



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 11:47 AM JST

PDB ID : 8IUF / pdb_00008iuf
EMDB ID : EMD-35720
Title : Cryo-EM structure of Euglena gracilis super-complex I+III2+IV, composite
Authors : Wu, M.C.; Tian, H.T.; He, Z.X.; Hu, Y.Q.; Zhou, L.
Deposited on : 2023-03-24
Resolution : 2.81 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 : 1.8.5 (274361), 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

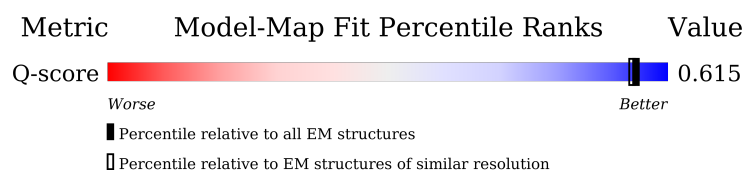
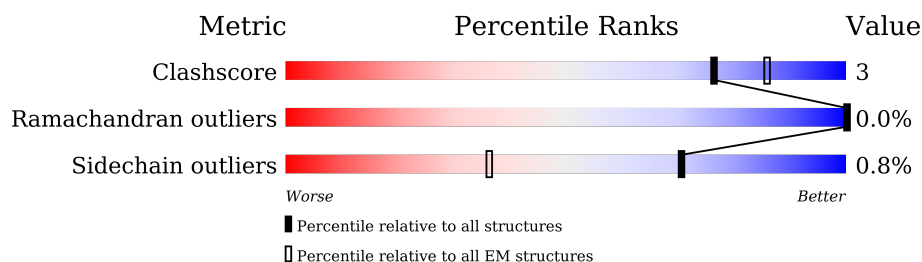
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

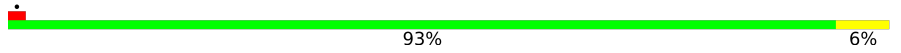
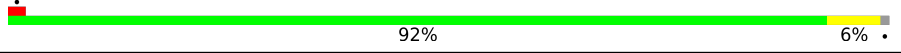
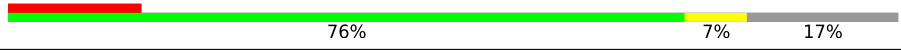
The reported resolution of this entry is 2.81 Å.

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	11740 (2.31 - 3.31)

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	385	
2	1B	527	
3	2B	142	
4	4A	246	

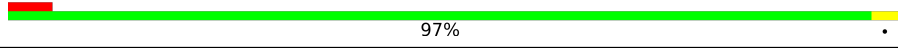
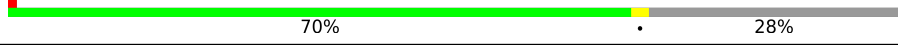
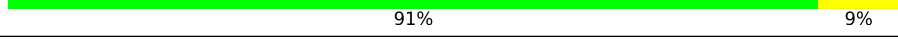
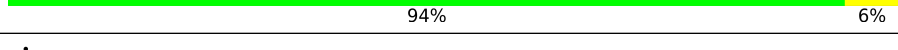
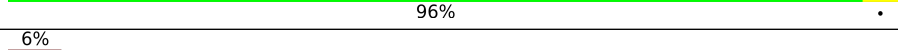
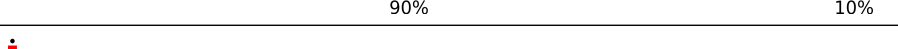
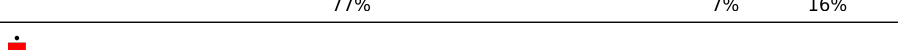
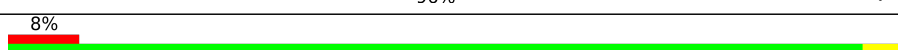
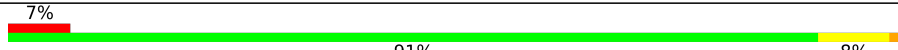
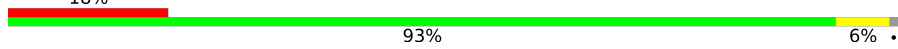
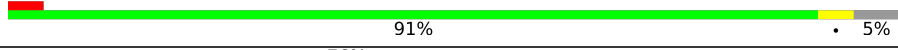
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Mol	Chain	Length	Quality of chain
5	4C	139	
6	4D	174	
7	4E	165	
8	4F	75	
9	4G	315	
10	4H	221	
11	4I	274	
12	4J	88	
13	4L	171	
14	5B	174	
15	5C	208	
16	6A	112	
17	6B	287	
18	7A	178	
19	7C	171	
20	A1	141	
21	A2	193	
22	A3	125	
23	A5	184	
24	A6	437	
25	A7	136	
26	A8	223	
27	A9	489	
28	AB	134	
29	AC	134	

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Mol	Chain	Length	Quality of chain
30	AL	281	
31	AM	198	
32	AN	287	
33	B2	145	
34	B3	62	
35	B4	171	
36	B5	140	
37	B6	91	
38	B7	97	
39	B8	176	
40	B9	158	
41	BL	144	
42	BM	112	
43	C1	495	
44	C2	196	
45	C3	161	
46	C4	185	
47	DC	179	
48	E1	483	
49	E2	472	
50	E3	594	
51	E4	368	
52	E5	290	
53	E6	371	
54	E7	246	

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Mol	Chain	Length	Quality of chain
55	E8	205	
56	E9	178	
57	EA	126	
58	EB	101	
59	EC	101	
60	ED	151	
61	FX	325	
62	G1	436	
63	G2	267	
64	G3	261	
65	N1	670	
66	N2	300	
67	N3	293	
67	N6	293	
68	N4	478	
69	N5	584	
70	QA	479	
70	Qa	479	
71	QB	474	
71	Qb	474	
72	QC	368	
72	Qc	368	
73	QD	243	
73	Qd	243	
74	QE	252	

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Mol	Chain	Length	Quality of chain
74	Qe	252	
75	QF	72	
75	Qf	72	
76	QG	228	
76	Qg	228	
77	QH	85	
77	Qh	85	
78	QI	70	
78	Qi	70	
79	QJ	154	
79	Qj	154	
80	QK	100	
80	Qk	100	
81	S2	395	
82	S3	277	
83	S4	208	
84	S5	122	
85	S6	147	
86	S7	207	
87	S8	212	
88	V1	526	
89	V2	225	
90	A	12	
90	B	12	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
107	HEC	QD	301	X	-	-	-
107	HEC	Qd	301	X	-	-	-

2 Entry composition

There are 108 unique types of molecules in this entry. The entry contains 368218 atoms, of which 183093 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 NDUFS1a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1A	352	Total	C	H	N	O	S	0	0
			5501	1753	2700	488	537	23		

- Molecule 2 is a protein called NDUFS1b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1B	525	Total	C	H	N	O	S	1	0
			8357	2679	4159	743	765	11		

- Molecule 3 is a protein called ND2b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2B	140	Total	C	H	N	O	S	0	0
			2059	712	989	172	183	3		

- Molecule 4 is a protein called COXEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4A	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		

- Molecule 5 is a protein called COXEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4C	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		

- Molecule 6 is a protein called COXEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	4D	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

- Molecule 7 is a protein called COXEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4E	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		

- Molecule 8 is a protein called COXEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4F	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		

- Molecule 9 is a protein called COXEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4G	297	Total	C	H	N	O	S	0	0
			4691	1478	2340	408	457	8		

- Molecule 10 is a protein called COXEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4H	205	Total	C	H	N	O	S	0	0
			3250	1040	1644	260	306			

- Molecule 11 is a protein called COXEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4I	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		

- Molecule 12 is a protein called COXEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	4J	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		

- Molecule 13 is a protein called ND4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	4L	108	Total	C	H	N	O	S	0	0
			1768	606	878	133	145	6		

- Molecule 14 is a protein called COX5b-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	5B	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		

- Molecule 15 is a protein called COX5c.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	5C	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		

- Molecule 16 is a protein called COX6a.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	6A	91	Total	C	H	N	O	S	0	0
			1497	498	747	128	120	4		

- Molecule 17 is a protein called COX6b-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	6B	282	Total	C	H	N	O	S	0	0
			4514	1455	2229	396	427	7		

- Molecule 18 is a protein called COX7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- Molecule 19 is a protein called COX7c.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	7C	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		

- Molecule 20 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	A1	137	Total	C	H	N	O	S	0	0
			2097	684	1026	192	192	3		

- Molecule 21 is a protein called NDUFA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	A2	192	Total	C	H	N	O	S	0	0
			2967	942	1474	267	280	4		

- Molecule 22 is a protein called NDUFA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A3	124	Total	C	H	N	O	S	0	0
			2089	678	1039	191	175	6		

- Molecule 23 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	A5	154	Total	C	H	N	O	S	0	0
			2509	794	1248	221	244	2		

- Molecule 24 is a protein called NDUFA6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A6	423	Total	C	H	N	O	S	0	0
			6608	2091	3280	601	632	4		

- Molecule 25 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	A7	136	Total	C	H	N	O	S	0	0
			2272	735	1118	219	194	6		

- Molecule 26 is a protein called NDUFA8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	A8	223	Total	C	H	N	O	S	0	0
			3548	1160	1726	315	334	13		

- Molecule 27 is a protein called NDUFA9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A9	484	Total	C	H	N	O	S	0	0
			7679	2449	3850	662	700	18		

- Molecule 28 is a protein called NDUFAB1-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AB	88	Total	C	H	N	O	S	0	0
			1367	437	673	114	139	4		

- Molecule 29 is a protein called NDUFAB1-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AC	92	Total	C	H	N	O	S	0	0
			1418	461	697	116	140	4		

- Molecule 30 is a protein called NDUFA12.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AL	265	Total	C	H	N	O	S	0	0
			4409	1439	2172	414	379	5		

- Molecule 31 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AM	184	Total	C	H	N	O	S	0	0
			2935	953	1448	264	263	7		

- Molecule 32 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AN	287	Total	C	H	N	O	S	0	0
			4573	1501	2267	396	399	10		

- Molecule 33 is a protein called NDUF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	B2	105	Total	C	H	N	O	S	0	0
			1770	604	857	142	166	1		

- Molecule 34 is a protein called NDUF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	B3	61	Total	C	H	N	O	S	0	0
			758	292	309	88	68	1		

- Molecule 35 is a protein called NDUF4.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	B4	171	Total	C	H	N	O	S	0	0
			2735	885	1358	250	236	6		

- Molecule 36 is a protein called NDUFB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	B5	140	Total	C	H	N	O	S	0	0
			2181	708	1069	207	195	2		

- Molecule 37 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	B6	91	Total	C	H	N	O	S	0	0
			1520	509	747	132	128	4		

- Molecule 38 is a protein called NDUFB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	B7	97	Total	C	H	N	O	S	0	0
			1692	536	835	165	149	7		

- Molecule 39 is a protein called NDUFB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	B8	147	Total	C	H	N	O	S	0	0
			2351	804	1127	199	213	8		

- Molecule 40 is a protein called NDUFB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	B9	151	Total	C	H	N	O	S	0	0
			2443	795	1207	216	222	3		

- Molecule 41 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	BL	144	Total	C	H	N	O	S	0	0
			2406	786	1179	215	216	10		

- Molecule 42 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	BM	112	Total	C	H	N	O	S	0	0
			1737	577	827	164	167	2		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	C1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	C2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		

- Molecule 45 is a protein called Putative NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	C3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		

- Molecule 46 is a protein called NDUFC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	C4	183	Total	C	H	N	O	S	0	0
			3062	1000	1517	268	271	6		

- Molecule 47 is a protein called COX4.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	DC	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		

- Molecule 48 is a protein called NDUEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	E1	450	Total	C	H	N	O	S	0	0
			7008	2244	3496	601	654	13		

- Molecule 49 is a protein called NDUEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	E2	466	Total	C	H	N	O	S	0	0
			7103	2286	3540	618	655	4		

- Molecule 50 is a protein called NDUEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	E3	432	Total	C	H	N	O	S	0	0
			6518	2071	3263	565	612	7		

- Molecule 51 is a protein called NDUEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	E4	351	Total	C	H	N	O	S	0	0
			5502	1774	2732	477	504	15		

- Molecule 52 is a protein called NDUEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	E5	276	Total	C	H	N	O	S	0	0
			4046	1265	2069	341	369	2		

- Molecule 53 is a protein called NDUEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	E6	342	Total	C	H	N	O	S	0	0
			5629	1839	2758	507	513	12		

- Molecule 54 is a protein called NDUEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	E7	246	Total	C	H	N	O	S	0	0
			3780	1205	1892	332	344	7		

- Molecule 55 is a protein called NDUEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	E8	205	Total	C	H	N	O	S	0	0
			3354	1100	1663	288	292	11		

- Molecule 56 is a protein called NDUEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	E9	165	Total	C	H	N	O	S	0	0
			2436	779	1224	213	217	3		

- Molecule 57 is a protein called NDUEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	EA	124	Total	C	H	N	O	S	0	0
			1793	630	832	172	156	3		

- Molecule 58 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	EB	101	Total	C	H	N	O	S	0	0
			1405	473	631	150	144	7		

- Molecule 59 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	EC	85	Total	C	H	N	O	S	0	0
			1323	424	663	116	118	2		

- Molecule 60 is a protein called NDUEG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	ED	138	Total	C	H	N	O	S	0	0
			2273	736	1131	205	196	5		

- Molecule 61 is a protein called NDUFEX.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	FX	237	Total	C	H	N	O	S	0	0
			3816	1263	1849	338	359	7		

- Molecule 62 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	G1	426	Total	C	H	N	O	S	0	0
			6552	2115	3205	593	623	16		

- Molecule 63 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	G2	236	Total	C	H	N	O	S	0	0
			3650	1138	1846	323	338	5		

- Molecule 64 is a protein called NDUCA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	G3	261	Total	C	H	N	O	S	0	0
			3905	1226	1944	356	373	6		

- Molecule 65 is a protein called ND1.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	N1	310	Total	C	H	N	O	S	0	0
			5331	1783	2726	380	435	7		

- Molecule 66 is a protein called ND2a.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	N2	296	Total	C	H	N	O	S	0	0
			5101	1725	2589	362	418	7		

- Molecule 67 is a protein called ND3.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	N3	121	Total	C	H	N	O	S	0	0
			2094	720	1057	143	172	2		
67	N6	154	Total	C	H	N	O	S	0	0
			2642	857	1385	187	210	3		

- Molecule 68 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	N4	478	Total	C	H	N	O	S	0	0
			8215	2743	4214	582	663	13		

- Molecule 69 is a protein called ND5.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	N5	584	Total	C	H	N	O	S	0	0
			9869	3293	5032	711	808	25		

- Molecule 70 is a protein called MPP-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	QA	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		
70	Qa	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		

- Molecule 71 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	QB	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		
71	Qb	423	Total	C	H	N	O	S	0	0
			6408	2057	3192	540	616	3		

- Molecule 72 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	QC	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		
72	Qc	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		

- Molecule 73 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	QD	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		
73	Qd	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		

- Molecule 74 is a protein called UQCRFS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	QE	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		
74	Qe	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		

- Molecule 75 is a protein called UQCRH.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	QF	64	Total	C	H	N	O	S	0	0
			1014	325	499	91	93	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
75	Qf	64	Total	C	H	N	O	S	0	0
			1018	325	503	91	93	6		

- Molecule 76 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	QG	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		
76	Qg	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		

- Molecule 77 is a protein called UQCRQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	QH	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		
77	Qh	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		

- Molecule 78 is a protein called UQCR9.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	QI	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		
78	Qi	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		

- Molecule 79 is a protein called UQCR10.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	QJ	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		
79	Qj	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		

- Molecule 80 is a protein called Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	QK	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
80	Qk	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

- Molecule 81 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	S2	394	Total	C	H	N	O	S	0	0
			6274	2041	3101	541	569	22		

- Molecule 82 is a protein called NDUFS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	S3	248	Total	C	H	N	O	S	0	0
			3978	1307	1928	346	384	13		

- Molecule 83 is a protein called NDUFS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	S4	190	Total	C	H	N	O	S	0	0
			3038	956	1502	300	273	7		

- Molecule 84 is a protein called NDUFS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	S5	122	Total	C	H	N	O	S	0	0
			1886	625	895	173	188	5		

- Molecule 85 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	S6	147	Total	C	H	N	O	S	0	0
			2392	759	1192	225	208	8		

- Molecule 86 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	S7	201	Total	C	H	N	O	S	0	0
			3045	975	1500	272	284	14		

- Molecule 87 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	S8	182	Total	C	H	N	O	S	0	0
			2843	915	1392	245	275	16		

- Molecule 88 is a protein called NDUFV1.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	V1	504	Total	C	H	N	O	S	0	0
			7724	2463	3827	680	727	27		

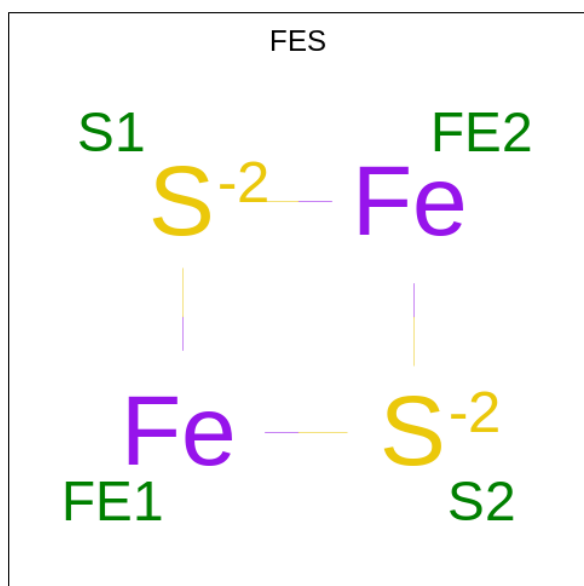
- Molecule 89 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	V2	225	Total	C	H	N	O	S	0	0
			3460	1124	1701	299	319	17		

- Molecule 90 is a protein called poly(UNK).

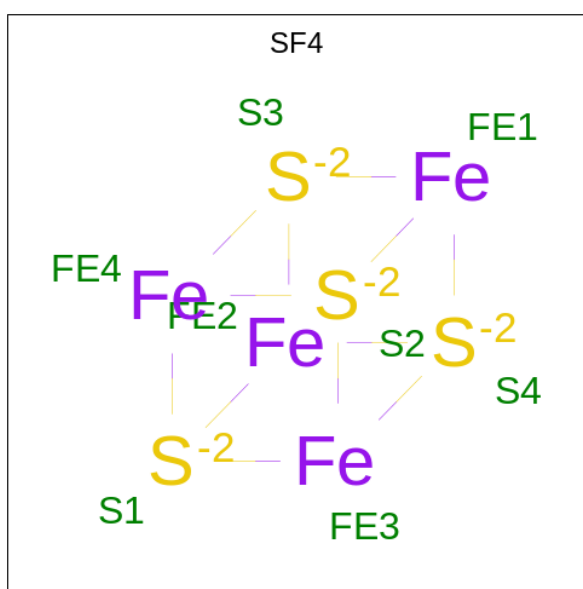
Mol	Chain	Residues	Atoms					AltConf	Trace
90	A	12	Total	C	H	N	O	0	0
			76	36	16	12	12		
90	B	12	Total	C	H	N	O	0	0
			76	36	16	12	12		

- Molecule 91 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
91	1A	1	Total	Fe	S	0
			4	2	2	
91	QE	1	Total	Fe	S	0
			4	2	2	
91	Qe	1	Total	Fe	S	0
			4	2	2	
91	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 92 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

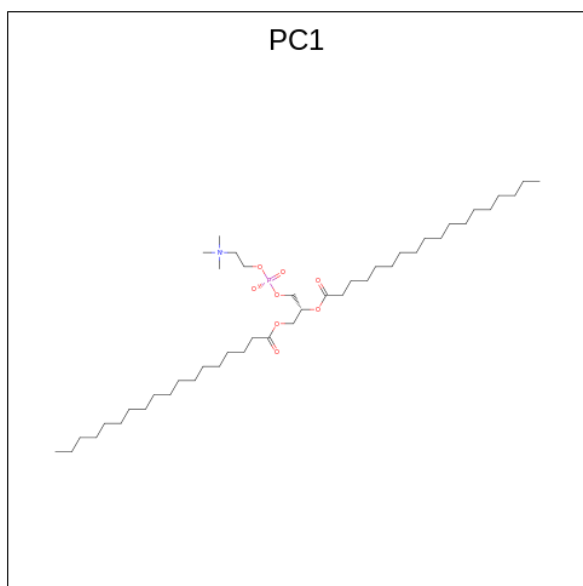


Mol	Chain	Residues	Atoms			AltConf
92	1A	1	Total	Fe	S	0
			8	4	4	
92	1A	1	Total	Fe	S	0
			8	4	4	
92	S7	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
93	1A	1	Total	K	0
			1	1	

- Molecule 94 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
94	4A	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
94	4A	1	Total	C	H	N	O	P	0
			112	36	66	1	8	1	
94	4E	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
94	7A	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
94	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
94	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
94	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
94	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
94	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
94	AM	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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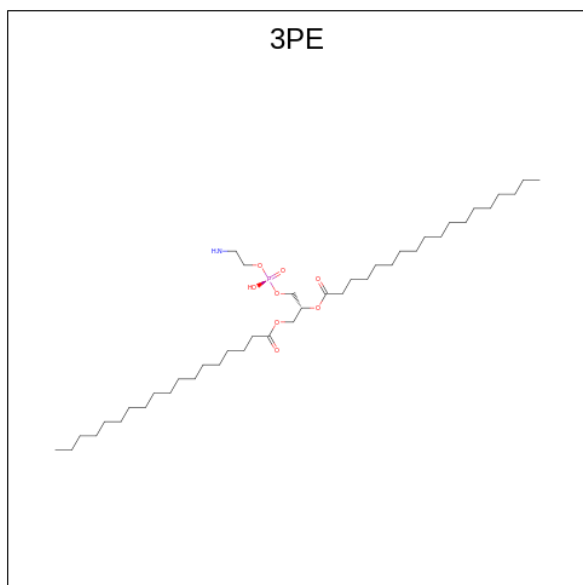
Mol	Chain	Residues	Atoms						AltConf
94	AM	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	AN	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B8	1	Total 85	C 27	H 48	N 1	O 8	P 1	0
94	C1	1	Total 127	C 40	H 77	N 1	O 8	P 1	0
94	C3	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
94	E4	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
94	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	E8	1	Total 73	C 23	H 40	N 1	O 8	P 1	0
94	E8	1	Total 64	C 20	H 34	N 1	O 8	P 1	0
94	E9	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
94	ED	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	ED	1	Total 97	C 31	H 56	N 1	O 8	P 1	0
94	G2	1	Total 88	C 28	H 50	N 1	O 8	P 1	0
94	N1	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
94	N1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
94	N3	1	Total 103	C 32	H 61	N 1	O 8	P 1	0
94	N4	1	Total 91	C 29	H 52	N 1	O 8	P 1	0
94	N4	1	Total 73	C 23	H 40	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
94	N4	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	N5	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	QC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	QD	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
94	QI	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	Qc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	Qc	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
94	Qe	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	Qg	1	Total 58	C 18	H 30	N 1	O 8	P 1	0
94	Qj	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 95 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



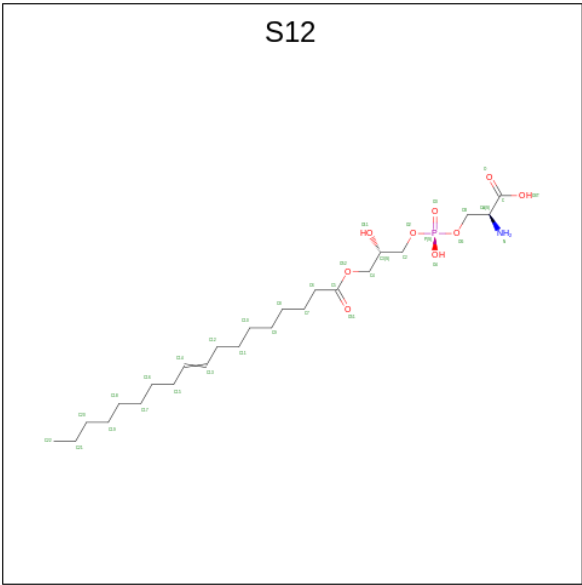
Mol	Chain	Residues	Atoms					AltConf	
95	4D	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	

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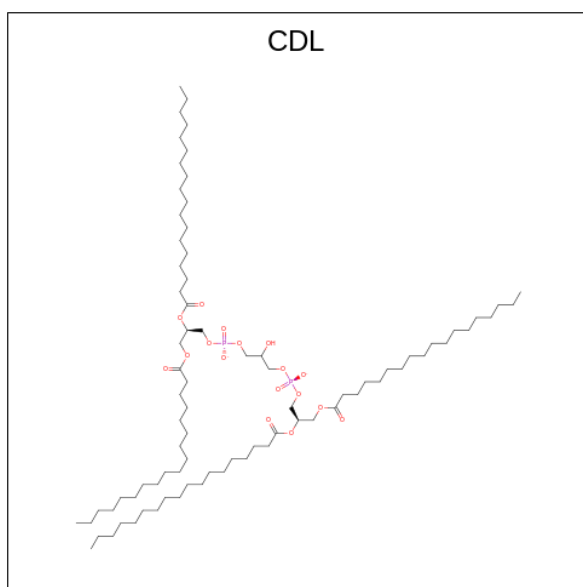
Mol	Chain	Residues	Atoms						AltConf
95	4D	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	7A	1	Total	C	H	N	O	P	0
			100	31	59	1	8	1	
95	B4	1	Total	C	H	N	O	P	0
			97	30	57	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	E9	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	N4	1	Total	C	H	N	O	P	0
			97	31	56	1	8	1	
95	N5	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 96 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (CCD ID: S12) (formula: C₂₄H₄₆NO₉P).



Mol	Chain	Residues	Atoms						AltConf
96	4D	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	

- Molecule 97 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms					AltConf
97	4E	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	7C	1	Total	C	H	O	P	0
			220	71	130	17	2	
97	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	A9	1	Total	C	H	O	P	0
			136	45	72	17	2	
97	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
97	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
97	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	B3	1	Total	C	H	O	P	0
			139	46	74	17	2	
97	B8	1	Total	C	H	O	P	0
			157	51	87	17	2	
97	BM	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	C4	1	Total	C	H	O	P	0
			235	75	141	17	2	
97	C4	1	Total	C	H	O	P	0
			151	50	82	17	2	
97	C4	1	Total	C	H	O	P	0
			247	79	149	17	2	

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Mol	Chain	Residues	Atoms					AltConf
97	E4	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	E6	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	
97	EA	1	Total	C	H	O	P	0
			121	40	62	17	2	
97	EA	1	Total	C	H	O	P	0
			109	36	54	17	2	
97	N1	1	Total	C	H	O	P	0
			154	51	84	17	2	
97	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
97	QC	1	Total	C	H	O	P	0
			112	37	56	17	2	
97	QD	1	Total	C	H	O	P	0
			151	50	82	17	2	
97	QH	1	Total	C	H	O	P	0
			175	57	99	17	2	
97	QH	1	Total	C	H	O	P	0
			124	41	64	17	2	
97	QJ	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	Qc	1	Total	C	H	O	P	0
			106	35	52	17	2	
97	Qd	1	Total	C	H	O	P	0
			256	81	156	17	2	
97	Qe	1	Total	C	H	O	P	0
			124	41	64	17	2	
97	Qh	1	Total	C	H	O	P	0
			139	46	74	17	2	
97	Qj	1	Total	C	H	O	P	0
			88	29	40	17	2	

- Molecule 98 is ZINC ION (CCD ID: ZN) (formula: Zn).

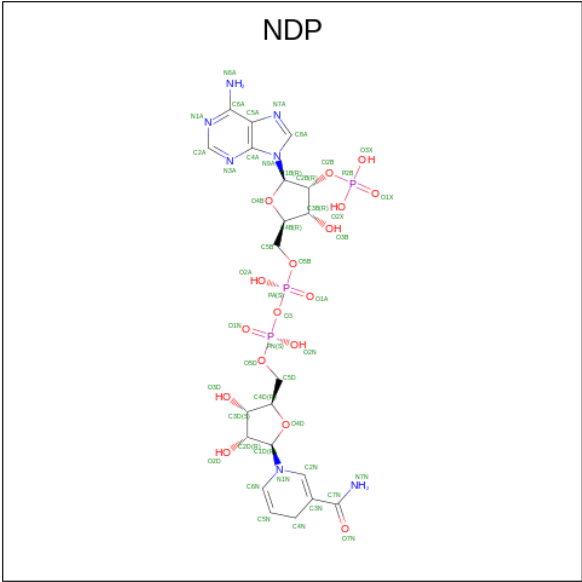
Mol	Chain	Residues	Atoms		AltConf
98	5B	1	Total	Zn	0
			1	1	
98	E7	1	Total	Zn	0
			1	1	

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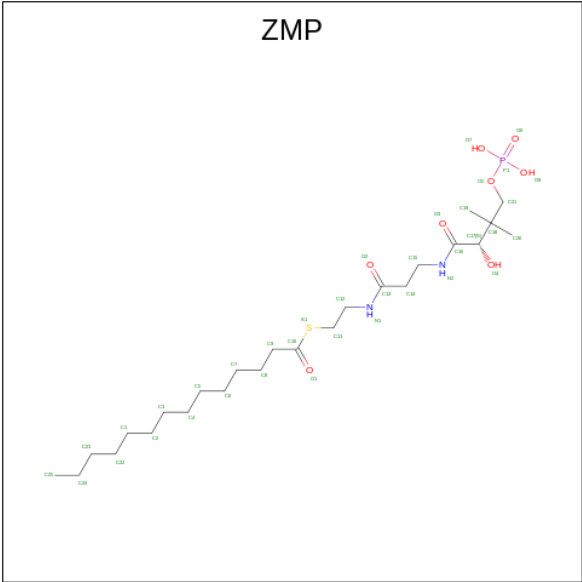
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
98	S6	1	1	1	0

- Molecule 99 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



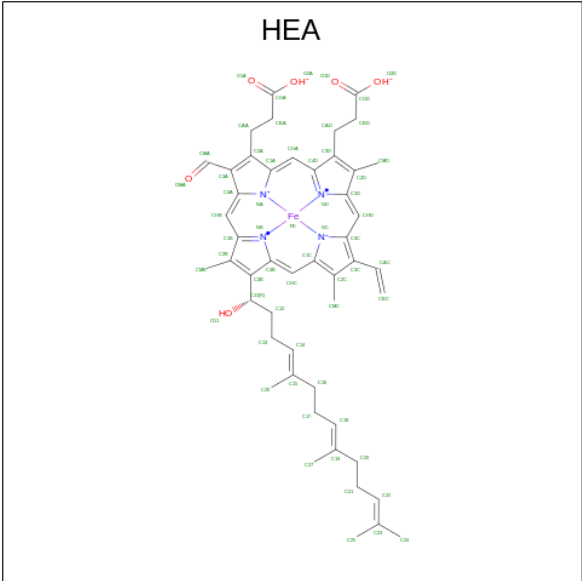
Mol	Chain	Residues	Atoms						AltConf
99	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 100 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
100	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
100	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 101 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
101	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
101	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

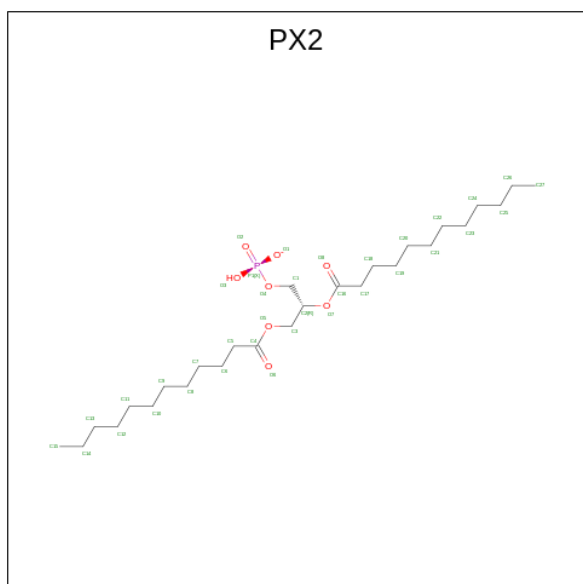
- Molecule 102 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
102	C1	1	Total	Cu	0
			1	1	
102	C2	2	Total	Cu	0
			2	2	

- Molecule 103 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
103	C1	1	Total	Mg	0
			1	1	

- Molecule 104 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: C₂₇H₅₂O₈P).



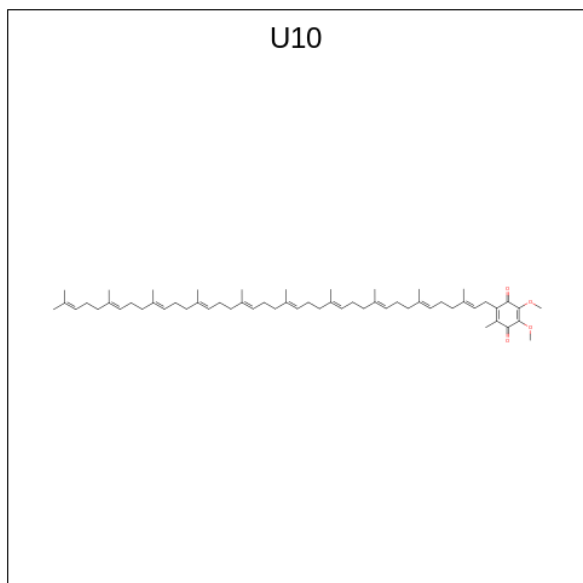
Mol	Chain	Residues	Atoms				AltConf
104	C2	1	Total	C	O	P	0
			36	27	8	1	

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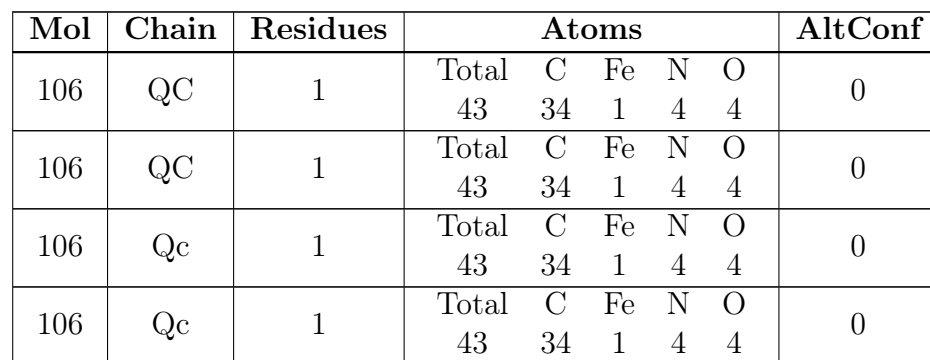
Mol	Chain	Residues	Atoms				AltConf
104	QJ	1	Total	C	O	P	0
			36	27	8	1	
104	QJ	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 105 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
105	N4	1	Total	C	H	O	0
			98	39	55	4	

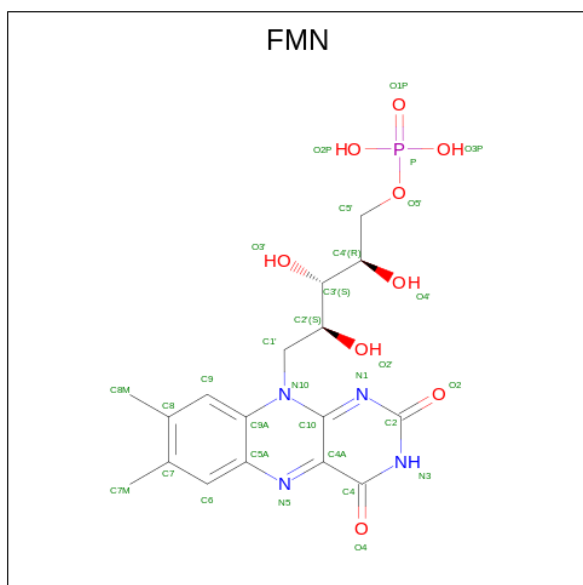
- Molecule 106 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- # HEC
-
- The chemical structure of HEC (Hexaethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains: CMC, CBC, CAC, C2C, C3C, C4C, CHC, C3B, C4B, CMB, C2B, C1B, CHB, C4A, C3A, CMA, C2A, C1A, CBA, CAA, CGA, CBA, CBA, CAA, CGA, CBA, CBA, CAA, CGA. Two carboxylic acid groups are attached to the ring, labeled O2D, O1D, O2A, and O1A.

Mol	Chain	Residues	Atoms					AltConf
107	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
107	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 108 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

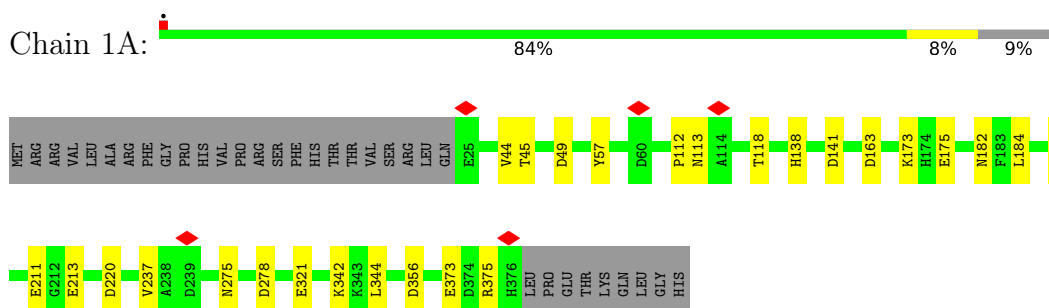


Mol	Chain	Residues	Atoms					AltConf
108	V1	1	Total	C	H	N	O	P
			50	17	19	4	9	1
								0

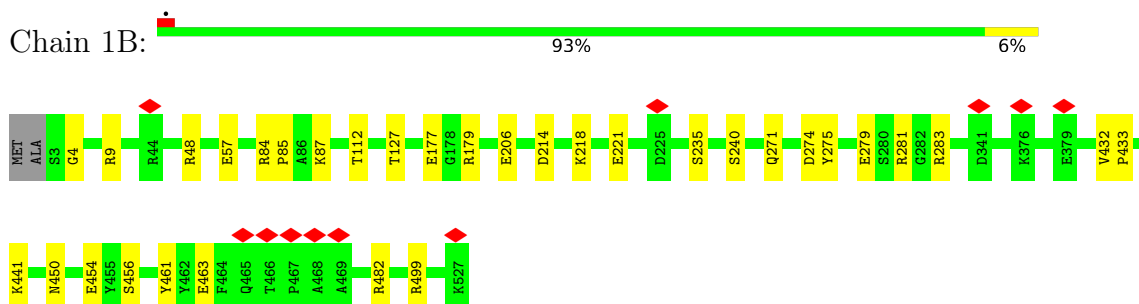
3 Residue-property plots

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.

