu	0
			2	2	
85	3C	1	Total	Cu	0
			2	2	

- Molecule 86 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
86	A	1	Total	Fe	S	0
			4	2	2	
86	C	1	Total	Fe	S	0
			4	2	2	

-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The ring atoms are labeled: N1, N5, N10 for the nitrogen atoms and C2, C4, C6, C7, C8, C9, C10 for the carbon atoms. Substituents on the ring include a dimethylaminomethyl group at C2 (C7M, C8M) and a ribityl chain at N10 (C1', C2', C3', C4'). The ribityl chain is shown with stereochemistry: C2' is (S) and C3' is (S). C4' is a chiral center with a hydroxyl group (OH) shown in red. The chain terminates in a phosphate group (O1P) with a central phosphorus atom (P) bonded to four oxygen atoms (O2', O3', O4', O5').

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

-
- The diagram shows a cubane-like complex with four iron (Fe) atoms at the corners of a cube and four sulfur (S) atoms at the centers of the edges. The iron atoms are labeled FE1, FE2, FE3, and FE4. The sulfur atoms are labeled S1, S2, S3, and S4. Each sulfur atom is bonded to two iron atoms, and each iron atom is bonded to three sulfur atoms. The bonds are represented by lines connecting the atoms. The sulfur atoms are colored yellow, and the iron atoms are colored purple. The labels are in green. The overall structure is a cube with the iron atoms at the vertices and the sulfur atoms at the midpoints of the edges.

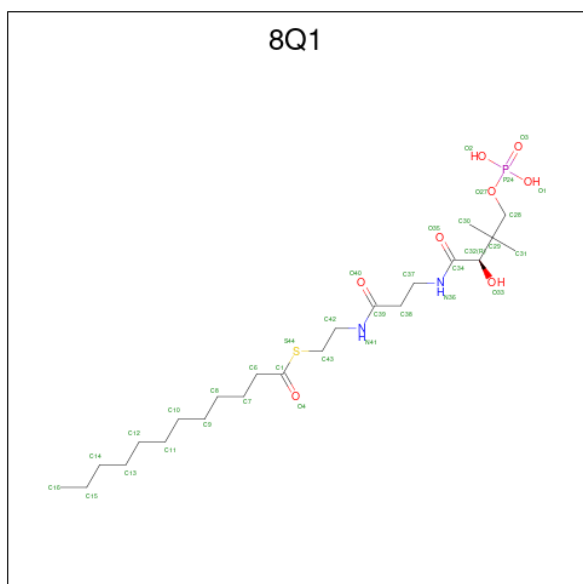
Mol	Chain	Residues	Atoms			AltConf
88	B	1	Total 8	Fe 4	S 4	0
88	C	1	Total 8	Fe 4	S 4	0

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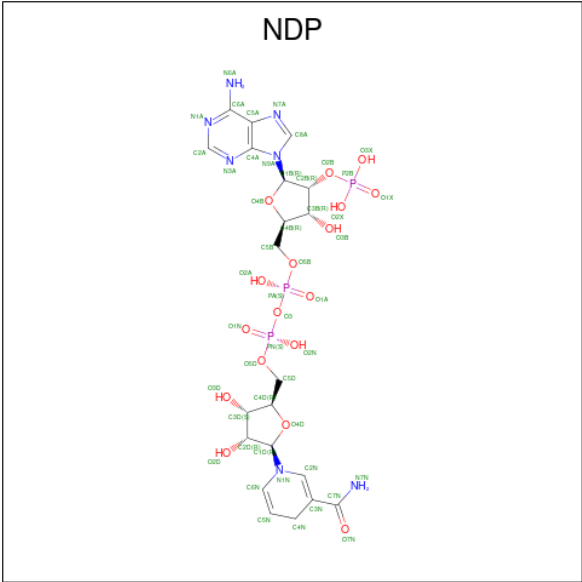
Mol	Chain	Residues	Atoms			AltConf
88	C	1	Total	Fe	S	0
			8	4	4	
88	F	1	Total	Fe	S	0
			8	4	4	
88	G	1	Total	Fe	S	0
			8	4	4	
88	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 89 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



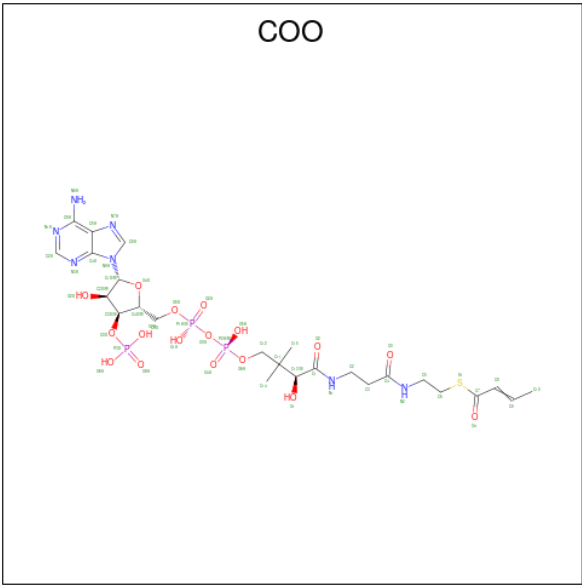
Mol	Chain	Residues	Atoms						AltConf
89	J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
89	r	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 90 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 91 is CROTONYL COENZYME A (CCD ID: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms					AltConf
91	s	1	Total	C	N	O	P	0
			53	25	7	17	3	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	1A	48	Total 48	O 48	0
92	1B	52	Total 52	O 52	0
92	1C	13	Total 13	O 13	0
92	1D	12	Total 12	O 12	0
92	1E	51	Total 51	O 51	0
92	1F	34	Total 34	O 34	0
92	1G	7	Total 7	O 7	0
92	1H	9	Total 9	O 9	0
92	1I	11	Total 11	O 11	0
92	1J	3	Total 3	O 3	0
92	1K	12	Total 12	O 12	0
92	1L	12	Total 12	O 12	0
92	1M	76	Total 76	O 76	0
92	1N	74	Total 74	O 74	0
92	1O	4	Total 4	O 4	0
92	1P	6	Total 6	O 6	0
92	1Q	27	Total 27	O 27	0
92	1R	32	Total 32	O 32	0
92	1S	29	Total 29	O 29	0
92	1T	28	Total 28	O 28	0
92	A	24	Total 24	O 24	0
92	B	66	Total 66	O 66	0

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Mol	Chain	Residues	Atoms		AltConf
92	C	168	Total 168	O 168	0
92	D	66	Total 66	O 66	0
92	E	87	Total 87	O 87	0
92	F	39	Total 39	O 39	0
92	G	62	Total 62	O 62	0
92	H	16	Total 16	O 16	0
92	I	19	Total 19	O 19	0
92	K	16	Total 16	O 16	0
92	L	68	Total 68	O 68	0
92	M	30	Total 30	O 30	0
92	N	53	Total 53	O 53	0
92	O	6	Total 6	O 6	0
92	P	69	Total 69	O 69	0
92	Q	24	Total 24	O 24	0
92	R	64	Total 64	O 64	0
92	S	22	Total 22	O 22	0
92	T	85	Total 85	O 85	0
92	U	14	Total 14	O 14	0
92	V	99	Total 99	O 99	0
92	W	25	Total 25	O 25	0
92	X	50	Total 50	O 50	0

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Mol	Chain	Residues	Atoms		AltConf
92	Y	4	Total 4	O 4	0
92	Z	20	Total 20	O 20	0
92	a	6	Total 6	O 6	0
92	b	24	Total 24	O 24	0
92	c	1	Total 1	O 1	0
92	d	12	Total 12	O 12	0
92	e	55	Total 55	O 55	0
92	f	10	Total 10	O 10	0
92	g	7	Total 7	O 7	0
92	h	38	Total 38	O 38	0
92	i	30	Total 30	O 30	0
92	j	29	Total 29	O 29	0
92	k	51	Total 51	O 51	0
92	l	17	Total 17	O 17	0
92	m	32	Total 32	O 32	0
92	n	7	Total 7	O 7	0
92	o	51	Total 51	O 51	0
92	p	21	Total 21	O 21	0
92	q	24	Total 24	O 24	0
92	r	12	Total 12	O 12	0
92	s	39	Total 39	O 39	0

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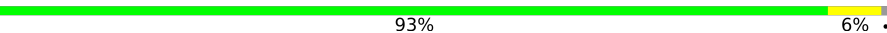
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Mol	Chain	Residues	Atoms		AltConf
92	t	55	Total 55	O 55	0
92	u	41	Total 41	O 41	0
92	v	2	Total 2	O 2	0
92	w	16	Total 16	O 16	0
92	x	22	Total 22	O 22	0
92	y	29	Total 29	O 29	0

3 Residue-property plots

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

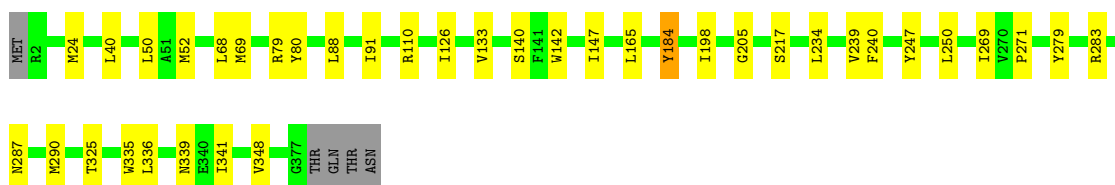
- Molecule 1: Cytochrome b

Chain 1A: 



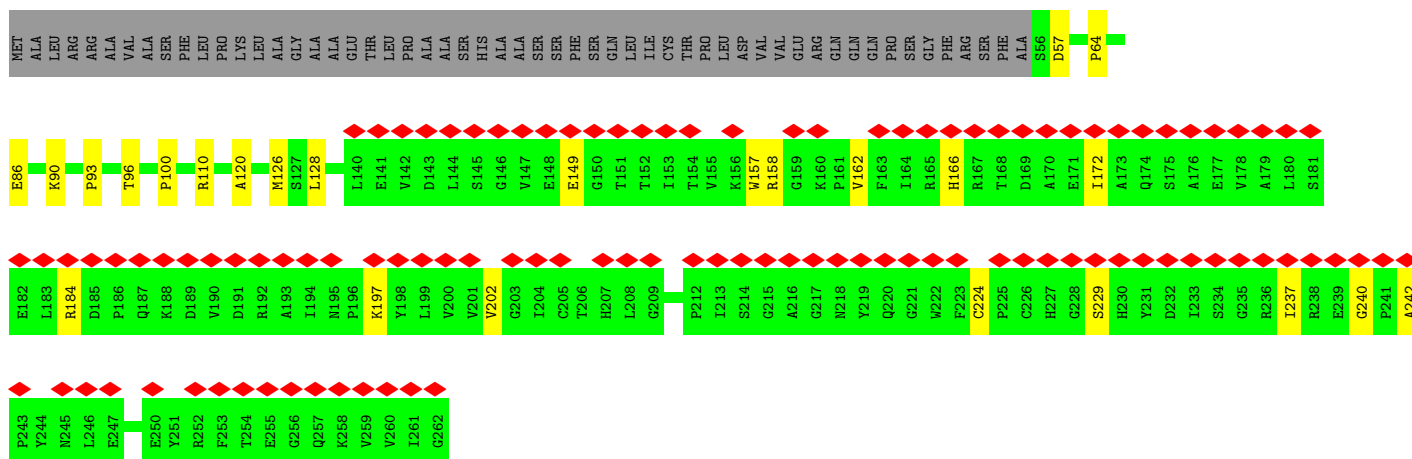
- Molecule 1: Cytochrome b

Chain 1B: 

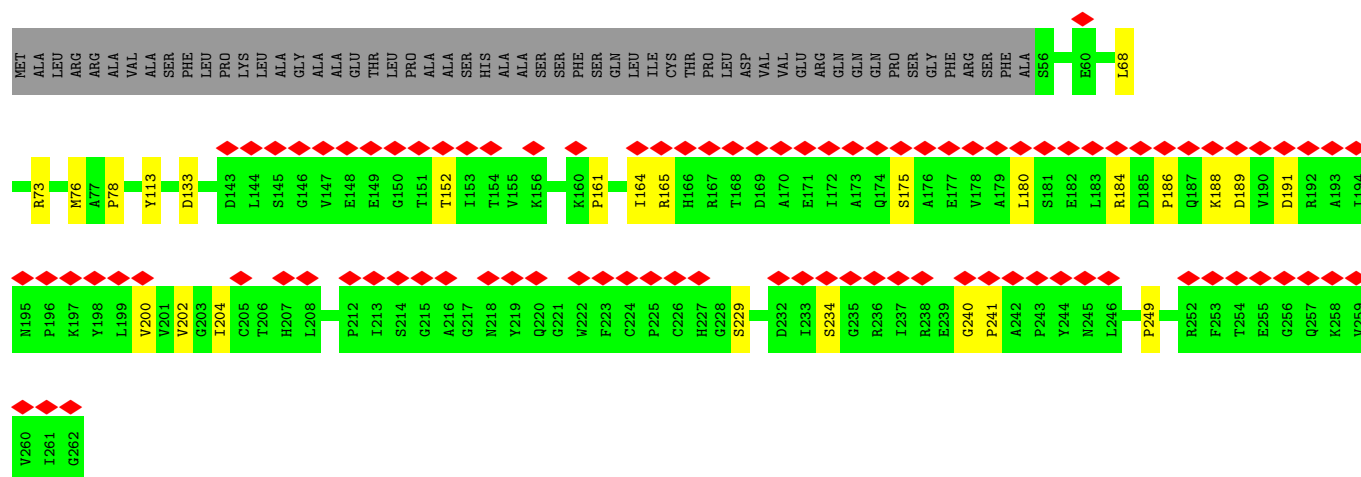


- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

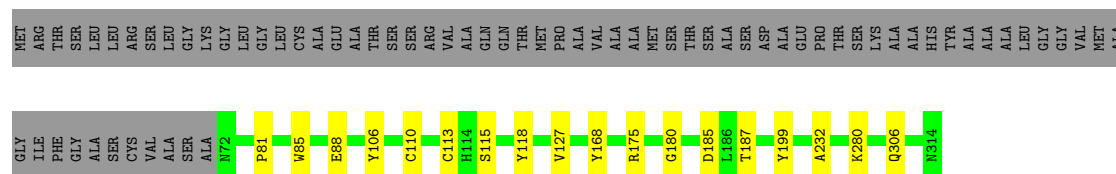
Chain 1C: 



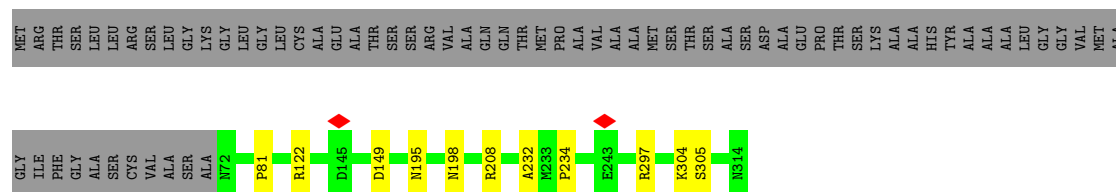
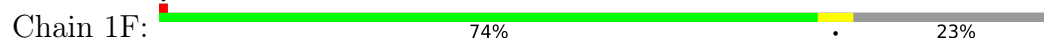
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



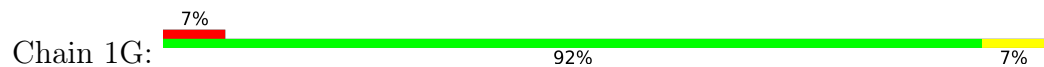
• Molecule 3: Cytochrome c1



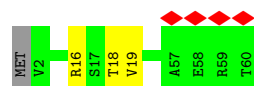
• Molecule 3: Cytochrome c1



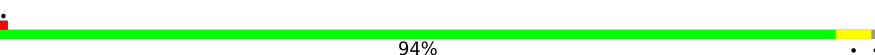
• Molecule 4: Complex III subunit 9

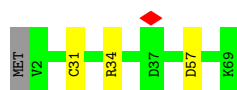


• Molecule 4: Complex III subunit 9

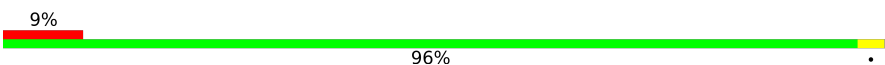


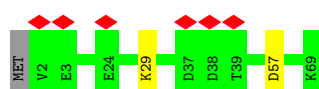
- Molecule 5: Cytochrome b-c1 complex subunit 6

Chain 1I:  94%



- Molecule 5: Cytochrome b-c1 complex subunit 6

Chain 1J:  96%



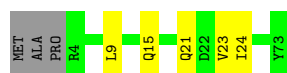
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1K:  90%



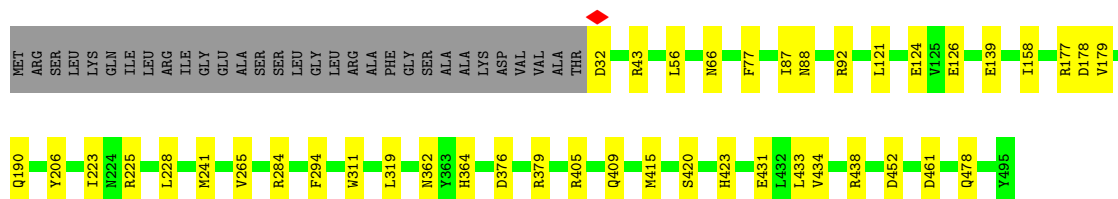
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1L:  89%



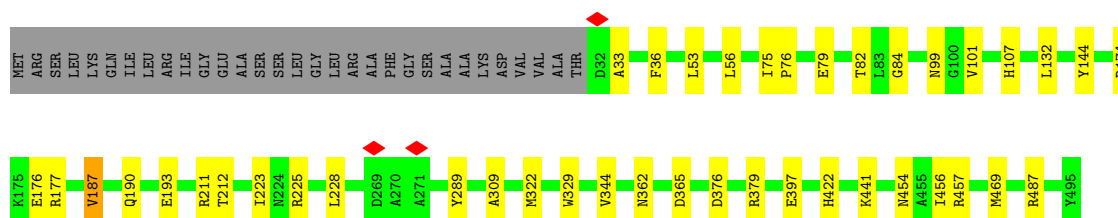
- Molecule 7: MPP-Beta

Chain 1M:  85%

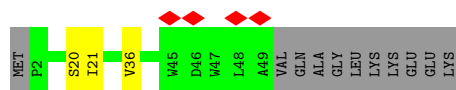
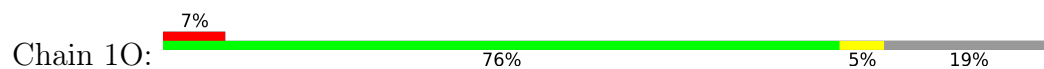


- Molecule 7: MPP-Beta

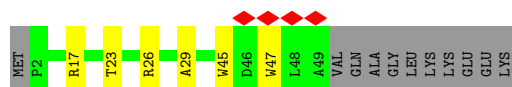
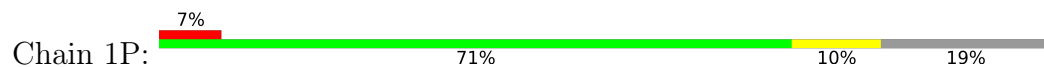
Chain 1N:  85%



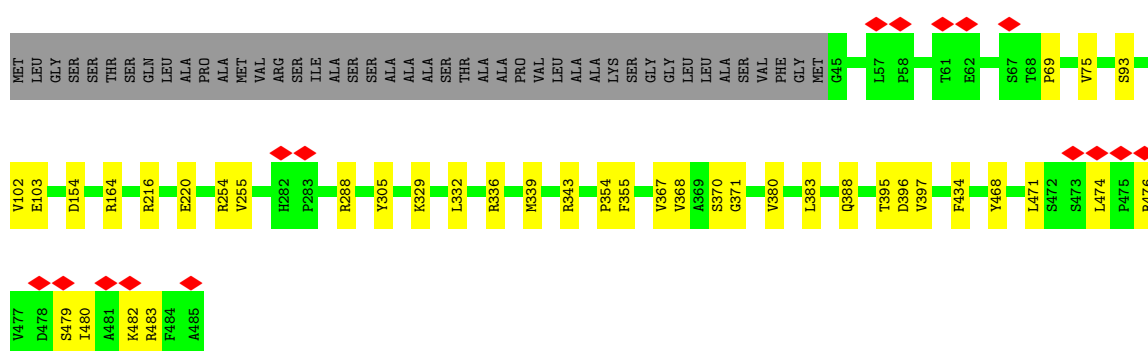
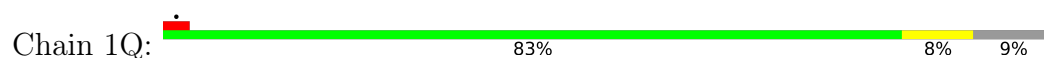
- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



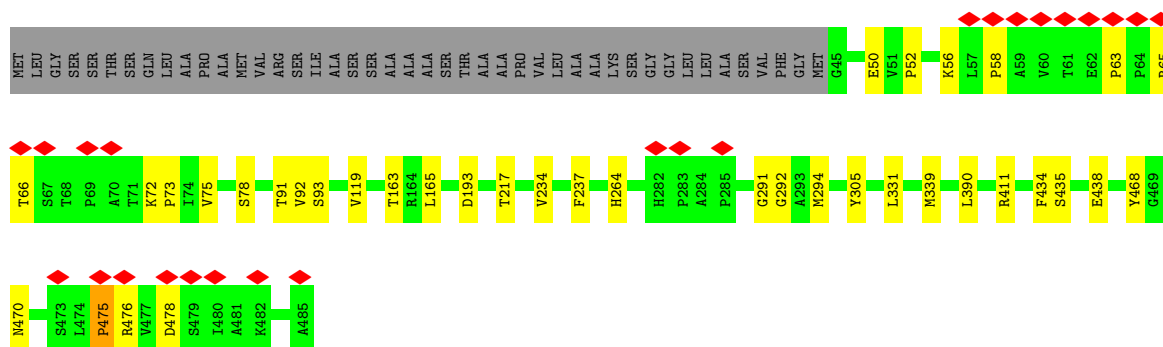
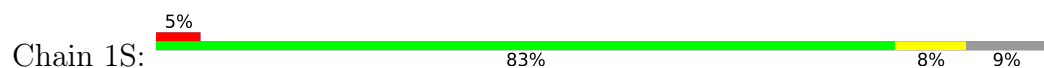
- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



- Molecule 9: Alpha-MPP

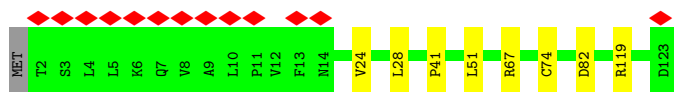


- Molecule 9: Alpha-MPP



- Molecule 10: Cytochrome b-c1 complex subunit 7

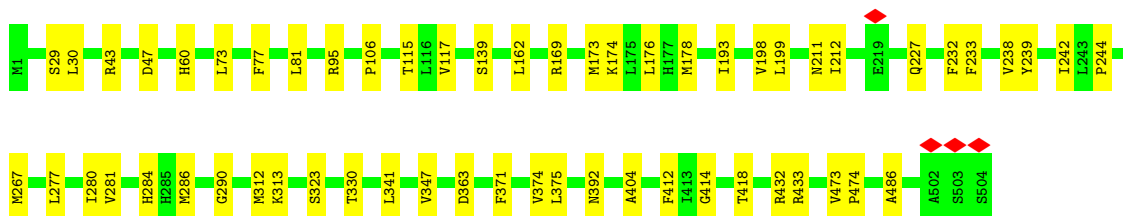
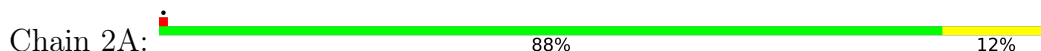




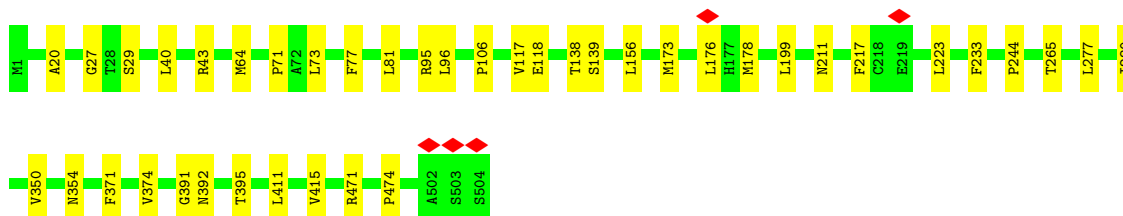
- Molecule 10: Cytochrome b-c1 complex subunit 7



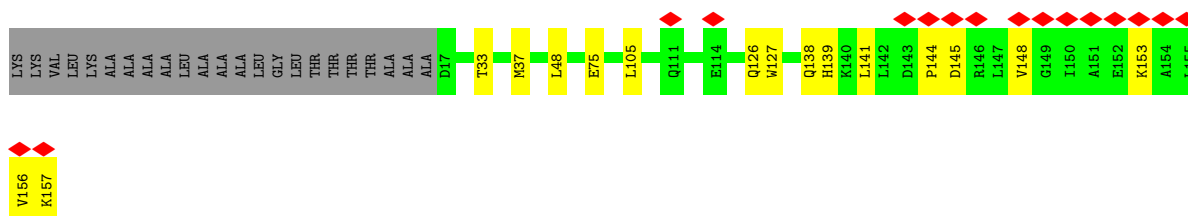
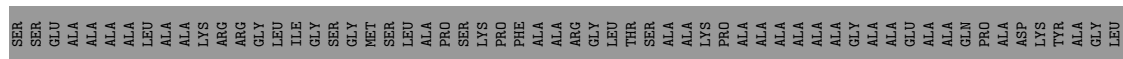
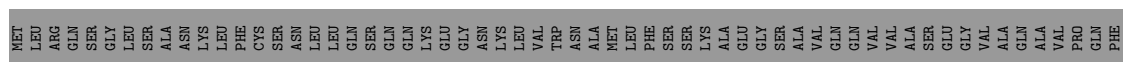
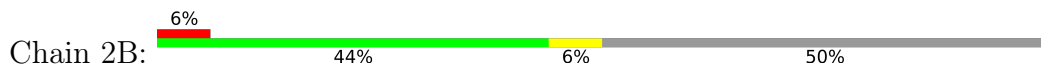
- Molecule 11: Cytochrome c oxidase subunit 1



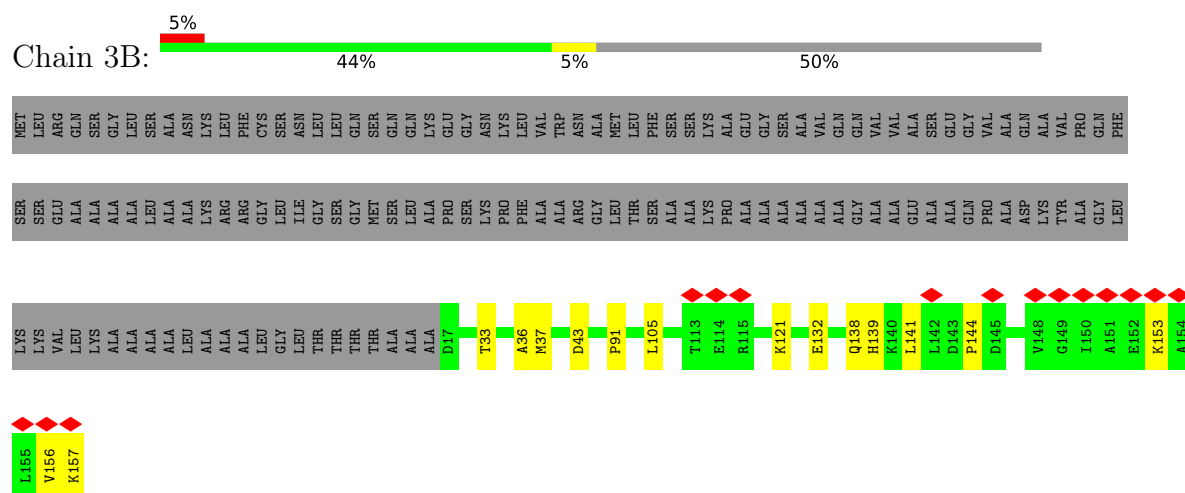
- Molecule 11: Cytochrome c oxidase subunit 1

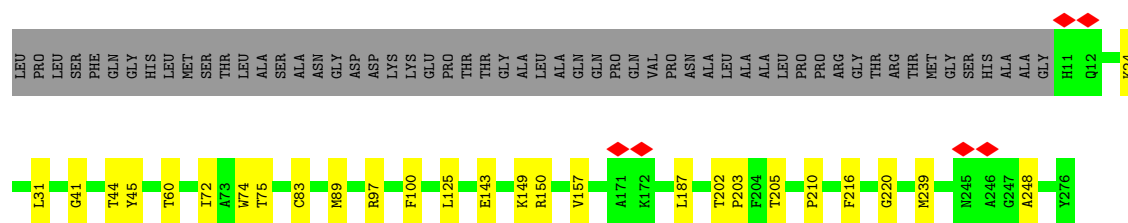


- Molecule 12: Cytochrome c oxidase polypeptide II

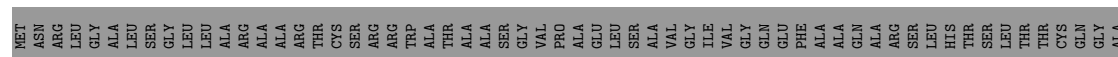


• Molecule 12: Cytochrome c oxidase polypeptide II

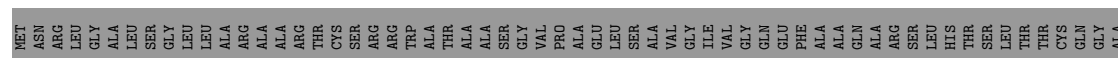




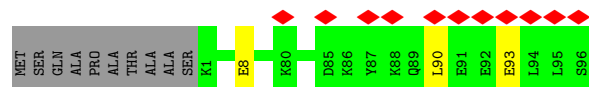
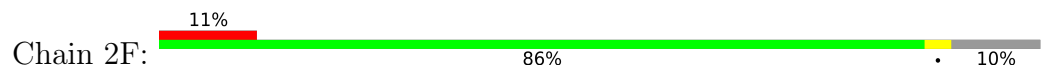
• Molecule 15: Cox5b



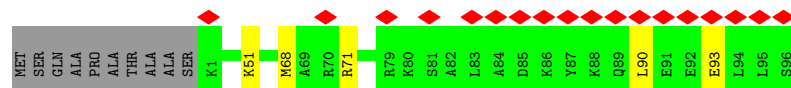
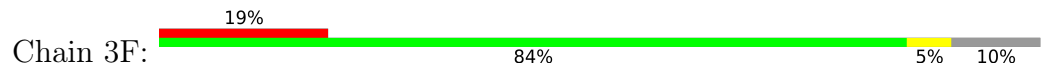
• Molecule 15: Cox5b



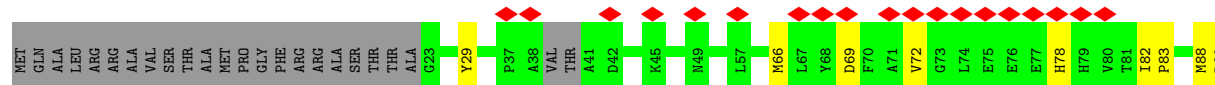
• Molecule 16: Cox5c

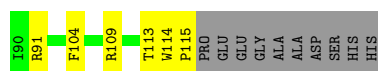


• Molecule 16: Cox5c

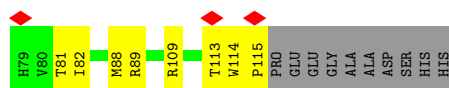
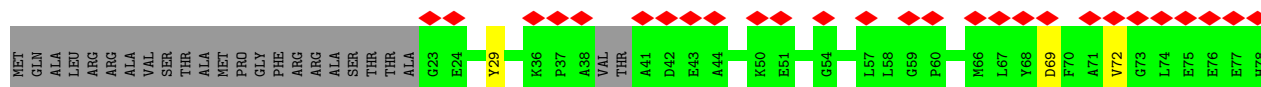


• Molecule 17: Cox6a

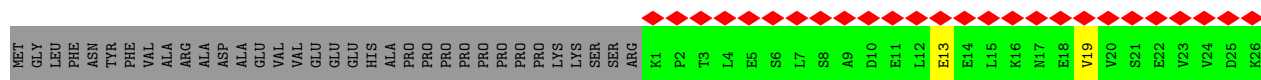
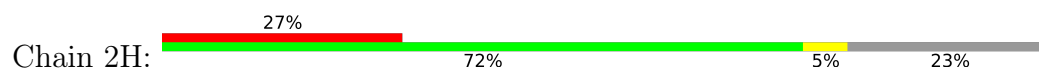




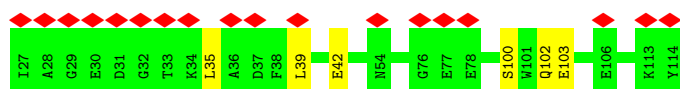
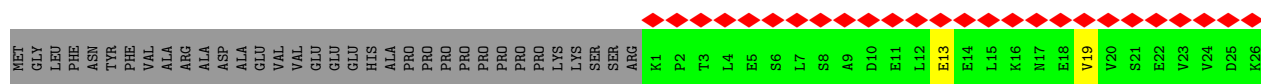
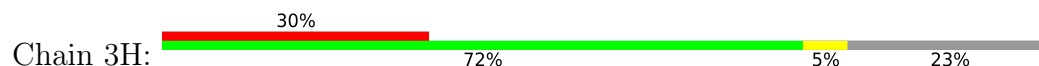
- Molecule 17: Cox6a



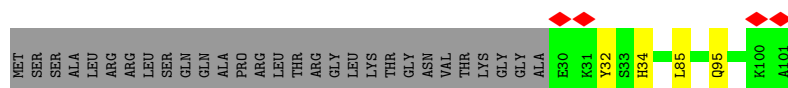
- Molecule 18: Cox6b



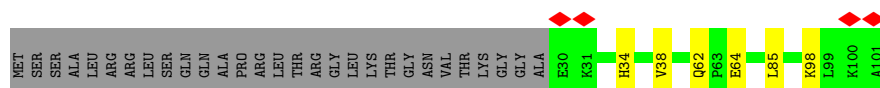
- Molecule 18: Cox6b



- Molecule 19: Cox7c

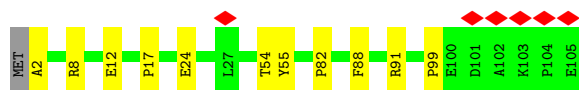


- Molecule 19: Cox7c

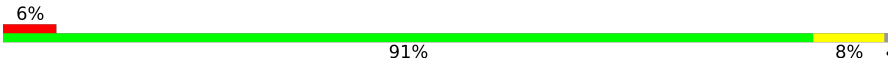


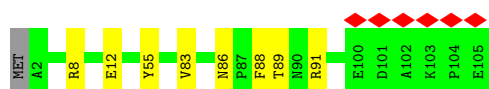
- Molecule 20: Cytochrome c oxidase subunit

Chain 2J:  6% 89% 10%



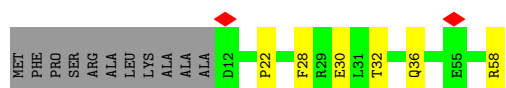
- Molecule 20: Cytochrome c oxidase subunit

Chain 3J:  6% 91% 8%



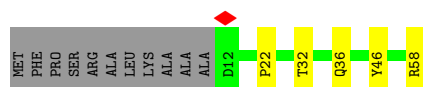
- Molecule 21: Cox7a

Chain 2K:  1% 71% 10% 19%



- Molecule 21: Cox7a

Chain 3K:  1% 72% 9% 19%



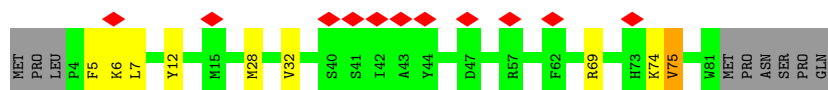
- Molecule 22: CoxIn

Chain 2L:  1% 80% 6% 13%



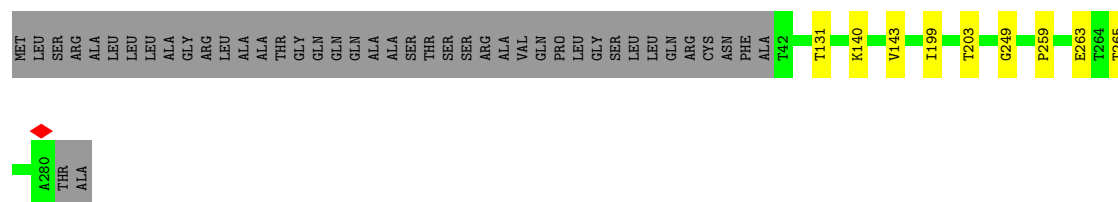
- Molecule 22: CoxIn

Chain 3L:  13% 79% 9% 10%

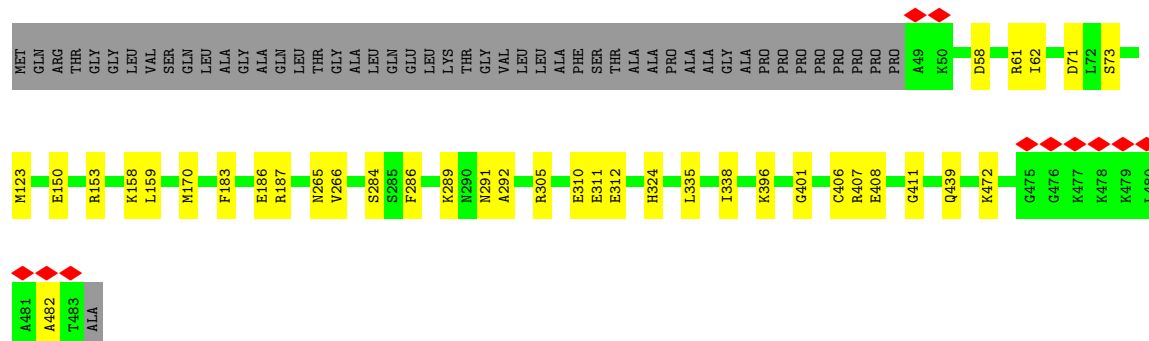
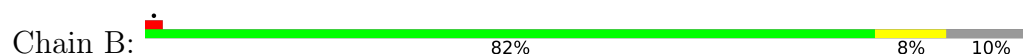


- Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

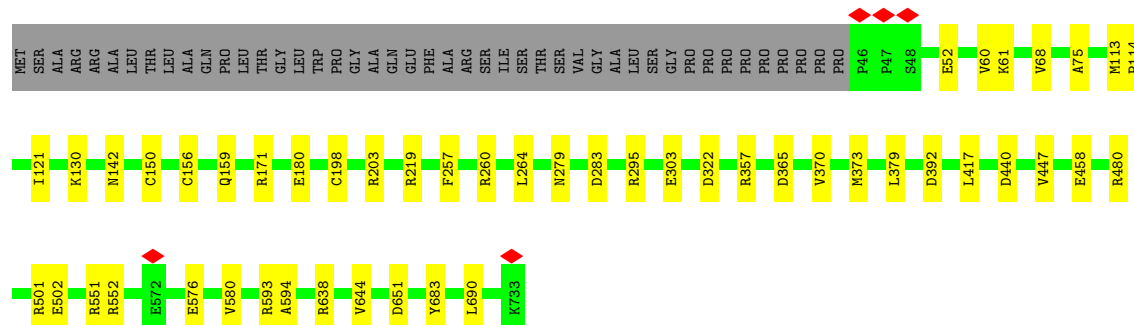
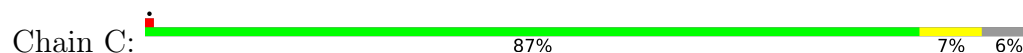
Chain A:  82% 15%



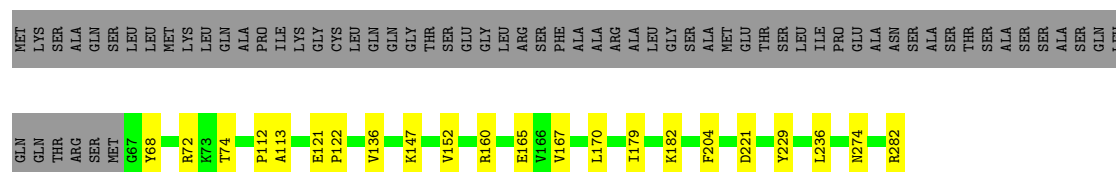
- Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



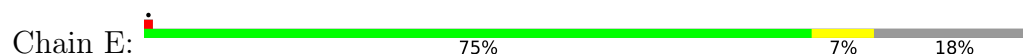
- Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

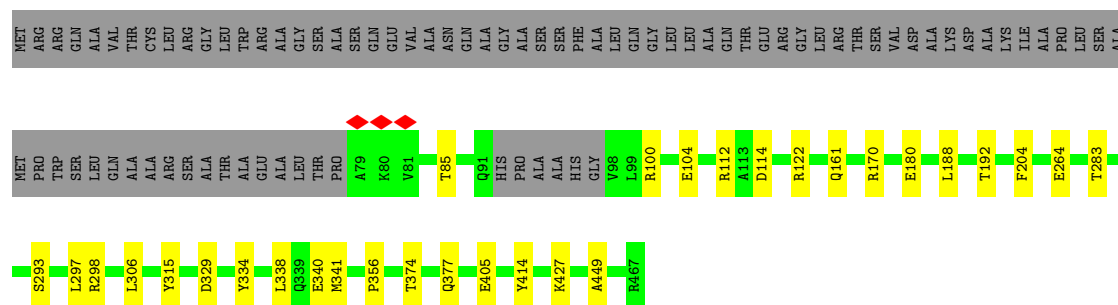


- Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

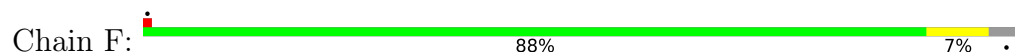


- Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit

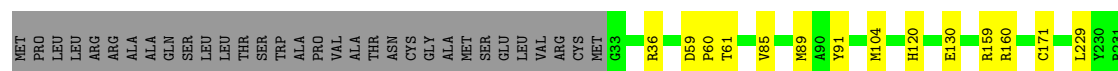
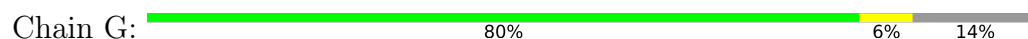




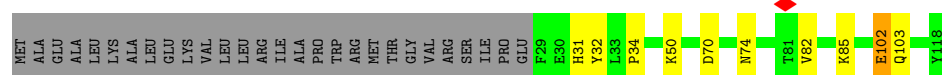
- Molecule 28: NADH:ubiquinone oxidoreductase subunit 10



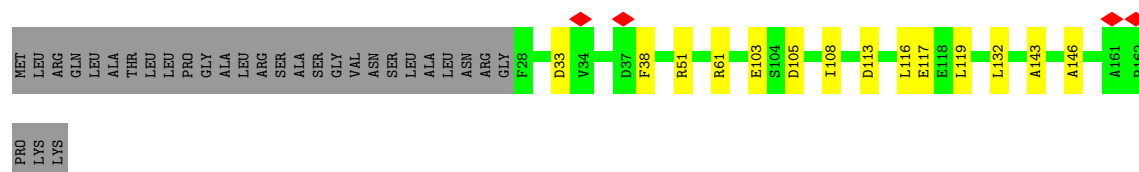
- Molecule 29: NADH:ubiquinone oxidoreductase subunit 8



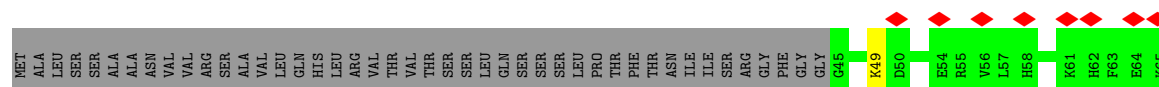
- Molecule 30: B14.5a

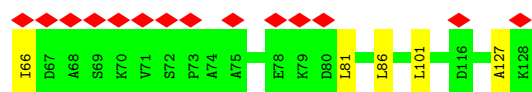


- Molecule 31: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit

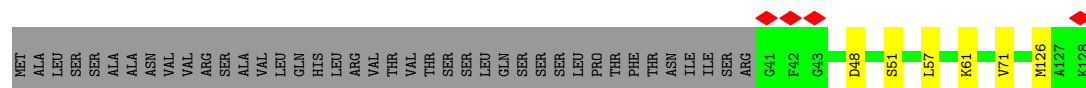


- Molecule 32: Acyl carrier protein

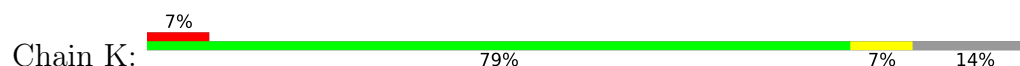




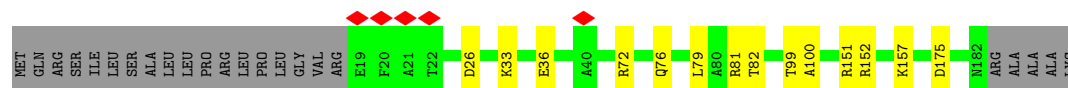
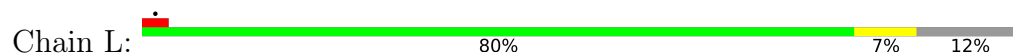
- Molecule 32: Acyl carrier protein



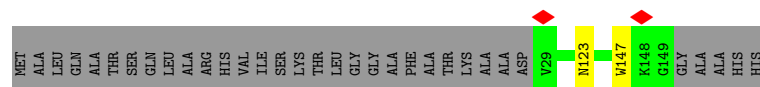
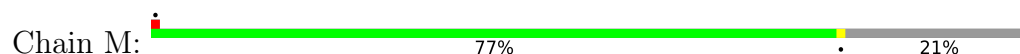
- Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit



- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



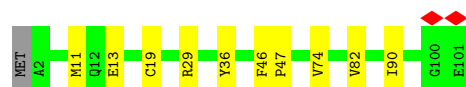
- Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

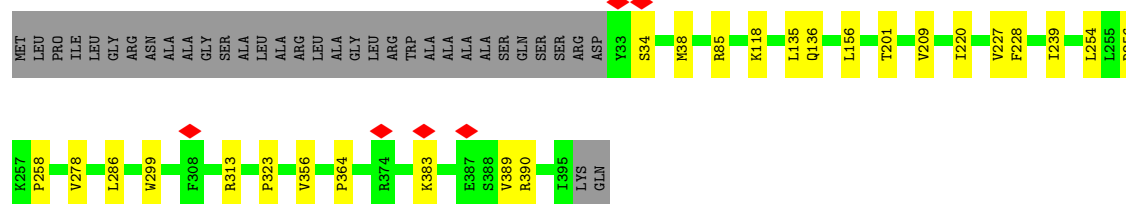


- Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit



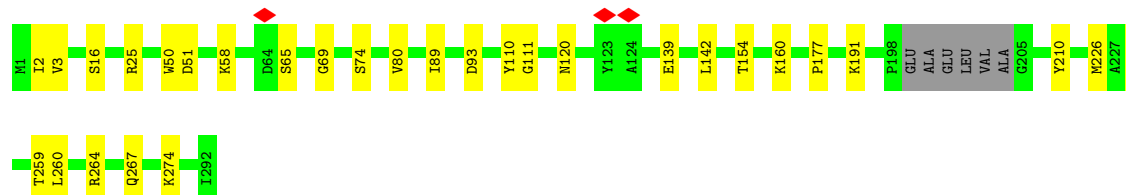
- Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

Chain P: 



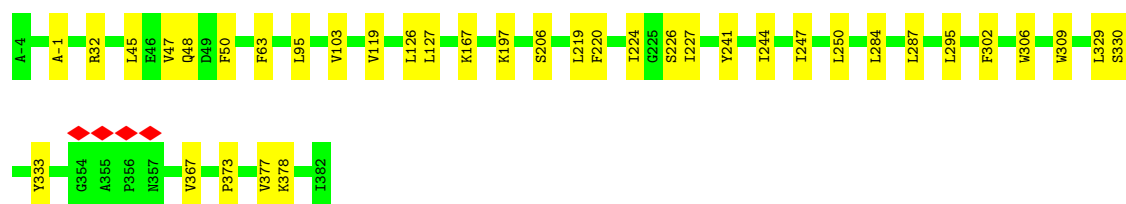
- Molecule 39: NADH-ubiquinone oxidoreductase chain 1

Chain Q: 



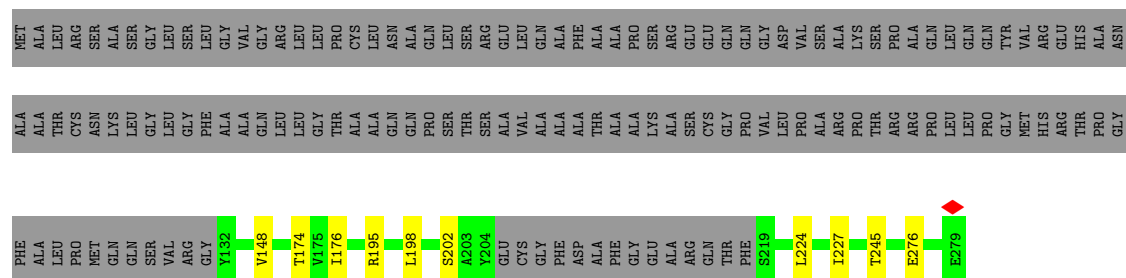
- Molecule 40: NADH-ubiquinone oxidoreductase chain 2

Chain R: 



- Molecule 41: NADH-ubiquinone oxidoreductase chain 3

Chain S: 



- Molecule 42: NADH-ubiquinone oxidoreductase chain 4

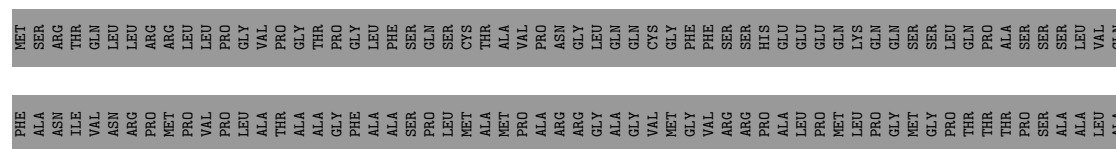
Chain T: 





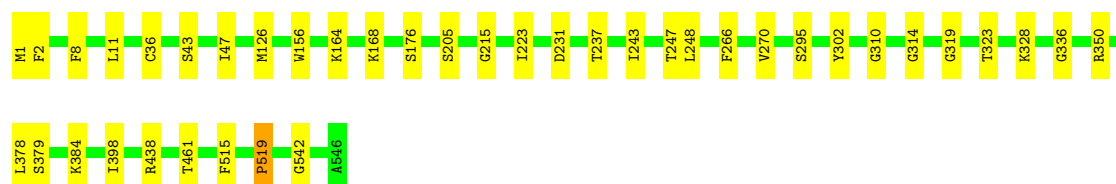
- Molecule 43: NADH dehydrogenase subunit 4L

Chain U: 41% 5% 54%



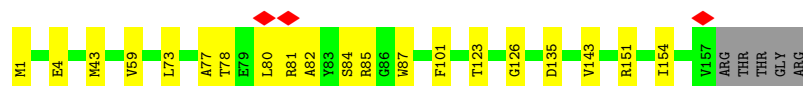
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain V: 93% 7%



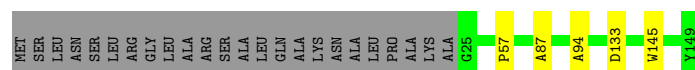
- Molecule 45: NADH-ubiquinone oxidoreductase chain 6

Chain W: 85% 12%



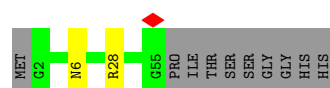
- Molecule 46: ASHI

Chain X: 81% 16%



- Molecule 47: P9

Chain Y: 81% 16%

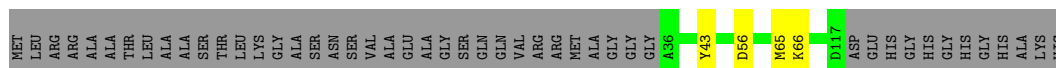


- Molecule 48: KFYI

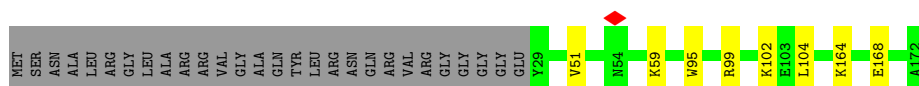
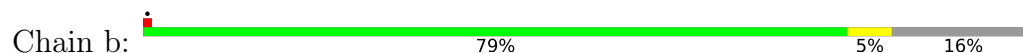
Chain Z: 83% 14%



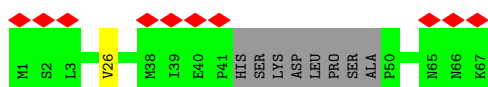
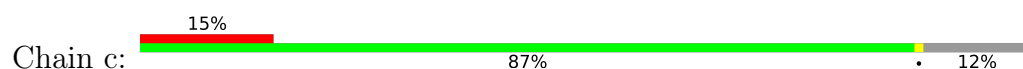
- Molecule 49: AGGG



- Molecule 50: ESSS



- Molecule 51: B9



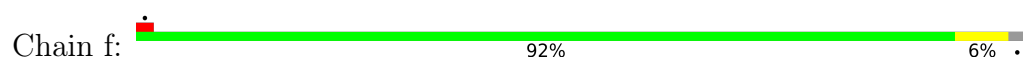
- Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit



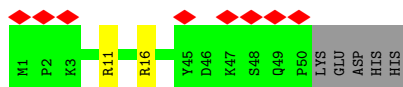
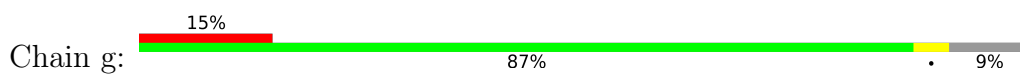
- Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit



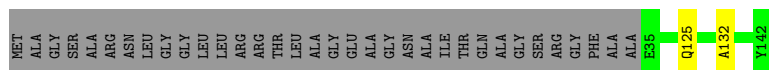
- Molecule 54: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit



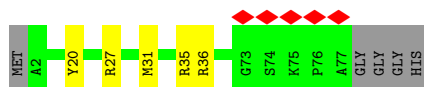
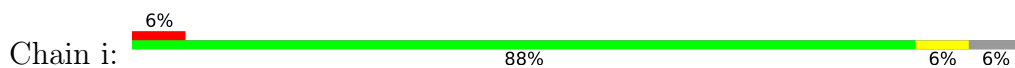
- Molecule 55: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit



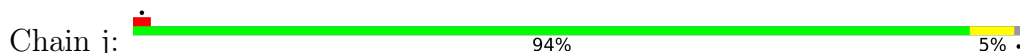
- Molecule 56: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit



- Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like



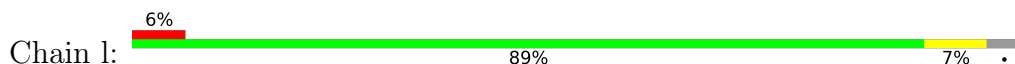
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



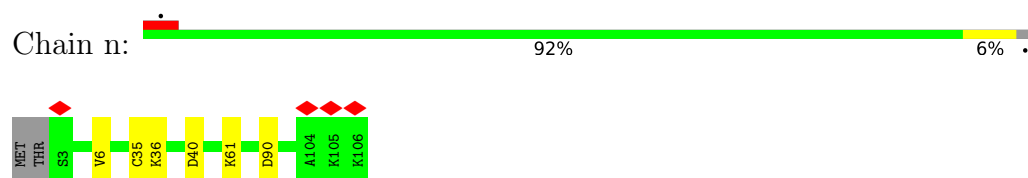
- Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit



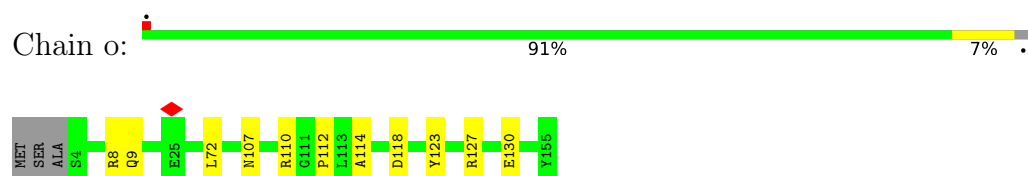
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



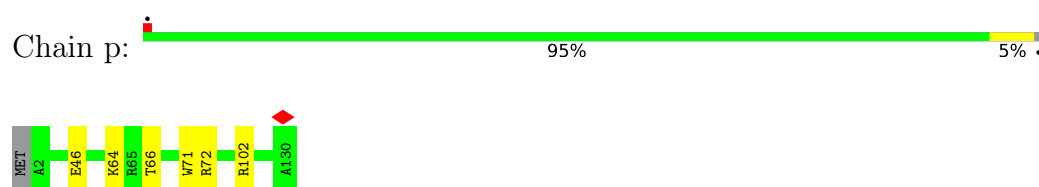
- Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit



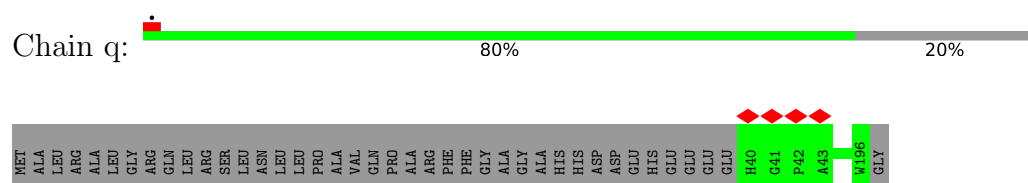
- Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit



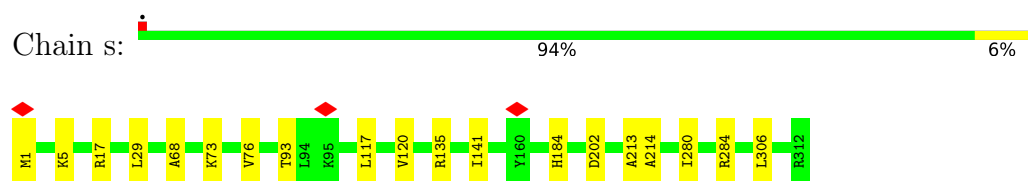
- Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit



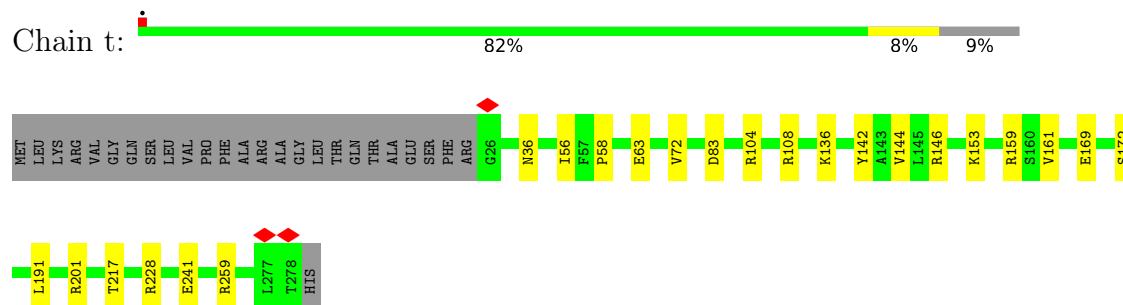
- Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit



- Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit



- Molecule 67: CAG2 - CA-like



- Molecule 68: CAG1

Chain u:  94% 6%



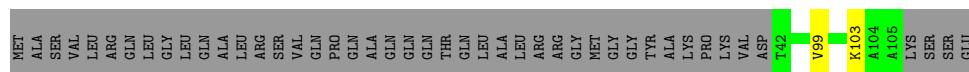
- Molecule 69: P10

Chain v:  100%



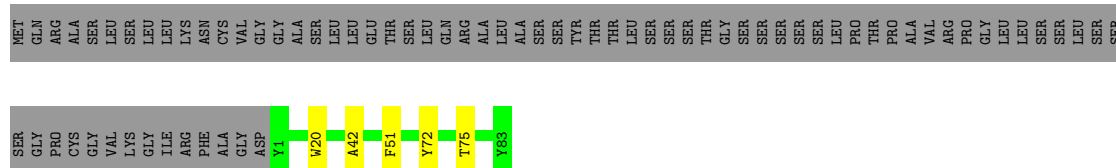
- Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit

Chain w:  57% 41%

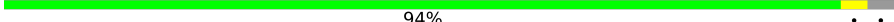


- Molecule 71: NUOP8

Chain x:  50% 47%



- Molecule 72: NUOP7

Chain y:  94%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.068	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.126	Depositor
Map size (Å)	589.6, 589.6, 589.6	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0027211, 1.0027211, 1.0027211	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8Q1, PC7, CUA, HEM, ZN, UQ5, SF4, FMN, 3PH, COO, MG, HEC, CU, NDP, PTY, CDL, HEA, FES, PGT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.25	0/3060	0.48	1/4187 (0.0%)
1	1B	0.26	0/3060	0.48	1/4187 (0.0%)
2	1C	0.18	0/1643	0.36	0/2233
2	1D	0.17	0/1643	0.33	0/2233
3	1E	0.24	0/1953	0.43	1/2654 (0.0%)
3	1F	0.22	0/1953	0.38	0/2654
4	1G	0.23	0/496	0.41	0/667
4	1H	0.22	0/496	0.39	0/667
5	1I	0.23	0/567	0.45	0/766
5	1J	0.21	0/567	0.39	0/766
6	1K	0.25	0/609	0.44	0/817
6	1L	0.22	0/609	0.42	0/817
7	1M	0.23	0/3723	0.42	0/5046
7	1N	0.22	0/3723	0.38	0/5046
8	1O	0.19	0/385	0.44	0/531
8	1P	0.21	0/385	0.52	0/531
9	1Q	0.21	0/3258	0.43	0/4439
9	1S	0.21	0/3258	0.43	1/4439 (0.0%)
10	1R	0.21	0/996	0.35	0/1349
10	1T	0.23	0/996	0.41	0/1349
11	2A	0.26	0/4011	0.51	3/5484 (0.1%)
11	3A	0.27	0/4011	0.54	1/5484 (0.0%)
12	2B	0.23	0/1204	0.45	0/1641
12	3B	0.24	0/1204	0.46	0/1641
13	2C	0.21	0/1237	0.41	0/1676
13	3C	0.24	0/1237	0.46	0/1676
14	2D	0.23	0/2152	0.47	0/2937
14	3D	0.24	0/2152	0.49	0/2937
15	2E	0.24	0/757	0.62	3/1029 (0.3%)
15	3E	0.24	0/757	0.61	2/1029 (0.2%)
16	2F	0.18	0/726	0.35	0/974

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
16	3F	0.18	0/726	0.38	0/974
17	2G	0.27	0/762	0.57	0/1038
17	3G	0.27	0/762	0.52	0/1038
18	2H	0.19	0/980	0.42	0/1325
18	3H	0.22	0/980	0.52	1/1325 (0.1%)
19	2I	0.23	0/619	0.46	0/839
19	3I	0.21	0/619	0.45	0/839
20	2J	0.21	0/839	0.39	0/1143
20	3J	0.22	0/839	0.43	0/1143
21	2K	0.19	0/392	0.39	0/531
21	3K	0.23	0/392	0.41	0/531
22	2L	0.25	0/621	0.59	1/841 (0.1%)
22	3L	0.27	0/645	0.57	1/875 (0.1%)
23	A	0.22	0/1878	0.47	0/2549
24	B	0.24	0/3400	0.45	0/4573
25	C	0.23	0/5272	0.42	0/7143
26	D	0.27	0/1843	0.49	0/2506
27	E	0.29	0/3158	0.49	0/4270
28	F	0.30	0/1258	0.48	0/1706
29	G	0.25	0/1648	0.50	0/2222
30	H	0.24	0/773	0.58	2/1046 (0.2%)
31	I	0.21	0/1061	0.38	0/1441
32	J	0.20	0/649	0.47	0/875
32	r	0.22	0/673	0.40	0/906
33	K	0.24	0/1007	0.54	1/1348 (0.1%)
34	L	0.23	0/1306	0.47	0/1769
35	M	0.23	0/936	0.43	0/1276
36	N	0.21	0/1277	0.37	0/1735
37	O	0.18	0/772	0.45	0/1037
38	P	0.22	0/2879	0.44	0/3905
39	Q	0.29	0/2234	0.52	0/3034
40	R	0.30	0/3100	0.54	0/4226
41	S	0.28	0/1106	0.49	0/1512
42	T	0.31	0/3533	0.55	0/4825
43	U	0.28	0/819	0.48	0/1112
44	V	0.29	0/4258	0.52	0/5792
45	W	0.26	0/1239	0.52	0/1686
46	X	0.27	0/1081	0.51	0/1479
47	Y	0.24	0/411	0.41	0/557
48	Z	0.23	0/894	0.42	0/1218
49	a	0.21	0/698	0.43	0/949
50	b	0.26	0/1201	0.49	0/1623
51	c	0.22	0/463	0.50	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
52	d	0.27	0/721	0.41	0/968
53	e	0.27	0/1688	0.46	0/2301
54	f	0.25	0/547	0.42	0/740
55	g	0.20	0/433	0.46	0/587
56	h	0.24	0/948	0.49	0/1285
57	i	0.22	0/644	0.40	0/860
58	j	0.23	0/732	0.38	0/983
59	k	0.25	0/1011	0.43	0/1361
60	l	0.25	0/936	0.43	0/1278
61	m	0.27	0/1155	0.41	0/1558
62	n	0.23	0/886	0.39	0/1188
63	o	0.27	0/1265	0.50	0/1705
64	p	0.22	0/1095	0.39	0/1480
65	q	0.23	0/1308	0.38	0/1779
66	s	0.22	0/2353	0.42	0/3202
67	t	0.25	0/2043	0.48	0/2778
68	u	0.25	0/1730	0.47	0/2341
69	v	0.22	0/369	0.37	0/498
70	w	0.24	0/521	0.41	0/702
71	x	0.23	0/727	0.39	0/994
72	y	0.25	0/963	0.48	0/1313
All	All	0.24	0/134906	0.46	19/183172 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1A	0	1
1	1B	0	1
17	3G	0	1
53	e	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	102	GLU	CA-C-N	7.46	135.79	121.54
30	H	102	GLU	C-N-CA	7.46	135.79	121.54
22	3L	75	VAL	N-CA-C	-7.07	106.11	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2L	75	VAL	N-CA-C	-6.75	106.22	112.43
15	2E	27	ALA	CA-C-N	6.59	134.13	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	184	TYR	Sidechain
1	1B	184	TYR	Sidechain
17	3G	114	TRP	Peptide
53	e	147	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2958	0	2955	15	0
1	1B	2958	0	2953	25	0
2	1C	1602	0	1577	16	0
2	1D	1602	0	1577	15	0
3	1E	1898	0	1800	11	0
3	1F	1898	0	1800	10	0
4	1G	486	0	490	4	0
4	1H	486	0	490	2	0
5	1I	550	0	501	2	0
5	1J	550	0	501	2	0
6	1K	594	0	590	4	0
6	1L	594	0	590	5	0
7	1M	3646	0	3555	30	0
7	1N	3646	0	3555	28	0
8	1O	371	0	372	2	0
8	1P	371	0	372	5	0
9	1Q	3204	0	3271	26	0
9	1S	3204	0	3271	23	0
10	1R	980	0	1004	7	0
10	1T	980	0	1005	7	0
11	2A	3888	0	3936	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	3A	3888	0	3936	33	0
12	2B	1169	0	1191	14	0
12	3B	1169	0	1191	12	0
13	2C	1212	0	1243	11	0
13	3C	1212	0	1243	13	0
14	2D	2079	0	2039	15	0
14	3D	2079	0	2039	20	0
15	2E	737	0	706	0	0
15	3E	737	0	706	1	0
16	2F	706	0	685	2	0
16	3F	706	0	685	3	0
17	2G	733	0	708	12	0
17	3G	733	0	708	6	0
18	2H	954	0	900	6	0
18	3H	954	0	900	6	0
19	2I	594	0	553	4	0
19	3I	594	0	553	6	0
20	2J	816	0	807	8	0
20	3J	816	0	807	6	0
21	2K	382	0	367	6	0
21	3K	382	0	367	5	0
22	2L	605	0	588	4	0
22	3L	627	0	604	16	0
23	A	1839	0	1827	6	0
24	B	3331	0	3328	23	0
25	C	5175	0	5182	32	0
26	D	1790	0	1740	16	0
27	E	3085	0	3058	20	0
28	F	1225	0	1224	11	0
29	G	1615	0	1551	11	0
30	H	750	0	751	8	0
31	I	1044	0	1046	10	0
32	J	640	0	629	5	0
32	r	663	0	647	5	0
33	K	986	0	1017	7	0
34	L	1275	0	1243	12	0
35	M	913	0	909	2	0
36	N	1235	0	1161	9	0
37	O	761	0	759	6	0
38	P	2823	0	2854	15	0
39	Q	2179	0	2241	26	0
40	R	3014	0	3102	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	S	1071	0	1035	12	0
42	T	3434	0	3590	36	0
43	U	805	0	812	9	0
44	V	4152	0	4212	27	0
45	W	1210	0	1275	19	0
46	X	1037	0	981	5	0
47	Y	405	0	404	2	0
48	Z	861	0	826	3	0
49	a	674	0	620	2	0
50	b	1169	0	1144	6	0
51	c	453	0	475	1	0
52	d	699	0	670	4	0
53	e	1639	0	1618	12	0
54	f	532	0	524	5	0
55	g	416	0	402	2	0
56	h	915	0	866	1	0
57	i	633	0	612	3	0
58	j	712	0	684	3	0
59	k	984	0	980	5	0
60	l	904	0	875	4	0
61	m	1126	0	1148	11	0
62	n	864	0	839	6	0
63	o	1240	0	1222	9	0
64	p	1069	0	1014	5	0
65	q	1268	0	1209	0	0
66	s	2302	0	2299	15	0
67	t	1997	0	1985	17	0
68	u	1698	0	1686	9	0
69	v	361	0	359	0	0
70	w	508	0	494	2	0
71	x	699	0	662	4	0
72	y	932	0	950	3	0
73	1A	76	0	100	2	0
73	1B	76	0	100	8	0
73	Q	38	0	50	2	0
74	1A	86	0	60	0	0
74	1B	86	0	60	2	0
75	1A	59	0	62	1	0
75	1B	135	0	159	6	0
75	1E	53	0	50	1	0
75	1F	56	0	56	1	0
75	1K	79	0	105	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	1L	59	0	62	0	0
75	1M	54	0	52	0	0
75	R	63	0	70	1	0
75	V	64	0	72	1	0
75	W	95	0	143	8	0
75	h	77	0	98	4	0
75	u	154	0	205	5	0
75	x	92	0	137	9	0
75	y	55	0	54	4	0
76	1A	31	0	35	0	0
76	1B	96	0	150	1	0
76	1E	40	0	56	1	0
76	1K	48	0	75	1	0
76	1R	37	0	50	1	0
76	2D	32	0	37	0	0
76	2I	42	0	60	0	0
76	3D	32	0	37	1	0
76	3I	42	0	60	0	0
76	R	32	0	37	1	0
76	S	37	0	47	0	0
76	V	83	0	115	3	0
76	c	48	0	75	2	0
76	g	37	0	50	0	0
76	h	45	0	63	2	0
76	w	45	0	66	3	0
76	y	32	0	37	1	0
77	1E	34	0	41	2	0
77	1F	38	0	49	0	0
77	2D	35	0	43	1	0
77	2F	34	0	41	0	0
77	3D	35	0	43	2	0
77	3F	34	0	41	0	0
77	G	43	0	62	2	0
77	R	118	0	161	2	0
77	S	46	0	68	3	0
77	T	104	0	133	1	0
77	V	125	0	175	3	0
77	e	68	0	85	3	0
77	h	46	0	68	1	0
77	x	50	0	79	0	0
78	1E	43	0	32	2	0
78	1F	43	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	1G	36	0	46	3	0
79	1H	39	0	52	2	0
79	2A	27	0	28	1	0
79	3A	27	0	28	3	0
79	Q	33	0	40	1	0
79	R	44	0	62	0	0
79	T	52	0	84	3	0
79	u	42	0	58	2	0
80	1M	1	0	0	0	0
80	1N	1	0	0	0	0
80	s	1	0	0	0	0
81	2A	33	0	36	1	0
81	3A	33	0	36	1	0
81	T	88	0	122	3	0
81	b	44	0	58	1	0
81	l	51	0	78	1	0
82	2A	120	0	108	2	0
82	3A	120	0	108	3	0
83	2A	1	0	0	0	0
83	3A	1	0	0	0	0
84	2A	1	0	0	0	0
84	3A	1	0	0	0	0
85	2C	2	0	0	3	0
85	3C	2	0	0	2	0
86	A	4	0	0	0	0
86	C	4	0	0	0	0
87	B	31	0	19	1	0
88	B	8	0	0	1	0
88	C	16	0	0	0	0
88	F	8	0	0	1	0
88	G	16	0	0	0	0
89	J	35	0	0	0	0
89	r	35	0	0	0	0
90	P	48	0	26	2	0
91	s	53	0	37	5	0
92	1A	48	0	0	1	0
92	1B	52	0	0	0	0
92	1C	13	0	0	0	0
92	1D	12	0	0	0	0
92	1E	51	0	0	0	0
92	1F	34	0	0	0	0
92	1G	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	1H	9	0	0	0	0
92	1I	11	0	0	0	0
92	1J	3	0	0	0	0
92	1K	12	0	0	0	0
92	1L	12	0	0	0	0
92	1M	76	0	0	1	0
92	1N	74	0	0	0	0
92	1O	4	0	0	0	0
92	1P	6	0	0	0	0
92	1Q	27	0	0	0	0
92	1R	32	0	0	0	0
92	1S	29	0	0	0	0
92	1T	28	0	0	0	0
92	A	24	0	0	0	0
92	B	66	0	0	1	0
92	C	168	0	0	1	0
92	D	66	0	0	0	0
92	E	87	0	0	1	0
92	F	39	0	0	0	0
92	G	62	0	0	0	0
92	H	16	0	0	0	0
92	I	19	0	0	0	0
92	K	16	0	0	0	0
92	L	68	0	0	1	0
92	M	30	0	0	0	0
92	N	53	0	0	0	0
92	O	6	0	0	0	0
92	P	69	0	0	0	0
92	Q	24	0	0	0	0
92	R	64	0	0	0	0
92	S	22	0	0	1	0
92	T	85	0	0	1	0
92	U	14	0	0	1	0
92	V	99	0	0	1	0
92	W	25	0	0	0	0
92	X	50	0	0	0	0
92	Y	4	0	0	0	0
92	Z	20	0	0	0	0
92	a	6	0	0	0	0
92	b	24	0	0	0	0
92	c	1	0	0	0	0
92	d	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	e	55	0	0	1	0
92	f	10	0	0	0	0
92	g	7	0	0	1	0
92	h	38	0	0	0	0
92	i	30	0	0	0	0
92	j	29	0	0	0	0
92	k	51	0	0	0	0
92	l	17	0	0	0	0
92	m	32	0	0	1	0
92	n	7	0	0	0	0
92	o	51	0	0	0	0
92	p	21	0	0	0	0
92	q	24	0	0	0	0
92	r	12	0	0	0	0
92	s	39	0	0	0	0
92	t	55	0	0	0	0
92	u	41	0	0	0	0
92	v	2	0	0	0	0
92	w	16	0	0	0	0
92	x	22	0	0	0	0
92	y	29	0	0	0	0
All	All	137999	0	135356	849	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 3.

The worst 5 of 849 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)
11:3A:265:THR:HG21	22:3L:5:PHE:CE2	1.39	1.53
13:2C:120:CYS:SG	85:2C:301:CUA:CU2	1.01	1.51
13:3C:124:CYS:SG	85:3C:301:CUA:CU1	1.27	1.24
11:3A:265:THR:CG2	22:3L:5:PHE:CE2	2.35	1.10
17:2G:78:HIS:O	17:2G:109:ARG:NH1	1.85	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	1B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
2	1C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	1D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
3	1E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	1F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
4	1G	57/60 (95%)	57 (100%)	0	0	100	100
4	1H	57/60 (95%)	57 (100%)	0	0	100	100
5	1I	66/69 (96%)	66 (100%)	0	0	100	100
5	1J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	1K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	1L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
7	1M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	1N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	71
8	1O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	1P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
9	1Q	439/485 (90%)	418 (95%)	20 (5%)	1 (0%)	43	71
9	1S	439/485 (90%)	425 (97%)	12 (3%)	2 (0%)	24	53
10	1R	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
10	1T	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
11	2A	502/504 (100%)	489 (97%)	13 (3%)	0	100	100
11	3A	502/504 (100%)	490 (98%)	12 (2%)	0	100	100
12	2B	139/284 (49%)	136 (98%)	3 (2%)	0	100	100
12	3B	139/284 (49%)	135 (97%)	4 (3%)	0	100	100
13	2C	151/153 (99%)	144 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	3C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
14	2D	264/382 (69%)	255 (97%)	9 (3%)	0	100	100
14	3D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
15	2E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	34
15	3E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	34
16	2F	84/96 (88%)	81 (96%)	3 (4%)	0	100	100
16	3F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
17	2G	87/125 (70%)	78 (90%)	9 (10%)	0	100	100
17	3G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
18	2H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	3H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
19	2I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	3I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
20	2J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	3J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
21	2K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	3K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
22	2L	74/87 (85%)	70 (95%)	4 (5%)	0	100	100
22	3L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
23	A	237/282 (84%)	228 (96%)	9 (4%)	0	100	100
24	B	433/484 (90%)	417 (96%)	16 (4%)	0	100	100
25	C	686/733 (94%)	667 (97%)	19 (3%)	0	100	100
26	D	214/282 (76%)	204 (95%)	10 (5%)	0	100	100
27	E	379/467 (81%)	368 (97%)	11 (3%)	0	100	100
28	F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
29	G	197/231 (85%)	189 (96%)	8 (4%)	0	100	100
30	H	88/118 (75%)	81 (92%)	7 (8%)	0	100	100
31	I	133/165 (81%)	130 (98%)	3 (2%)	0	100	100
32	J	82/128 (64%)	76 (93%)	6 (7%)	0	100	100
32	r	86/128 (67%)	84 (98%)	2 (2%)	0	100	100
33	K	117/138 (85%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	L	162/187 (87%)	155 (96%)	7 (4%)	0	100	100
35	M	119/154 (77%)	111 (93%)	8 (7%)	0	100	100
36	N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
37	O	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	P	361/397 (91%)	350 (97%)	11 (3%)	0	100	100
39	Q	282/292 (97%)	274 (97%)	8 (3%)	0	100	100
40	R	385/387 (100%)	369 (96%)	16 (4%)	0	100	100
41	S	130/279 (47%)	128 (98%)	2 (2%)	0	100	100
42	T	441/443 (100%)	431 (98%)	10 (2%)	0	100	100
43	U	103/227 (45%)	102 (99%)	1 (1%)	0	100	100
44	V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	43	71
45	W	155/162 (96%)	151 (97%)	4 (3%)	0	100	100
46	X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
47	Y	52/64 (81%)	52 (100%)	0	0	100	100
48	Z	105/124 (85%)	100 (95%)	5 (5%)	0	100	100
49	a	80/129 (62%)	78 (98%)	1 (1%)	1 (1%)	9	29
50	b	142/172 (83%)	139 (98%)	3 (2%)	0	100	100
51	c	55/67 (82%)	52 (94%)	3 (6%)	0	100	100
52	d	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
53	e	216/219 (99%)	214 (99%)	1 (0%)	1 (0%)	24	53
54	f	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	g	48/55 (87%)	42 (88%)	6 (12%)	0	100	100
56	h	106/142 (75%)	97 (92%)	9 (8%)	0	100	100
57	i	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
58	j	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
59	k	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
60	l	114/121 (94%)	110 (96%)	4 (4%)	0	100	100
61	m	134/142 (94%)	133 (99%)	1 (1%)	0	100	100
62	n	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
63	o	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
64	p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	q	155/197 (79%)	149 (96%)	6 (4%)	0	100	100
66	s	310/312 (99%)	303 (98%)	7 (2%)	0	100	100
67	t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
68	u	226/229 (99%)	220 (97%)	6 (3%)	0	100	100
69	v	43/45 (96%)	43 (100%)	0	0	100	100
70	w	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
71	x	81/157 (52%)	81 (100%)	0	0	100	100
72	y	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
All	All	16540/19385 (85%)	16027 (97%)	504 (3%)	9 (0%)	49	75

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	1Q	396	ASP
15	2E	28	TRP
15	3E	28	TRP
49	a	43	TYR
9	1S	66	THR

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	312/317 (98%)	312 (100%)	0	100	100
1	1B	312/317 (98%)	312 (100%)	0	100	100
2	1C	171/213 (80%)	171 (100%)	0	100	100
2	1D	171/213 (80%)	171 (100%)	0	100	100
3	1E	191/238 (80%)	191 (100%)	0	100	100
3	1F	191/238 (80%)	191 (100%)	0	100	100
4	1G	52/53 (98%)	52 (100%)	0	100	100
4	1H	52/53 (98%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1I	58/59 (98%)	58 (100%)	0	100	100
5	1J	58/59 (98%)	58 (100%)	0	100	100
6	1K	62/64 (97%)	62 (100%)	0	100	100
6	1L	62/64 (97%)	62 (100%)	0	100	100
7	1M	390/413 (94%)	390 (100%)	0	100	100
7	1N	390/413 (94%)	390 (100%)	0	100	100
8	1O	38/47 (81%)	38 (100%)	0	100	100
8	1P	38/47 (81%)	38 (100%)	0	100	100
9	1Q	333/362 (92%)	333 (100%)	0	100	100
9	1S	333/362 (92%)	333 (100%)	0	100	100
10	1R	106/107 (99%)	106 (100%)	0	100	100
10	1T	106/107 (99%)	106 (100%)	0	100	100
11	2A	408/408 (100%)	408 (100%)	0	100	100
11	3A	408/408 (100%)	408 (100%)	0	100	100
12	2B	132/224 (59%)	132 (100%)	0	100	100
12	3B	132/224 (59%)	132 (100%)	0	100	100
13	2C	137/137 (100%)	137 (100%)	0	100	100
13	3C	137/137 (100%)	137 (100%)	0	100	100
14	2D	211/294 (72%)	211 (100%)	0	100	100
14	3D	211/294 (72%)	211 (100%)	0	100	100
15	2E	79/137 (58%)	79 (100%)	0	100	100
15	3E	79/137 (58%)	79 (100%)	0	100	100
16	2F	66/72 (92%)	66 (100%)	0	100	100
16	3F	66/72 (92%)	66 (100%)	0	100	100
17	2G	75/100 (75%)	75 (100%)	0	100	100
17	3G	75/100 (75%)	75 (100%)	0	100	100
18	2H	103/132 (78%)	103 (100%)	0	100	100
18	3H	103/132 (78%)	103 (100%)	0	100	100
19	2I	58/80 (72%)	58 (100%)	0	100	100
19	3I	58/80 (72%)	58 (100%)	0	100	100
20	2J	83/84 (99%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	3J	83/84 (99%)	83 (100%)	0	100	100
21	2K	39/46 (85%)	39 (100%)	0	100	100
21	3K	39/46 (85%)	39 (100%)	0	100	100
22	2L	63/74 (85%)	63 (100%)	0	100	100
22	3L	65/74 (88%)	65 (100%)	0	100	100
23	A	197/228 (86%)	197 (100%)	0	100	100
24	B	344/377 (91%)	344 (100%)	0	100	100
25	C	537/572 (94%)	537 (100%)	0	100	100
26	D	196/248 (79%)	196 (100%)	0	100	100
27	E	329/388 (85%)	329 (100%)	0	100	100
28	F	129/133 (97%)	129 (100%)	0	100	100
29	G	172/198 (87%)	172 (100%)	0	100	100
30	H	82/105 (78%)	82 (100%)	0	100	100
31	I	111/134 (83%)	111 (100%)	0	100	100
32	J	71/108 (66%)	71 (100%)	0	100	100
32	r	72/108 (67%)	72 (100%)	0	100	100
33	K	106/122 (87%)	106 (100%)	0	100	100
34	L	130/148 (88%)	130 (100%)	0	100	100
35	M	100/121 (83%)	100 (100%)	0	100	100
36	N	128/132 (97%)	128 (100%)	0	100	100
37	O	80/81 (99%)	80 (100%)	0	100	100
38	P	305/327 (93%)	305 (100%)	0	100	100
39	Q	230/234 (98%)	230 (100%)	0	100	100
40	R	321/321 (100%)	321 (100%)	0	100	100
41	S	111/217 (51%)	111 (100%)	0	100	100
42	T	374/374 (100%)	374 (100%)	0	100	100
43	U	84/180 (47%)	84 (100%)	0	100	100
44	V	439/439 (100%)	439 (100%)	0	100	100
45	W	131/135 (97%)	131 (100%)	0	100	100
46	X	105/122 (86%)	105 (100%)	0	100	100
47	Y	38/46 (83%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Z	93/102 (91%)	93 (100%)	0	100	100
49	a	68/98 (69%)	68 (100%)	0	100	100
50	b	119/138 (86%)	119 (100%)	0	100	100
51	c	49/56 (88%)	49 (100%)	0	100	100
52	d	63/64 (98%)	63 (100%)	0	100	100
53	e	163/164 (99%)	163 (100%)	0	100	100
54	f	52/53 (98%)	52 (100%)	0	100	100
55	g	40/45 (89%)	40 (100%)	0	100	100
56	h	91/110 (83%)	91 (100%)	0	100	100
57	i	65/67 (97%)	65 (100%)	0	100	100
58	j	72/73 (99%)	72 (100%)	0	100	100
59	k	102/102 (100%)	102 (100%)	0	100	100
60	l	94/99 (95%)	94 (100%)	0	100	100
61	m	118/122 (97%)	118 (100%)	0	100	100
62	n	92/94 (98%)	92 (100%)	0	100	100
63	o	130/132 (98%)	130 (100%)	0	100	100
64	p	109/110 (99%)	109 (100%)	0	100	100
65	q	135/165 (82%)	135 (100%)	0	100	100
66	s	243/243 (100%)	243 (100%)	0	100	100
67	t	212/233 (91%)	212 (100%)	0	100	100
68	u	180/181 (99%)	180 (100%)	0	100	100
69	v	38/38 (100%)	38 (100%)	0	100	100
70	w	55/91 (60%)	55 (100%)	0	100	100
71	x	70/130 (54%)	70 (100%)	0	100	100
72	y	102/106 (96%)	102 (100%)	0	100	100
All	All	13813/15736 (88%)	13813 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
24	B	241	GLN

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Mol	Chain	Res	Type
33	K	95	HIS
68	u	147	ASN
62	n	29	HIS
24	B	462	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 107 ligands modelled in this entry, 7 are monoatomic - leaving 100 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	1M	501	-	53,53,99	0.49	1 (1%)	59,65,111	0.26	0
77	PTY	S	302	-	45,45,49	0.49	0	48,50,54	0.41	0
88	SF4	C	802	25	0,12,12	-	-	-	-	-
77	PTY	V	606	-	34,34,49	0.56	0	37,39,54	0.44	0
73	UQ5	1B	401	-	38,38,38	0.46	0	46,49,49	0.73	1 (2%)
75	CDL	1B	405	-	63,63,99	0.44	1 (1%)	69,75,111	0.25	0
88	SF4	C	803	25	0,12,12	-	-	-	-	-
91	COO	s	401	-	48,55,55	1.10	4 (8%)	68,81,81	4.02	17 (25%)
78	HEC	1E	404	3	50,50,50	1.84	5 (10%)	68,82,82	1.45	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	PTY	1E	403	-	33,33,49	0.55	0	36,38,54	0.50	0
77	PTY	T	501	-	49,49,49	0.46	0	52,54,54	0.62	1 (1%)
75	CDL	y	202	-	54,54,99	0.53	1 (1%)	60,66,111	0.32	0
77	PTY	T	504	-	27,27,49	0.65	0	30,32,54	0.48	0
81	PGT	b	601	-	43,43,50	0.53	0	46,49,56	0.51	0
75	CDL	V	603	-	63,63,99	0.41	0	69,75,111	0.25	0
87	FMN	B	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.25	8 (16%)
76	3PH	1R	201	10	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
75	CDL	1F	401	-	55,55,99	0.42	0	61,67,111	0.27	0
85	CUA	3C	301	13	0,1,1	-	-	-	-	-
76	3PH	S	301	-	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
75	CDL	R	405	-	62,62,99	0.40	0	68,74,111	0.28	0
75	CDL	1B	408	1	70,70,99	0.34	0	76,82,111	0.34	0
76	3PH	1B	407	-	47,47,47	0.63	1 (2%)	51,52,52	0.60	0
75	CDL	h	203	-	76,76,99	0.37	0	82,88,111	0.25	0
77	PTY	3F	101	-	33,33,49	0.55	0	36,38,54	0.47	0
74	HEM	1B	404	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	7 (10%)
73	UQ5	1A	401	-	38,38,38	0.53	0	46,49,49	1.08	4 (8%)
76	3PH	R	401	-	31,31,47	0.75	1 (3%)	35,36,52	0.73	2 (5%)
76	3PH	w	201	-	44,44,47	0.64	1 (2%)	48,49,52	0.75	3 (6%)
81	PGT	T	502	-	47,47,50	0.53	0	50,53,56	0.56	1 (2%)
74	HEM	1A	403	1	50,50,50	1.49	6 (12%)	66,82,82	1.38	8 (12%)
77	PTY	T	506	-	25,25,49	0.64	0	28,30,54	0.47	0
76	3PH	3I	201	-	41,41,47	0.65	1 (2%)	45,46,52	0.66	1 (2%)
76	3PH	V	601	-	41,41,47	0.66	1 (2%)	45,46,52	0.63	1 (2%)
77	PTY	2D	301	-	34,34,49	0.56	0	37,39,54	0.56	0
76	3PH	2I	201	-	41,41,47	0.67	1 (2%)	45,46,52	0.67	1 (2%)
89	8Q1	J	200	-	31,34,34	1.69	5 (16%)	40,43,43	1.71	5 (12%)
81	PGT	l	701	-	50,50,50	0.48	0	53,56,56	0.59	1 (1%)
73	UQ5	Q	301	-	38,38,38	0.51	0	46,49,49	0.83	3 (6%)
77	PTY	e	302	-	42,42,49	0.52	0	45,47,54	0.42	0
77	PTY	3D	301	-	34,34,49	0.57	0	37,39,54	0.47	0
74	HEM	1A	404	1	50,50,50	1.31	7 (14%)	66,82,82	1.29	8 (12%)
90	NDP	P	401	-	49,52,52	2.19	6 (12%)	66,80,80	1.56	15 (22%)
76	3PH	1K	102	-	47,47,47	0.64	1 (2%)	51,52,52	0.60	2 (3%)
75	CDL	u	602	-	82,82,99	0.38	0	88,94,111	0.30	0
78	HEC	1F	402	3	50,50,50	1.76	4 (8%)	68,82,82	1.52	12 (17%)
76	3PH	1E	402	-	39,39,47	0.69	1 (2%)	43,44,52	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	HEA	2A	603	11	66,67,67	2.46	24 (36%)	78,103,103	2.58	32 (41%)
77	PTY	2F	101	-	33,33,49	0.55	0	36,38,54	0.45	0
81	PGT	T	505	-	39,39,50	0.54	0	42,45,56	0.50	0
76	3PH	2D	302	-	31,31,47	0.77	1 (3%)	35,36,52	0.72	1 (2%)
75	CDL	1A	405	-	58,58,99	0.44	0	64,70,111	0.27	0
88	SF4	B	502	24	0,12,12	-	-	-	-	-
75	CDL	W	701	-	94,94,99	0.35	0	100,106,111	0.28	0
77	PTY	R	404	-	43,43,49	0.51	0	46,48,54	0.46	0
77	PTY	V	604	-	39,39,49	0.54	0	42,44,54	0.50	0
79	PC7	T	503	-	51,51,51	0.50	0	57,59,59	0.59	0
88	SF4	F	201	28	0,12,12	-	-	-	-	-
88	SF4	G	302	29	0,12,12	-	-	-	-	-
77	PTY	V	605	-	49,49,49	0.46	0	52,54,54	0.38	0
76	3PH	V	602	-	40,40,47	0.67	1 (2%)	44,45,52	0.82	1 (2%)
79	PC7	1G	301	-	35,35,51	0.61	0	41,43,59	0.60	1 (2%)
75	CDL	x	101	-	91,91,99	0.40	1 (1%)	97,103,111	0.24	0
81	PGT	3A	601	-	32,32,50	0.59	0	35,38,56	0.52	0
79	PC7	u	601	-	41,41,51	0.55	0	47,49,59	0.68	2 (4%)
76	3PH	3D	302	-	31,31,47	0.75	1 (3%)	35,36,52	0.80	1 (2%)
77	PTY	G	303	-	42,42,49	0.49	0	45,47,54	0.44	0
73	UQ5	1A	402	-	38,38,38	0.52	0	46,49,49	0.66	1 (2%)
76	3PH	g	101	-	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
82	HEA	3A	603	11	66,67,67	2.39	23 (34%)	78,103,103	2.59	30 (38%)
88	SF4	G	301	29	0,12,12	-	-	-	-	-
77	PTY	h	202	-	45,45,49	0.47	0	48,50,54	0.46	0
77	PTY	x	102	-	49,49,49	0.46	0	52,54,54	0.40	0
76	3PH	h	201	-	44,44,47	0.65	1 (2%)	48,49,52	3.77	5 (10%)
77	PTY	1F	403	-	37,37,49	0.51	0	40,42,54	0.44	0
86	FES	C	801	25	0,4,4	-	-	-	-	-
89	8Q1	r	200	-	31,34,34	1.76	5 (16%)	40,43,43	1.88	10 (25%)
77	PTY	R	402	-	33,33,49	0.53	0	36,38,54	0.43	0
75	CDL	1E	401	-	52,52,99	0.44	0	58,64,111	0.25	0
79	PC7	3A	606	-	26,26,51	0.66	0	32,34,59	0.65	0
77	PTY	e	301	-	24,24,49	0.64	0	27,29,54	0.52	0
76	3PH	y	201	-	31,31,47	0.78	1 (3%)	35,36,52	0.66	1 (2%)
79	PC7	1H	101	-	38,38,51	0.57	0	44,46,59	0.56	0
79	PC7	Q	302	-	32,32,51	0.59	0	38,40,59	0.69	0
75	CDL	1L	101	-	58,58,99	0.43	0	64,70,111	0.35	0
76	3PH	c	101	-	47,47,47	0.62	1 (2%)	51,52,52	0.63	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
73	UQ5	1B	402	-	38,38,38	0.51	0	46,49,49	1.51	6 (13%)
82	HEA	3A	602	11	66,67,67	2.39	25 (37%)	78,103,103	2.55	33 (42%)
76	3PH	1A	406	-	30,30,47	0.78	1 (3%)	34,35,52	0.69	1 (2%)
75	CDL	u	603	-	70,70,99	0.43	0	76,82,111	0.28	0
74	HEM	1B	403	1	50,50,50	1.42	8 (16%)	66,82,82	1.36	10 (15%)
82	HEA	2A	602	11	66,67,67	2.44	26 (39%)	78,103,103	2.54	32 (41%)
79	PC7	2A	606	-	26,26,51	0.66	0	32,34,59	0.70	0
79	PC7	R	403	-	43,43,51	0.53	0	49,51,59	0.61	0
77	PTY	R	406	-	39,39,49	0.53	0	42,44,54	0.51	0
85	CUA	2C	301	-	0,1,1	-	-	-	-	-
76	3PH	1B	406	-	47,47,47	0.62	1 (2%)	51,52,52	0.60	1 (1%)
75	CDL	1K	101	-	78,78,99	0.43	0	84,90,111	0.28	0
86	FES	A	301	23	0,4,4	-	-	-	-	-
81	PGT	2A	601	-	32,32,50	0.61	0	35,38,56	0.60	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	1M	501	-	-	31/64/64/110	-
77	PTY	S	302	-	-	21/49/49/53	-
88	SF4	C	802	25	-	-	0/6/5/5
77	PTY	V	606	-	-	18/38/38/53	-
73	UQ5	1B	401	-	-	7/33/57/57	0/1/1/1
75	CDL	1B	405	-	-	49/74/74/110	-
88	SF4	C	803	25	-	-	0/6/5/5
91	COO	s	401	-	-	22/54/70/70	0/3/3/3
78	HEC	1E	404	3	1/1/3/7	2/14/54/54	-
77	PTY	1E	403	-	-	15/37/37/53	-
77	PTY	T	501	-	-	19/53/53/53	-
75	CDL	y	202	-	-	30/65/65/110	-
77	PTY	T	504	-	-	11/31/31/53	-
81	PGT	b	601	-	-	27/48/48/55	-
75	CDL	V	603	-	-	42/74/74/110	-
87	FMN	B	501	-	-	4/18/18/18	0/3/3/3
76	3PH	1R	201	10	-	13/38/38/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	1F	401	-	-	32/66/66/110	-
76	3PH	S	301	-	-	13/38/38/49	-
75	CDL	R	405	-	-	43/73/73/110	-
75	CDL	1B	408	1	-	45/81/81/110	-
76	3PH	1B	407	-	-	18/49/49/49	-
75	CDL	h	203	-	-	58/87/87/110	-
77	PTY	3F	101	-	-	10/37/37/53	-
74	HEM	1B	404	1	-	4/14/54/54	-
73	UQ5	1A	401	-	-	10/33/57/57	0/1/1/1
76	3PH	R	401	-	-	13/33/33/49	-
76	3PH	w	201	-	-	21/46/46/49	-
81	PGT	T	502	-	-	20/52/52/55	-
74	HEM	1A	403	1	-	3/14/54/54	-
77	PTY	T	506	-	-	15/29/29/53	-
76	3PH	3I	201	-	-	9/43/43/49	-
76	3PH	V	601	-	-	18/43/43/49	-
77	PTY	2D	301	-	-	13/38/38/53	-
76	3PH	2I	201	-	-	14/43/43/49	-
89	8Q1	J	200	-	-	11/41/41/41	-
81	PGT	l	701	-	-	27/55/55/55	-
73	UQ5	Q	301	-	-	4/33/57/57	0/1/1/1
77	PTY	e	302	-	-	22/46/46/53	-
77	PTY	3D	301	-	-	15/38/38/53	-
74	HEM	1A	404	1	-	4/14/54/54	-
90	NDP	P	401	-	-	11/34/77/77	0/5/5/5
76	3PH	1K	102	-	-	15/49/49/49	-
75	CDL	u	602	-	-	51/93/93/110	-
78	HEC	1F	402	3	1/1/3/7	2/14/54/54	-
76	3PH	1E	402	-	-	17/41/41/49	-
82	HEA	2A	603	11	-	7/36/76/76	-
77	PTY	2F	101	-	-	15/37/37/53	-
81	PGT	T	505	-	-	18/44/44/55	-
76	3PH	2D	302	-	-	19/33/33/49	-
75	CDL	1A	405	-	-	34/69/69/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SF4	B	502	24	-	-	0/6/5/5
75	CDL	W	701	-	-	62/105/105/110	-
77	PTY	R	404	-	-	21/47/47/53	-
77	PTY	V	604	-	-	15/43/43/53	-
79	PC7	T	503	-	-	22/55/55/55	-
88	SF4	F	201	28	-	-	0/6/5/5
88	SF4	G	302	29	-	-	0/6/5/5
77	PTY	V	605	-	-	25/53/53/53	-
76	3PH	V	602	-	-	17/42/42/49	-
79	PC7	1G	301	-	-	16/39/39/55	-
75	CDL	x	101	-	-	65/102/102/110	-
81	PGT	3A	601	-	-	12/37/37/55	-
79	PC7	u	601	-	-	15/45/45/55	-
76	3PH	3D	302	-	-	10/33/33/49	-
77	PTY	G	303	-	-	6/46/46/53	-
73	UQ5	1A	402	-	-	9/33/57/57	0/1/1/1
76	3PH	g	101	-	-	10/38/38/49	-
82	HEA	3A	603	11	-	4/36/76/76	-
88	SF4	G	301	29	-	-	0/6/5/5
77	PTY	h	202	-	-	20/49/49/53	-
77	PTY	x	102	-	-	18/53/53/53	-
76	3PH	h	201	-	-	19/46/46/49	-
77	PTY	1F	403	-	-	17/41/41/53	-
89	8Q1	r	200	-	-	19/41/41/41	-
86	FES	C	801	25	-	-	0/1/1/1
77	PTY	R	402	-	-	11/37/37/53	-
75	CDL	1E	401	-	-	41/63/63/110	-
79	PC7	3A	606	-	-	22/30/30/55	-
77	PTY	e	301	-	-	9/28/28/53	-
76	3PH	y	201	-	-	13/33/33/49	-
79	PC7	1H	101	-	-	19/42/42/55	-
79	PC7	Q	302	-	-	14/36/36/55	-
75	CDL	1L	101	-	-	43/69/69/110	-
76	3PH	c	101	-	-	13/49/49/49	-
73	UQ5	1B	402	-	-	10/33/57/57	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	HEA	3A	602	11	-	9/36/76/76	-
76	3PH	1A	406	-	-	13/32/32/49	-
75	CDL	u	603	-	-	57/81/81/110	-
74	HEM	1B	403	1	-	4/14/54/54	-
82	HEA	2A	602	11	-	10/36/76/76	-
79	PC7	2A	606	-	-	10/30/30/55	-
79	PC7	R	403	-	-	15/47/47/55	-
77	PTY	R	406	-	-	15/43/43/53	-
76	3PH	1B	406	-	-	22/49/49/49	-
75	CDL	1K	101	-	-	59/89/89/110	-
86	FES	A	301	23	-	-	0/1/1/1
81	PGT	2A	601	-	-	10/37/37/55	-

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	P	401	NDP	P2B-O2B	12.34	1.82	1.59
78	1E	404	HEC	C3D-C2D	7.83	1.53	1.36
78	1F	402	HEC	C3D-C2D	7.74	1.53	1.36
89	r	200	8Q1	C34-N36	5.99	1.46	1.33
82	2A	603	HEA	C3B-C2B	5.65	1.47	1.34

The worst 5 of 280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	s	401	COO	C15-C11-C12	-19.13	77.03	108.23
76	h	201	3PH	O31-C31-O32	-17.93	78.33	123.59
91	s	401	COO	C15-C11-C13	-16.74	79.80	108.82
91	s	401	COO	C15-C11-C14	-15.18	78.23	109.17
76	h	201	3PH	O31-C31-C32	14.35	156.94	111.91

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
78	1E	404	HEC	NA
78	1F	402	HEC	NA

5 of 1763 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
73	1A	401	UQ5	C1-C6-C7-C8
73	1A	401	UQ5	C5-C6-C7-C8
73	1A	401	UQ5	C9-C11-C12-C13
73	1A	401	UQ5	C24-C26-C27-C28
73	1A	402	UQ5	C14-C16-C17-C18

There are no ring outliers.