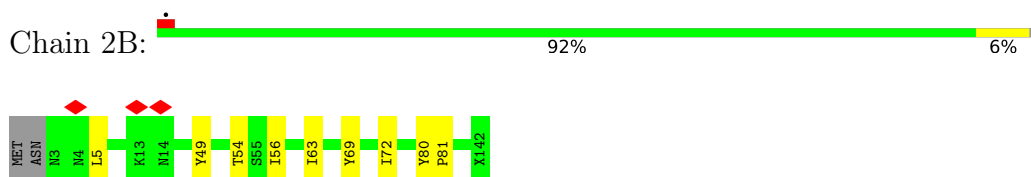
• Molecule 1: NDUFS1a



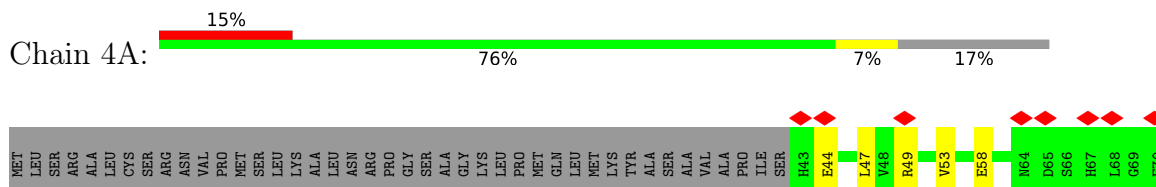
• Molecule 2: NDUFS1b

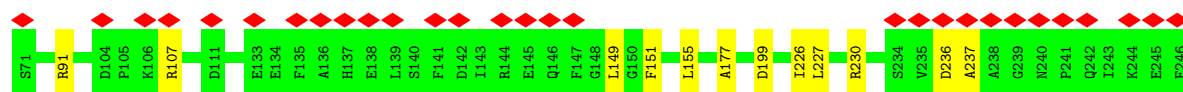


• Molecule 3: ND2b

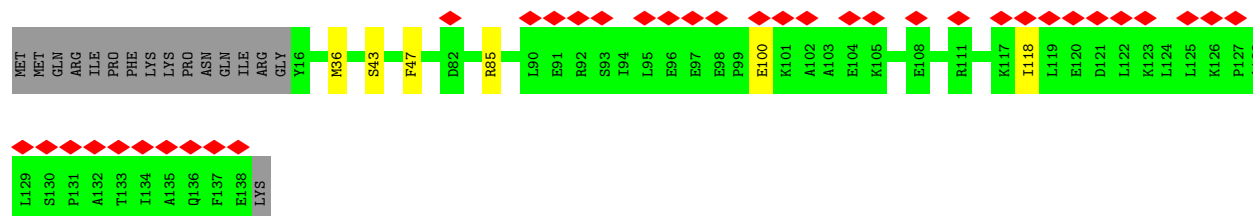
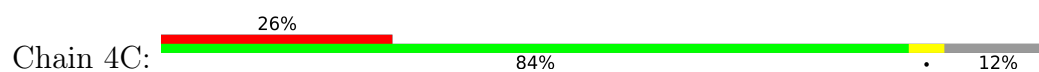


• Molecule 4: COXEG1

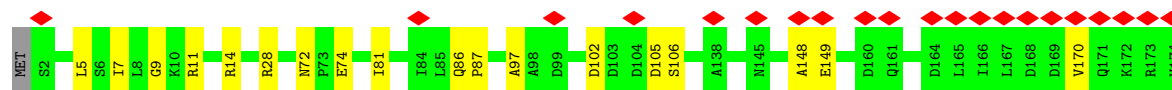
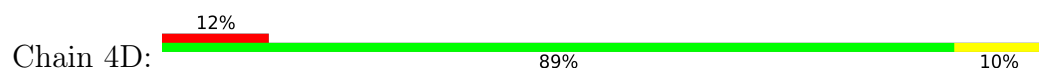




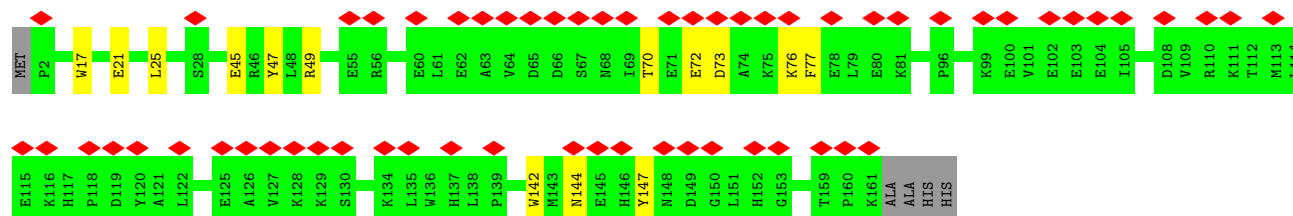
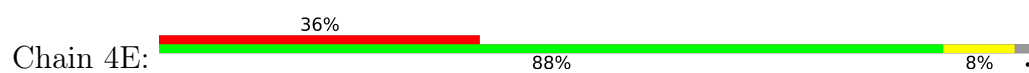
• Molecule 5: COXEG3



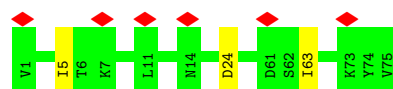
• Molecule 6: COXEG4



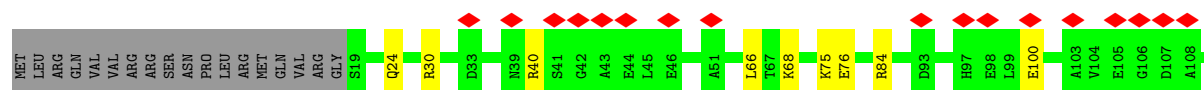
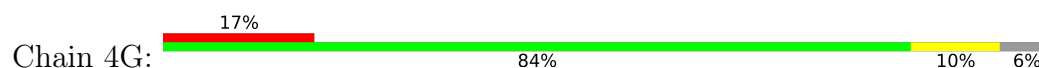
• Molecule 7: COXEG5

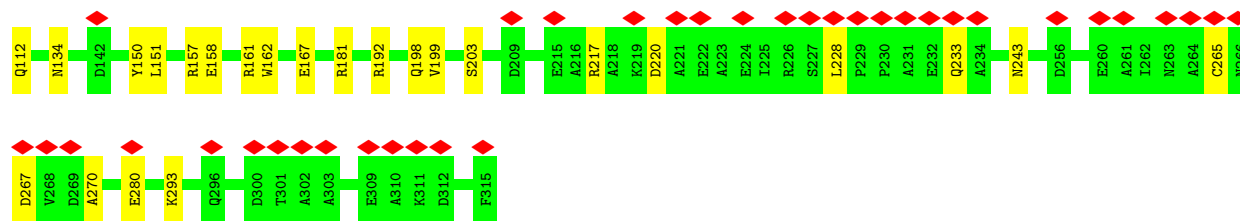


• Molecule 8: COXEG6

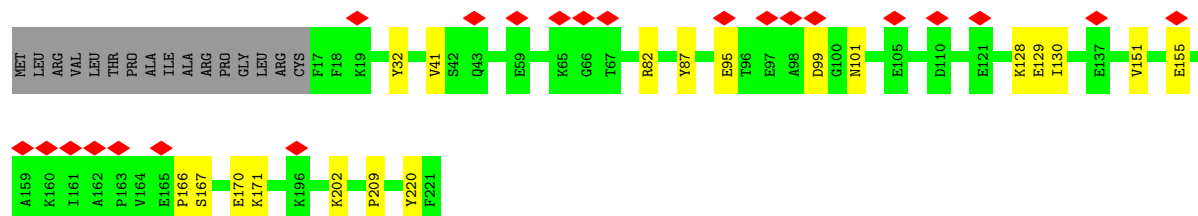
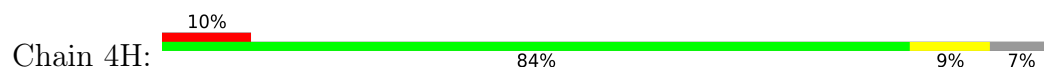


• Molecule 9: COXEG7

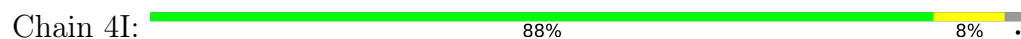




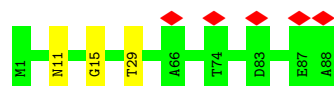
• Molecule 10: COXEG8



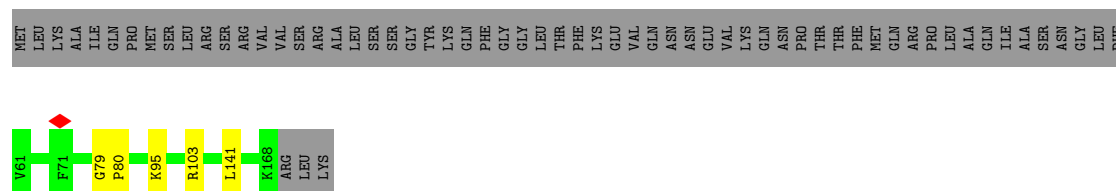
• Molecule 11: COXEG9



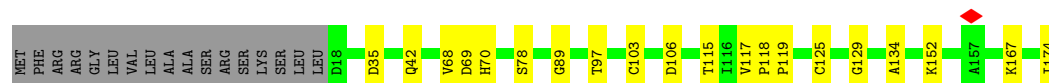
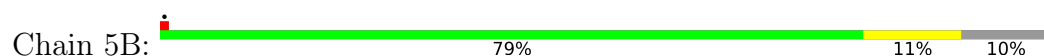
• Molecule 12: COXEG10



• Molecule 13: ND4L

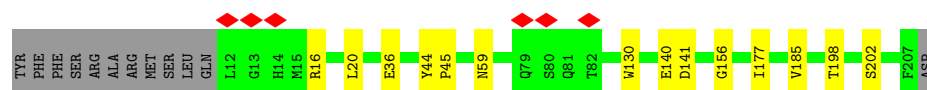


• Molecule 14: COX5b-2

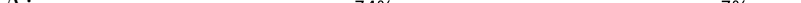


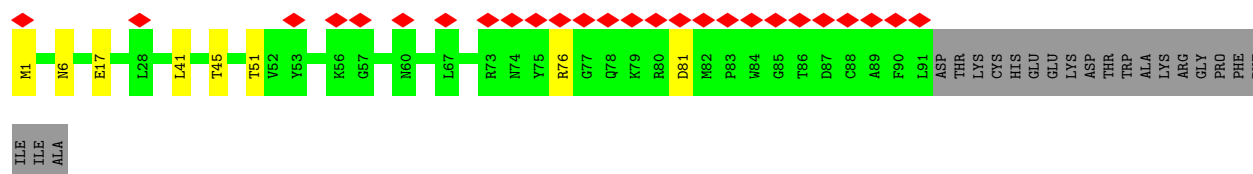
- Molecule 15: COX5c

Chain 5C: 88% 7% 6%

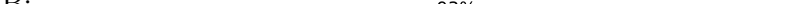


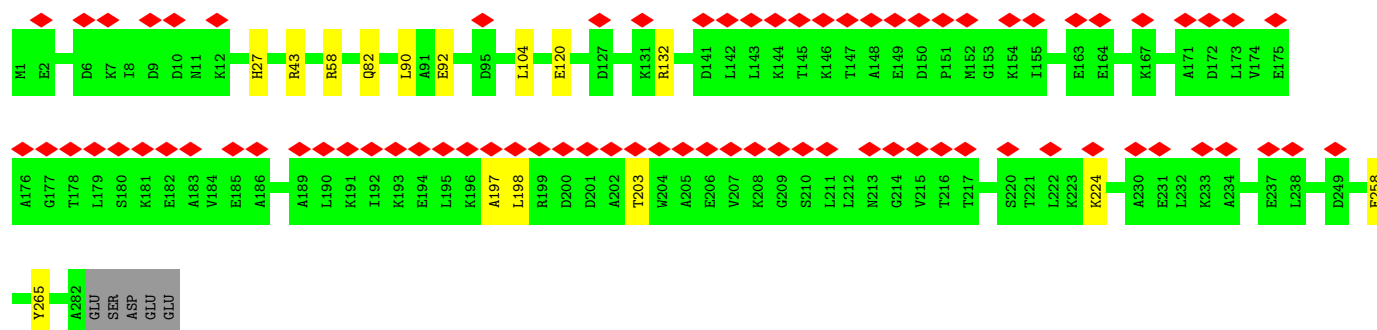
- Molecule 16: COX6a

Chain 6A: 

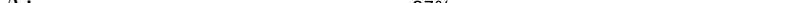


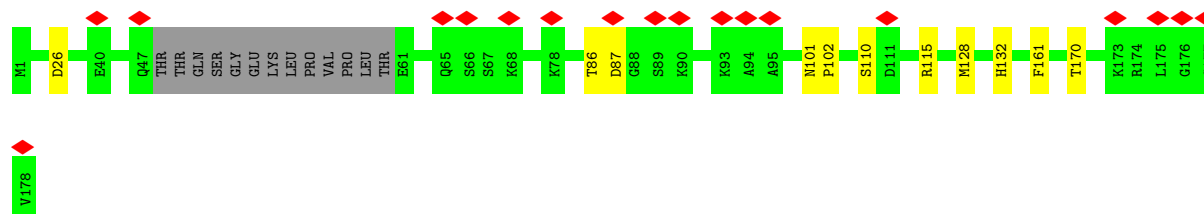
- Molecule 17: COX6b-1

Chain 6B: 

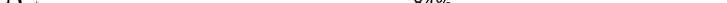


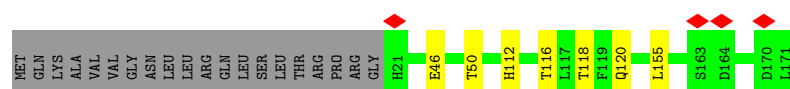
- Molecule 18: COX7a

Chain 7A: 

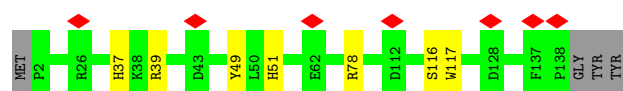


- Molecule 19: COX7c

Chain 7C:  84% 12%



- Molecule 20: NDUFA1



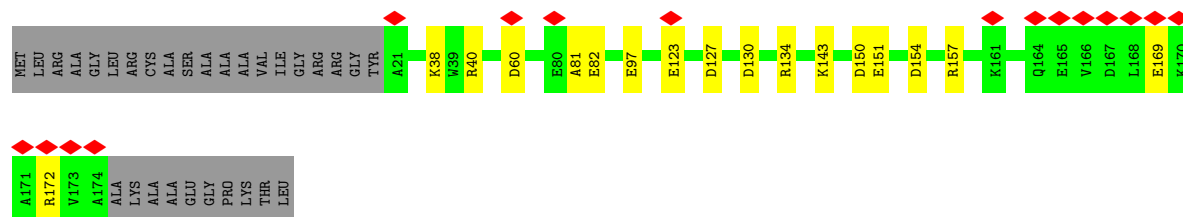
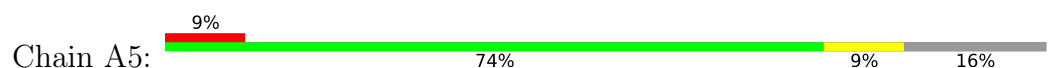
• Molecule 21: NDUFA2



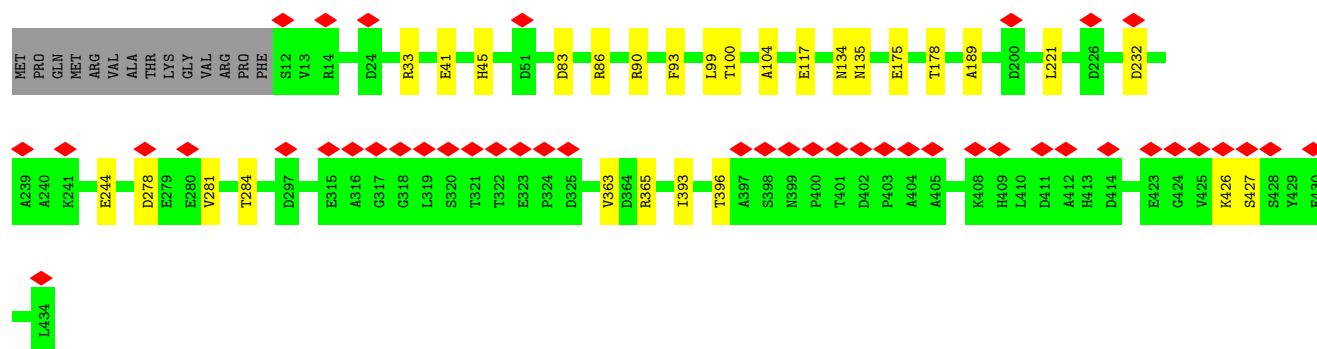
• Molecule 22: NDUFA3



• Molecule 23: NDUFA5



• Molecule 24: NDUFA6

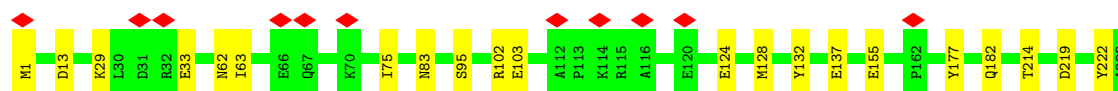


• Molecule 25: NDUFA7

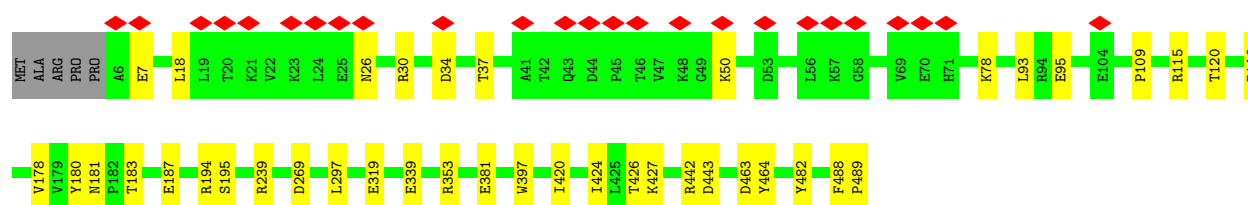




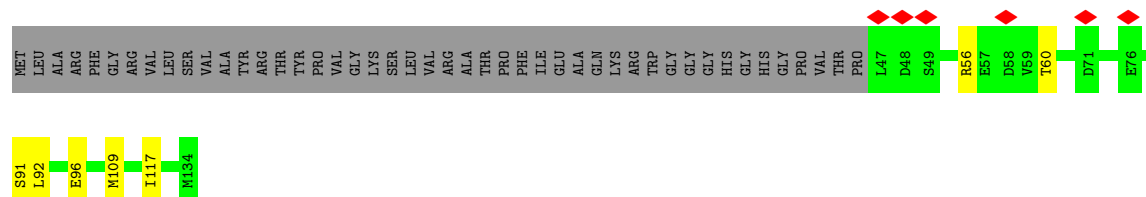
• Molecule 26: NDUFA8



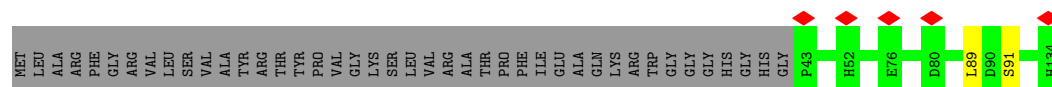
• Molecule 27: NDUFA9



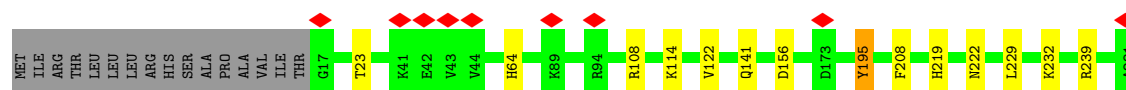
• Molecule 28: NDUFAB1-alpha



• Molecule 29: NDUFAB1-beta

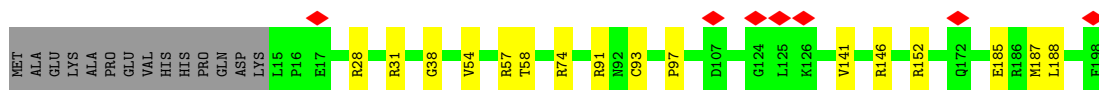


• Molecule 30: NDUFA12

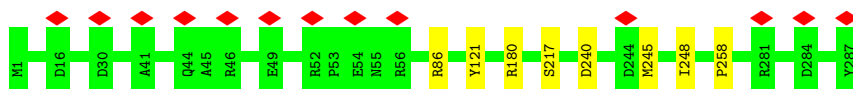


• Molecule 31: NDUFA13

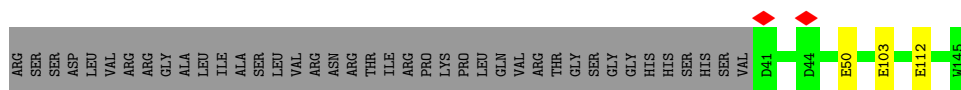




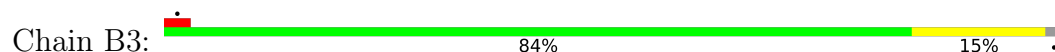
• Molecule 32: NDUFA11



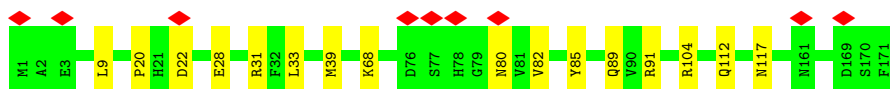
• Molecule 33: NDUFB2



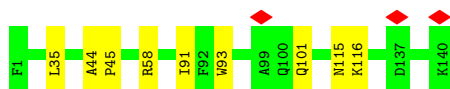
• Molecule 34: NDUFB3



• Molecule 35: NDUFB4



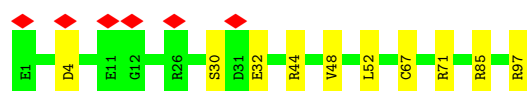
• Molecule 36: NDUFB5



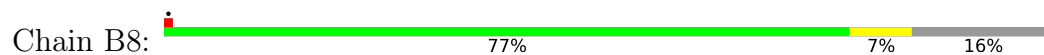
• Molecule 37: NDUFB6



• Molecule 38: NDUFB7



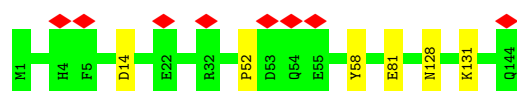
• Molecule 39: NDUFB8



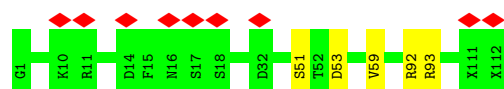
• Molecule 40: NDUFB9



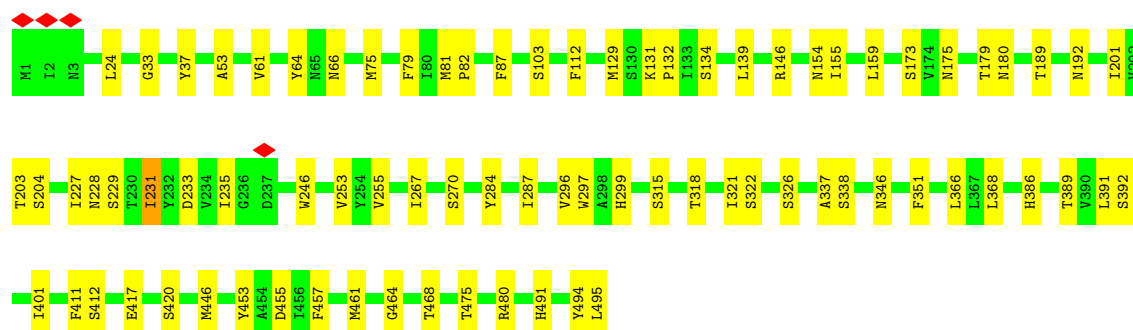
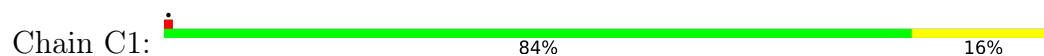
• Molecule 41: NDUFB10



• Molecule 42: NDUFB11



• Molecule 43: Cytochrome c oxidase subunit 1

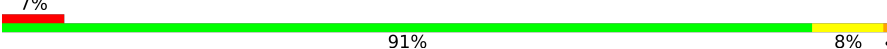


• Molecule 44: Cytochrome c oxidase subunit 2

Chain C2:  88% 11% .



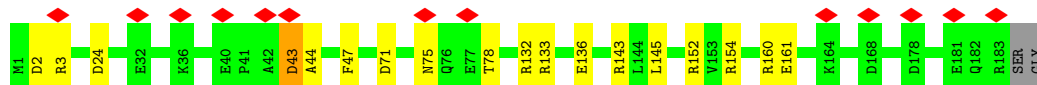
- Molecule 45: Putative NADH dehydrogenase subunit 6

Chain C3:  7% 91% 8% .



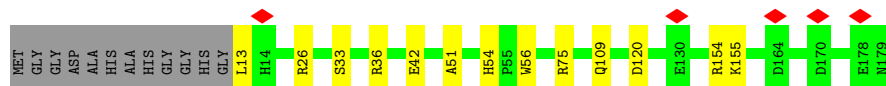
- Molecule 46: NDUFC2

Chain C4:  7% 89% 9% ..



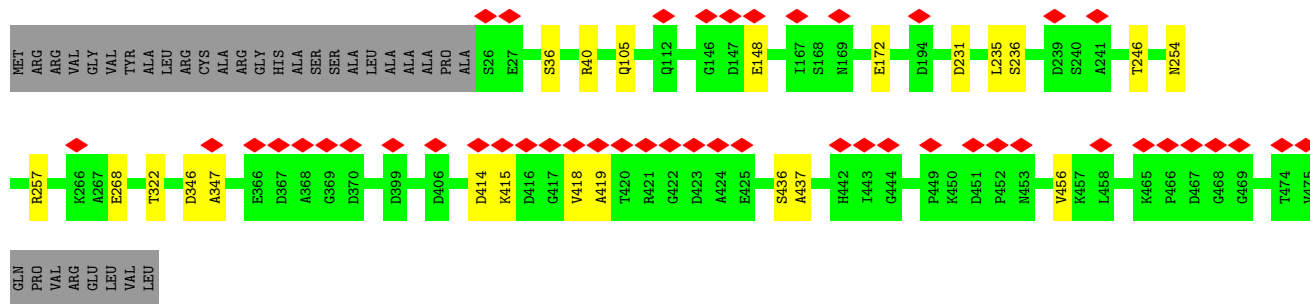
- Molecule 47: COX4

Chain DC:  86% 7% 7%

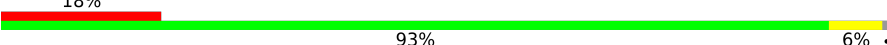


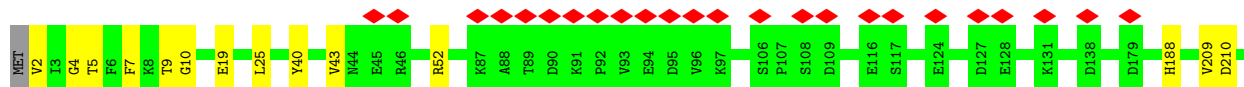
- Molecule 48: NDUEG1

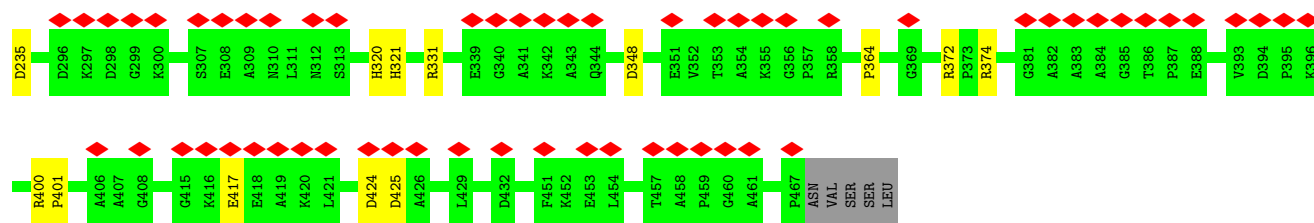
Chain E1:  10% 89% 5% 7%



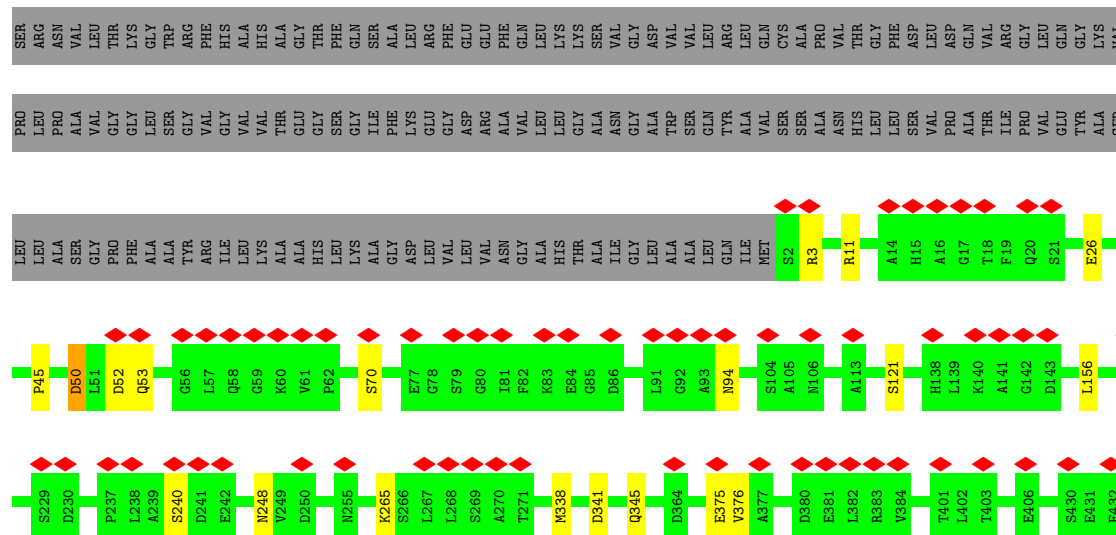
- Molecule 49: NDUEG2

Chain E2:  18% 93% 6% .

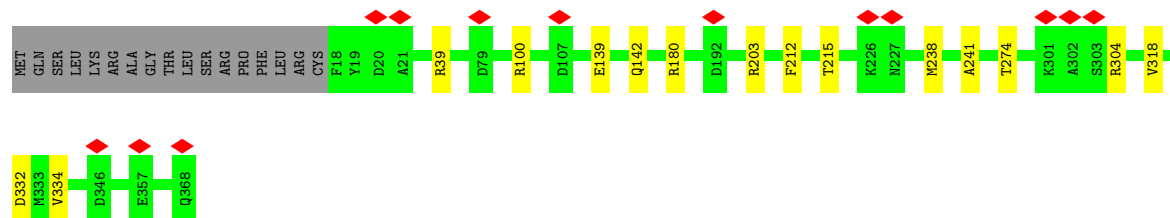




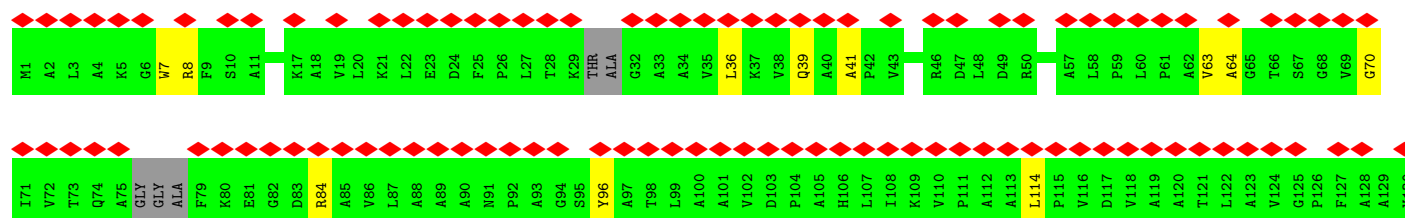
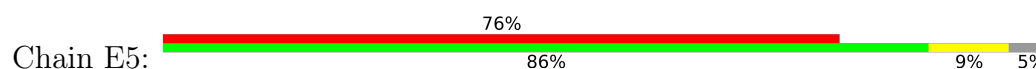
• Molecule 50: NDUEG3

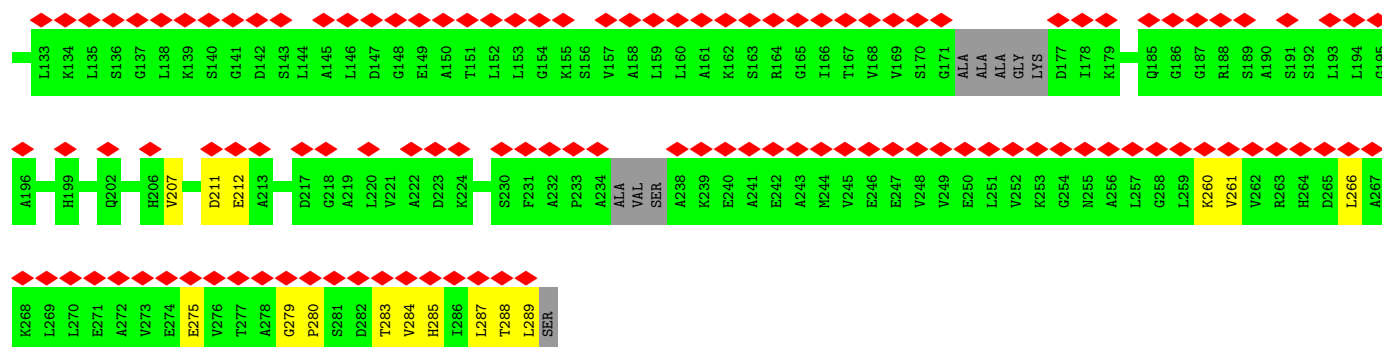


• Molecule 51: NDUEG4

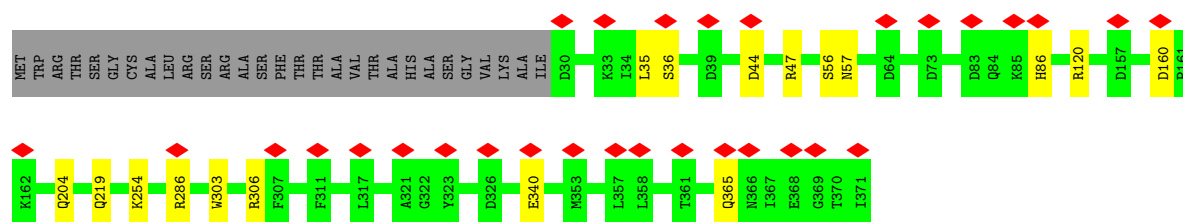
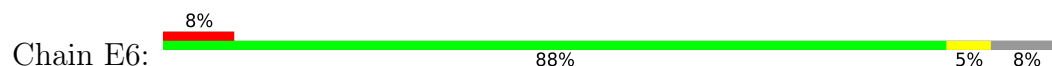


• Molecule 52: NDUEG5

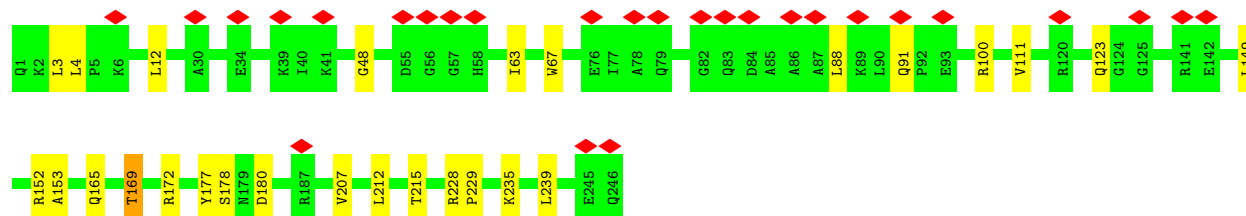
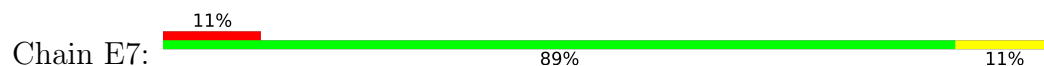




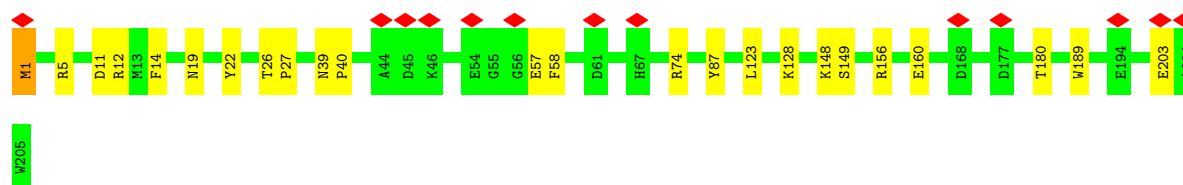
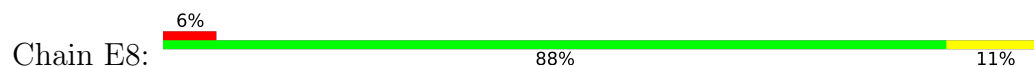
• Molecule 53: NDUEG6



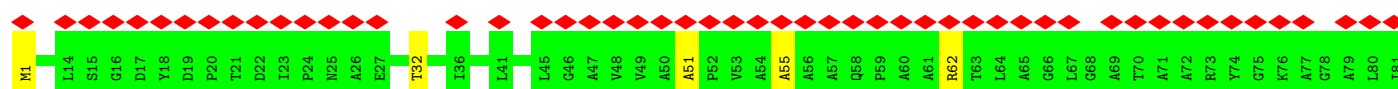
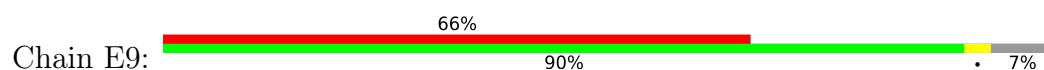
• Molecule 54: NDUEG7

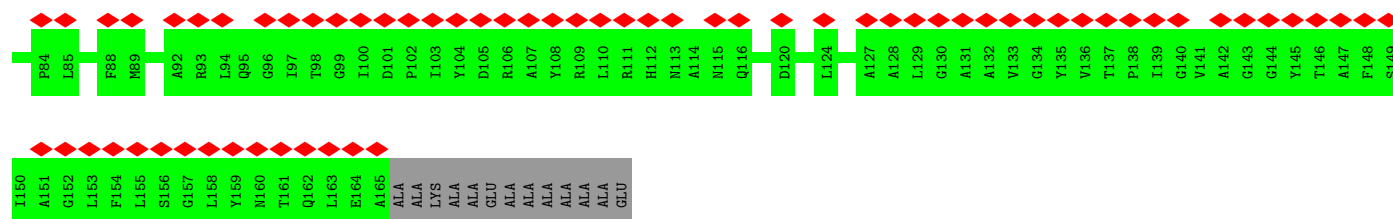


• Molecule 55: NDUEG8

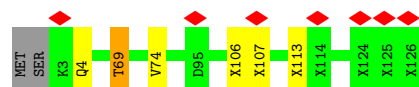


• Molecule 56: NDUEG9

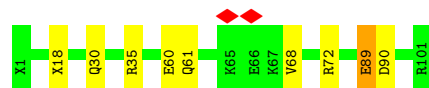
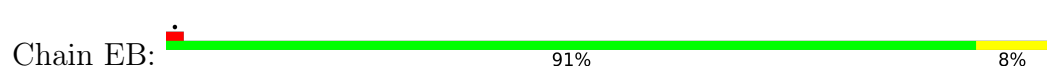




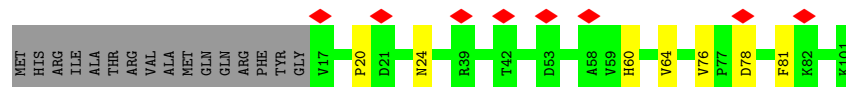
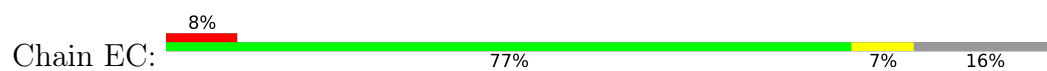
• Molecule 57: NDUEG10



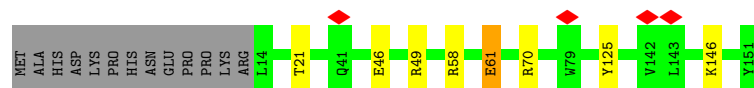
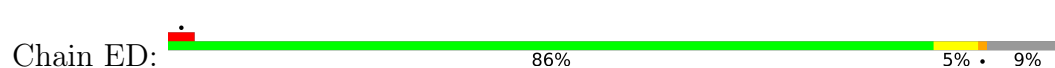
• Molecule 58: NDUEG11



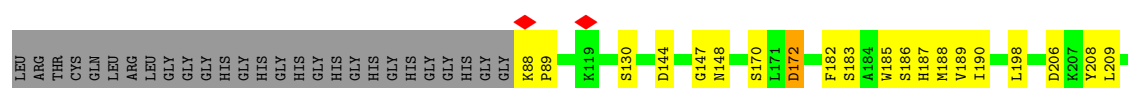
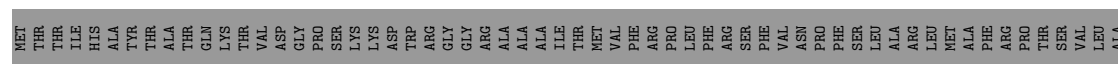
• Molecule 59: NDUEG11



• Molecule 60: NDUEG13



• Molecule 61: NDUFX



Chain G1:

MTT
ALA
LVS
LEU
THR
TRP
LEU
LVS
ASN
LEU
L11
N12
T21
R28
S35
A36
E37
R38
D39
H105
R108
G112
R113
W114
F123
D124
F127
R133
W169
N184
A187
P205
K206
S207
E211
G228
G233
A246
D251
V278

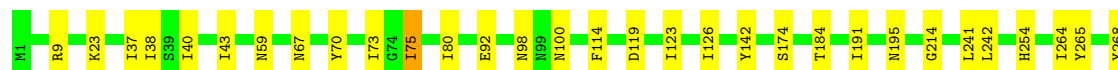
R294
P295
A296
R297
D304
H321
E326
D339
Q354
A355
H356
R360
K370
D388
D389
R403
M413
Q416
R419
P420
V421
Y426
A436

Chain G2:

Position	Residue	Category
1	MET	Grey
2	P2	Green
3	ARG	Green
4	SER	Green
5	HIS	Green
6	VAL	Yellow
7	ALA	Yellow
8	ARG	Yellow
9	ALA	Yellow
10	ALA	Yellow
11	PRO	Yellow
12	ASN	Yellow
13	VAL	Yellow
14	SER	Yellow
15	PRO	Yellow
16	GLY	Yellow
17	ASN	Yellow
18	ILE	Yellow
19	ALA	Yellow
20	ALA	Yellow
21	GLY	Yellow
22	P133	Yellow
23	SER	Green
24	C134	Green
25	ALA	Green
26	Q135	Green
27	ALA	Green
28	Y141	Green
29	ALA	Green
30	K153	Green
31	L172	Green
32	V181	Green
33	K184	Green
34	S185	Green
35	T190	Green
36	T191	Green
37	E192	Green
38	ALA	Green
39	E195	Green
40	E203	Green
41	ALA	Green
42	N215	Yellow
43	L218	Yellow
44	I219	Yellow
45	ALA	Yellow
46	D231	Yellow
47	Q236	Green
48	L237	Green
49	ASN	Grey
50	GLU	Grey
51	GLY	Grey
52	ASN	Grey
53	GLU	Grey
54	PHE	Grey
55	TYP	Grey

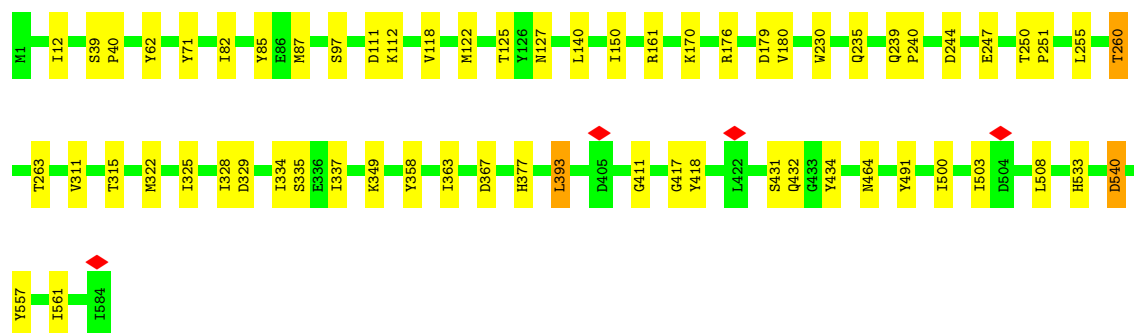
Chain G3:

[illegible]





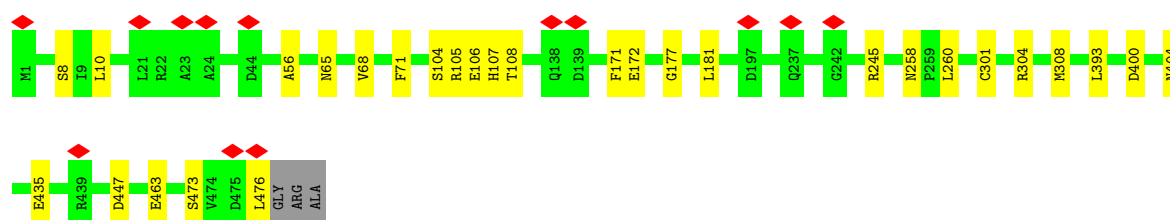
• Molecule 69: ND5



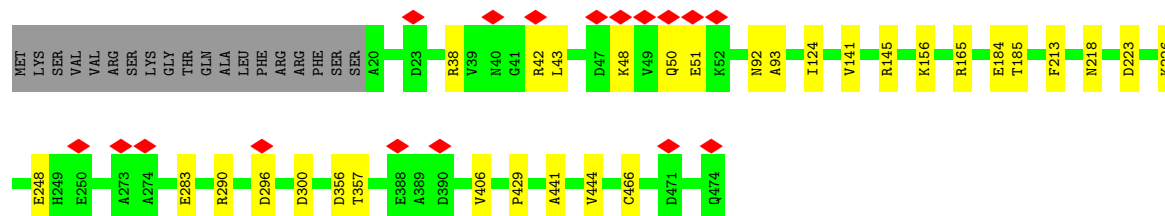
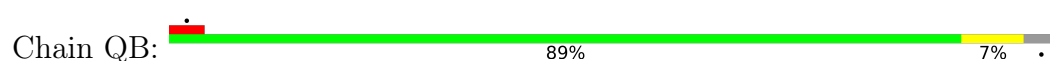
• Molecule 70: MPP-beta



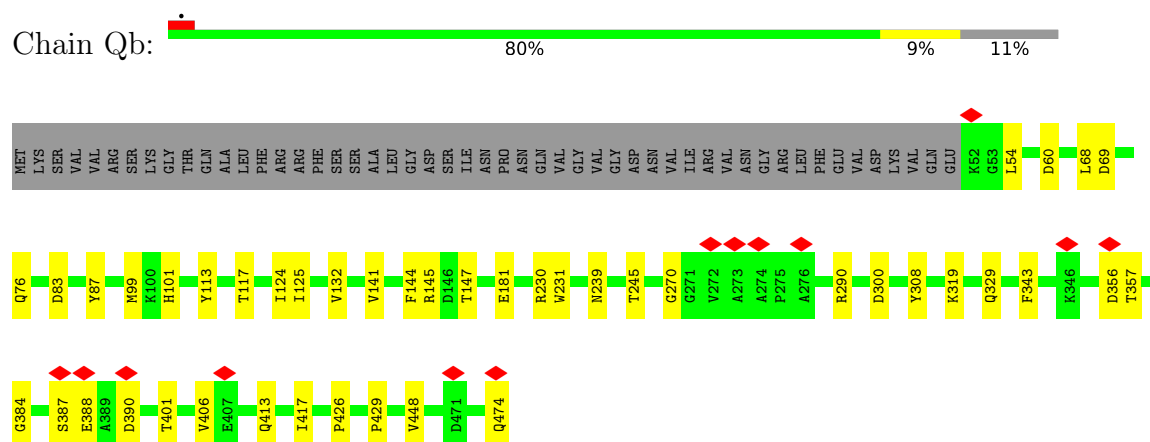
• Molecule 70: MPP-beta



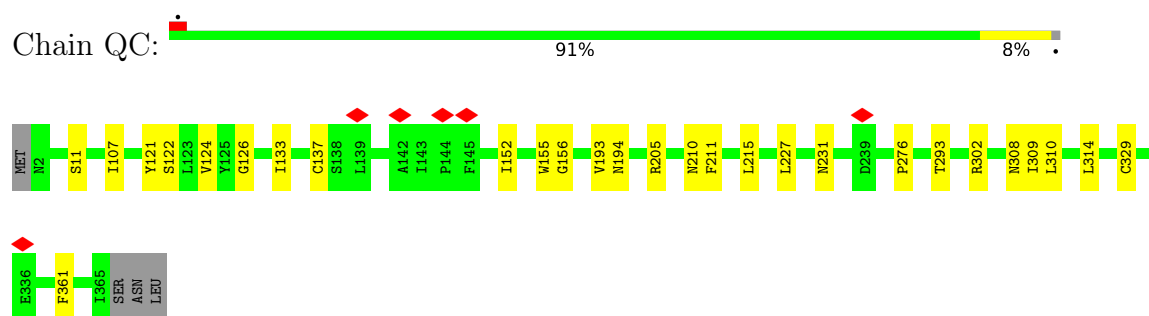
• Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



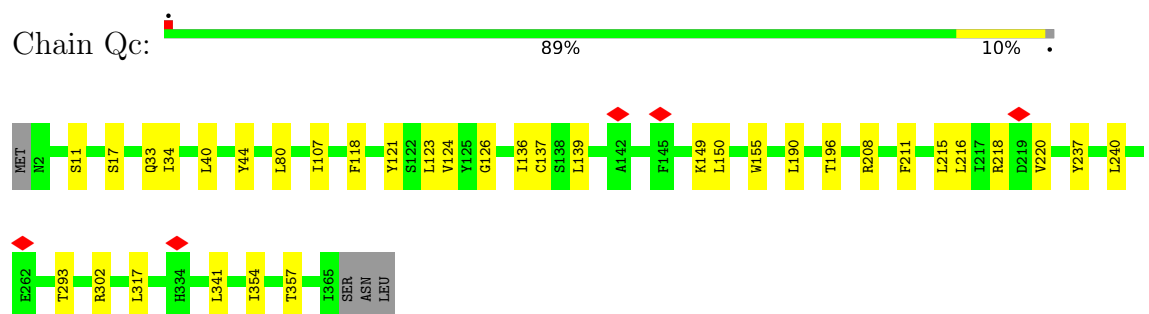
- Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



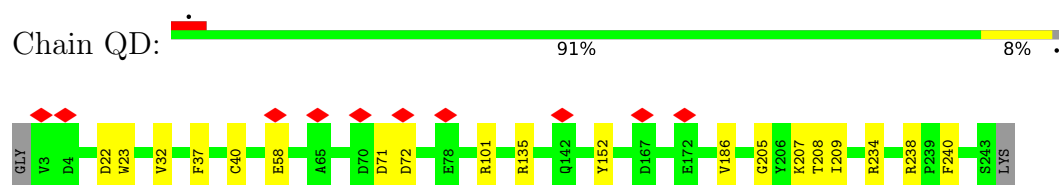
- Molecule 72: Cytochrome b



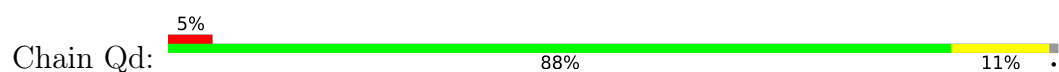
- Molecule 72: Cytochrome b

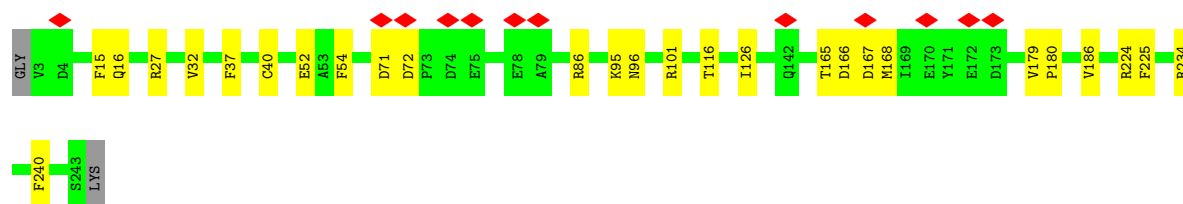


- Molecule 73: Cytochrome c1, heme protein

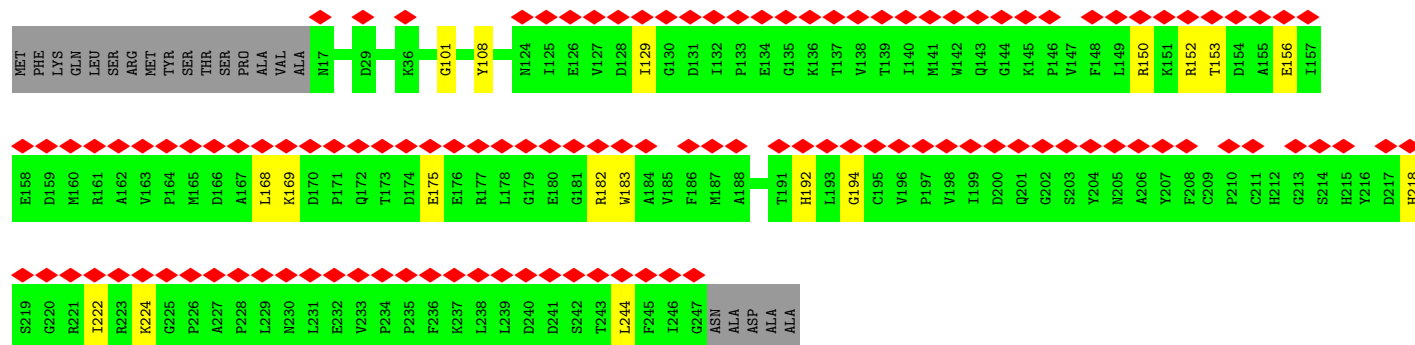
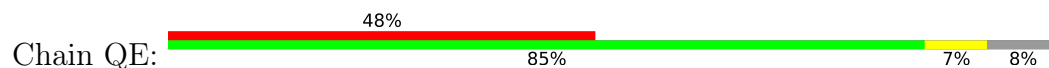


- Molecule 73: Cytochrome c1, heme protein

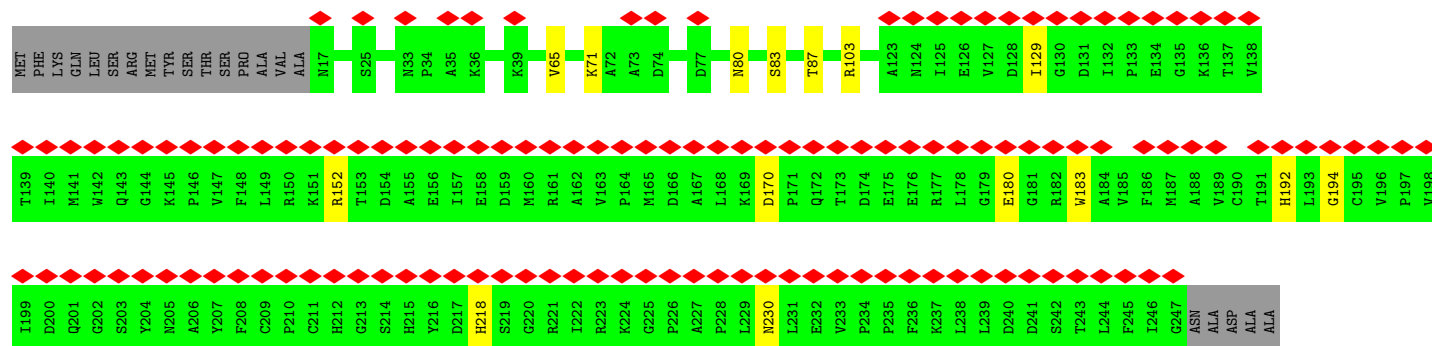
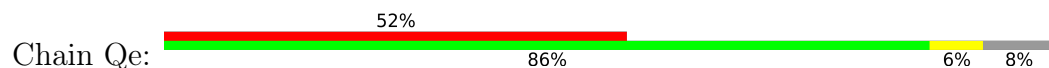




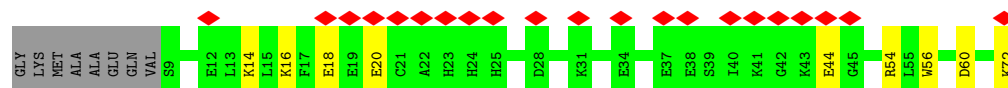
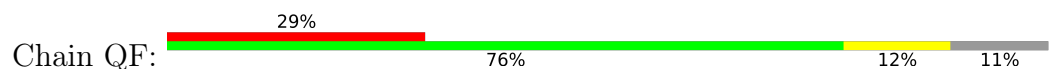
• Molecule 74: UQCRFS1



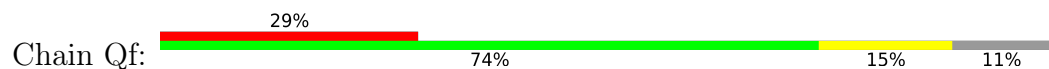
• Molecule 74: UQCRFS1

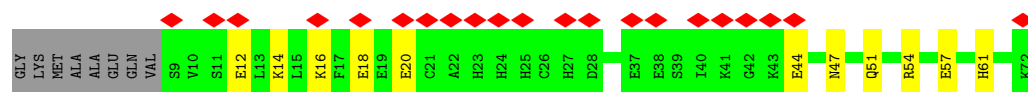


• Molecule 75: UQCRH

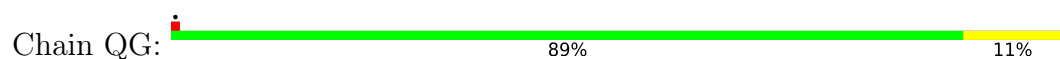


• Molecule 75: UQCRH

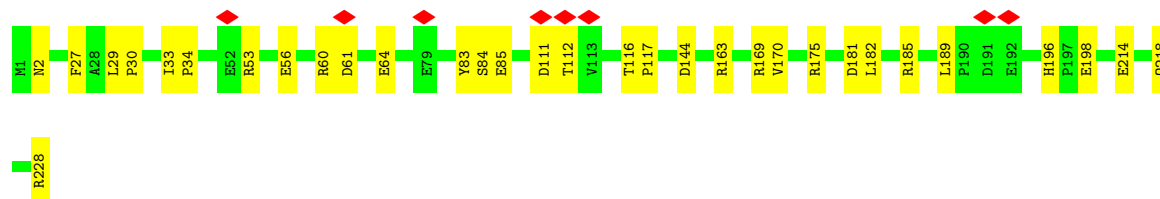




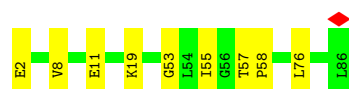
• Molecule 76: UQCRB



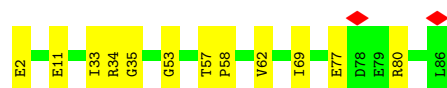
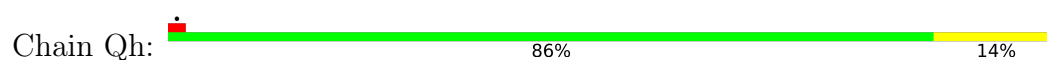
• Molecule 76: UQCRB



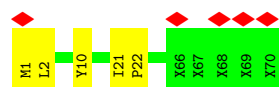
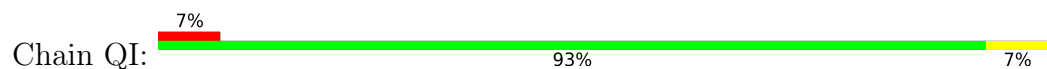
• Molecule 77: UQCRQ



• Molecule 77: UQCRQ

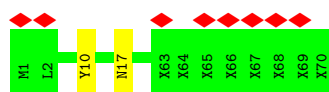


• Molecule 78: UQCR9

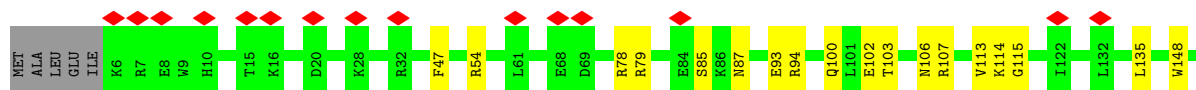
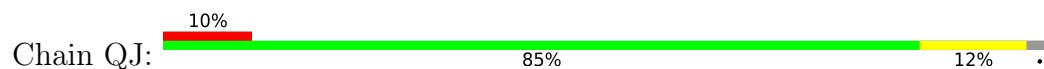


• Molecule 78: UQCR9

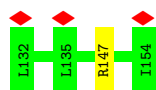
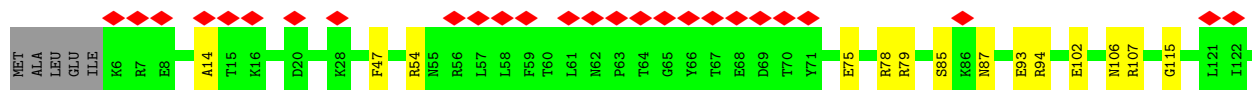
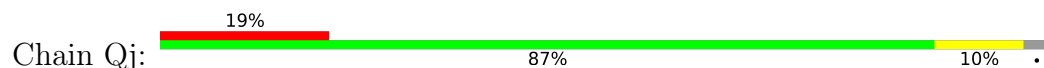




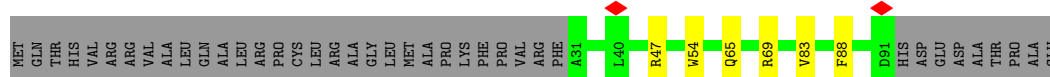
• Molecule 79: UQCR10



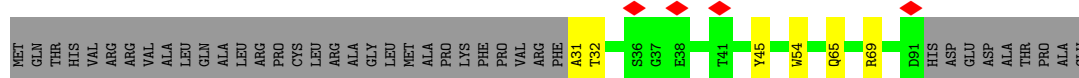
• Molecule 79: UQCR10



• Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial



• Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

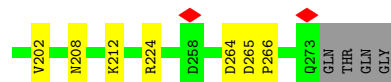
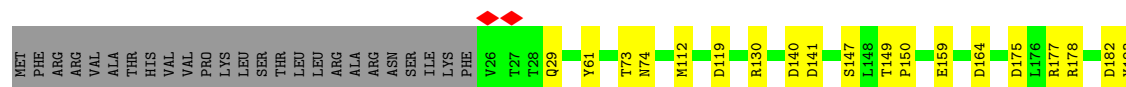
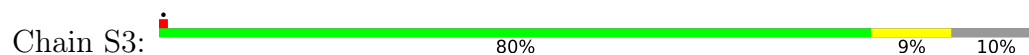


• Molecule 81: NDUFS2

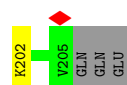
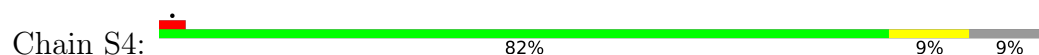




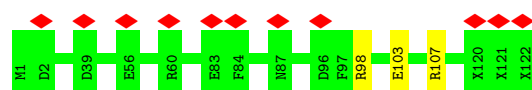
- Molecule 82: NDUFS3



- Molecule 83: NDUFS4



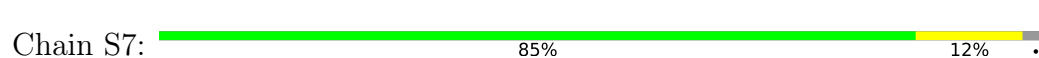
- Molecule 84: NDUFS5



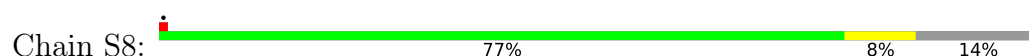
- Molecule 85: NDUFS6

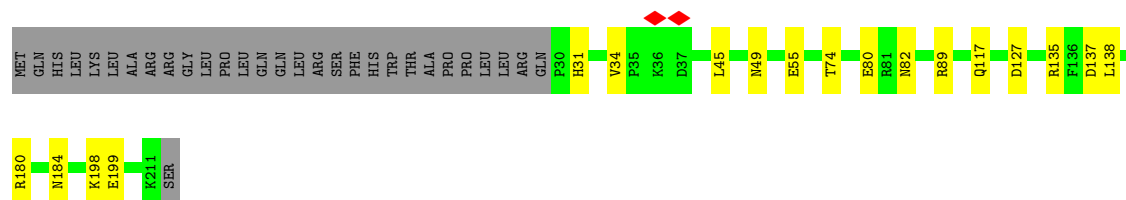


- Molecule 86: NDUFS7

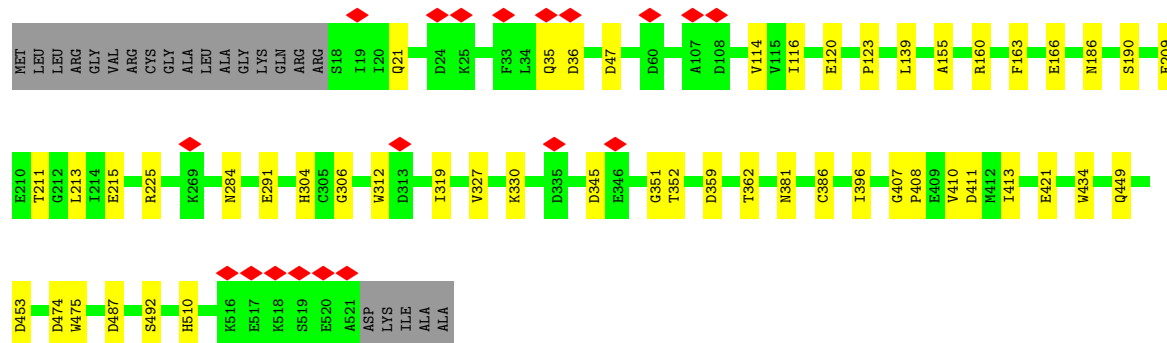


- Molecule 87: NDUFS8

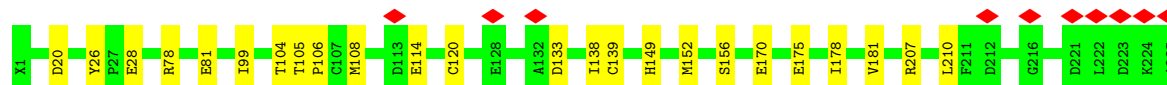
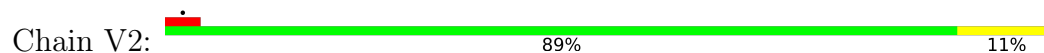




• Molecule 88: NDUFV1



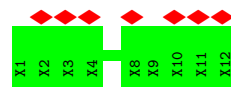
• Molecule 89: NDUFV2



• Molecule 90: poly(UNK)



• Molecule 90: poly(UNK)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	345048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	37.689	Depositor
Minimum map value	-25.803	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.049	Depositor
Recommended contour level	5	Depositor
Map size (Å)	537.60004, 537.60004, 537.60004	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FES, HEA, K, PC1, HEM, HEC, PX2, U10, FMN, 2MR, CU, MG, CDL, S12, SF4, NDP, 3PE, ZMP

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	0.28	0/2858	0.36	0/3878
2	1B	0.25	0/4306	0.30	0/5854
3	2B	0.28	0/958	0.36	0/1306
4	4A	0.18	0/1650	0.25	0/2235
5	4C	0.20	0/1051	0.27	0/1432
6	4D	0.21	0/1379	0.31	0/1867
7	4E	0.16	0/1376	0.26	0/1864
8	4F	0.19	0/641	0.28	0/867
9	4G	0.21	0/2391	0.28	0/3240
10	4H	0.20	0/1640	0.29	0/2224
11	4I	0.27	0/2255	0.32	0/3059
12	4J	0.25	0/736	0.29	0/1008
13	4L	0.26	0/924	0.30	0/1261
14	5B	0.29	0/1294	0.37	0/1759
15	5C	0.24	0/1616	0.30	0/2192
16	6A	0.19	0/777	0.28	0/1055
17	6B	0.20	0/2343	0.26	0/3174
18	7A	0.21	0/1359	0.30	0/1835
19	7C	0.25	0/1299	0.30	0/1777
20	A1	0.20	0/1108	0.28	0/1511
21	A2	0.22	0/1530	0.30	0/2089
22	A3	0.23	0/1079	0.30	0/1453
23	A5	0.23	0/1282	0.28	0/1737
24	A6	0.22	0/3395	0.28	0/4608
25	A7	0.25	0/1194	0.33	0/1619
26	A8	0.21	0/1879	0.27	0/2543
27	A9	0.25	0/3920	0.32	0/5335
28	AB	0.21	0/704	0.25	0/951
29	AC	0.25	0/736	0.28	0/1000
30	AL	0.25	0/2317	0.32	0/3136
31	AM	0.22	0/1533	0.26	0/2079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AN	0.22	0/2382	0.26	0/3249
33	B2	0.24	0/947	0.27	0/1291
34	B3	0.27	0/326	0.29	0/441
35	B4	0.25	0/1419	0.30	0/1922
36	B5	0.26	0/1111	0.32	0/1505
37	B6	0.24	0/803	0.29	0/1087
38	B7	0.23	0/877	0.27	0/1172
39	B8	0.25	0/1273	0.29	0/1733
40	B9	0.25	0/1274	0.32	0/1728
41	BL	0.25	0/1266	0.29	0/1710
42	BM	0.24	0/876	0.30	0/1192
43	C1	0.29	0/4054	0.38	0/5516
44	C2	0.26	0/1620	0.36	0/2207
45	C3	0.22	0/1416	0.31	0/1945
46	C4	0.24	0/1592	0.30	0/2158
47	DC	0.25	0/1410	0.31	0/1914
48	E1	0.21	0/3596	0.29	0/4879
49	E2	0.18	0/3658	0.26	0/4983
50	E3	0.19	0/3320	0.28	0/4520
51	E4	0.22	0/2850	0.27	0/3884
52	E5	0.14	0/2004	0.35	0/2721
53	E6	0.23	0/2954	0.29	0/4004
54	E7	0.22	0/1931	0.32	0/2618
55	E8	0.24	0/1747	0.31	0/2367
56	E9	0.13	0/1239	0.25	0/1690
57	EA	0.27	0/858	0.28	0/1163
58	EB	0.20	0/650	0.25	0/863
59	EC	0.19	0/676	0.30	0/925
60	ED	0.22	0/1176	0.29	0/1590
61	FX	0.29	0/2035	0.36	0/2763
62	G1	0.25	0/3443	0.33	0/4686
63	G2	0.23	0/1832	0.32	0/2476
64	G3	0.22	0/1957	0.34	0/2646
65	N1	0.24	0/2672	0.35	0/3639
66	N2	0.28	0/2582	0.36	0/3530
67	N3	0.26	0/1068	0.37	0/1456
67	N6	0.23	0/1275	0.35	0/1730
68	N4	0.27	0/4105	0.38	0/5594
69	N5	0.27	0/4963	0.38	0/6758
70	QA	0.23	0/3838	0.31	0/5193
70	Qa	0.22	0/3838	0.30	0/5193
71	QB	0.24	0/3532	0.31	0/4805
71	Qb	0.24	0/3288	0.30	0/4474

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
72	QC	0.26	0/3058	0.33	0/4178
72	Qc	0.27	0/3058	0.33	0/4178
73	QD	0.25	0/2027	0.31	0/2760
73	Qd	0.24	0/2027	0.33	0/2760
74	QE	0.18	0/1842	0.30	0/2502
74	Qe	0.17	0/1842	0.29	0/2502
75	QF	0.18	0/526	0.27	0/702
75	Qf	0.17	0/526	0.27	0/702
76	QG	0.28	0/1987	0.34	0/2696
76	Qg	0.27	0/1987	0.34	0/2696
77	QH	0.24	0/717	0.31	0/966
77	Qh	0.23	0/717	0.33	0/966
78	QI	0.25	0/251	0.28	0/340
78	Qi	0.22	0/251	0.27	0/340
79	QJ	0.20	0/1243	0.27	0/1693
79	Qj	0.19	0/1243	0.27	0/1693
80	QK	0.22	0/498	0.28	0/677
80	Qk	0.21	0/498	0.27	0/677
81	S2	0.29	0/3244	0.35	0/4403
82	S3	0.28	0/2112	0.37	0/2874
83	S4	0.24	0/1573	0.32	0/2107
84	S5	0.19	0/960	0.25	0/1291
85	S6	0.26	0/1232	0.32	0/1659
86	S7	0.28	0/1558	0.33	0/2120
87	S8	0.29	0/1485	0.33	0/2010
88	V1	0.22	0/3990	0.32	0/5394
89	V2	0.21	0/1787	0.30	0/2428
All	All	0.24	0/183502	0.31	0/249182

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2801	2700	2710	20	0
2	1B	4198	4159	4175	26	0
3	2B	1070	989	1009	6	0
4	4A	1612	1608	1617	12	0
5	4C	1022	1027	1029	6	0
6	4D	1349	1359	1363	11	0
7	4E	1333	1279	1283	8	0
8	4F	620	626	627	1	0
9	4G	2351	2340	2343	20	0
10	4H	1606	1644	1648	12	0
11	4I	2178	2046	2058	17	0
12	4J	711	688	689	1	0
13	4L	890	878	880	5	0
14	5B	1258	1184	1192	14	0
15	5C	1571	1546	1550	10	0
16	6A	750	747	749	9	0
17	6B	2285	2229	2239	14	0
18	7A	1319	1284	1295	9	0
19	7C	1254	1183	1190	4	0
20	A1	1071	1026	1030	5	0
21	A2	1493	1474	1478	10	0
22	A3	1050	1039	1041	4	0
23	A5	1261	1248	1251	9	0
24	A6	3328	3280	3293	23	0
25	A7	1154	1118	1123	14	0
26	A8	1822	1726	1736	25	0
27	A9	3829	3850	3857	27	0
28	AB	694	673	677	4	0
29	AC	721	697	702	2	0
30	AL	2237	2172	2180	11	0
31	AM	1487	1448	1452	17	0
32	AN	2306	2267	2275	6	0
33	B2	913	857	858	3	0
34	B3	449	309	312	6	0
35	B4	1377	1358	1364	10	0
36	B5	1112	1069	1075	8	0
37	B6	773	747	751	3	0
38	B7	857	835	841	6	0
39	B8	1224	1127	1136	9	0
40	B9	1236	1207	1212	11	0
41	BL	1227	1179	1185	4	0
42	BM	910	827	829	4	0
43	C1	3938	3980	3999	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	C2	1585	1647	1652	16	0
45	C3	1378	1413	1419	10	0
46	C4	1545	1517	1519	12	0
47	DC	1366	1362	1366	9	0
48	E1	3512	3496	3510	13	0
49	E2	3563	3540	3554	18	0
50	E3	3255	3263	3279	15	0
51	E4	2770	2732	2742	8	0
52	E5	1977	2069	2075	21	0
53	E6	2871	2758	2767	11	0
54	E7	1888	1892	1903	16	0
55	E8	1691	1663	1668	19	0
56	E9	1212	1224	1228	3	0
57	EA	961	832	835	5	0
58	EB	774	631	635	6	0
59	EC	660	663	666	5	0
60	ED	1142	1131	1134	5	0
61	FX	1967	1849	1858	28	0
62	G1	3347	3205	3222	29	0
63	G2	1804	1846	1850	12	0
64	G3	1961	1944	1950	13	0
65	N1	2605	2726	2729	25	0
66	N2	2512	2589	2592	31	0
67	N3	1037	1057	1057	11	0
67	N6	1257	1385	1385	13	0
68	N4	4001	4214	4224	27	0
69	N5	4837	5032	5046	38	0
70	QA	3750	3658	3668	23	0
70	Qa	3750	3658	3668	20	0
71	QB	3458	3431	3443	18	0
71	Qb	3216	3192	3204	27	0
72	QC	2975	3064	3076	16	0
72	Qc	2975	3064	3076	30	0
73	QD	1959	1858	1864	17	0
73	Qd	1959	1858	1865	25	0
74	QE	1795	1776	1780	12	0
74	Qe	1795	1776	1780	10	0
75	QF	515	499	505	5	0
75	Qf	515	503	509	5	0
76	QG	1932	1870	1880	21	0
76	Qg	1932	1870	1880	25	0
77	QH	701	692	694	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
77	Qh	701	692	694	13	0
78	QI	449	293	293	4	0
78	Qi	449	293	293	2	0
79	QJ	1206	1212	1216	14	0
79	Qj	1206	1212	1216	14	0
80	QK	485	499	500	6	0
80	Qk	485	499	500	6	0
81	S2	3173	3101	3114	28	0
82	S3	2050	1928	1936	16	0
83	S4	1536	1502	1505	15	0
84	S5	991	895	898	2	0
85	S6	1200	1192	1198	10	0
86	S7	1545	1500	1503	19	0
87	S8	1451	1392	1397	15	0
88	V1	3897	3827	3837	31	0
89	V2	1759	1701	1710	13	0
90	A	60	16	16	0	0
90	B	60	16	16	0	0
91	1A	4	0	0	0	0
91	QE	4	0	0	0	0
91	Qe	4	0	0	0	0
91	V2	4	0	0	0	0
92	1A	16	0	0	0	0
92	S7	8	0	0	1	0
92	S8	16	0	0	0	0
92	V1	8	0	0	0	0
93	1A	1	0	0	0	0
94	4A	93	137	137	0	0
94	4E	35	44	44	0	0
94	7A	36	46	46	0	0
94	A1	80	111	111	1	0
94	A9	66	80	80	0	0
94	AL	50	77	77	0	0
94	AM	97	148	148	1	0
94	AN	48	73	73	0	0
94	B5	108	176	176	3	0
94	B8	37	48	48	0	0
94	C1	50	77	77	0	0
94	C3	51	79	79	0	0
94	E4	51	79	79	0	0
94	E8	171	250	250	0	0
94	E9	35	44	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	ED	95	144	144	0	0
94	G2	38	50	50	0	0
94	N1	89	129	129	0	0
94	N3	42	61	61	0	0
94	N4	126	180	180	0	0
94	N5	36	46	46	0	0
94	QC	54	88	88	0	0
94	QD	31	36	36	0	0
94	QI	36	46	46	1	0
94	Qc	85	124	124	0	0
94	Qe	36	46	46	0	0
94	Qg	28	30	30	0	0
94	Qj	54	88	88	0	0
95	4D	86	126	126	0	0
95	7A	41	59	59	0	0
95	B4	40	57	57	1	0
95	C1	80	108	108	0	0
95	E9	51	82	82	0	0
95	N4	41	56	56	0	0
95	N5	51	82	82	0	0
96	4D	35	44	44	0	0
97	4E	72	91	91	0	0
97	7C	90	130	130	1	0
97	A3	58	60	60	1	0
97	A9	64	72	72	1	0
97	AL	132	152	152	0	0
97	AM	144	182	182	4	0
97	B3	65	74	74	1	0
97	B8	70	87	87	1	0
97	BM	58	60	60	0	0
97	C4	261	372	372	2	0
97	E4	72	91	91	2	0
97	E6	58	60	60	1	0
97	E7	68	80	80	0	0
97	EA	114	116	116	1	0
97	N1	70	84	84	1	0
97	N5	93	136	136	0	0
97	QC	56	56	56	0	0
97	QD	69	82	82	0	0
97	QH	136	163	163	2	0
97	QJ	58	60	60	1	0
97	Qc	54	52	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	Qd	100	156	156	2	0
97	Qe	60	64	64	0	0
97	Qh	65	74	74	0	0
97	Qj	48	40	40	1	0
98	5B	1	0	0	0	0
98	E7	1	0	0	0	0
98	S6	1	0	0	0	0
99	A9	48	26	26	0	0
100	AB	36	0	47	3	0
100	AC	36	0	47	7	0
101	C1	120	0	108	21	0
102	C1	1	0	0	0	0
102	C2	2	0	0	0	0
103	C1	1	0	0	0	0
104	C2	36	0	52	4	0
104	QJ	72	0	104	8	0
105	N4	43	55	55	4	0
106	QC	86	0	60	2	0
106	Qc	86	0	60	10	0
107	QD	43	0	31	5	0
107	Qd	43	0	32	6	0
108	V1	31	19	19	0	0
All	All	185125	183093	184288	1123	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 1123 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)
73:Qd:40:CYS:SG	107:Qd:301:HEC:HAC	1.36	1.63
73:QD:40:CYS:SG	107:QD:301:HEC:CAC	2.03	1.45
73:Qd:40:CYS:SG	107:Qd:301:HEC:CAC	2.07	1.43
101:C1:501:HEA:HBC1	101:C1:501:HEA:HHD	1.46	0.97
52:E5:287:LEU:O	52:E5:289:LEU:N	1.98	0.94