67 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	S	302	PTY	3	0
77	V	606	PTY	1	0
73	1B	401	UQ5	4	0
75	1B	405	CDL	4	0
91	s	401	COO	5	0
78	1E	404	HEC	2	0
77	1E	403	PTY	2	0
77	T	501	PTY	1	0
75	y	202	CDL	4	0
81	b	601	PGT	1	0
75	V	603	CDL	1	0
87	B	501	FMN	1	0
76	1R	201	3PH	1	0
75	1F	401	CDL	1	0
85	3C	301	CUA	2	0
75	R	405	CDL	1	0
75	1B	408	CDL	2	0
75	h	203	CDL	4	0
76	R	401	3PH	1	0
76	w	201	3PH	3	0
81	T	502	PGT	3	0
77	2D	301	PTY	1	0
81	l	701	PGT	1	0
73	Q	301	UQ5	2	0
77	e	302	PTY	3	0
77	3D	301	PTY	2	0
90	P	401	NDP	2	0
76	1K	102	3PH	1	0
75	u	602	CDL	2	0
78	1F	402	HEC	2	0
76	1E	402	3PH	1	0
82	2A	603	HEA	1	0
75	1A	405	CDL	1	0

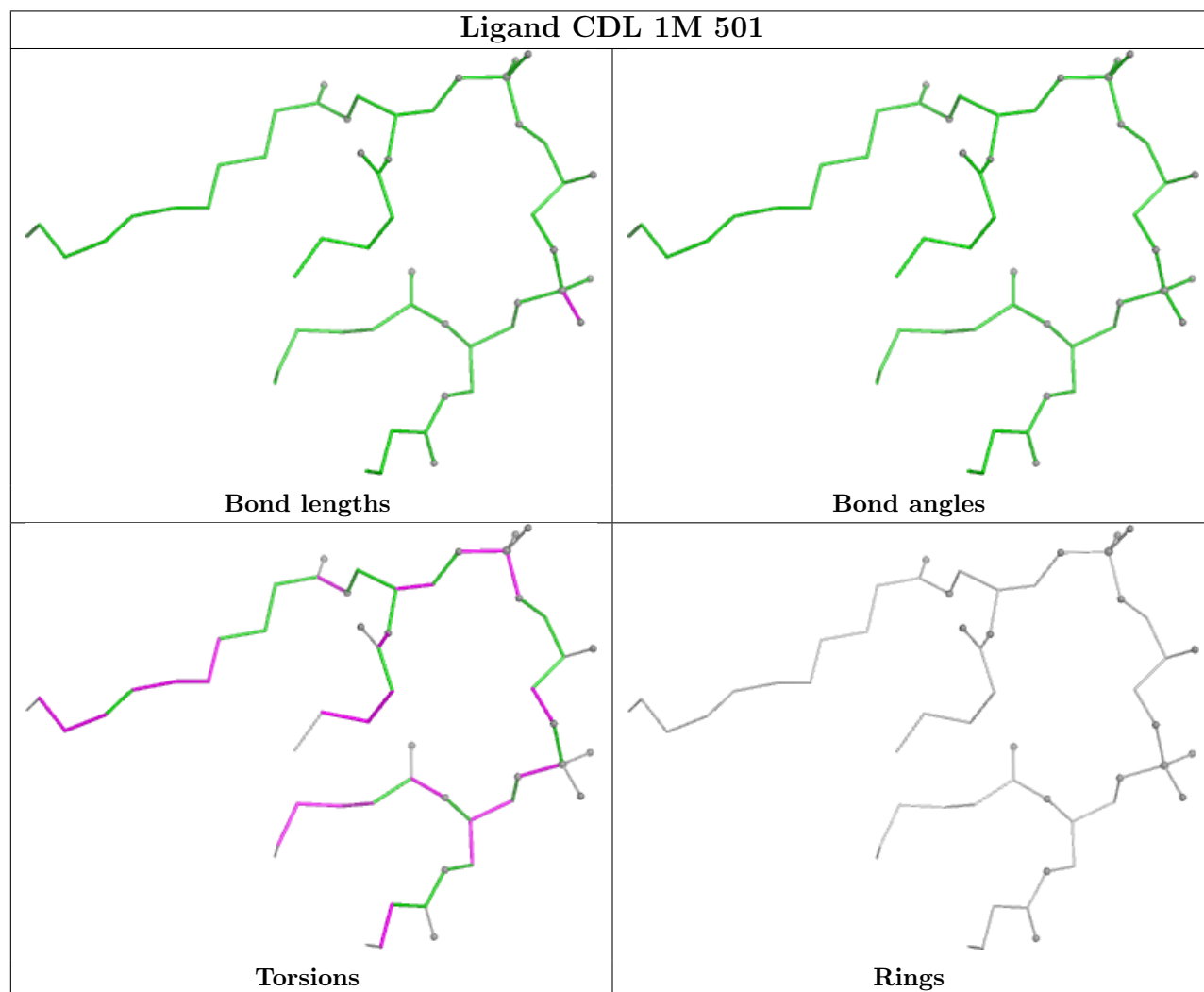
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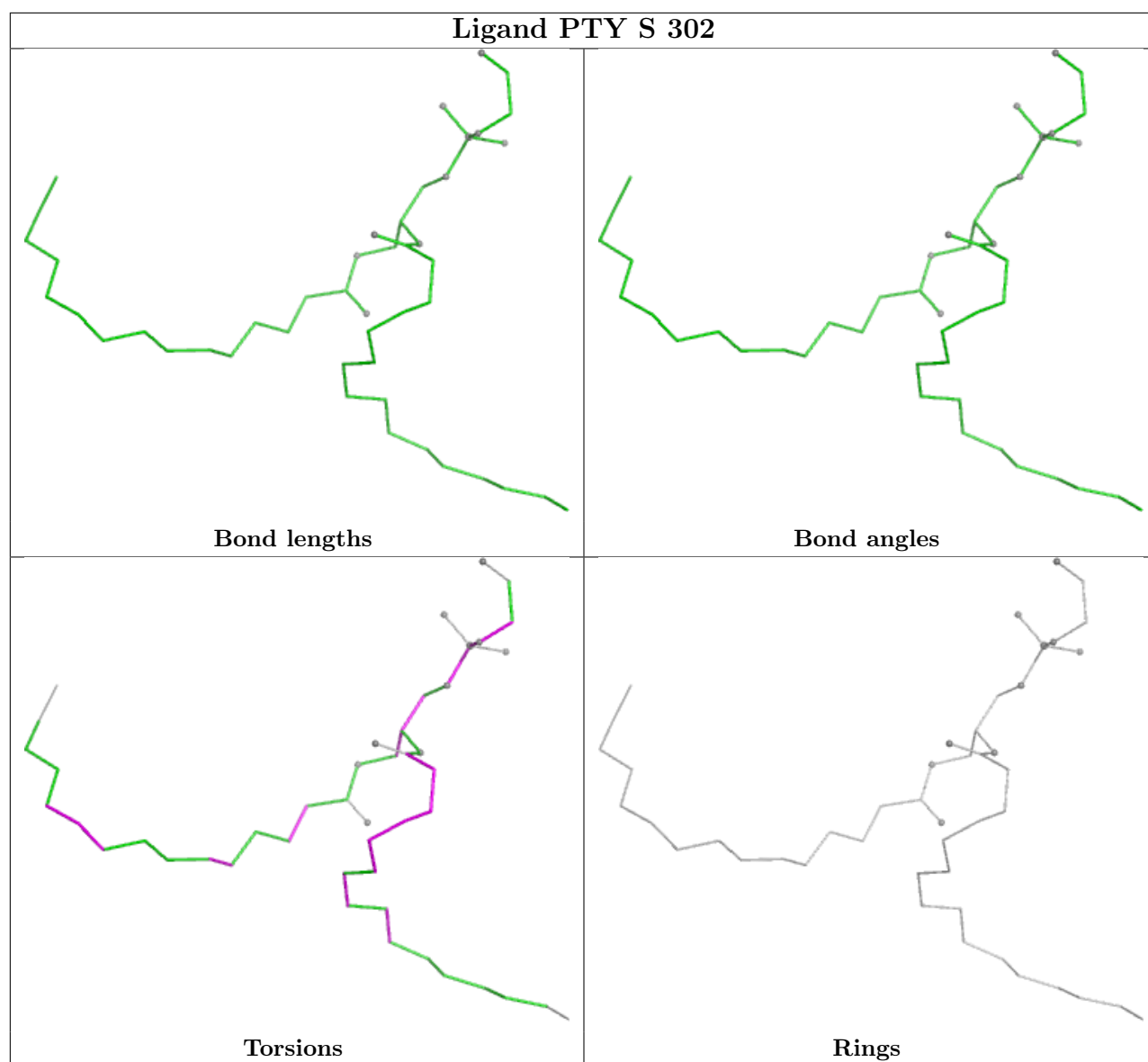
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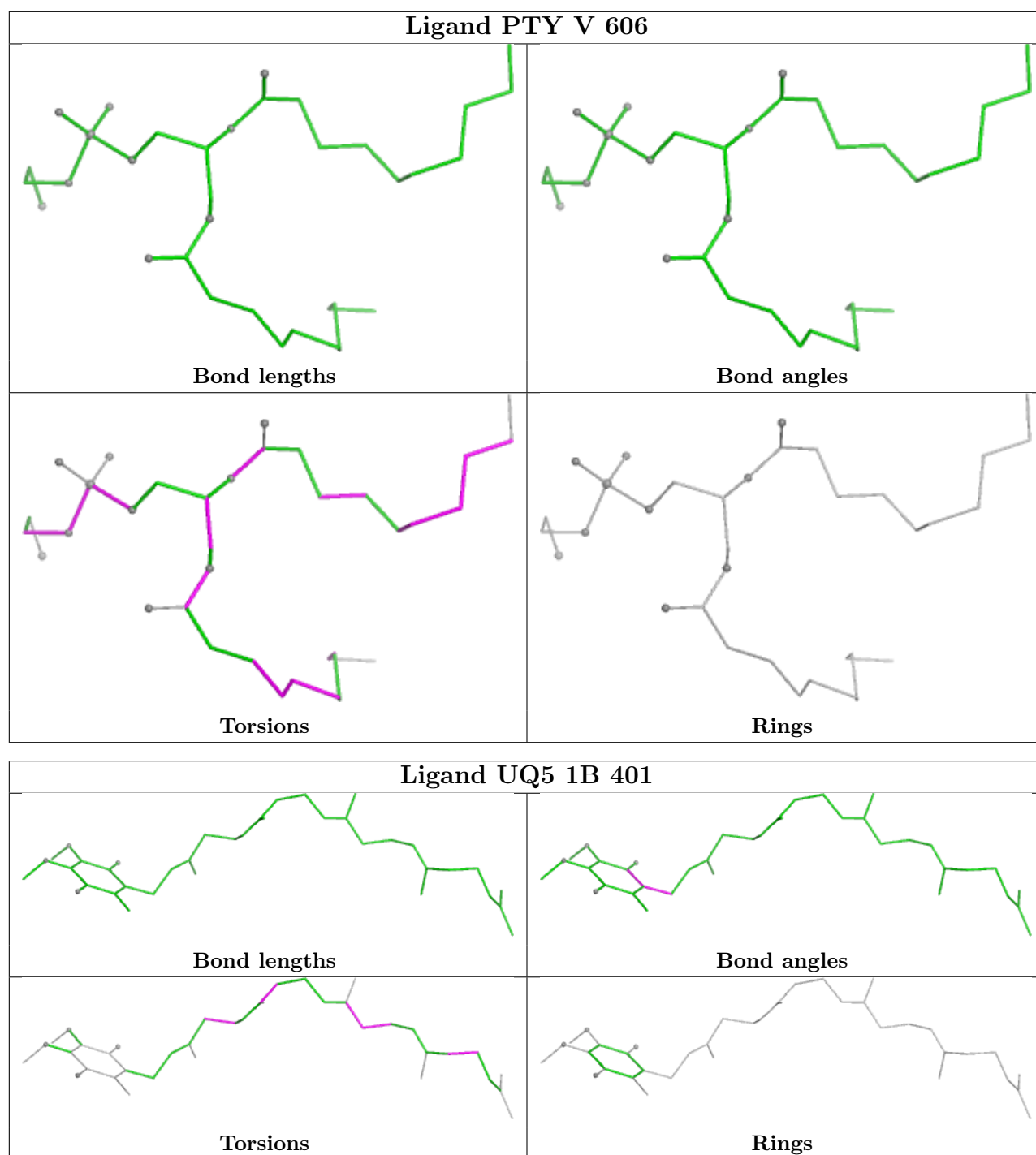
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	B	502	SF4	1	0
75	W	701	CDL	8	0
77	R	404	PTY	1	0
79	T	503	PC7	3	0
88	F	201	SF4	1	0
77	V	605	PTY	2	0
76	V	602	3PH	3	0
79	1G	301	PC7	3	0
75	x	101	CDL	9	0
81	3A	601	PGT	1	0
79	u	601	PC7	2	0
76	3D	302	3PH	1	0
77	G	303	PTY	2	0
73	1A	402	UQ5	2	0
82	3A	603	HEA	2	0
77	h	202	PTY	1	0
76	h	201	3PH	2	0
75	1E	401	CDL	1	0
79	3A	606	PC7	3	0
76	y	201	3PH	1	0
79	1H	101	PC7	2	0
79	Q	302	PC7	1	0
76	c	101	3PH	2	0
73	1B	402	UQ5	4	0
82	3A	602	HEA	1	0
75	u	603	CDL	3	0
74	1B	403	HEM	2	0
82	2A	602	HEA	1	0
79	2A	606	PC7	1	0
77	R	406	PTY	1	0
85	2C	301	CUA	3	0
76	1B	406	3PH	1	0
75	1K	101	CDL	5	0
81	2A	601	PGT	1	0

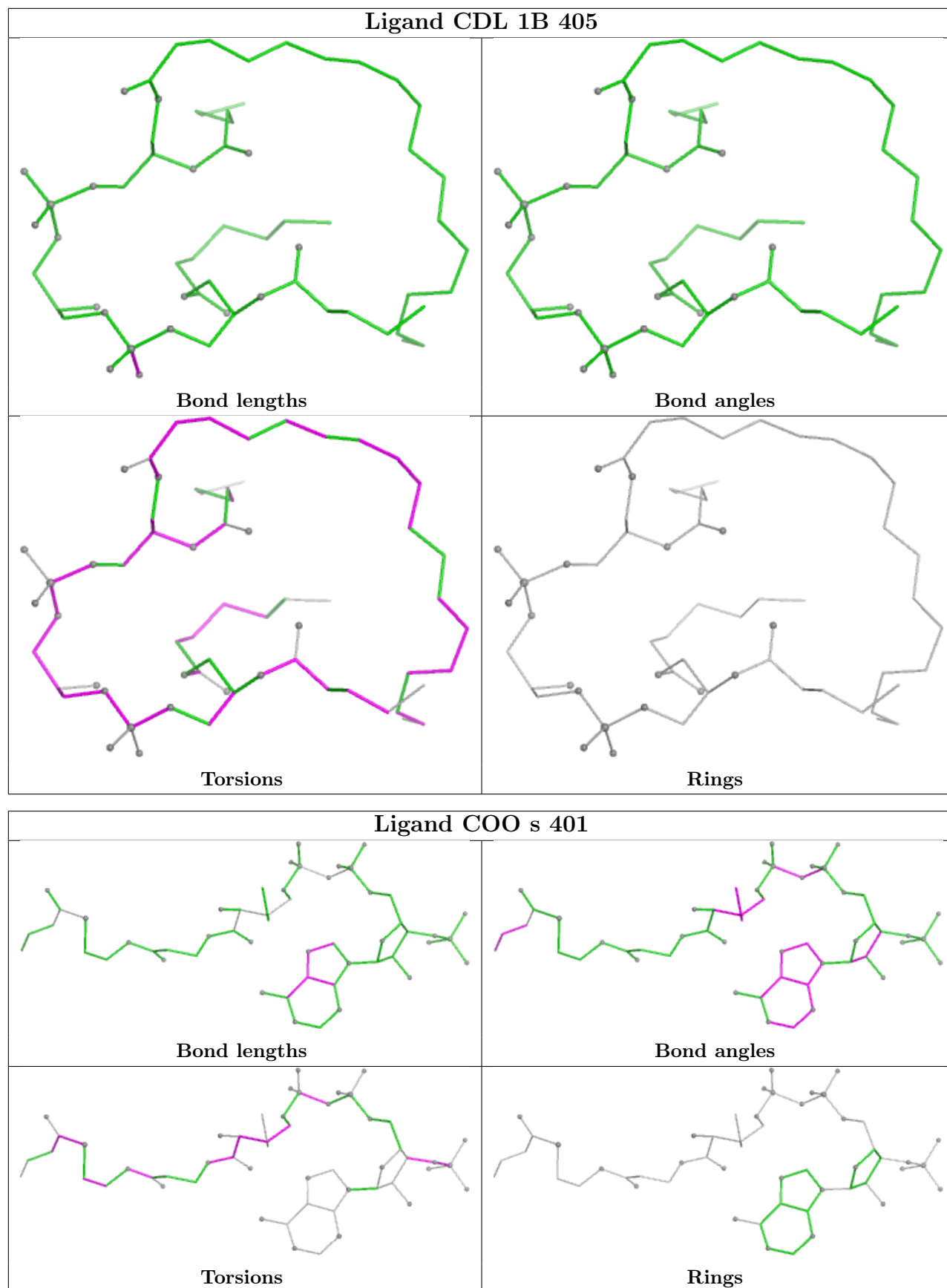
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

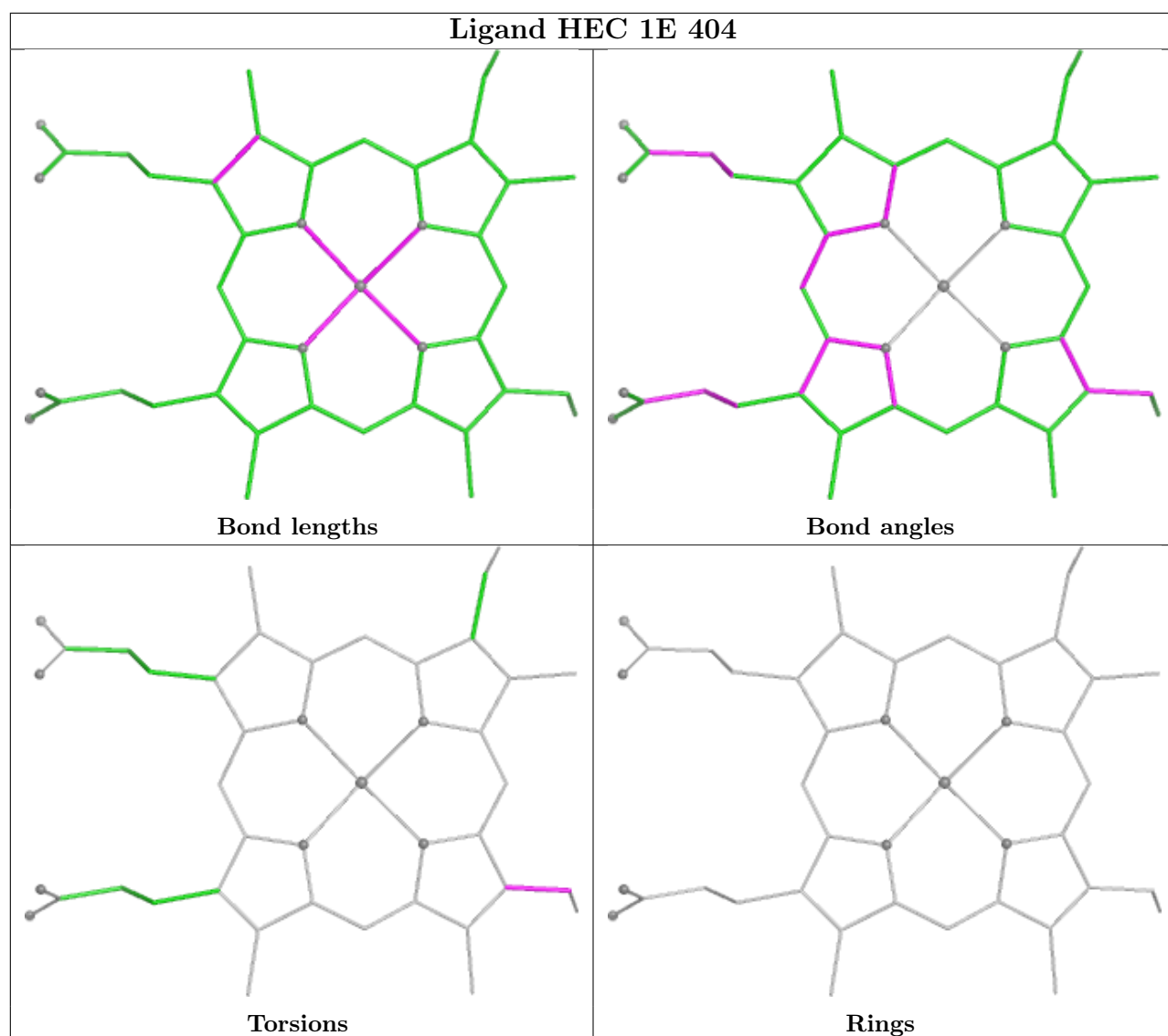
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

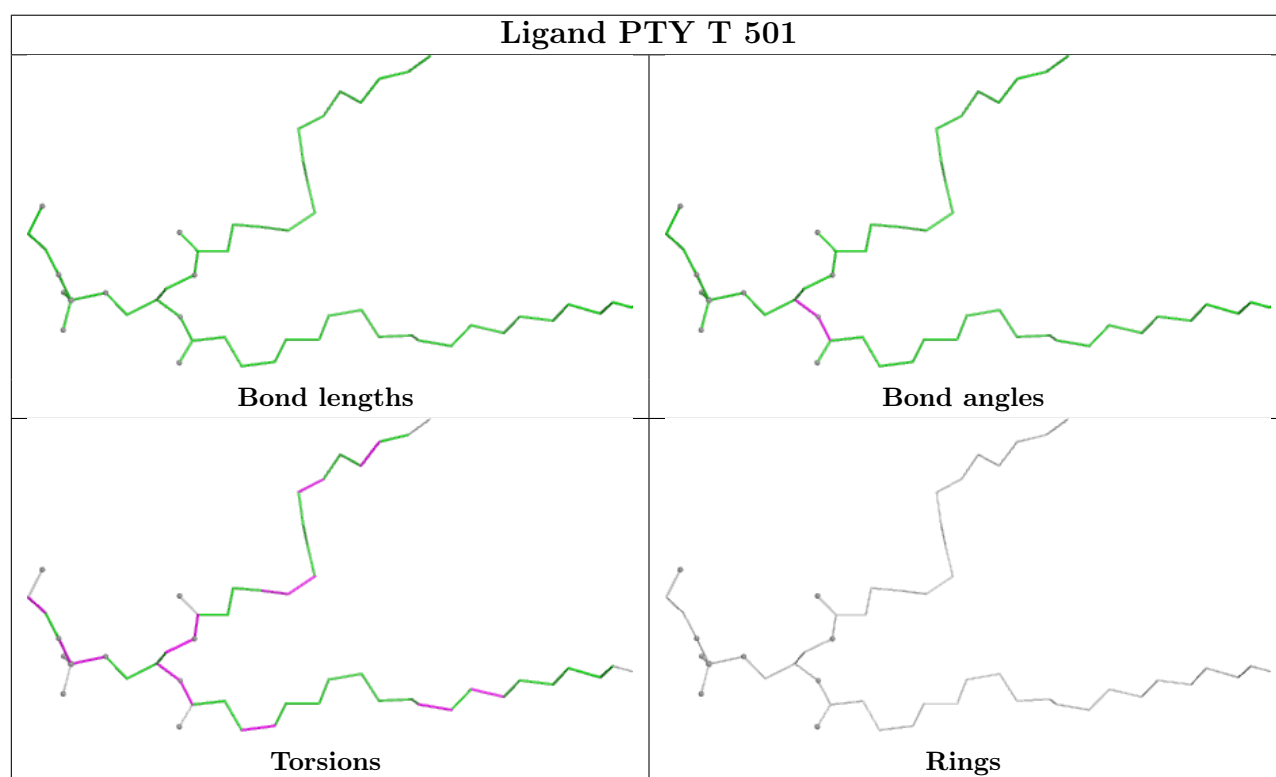
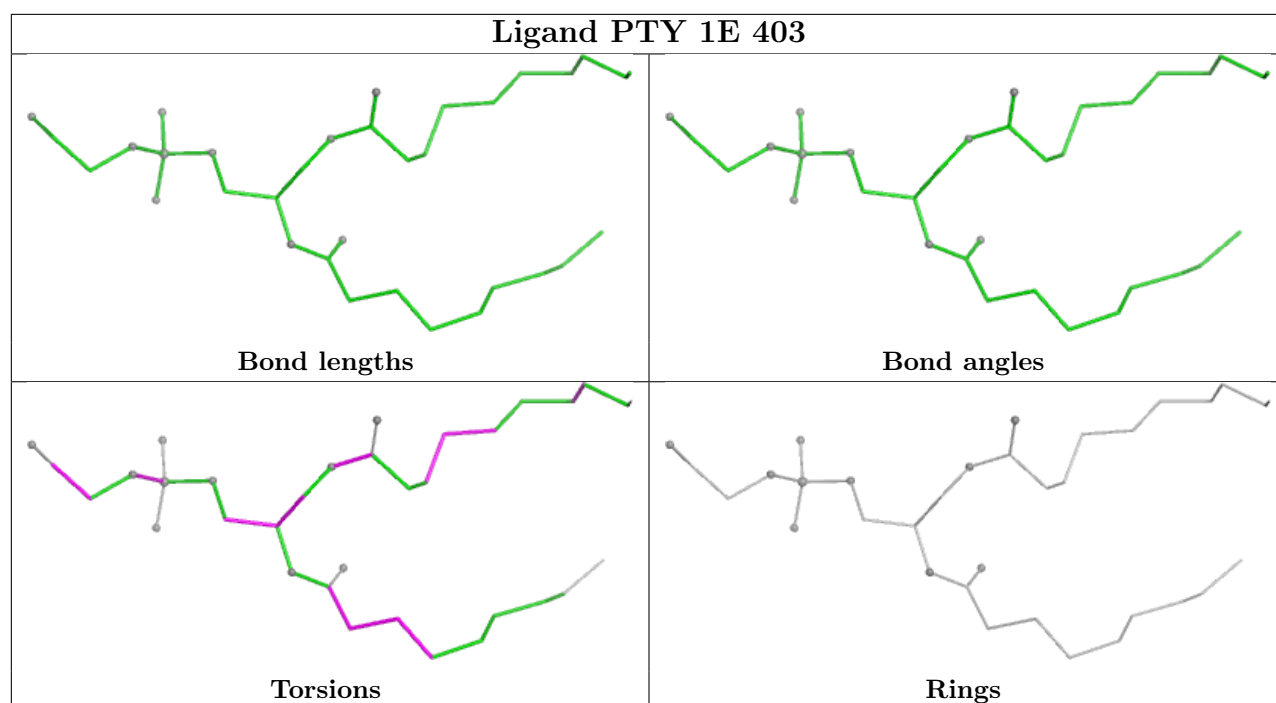


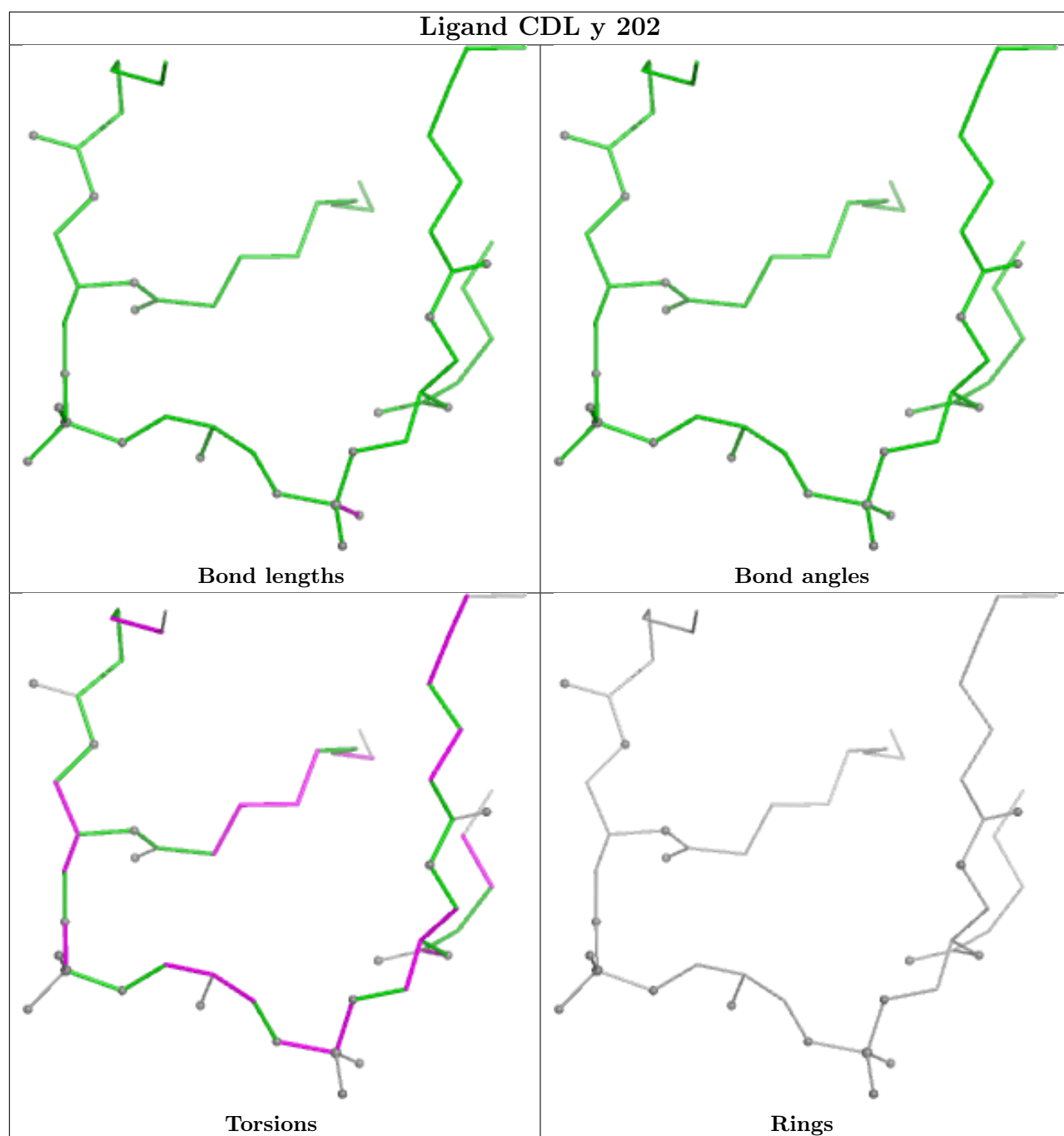


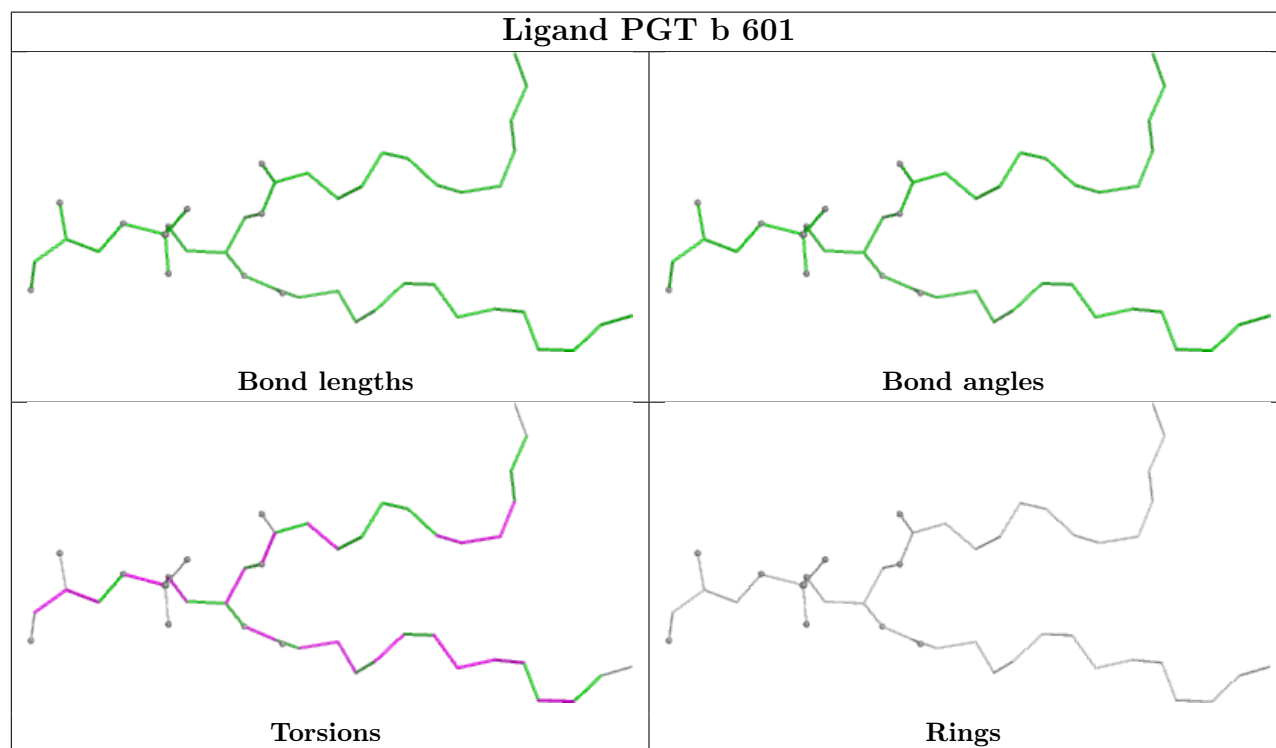
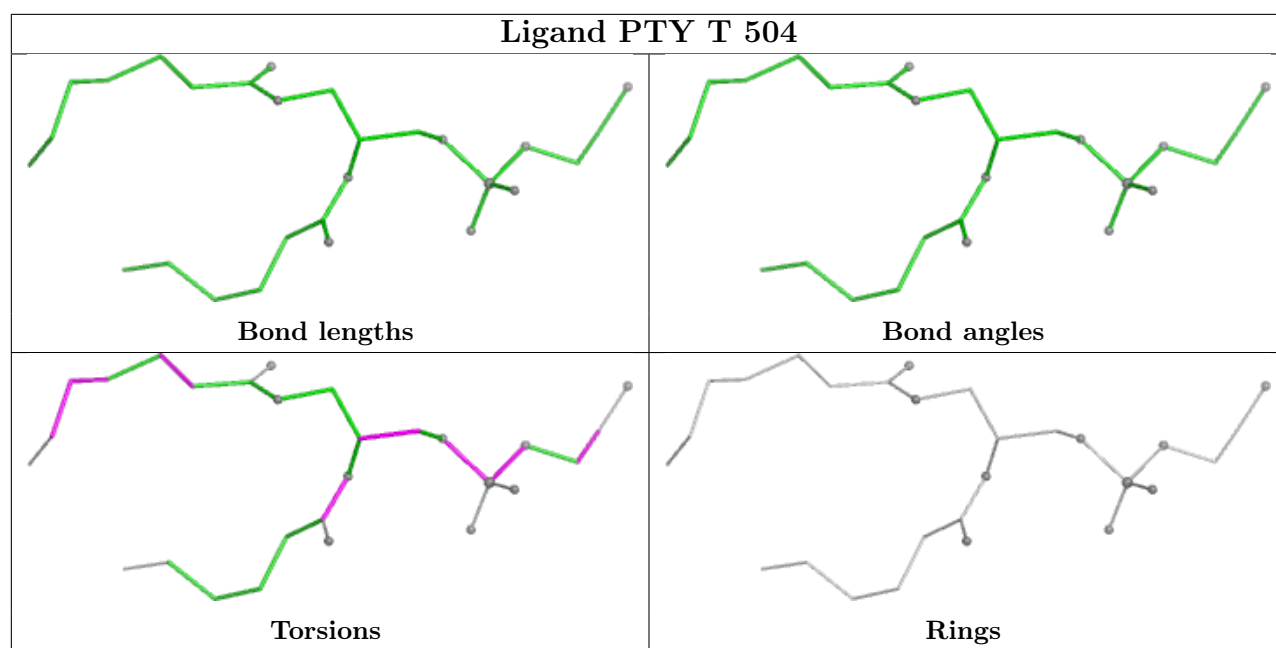


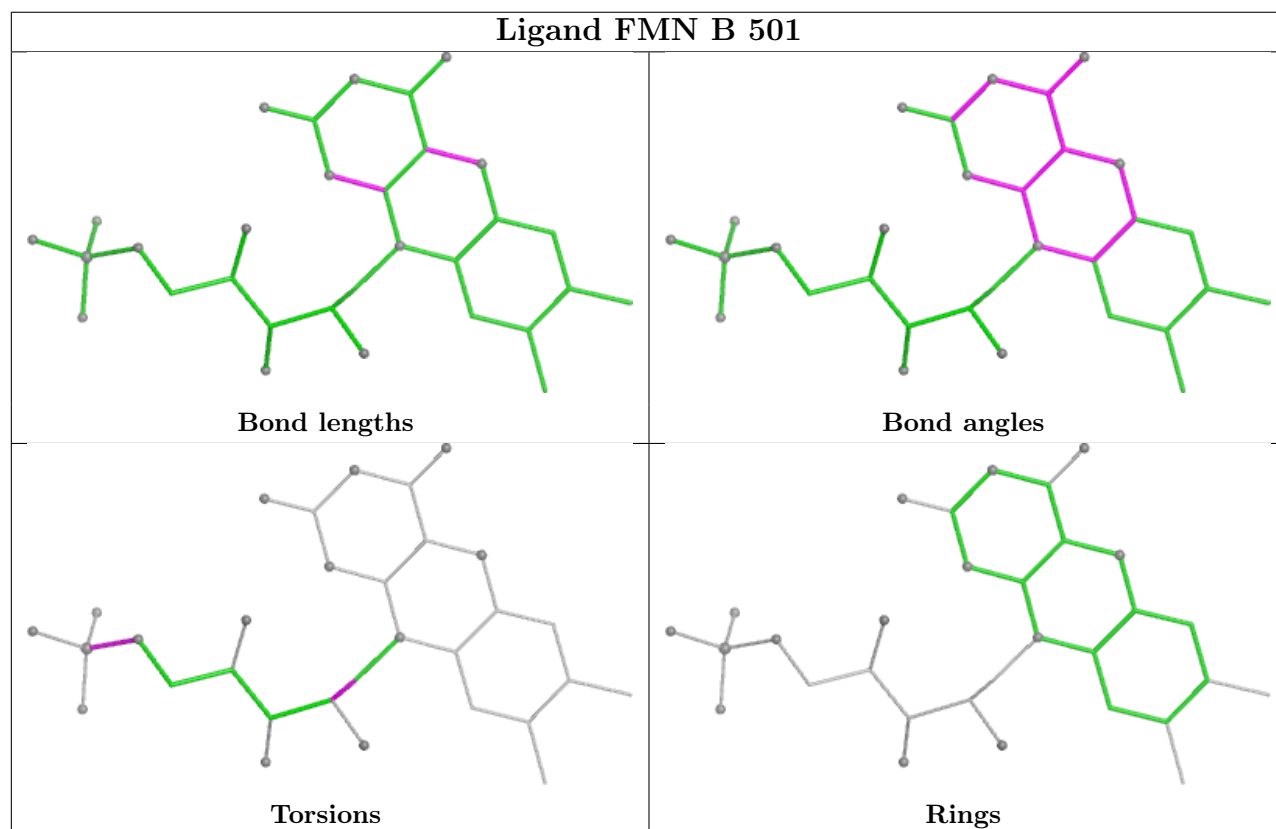
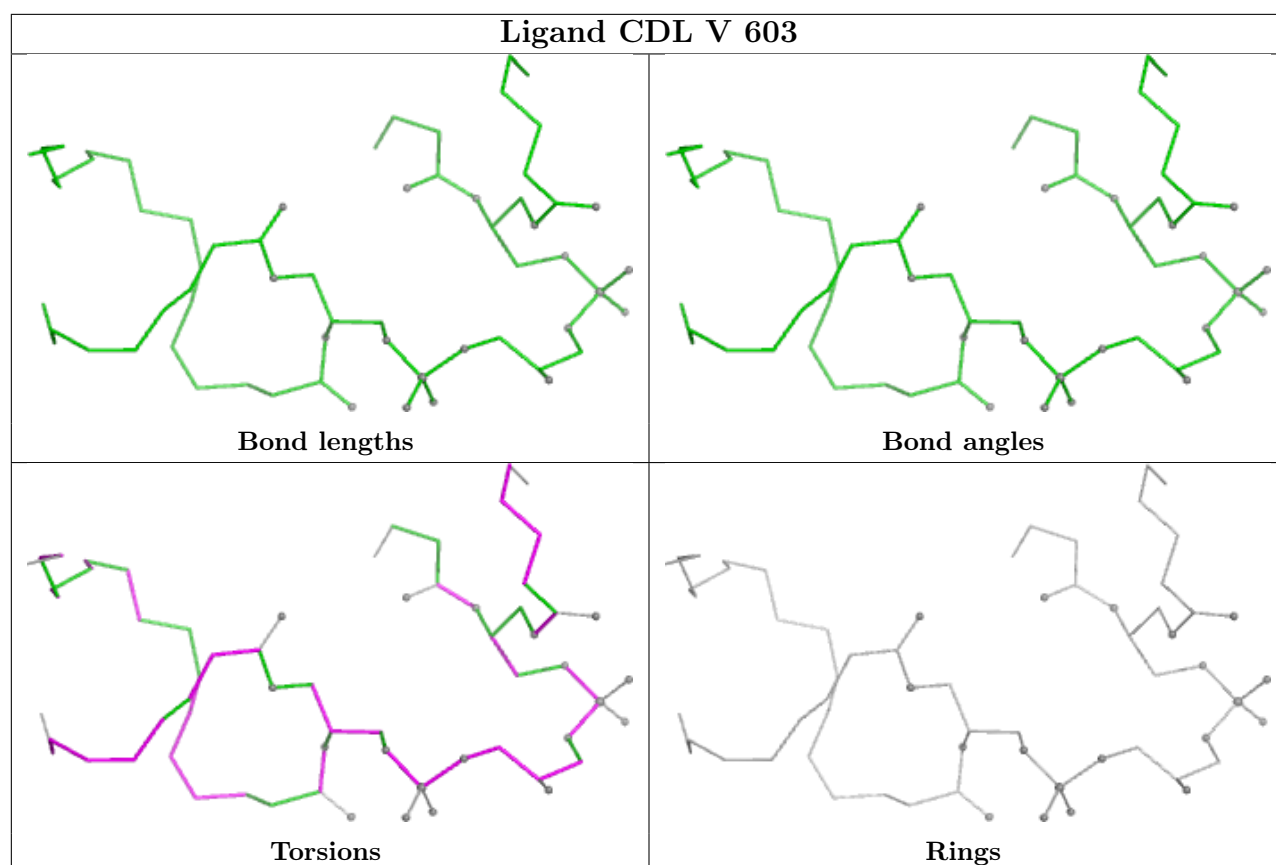