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	350/385 (91%)	333 (95%)	17 (5%)	0	100	100
2	1B	523/527 (99%)	509 (97%)	14 (3%)	0	100	100
3	2B	112/142 (79%)	102 (91%)	10 (9%)	0	100	100
4	4A	202/246 (82%)	197 (98%)	5 (2%)	0	100	100
5	4C	121/139 (87%)	119 (98%)	2 (2%)	0	100	100
6	4D	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
7	4E	158/165 (96%)	155 (98%)	3 (2%)	0	100	100
8	4F	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
9	4G	295/315 (94%)	288 (98%)	7 (2%)	0	100	100
10	4H	203/221 (92%)	195 (96%)	8 (4%)	0	100	100
11	4I	263/274 (96%)	256 (97%)	7 (3%)	0	100	100
12	4J	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
13	4L	106/171 (62%)	105 (99%)	1 (1%)	0	100	100
14	5B	155/174 (89%)	152 (98%)	3 (2%)	0	100	100
15	5C	194/208 (93%)	187 (96%)	7 (4%)	0	100	100
16	6A	89/112 (80%)	82 (92%)	7 (8%)	0	100	100
17	6B	280/287 (98%)	276 (99%)	4 (1%)	0	100	100
18	7A	161/178 (90%)	158 (98%)	3 (2%)	0	100	100
19	7C	149/171 (87%)	146 (98%)	3 (2%)	0	100	100
20	A1	135/141 (96%)	126 (93%)	9 (7%)	0	100	100
21	A2	190/193 (98%)	187 (98%)	3 (2%)	0	100	100
22	A3	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
23	A5	152/184 (83%)	147 (97%)	5 (3%)	0	100	100
24	A6	421/437 (96%)	396 (94%)	25 (6%)	0	100	100
25	A7	134/136 (98%)	128 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	A8	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
27	A9	482/489 (99%)	462 (96%)	20 (4%)	0	100	100
28	AB	86/134 (64%)	86 (100%)	0	0	100	100
29	AC	90/134 (67%)	90 (100%)	0	0	100	100
30	AL	263/281 (94%)	249 (95%)	14 (5%)	0	100	100
31	AM	182/198 (92%)	178 (98%)	4 (2%)	0	100	100
32	AN	285/287 (99%)	279 (98%)	6 (2%)	0	100	100
33	B2	103/145 (71%)	103 (100%)	0	0	100	100
34	B3	32/62 (52%)	30 (94%)	2 (6%)	0	100	100
35	B4	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
36	B5	132/140 (94%)	130 (98%)	2 (2%)	0	100	100
37	B6	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
38	B7	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
39	B8	145/176 (82%)	142 (98%)	3 (2%)	0	100	100
40	B9	149/158 (94%)	143 (96%)	6 (4%)	0	100	100
41	BL	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
42	BM	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
43	C1	493/495 (100%)	474 (96%)	19 (4%)	0	100	100
44	C2	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
45	C3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
46	C4	181/185 (98%)	175 (97%)	6 (3%)	0	100	100
47	DC	165/179 (92%)	156 (94%)	9 (6%)	0	100	100
48	E1	448/483 (93%)	431 (96%)	17 (4%)	0	100	100
49	E2	464/472 (98%)	447 (96%)	17 (4%)	0	100	100
50	E3	430/594 (72%)	419 (97%)	11 (3%)	0	100	100
51	E4	349/368 (95%)	339 (97%)	10 (3%)	0	100	100
52	E5	266/290 (92%)	246 (92%)	19 (7%)	1 (0%)	30	58
53	E6	340/371 (92%)	336 (99%)	4 (1%)	0	100	100
54	E7	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
55	E8	203/205 (99%)	190 (94%)	13 (6%)	0	100	100
56	E9	163/178 (92%)	149 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	EA	96/126 (76%)	91 (95%)	5 (5%)	0	100	100
58	EB	73/101 (72%)	73 (100%)	0	0	100	100
59	EC	83/101 (82%)	77 (93%)	6 (7%)	0	100	100
60	ED	136/151 (90%)	132 (97%)	4 (3%)	0	100	100
61	FX	235/325 (72%)	224 (95%)	11 (5%)	0	100	100
62	G1	424/436 (97%)	408 (96%)	16 (4%)	0	100	100
63	G2	234/267 (88%)	221 (94%)	13 (6%)	0	100	100
64	G3	253/261 (97%)	238 (94%)	15 (6%)	0	100	100
65	N1	308/670 (46%)	292 (95%)	16 (5%)	0	100	100
66	N2	294/300 (98%)	274 (93%)	20 (7%)	0	100	100
67	N3	119/293 (41%)	116 (98%)	2 (2%)	1 (1%)	16	41
67	N6	152/293 (52%)	145 (95%)	7 (5%)	0	100	100
68	N4	476/478 (100%)	462 (97%)	14 (3%)	0	100	100
69	N5	582/584 (100%)	560 (96%)	22 (4%)	0	100	100
70	QA	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
70	Qa	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
71	QB	453/474 (96%)	443 (98%)	10 (2%)	0	100	100
71	Qb	421/474 (89%)	410 (97%)	11 (3%)	0	100	100
72	QC	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
72	Qc	362/368 (98%)	353 (98%)	9 (2%)	0	100	100
73	QD	239/243 (98%)	224 (94%)	15 (6%)	0	100	100
73	Qd	239/243 (98%)	215 (90%)	24 (10%)	0	100	100
74	QE	229/252 (91%)	218 (95%)	11 (5%)	0	100	100
74	Qe	229/252 (91%)	215 (94%)	14 (6%)	0	100	100
75	QF	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
75	Qf	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
76	QG	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
76	Qg	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
77	QH	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
77	Qh	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
78	QI	28/70 (40%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Qi	28/70 (40%)	28 (100%)	0	0	100	100
79	QJ	147/154 (96%)	143 (97%)	4 (3%)	0	100	100
79	Qj	147/154 (96%)	138 (94%)	9 (6%)	0	100	100
80	QK	59/100 (59%)	58 (98%)	1 (2%)	0	100	100
80	Qk	59/100 (59%)	58 (98%)	1 (2%)	0	100	100
81	S2	391/395 (99%)	373 (95%)	18 (5%)	0	100	100
82	S3	246/277 (89%)	235 (96%)	11 (4%)	0	100	100
83	S4	188/208 (90%)	179 (95%)	9 (5%)	0	100	100
84	S5	110/122 (90%)	105 (96%)	5 (4%)	0	100	100
85	S6	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
86	S7	195/207 (94%)	187 (96%)	8 (4%)	0	100	100
87	S8	180/212 (85%)	174 (97%)	6 (3%)	0	100	100
88	V1	502/526 (95%)	477 (95%)	25 (5%)	0	100	100
89	V2	220/225 (98%)	212 (96%)	8 (4%)	0	100	100
All	All	22046/24488 (90%)	21217 (96%)	827 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	E5	288	THR
67	N3	214	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	310/340 (91%)	308 (99%)	2 (1%)	78	92
2	1B	453/454 (100%)	453 (100%)	0	100	100
3	2B	109/111 (98%)	108 (99%)	1 (1%)	70	89
4	4A	173/207 (84%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4C	112/127 (88%)	112 (100%)	0	100	100
6	4D	146/147 (99%)	143 (98%)	3 (2%)	47	78
7	4E	142/145 (98%)	141 (99%)	1 (1%)	76	91
8	4F	62/62 (100%)	61 (98%)	1 (2%)	55	82
9	4G	247/264 (94%)	244 (99%)	3 (1%)	63	86
10	4H	176/189 (93%)	175 (99%)	1 (1%)	78	92
11	4I	230/238 (97%)	228 (99%)	2 (1%)	70	89
12	4J	75/75 (100%)	74 (99%)	1 (1%)	61	85
13	4L	96/151 (64%)	96 (100%)	0	100	100
14	5B	134/148 (90%)	132 (98%)	2 (2%)	57	83
15	5C	167/178 (94%)	166 (99%)	1 (1%)	78	92
16	6A	79/97 (81%)	79 (100%)	0	100	100
17	6B	238/243 (98%)	237 (100%)	1 (0%)	84	94
18	7A	138/150 (92%)	138 (100%)	0	100	100
19	7C	135/152 (89%)	134 (99%)	1 (1%)	76	91
20	A1	115/118 (98%)	114 (99%)	1 (1%)	70	89
21	A2	159/160 (99%)	159 (100%)	0	100	100
22	A3	104/104 (100%)	104 (100%)	0	100	100
23	A5	134/152 (88%)	131 (98%)	3 (2%)	45	77
24	A6	346/358 (97%)	346 (100%)	0	100	100
25	A7	119/119 (100%)	119 (100%)	0	100	100
26	A8	196/196 (100%)	196 (100%)	0	100	100
27	A9	420/424 (99%)	418 (100%)	2 (0%)	81	93
28	AB	79/114 (69%)	78 (99%)	1 (1%)	61	85
29	AC	80/111 (72%)	79 (99%)	1 (1%)	61	85
30	AL	228/242 (94%)	225 (99%)	3 (1%)	61	85
31	AM	156/168 (93%)	156 (100%)	0	100	100
32	AN	241/241 (100%)	240 (100%)	1 (0%)	84	94
33	B2	97/131 (74%)	97 (100%)	0	100	100
34	B3	30/31 (97%)	30 (100%)	0	100	100
35	B4	144/144 (100%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	B5	108/108 (100%)	108 (100%)	0	100	100
37	B6	82/82 (100%)	82 (100%)	0	100	100
38	B7	93/93 (100%)	92 (99%)	1 (1%)	65	86
39	B8	127/148 (86%)	126 (99%)	1 (1%)	73	90
40	B9	132/139 (95%)	130 (98%)	2 (2%)	57	83
41	BL	132/132 (100%)	132 (100%)	0	100	100
42	BM	93/93 (100%)	93 (100%)	0	100	100
43	C1	438/438 (100%)	434 (99%)	4 (1%)	70	89
44	C2	178/178 (100%)	176 (99%)	2 (1%)	65	86
45	C3	155/155 (100%)	153 (99%)	2 (1%)	61	85
46	C4	166/167 (99%)	164 (99%)	2 (1%)	63	86
47	DC	148/153 (97%)	146 (99%)	2 (1%)	59	84
48	E1	381/404 (94%)	379 (100%)	2 (0%)	81	93
49	E2	379/385 (98%)	378 (100%)	1 (0%)	86	95
50	E3	339/460 (74%)	337 (99%)	2 (1%)	78	92
51	E4	302/317 (95%)	300 (99%)	2 (1%)	76	91
52	E5	200/205 (98%)	198 (99%)	2 (1%)	68	88
53	E6	293/314 (93%)	289 (99%)	4 (1%)	59	84
54	E7	192/192 (100%)	188 (98%)	4 (2%)	47	78
55	E8	179/179 (100%)	178 (99%)	1 (1%)	78	92
56	E9	115/118 (98%)	115 (100%)	0	100	100
57	EA	84/86 (98%)	83 (99%)	1 (1%)	63	86
58	EB	70/70 (100%)	68 (97%)	2 (3%)	37	71
59	EC	73/86 (85%)	73 (100%)	0	100	100
60	ED	121/133 (91%)	119 (98%)	2 (2%)	53	81
61	FX	212/276 (77%)	209 (99%)	3 (1%)	59	84
62	G1	356/365 (98%)	348 (98%)	8 (2%)	45	77
63	G2	192/214 (90%)	189 (98%)	3 (2%)	55	82
64	G3	202/202 (100%)	202 (100%)	0	100	100
65	N1	295/639 (46%)	294 (100%)	1 (0%)	86	95
66	N2	285/289 (99%)	283 (99%)	2 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	N3	116/281 (41%)	115 (99%)	1 (1%)	70	89
67	N6	147/281 (52%)	146 (99%)	1 (1%)	76	91
68	N4	455/455 (100%)	449 (99%)	6 (1%)	61	85
69	N5	546/546 (100%)	537 (98%)	9 (2%)	55	82
70	QA	400/401 (100%)	398 (100%)	2 (0%)	81	93
70	Qa	400/401 (100%)	399 (100%)	1 (0%)	86	95
71	QB	369/386 (96%)	367 (100%)	2 (0%)	81	93
71	Qb	342/386 (89%)	341 (100%)	1 (0%)	86	95
72	QC	337/341 (99%)	335 (99%)	2 (1%)	78	92
72	Qc	337/341 (99%)	336 (100%)	1 (0%)	86	95
73	QD	206/207 (100%)	206 (100%)	0	100	100
73	Qd	206/207 (100%)	206 (100%)	0	100	100
74	QE	193/209 (92%)	190 (98%)	3 (2%)	55	82
74	Qe	193/209 (92%)	192 (100%)	1 (0%)	81	93
75	QF	58/63 (92%)	56 (97%)	2 (3%)	32	66
75	Qf	58/63 (92%)	55 (95%)	3 (5%)	21	51
76	QG	207/207 (100%)	205 (99%)	2 (1%)	68	88
76	Qg	207/207 (100%)	206 (100%)	1 (0%)	81	93
77	QH	71/71 (100%)	70 (99%)	1 (1%)	59	84
77	Qh	71/71 (100%)	71 (100%)	0	100	100
78	QI	27/27 (100%)	26 (96%)	1 (4%)	30	63
78	Qi	27/27 (100%)	27 (100%)	0	100	100
79	QJ	124/128 (97%)	123 (99%)	1 (1%)	73	90
79	Qj	124/128 (97%)	124 (100%)	0	100	100
80	QK	50/82 (61%)	50 (100%)	0	100	100
80	Qk	50/82 (61%)	50 (100%)	0	100	100
81	S2	335/336 (100%)	332 (99%)	3 (1%)	70	89
82	S3	224/250 (90%)	222 (99%)	2 (1%)	70	89
83	S4	159/172 (92%)	156 (98%)	3 (2%)	50	79
84	S5	102/102 (100%)	102 (100%)	0	100	100
85	S6	130/130 (100%)	129 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	S7	165/171 (96%)	162 (98%)	3 (2%)	51	80
87	S8	160/187 (86%)	159 (99%)	1 (1%)	78	92
88	V1	412/427 (96%)	411 (100%)	1 (0%)	87	96
89	V2	190/190 (100%)	184 (97%)	6 (3%)	34	68
All	All	19190/20883 (92%)	19041 (99%)	149 (1%)	70	90

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
75	QF	72	LYS
89	V2	108	MET
78	QI	2	LEU
81	S2	147	TYR
48	E1	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 420 such sidechains are listed below:

Mol	Chain	Res	Type
60	ED	139	HIS
68	N4	254	HIS
84	S5	75	GLN
62	G1	105	HIS
65	N1	530	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	2MR	S2	154	81	10,12,13	2.39	2 (20%)	5,13,15	0.98	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
81	2MR	S2	154	81	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	S2	154	2MR	CZ-NH2	5.07	1.44	1.33
81	S2	154	2MR	CZ-NE	4.97	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	S2	154	2MR	CG-CD-NE-CZ
81	S2	154	2MR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 116 ligands modelled in this entry, 8 are monoatomic - leaving 108 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$
97	CDL	N5	603	-	92,92,99	0.31	0	98,104,111	0.31	0
95	3PE	4D	202	-	50,50,50	0.31	0	53,55,55	0.36	0
96	S12	4D	203	-	33,34,34	0.78	0	36,40,40	0.97	3 (8%)
94	PC1	QC	404	-	53,53,53	0.30	0	59,61,61	0.33	0
97	CDL	E6	401	-	57,57,99	0.39	0	63,69,111	0.45	0
94	PC1	N4	505	-	53,53,53	0.30	0	59,61,61	0.29	0
104	PX2	QJ	202	-	35,35,35	0.98	3 (8%)	39,40,40	1.08	2 (5%)
95	3PE	4D	201	-	34,34,50	0.37	0	37,39,55	0.34	0
94	PC1	B5	201	-	53,53,53	0.29	0	59,61,61	0.33	0
94	PC1	4A	302	-	45,45,53	0.32	0	51,53,61	0.33	0
97	CDL	Qh	101	-	64,64,99	0.38	0	70,76,111	0.33	0
97	CDL	Qe	302	-	59,59,99	0.38	0	65,71,111	0.34	0
100	ZMP	AC	201	29	29,35,36	0.83	1 (3%)	34,42,45	1.08	3 (8%)
94	PC1	QI	101	-	35,35,53	0.36	0	41,43,61	0.40	0
94	PC1	Qj	201	-	53,53,53	0.31	0	59,61,61	0.30	0
94	PC1	A1	201	-	48,48,53	0.32	0	54,56,61	0.35	0
91	FES	QE	301	74	0,4,4	-	-	-	-	-
91	FES	1A	401	1	0,4,4	-	-	-	-	-
92	SF4	1A	402	1	0,12,12	-	-	-	-	-
106	HEM	QC	402	72	50,50,50	1.37	8 (16%)	66,82,82	1.73	16 (24%)
94	PC1	A1	202	-	30,30,53	0.38	0	36,38,61	0.34	0
97	CDL	C4	203	-	97,97,99	0.32	0	103,109,111	0.34	0
91	FES	V2	301	89	0,4,4	-	-	-	-	-
97	CDL	Qd	302	-	99,99,99	0.31	0	105,111,111	0.27	0
97	CDL	EA	202	-	54,54,99	0.40	0	60,66,111	0.37	0
100	ZMP	AB	201	28	29,35,36	0.77	1 (3%)	34,42,45	1.21	5 (14%)
97	CDL	4E	202	-	71,71,99	0.36	0	77,83,111	0.34	0
94	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.32	0
94	PC1	B8	301	-	36,36,53	0.35	0	42,44,61	0.47	0
97	CDL	C4	201	-	93,93,99	0.32	0	99,105,111	0.36	0
106	HEM	Qc	402	72	50,50,50	1.35	9 (18%)	66,82,82	1.75	14 (21%)
97	CDL	QH	101	-	75,75,99	0.36	0	81,87,111	0.32	0
101	HEA	C1	501	43	66,67,67	2.22	24 (36%)	78,103,103	2.55	32 (41%)
97	CDL	C4	202	-	68,68,99	0.36	0	74,80,111	0.37	0
97	CDL	A3	201	-	57,57,99	0.39	0	63,69,111	0.37	0
94	PC1	Qc	401	-	53,53,53	0.30	0	59,61,61	0.32	0
95	3PE	N5	602	-	50,50,50	0.32	0	53,55,55	0.35	0
95	3PE	C1	506	-	39,39,50	0.36	0	42,44,55	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.28	0
94	PC1	AM	203	-	48,48,53	0.31	0	54,56,61	0.32	0
95	3PE	E9	201	-	50,50,50	0.30	0	53,55,55	0.28	0
92	SF4	1A	403	1	0,12,12	-	-	-		
94	PC1	N3	301	-	41,41,53	0.34	0	47,49,61	0.34	0
105	U10	N4	504	-	43,43,63	2.39	15 (34%)	52,55,79	1.84	14 (26%)
94	PC1	N1	703	-	39,39,53	0.34	0	45,47,61	0.29	0
94	PC1	E8	303	-	32,32,53	0.37	0	38,40,61	0.35	0
92	SF4	S8	302	87	0,12,12	-	-	-		
97	CDL	AL	303	-	63,63,99	0.38	0	69,75,111	0.33	0
104	PX2	C2	201	-	35,35,35	0.98	4 (11%)	39,40,40	1.07	2 (5%)
97	CDL	Qj	202	-	47,47,99	0.43	0	53,59,111	0.36	0
97	CDL	E4	401	-	71,71,99	0.36	0	77,83,111	0.38	0
94	PC1	A9	503	-	32,32,53	0.38	0	38,40,61	0.35	0
97	CDL	AL	302	-	67,67,99	0.37	0	73,79,111	0.33	0
104	PX2	QJ	201	-	35,35,35	0.99	3 (8%)	39,40,40	1.05	2 (5%)
92	SF4	S7	301	86	0,12,12	-	-	-		
106	HEM	QC	401	72	50,50,50	1.34	9 (18%)	66,82,82	1.72	13 (19%)
94	PC1	Qc	404	-	30,30,53	0.40	0	36,38,61	0.44	0
94	PC1	N4	501	-	38,38,53	0.33	0	44,46,61	0.29	0
94	PC1	G2	301	-	37,37,53	0.35	0	43,45,61	0.31	0
97	CDL	E7	301	-	67,67,99	0.37	0	73,79,111	0.33	0
97	CDL	B8	302	-	69,69,99	0.36	0	75,81,111	0.31	0
94	PC1	N4	502	-	32,32,53	0.37	0	38,40,61	0.38	0
94	PC1	7A	201	-	35,35,53	0.37	0	41,43,61	0.35	0
94	PC1	E8	302	-	53,53,53	0.30	0	59,61,61	0.30	0
95	3PE	C1	507	-	39,39,50	0.35	0	42,44,55	0.38	0
106	HEM	Qc	403	72	50,50,50	1.35	7 (14%)	66,82,82	1.75	16 (24%)
94	PC1	E9	202	-	34,34,53	0.36	0	40,42,61	0.42	0
95	3PE	7A	202	-	40,40,50	0.35	0	43,45,55	0.31	0
95	3PE	B4	201	-	39,39,50	0.34	0	42,44,55	0.36	0
94	PC1	Qe	303	-	35,35,53	0.36	0	41,43,61	0.34	0
97	CDL	7C	201	-	89,89,99	0.32	0	95,101,111	0.30	0
97	CDL	A9	504	-	63,63,99	0.39	0	69,75,111	0.35	0
97	CDL	QD	302	-	68,68,99	0.37	0	74,80,111	0.36	0
97	CDL	AM	201	-	71,71,99	0.36	0	77,83,111	0.32	0
94	PC1	4A	301	-	46,46,53	0.32	0	52,54,61	0.31	0
97	CDL	AM	202	-	71,71,99	0.36	0	77,83,111	0.32	0
92	SF4	S8	301	87	0,12,12	-	-	-		
97	CDL	EA	201	-	58,58,99	0.40	0	64,70,111	0.39	0
94	PC1	4E	201	-	34,34,53	0.37	0	40,42,61	0.34	0
97	CDL	QC	403	-	55,55,99	0.41	0	61,67,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	PC1	N5	601	-	35,35,53	0.35	0	41,43,61	0.30	0
91	FES	Qe	301	74	0,4,4	-	-	-		
95	3PE	N4	503	-	40,40,50	0.35	0	43,45,55	0.32	0
94	PC1	QD	303	-	30,30,53	0.39	0	36,38,61	0.38	0
99	NDP	A9	501	-	49,52,52	0.47	0	66,80,80	0.45	0
94	PC1	B5	202	-	53,53,53	0.30	0	59,61,61	0.28	0
94	PC1	N1	702	-	48,48,53	0.31	0	54,56,61	0.28	0
94	PC1	C3	201	-	50,50,53	0.31	0	56,58,61	0.30	0
107	HEC	Qd	301	73	50,50,50	1.31	5 (10%)	68,82,82	1.18	4 (5%)
94	PC1	AN	301	-	47,47,53	0.31	0	53,55,61	0.30	0
94	PC1	C1	505	-	49,49,53	0.32	0	55,57,61	0.32	0
94	PC1	Qg	301	-	27,27,53	0.40	0	33,35,61	0.34	0
101	HEA	C1	502	43	66,67,67	2.23	24 (36%)	78,103,103	2.59	24 (30%)
94	PC1	E4	402	-	50,50,53	0.30	0	56,58,61	0.29	0
97	CDL	QJ	203	-	57,57,99	0.40	0	63,69,111	0.32	0
94	PC1	A9	502	-	32,32,53	0.39	0	38,40,61	0.34	0
94	PC1	AM	204	-	47,47,53	0.32	0	53,55,61	0.26	0
94	PC1	AL	301	-	49,49,53	0.31	0	55,57,61	0.29	0
97	CDL	Qc	405	-	53,53,99	0.41	0	59,65,111	0.35	0
94	PC1	ED	201	-	53,53,53	0.30	0	59,61,61	0.31	0
92	SF4	V1	602	88	0,12,12	-	-	-		
94	PC1	ED	202	-	40,40,53	0.33	0	46,48,61	0.33	0
107	HEC	QD	301	73	50,50,50	1.31	4 (8%)	68,82,82	1.28	7 (10%)
108	FMN	V1	601	-	33,33,33	0.36	0	48,50,50	0.43	0
97	CDL	QH	102	-	59,59,99	0.39	0	65,71,111	0.35	0
97	CDL	B3	101	-	64,64,99	0.38	0	70,76,111	0.33	0
97	CDL	BM	201	-	57,57,99	0.39	0	63,69,111	0.36	0
97	CDL	N1	701	-	69,69,99	0.37	0	75,81,111	0.32	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
97	CDL	N5	603	-	-	30/103/103/110	-
95	3PE	4D	202	-	-	21/54/54/54	-
96	S12	4D	203	-	-	14/38/38/38	-
94	PC1	QC	404	-	-	8/57/57/57	-
97	CDL	E6	401	-	-	23/68/68/110	-
94	PC1	N4	505	-	-	13/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
104	PX2	QJ	202	-	-	24/37/37/37	-
95	3PE	4D	201	-	-	11/38/38/54	-
94	PC1	B5	201	-	-	15/57/57/57	-
94	PC1	4A	302	-	-	21/49/49/57	-
97	CDL	Qh	101	-	-	18/75/75/110	-
97	CDL	Qe	302	-	-	12/70/70/110	-
100	ZMP	AC	201	29	-	18/40/42/43	-
94	PC1	QI	101	-	-	3/39/39/57	-
94	PC1	Qj	201	-	-	16/57/57/57	-
94	PC1	A1	201	-	-	15/52/52/57	-
91	FES	QE	301	74	-	-	0/1/1/1
91	FES	1A	401	1	-	-	0/1/1/1
106	HEM	QC	402	72	-	6/14/54/54	-
92	SF4	1A	402	1	-	-	0/6/5/5
94	PC1	A1	202	-	-	7/34/34/57	-
97	CDL	C4	203	-	-	25/108/108/110	-
91	FES	V2	301	89	-	-	0/1/1/1
97	CDL	Qd	302	-	-	27/110/110/110	-
97	CDL	EA	202	-	-	17/65/65/110	-
100	ZMP	AB	201	28	-	20/40/42/43	-
97	CDL	4E	202	-	-	20/82/82/110	-
94	PC1	E8	304	-	-	11/33/33/57	-
94	PC1	B8	301	-	-	8/40/40/57	-
97	CDL	C4	201	-	-	23/104/104/110	-
106	HEM	Qc	402	72	-	7/14/54/54	-
97	CDL	QH	101	-	-	20/86/86/110	-
101	HEA	C1	501	43	-	17/36/76/76	-
97	CDL	C4	202	-	-	10/79/79/110	-
97	CDL	A3	201	-	-	7/68/68/110	-
94	PC1	Qc	401	-	-	17/57/57/57	-
95	3PE	N5	602	-	-	11/54/54/54	-
95	3PE	C1	506	-	-	16/43/43/54	-
94	PC1	E8	301	-	-	13/57/57/57	-
94	PC1	AM	203	-	-	18/52/52/57	-
95	3PE	E9	201	-	-	8/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	PC1	N3	301	-	-	8/45/45/57	-
92	SF4	1A	403	1	-	-	0/6/5/5
105	U10	N4	504	-	-	10/39/63/87	0/1/1/1
94	PC1	N1	703	-	-	17/43/43/57	-
94	PC1	E8	303	-	-	6/36/36/57	-
92	SF4	S8	302	87	-	-	0/6/5/5
97	CDL	AL	303	-	-	15/74/74/110	-
104	PX2	C2	201	-	-	20/37/37/37	-
97	CDL	Qj	202	-	-	19/58/58/110	-
97	CDL	E4	401	-	-	14/82/82/110	-
94	PC1	A9	503	-	-	6/36/36/57	-
97	CDL	AL	302	-	-	10/78/78/110	-
104	PX2	QJ	201	-	-	19/37/37/37	-
92	SF4	S7	301	86	-	-	0/6/5/5
106	HEM	QC	401	72	-	8/14/54/54	-
94	PC1	Qc	404	-	-	12/34/34/57	-
94	PC1	N4	501	-	-	13/42/42/57	-
94	PC1	G2	301	-	-	9/41/41/57	-
97	CDL	E7	301	-	-	18/78/78/110	-
97	CDL	B8	302	-	-	13/80/80/110	-
94	PC1	N4	502	-	-	10/36/36/57	-
94	PC1	7A	201	-	-	14/39/39/57	-
94	PC1	E8	302	-	-	13/57/57/57	-
95	3PE	C1	507	-	-	11/43/43/54	-
106	HEM	Qc	403	72	-	6/14/54/54	-
94	PC1	E9	202	-	-	8/38/38/57	-
95	3PE	7A	202	-	-	7/44/44/54	-
95	3PE	B4	201	-	-	16/43/43/54	-
94	PC1	Qe	303	-	-	6/39/39/57	-
97	CDL	7C	201	-	-	25/100/100/110	-
97	CDL	A9	504	-	-	25/74/74/110	-
97	CDL	QD	302	-	-	15/79/79/110	-
97	CDL	AM	201	-	-	14/82/82/110	-
94	PC1	4A	301	-	-	8/50/50/57	-
97	CDL	AM	202	-	-	20/82/82/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	SF4	S8	301	87	-	-	0/6/5/5
97	CDL	EA	201	-	-	14/69/69/110	-
94	PC1	4E	201	-	-	13/38/38/57	-
97	CDL	QC	403	-	-	17/66/66/110	-
94	PC1	N5	601	-	-	9/39/39/57	-
95	3PE	N4	503	-	-	8/44/44/54	-
91	FES	Qe	301	74	-	-	0/1/1/1
94	PC1	QD	303	-	-	11/34/34/57	-
99	NDP	A9	501	-	-	10/34/77/77	0/5/5/5
94	PC1	B5	202	-	-	19/57/57/57	-
94	PC1	N1	702	-	-	14/52/52/57	-
94	PC1	C3	201	-	-	9/54/54/57	-
107	HEC	Qd	301	73	1/1/3/7	7/14/54/54	-
94	PC1	AN	301	-	-	9/51/51/57	-
94	PC1	C1	505	-	-	10/53/53/57	-
94	PC1	Qg	301	-	-	3/31/31/57	-
101	HEA	C1	502	43	-	18/36/76/76	-
94	PC1	E4	402	-	-	9/54/54/57	-
97	CDL	QJ	203	-	-	19/68/68/110	-
94	PC1	A9	502	-	-	13/36/36/57	-
94	PC1	AM	204	-	-	10/51/51/57	-
94	PC1	AL	301	-	-	12/53/53/57	-
97	CDL	Qc	405	-	-	15/64/64/110	-
94	PC1	ED	201	-	-	11/57/57/57	-
94	PC1	ED	202	-	-	16/44/44/57	-
92	SF4	V1	602	88	-	-	0/6/5/5
107	HEC	QD	301	73	1/1/3/7	5/14/54/54	-
108	FMN	V1	601	-	-	3/18/18/18	0/3/3/3
97	CDL	QH	102	-	-	19/70/70/110	-
97	CDL	B3	101	-	-	10/75/75/110	-
97	CDL	BM	201	-	-	7/68/68/110	-
97	CDL	N1	701	-	-	24/80/80/110	-

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
105	N4	504	U10	C6-C1	10.22	1.53	1.35
101	C1	502	HEA	C3B-C2B	5.39	1.46	1.34
101	C1	501	HEA	FE-ND	4.90	2.10	1.94
101	C1	502	HEA	FE-ND	4.90	2.10	1.94
101	C1	501	HEA	C3B-C2B	4.80	1.45	1.34

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	C1	502	HEA	CAD-CBD-CGD	-8.14	96.09	113.60
101	C1	501	HEA	CAD-CBD-CGD	-6.75	99.07	113.60
101	C1	502	HEA	C3C-C4C-NC	6.57	114.29	110.25
101	C1	501	HEA	CAA-CBA-CGA	-6.39	99.85	113.60
101	C1	502	HEA	CAA-CBA-CGA	-6.32	100.01	113.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
107	QD	301	HEC	NA
107	Qd	301	HEC	NA

5 of 1329 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	4A	301	PC1	C11-O13-P-O12
94	4A	301	PC1	C1-O11-P-O14
94	4A	302	PC1	C11-O13-P-O14
94	4A	302	PC1	C1-O11-P-O12
94	4A	302	PC1	O21-C2-C3-O31

There are no ring outliers.

40 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	E6	401	CDL	1	0
104	QJ	202	PX2	4	0
94	B5	201	PC1	1	0
100	AC	201	ZMP	7	0
94	QI	101	PC1	1	0
106	QC	402	HEM	1	0
94	A1	202	PC1	1	0
97	C4	203	CDL	2	0

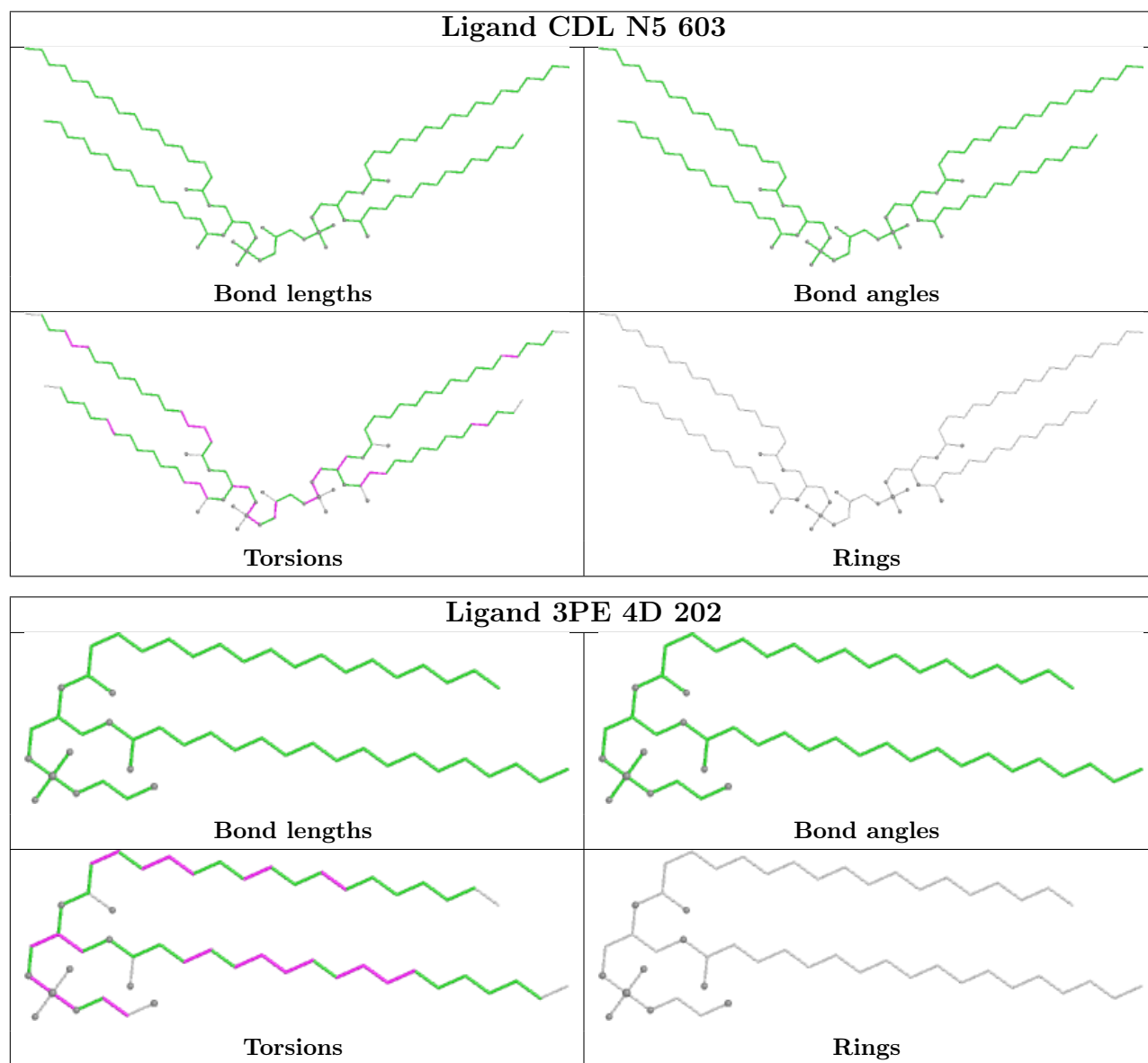
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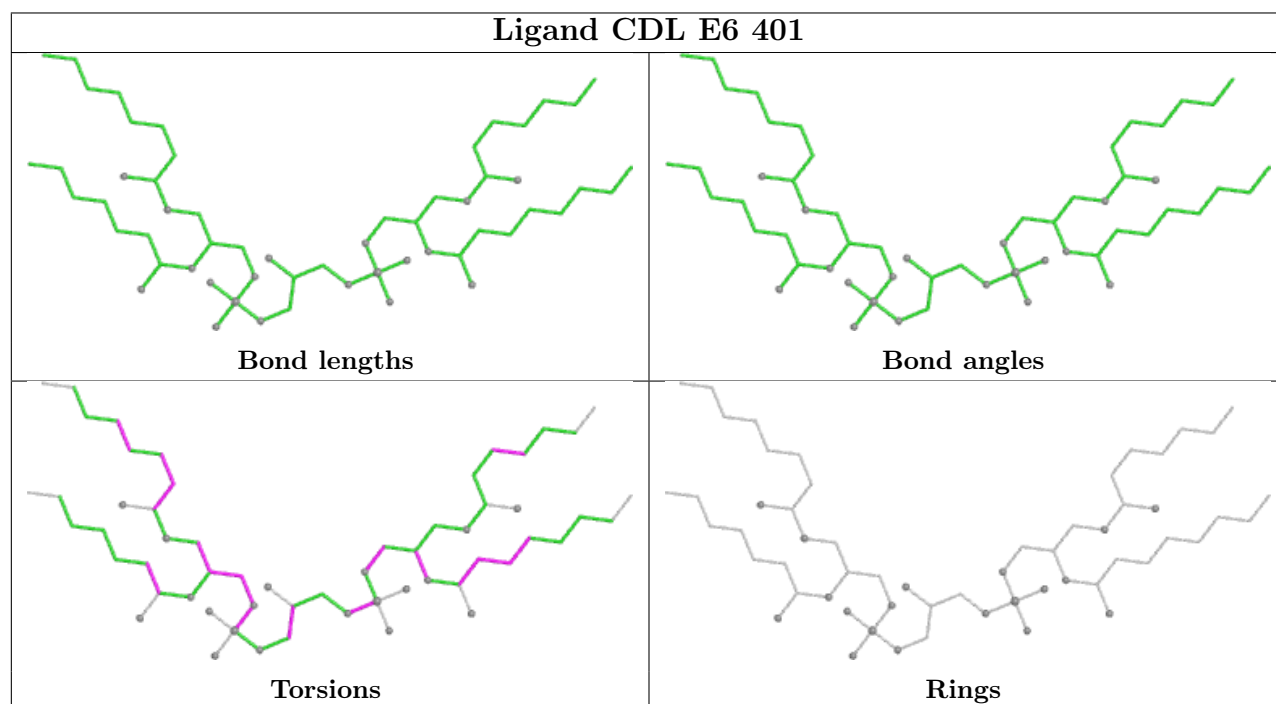
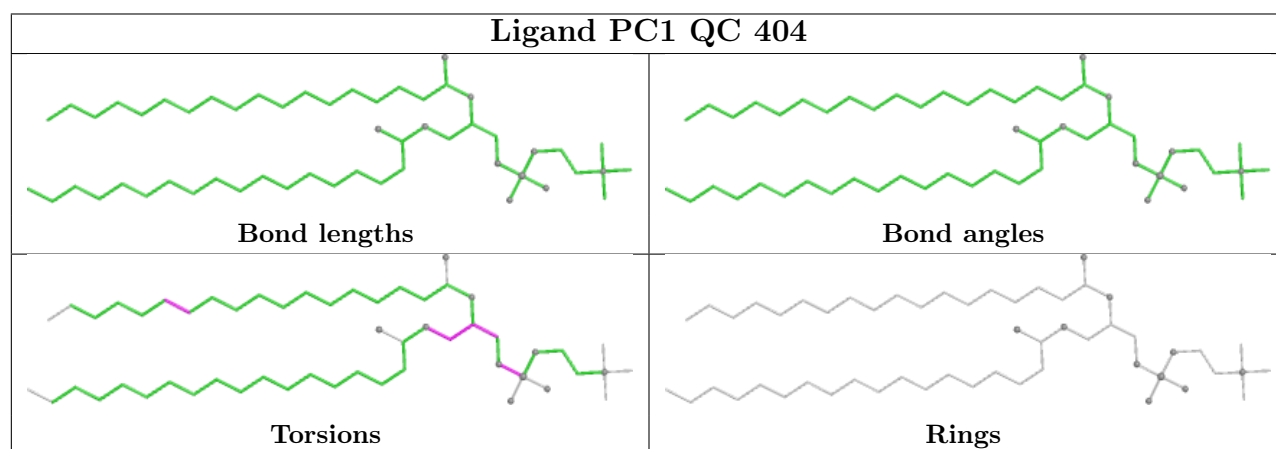
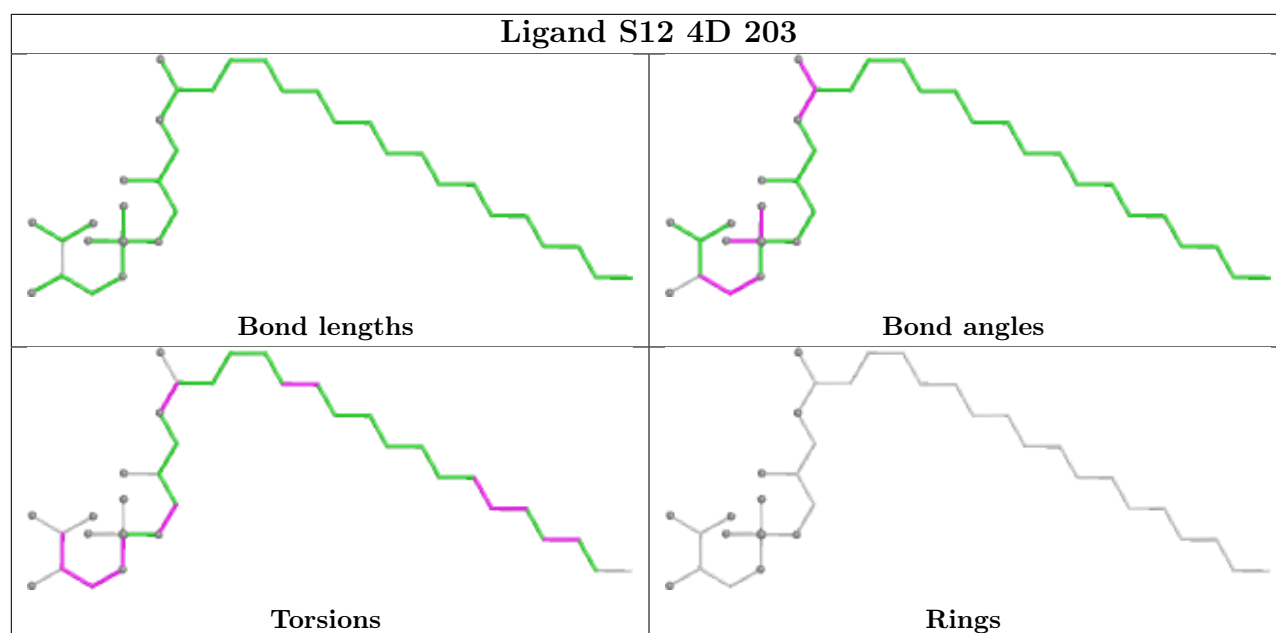
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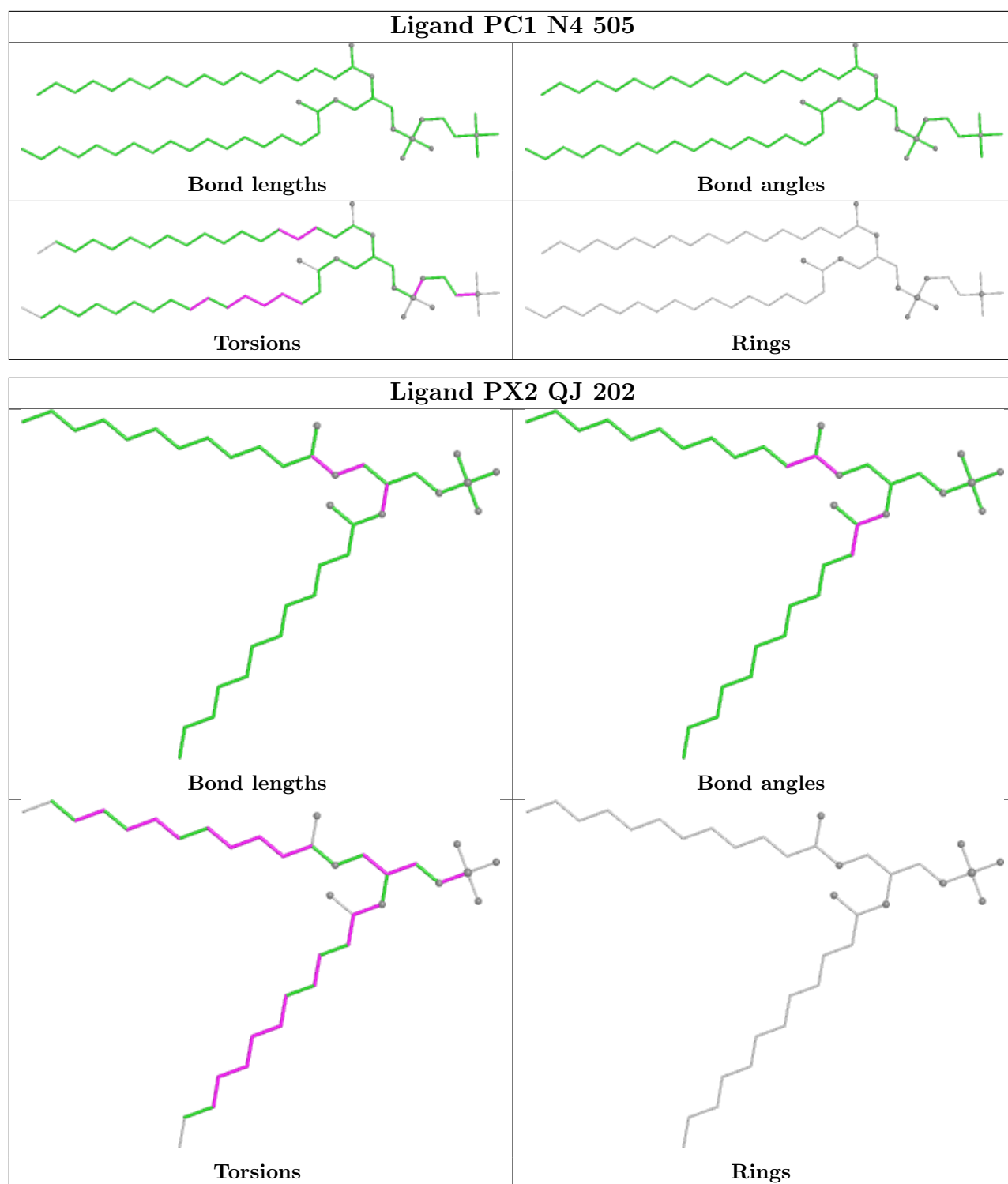
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	Qd	302	CDL	2	0
100	AB	201	ZMP	3	0
106	Qc	402	HEM	5	0
97	QH	101	CDL	1	0
101	C1	501	HEA	14	0
97	A3	201	CDL	1	0
105	N4	504	U10	4	0
104	C2	201	PX2	4	0
97	Qj	202	CDL	1	0
97	E4	401	CDL	2	0
104	QJ	201	PX2	4	0
92	S7	301	SF4	1	0
106	QC	401	HEM	1	0
97	B8	302	CDL	1	0
106	Qc	403	HEM	5	0
94	E9	202	PC1	1	0
95	B4	201	3PE	1	0
97	7C	201	CDL	1	0
97	A9	504	CDL	1	0
97	AM	201	CDL	1	0
97	AM	202	CDL	3	0
97	EA	201	CDL	1	0
94	B5	202	PC1	2	0
107	Qd	301	HEC	6	0
101	C1	502	HEA	7	0
97	QJ	203	CDL	1	0
94	AM	204	PC1	1	0
97	Qc	405	CDL	1	0
107	QD	301	HEC	5	0
97	QH	102	CDL	1	0
97	B3	101	CDL	1	0
97	N1	701	CDL	1	0

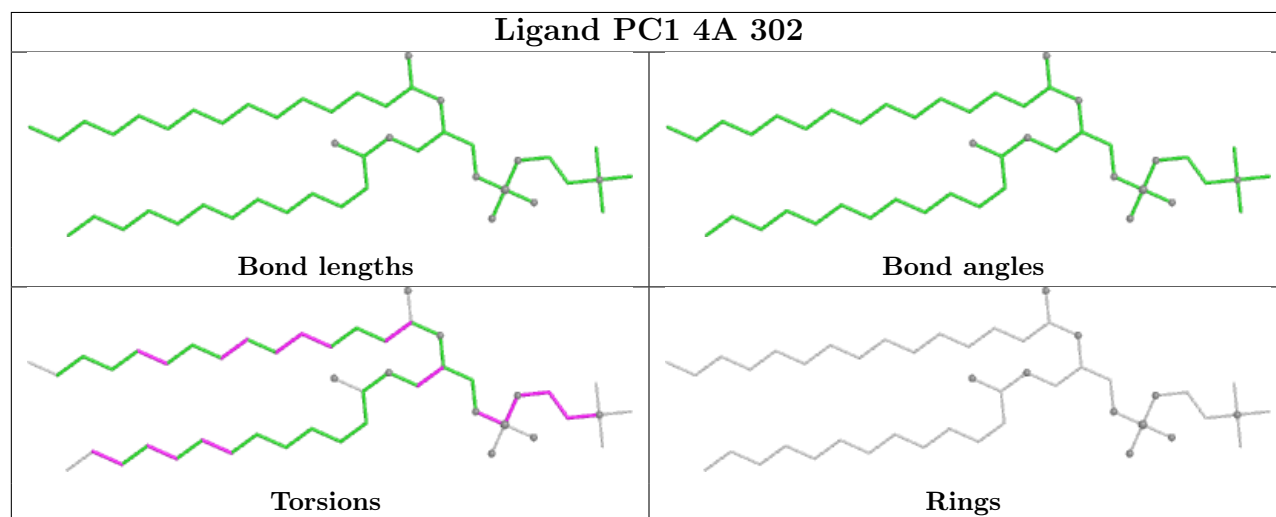
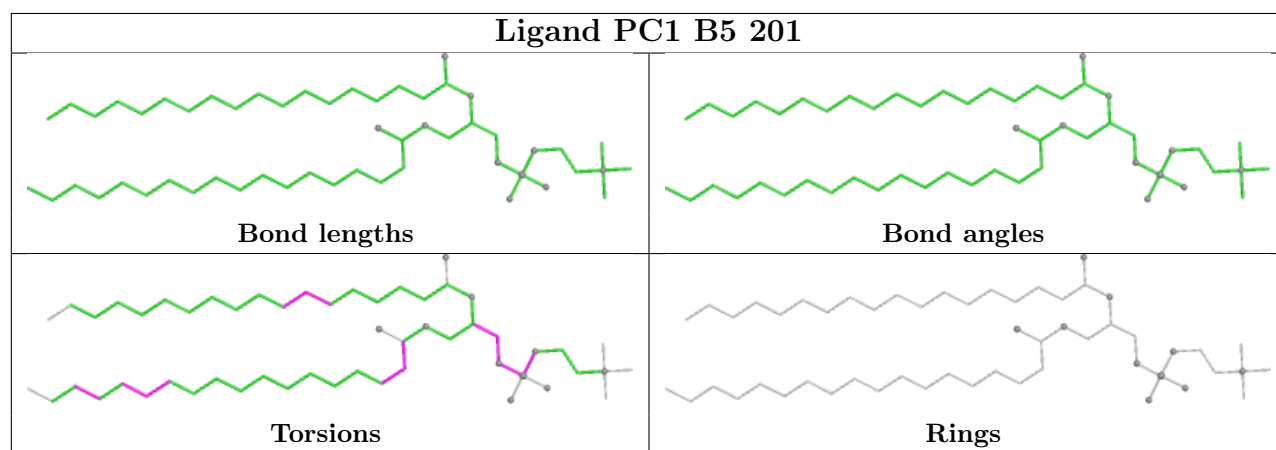
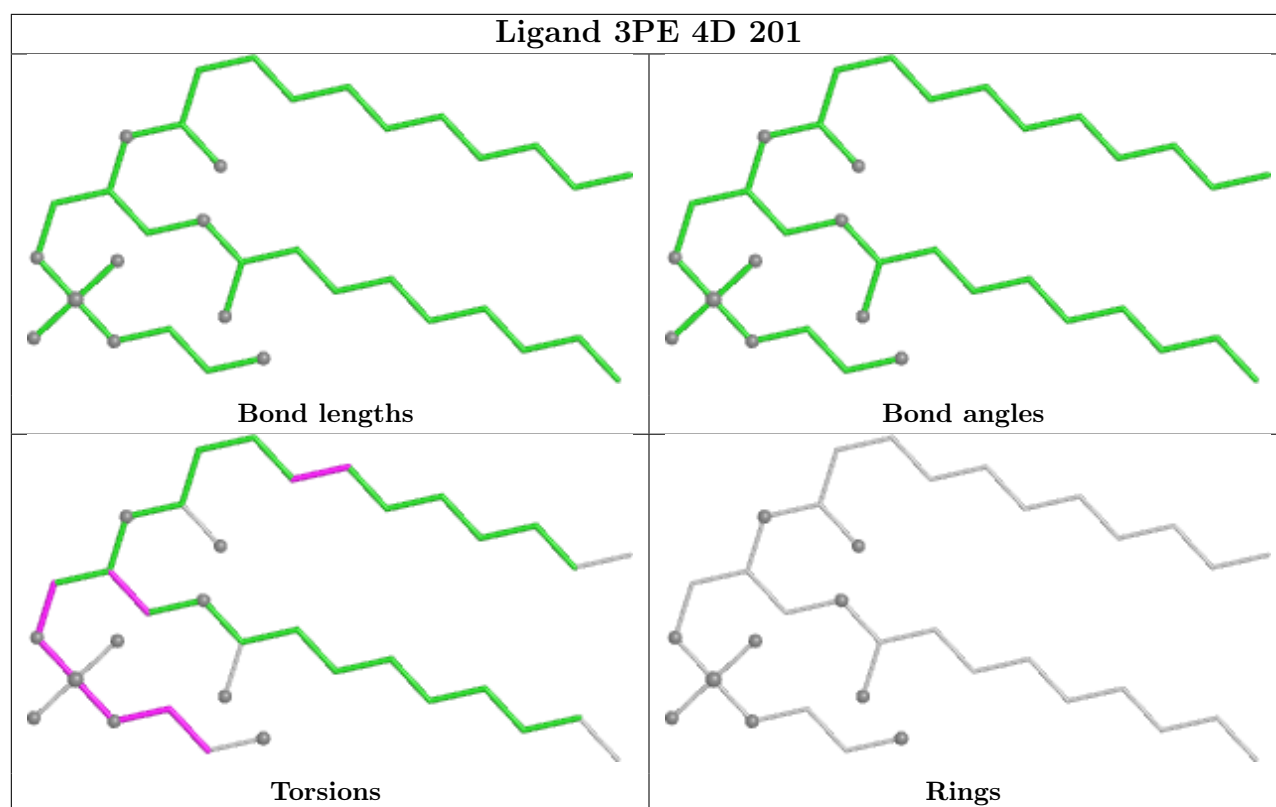
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

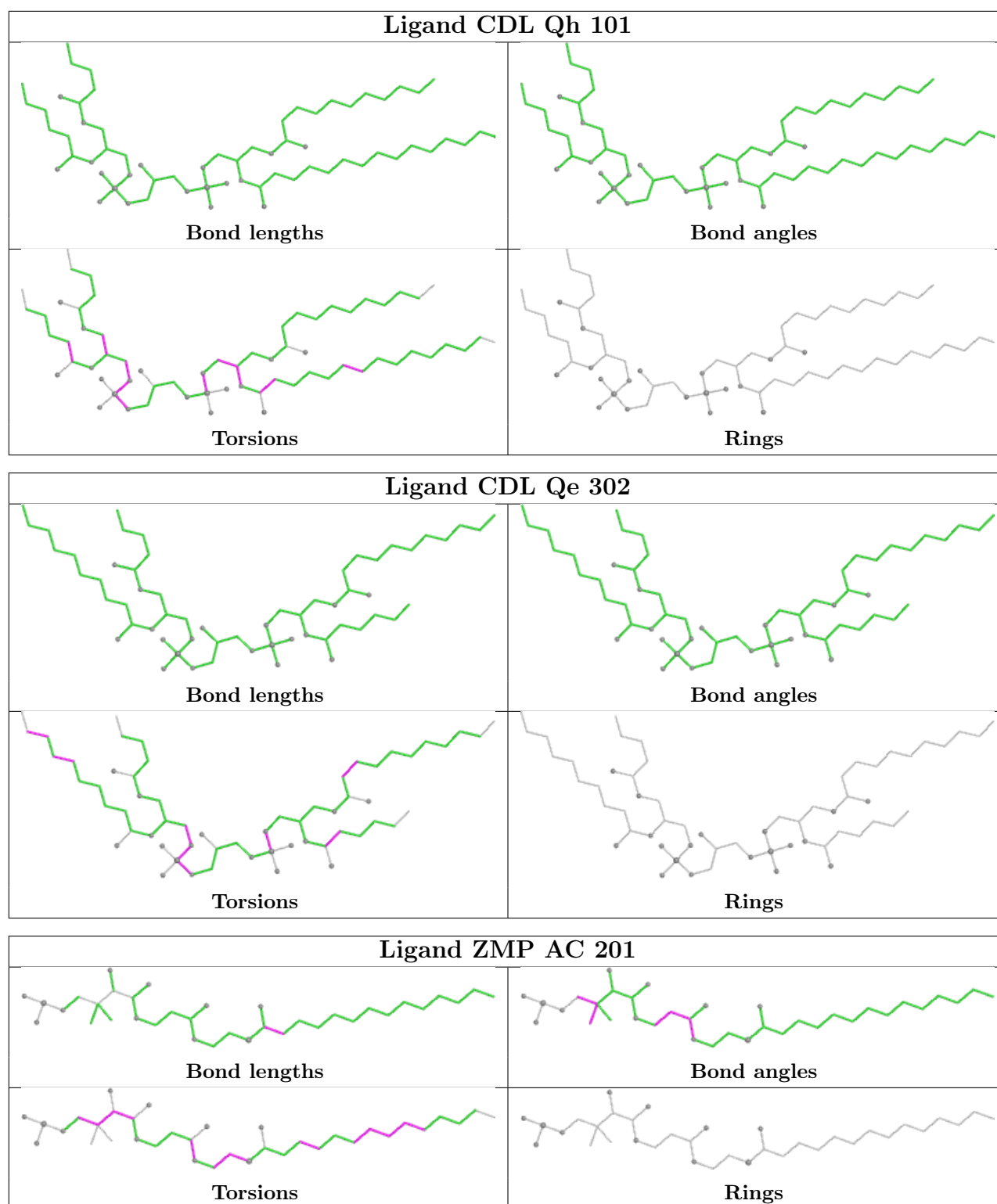
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

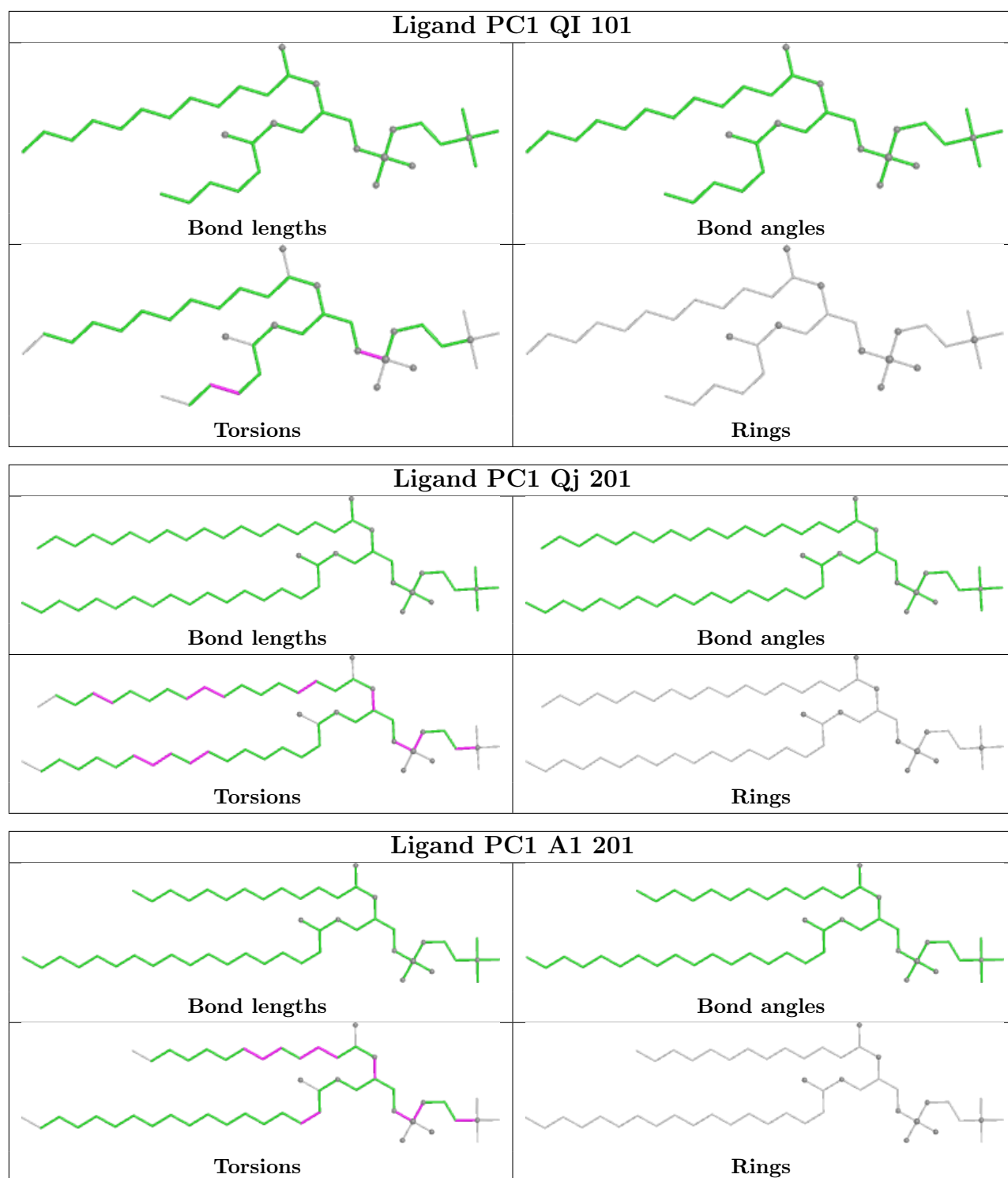


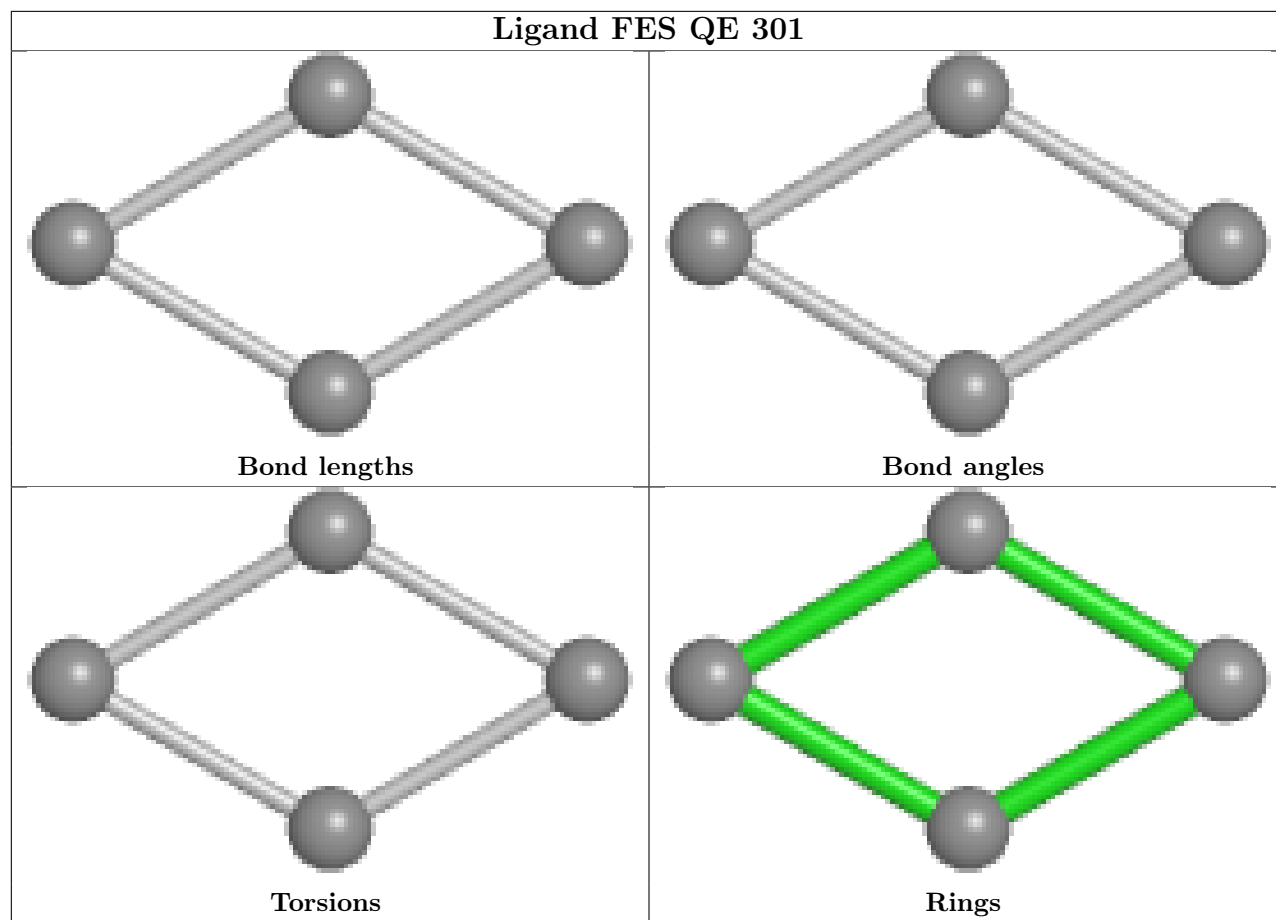


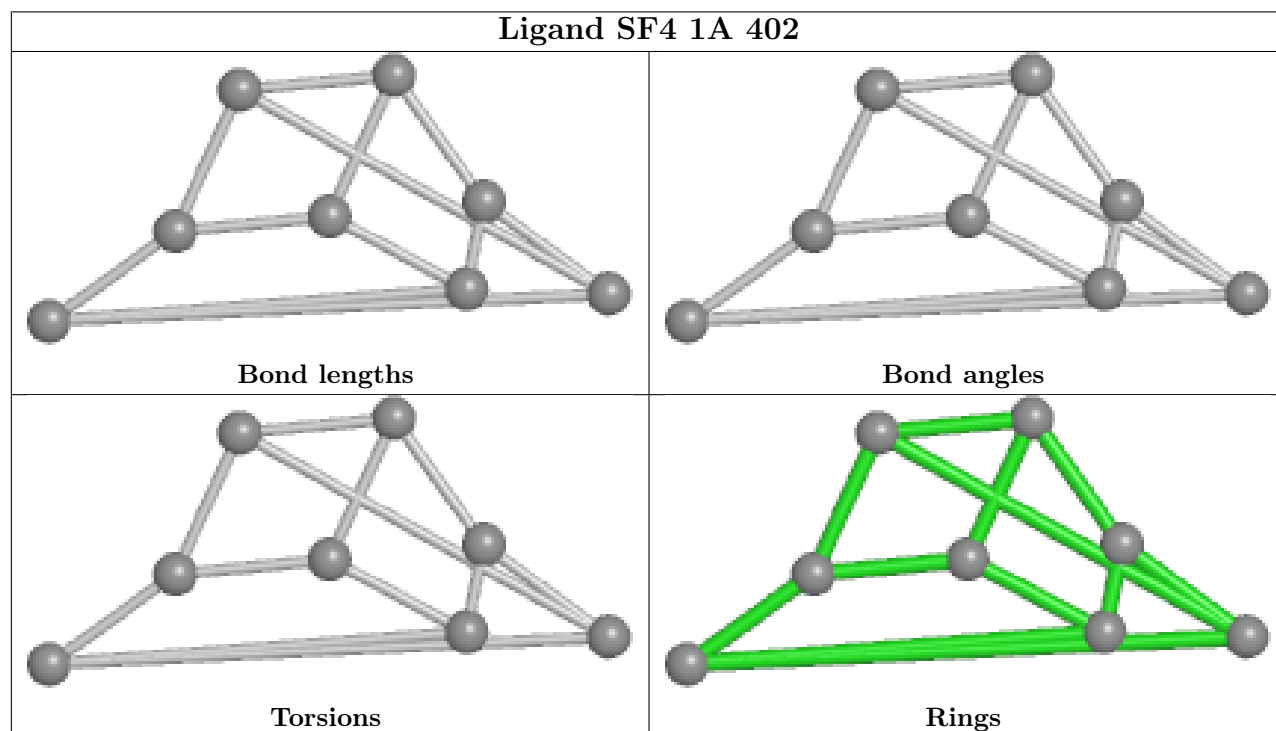
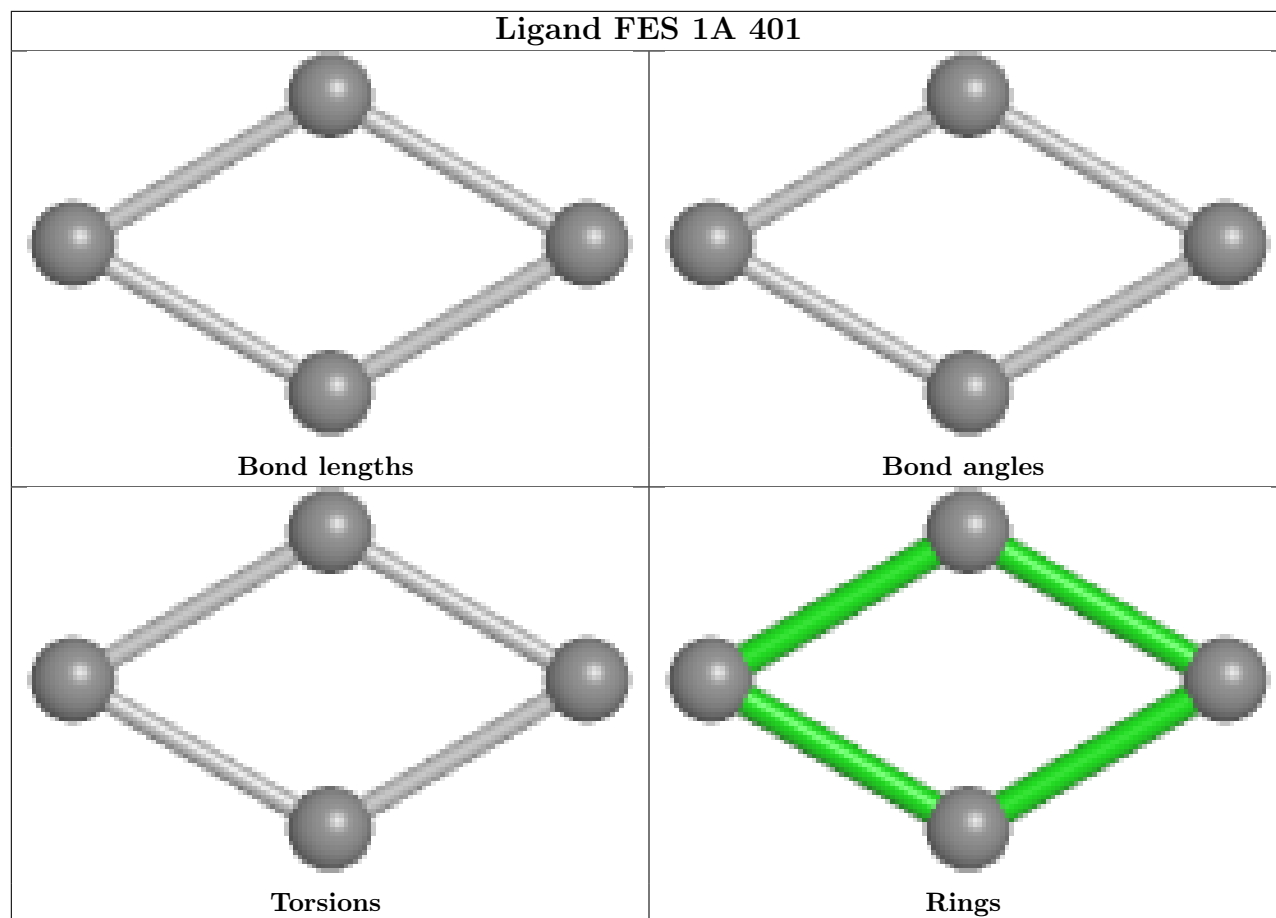


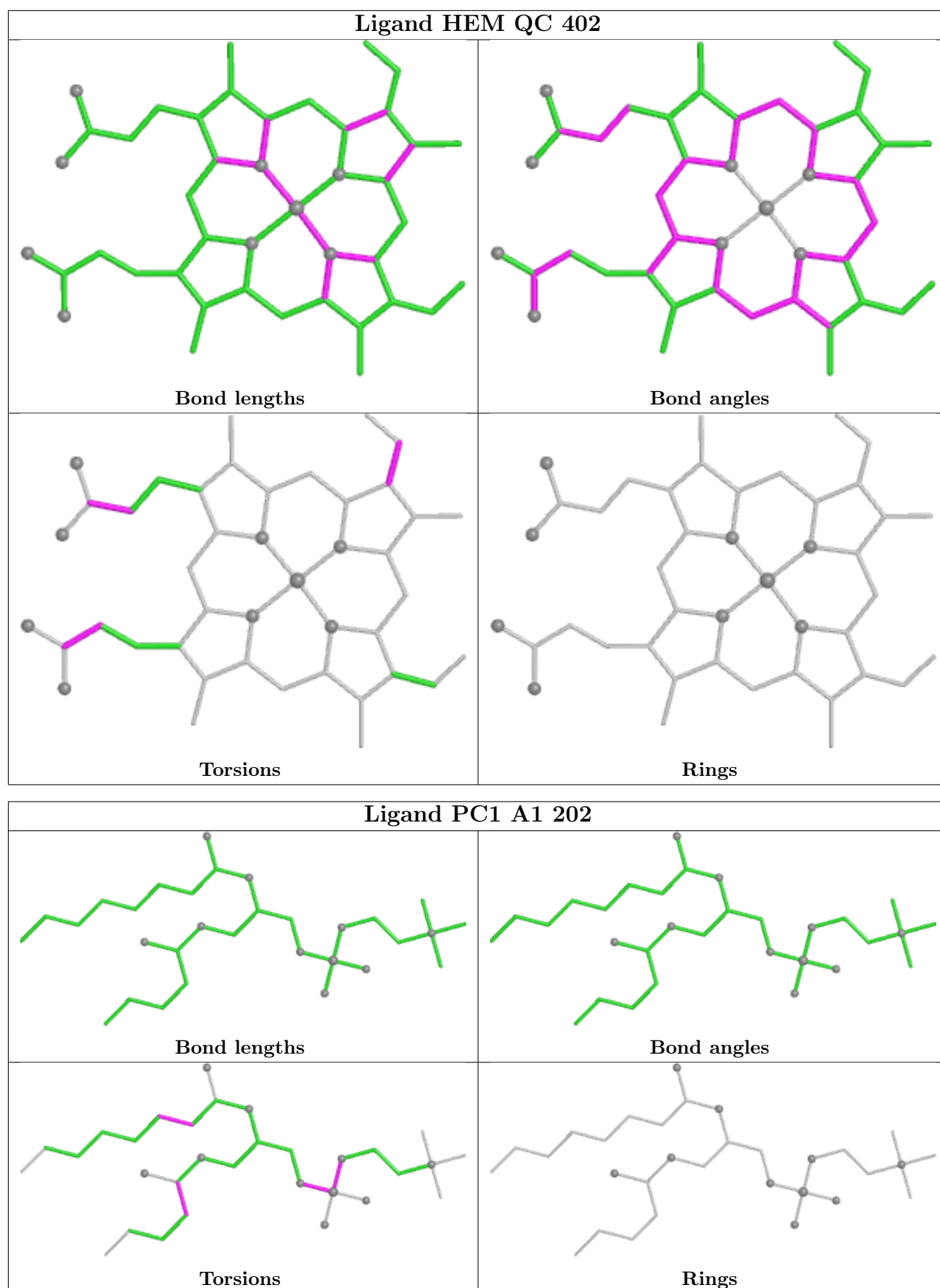


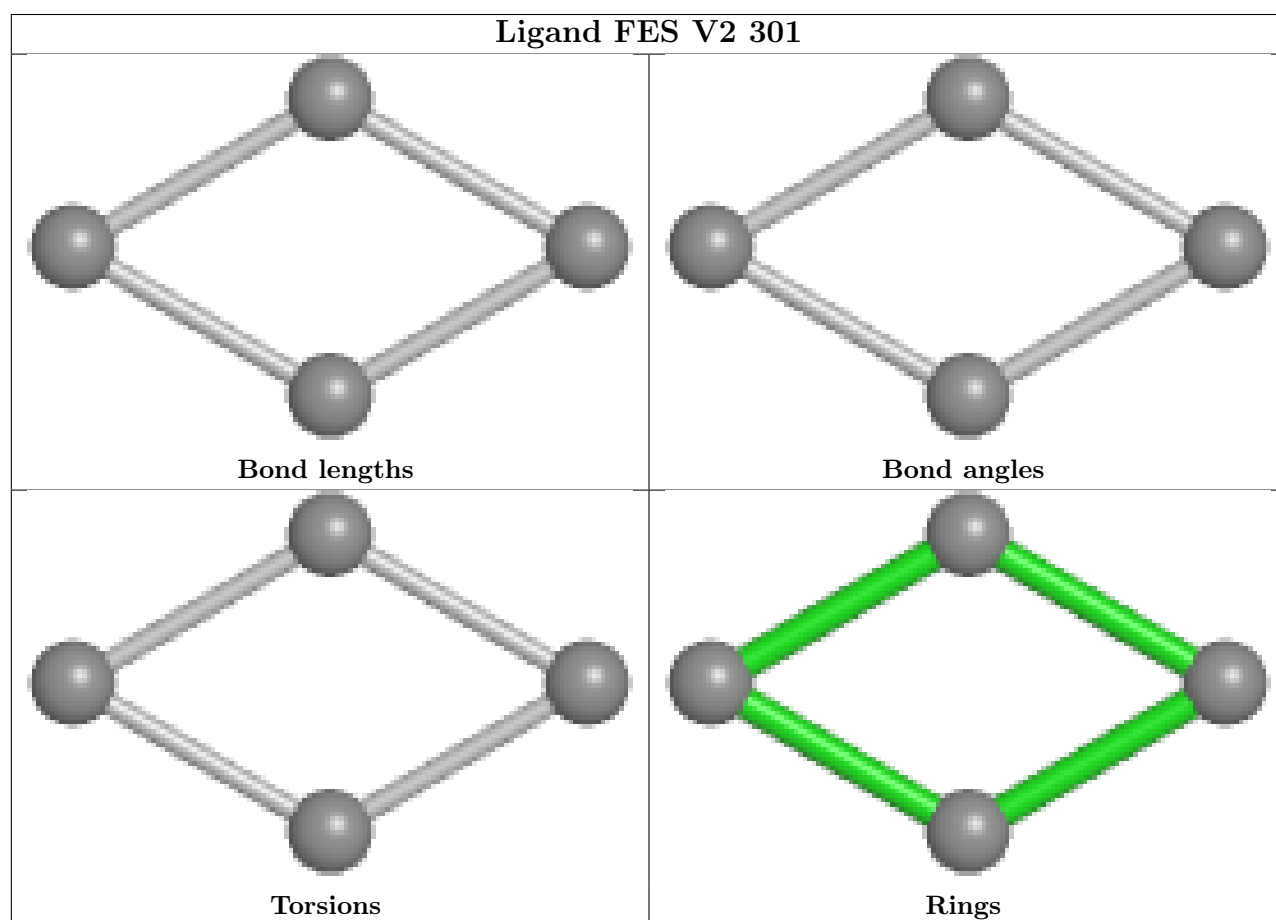
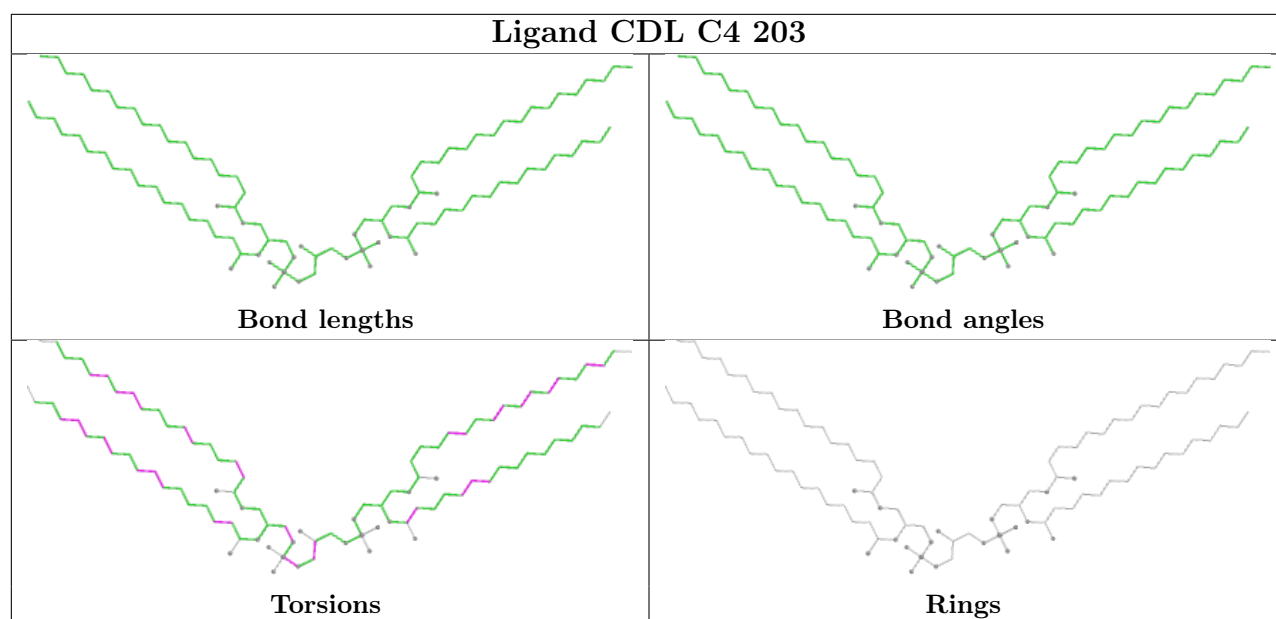


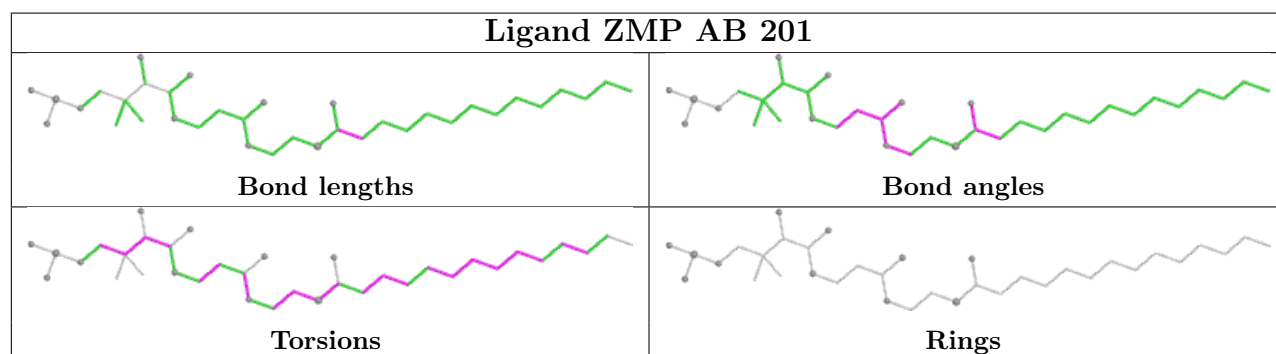
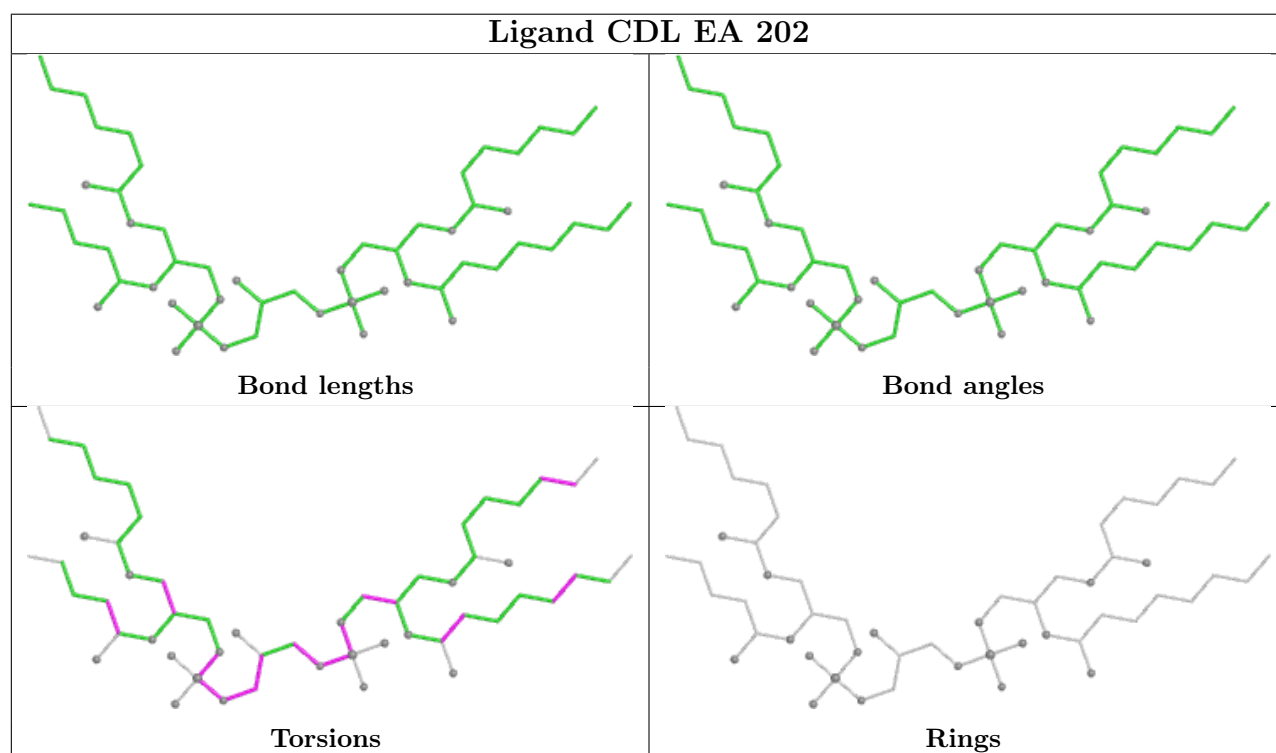
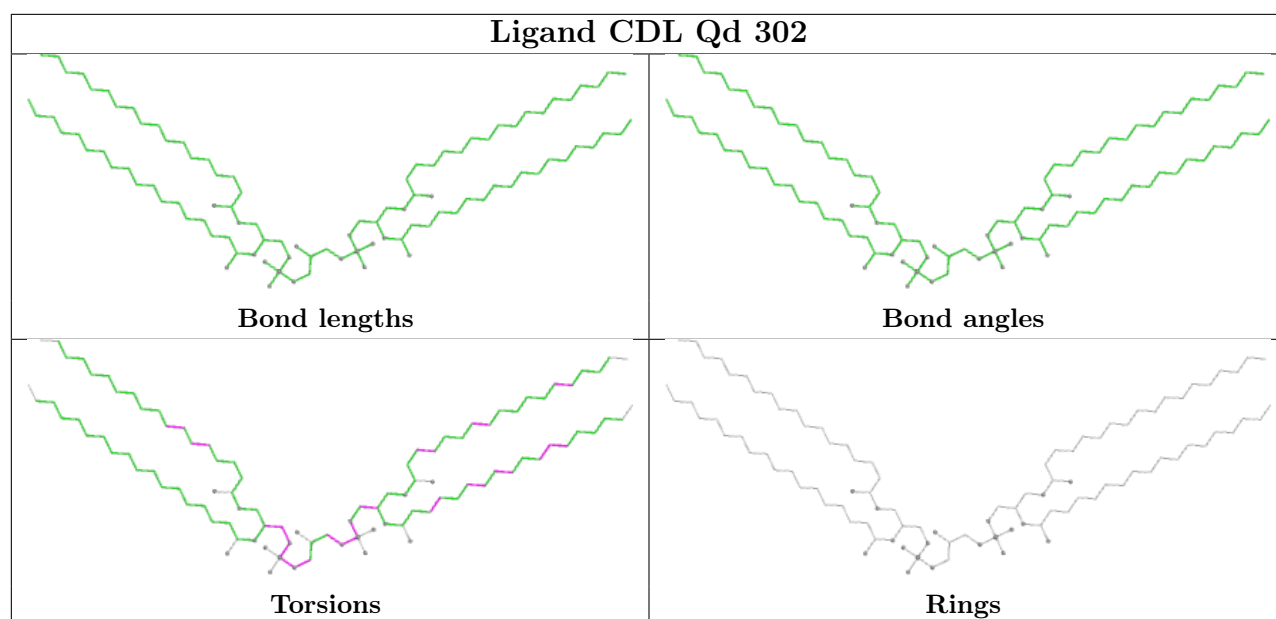