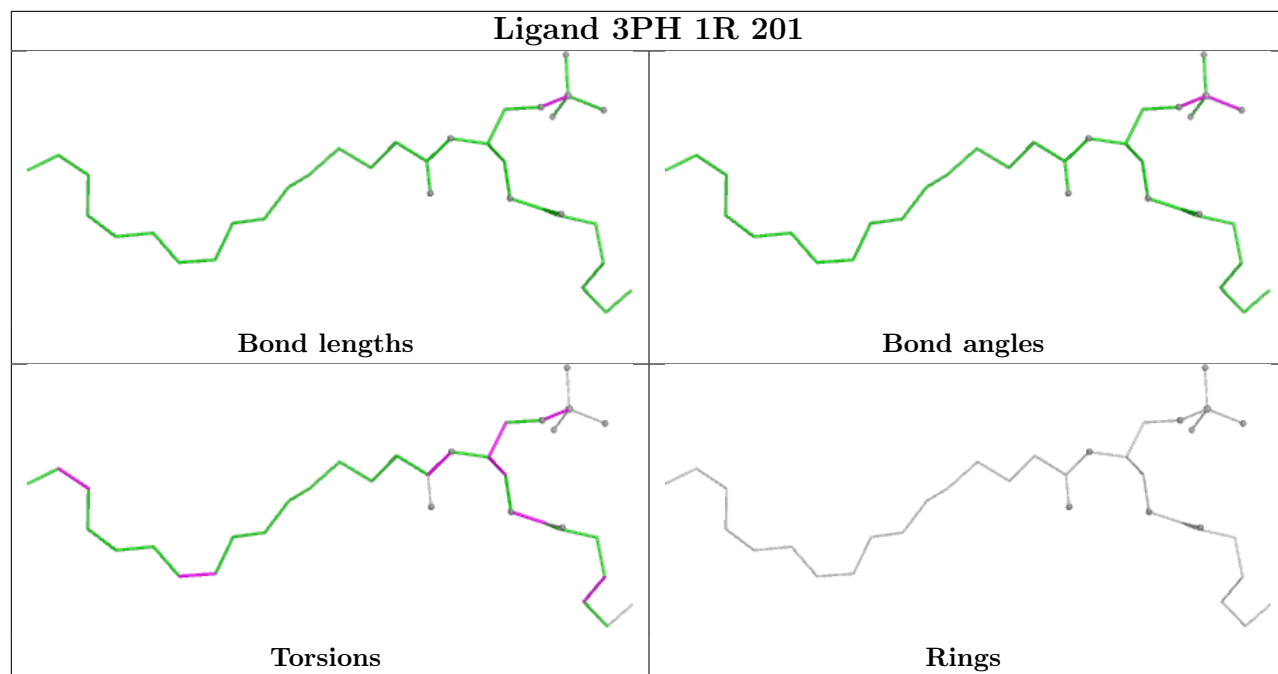


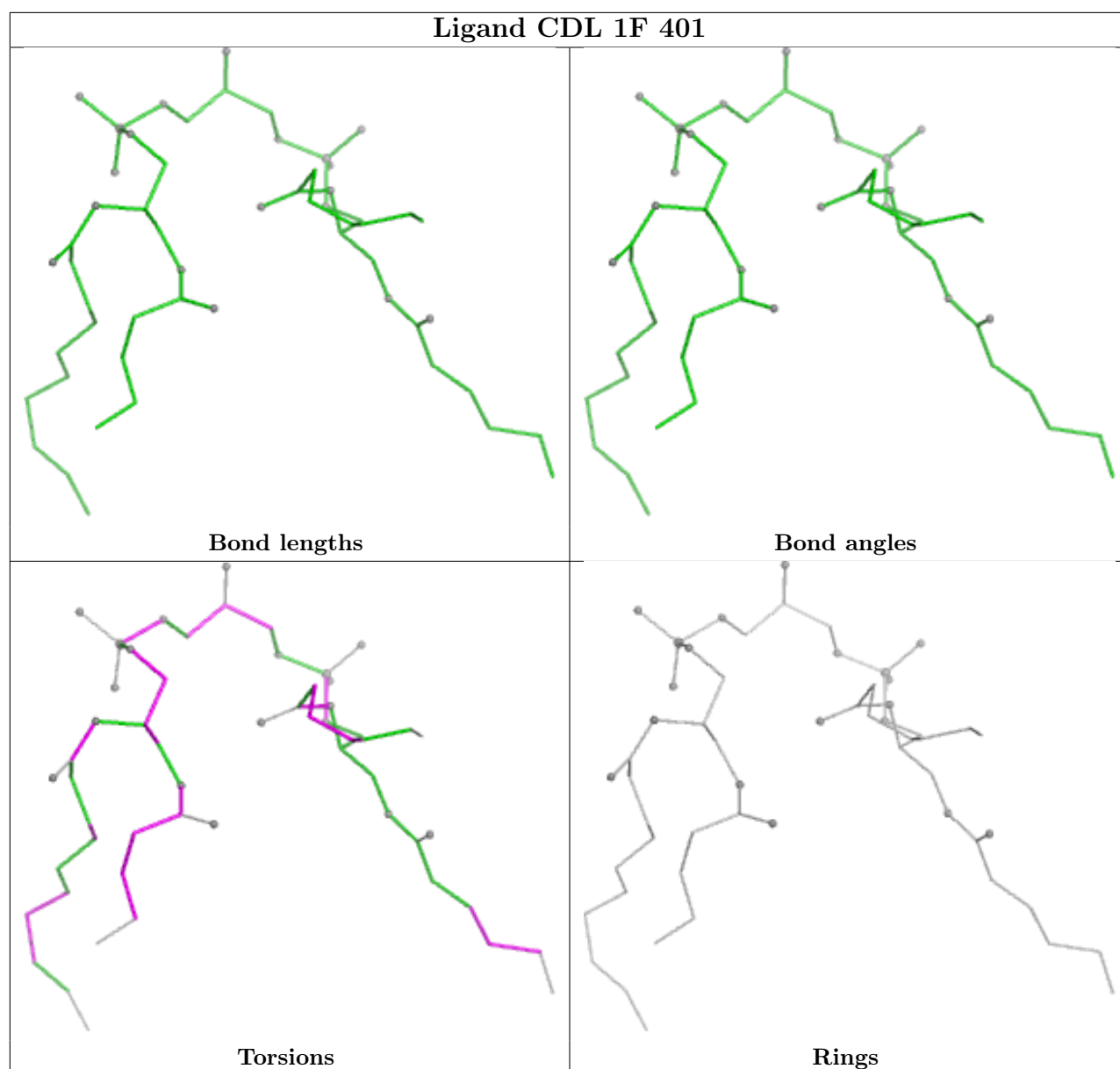


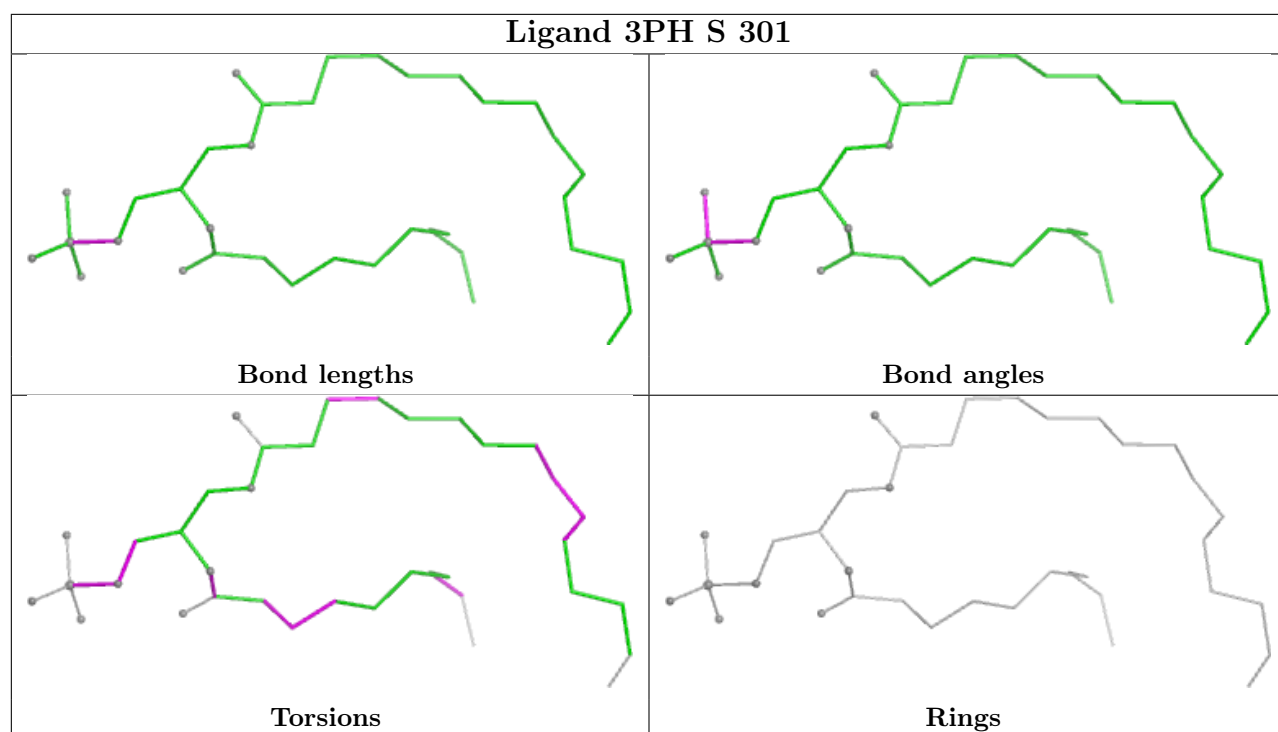


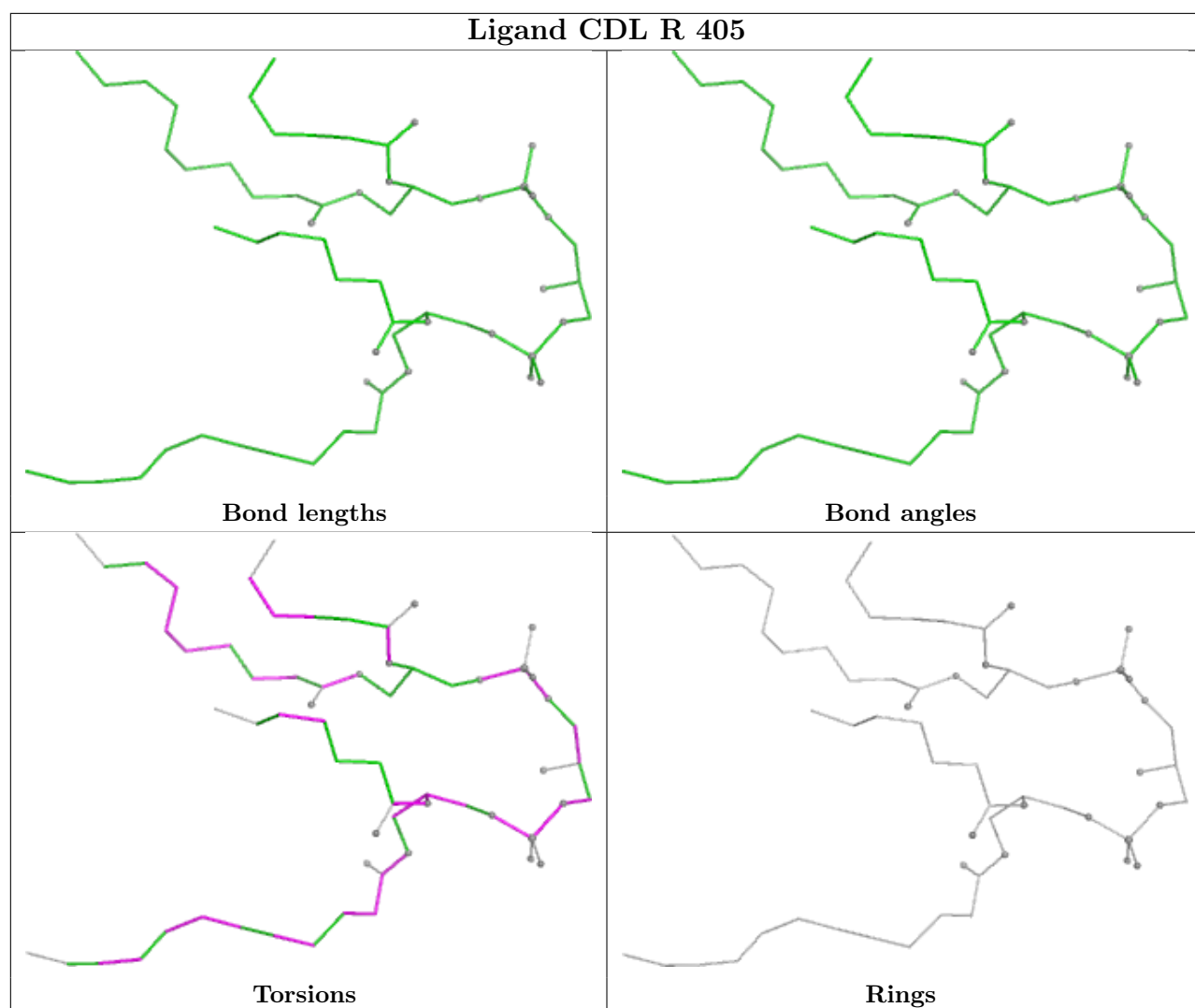


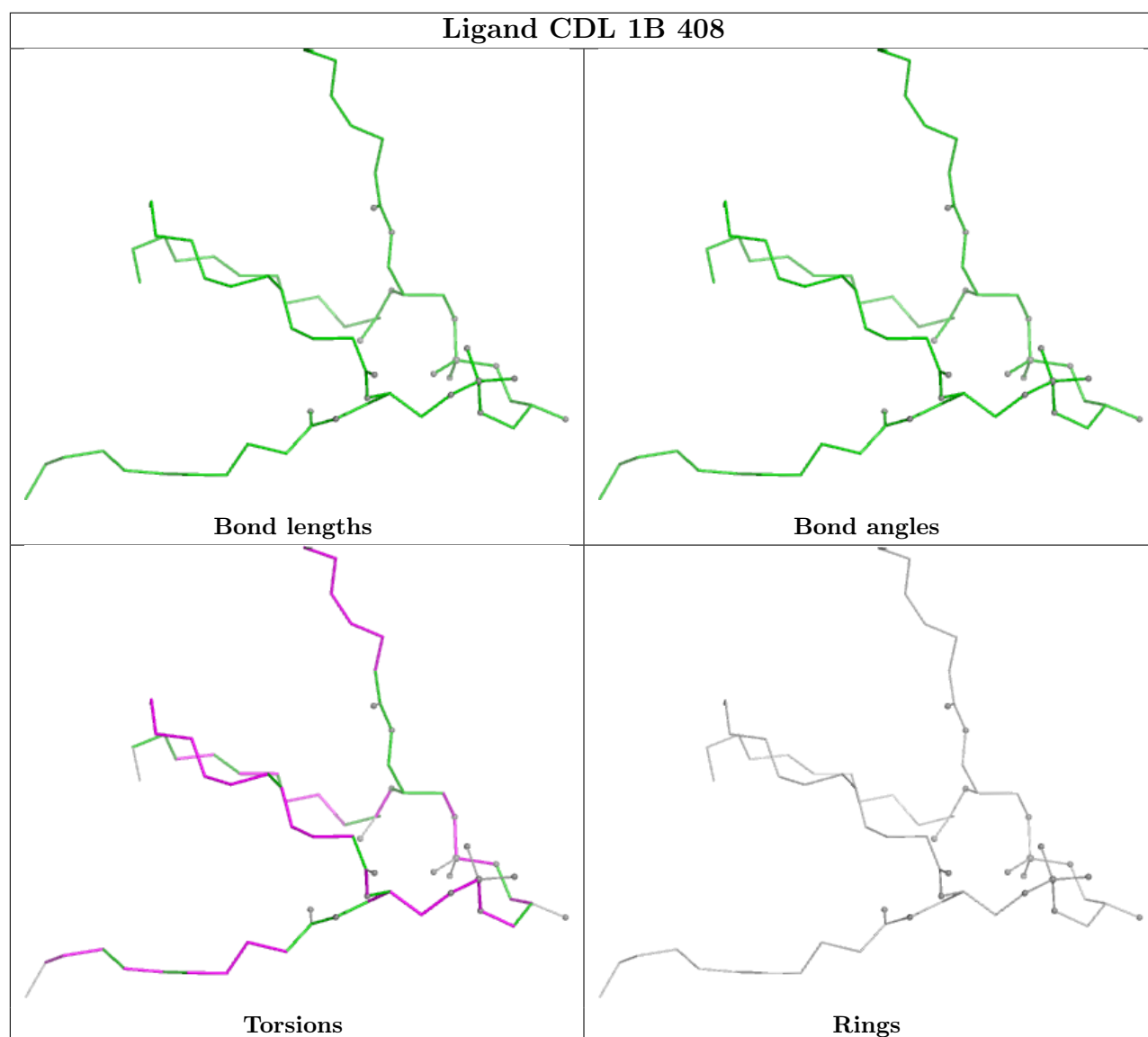


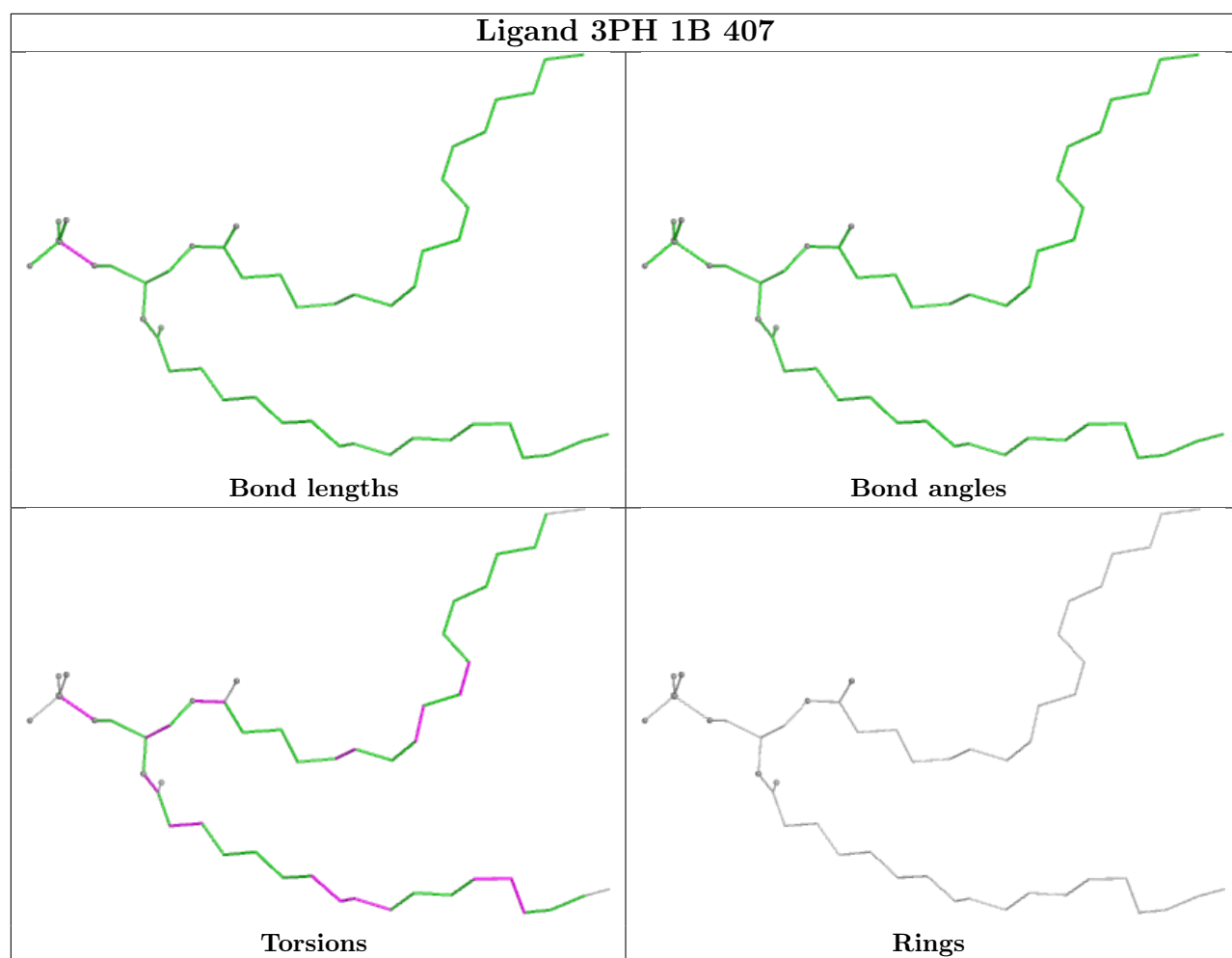


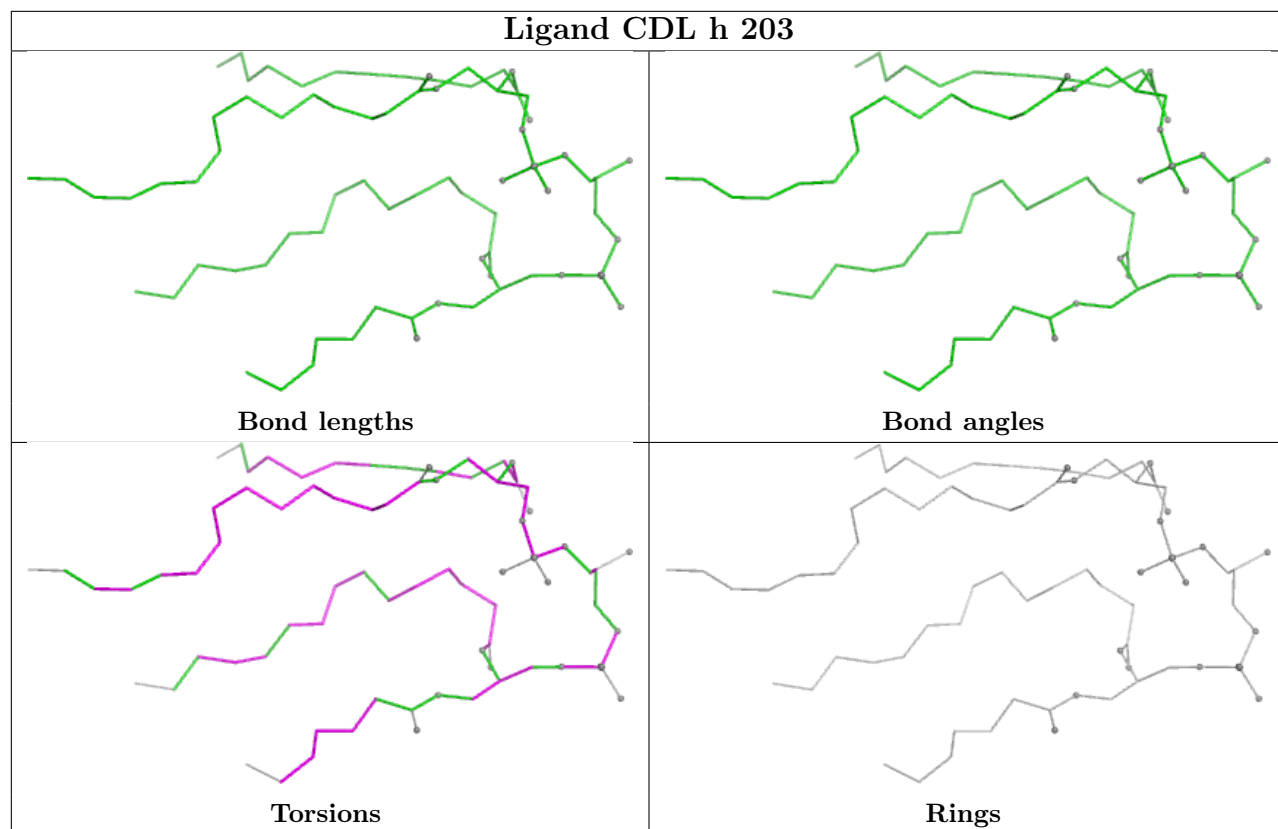


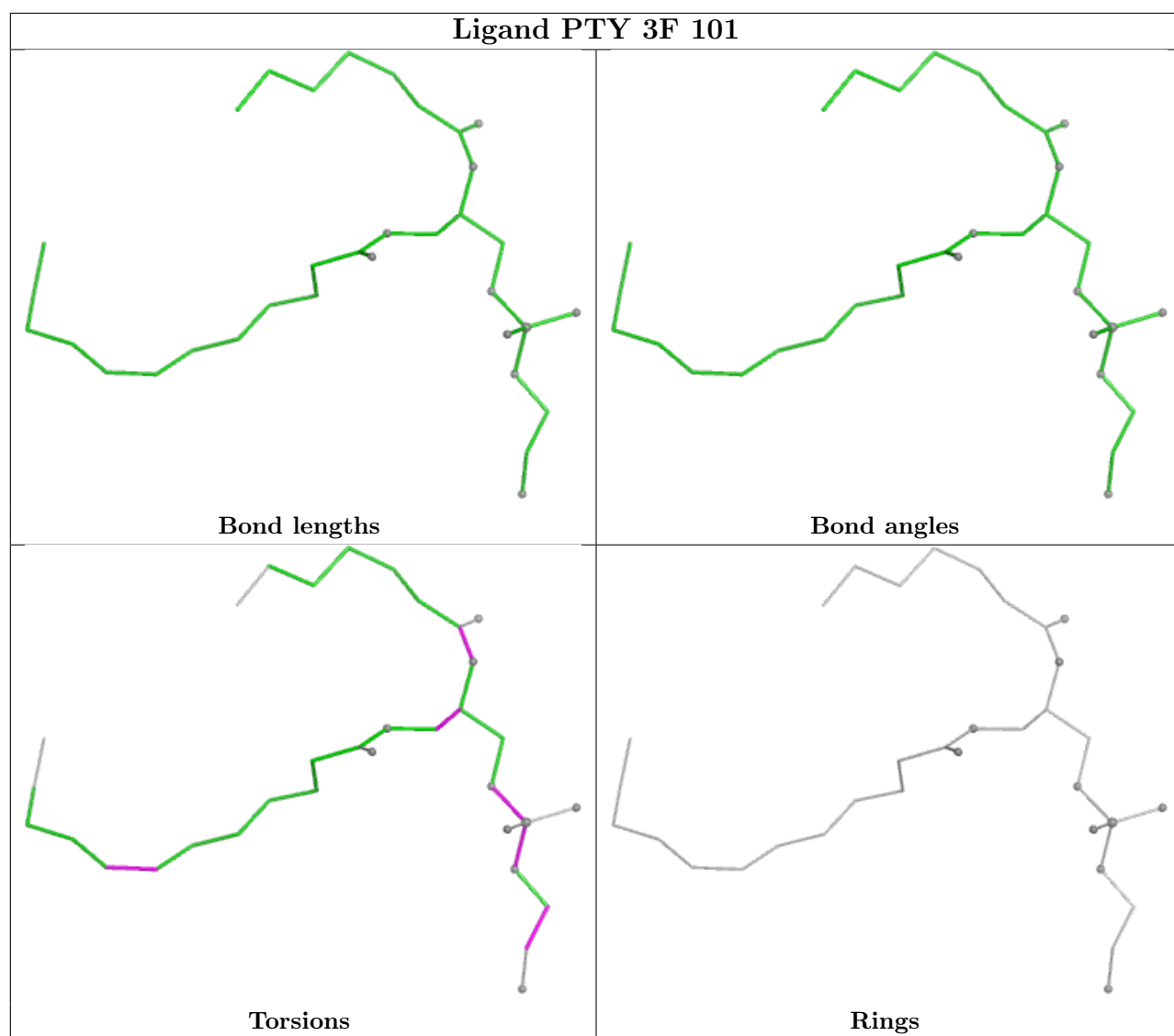




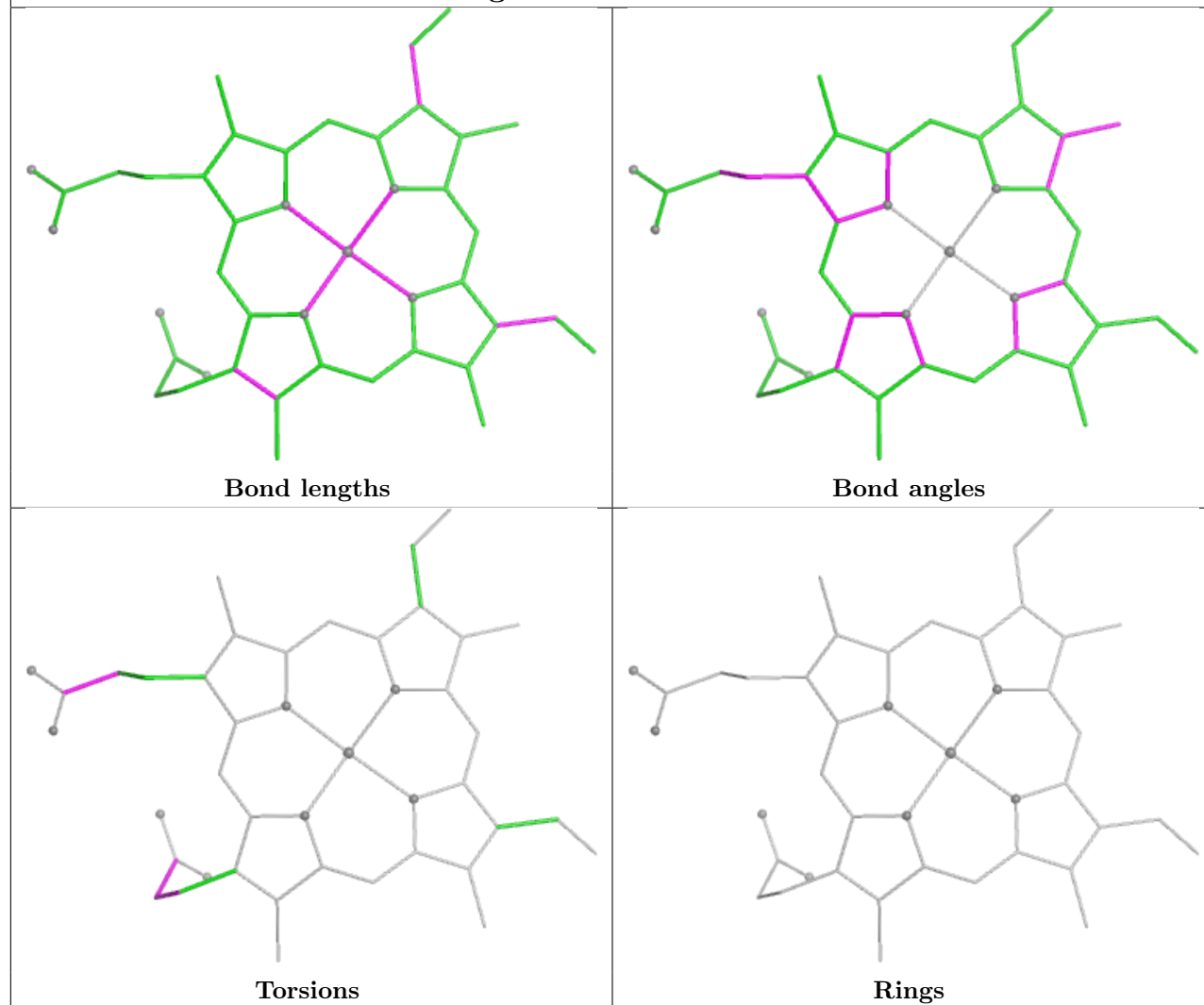




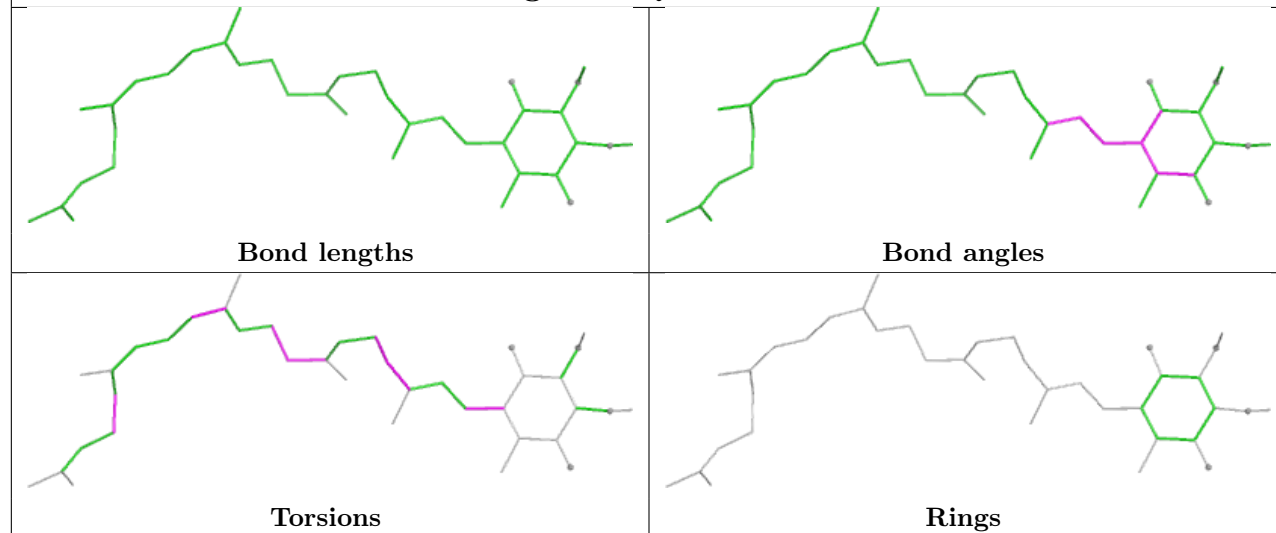


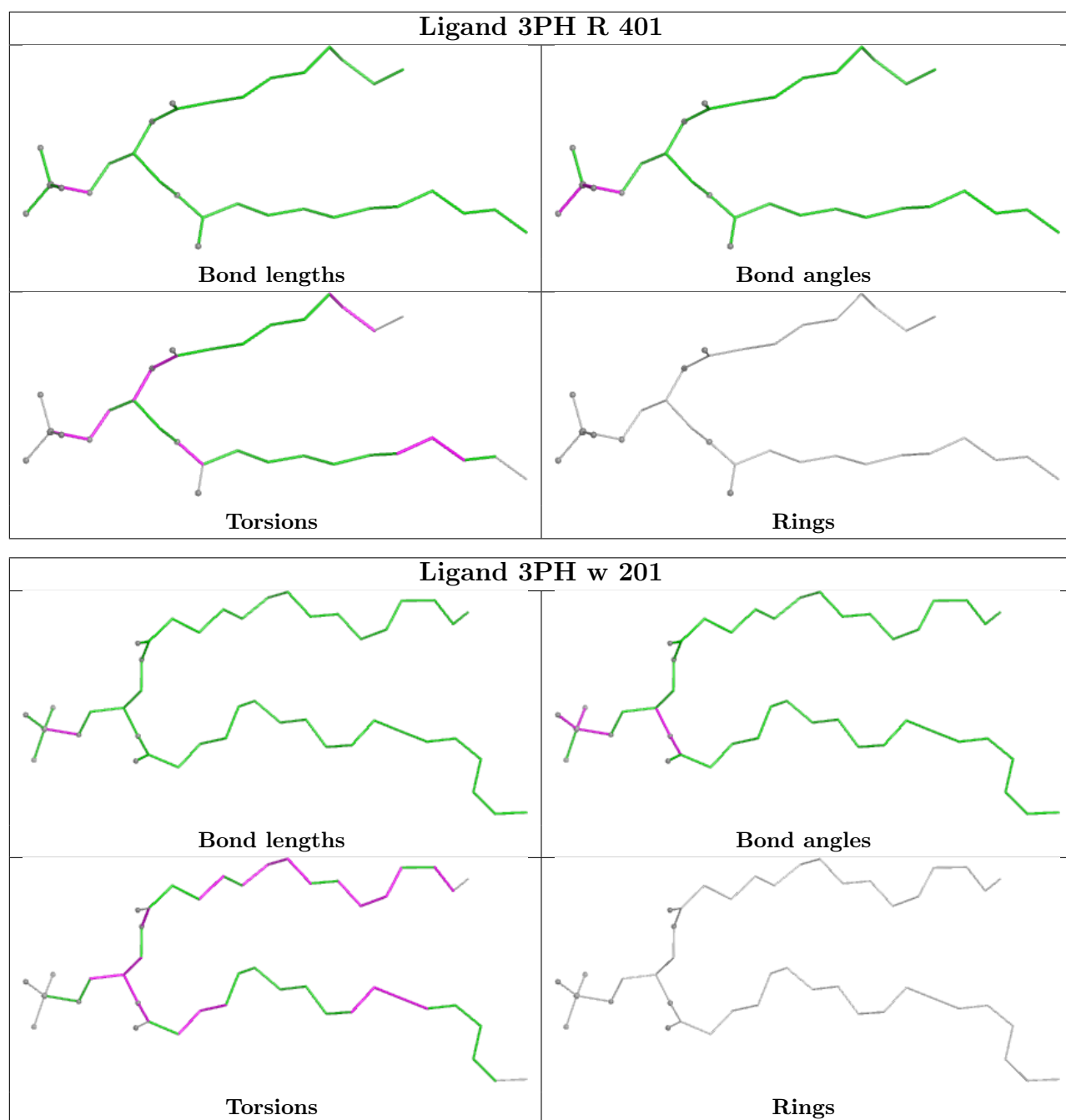


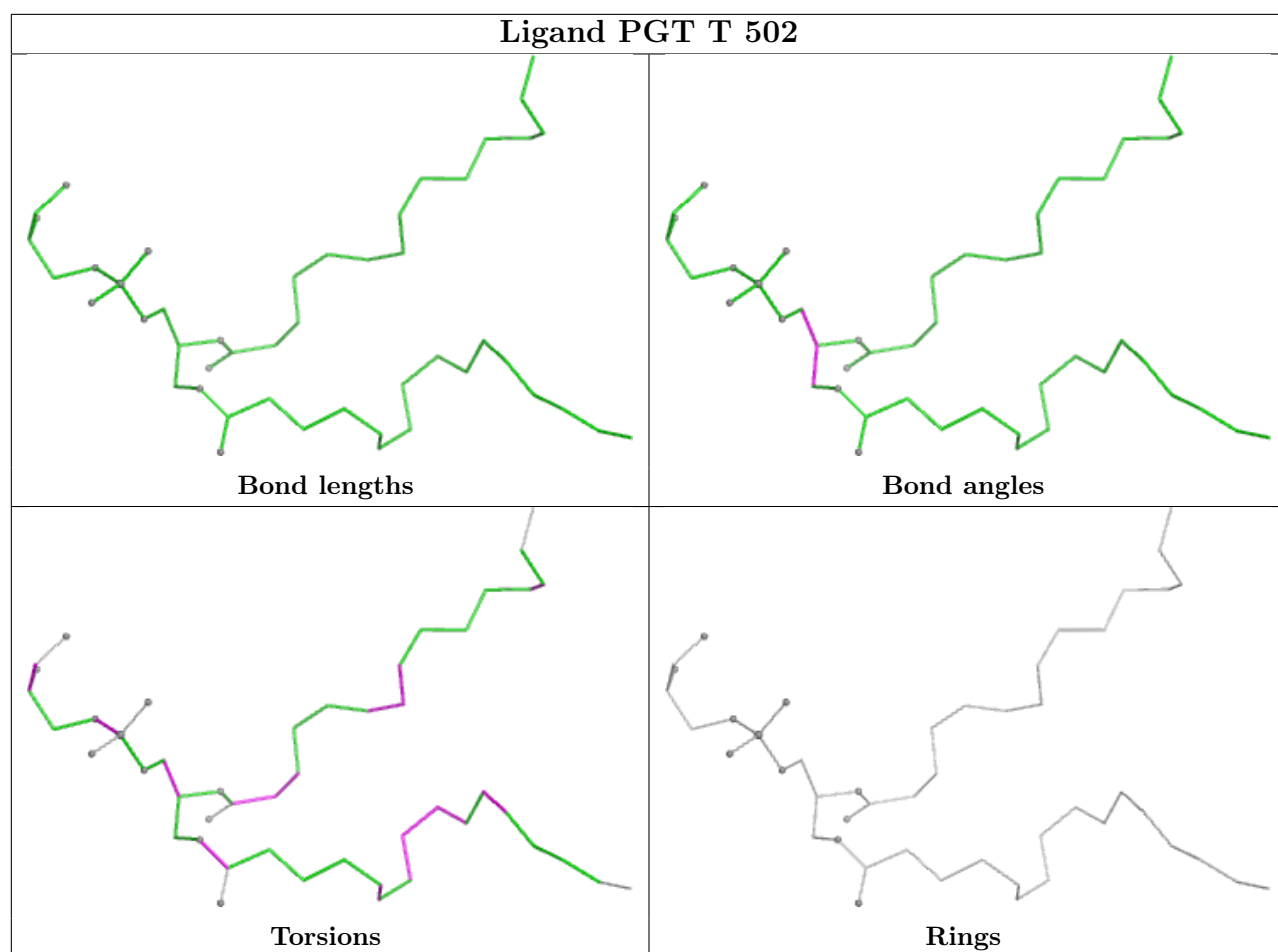
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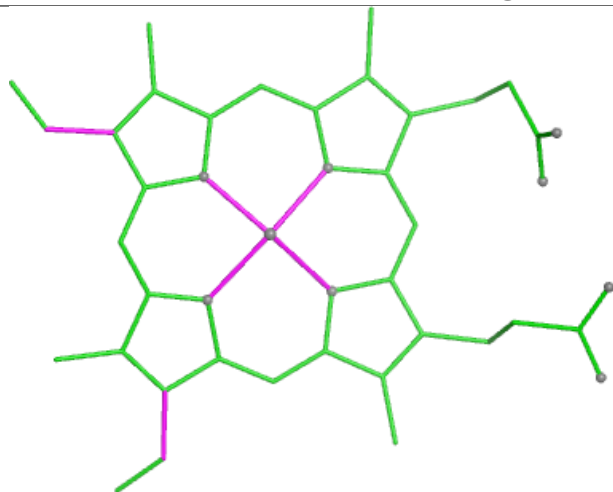
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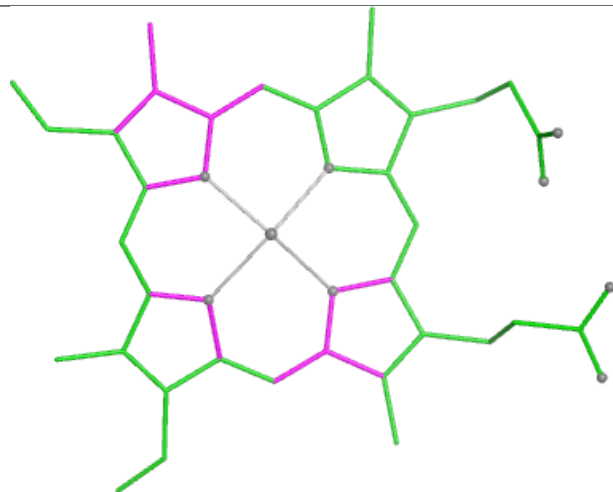




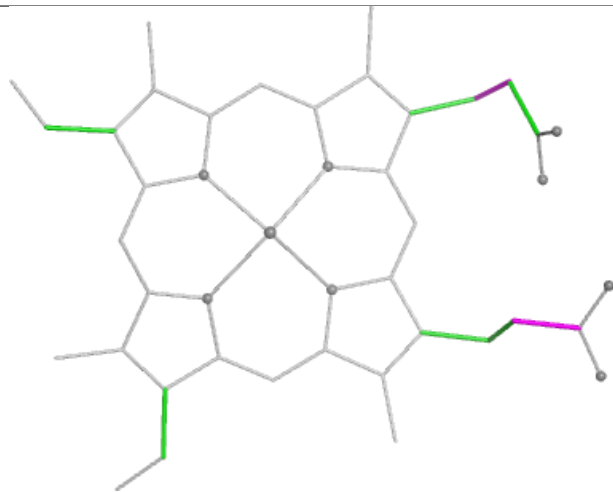
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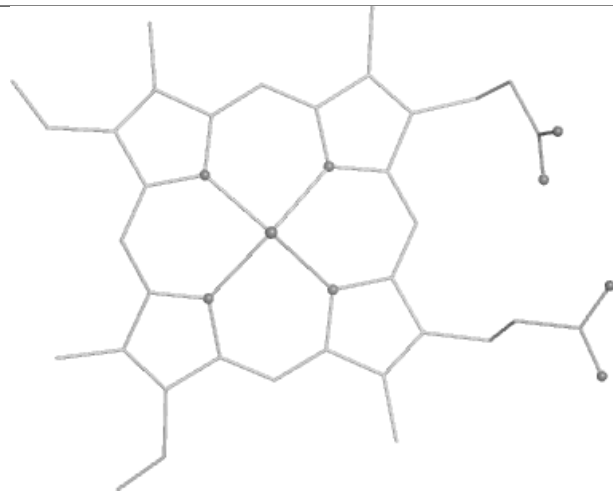
Bond lengths



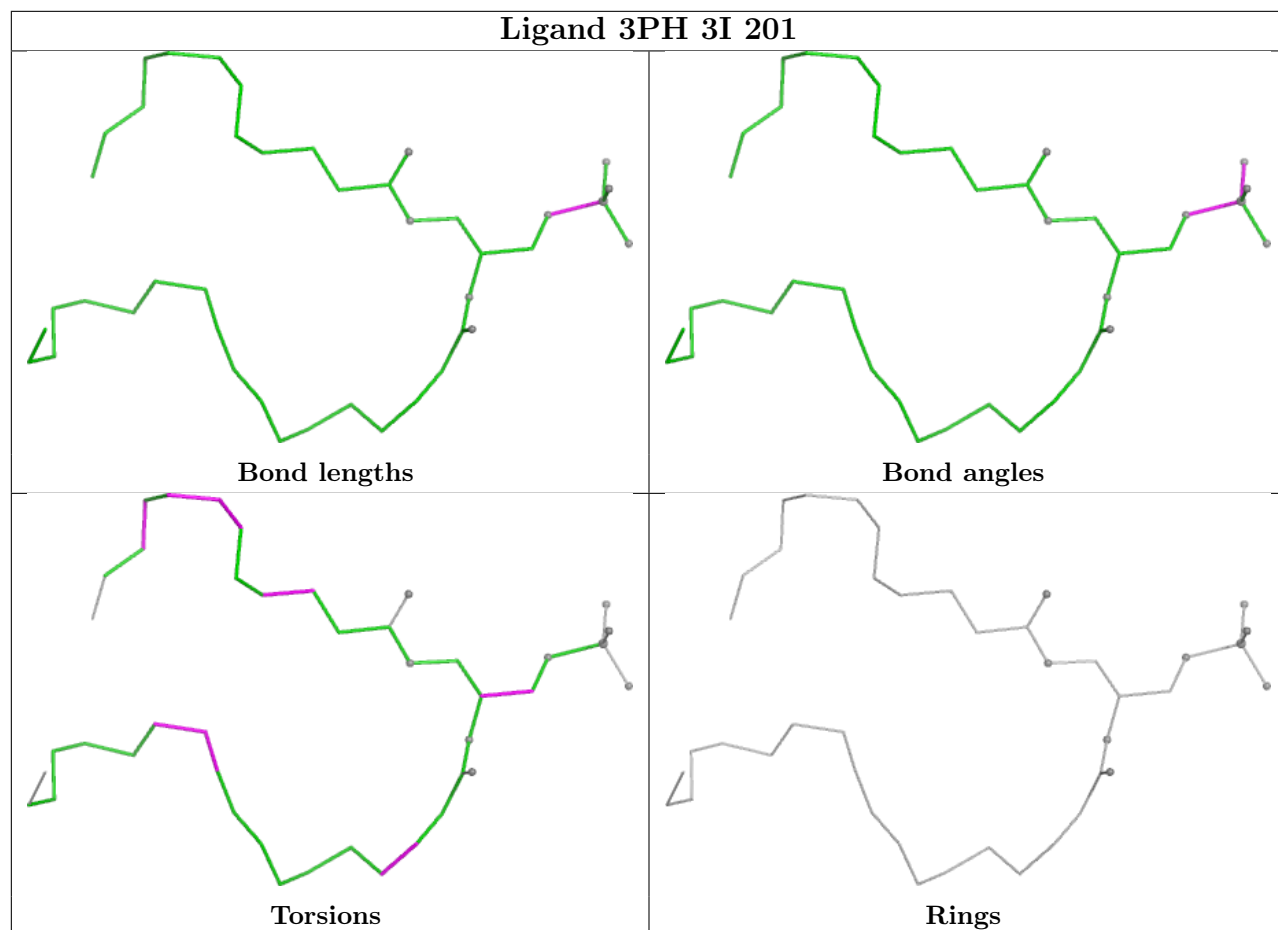
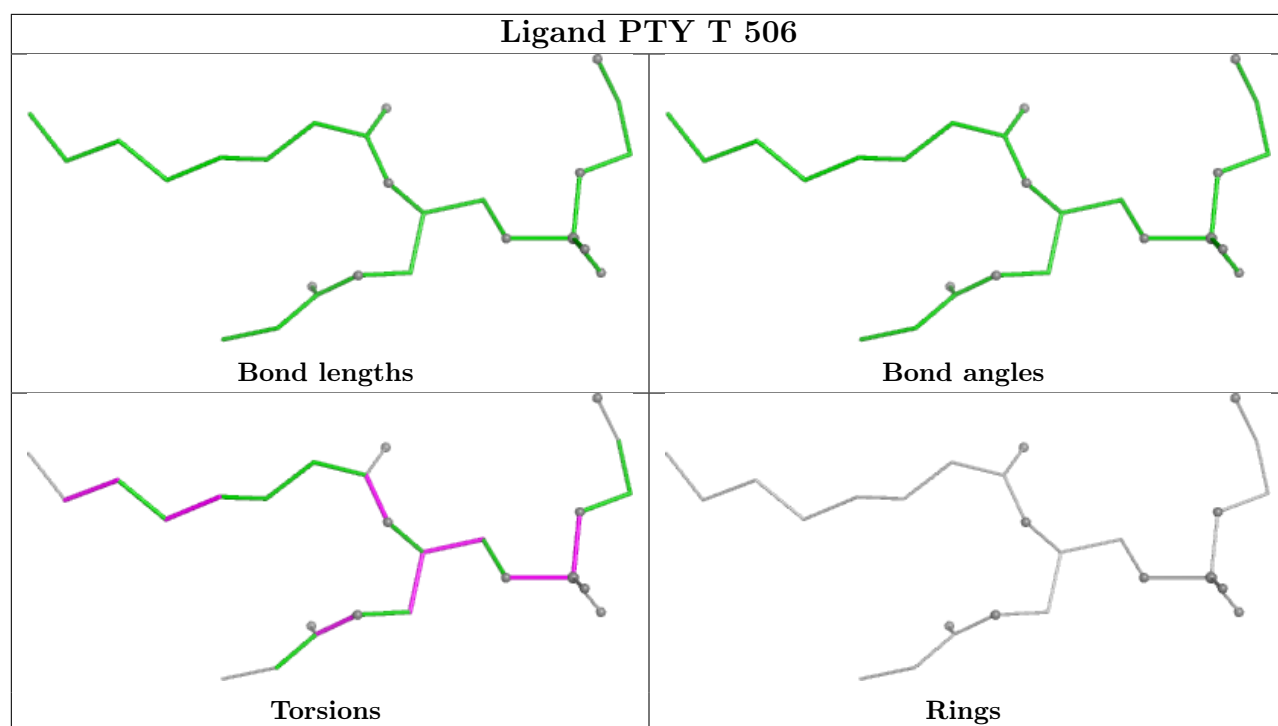
Bond angles

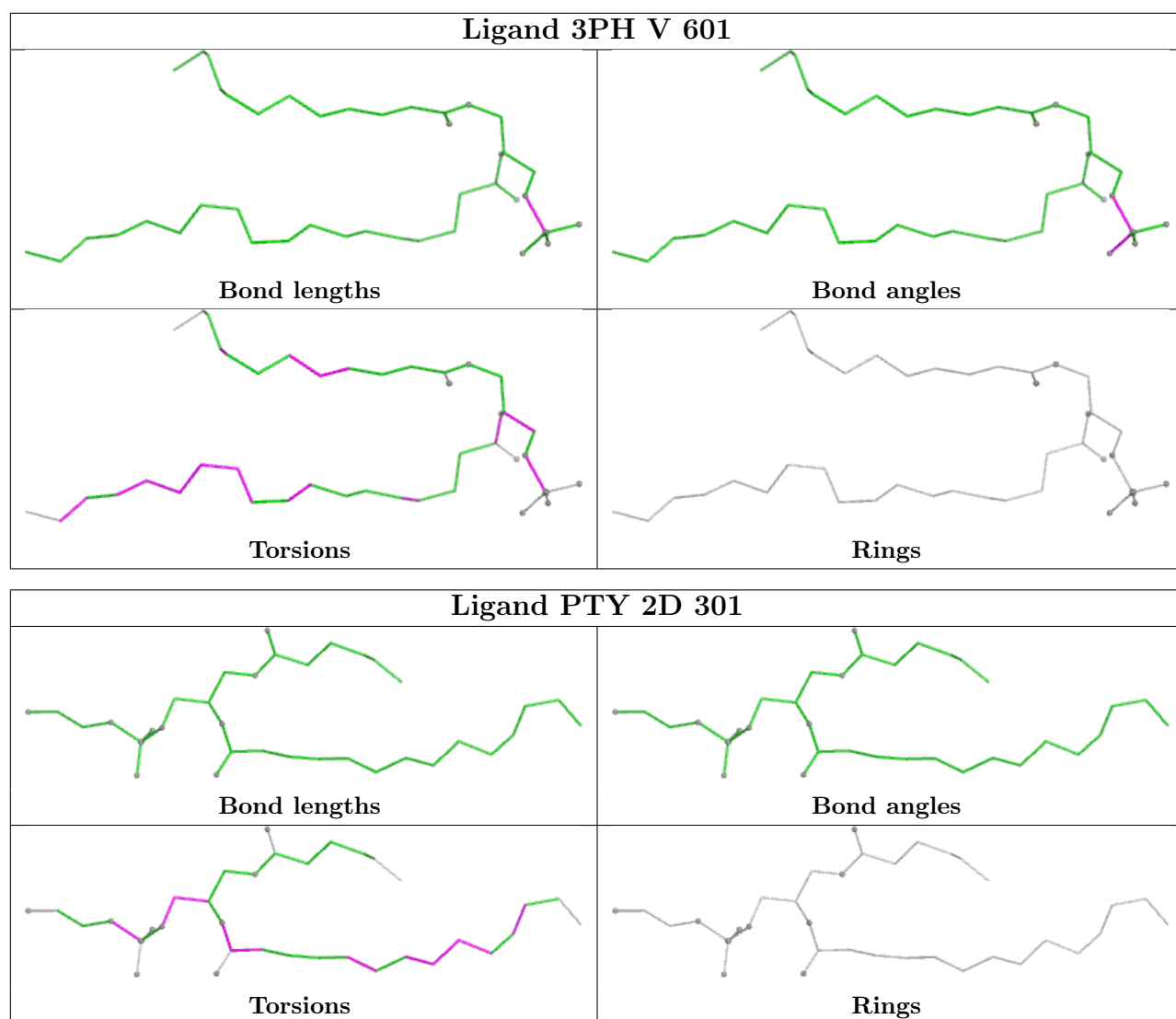


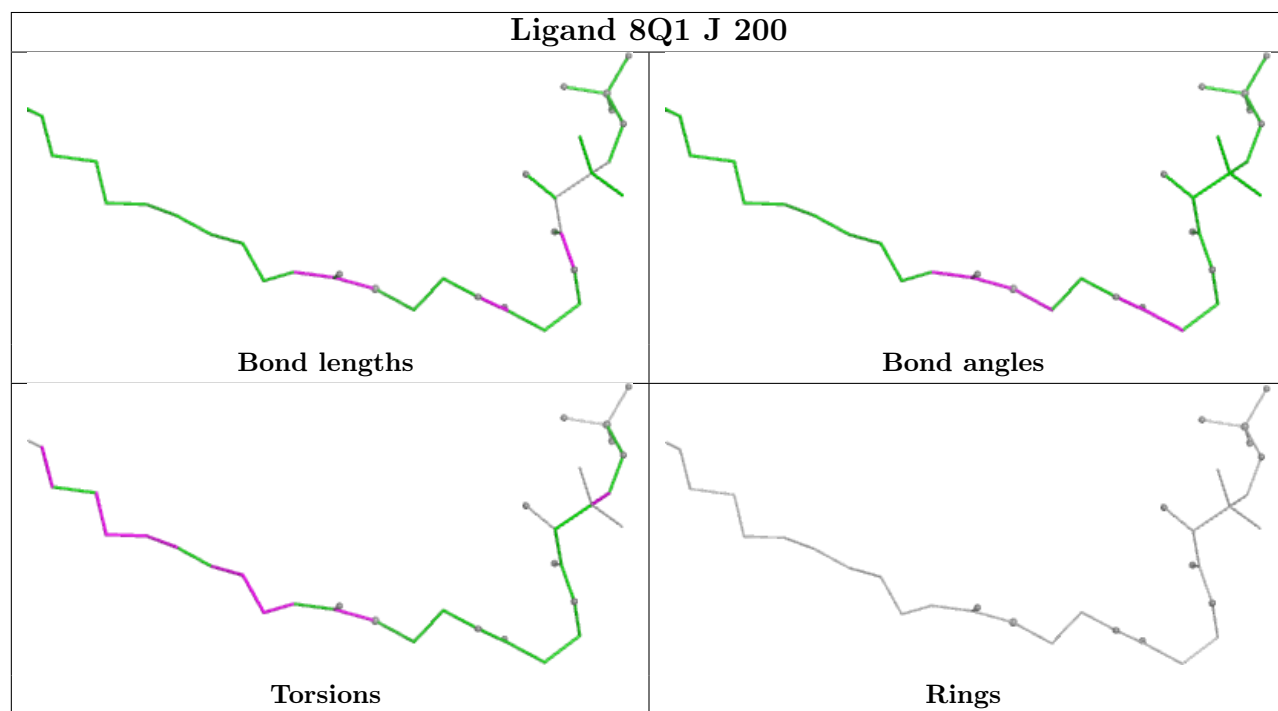
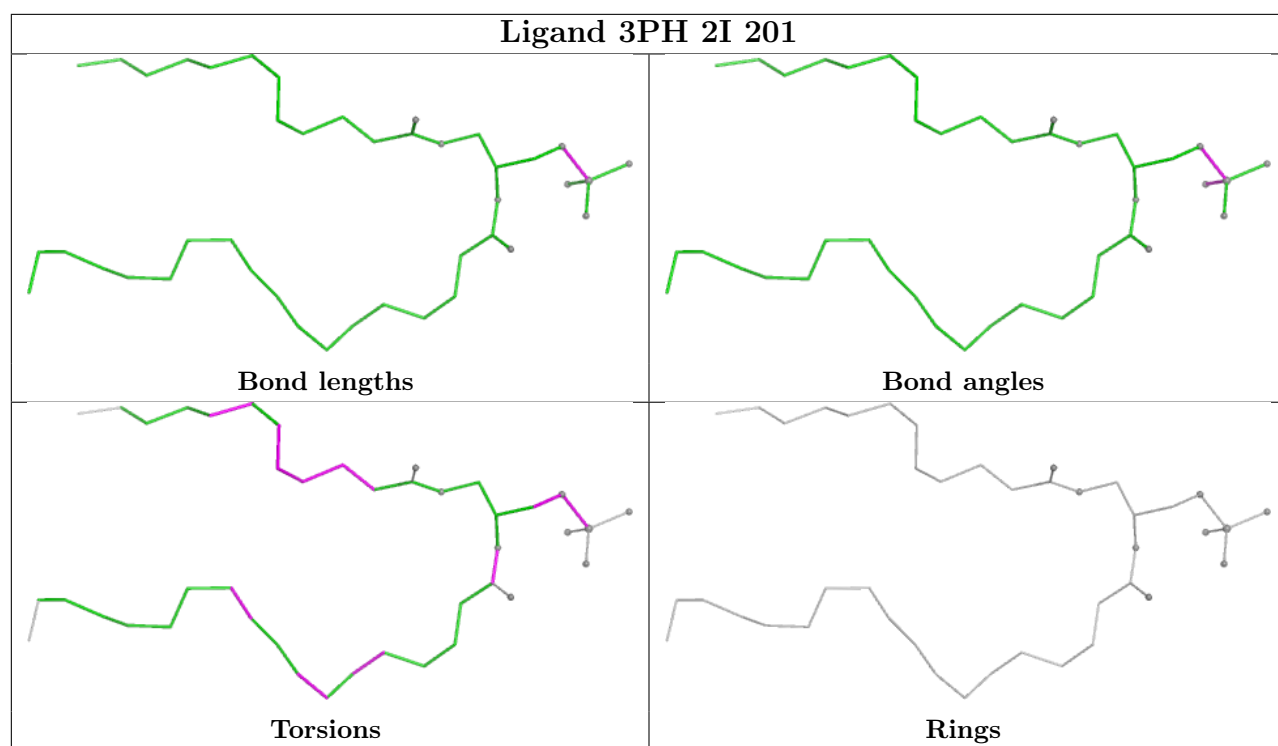
Torsions