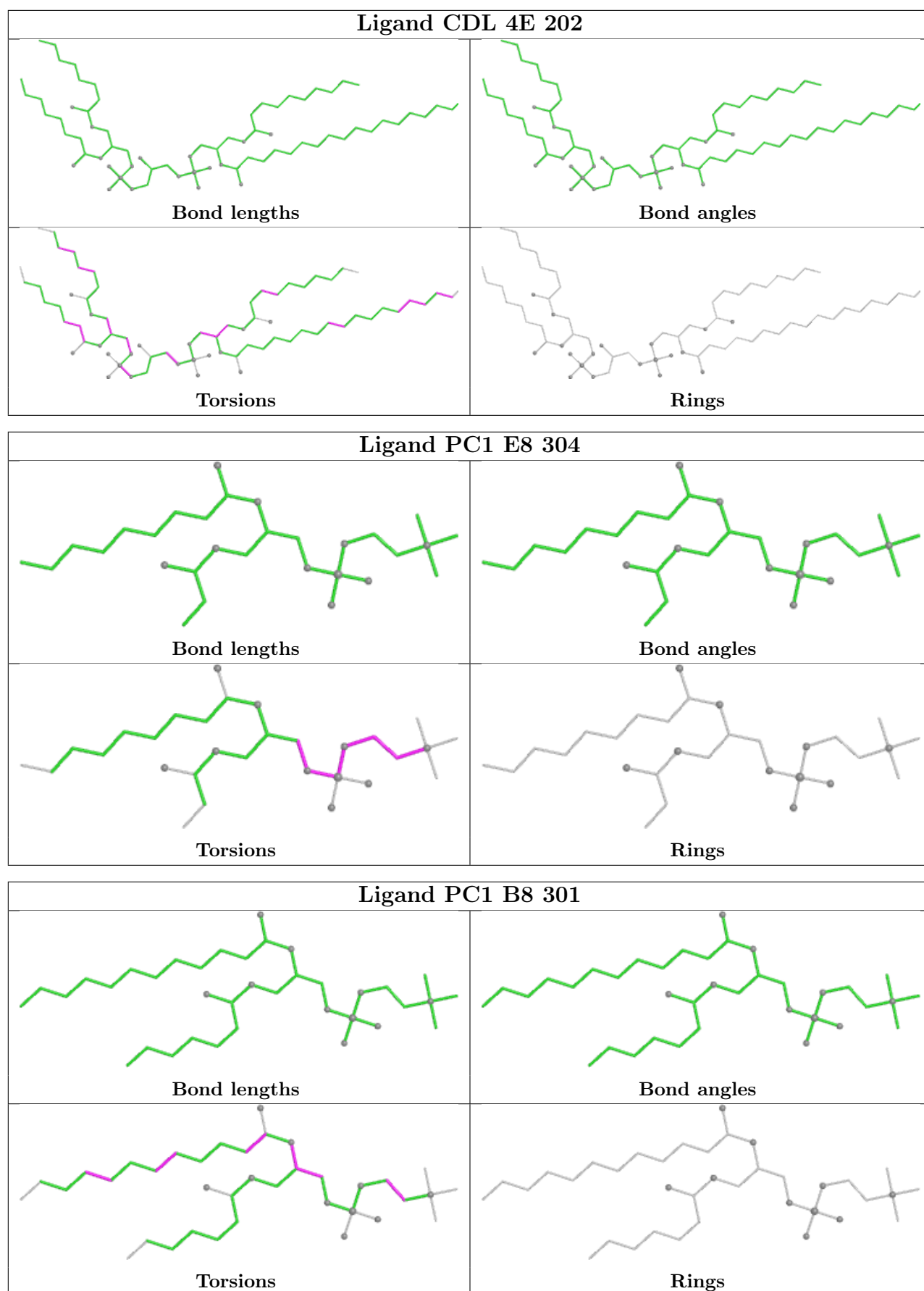


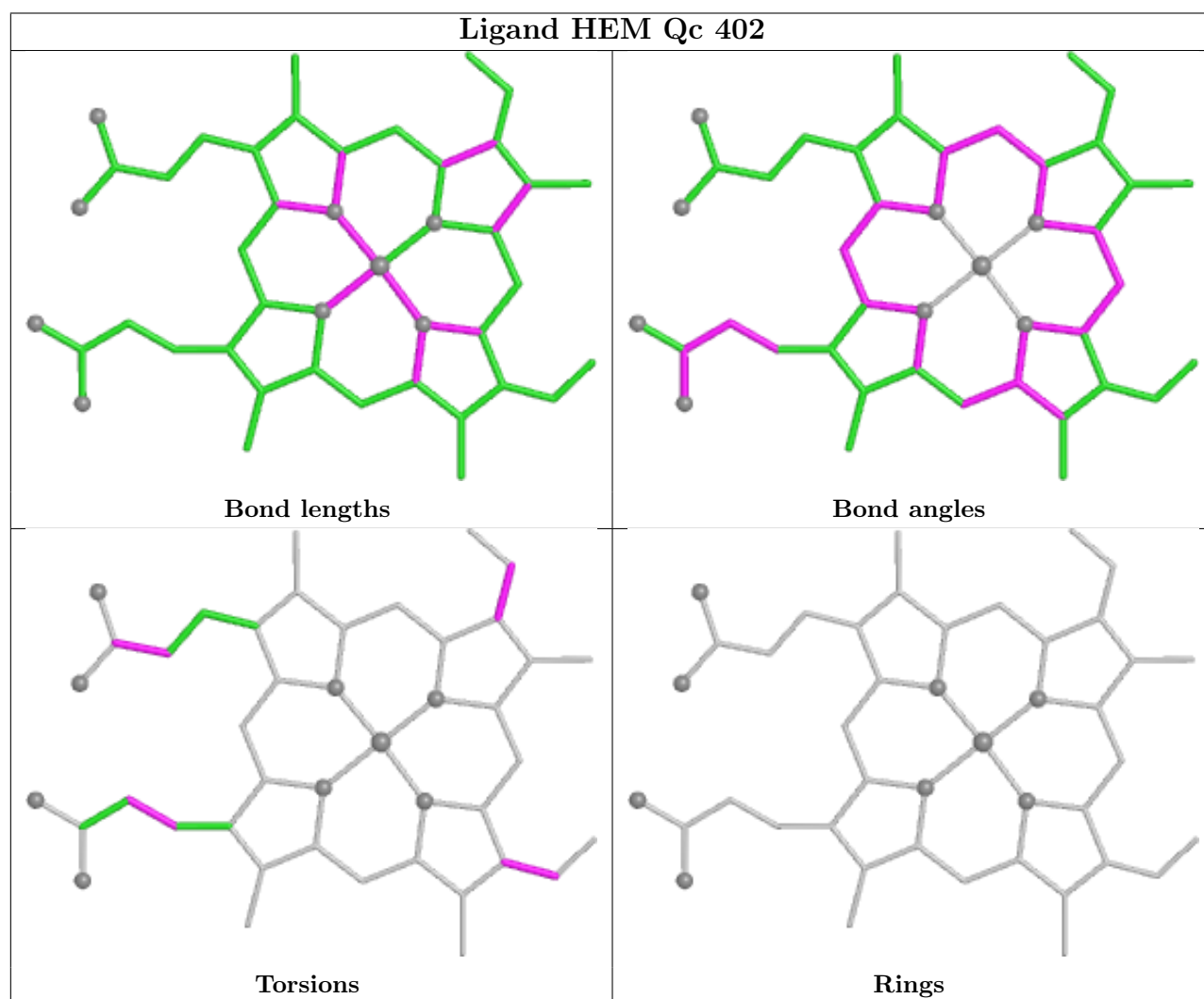
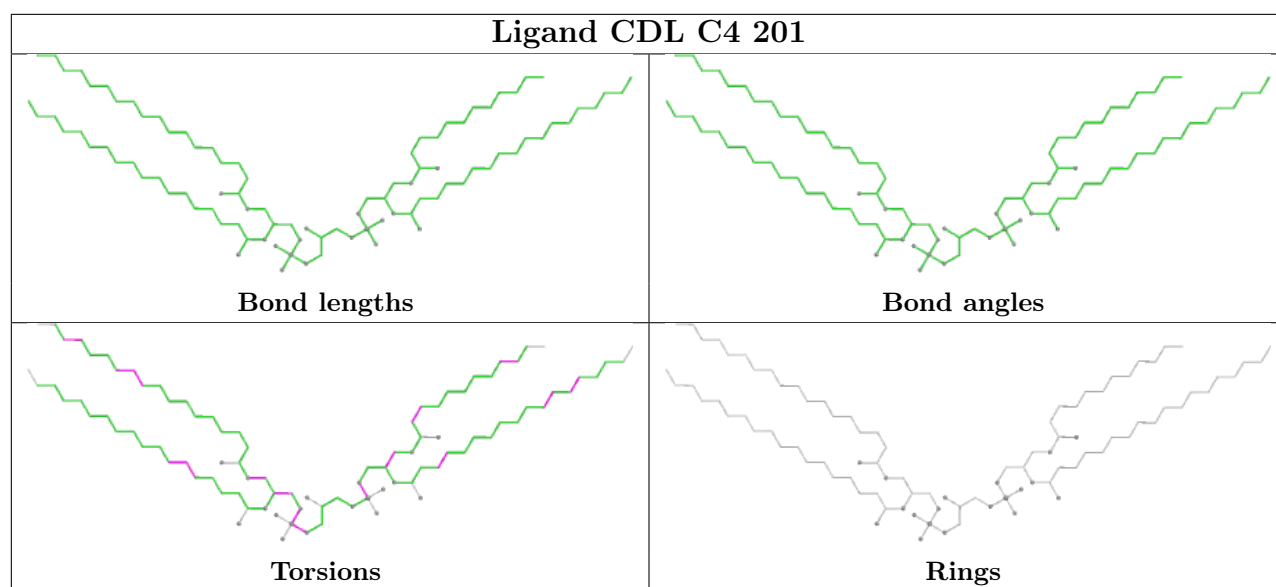


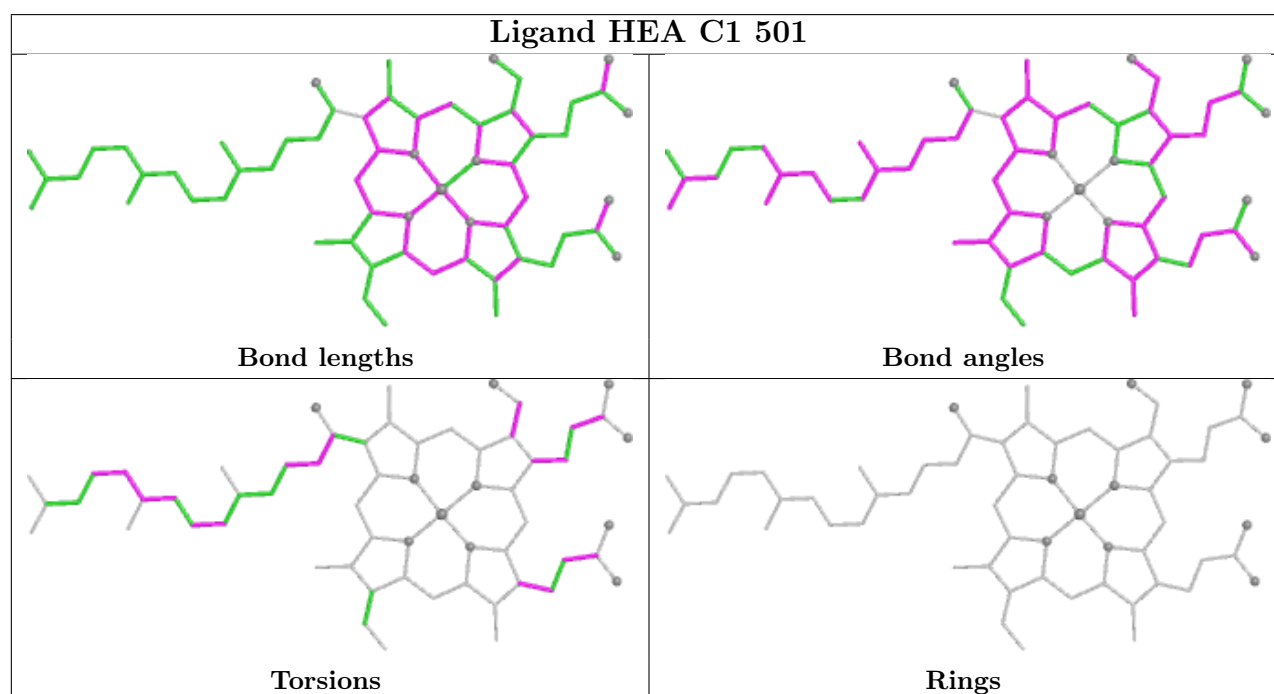
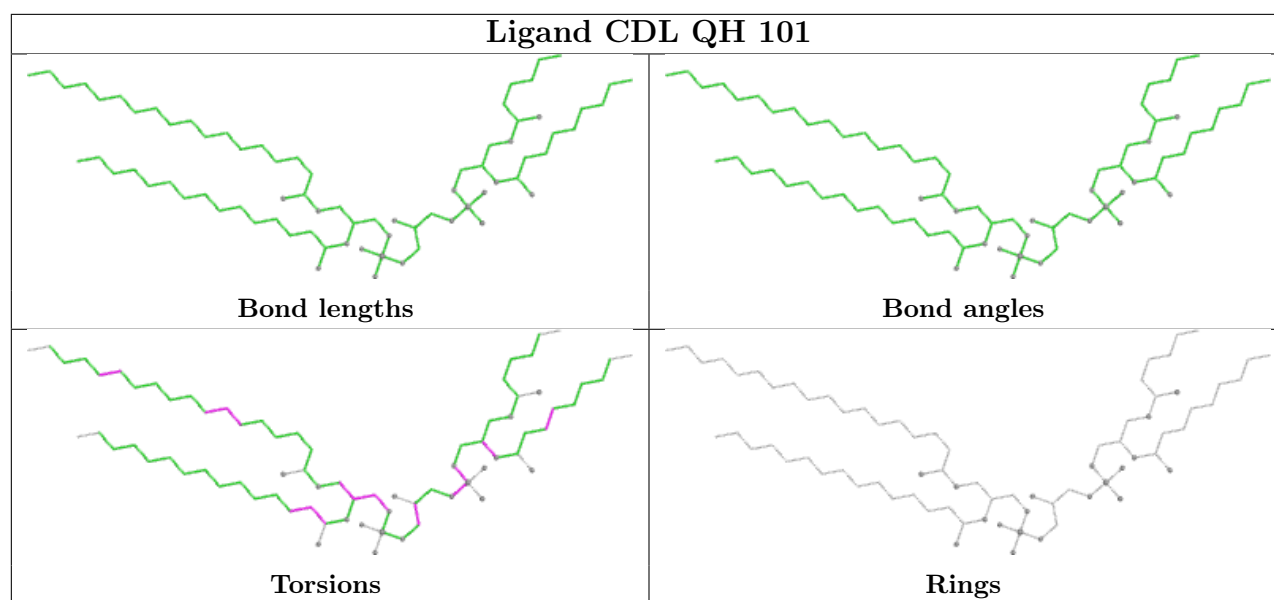


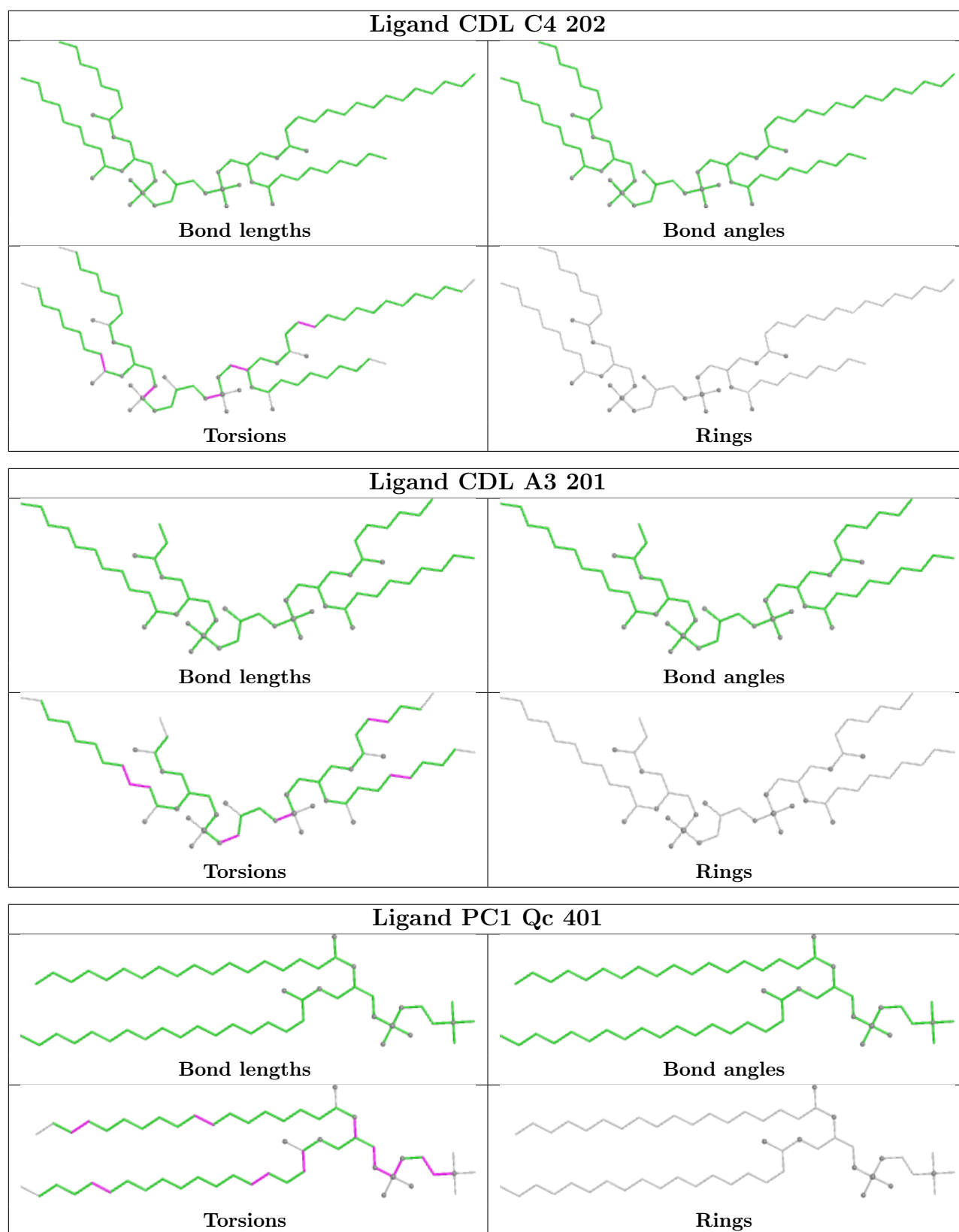


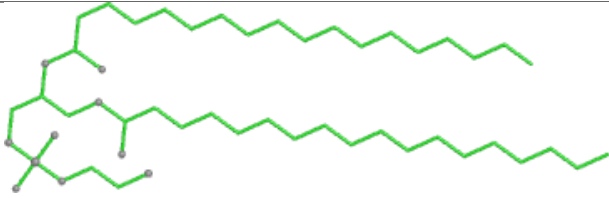
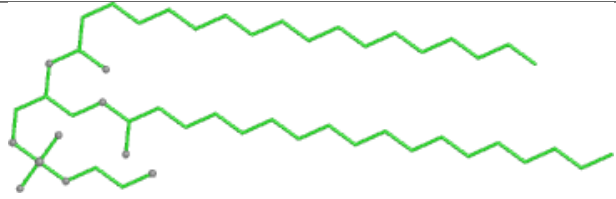
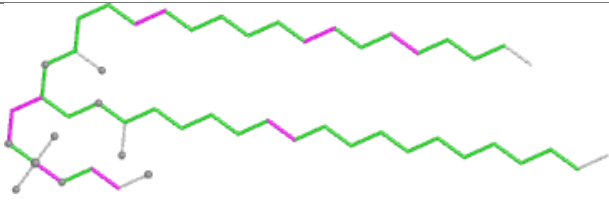
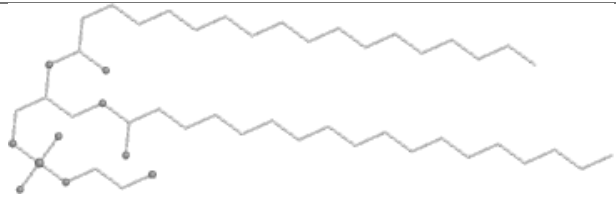


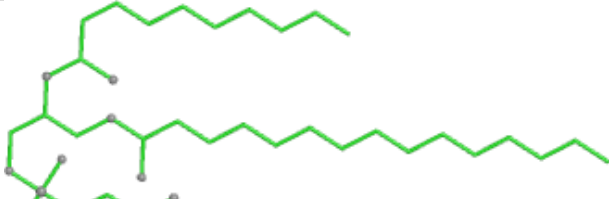
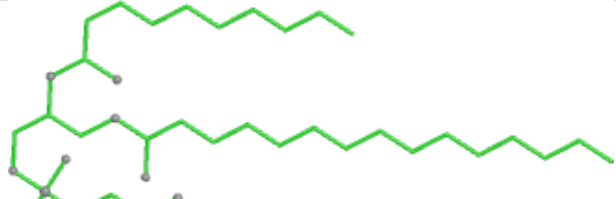
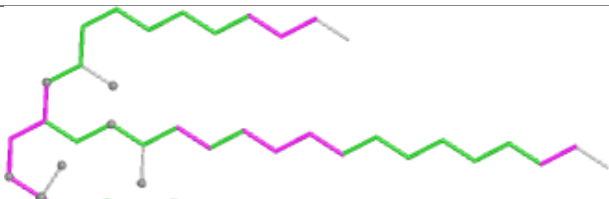
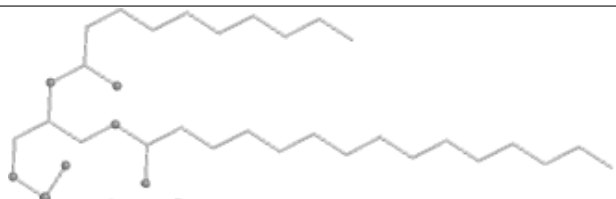


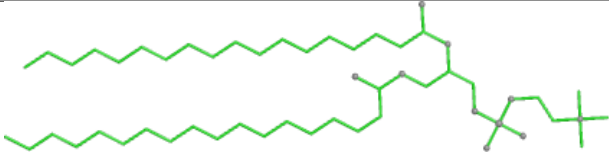
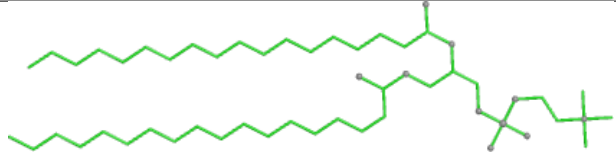
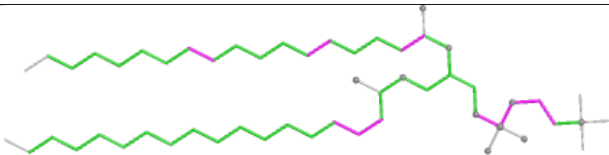
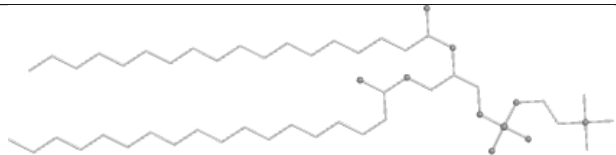


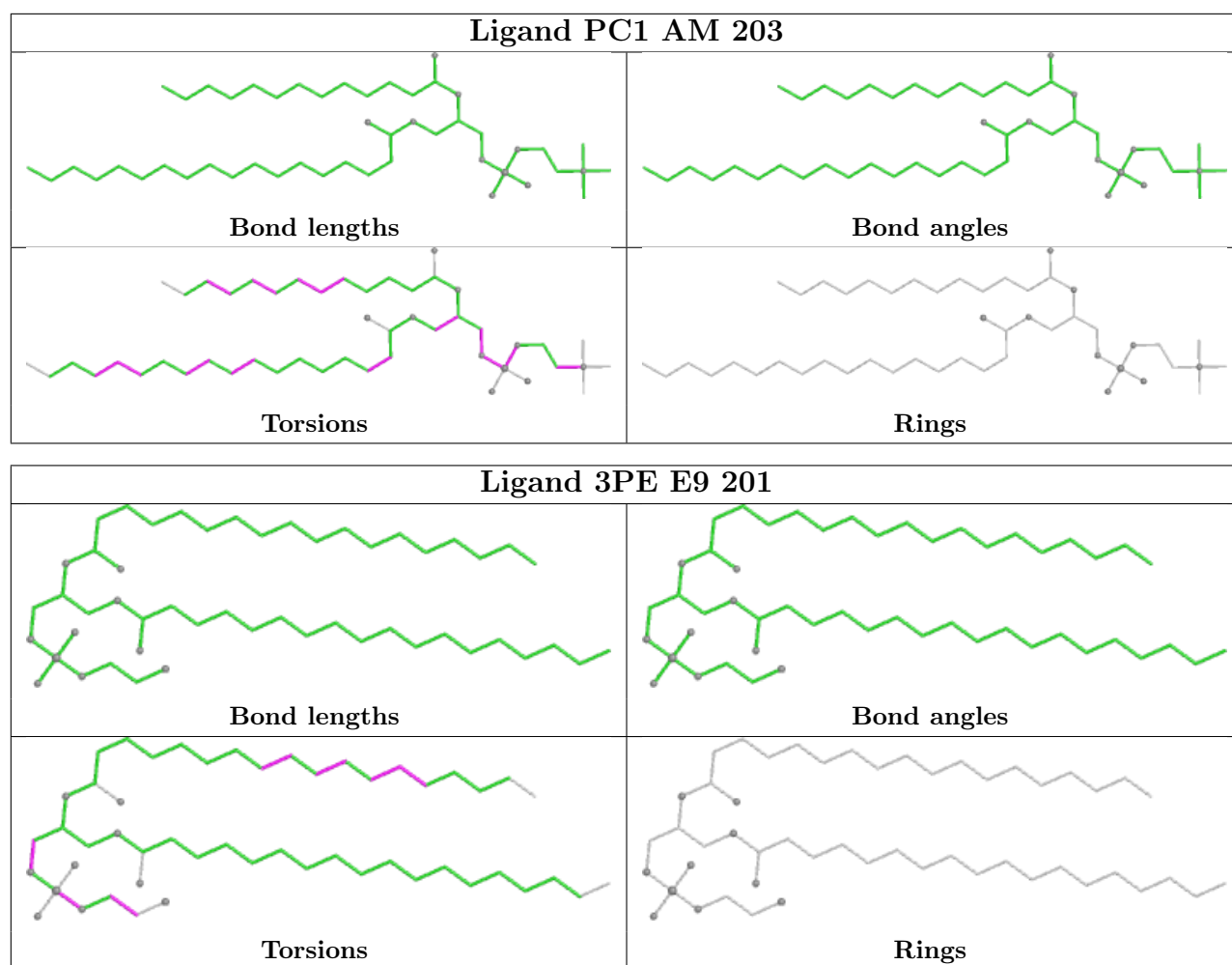


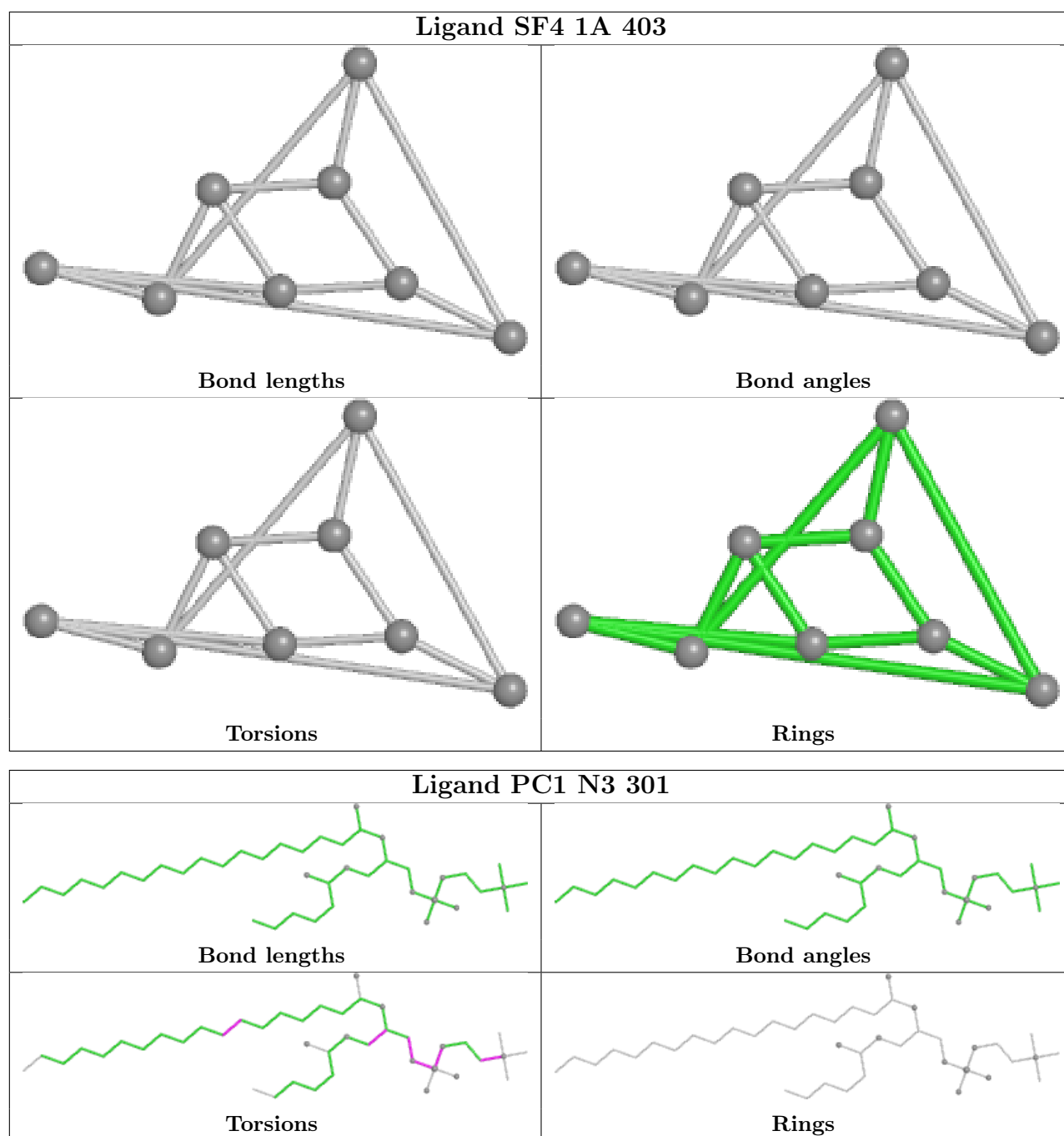


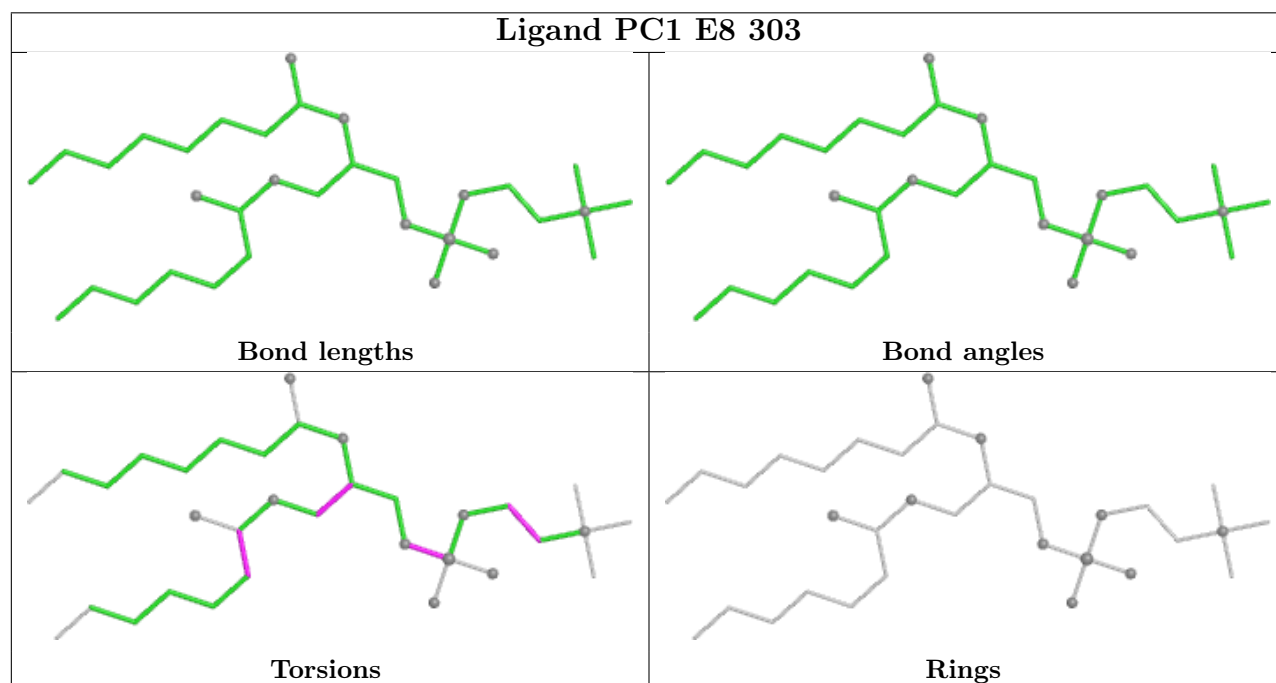
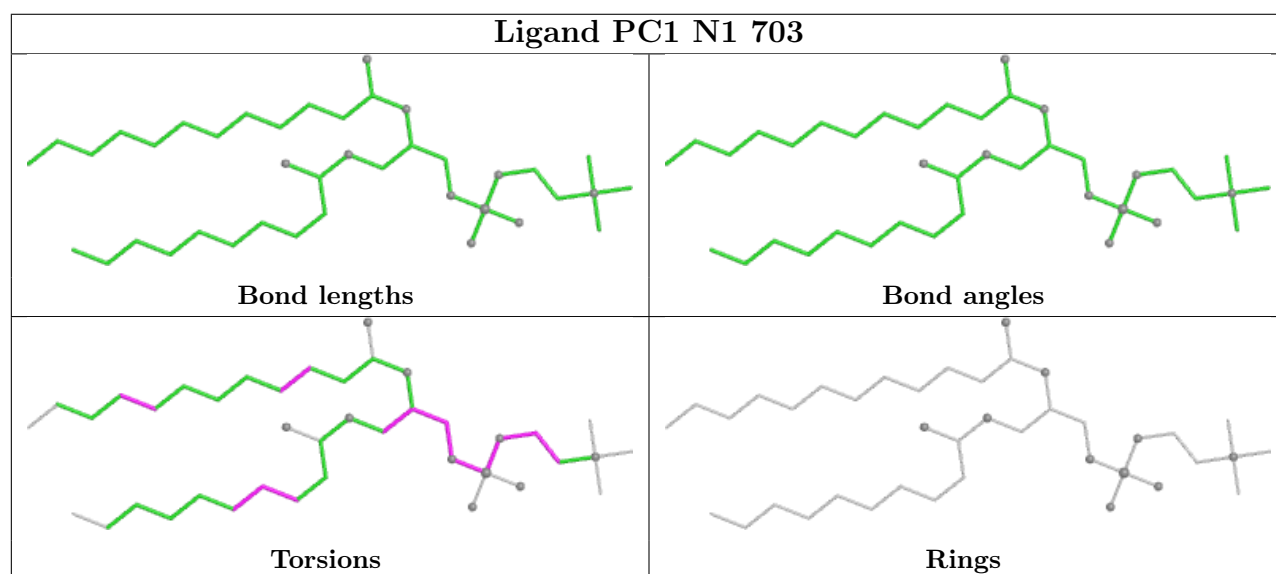
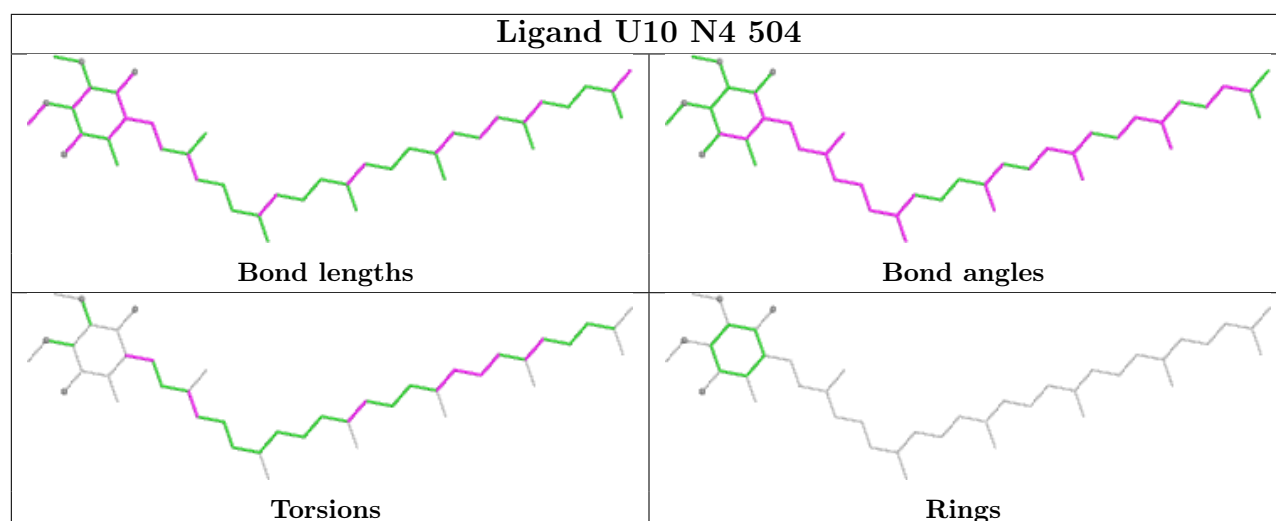
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Bond lengths	Bond angles
	
Torsions	Rings

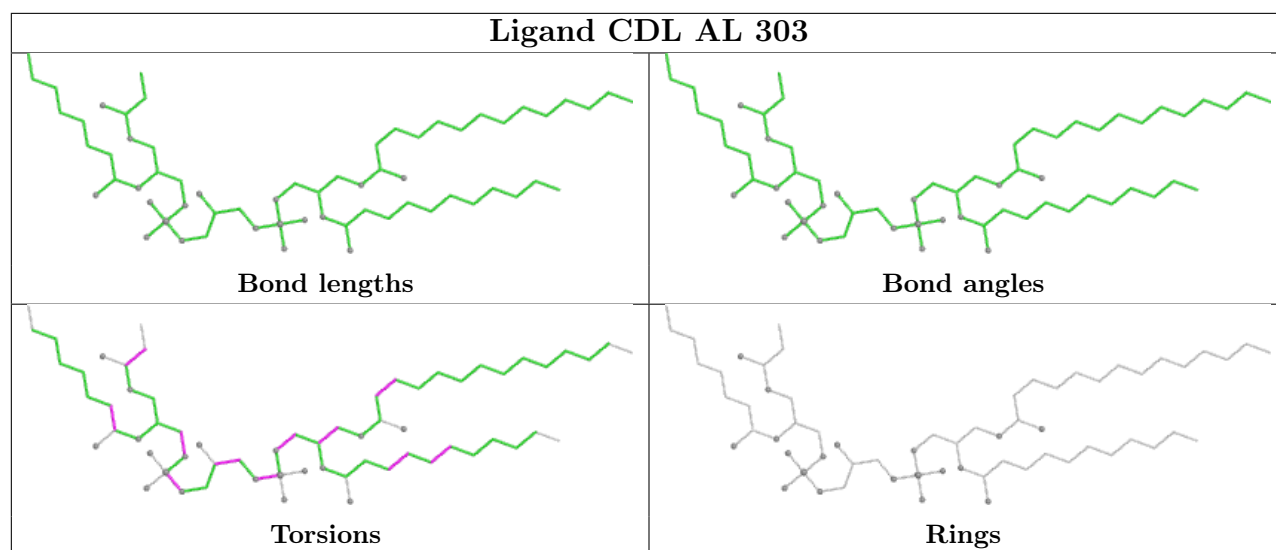
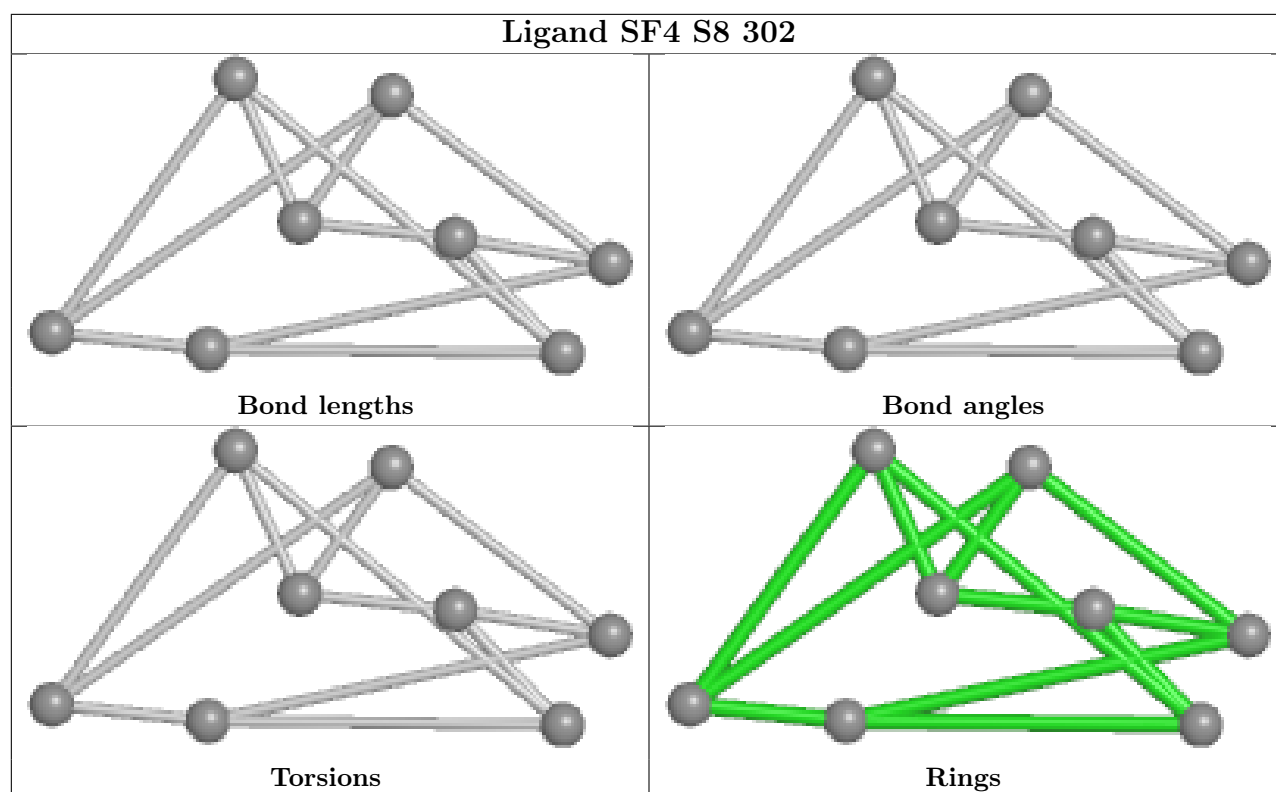
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Bond lengths	Bond angles
	
Torsions	Rings

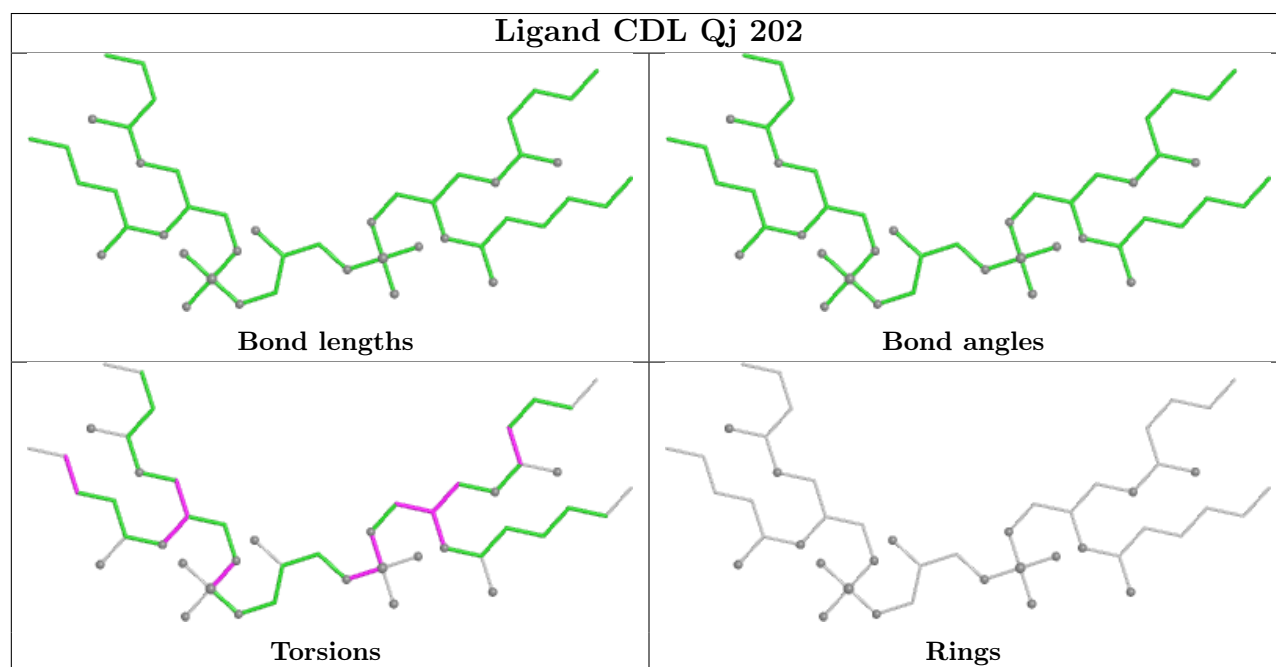
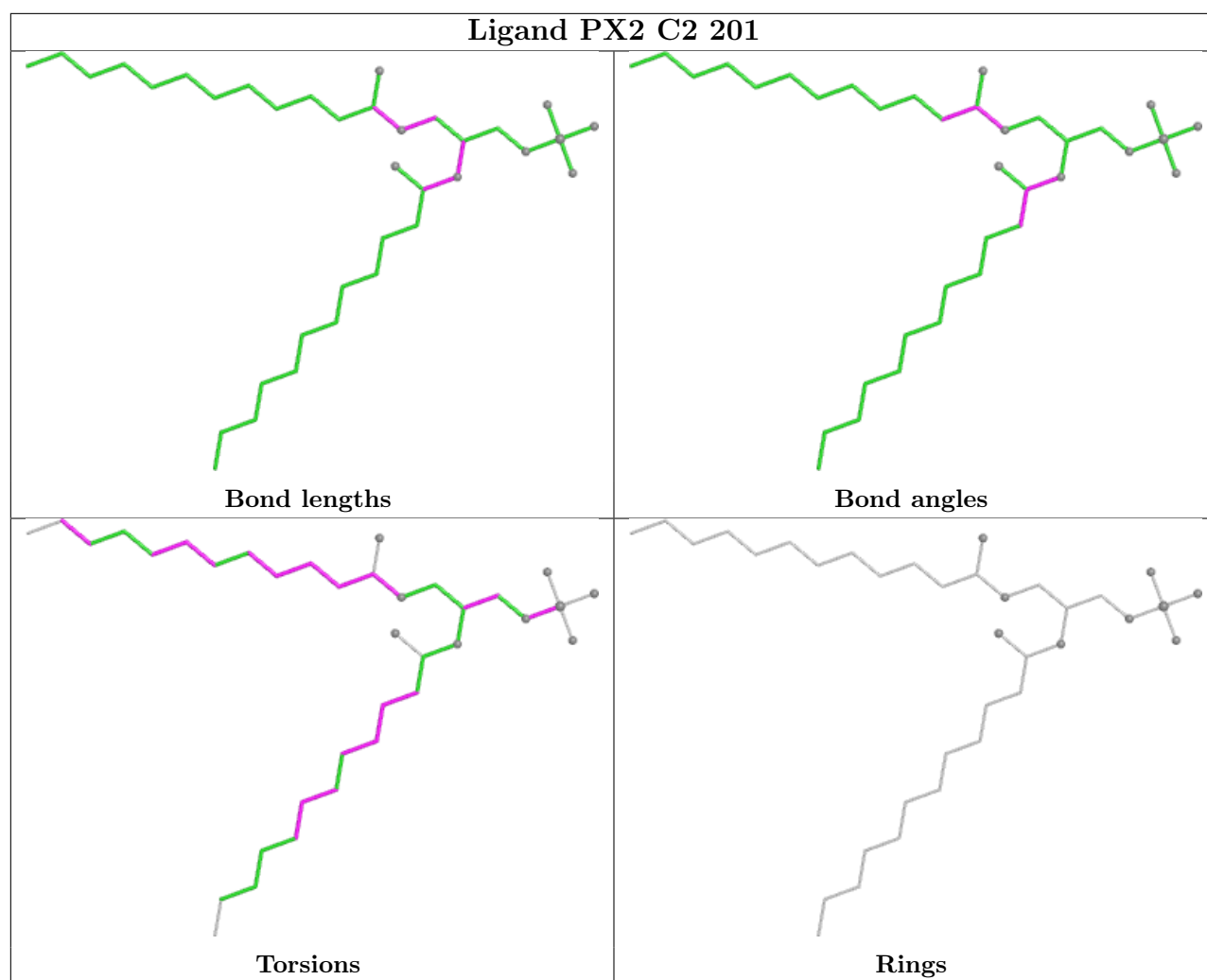
Ligand PC1 E8 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

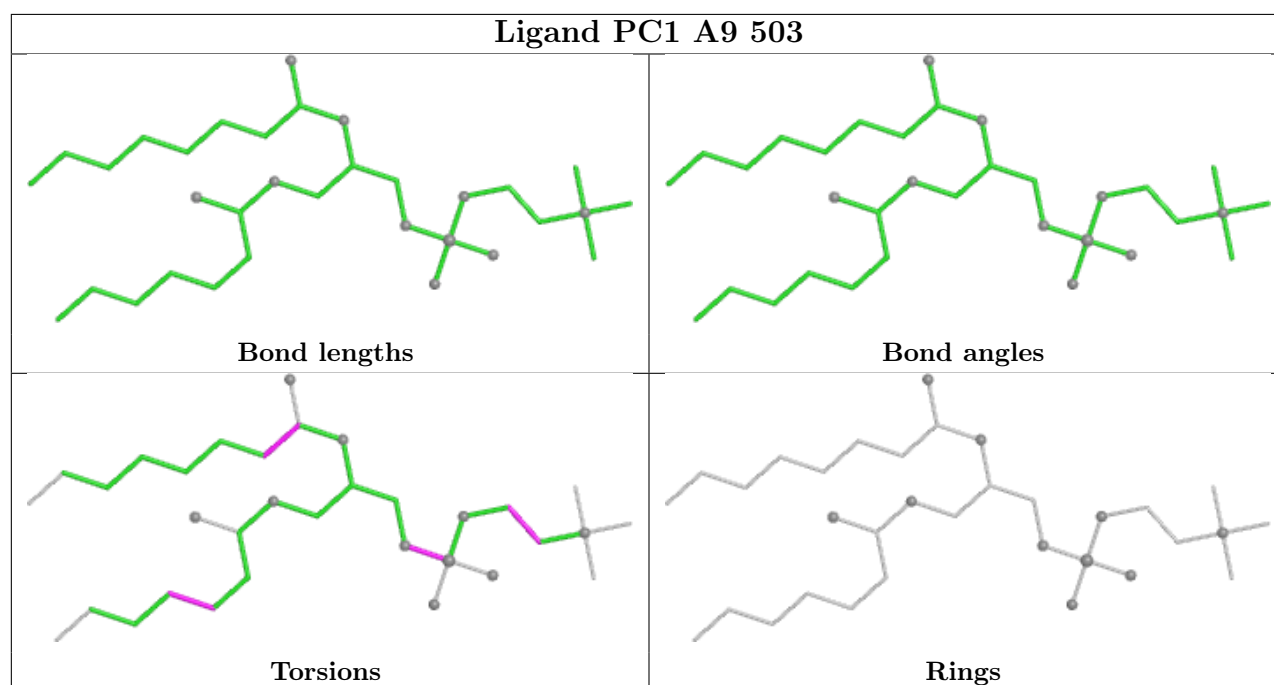
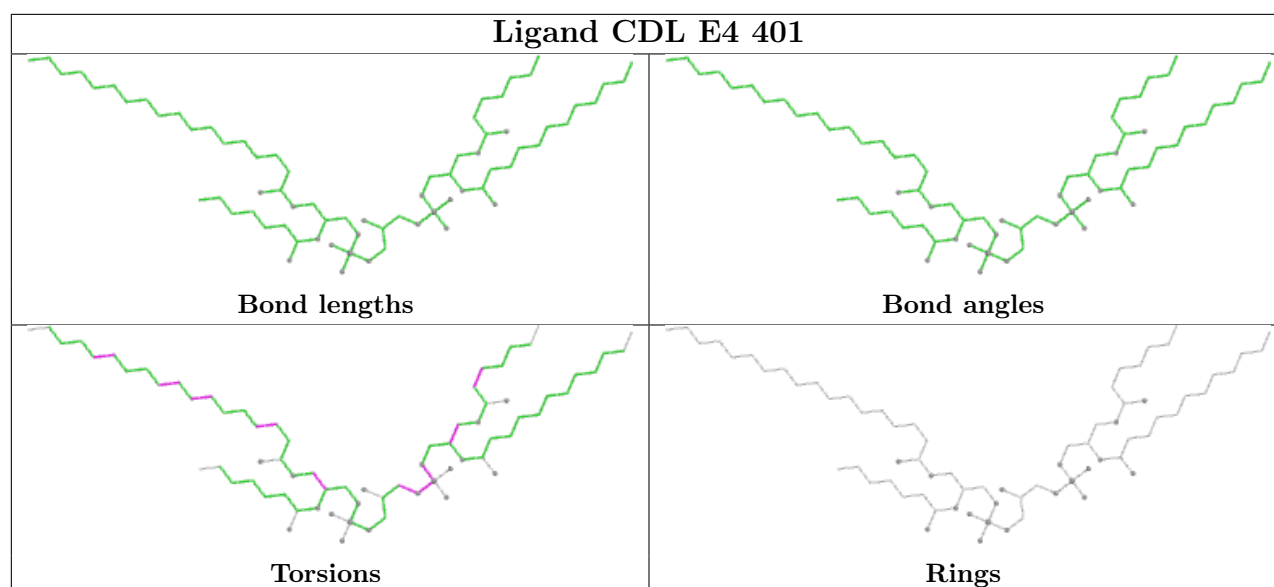


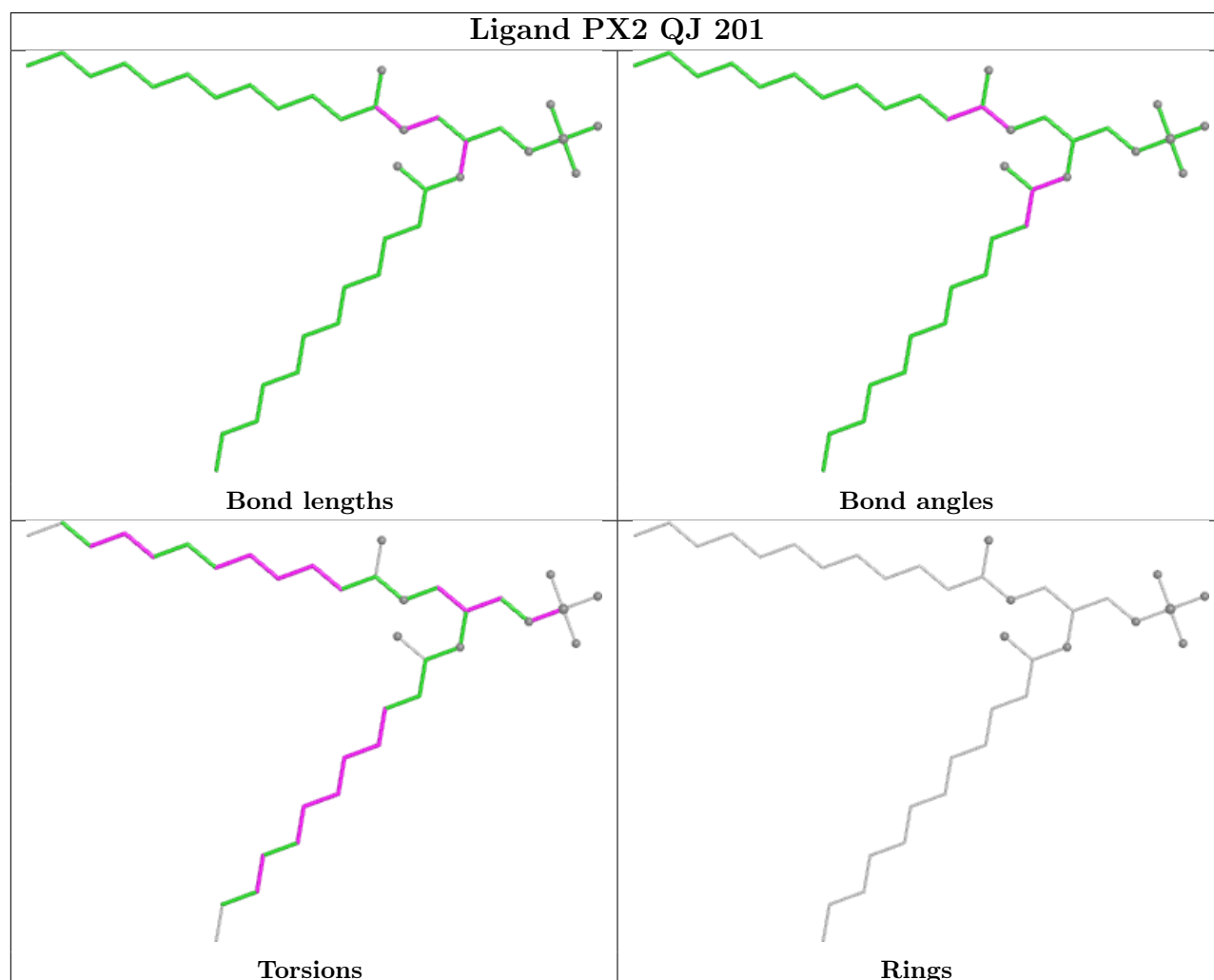
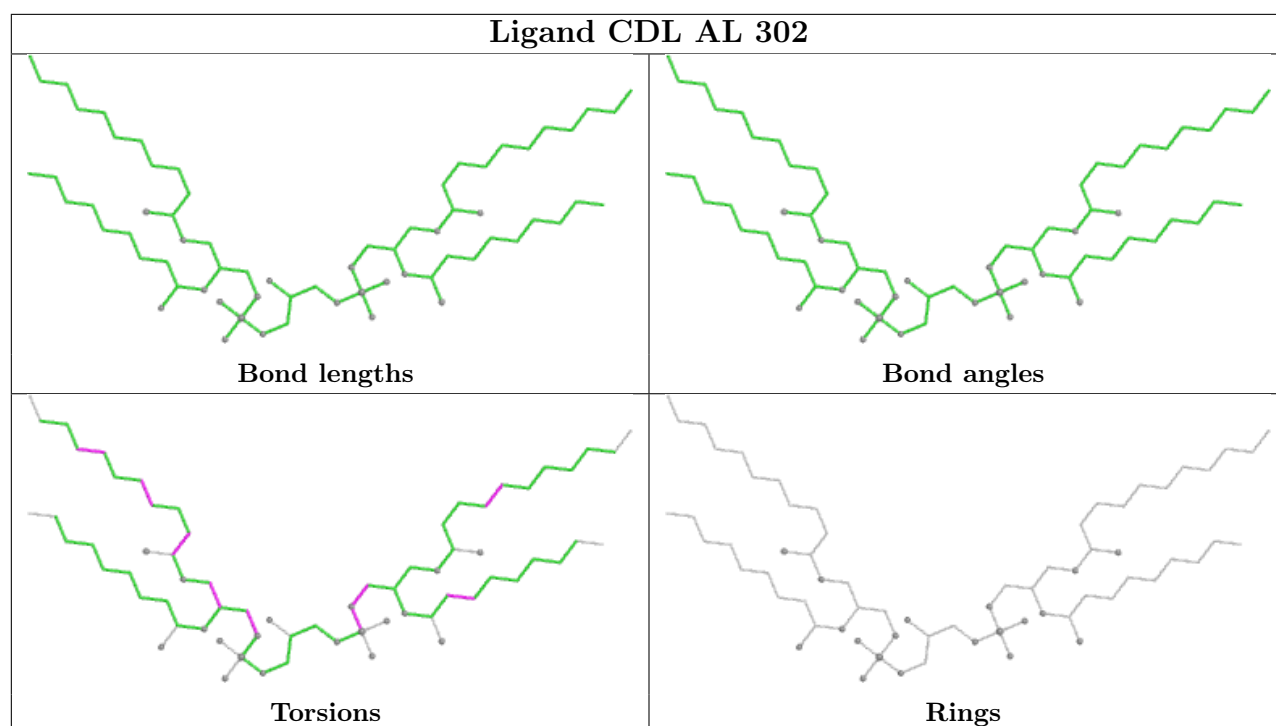




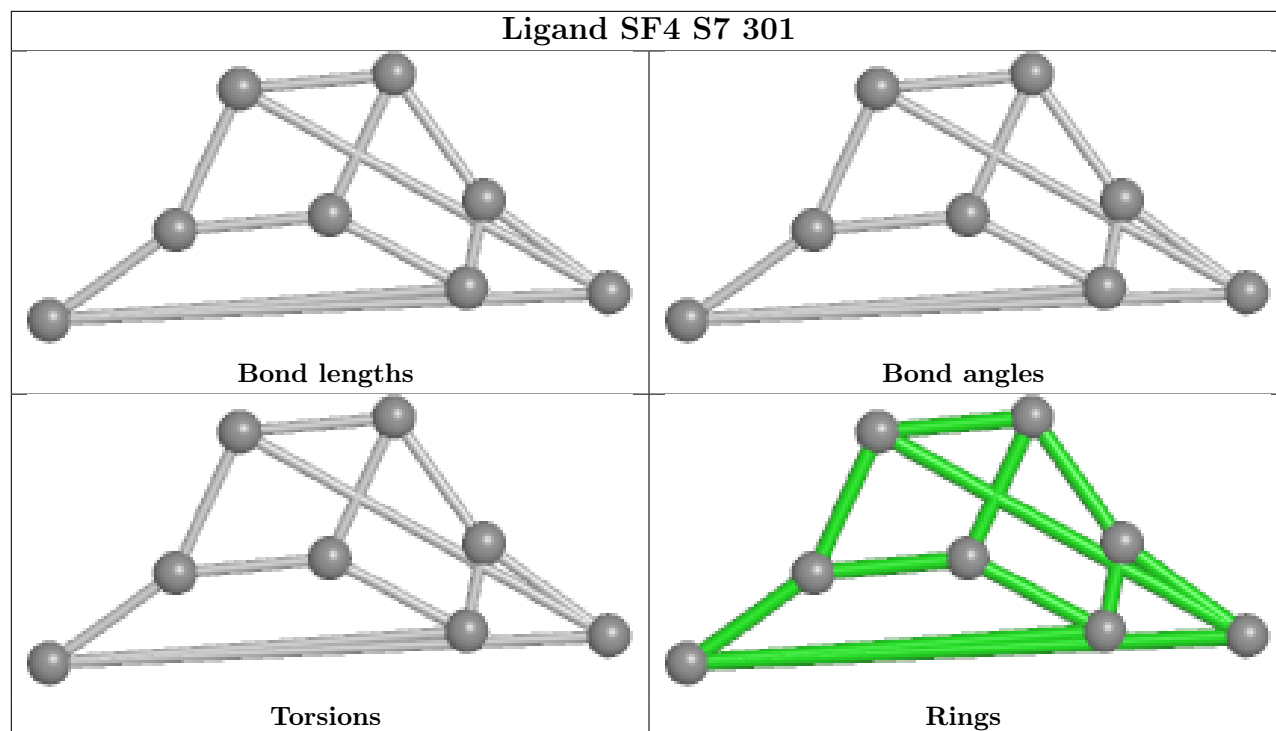




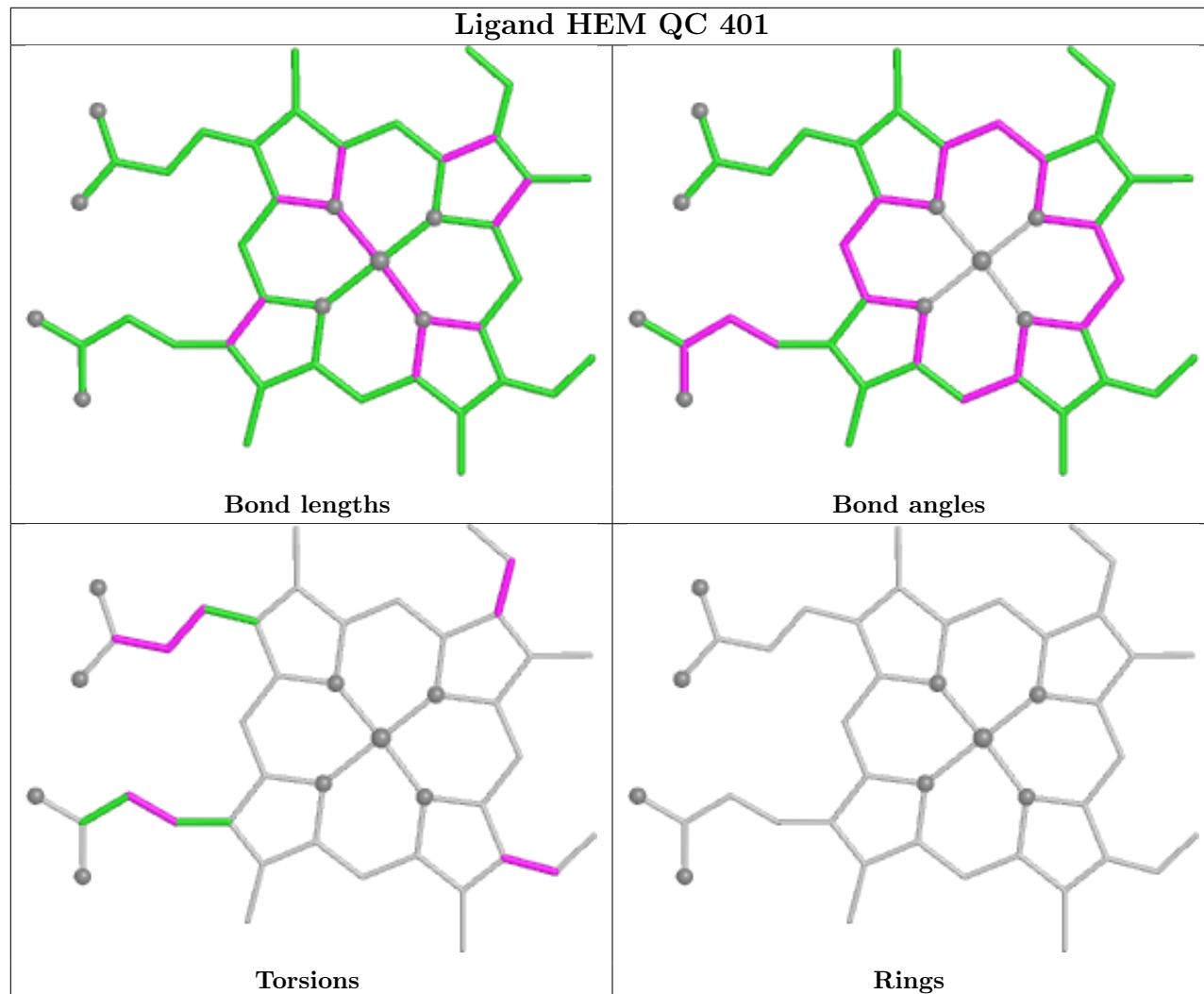


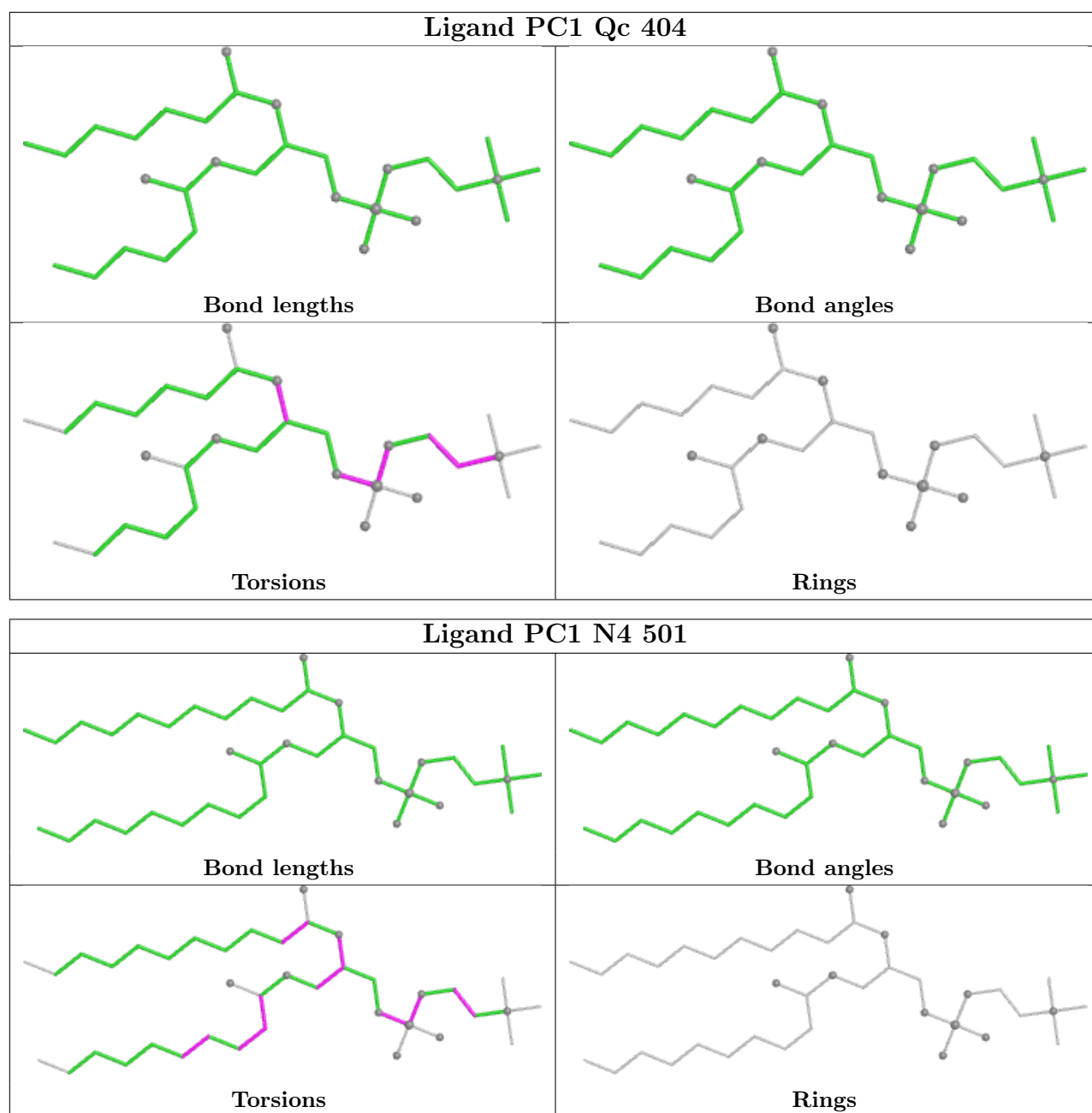


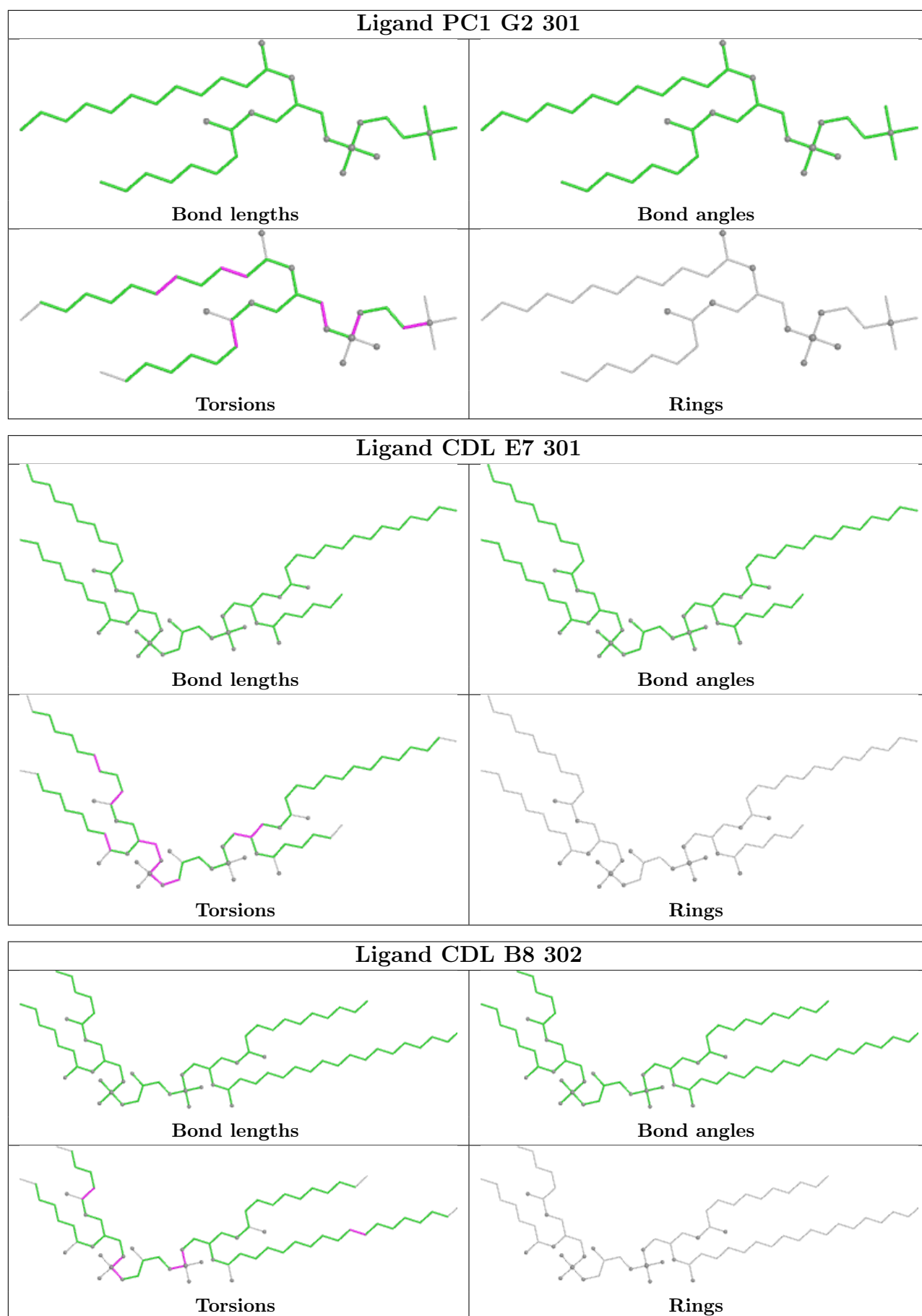
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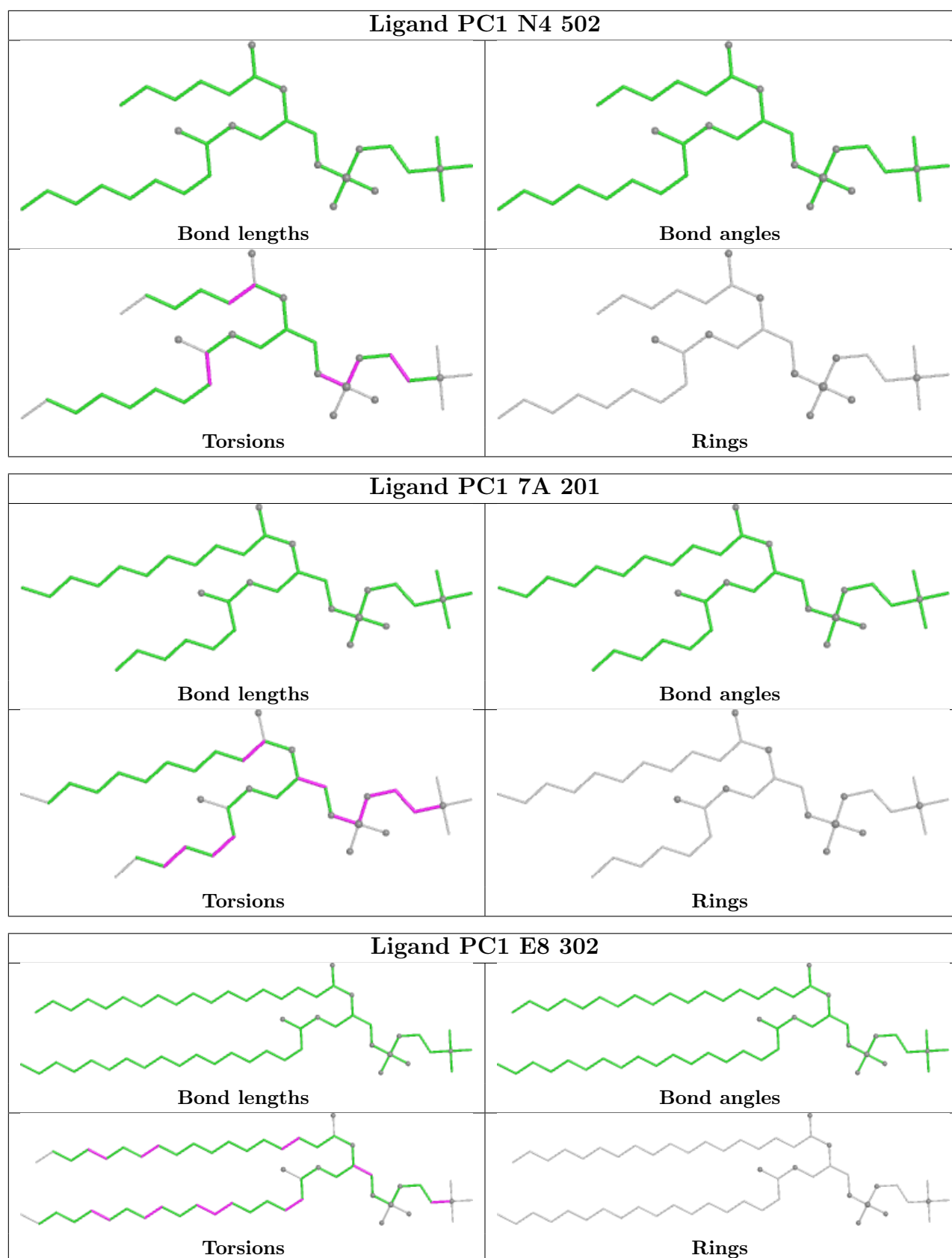