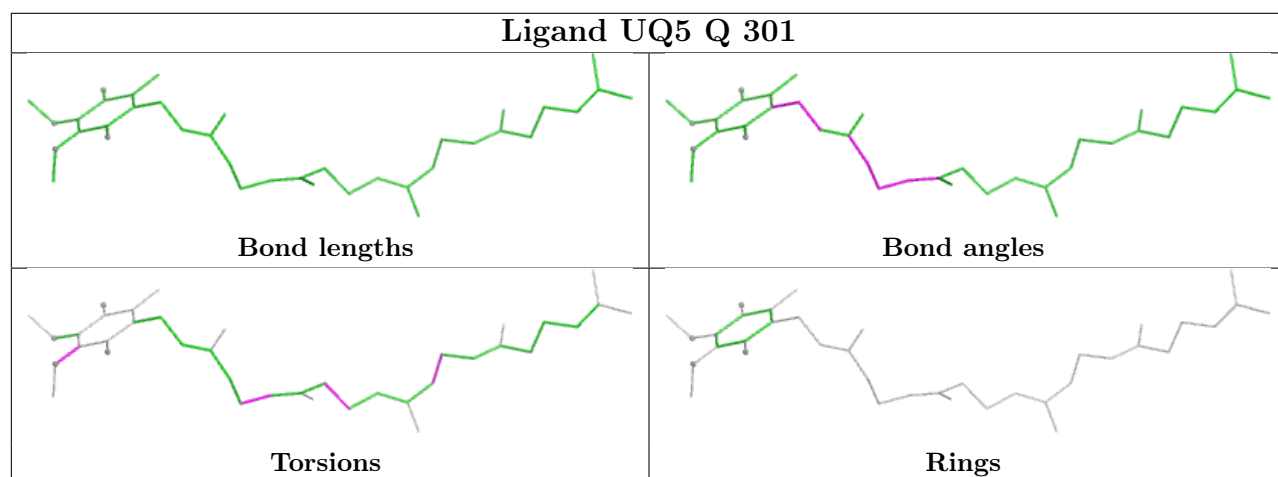
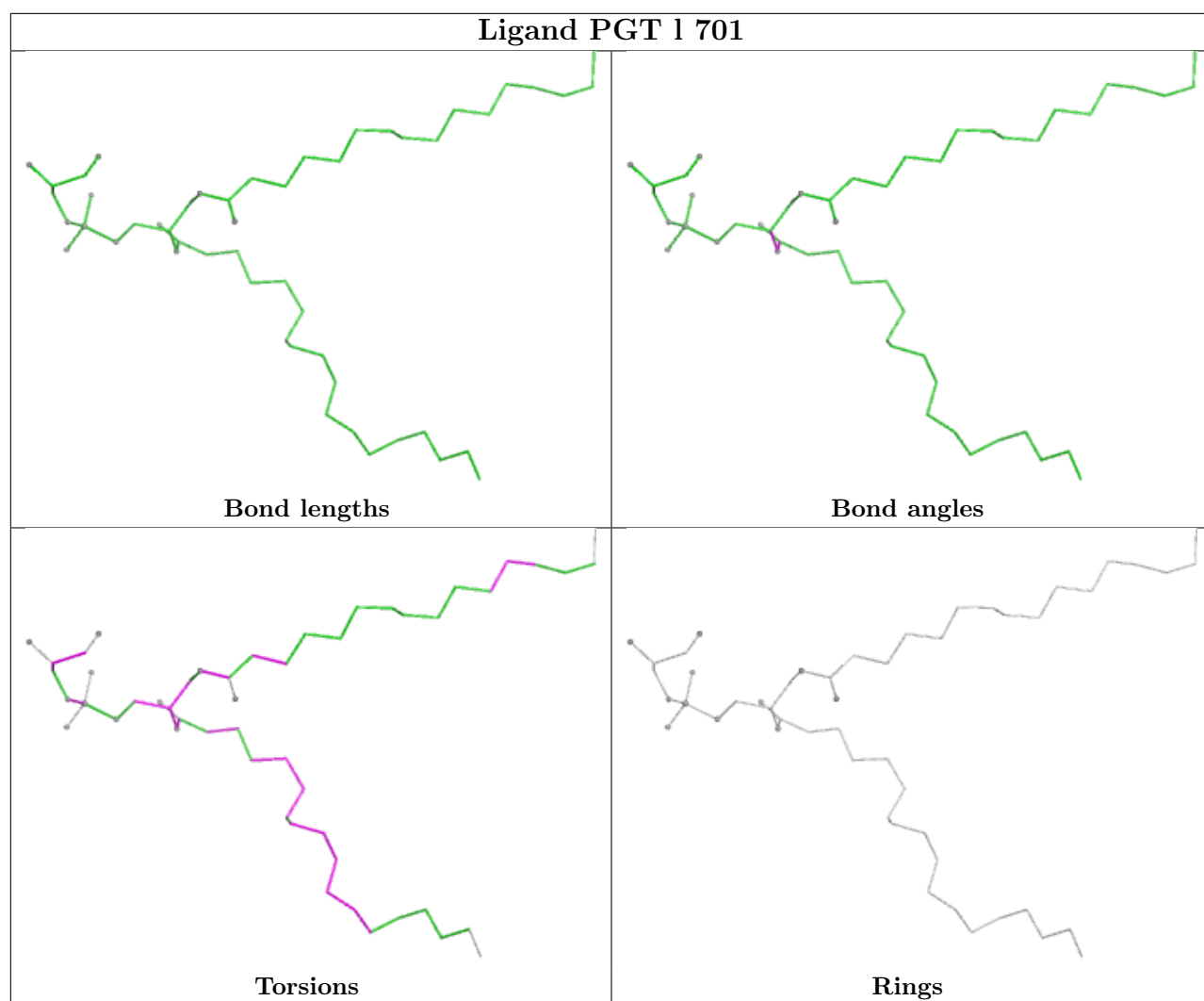


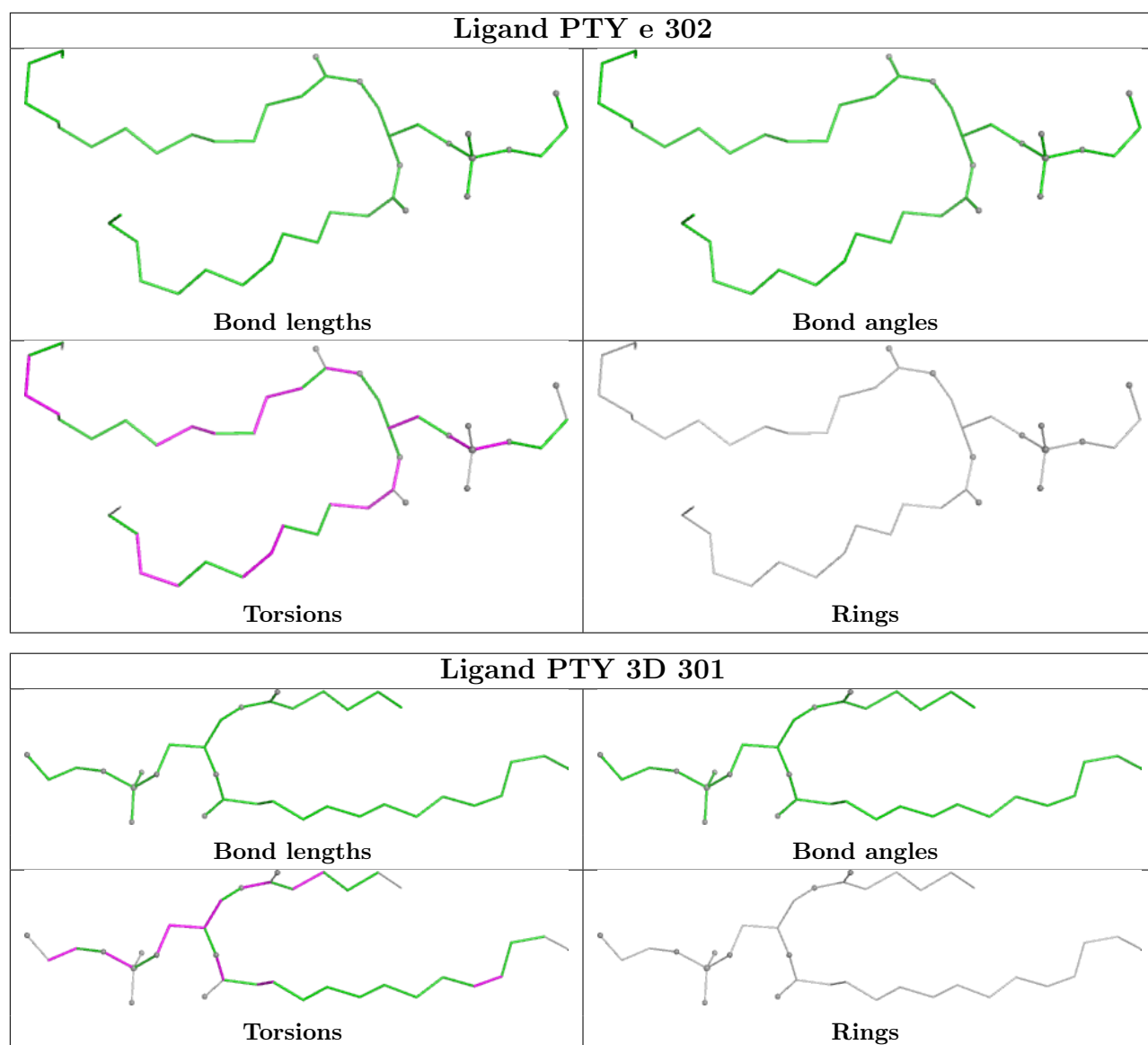
Rings



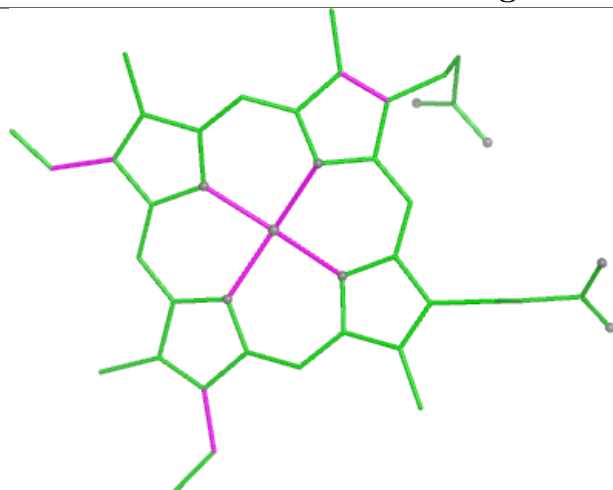




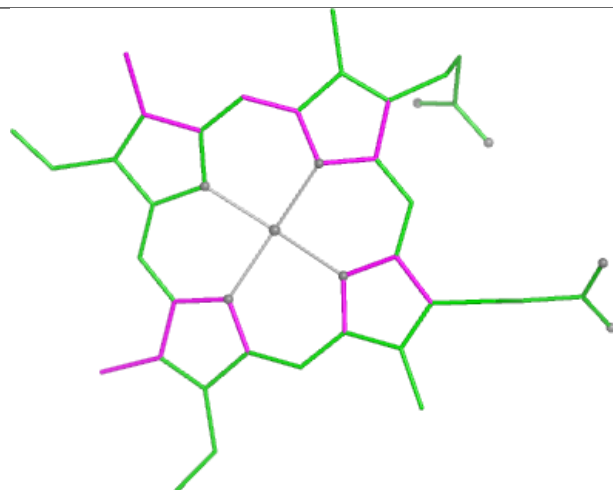




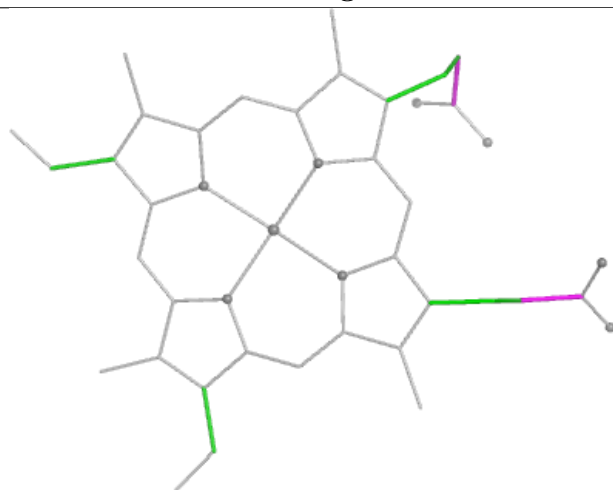
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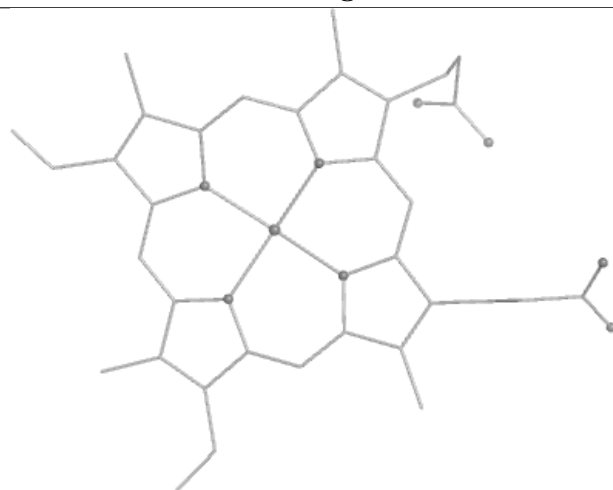
Bond lengths



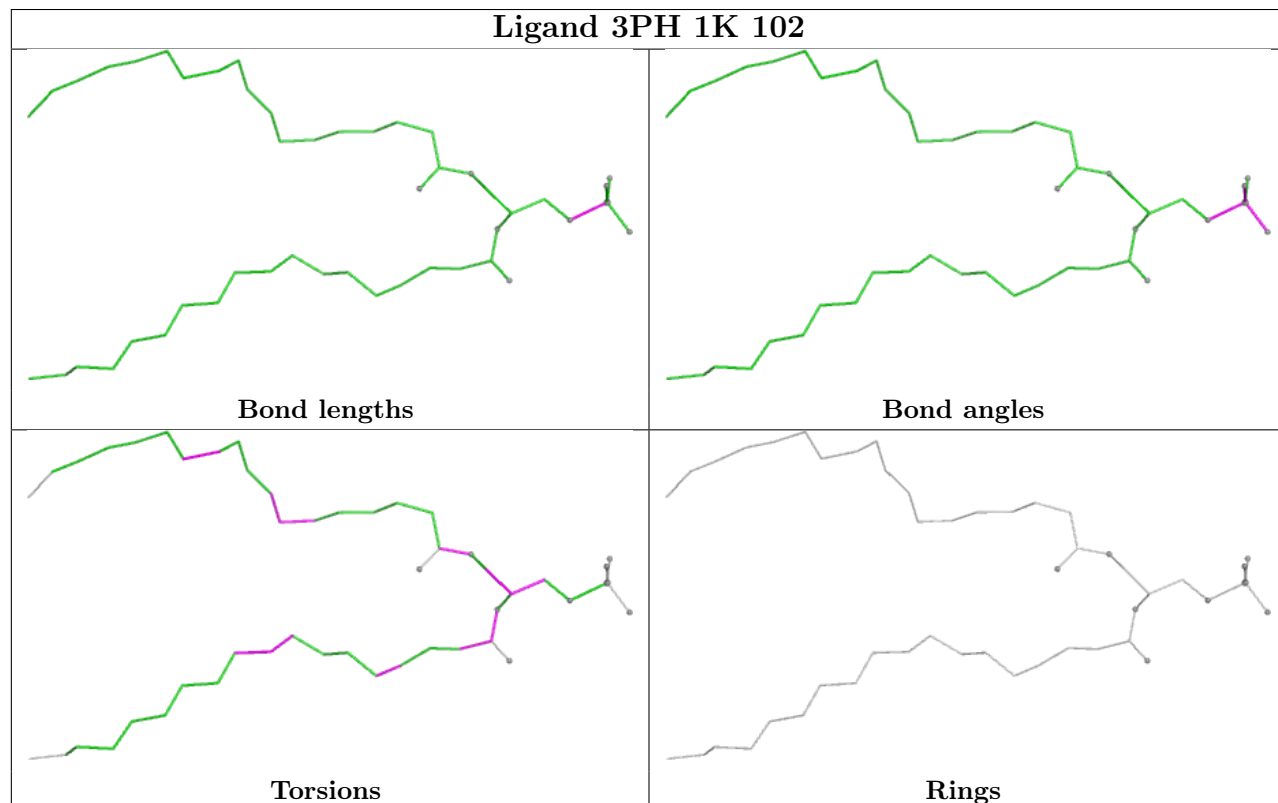
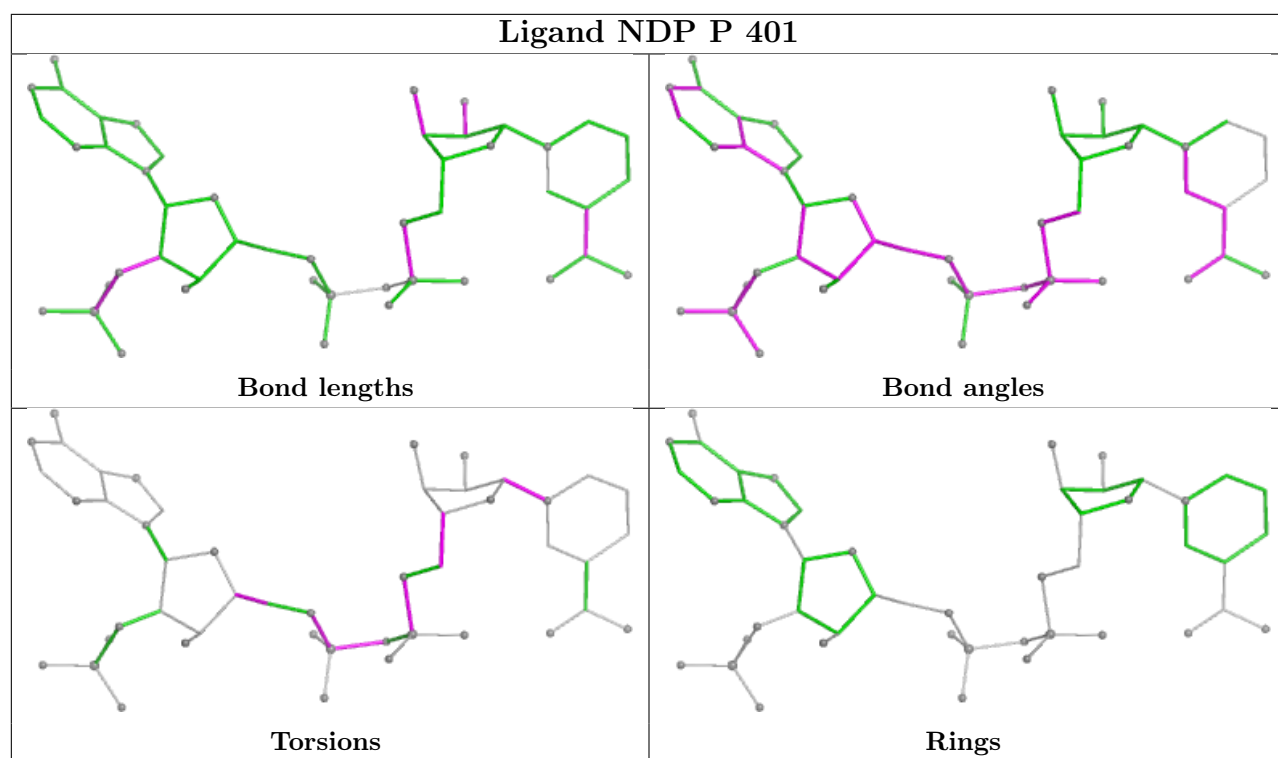
Bond angles

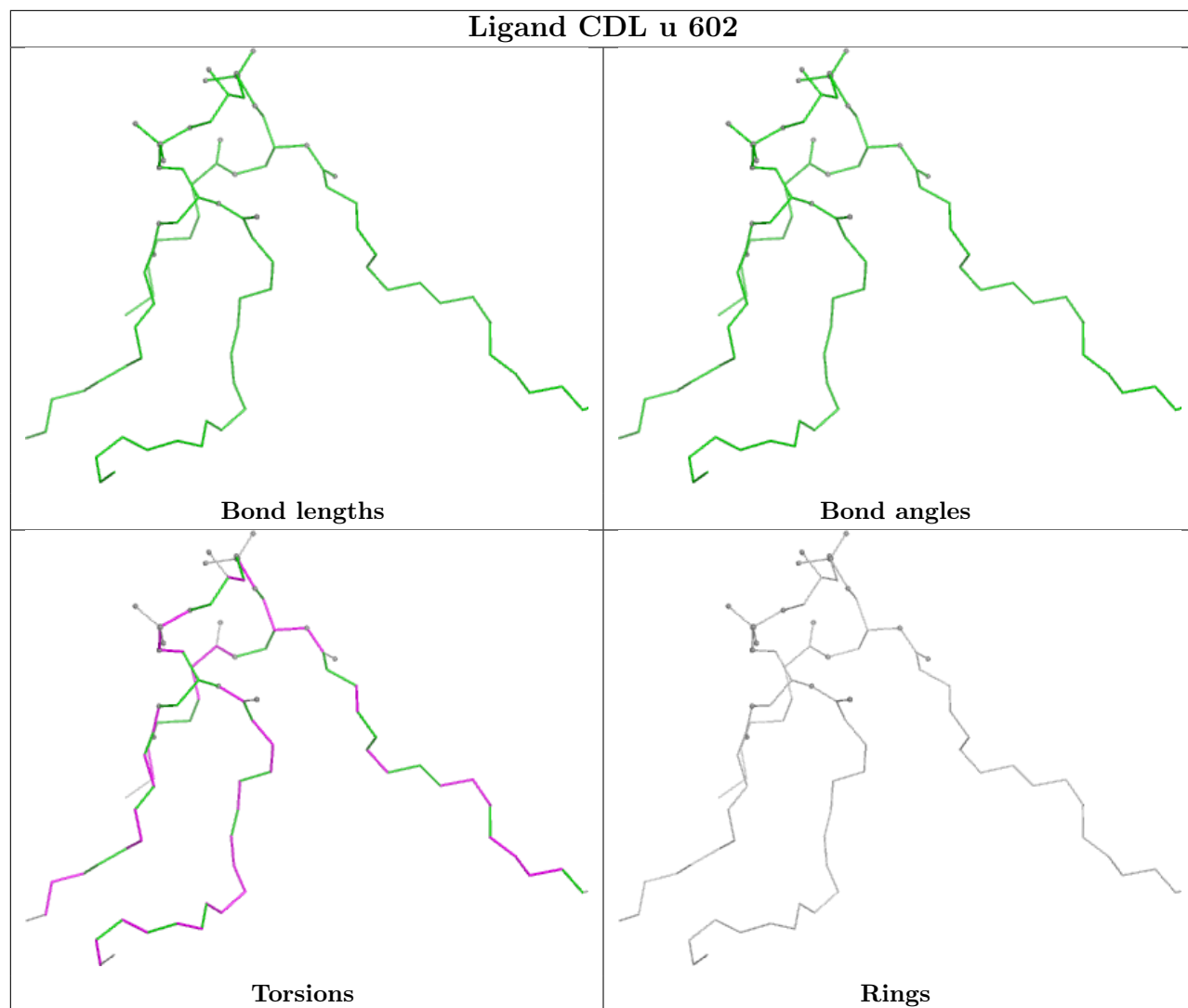


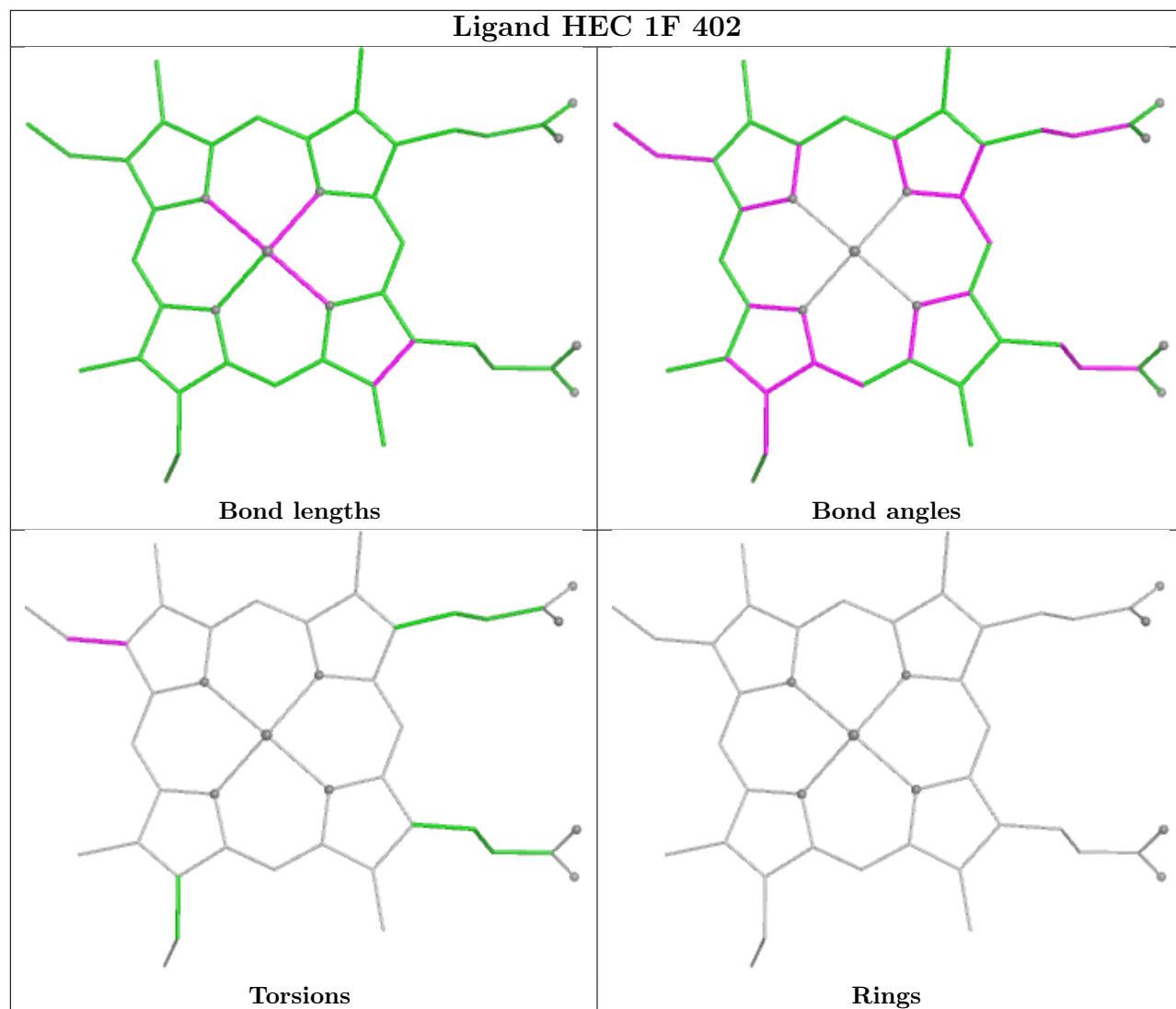
Torsions

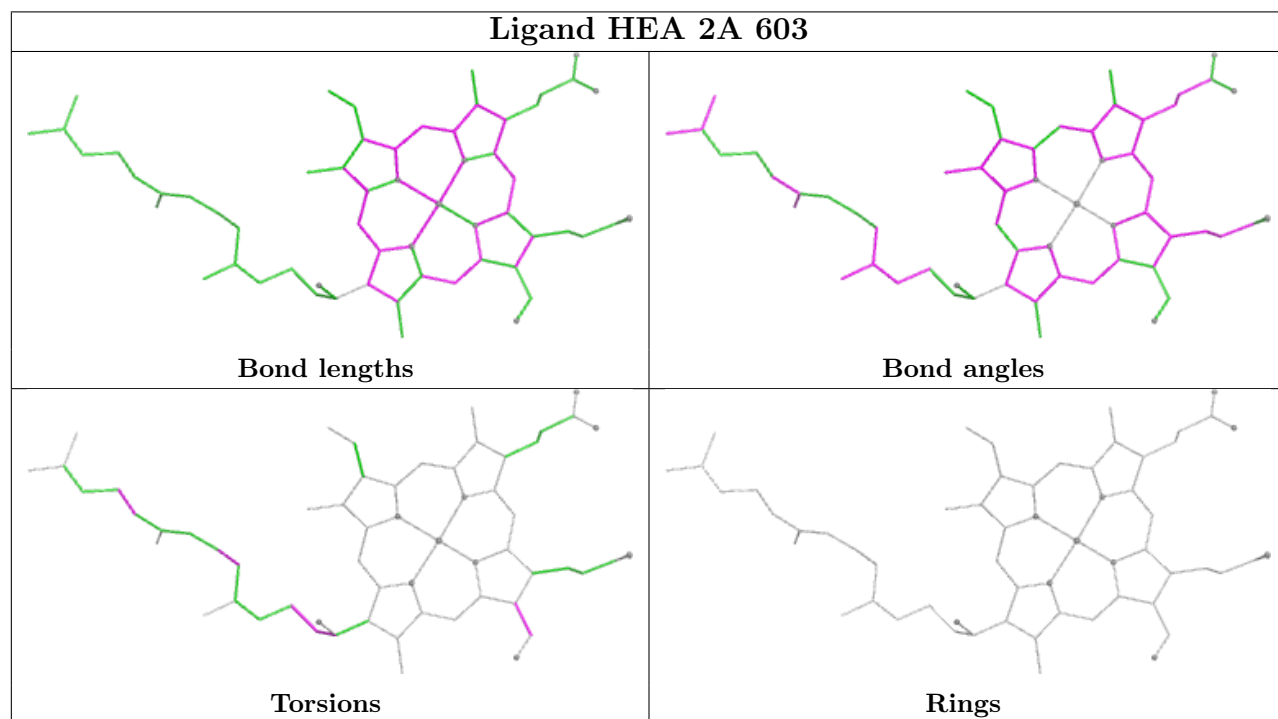
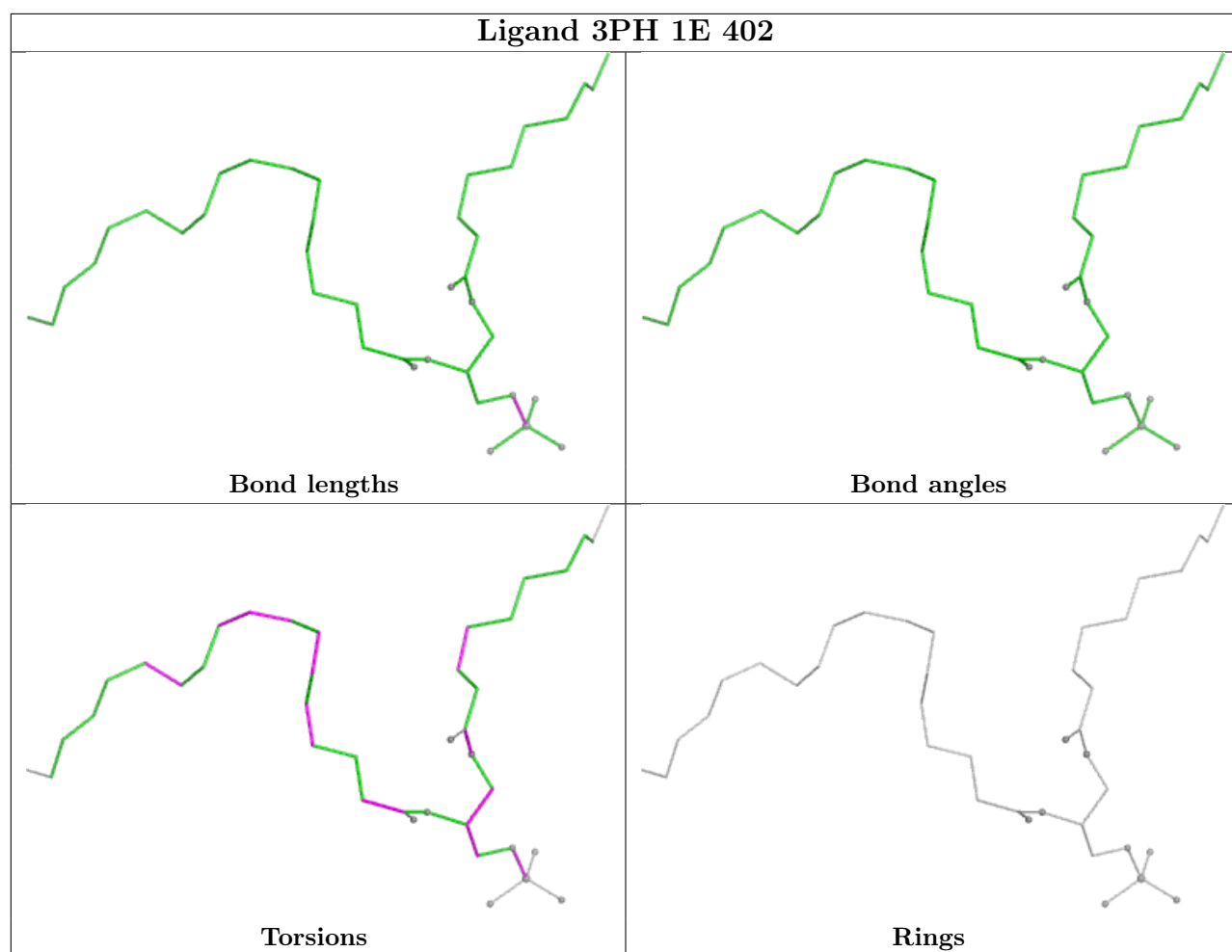


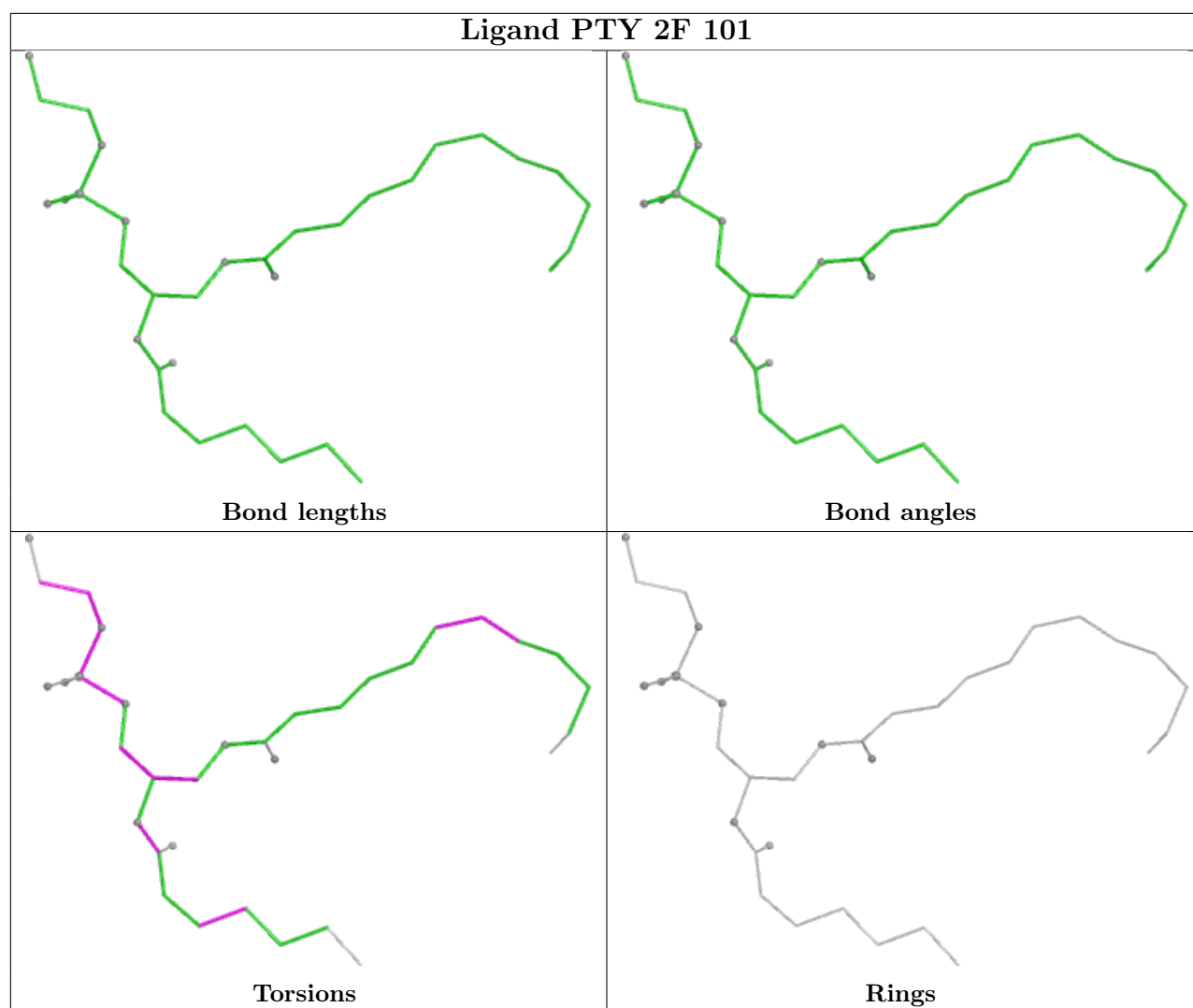
Rings

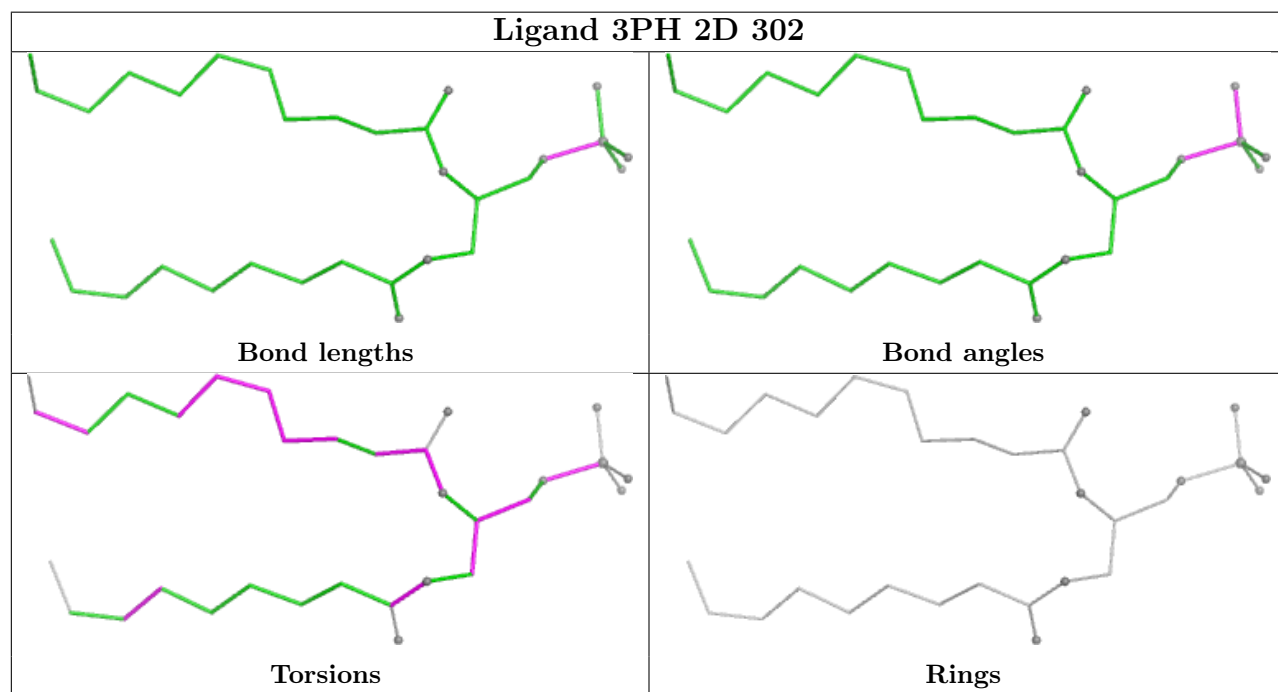
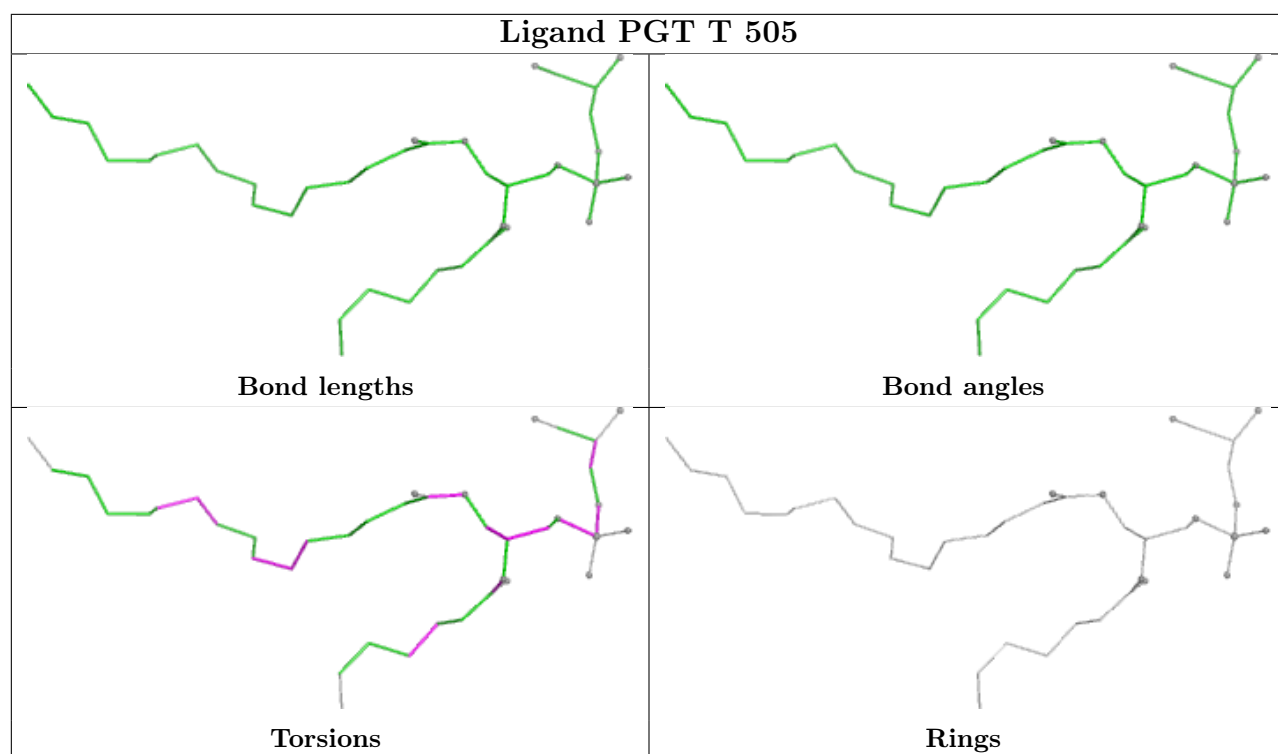


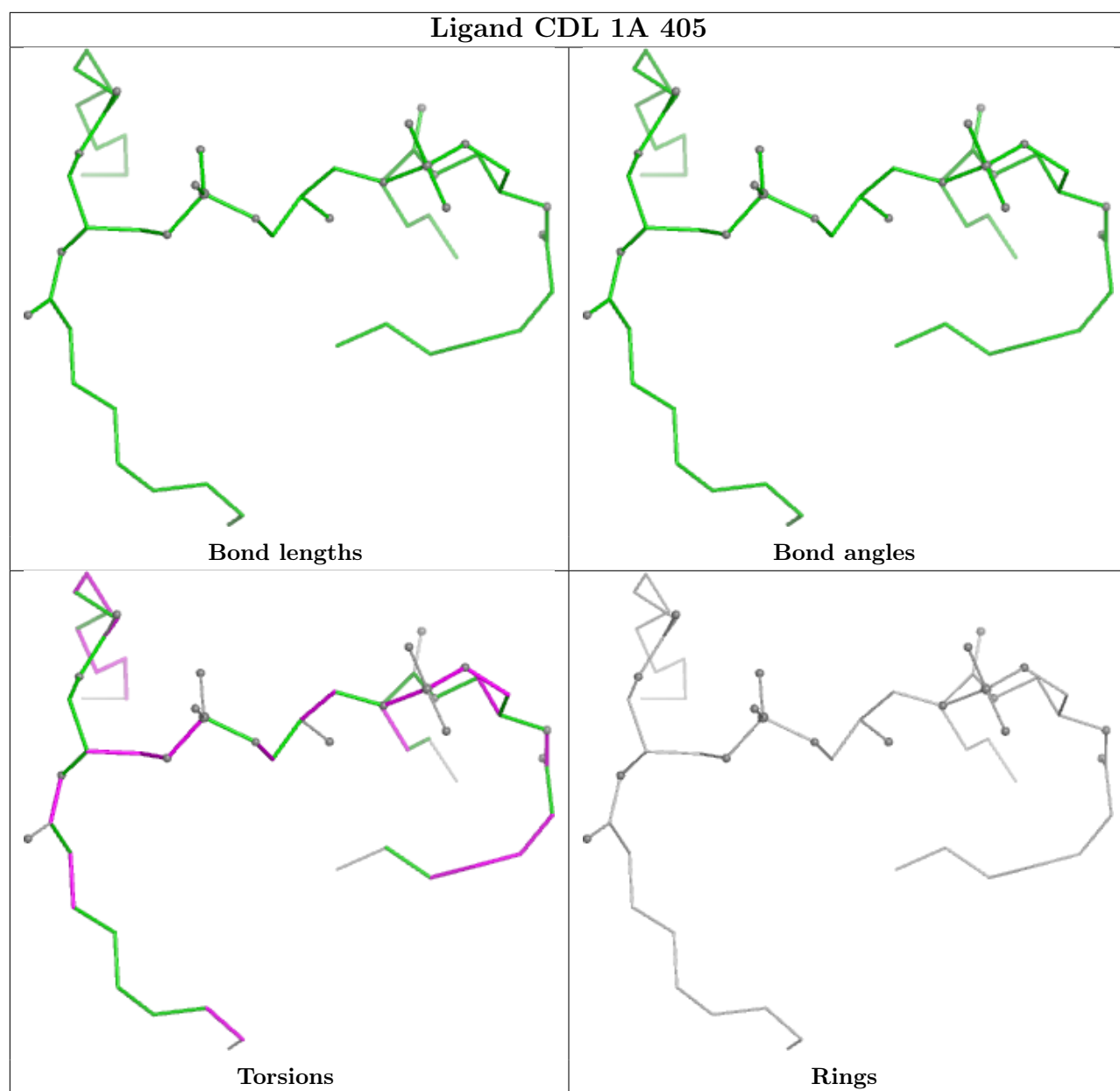


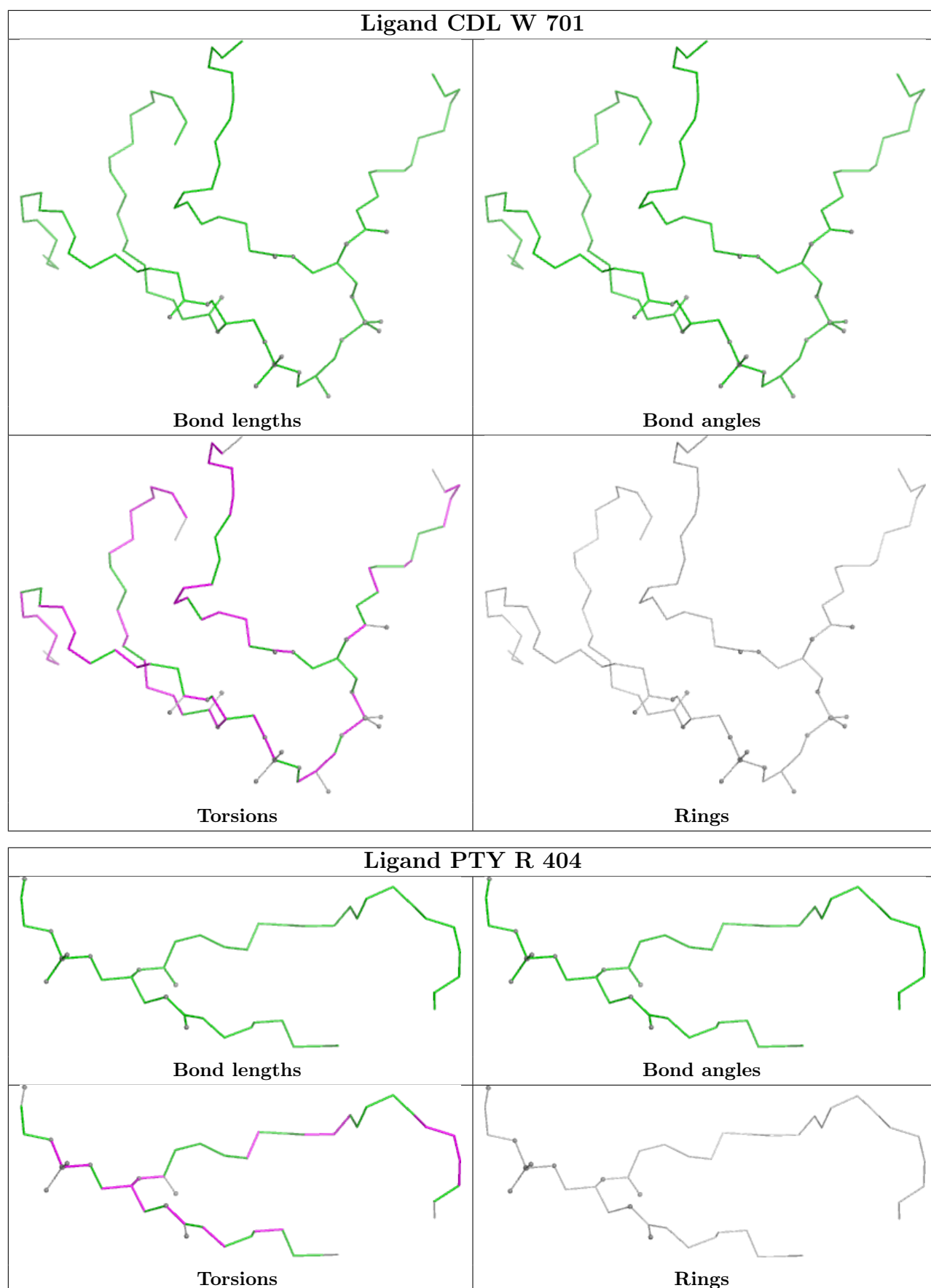


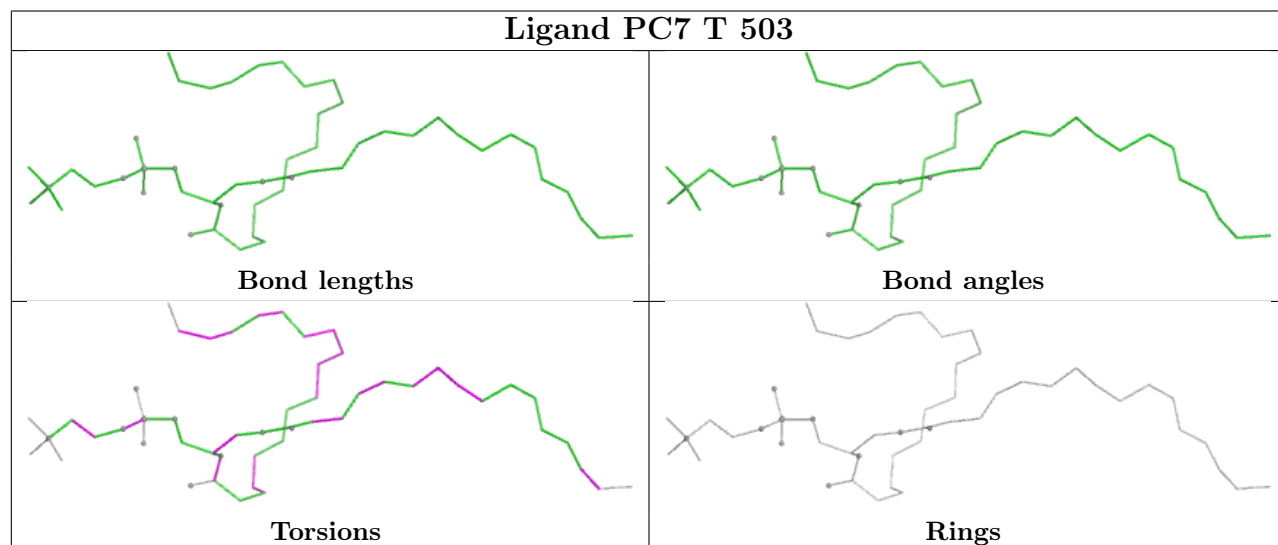
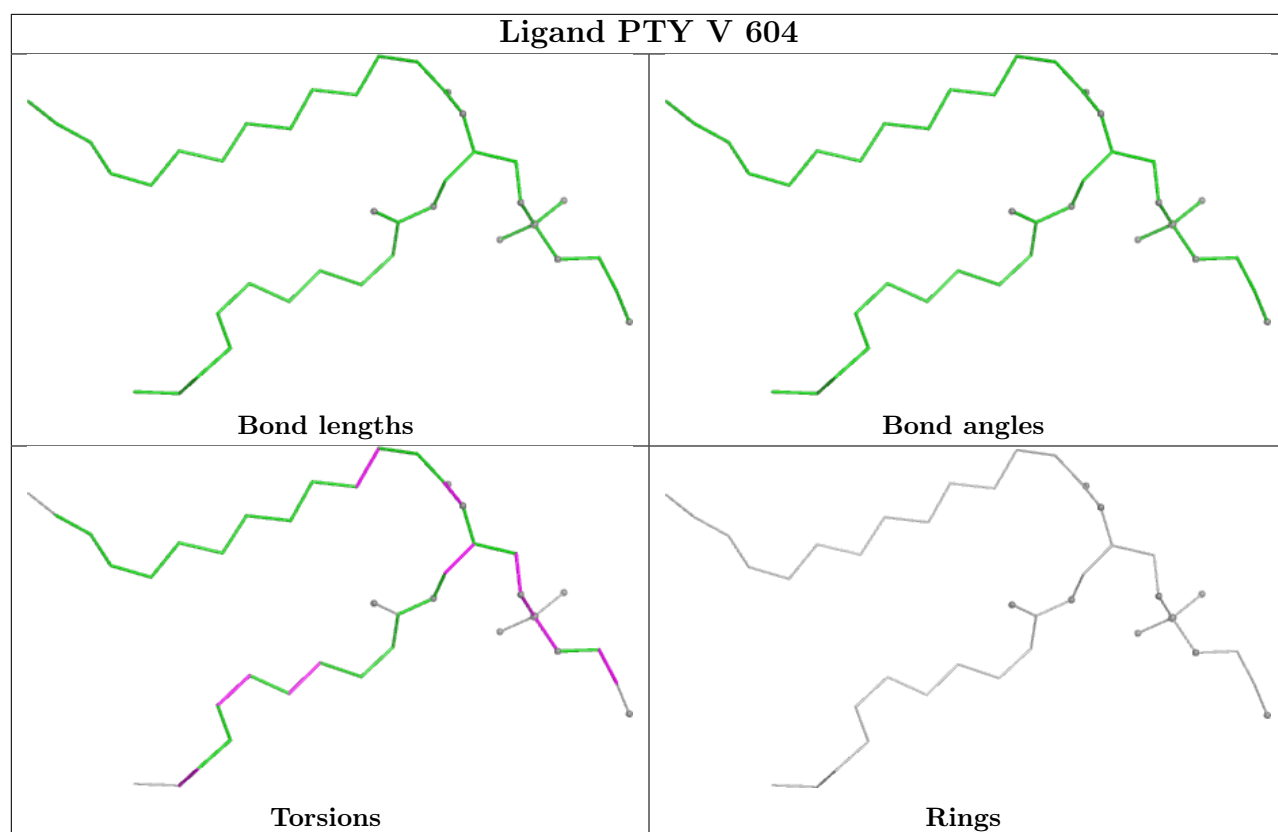


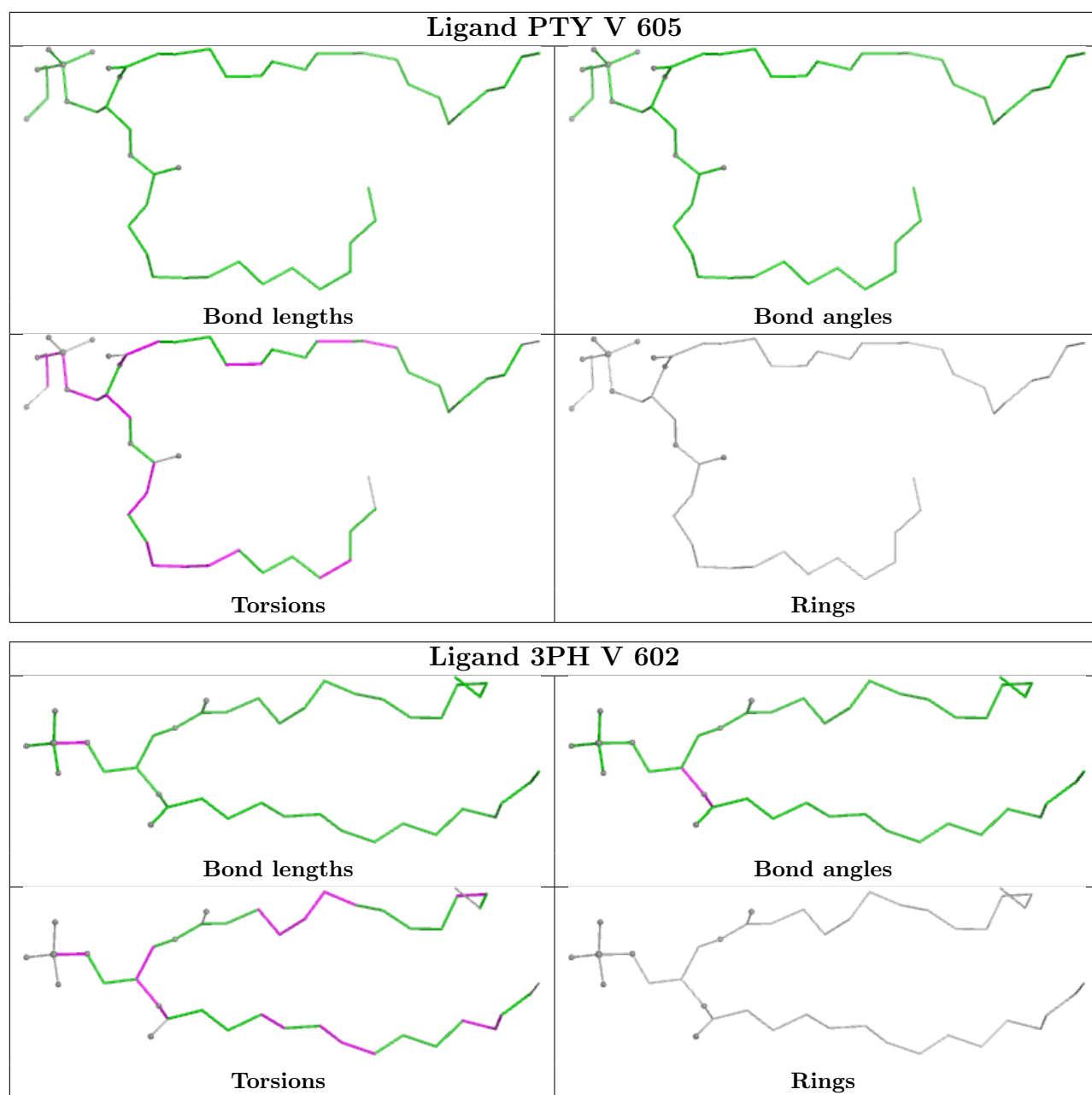


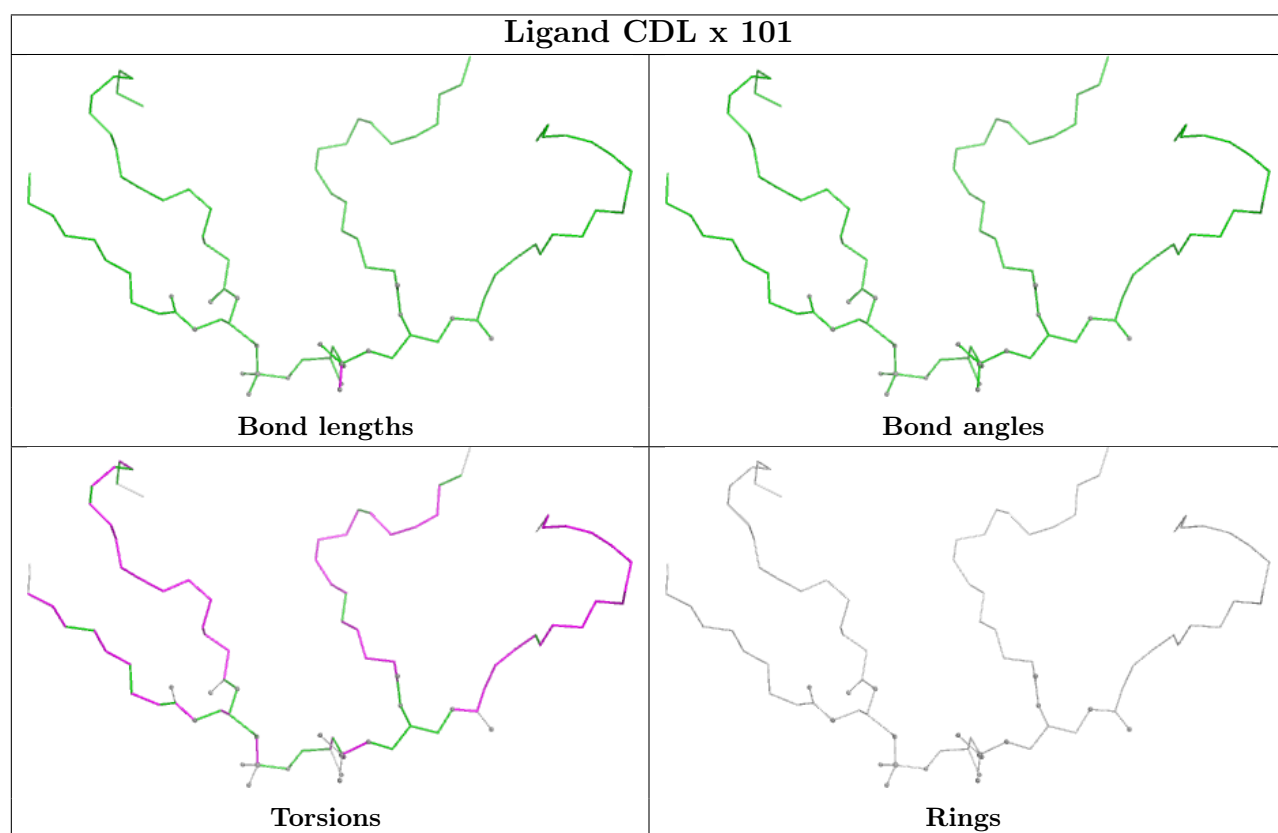
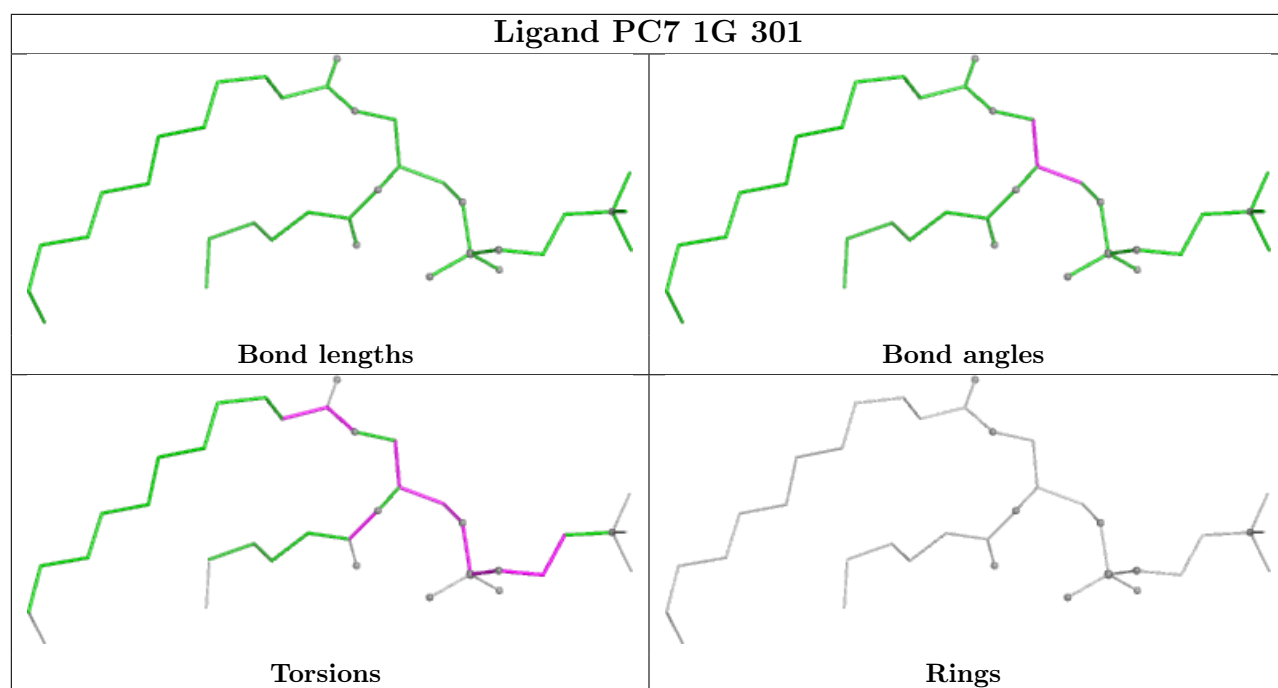


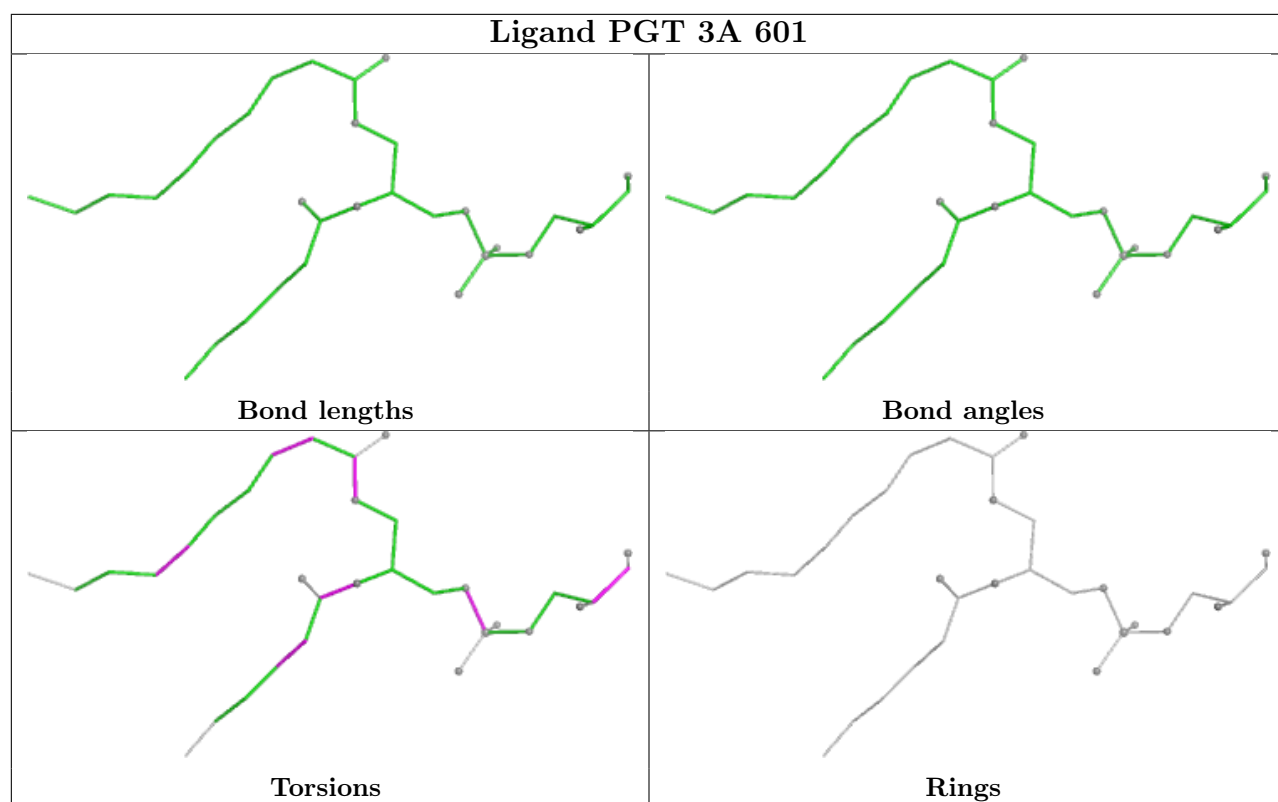


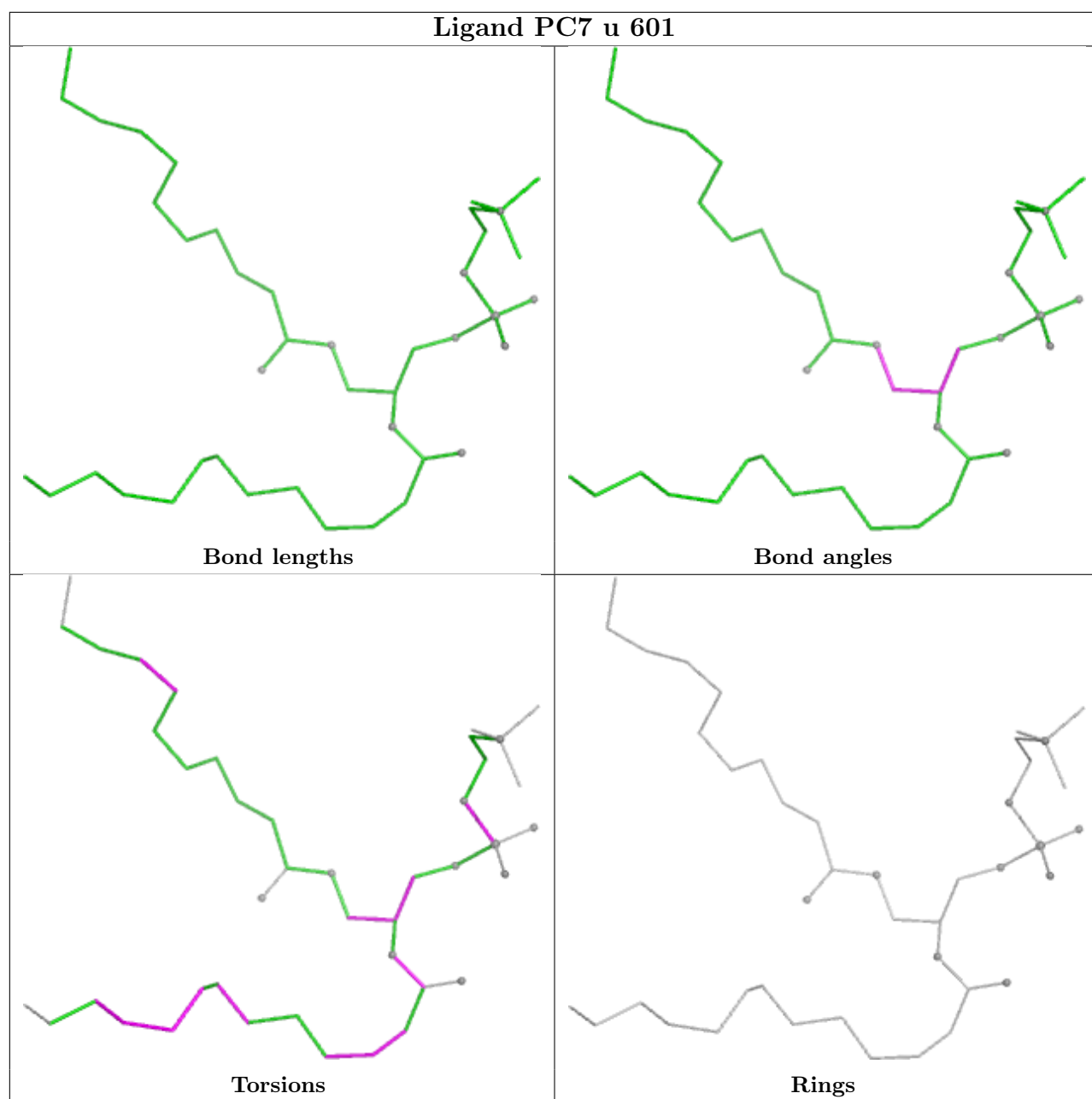


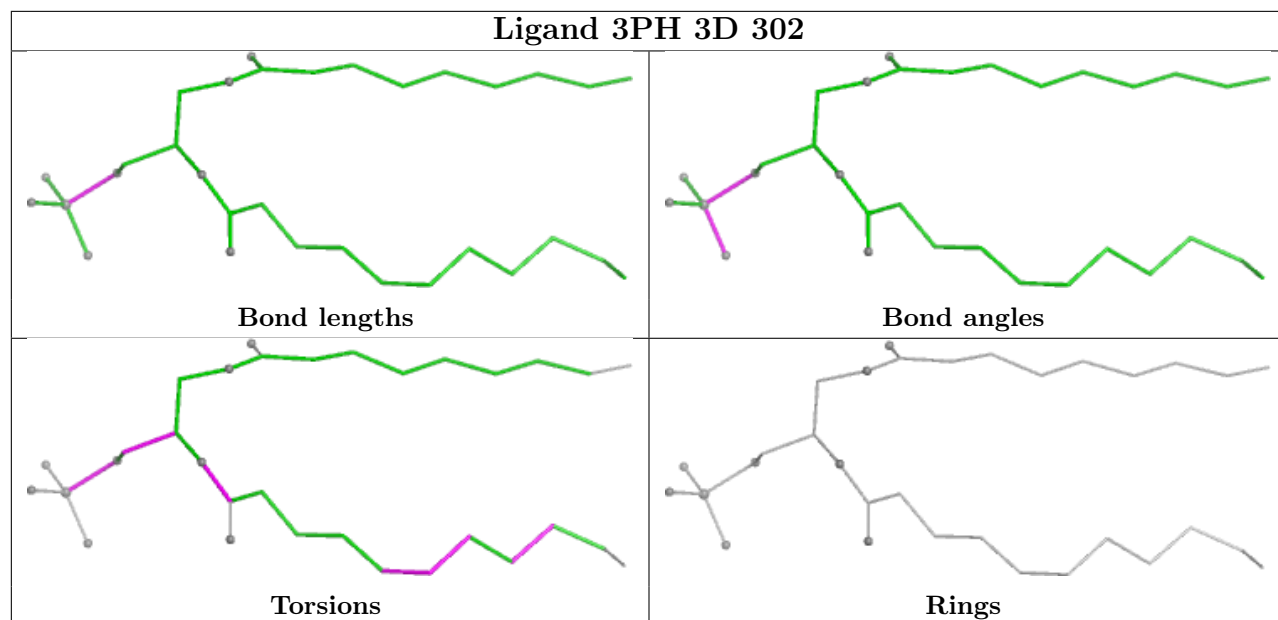


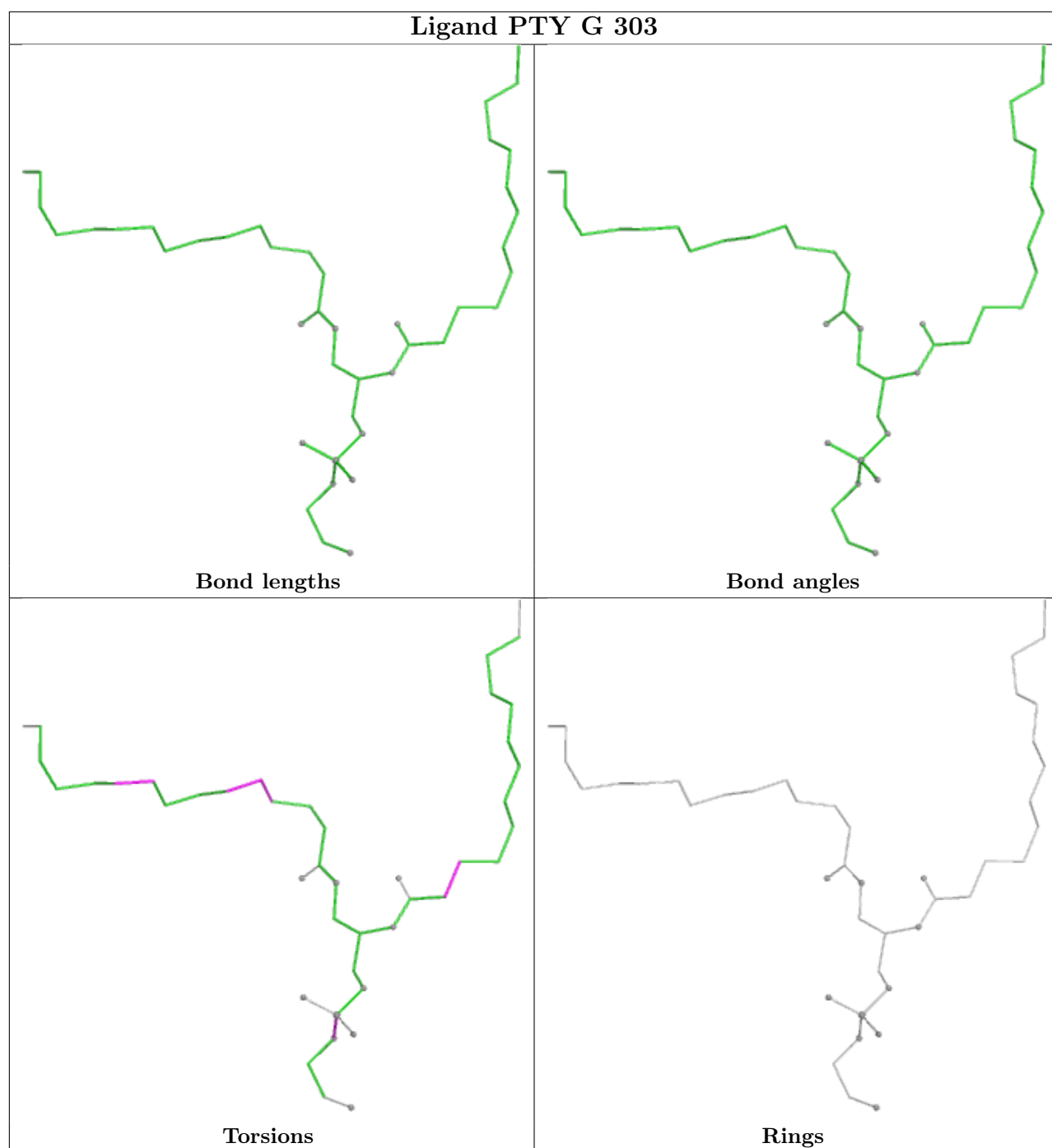


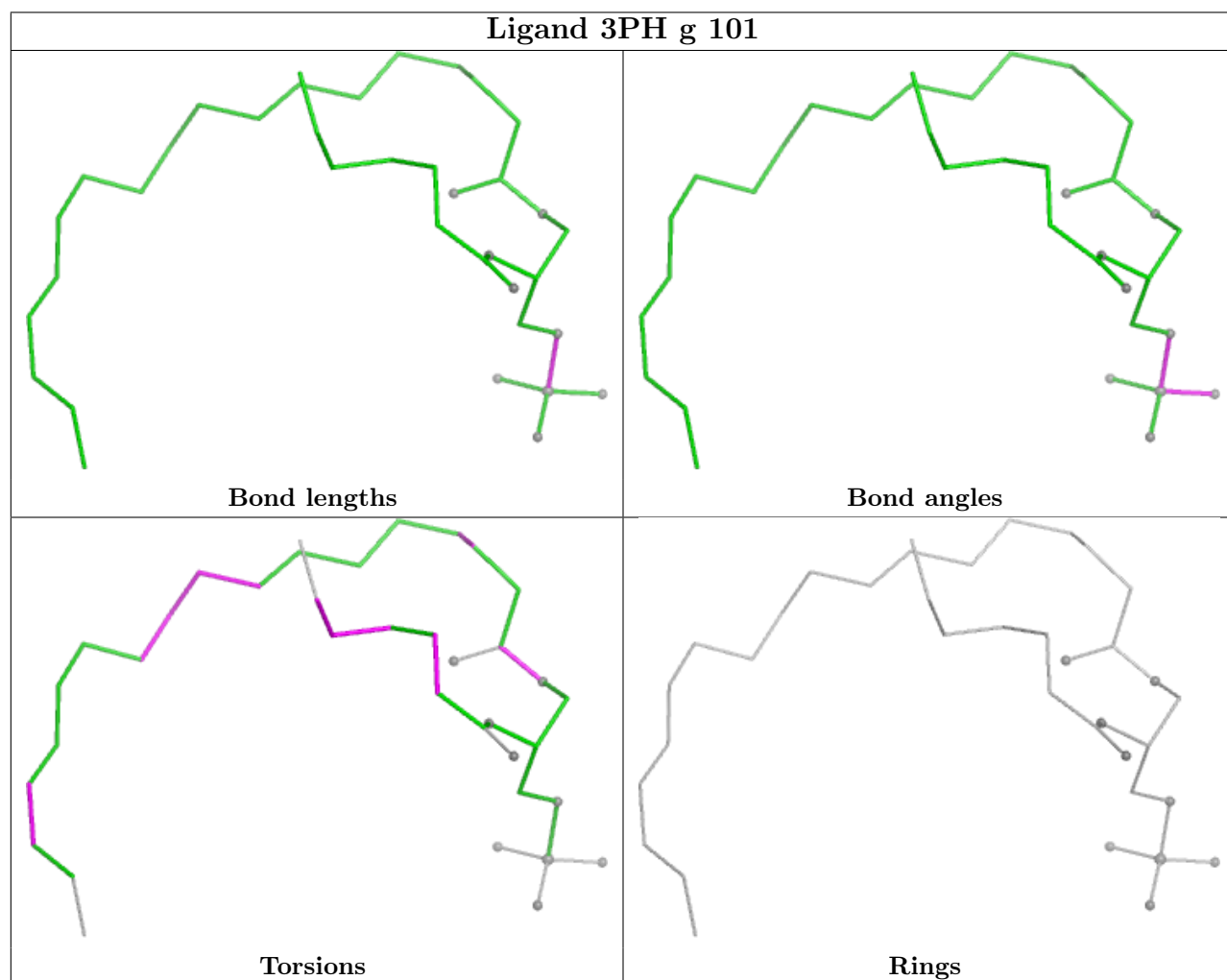
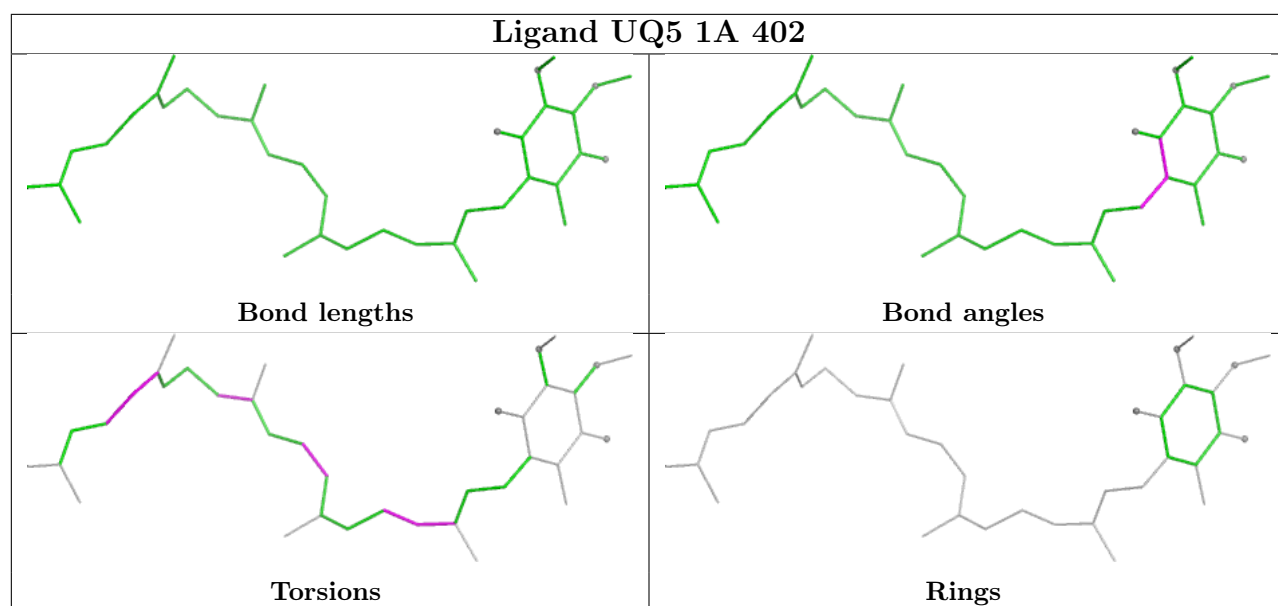


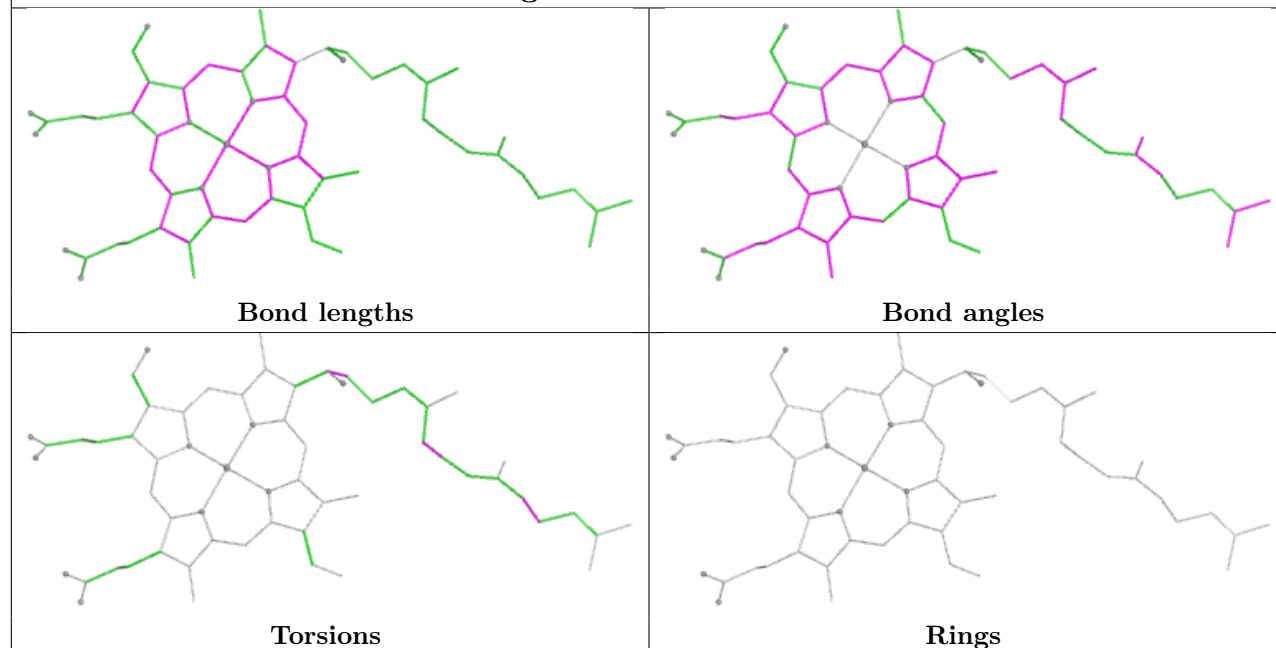
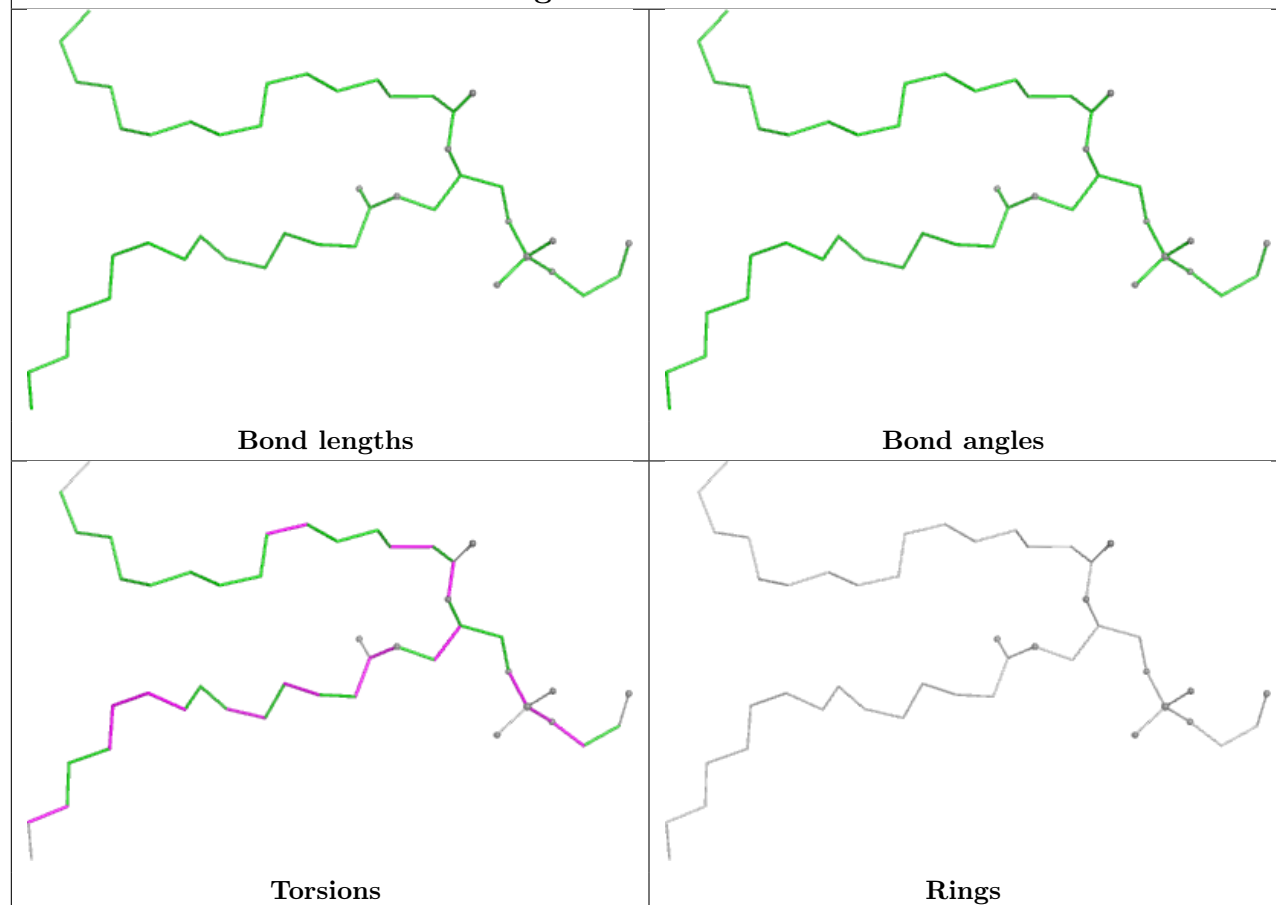


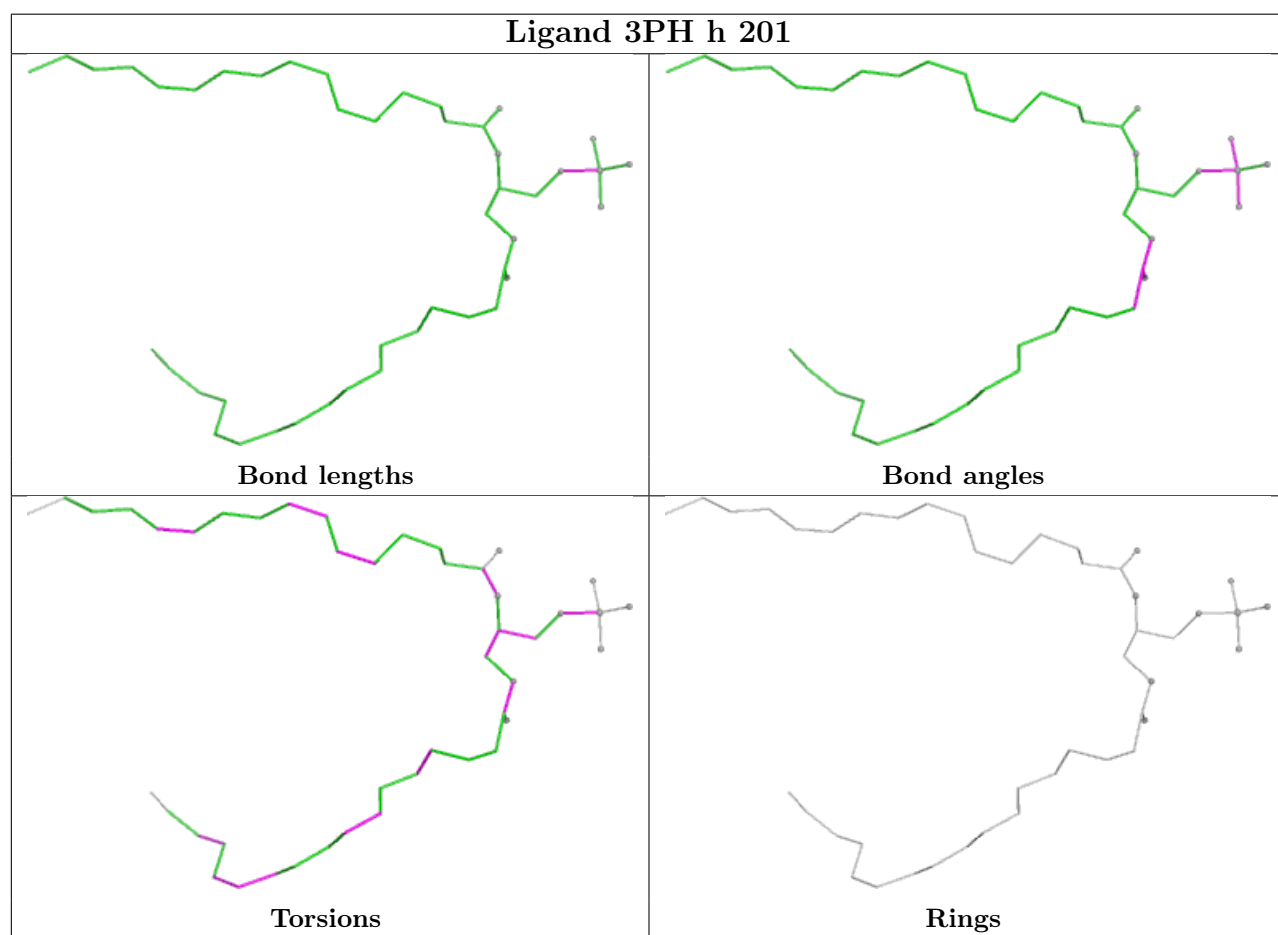
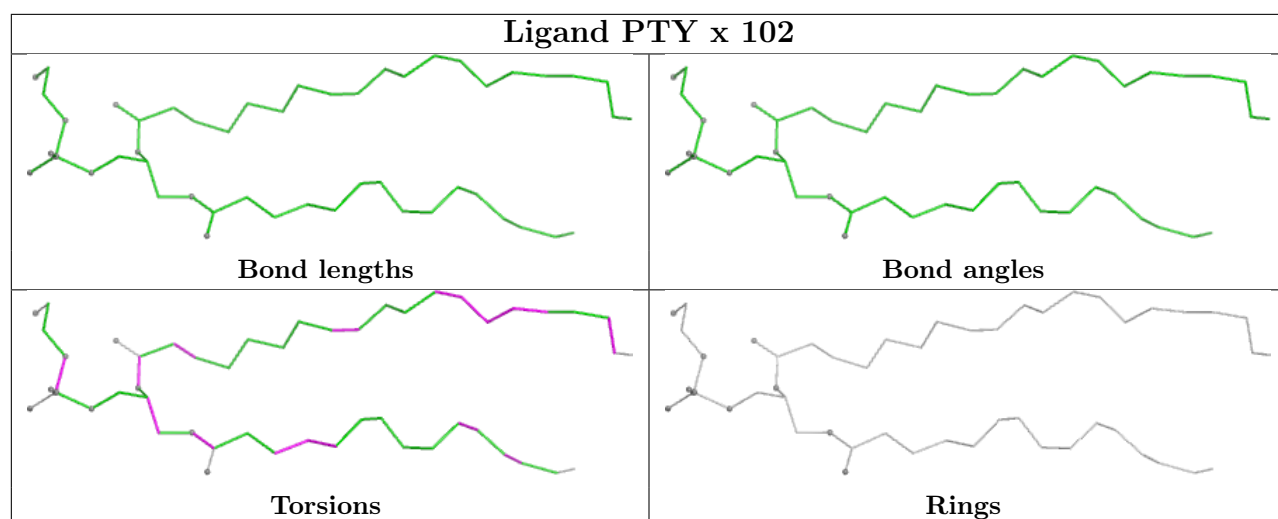


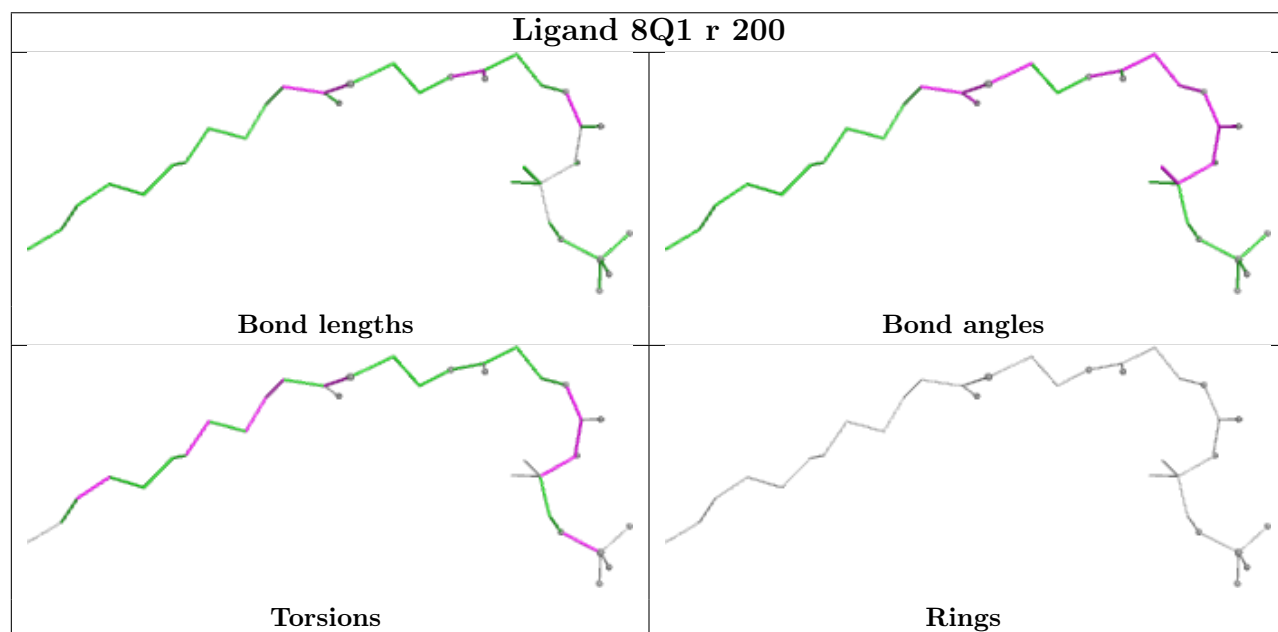
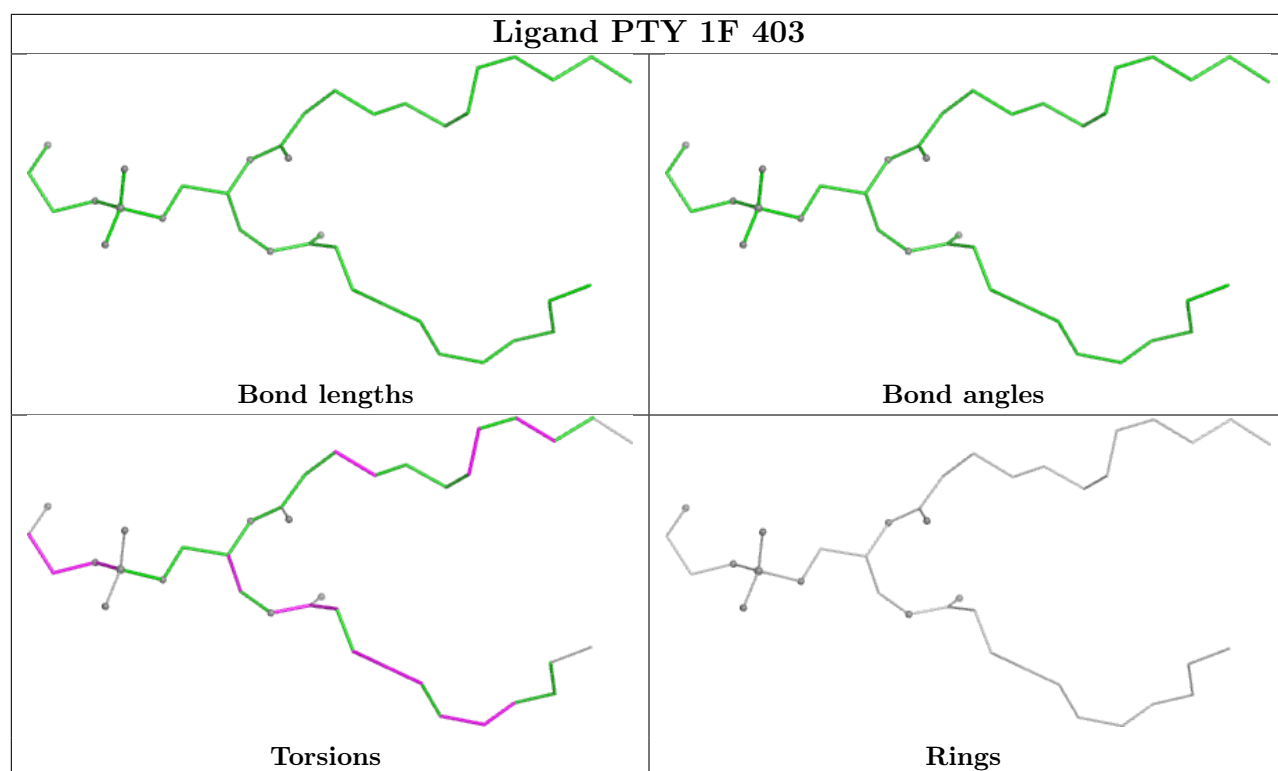


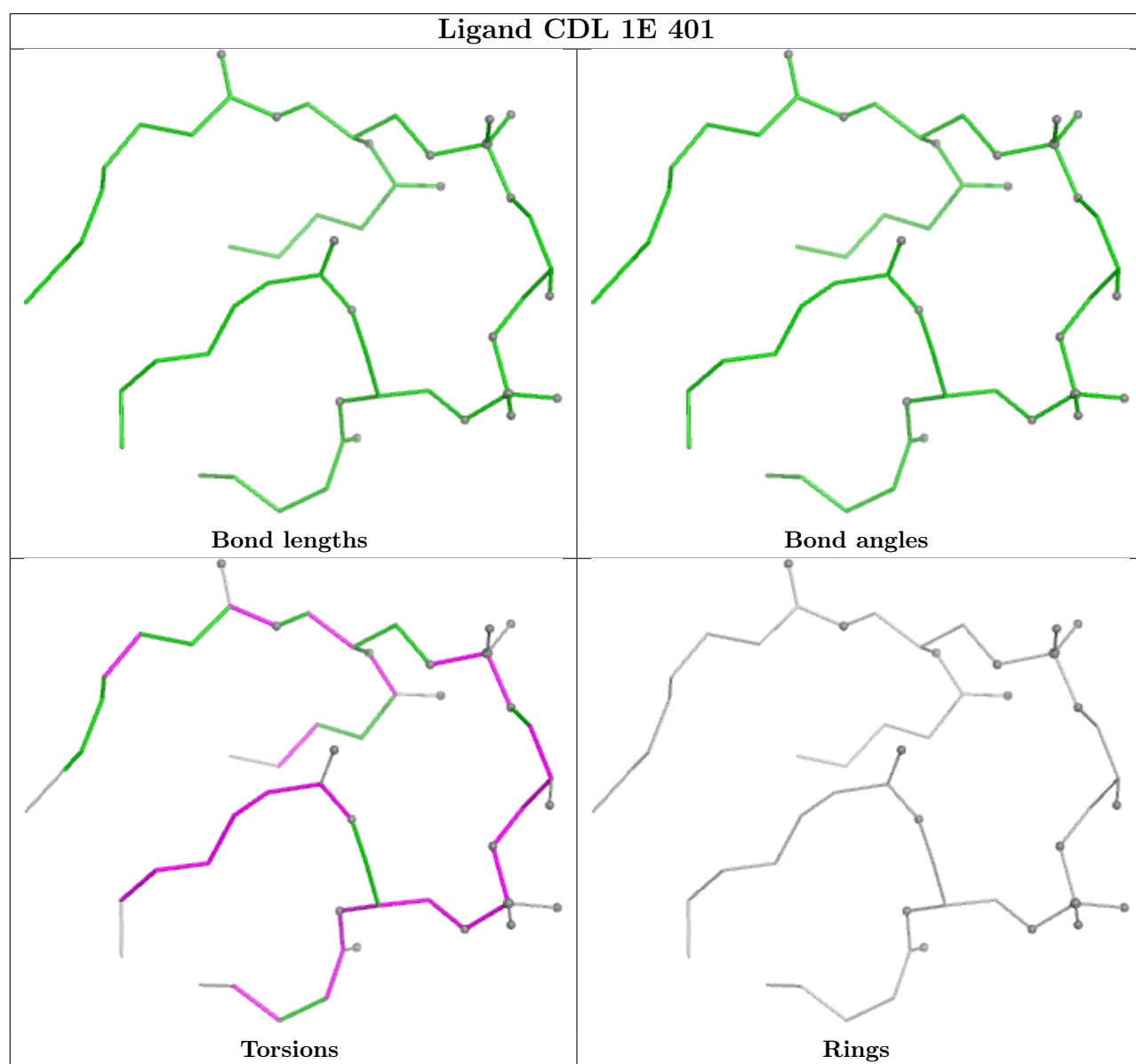
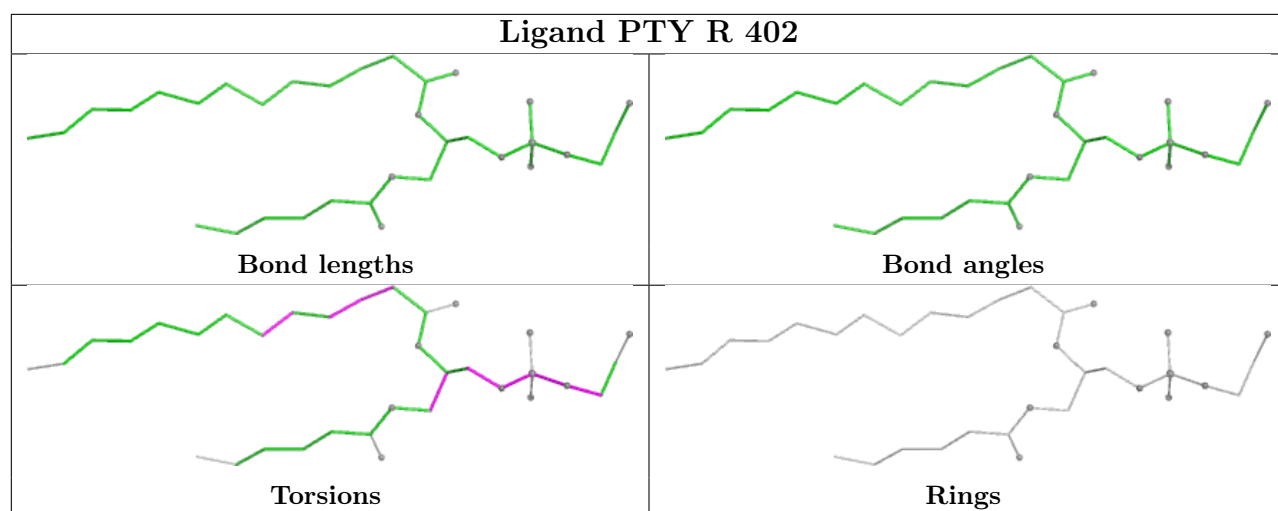


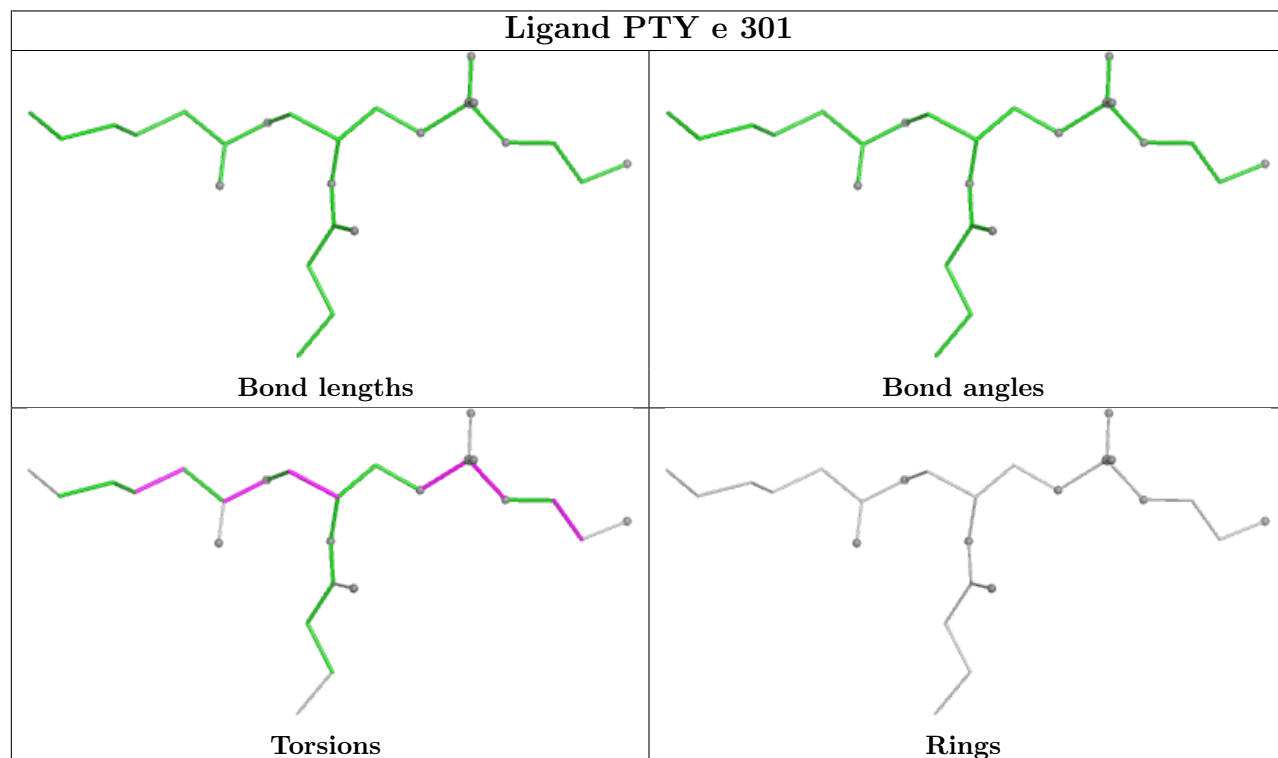
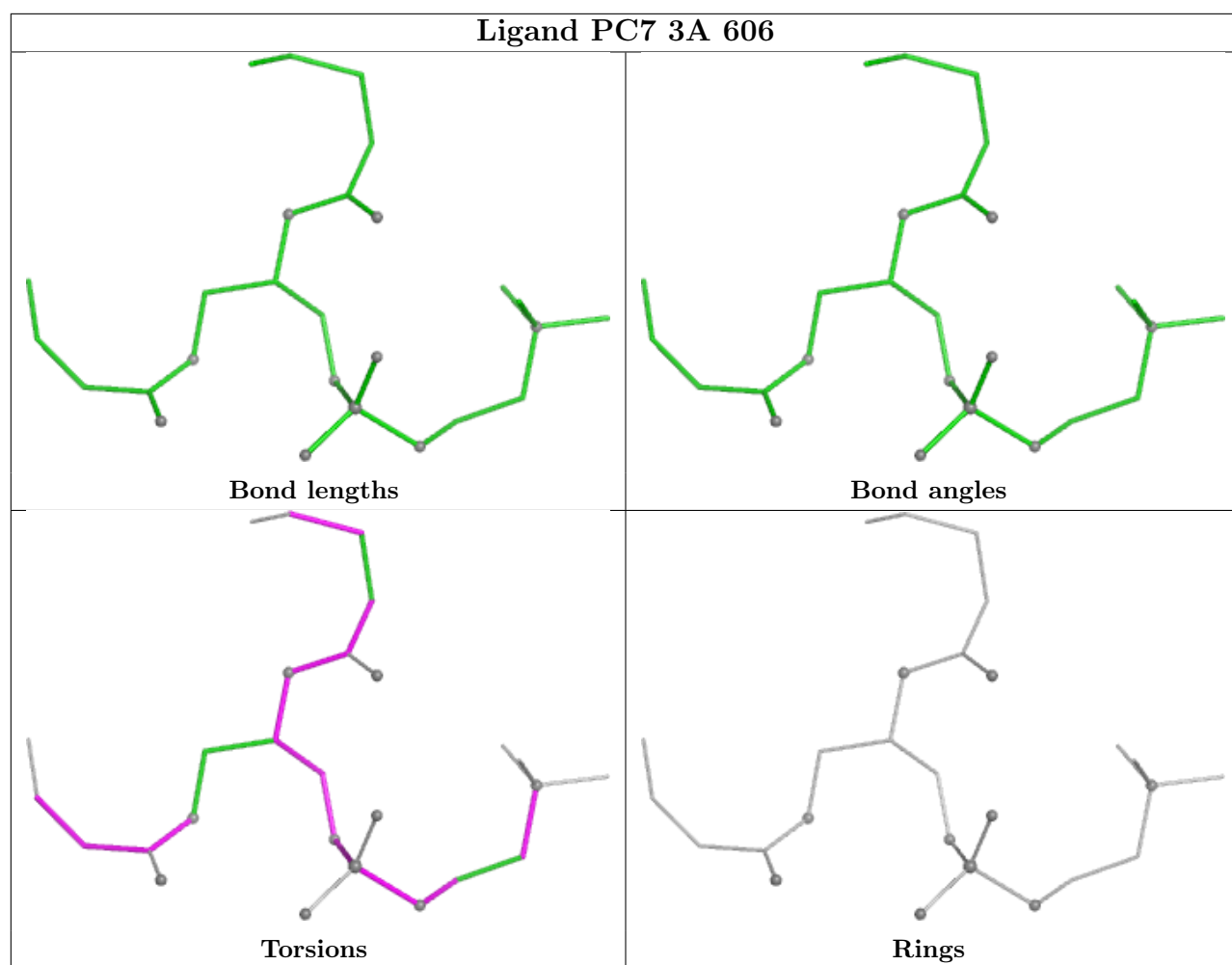


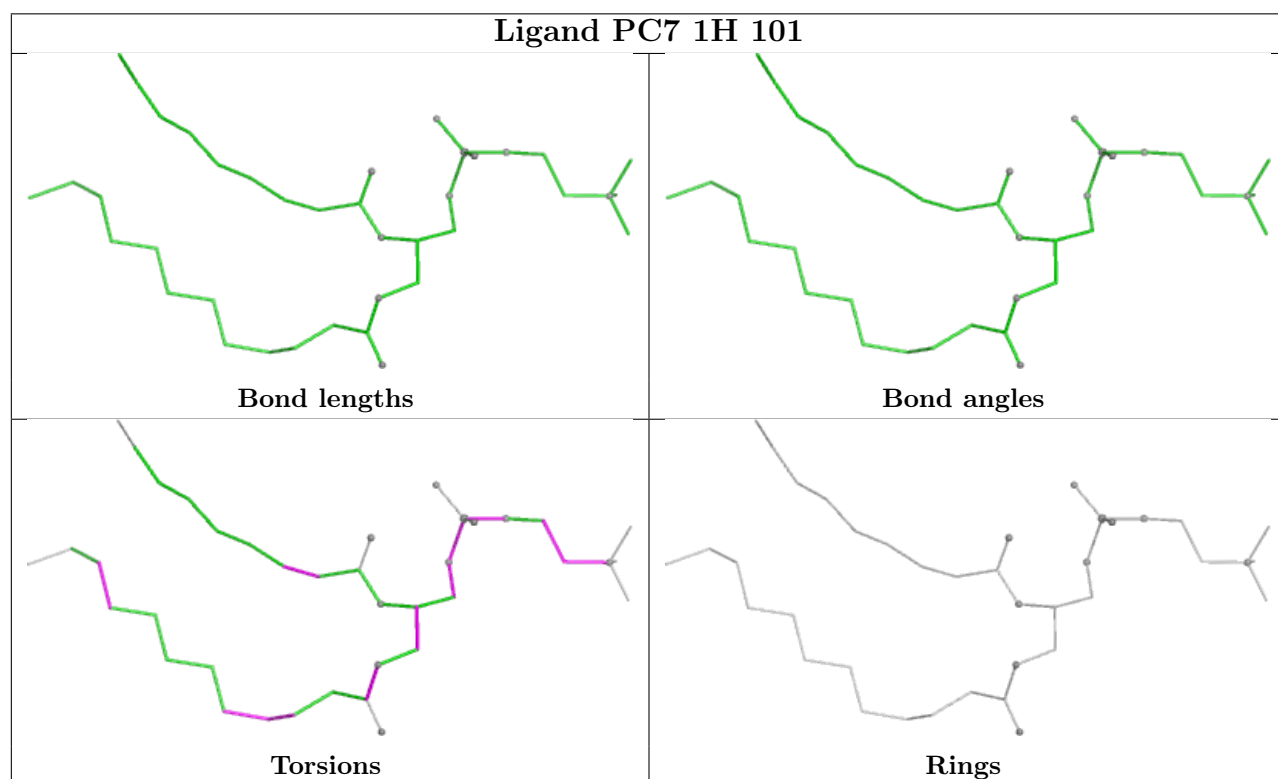
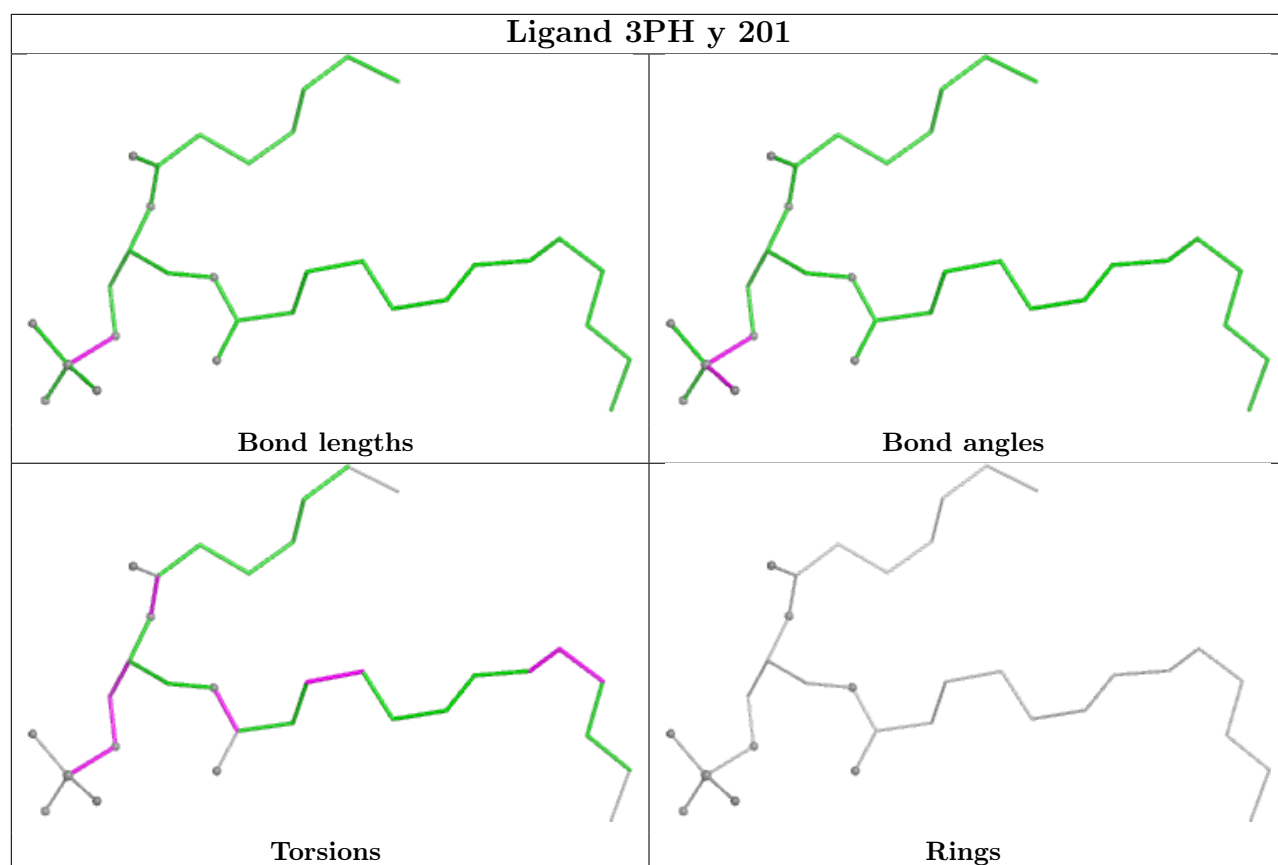
Ligand HEA 3A 603**Ligand PTY h 202**

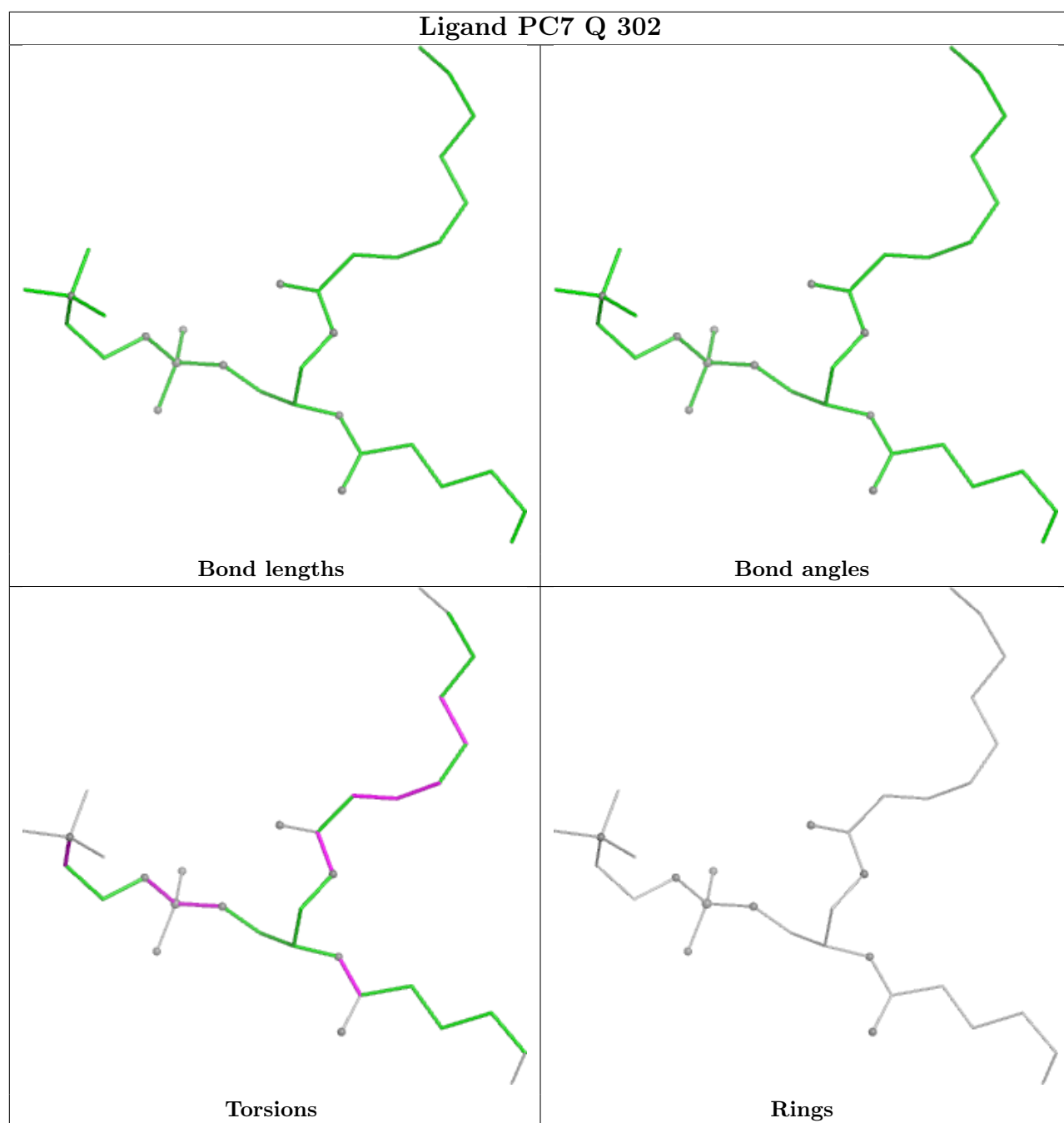


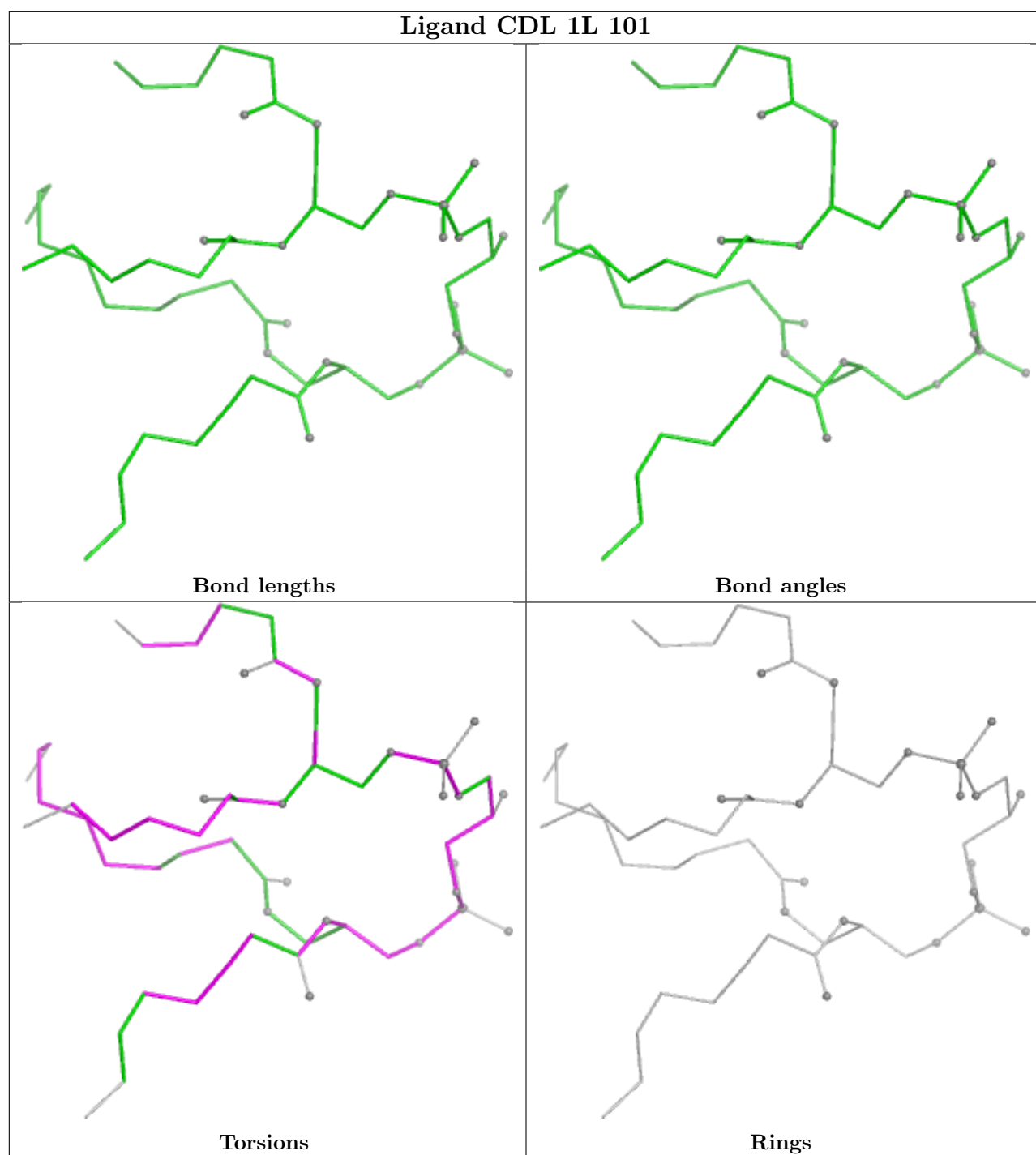


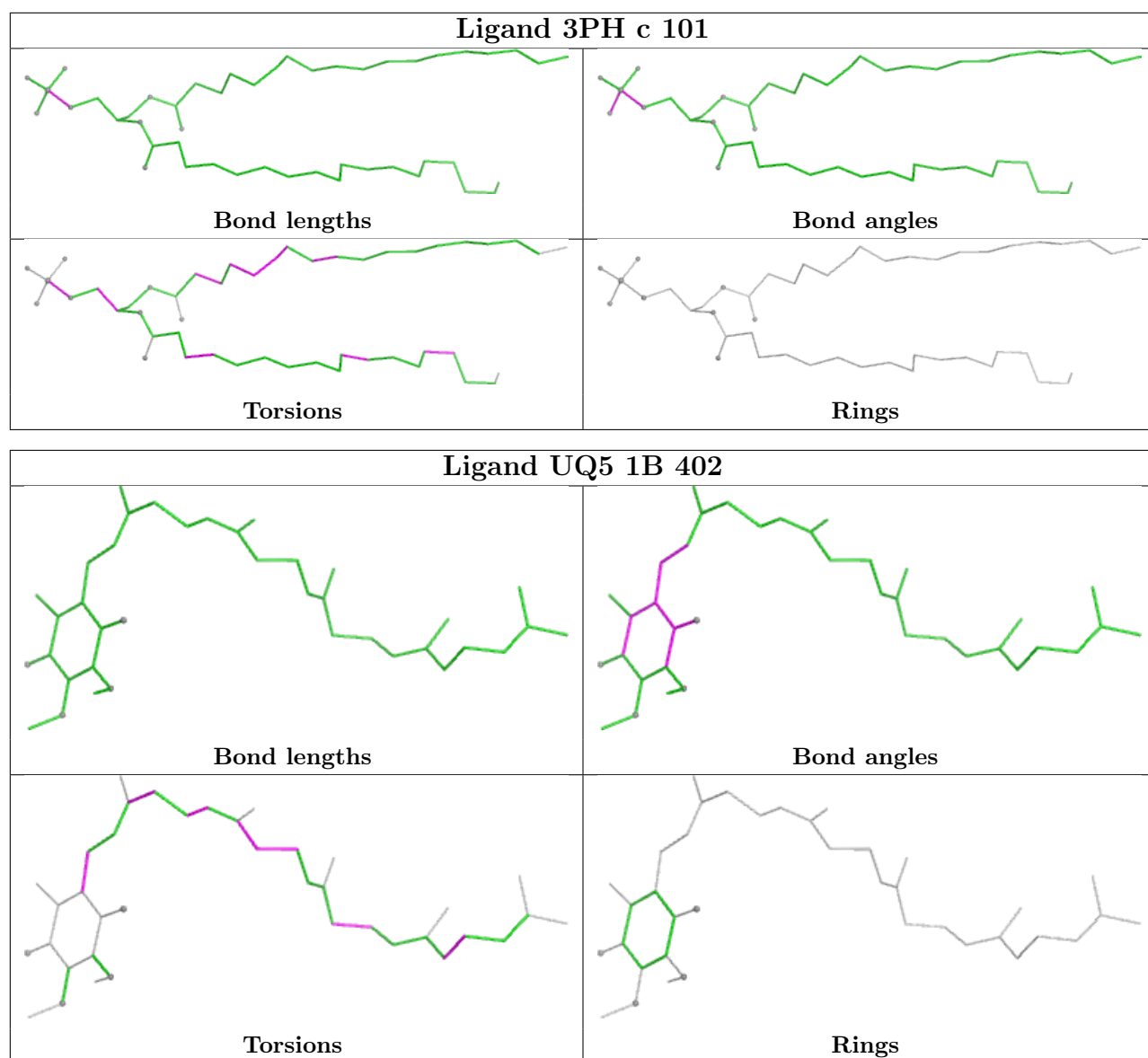


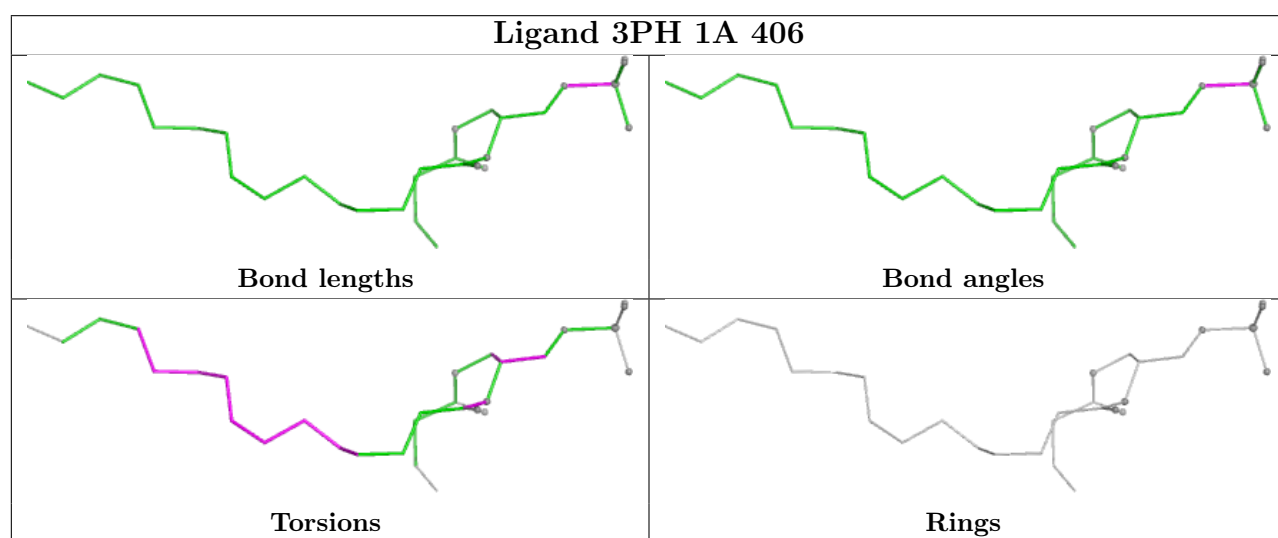
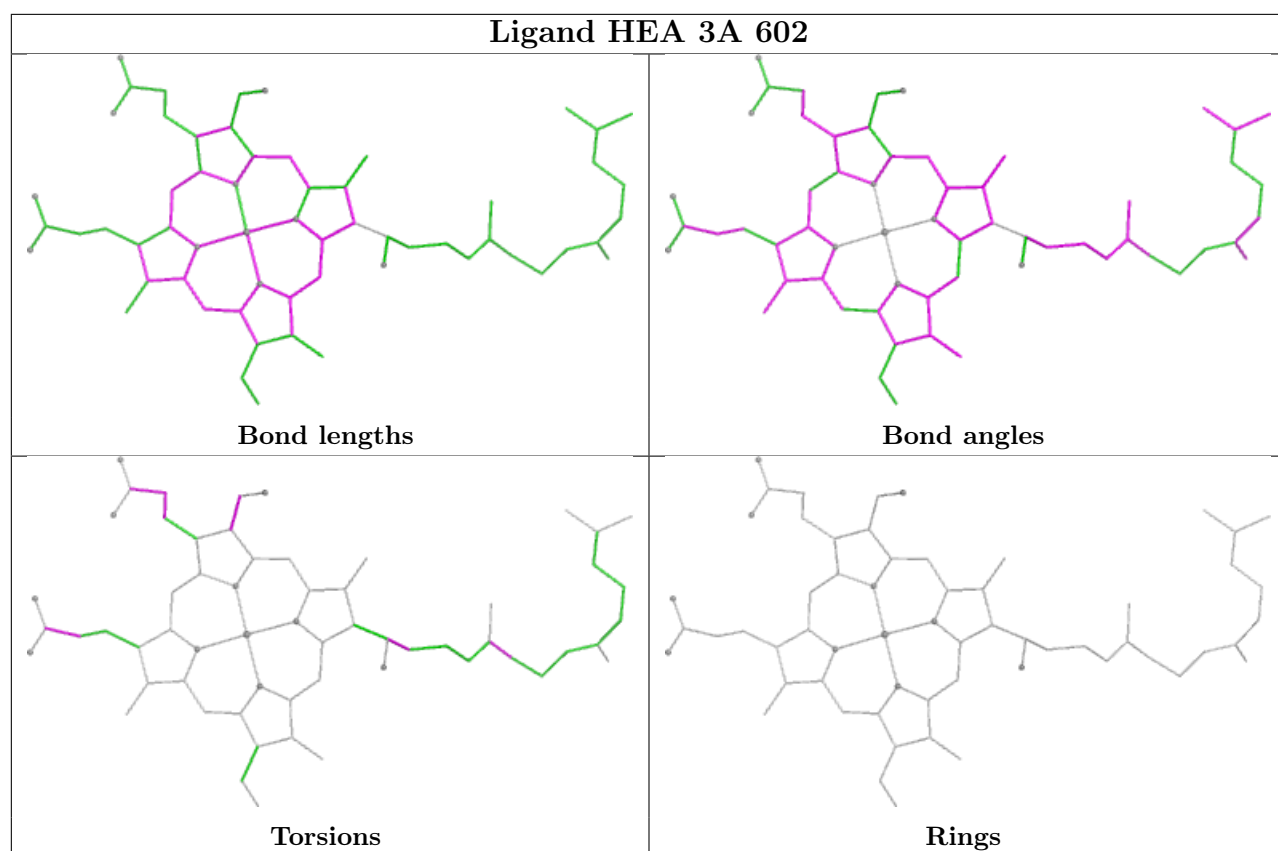


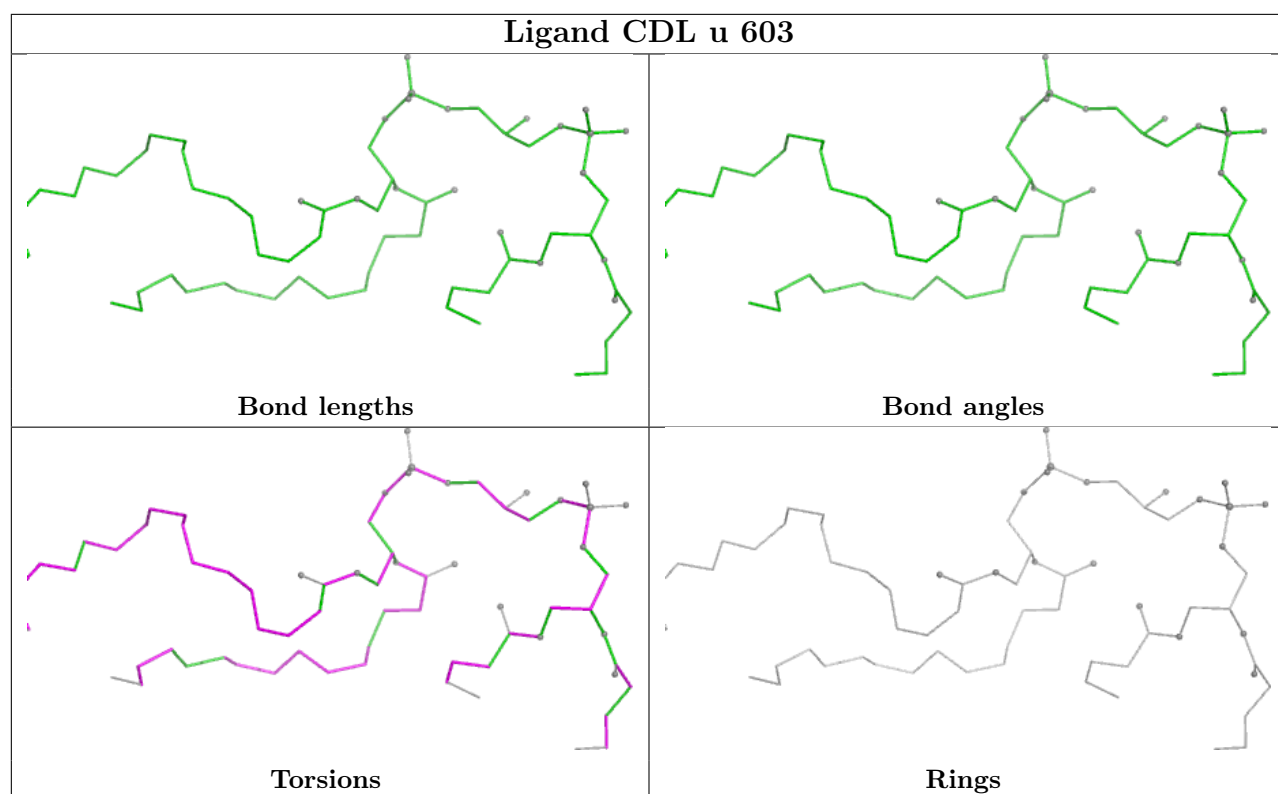




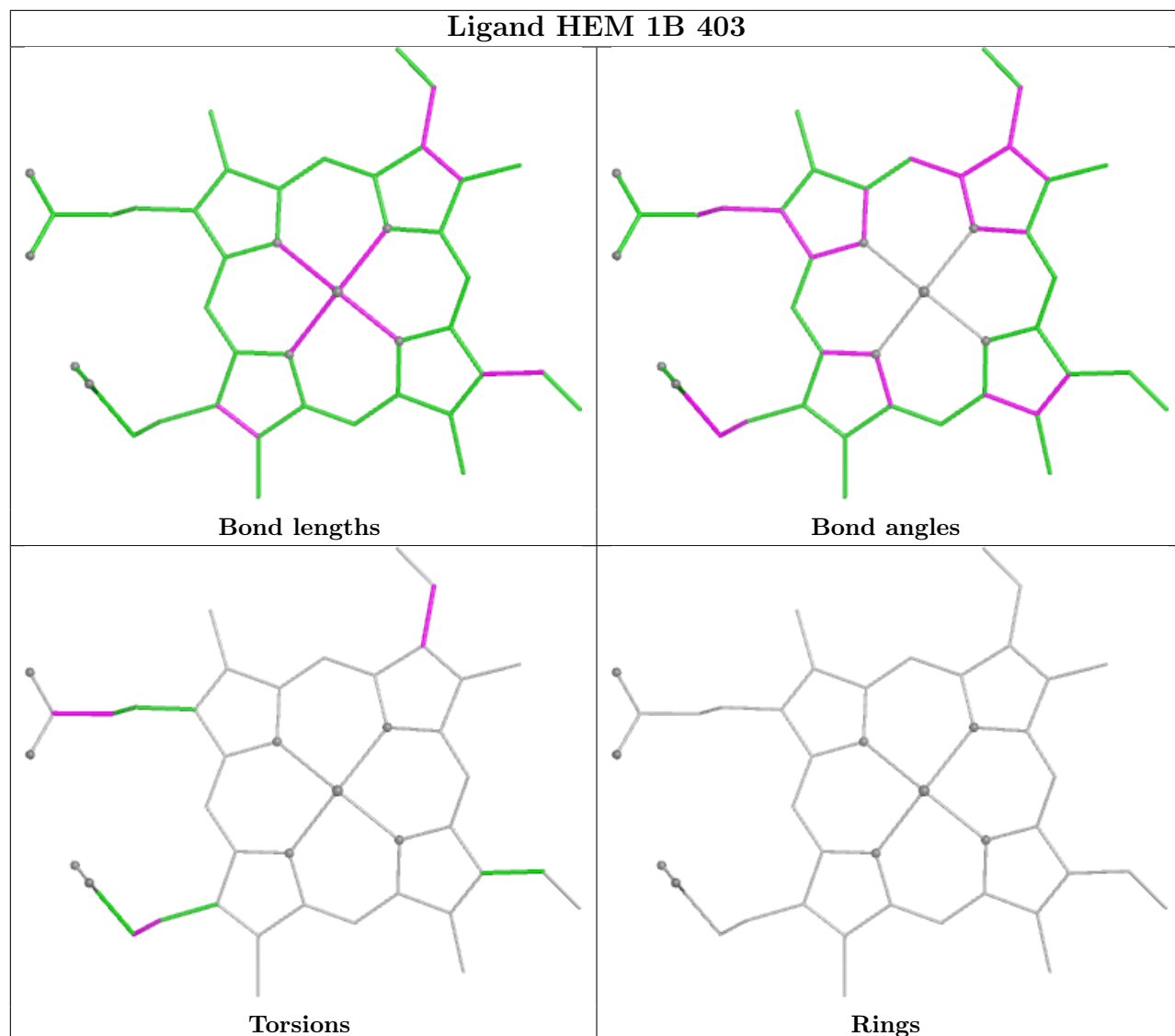


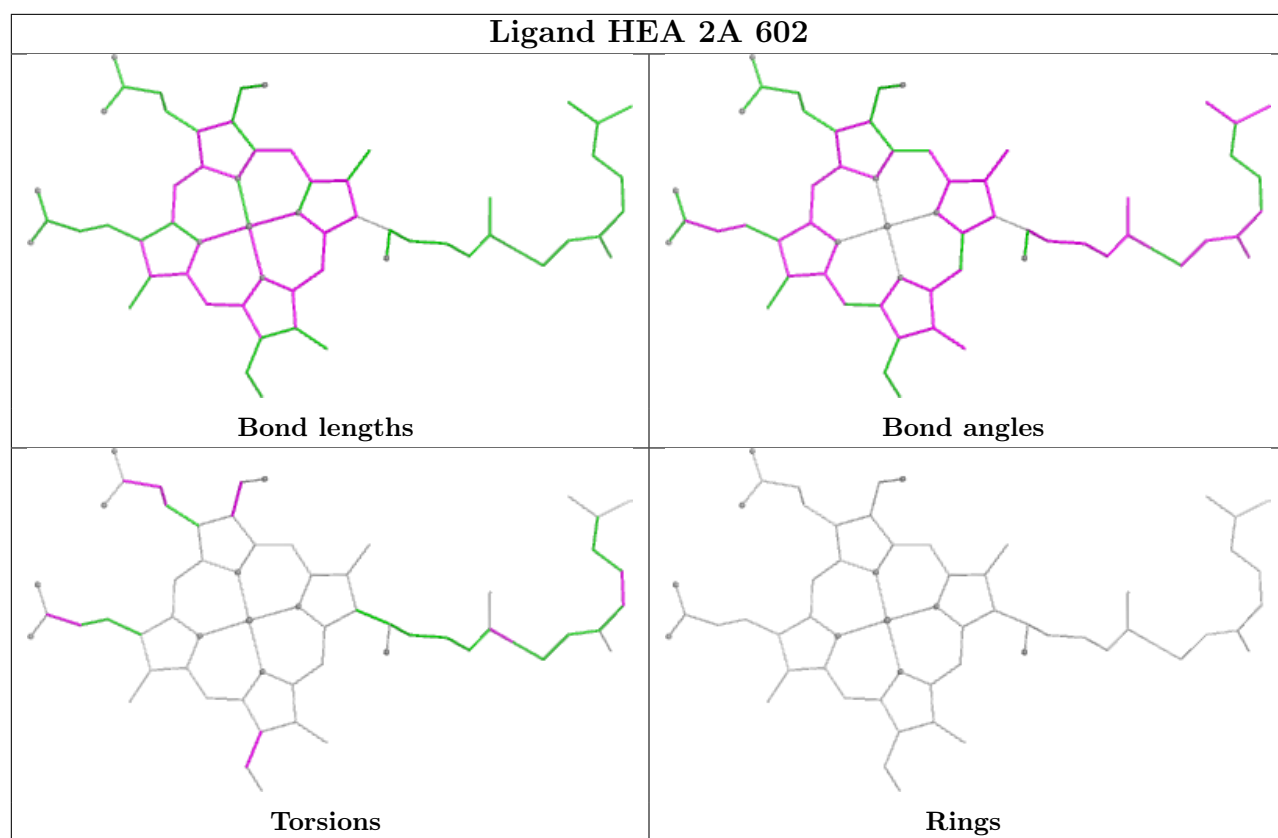


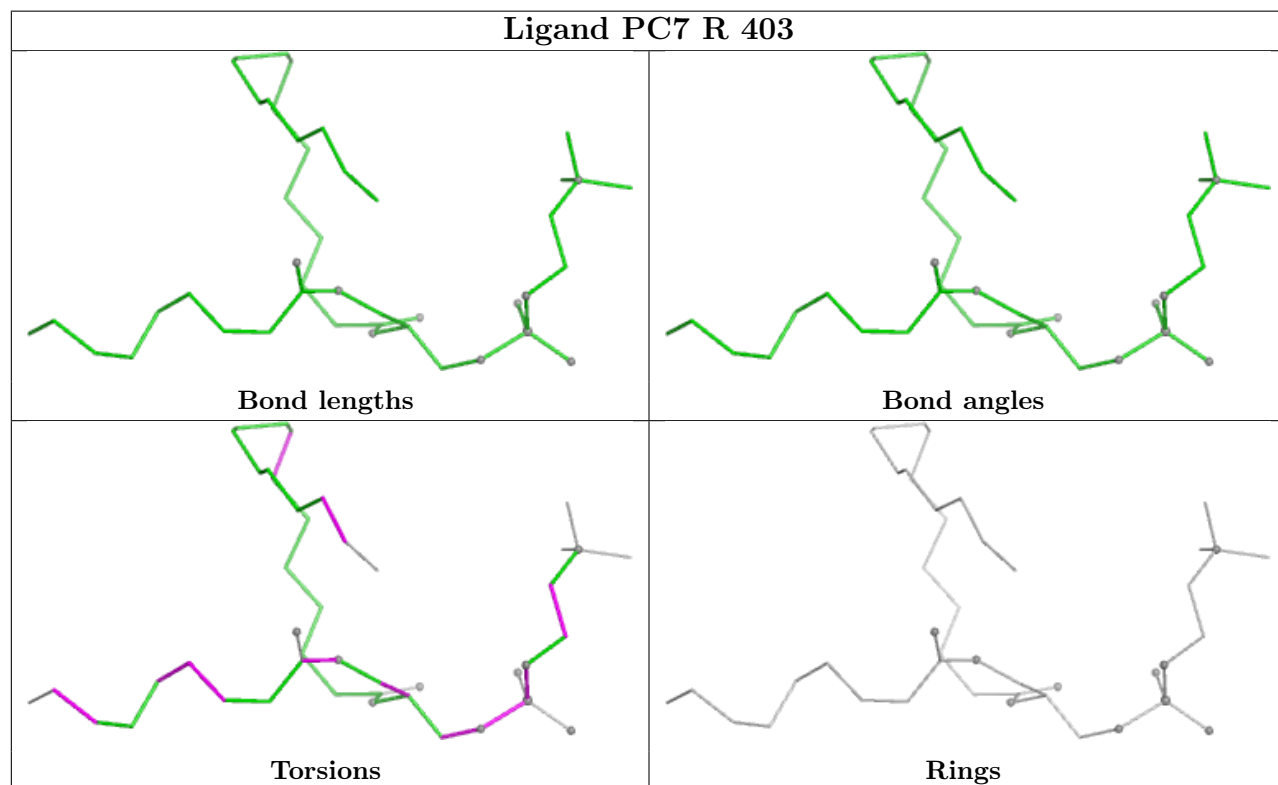
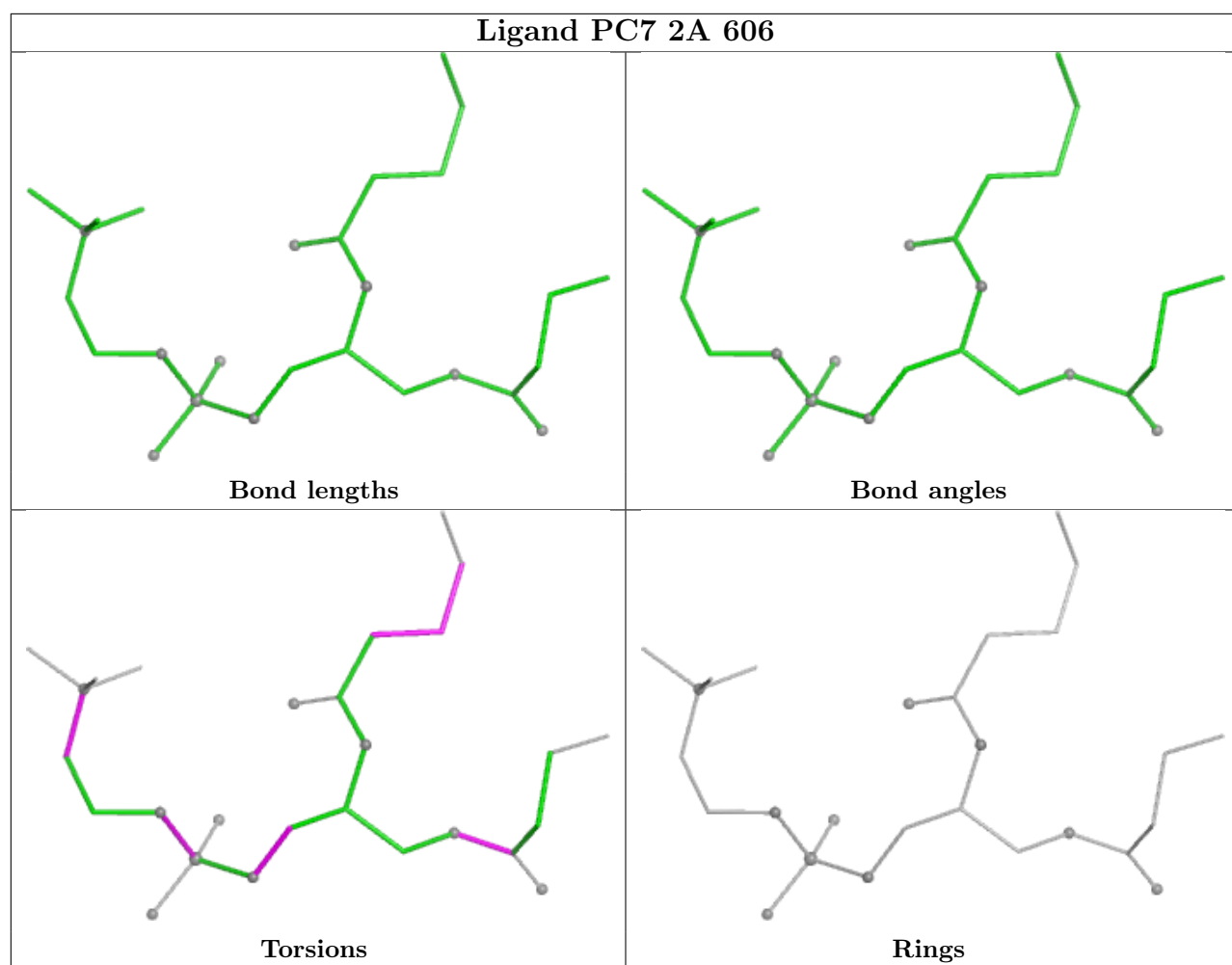


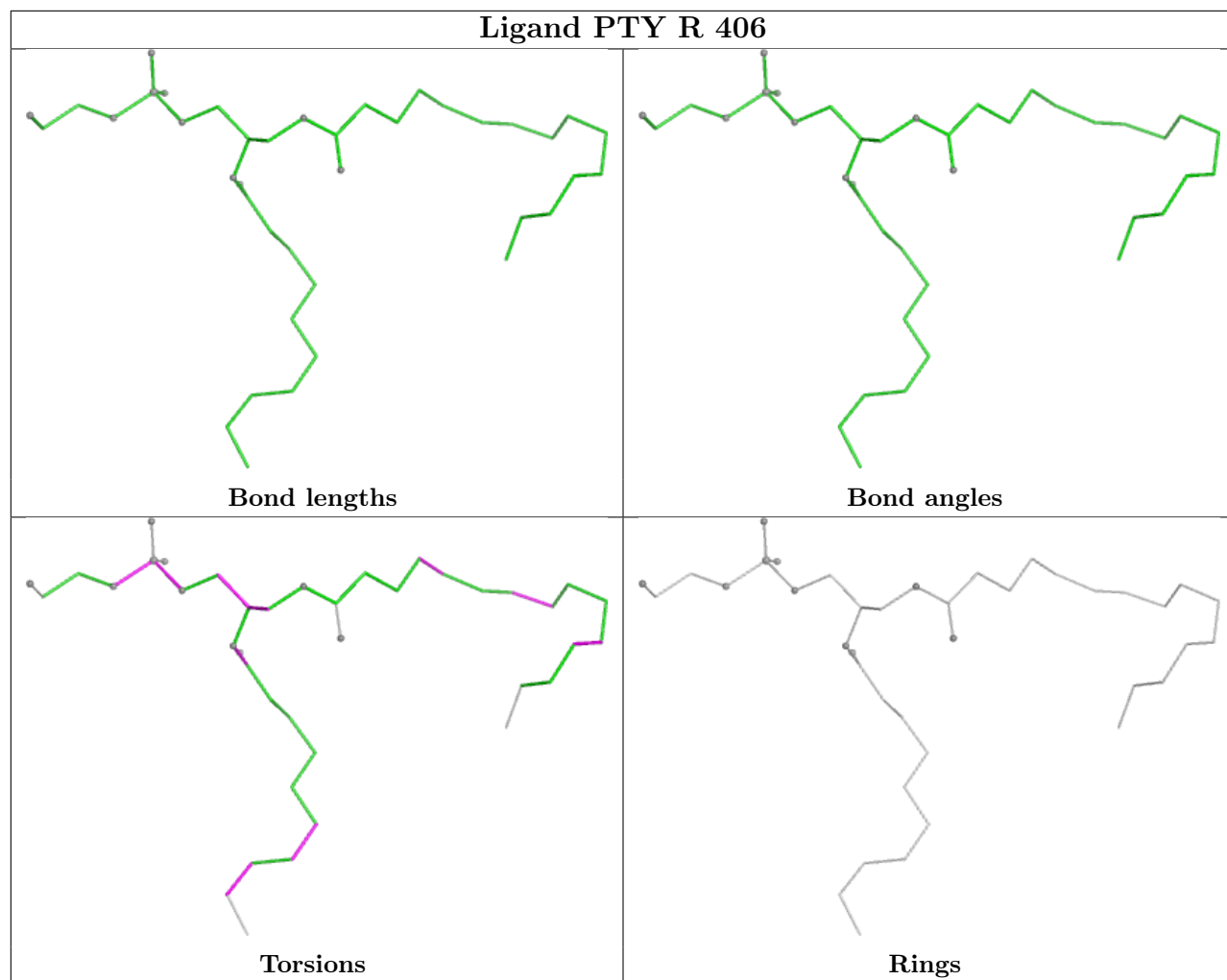


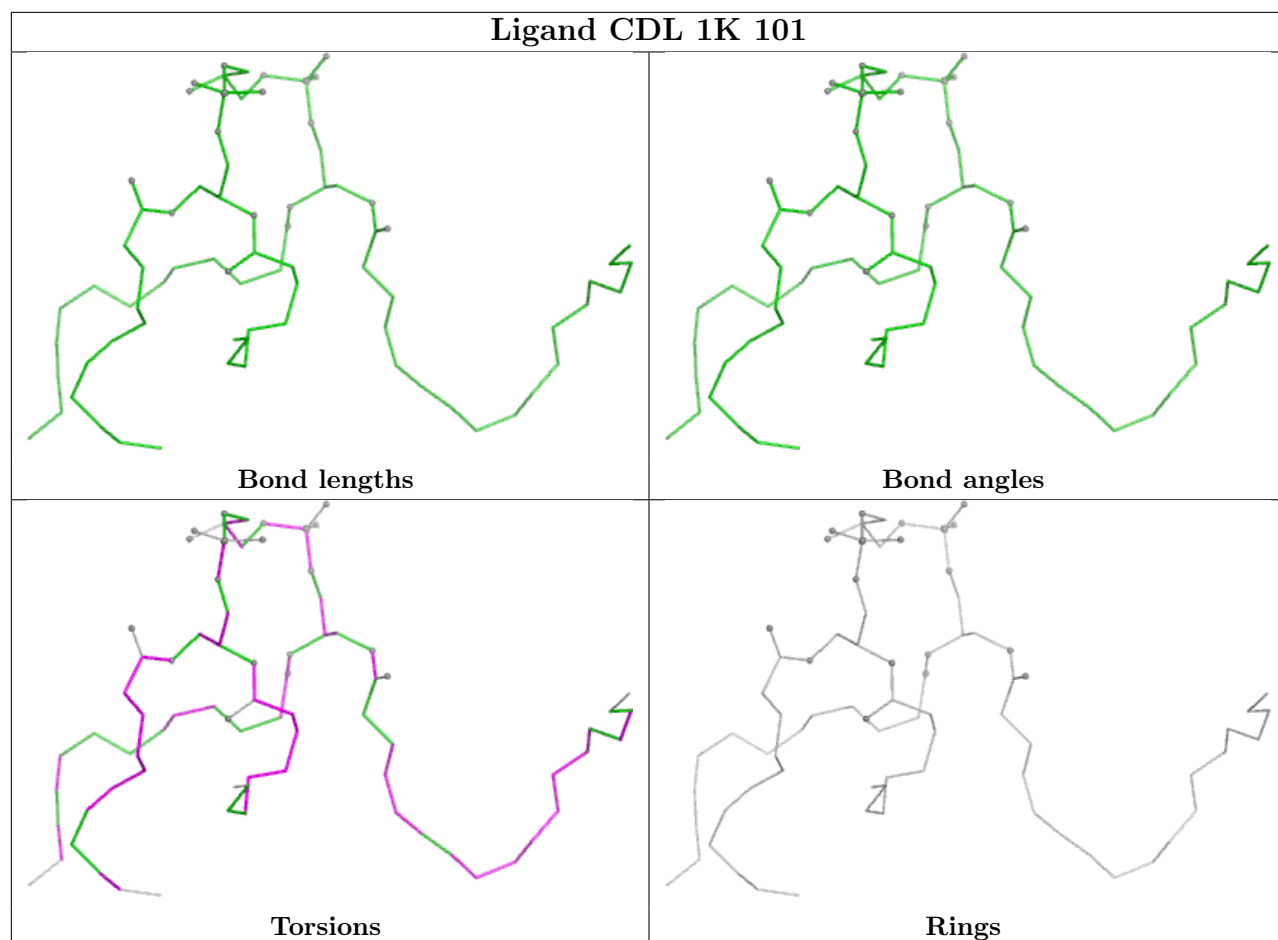
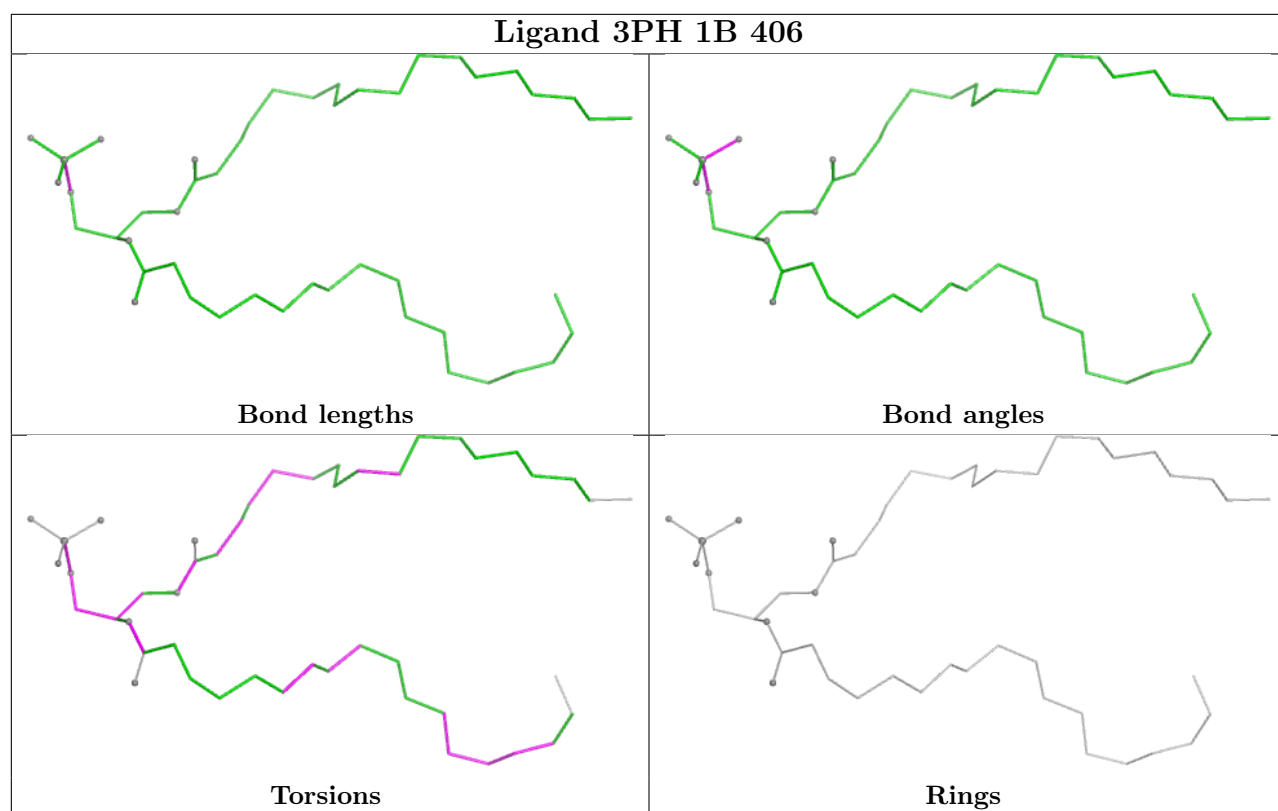
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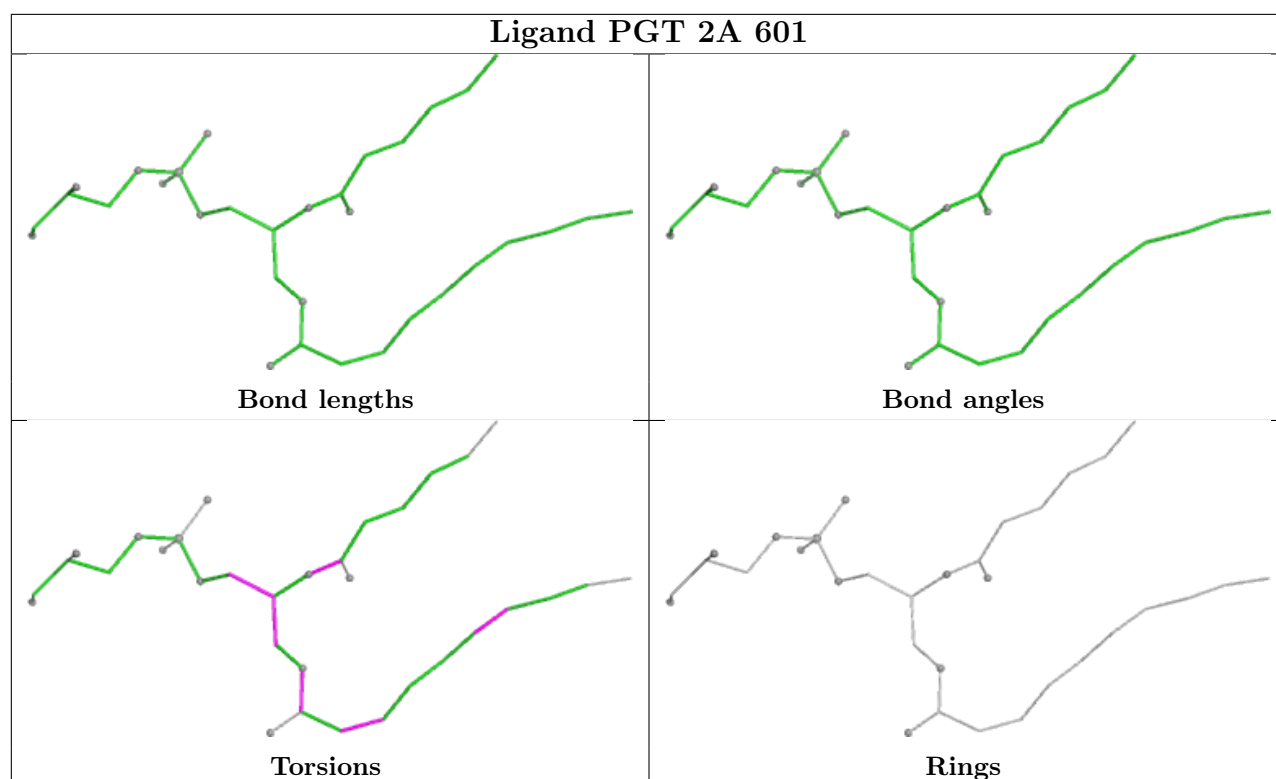












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

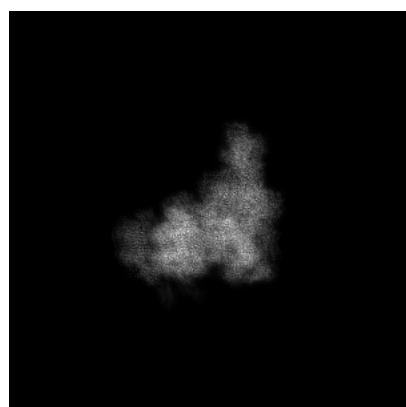
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50202. These allow visual inspection of the internal detail of the map and identification of artifacts.

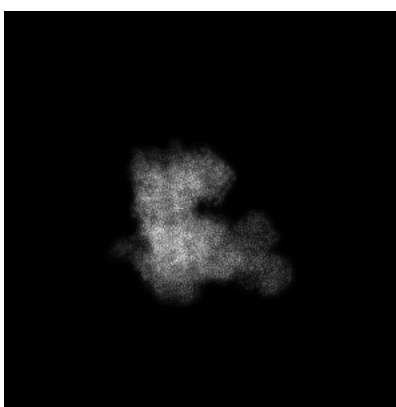
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

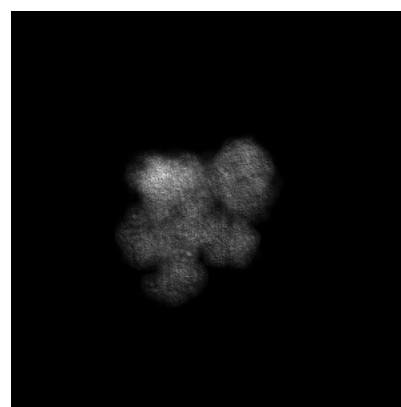
6.1.1 Primary map



X



Y

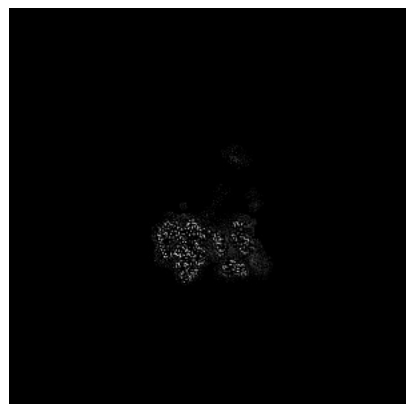


Z

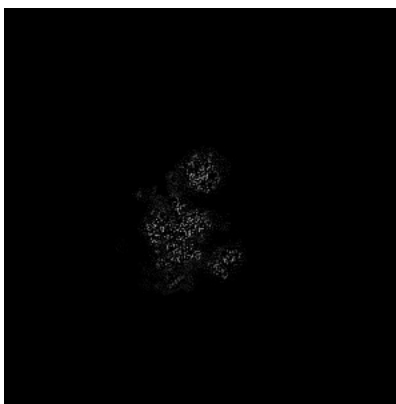
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

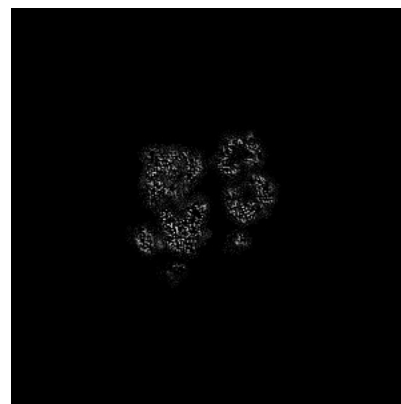
6.2.1 Primary map



X Index: 294



Y Index: 294

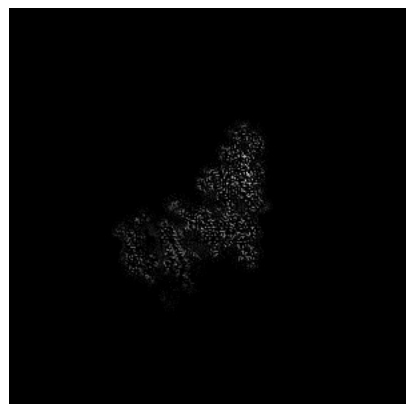


Z Index: 294

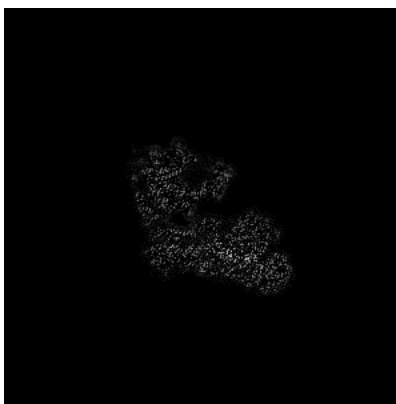
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

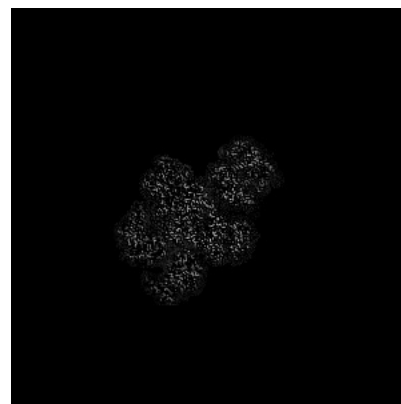
6.3.1 Primary map



X Index: 221



Y Index: 345

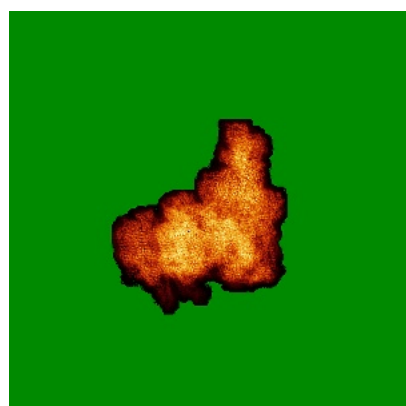


Z Index: 260

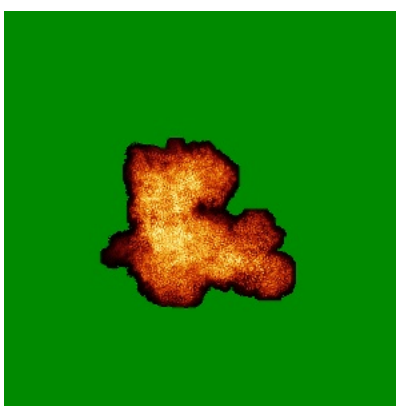
The images above show the largest variance slices of the map in three orthogonal directions.

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

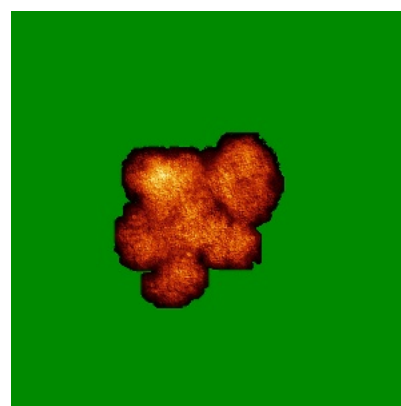
6.4.1 Primary map



X



Y

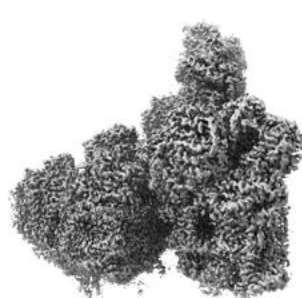


Z

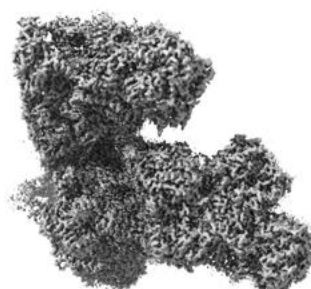
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

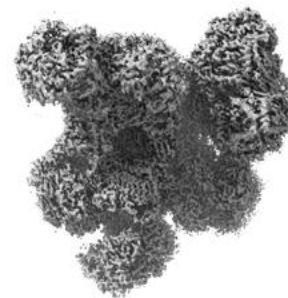
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

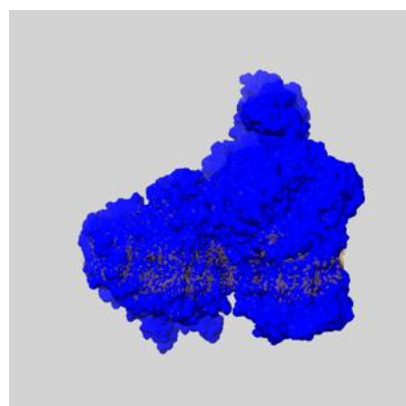
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

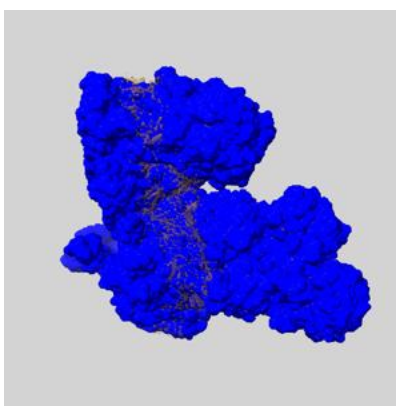
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

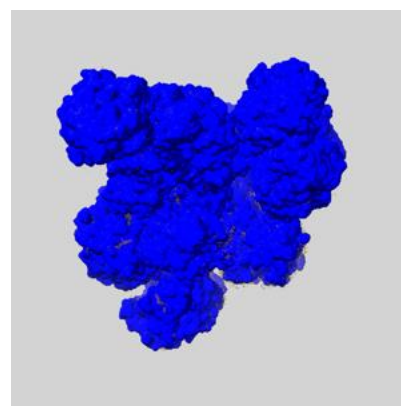
6.6.1 emd_50202_msk_1.map [i](#)



X



Y

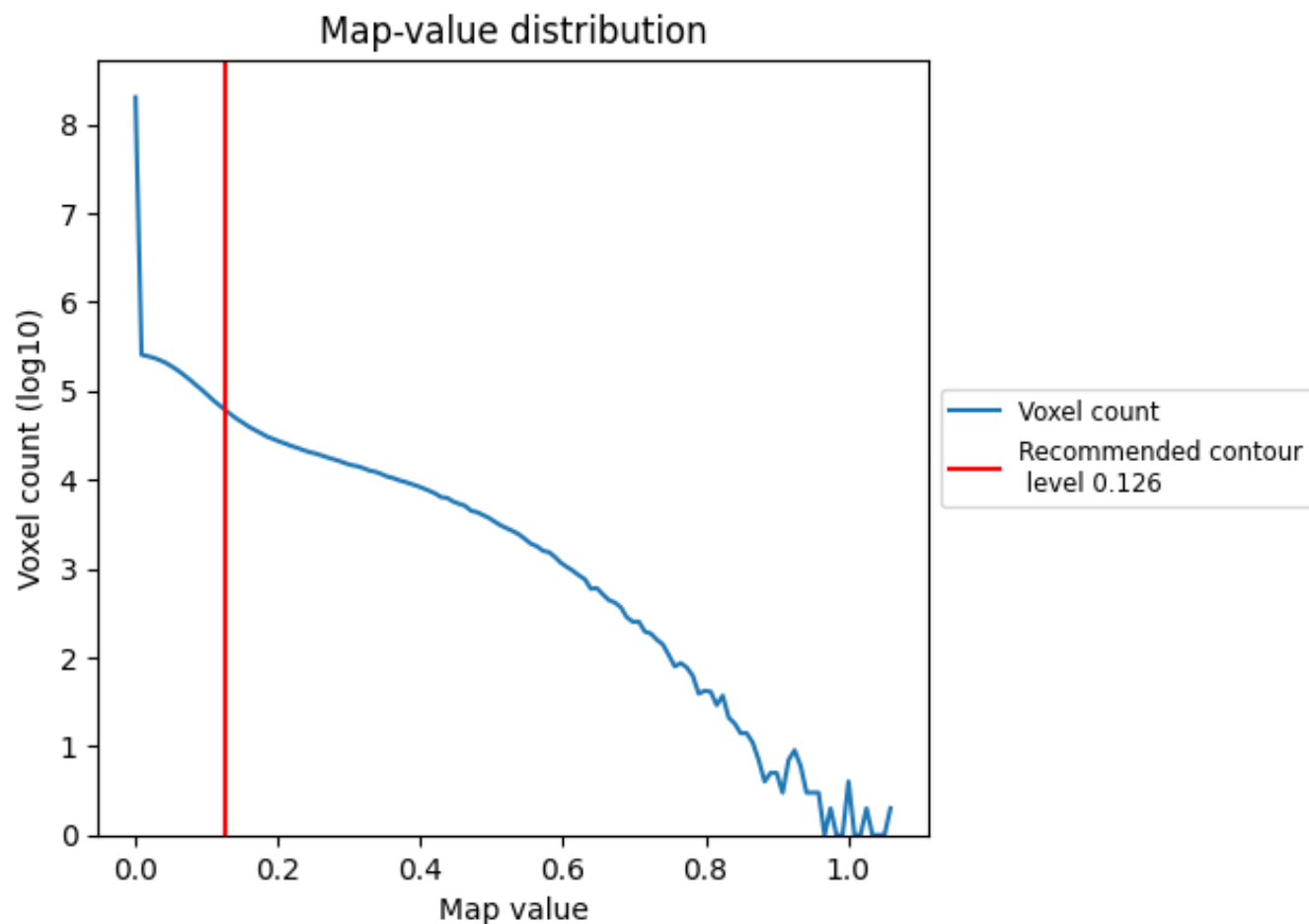


Z

7 Map analysis [i](#)

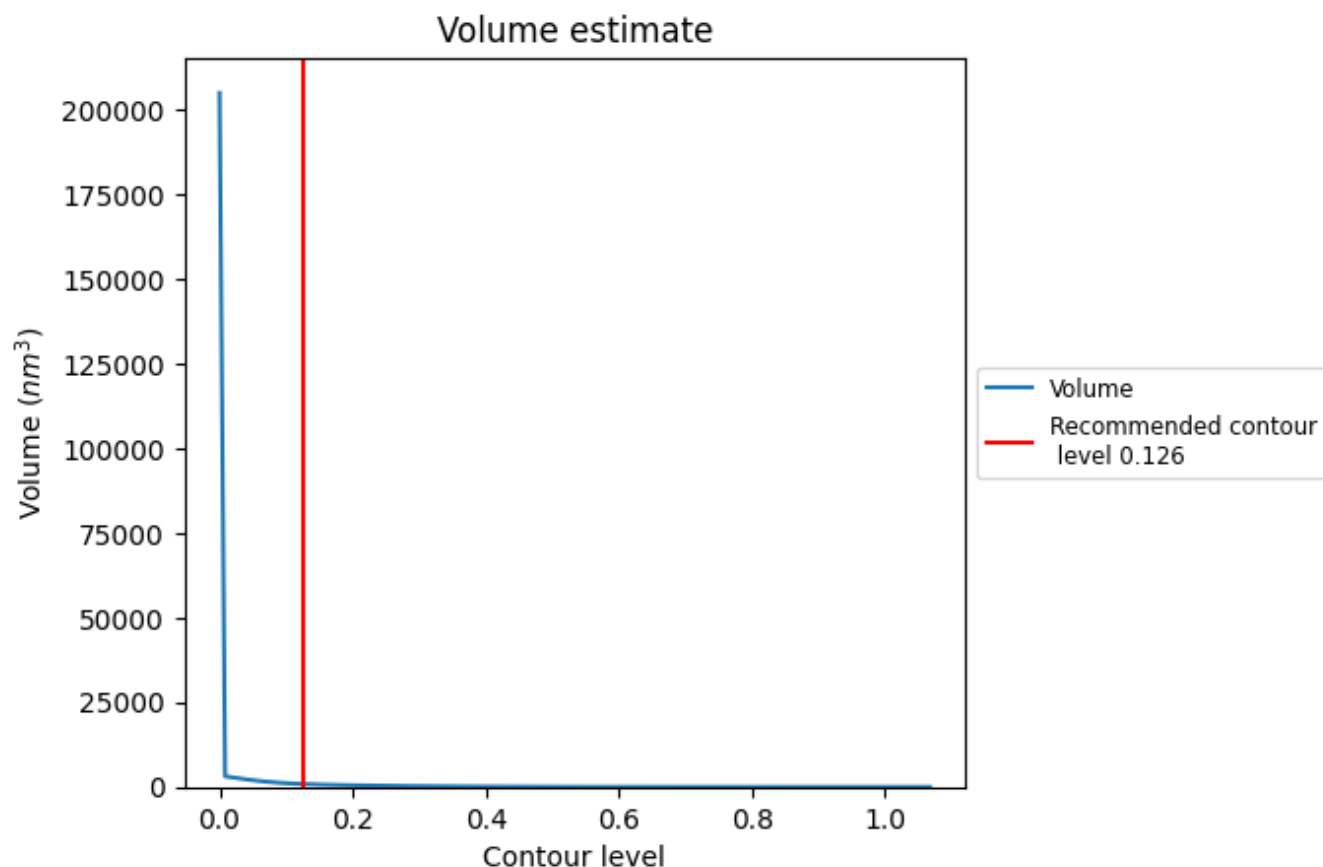
This section contains the results of statistical analysis of the map.

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.

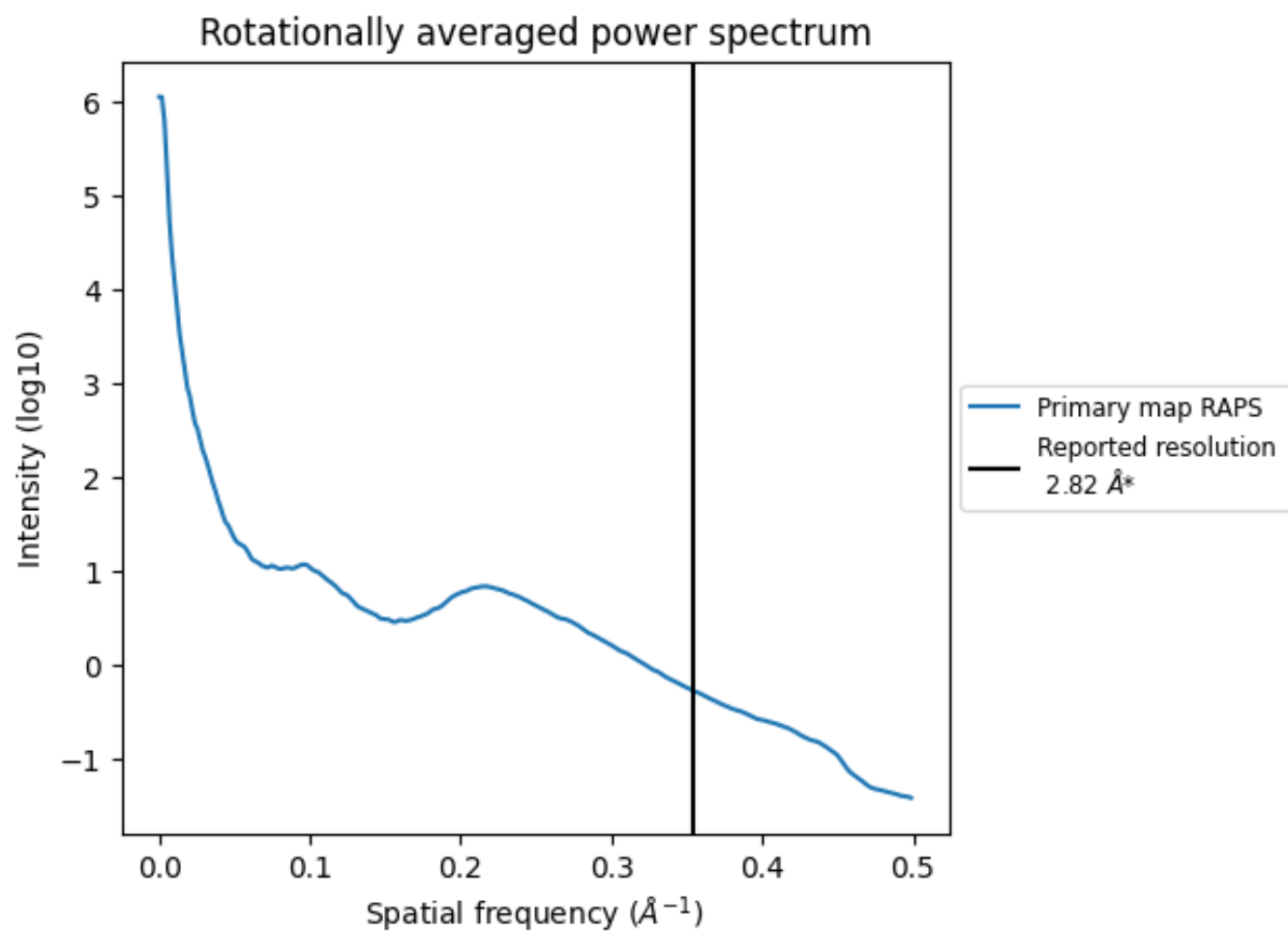
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 863 nm^3 ; this corresponds to an approximate mass of 780 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 ⓘ

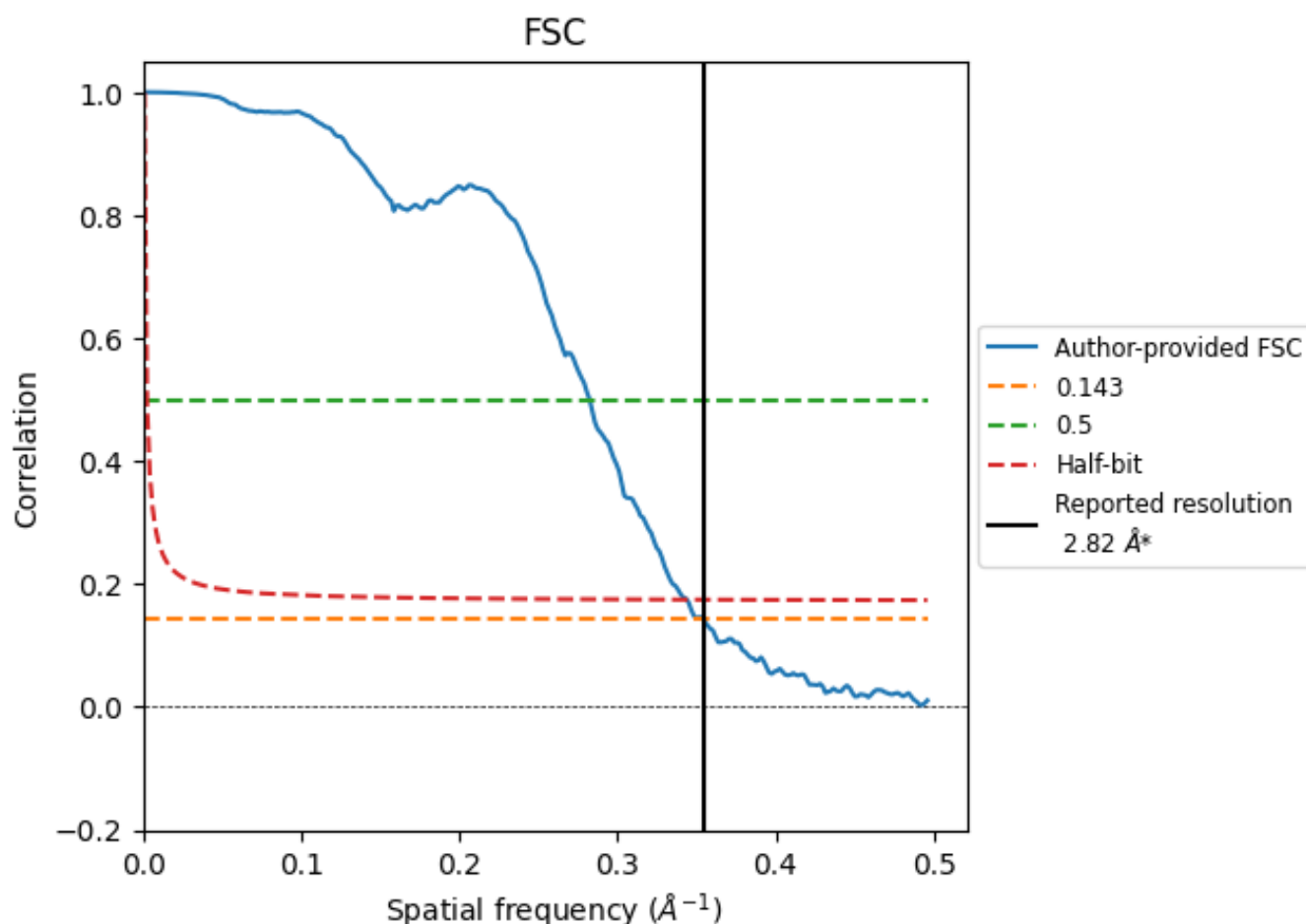


*Reported resolution corresponds to spatial frequency of 0.355 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.355 Å⁻¹

8.2 Resolution estimates [i](#)

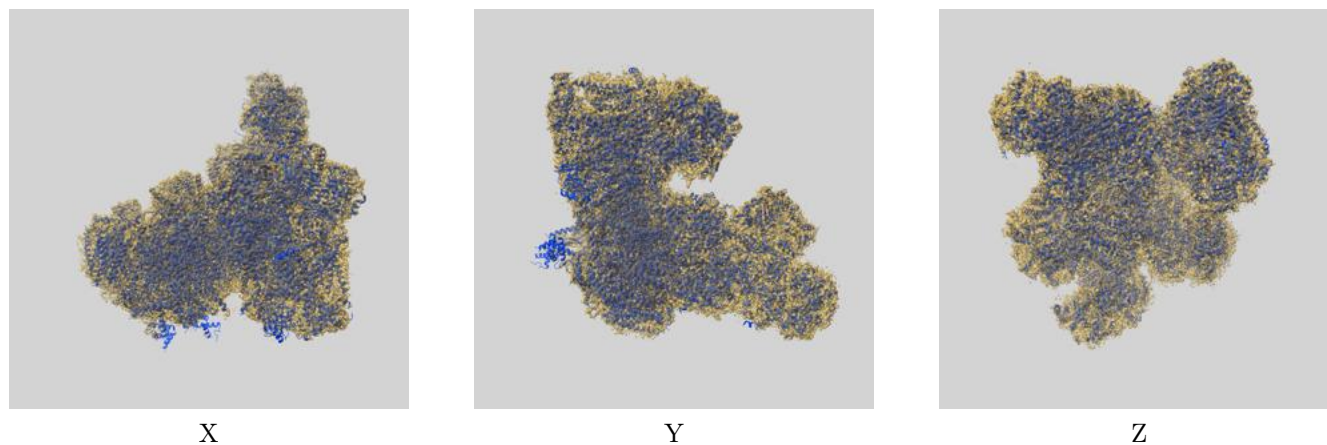
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.54	2.91
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

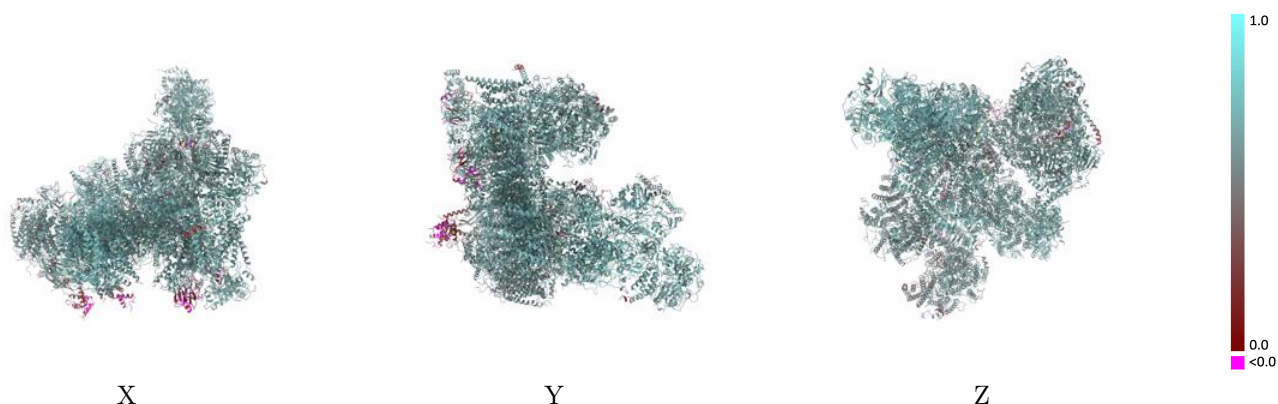
This section contains information regarding the fit between EMDB map EMD-50202 and PDB model 9F5X. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



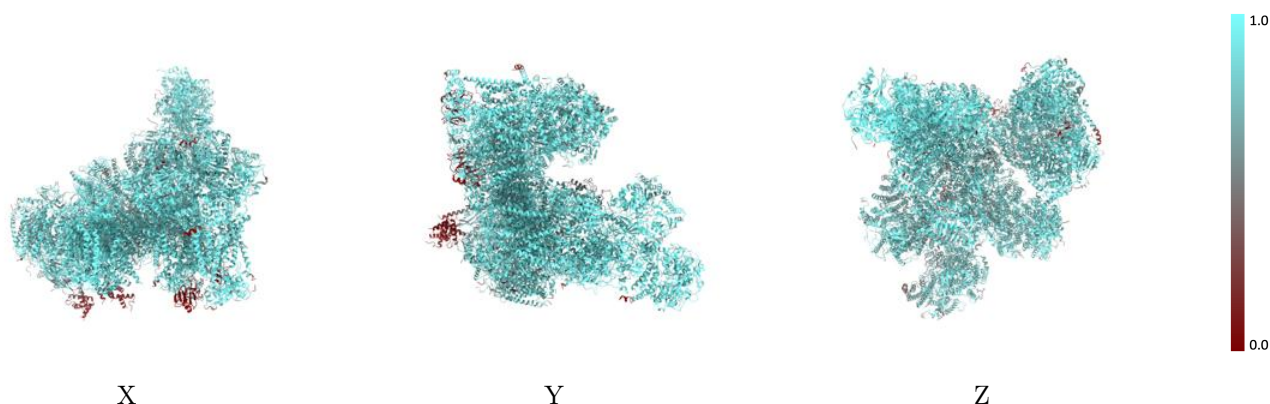
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



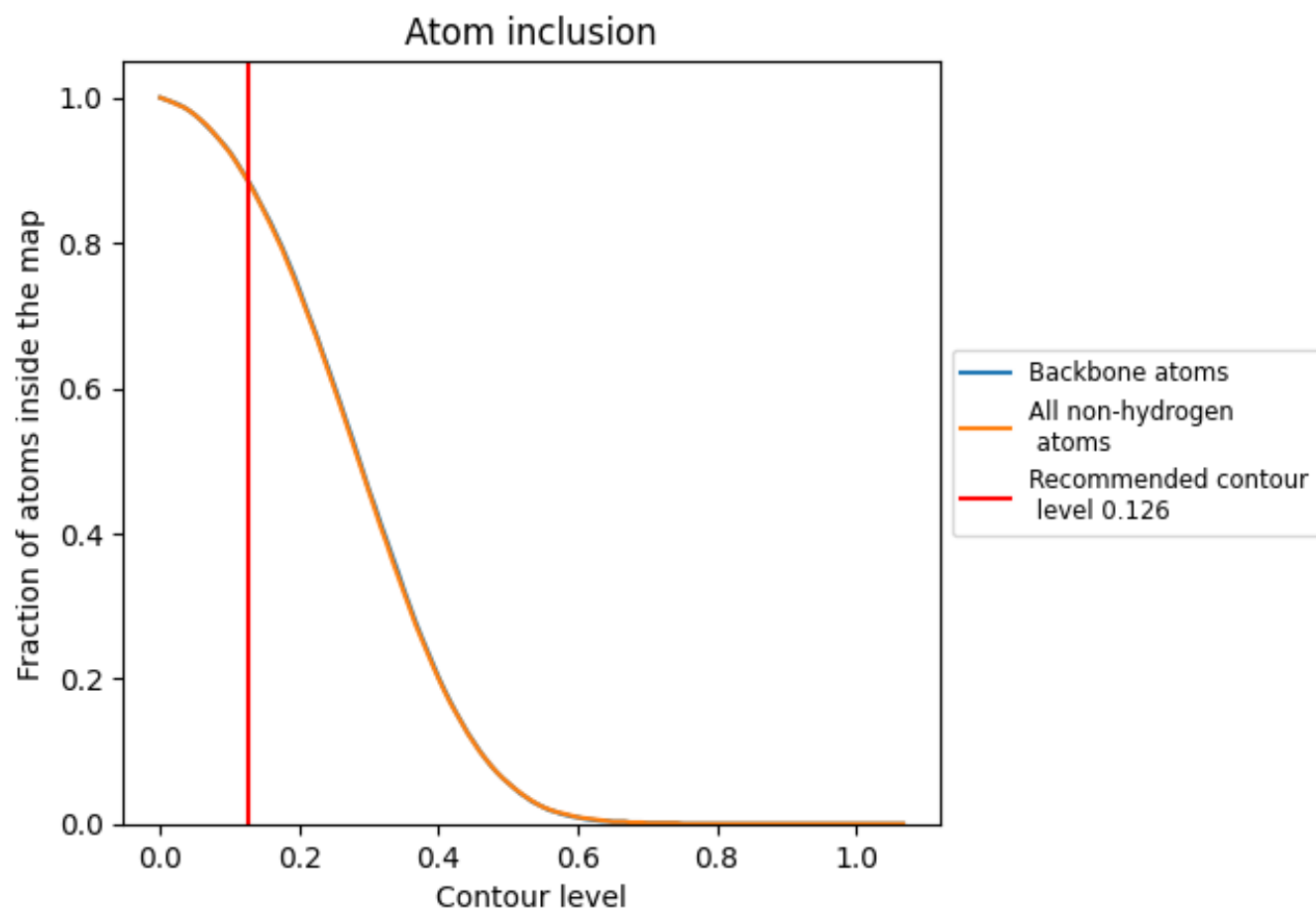
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.6230
1A	 0.9410	 0.6440
1B	 0.9420	 0.6500
1C	 0.4630	 0.3650
1D	 0.4960	 0.3770
1E	 0.9310	 0.6500
1F	 0.9100	 0.6300
1G	 0.8760	 0.6190
1H	 0.8610	 0.6110
1I	 0.8780	 0.6110
1J	 0.7920	 0.5780
1K	 0.9020	 0.6250
1L	 0.8810	 0.6040
1M	 0.9320	 0.6400
1N	 0.9060	 0.6250
1O	 0.8310	 0.5940
1P	 0.8390	 0.5720
1Q	 0.8550	 0.5790
1R	 0.8390	 0.6000
1S	 0.8300	 0.5750
1T	 0.9230	 0.6440
2A	 0.9310	 0.6240
2B	 0.8230	 0.5790
2C	 0.7240	 0.5260
2D	 0.8700	 0.5940
2E	 0.8260	 0.5690
2F	 0.7560	 0.5260
2G	 0.6610	 0.5220
2H	 0.5940	 0.4390
2I	 0.8200	 0.5860
2J	 0.8220	 0.5790
2K	 0.7820	 0.5640
2L	 0.7770	 0.5390
3A	 0.9150	 0.6090
3B	 0.7870	 0.5300



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Chain	Atom inclusion	Q-score
3C	 0.7250	 0.4970
3D	 0.8320	 0.5590
3E	 0.7380	 0.5220
3F	 0.6830	 0.4500
3G	 0.5820	 0.4570
3H	 0.5550	 0.3890
3I	 0.7850	 0.5550
3J	 0.8460	 0.5690
3K	 0.7680	 0.5180
3L	 0.6640	 0.4470
A	 0.9110	 0.6380
B	 0.9370	 0.6520
C	 0.9410	 0.6640
D	 0.9630	 0.6840
E	 0.9600	 0.6730
F	 0.9570	 0.6620
G	 0.9560	 0.6720
H	 0.9090	 0.6480
I	 0.8770	 0.6330
J	 0.5910	 0.4580
K	 0.8130	 0.5790
L	 0.9010	 0.6440
M	 0.9200	 0.6650
N	 0.9220	 0.6540
O	 0.8200	 0.5770
P	 0.9060	 0.6270
Q	 0.9470	 0.6520
R	 0.9570	 0.6840
S	 0.9340	 0.6560
T	 0.9800	 0.7050
U	 0.9650	 0.6910
V	 0.9730	 0.6990
W	 0.9350	 0.6630
X	 0.9720	 0.6950
Y	 0.9520	 0.6470
Z	 0.9340	 0.6820
a	 0.9080	 0.6360
b	 0.9360	 0.6870
c	 0.7420	 0.5460
d	 0.9420	 0.6700
e	 0.9650	 0.6790
f	 0.9170	 0.6490

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Chain	Atom inclusion	Q-score
g	 0.7730	 0.5720
h	 0.9290	 0.6740
i	 0.9070	 0.6610
j	 0.9480	 0.6780
k	 0.9520	 0.6800
l	 0.8750	 0.6300
m	 0.9080	 0.6450
n	 0.8620	 0.6300
o	 0.9500	 0.6840
p	 0.9370	 0.6610
q	 0.9330	 0.6730
r	 0.8830	 0.6350
s	 0.9200	 0.6520
t	 0.9650	 0.6930
u	 0.9260	 0.6680
v	 0.8970	 0.6370
w	 0.9230	 0.6680
x	 0.9340	 0.6660
y	 0.9470	 0.6750