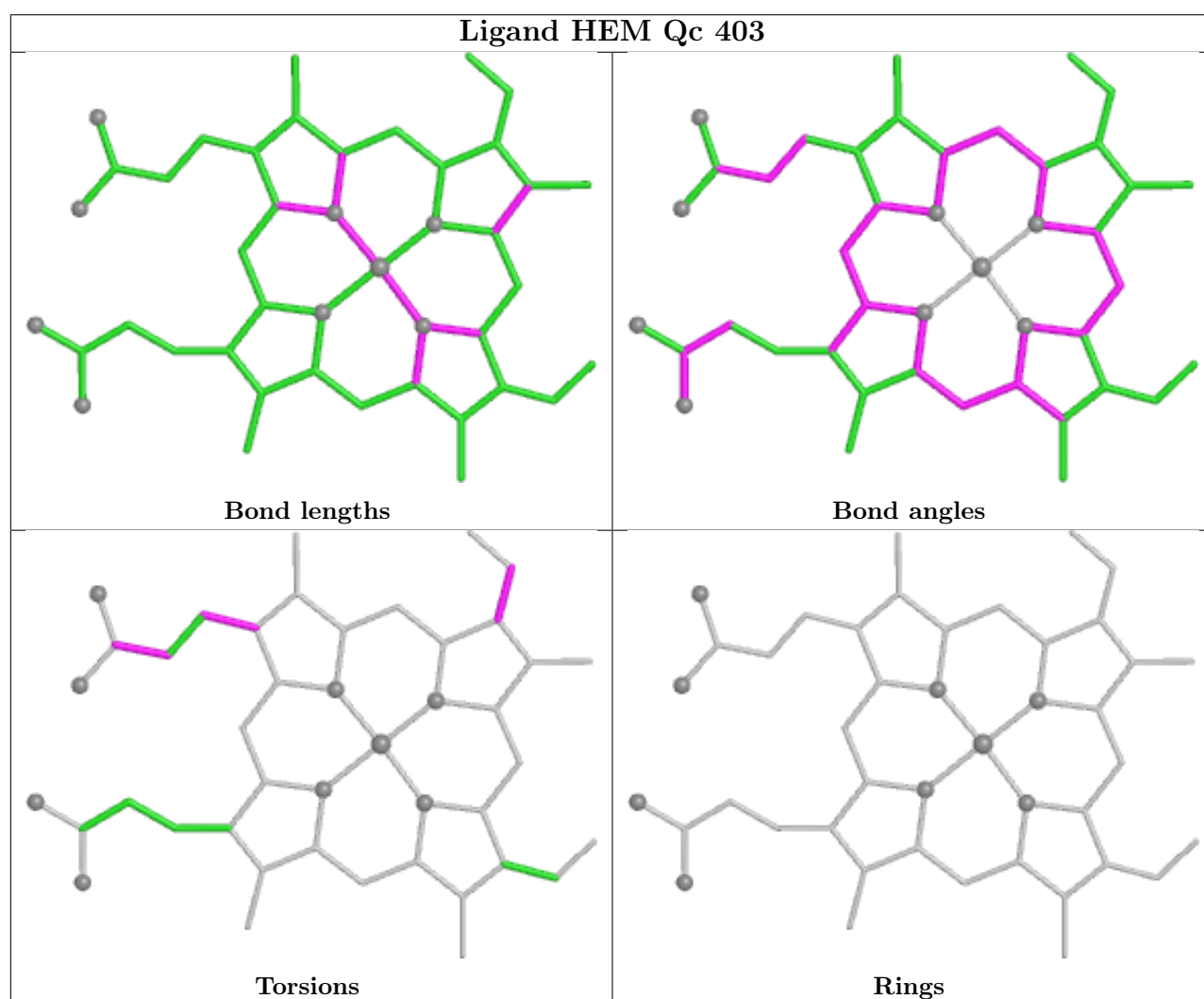
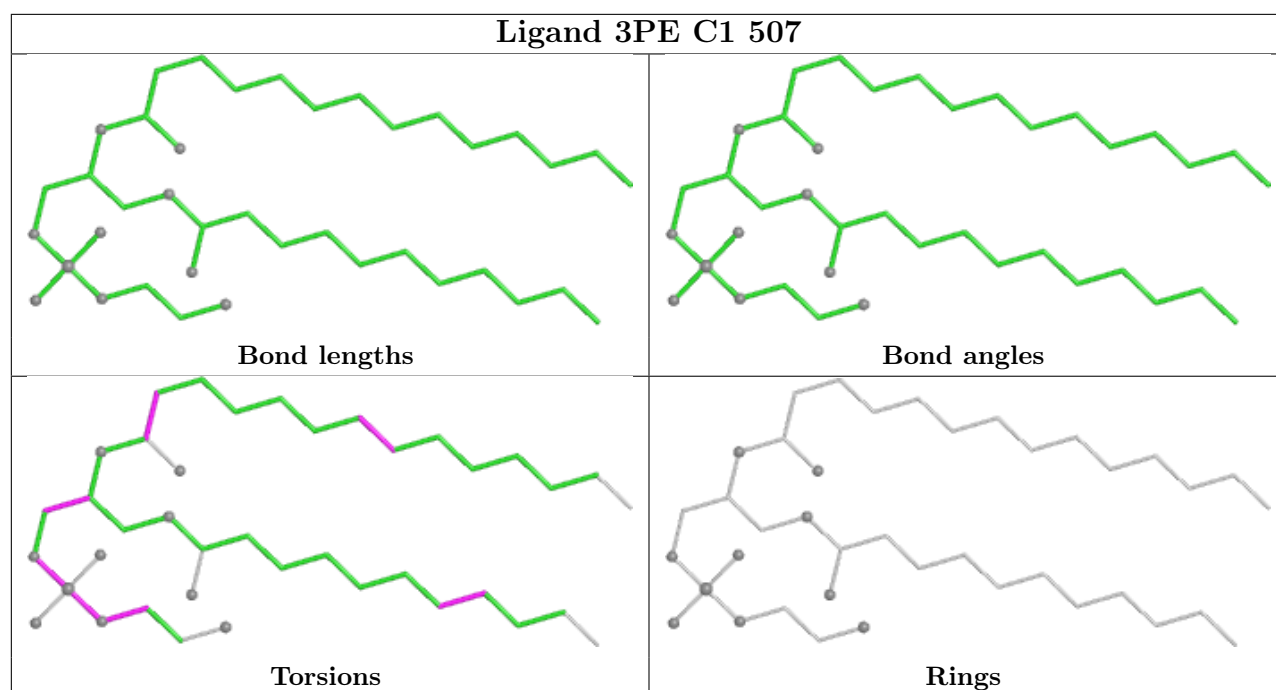
Ligand HEM QC 401

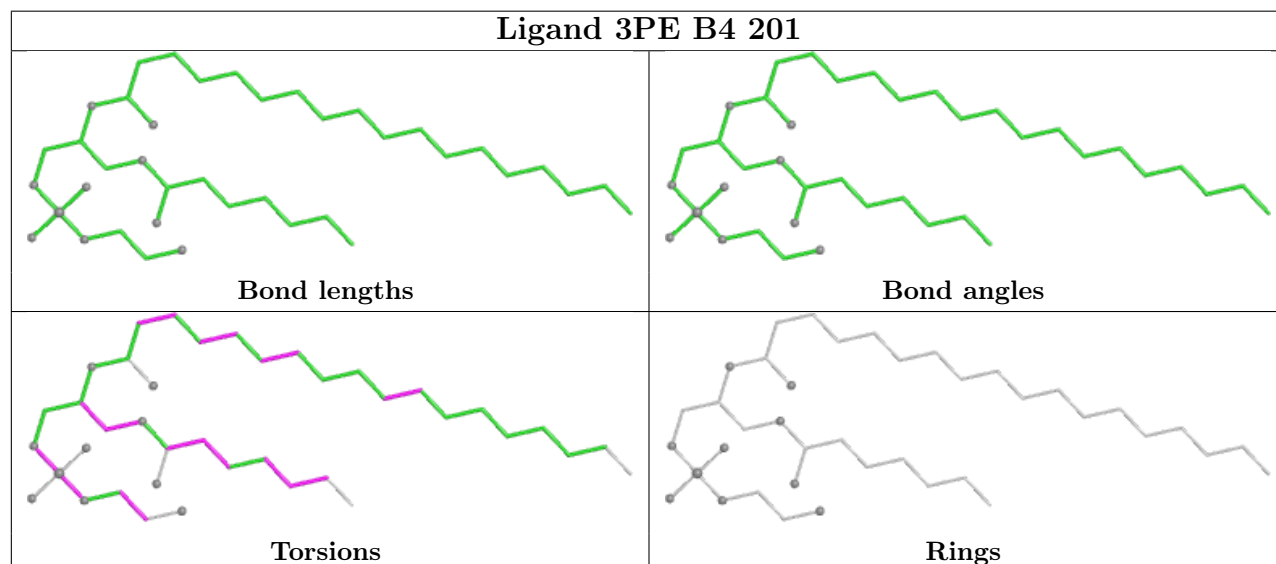
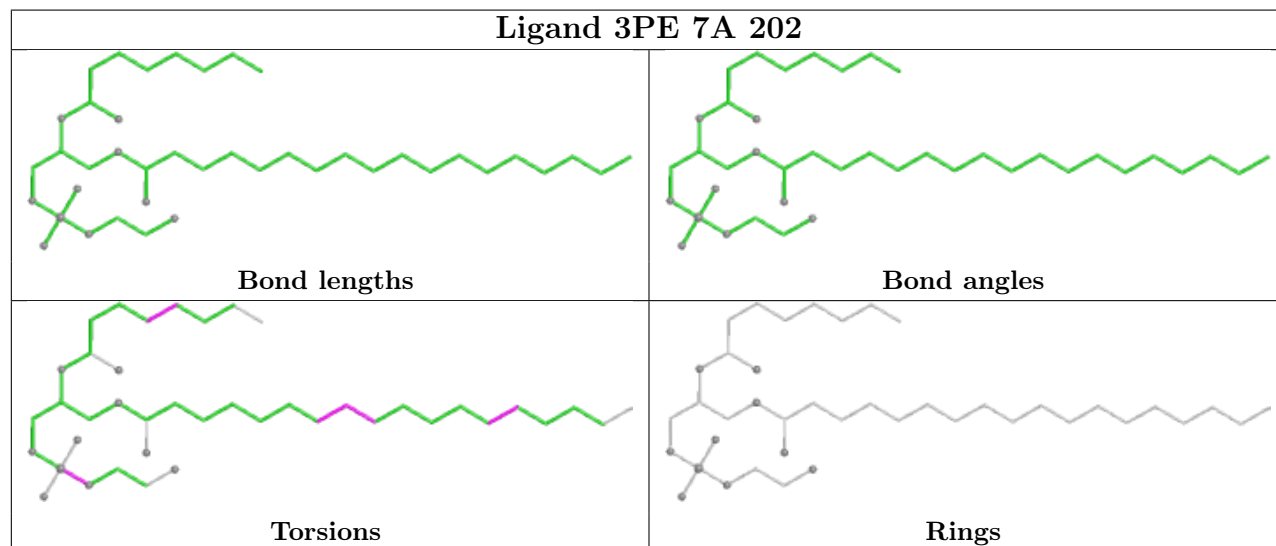
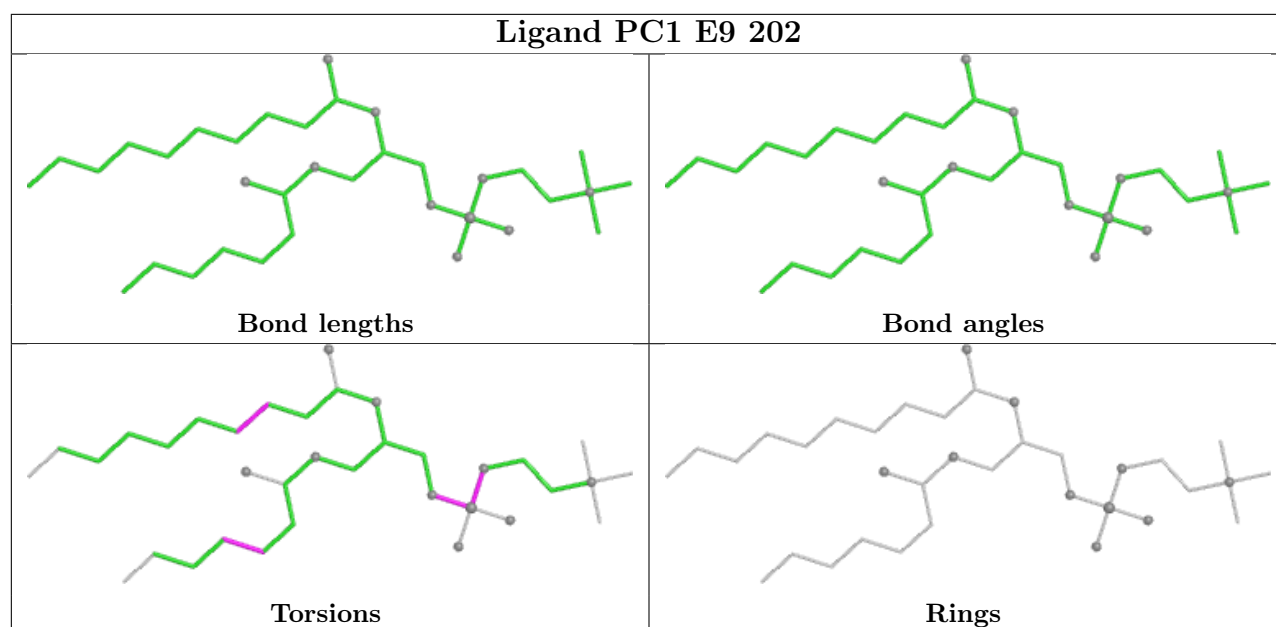


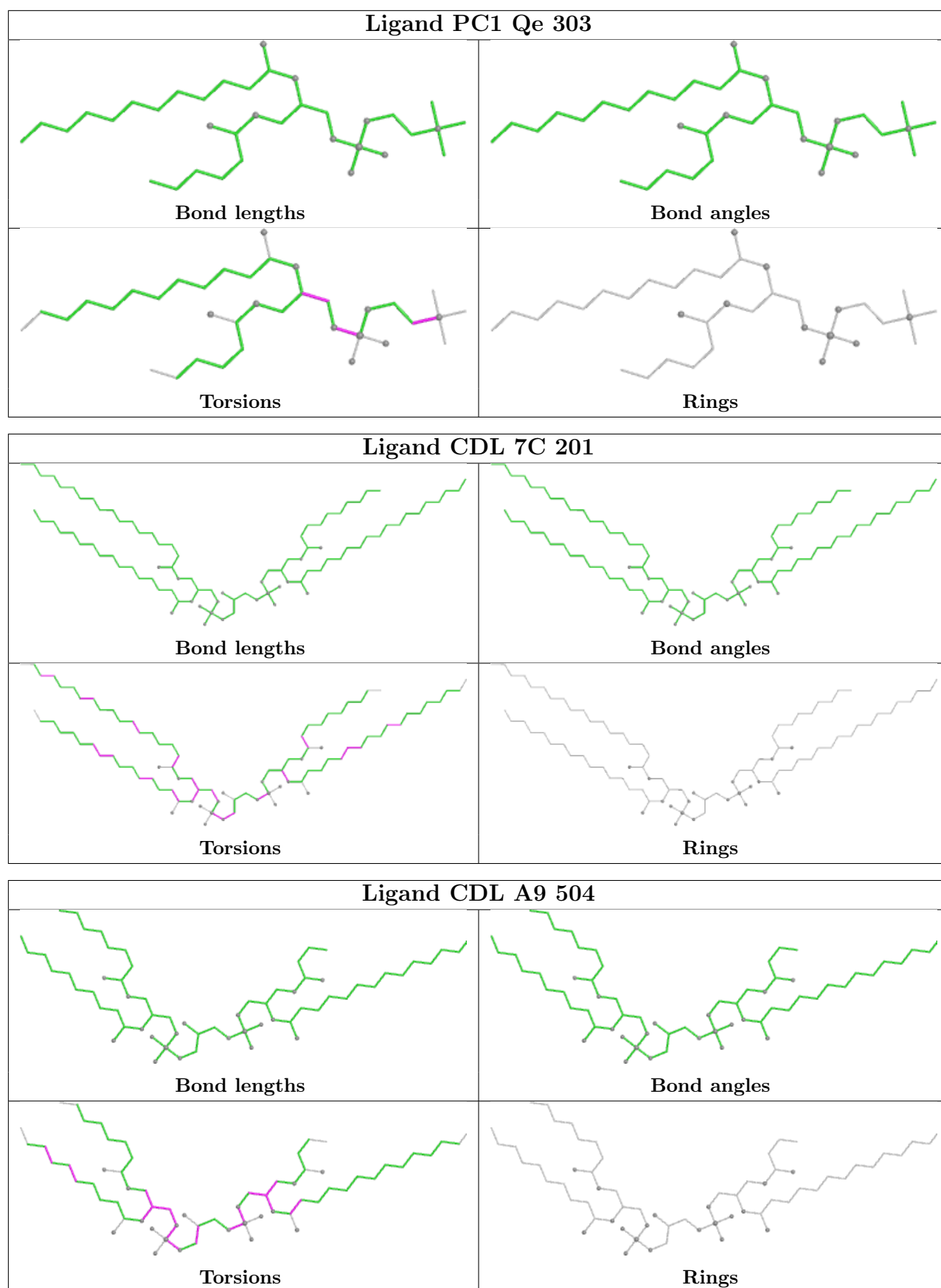


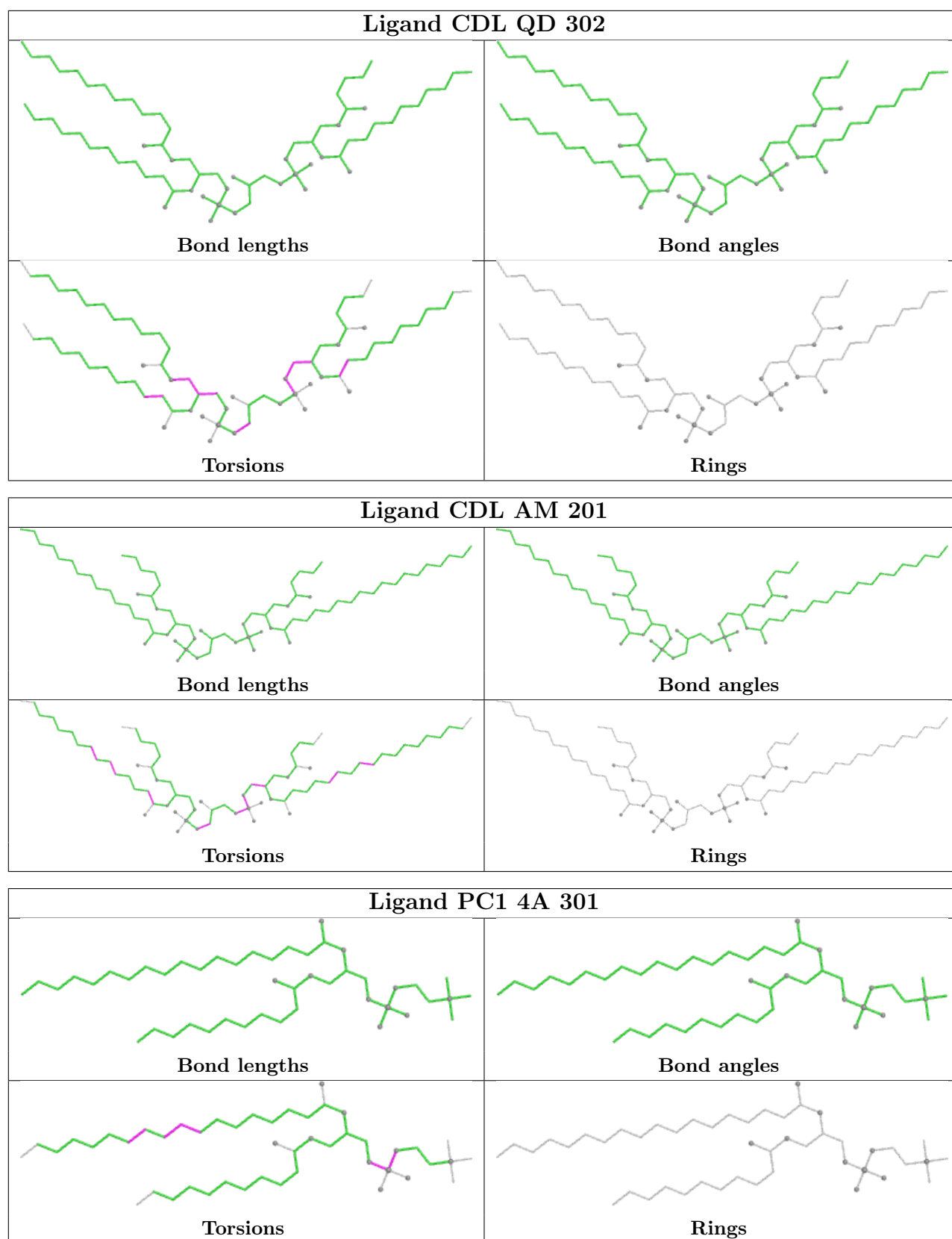


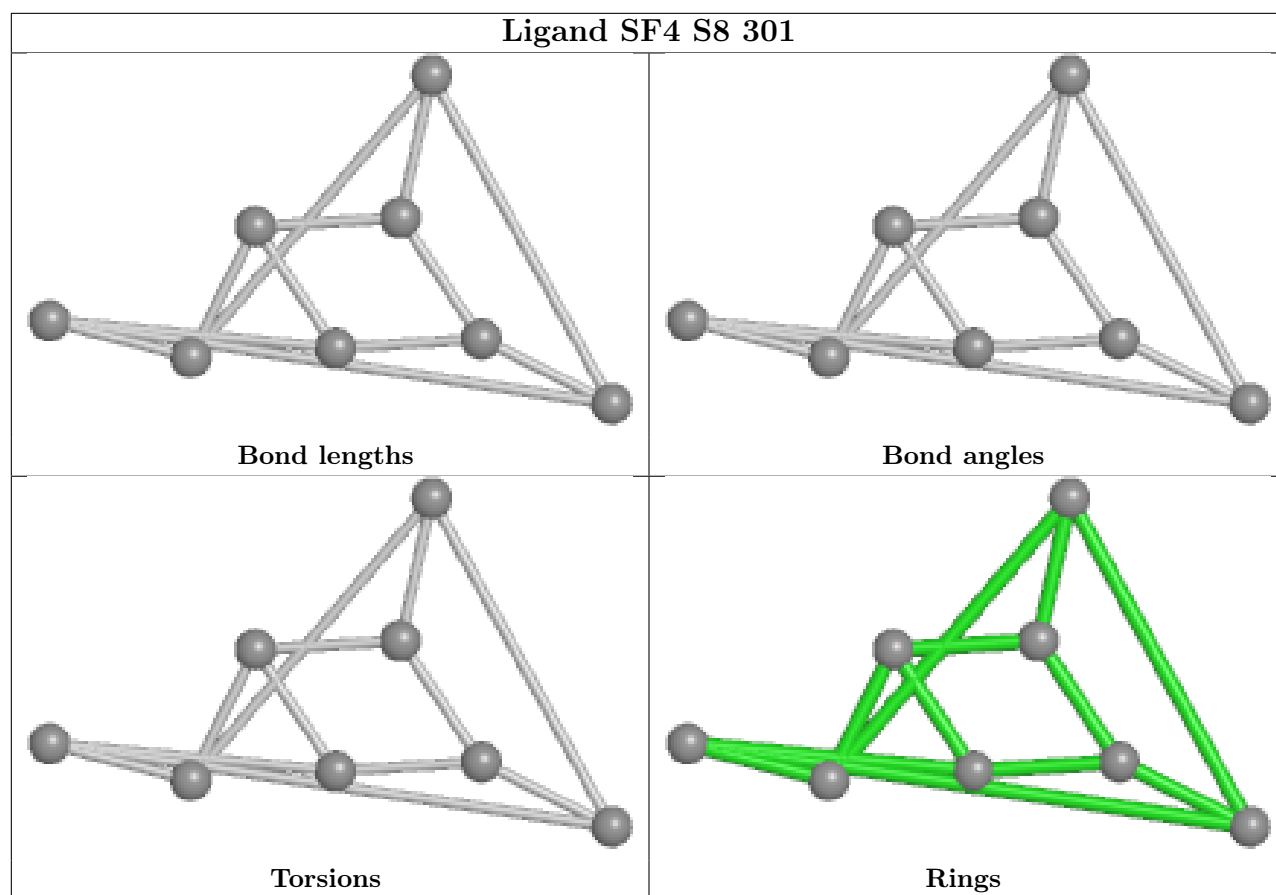
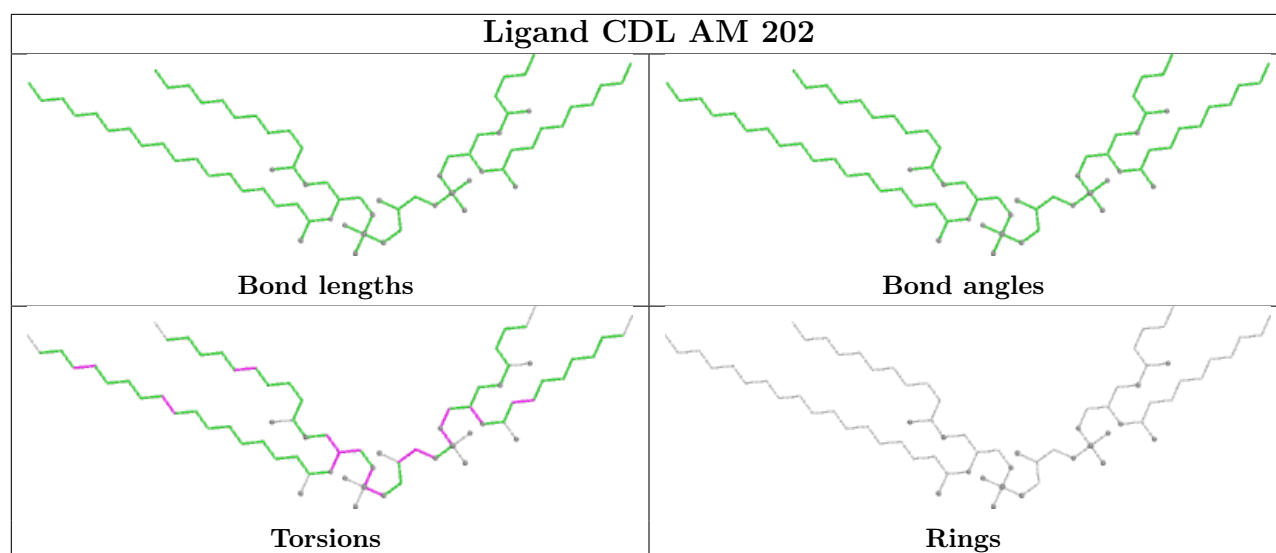


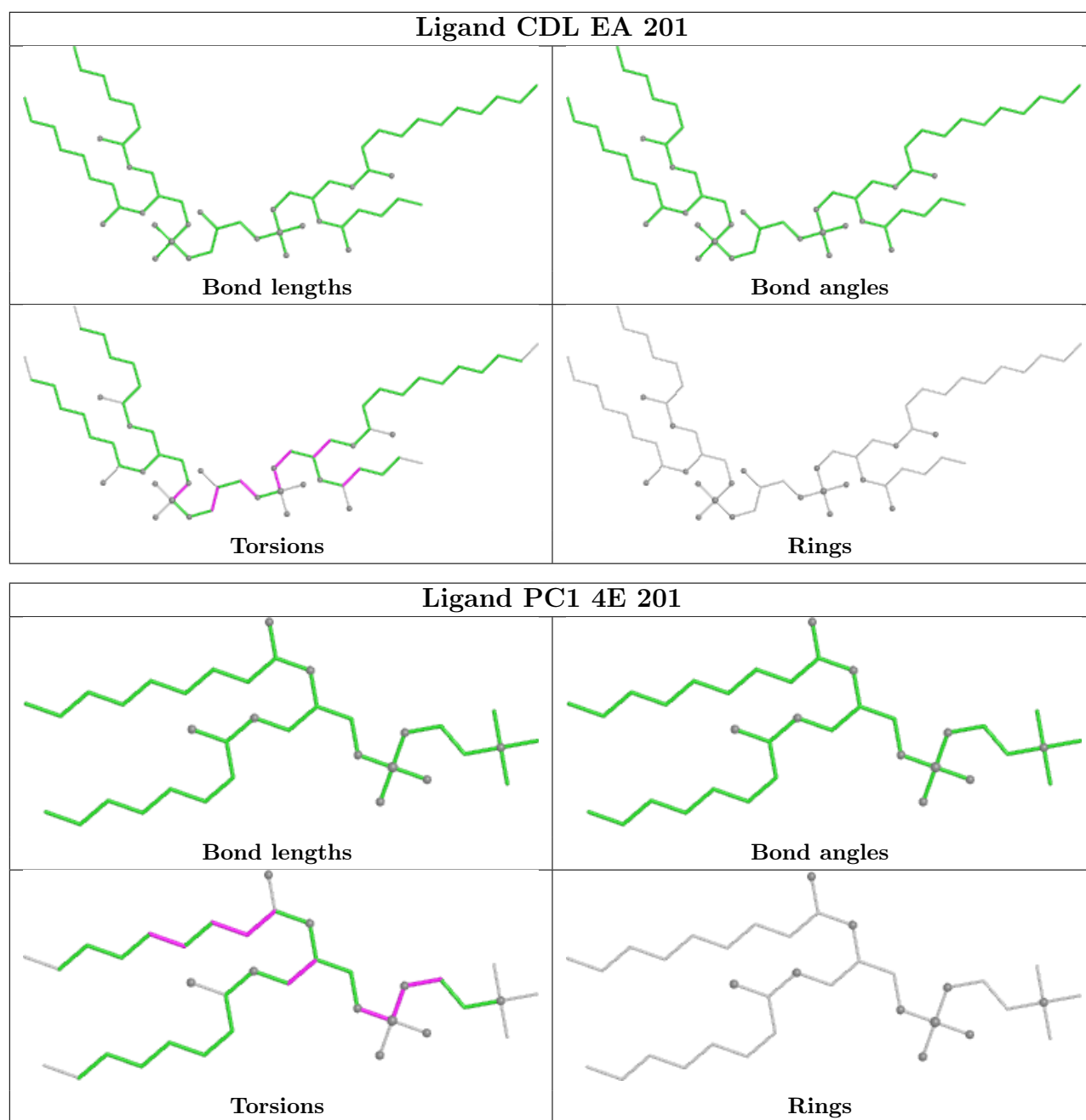


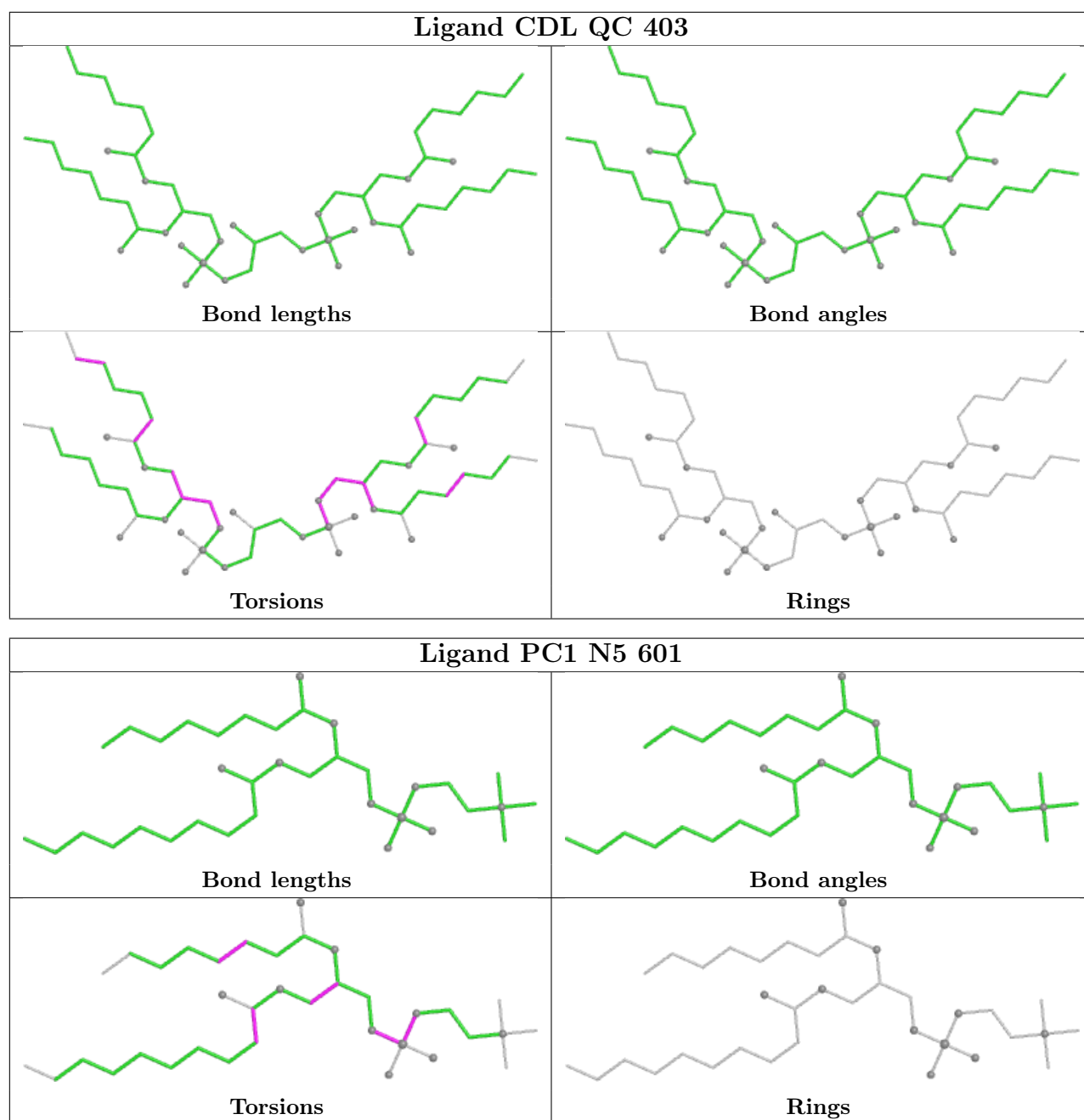


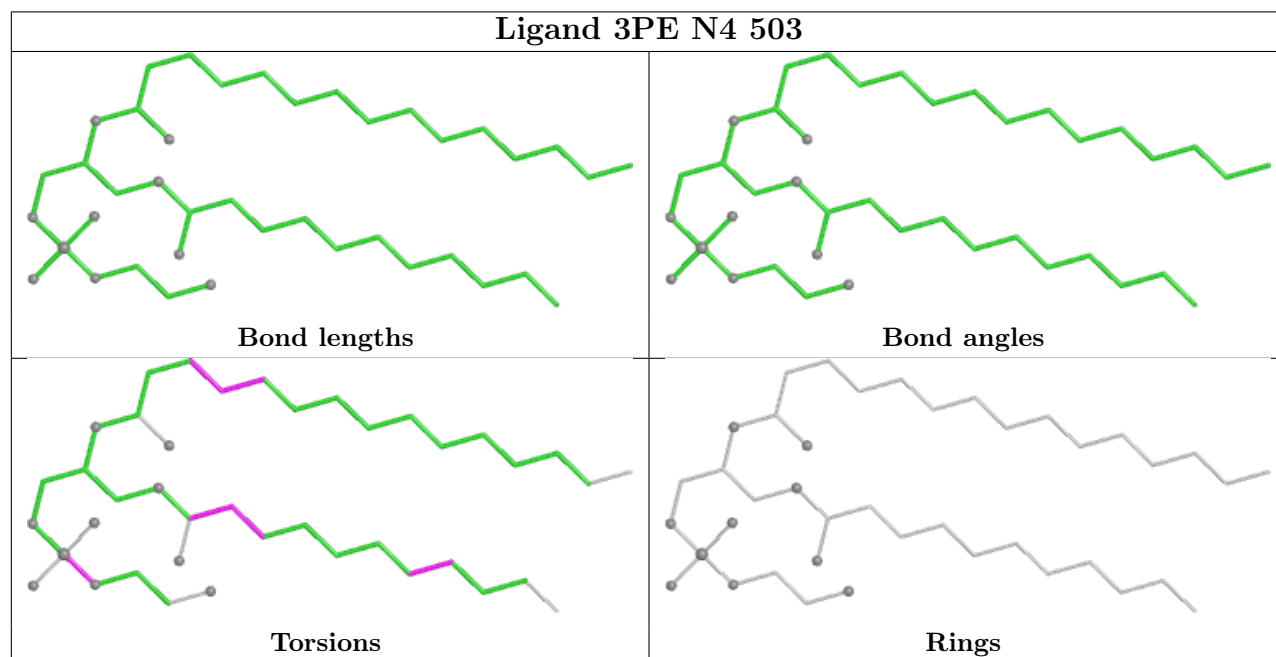
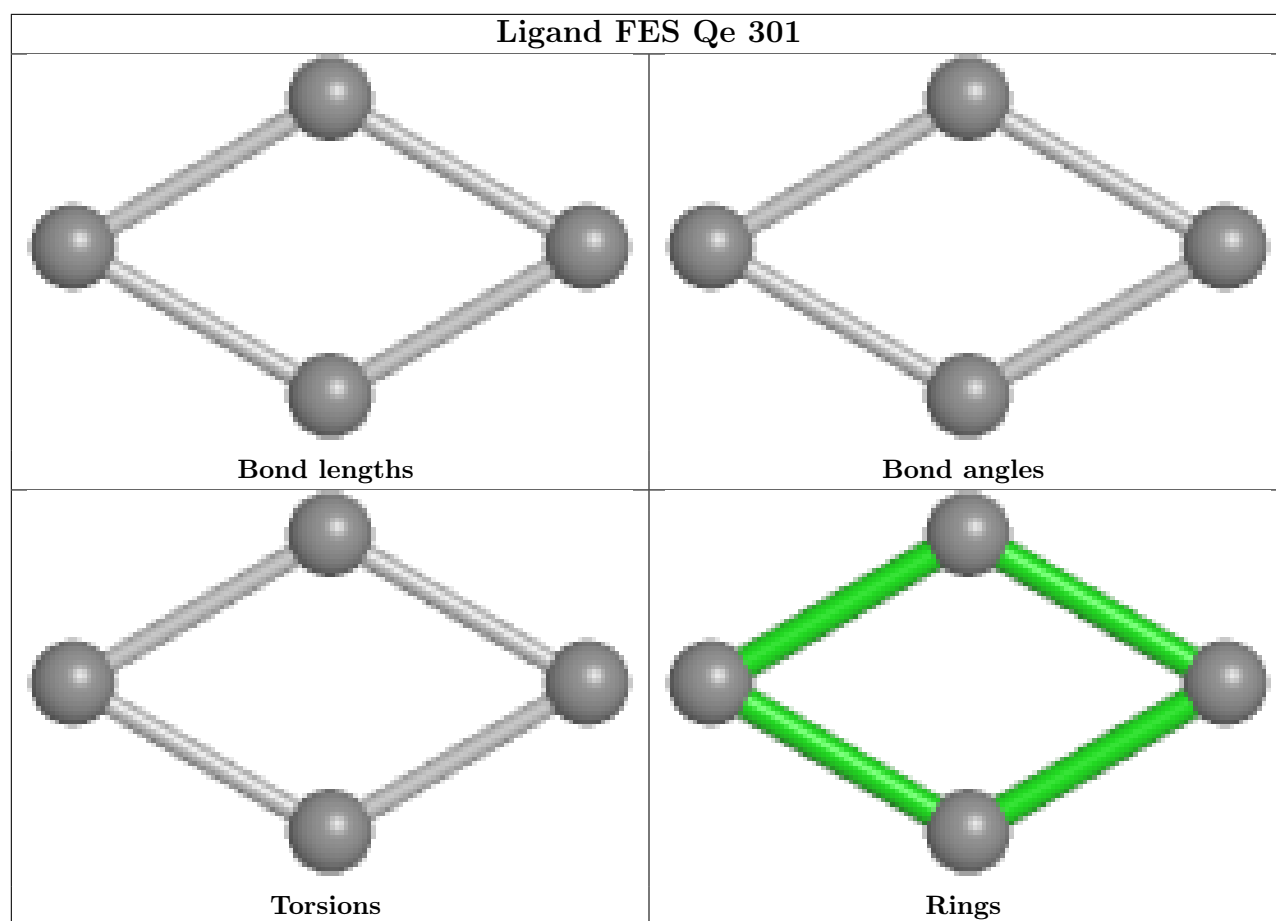


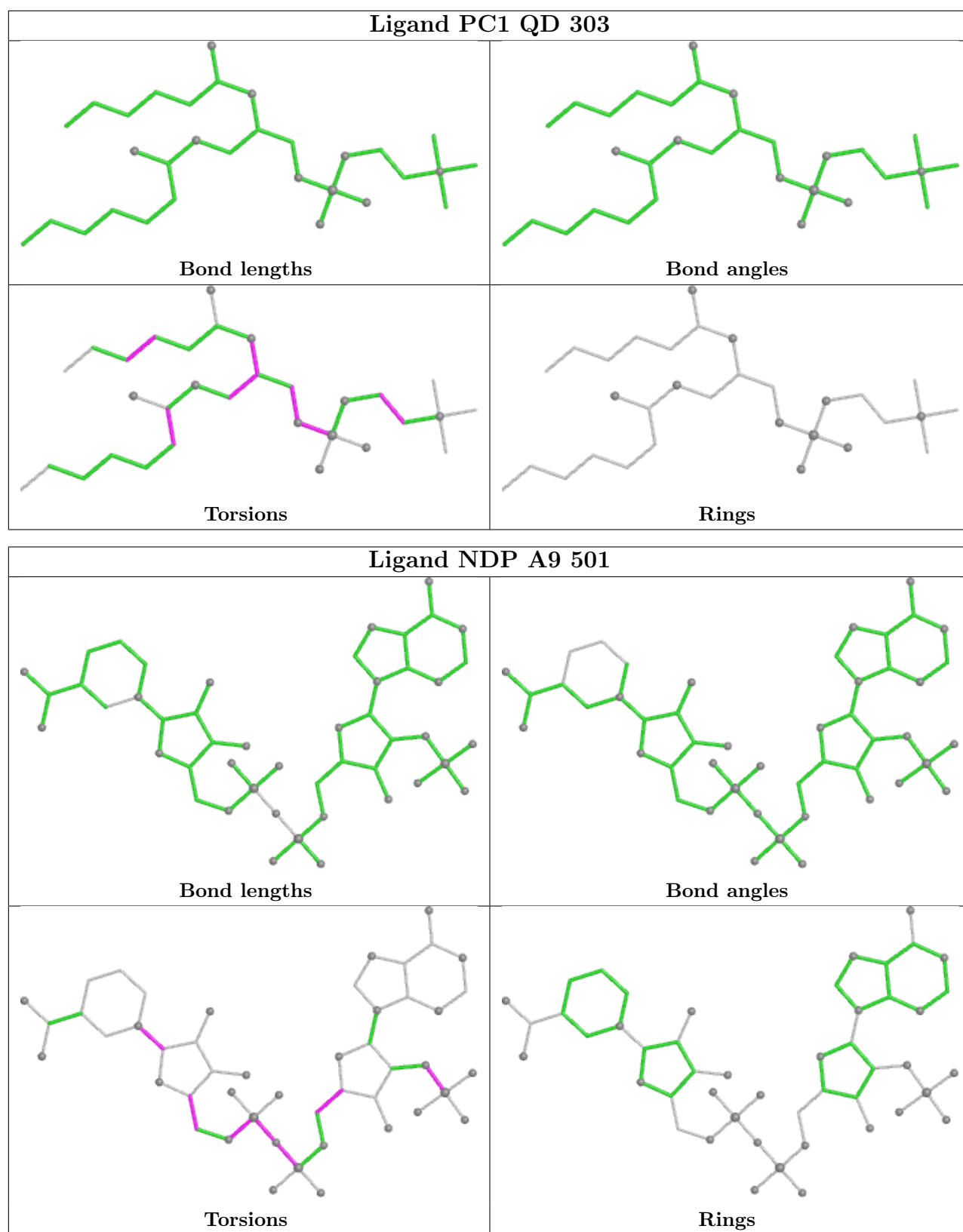


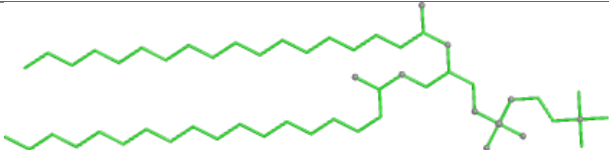
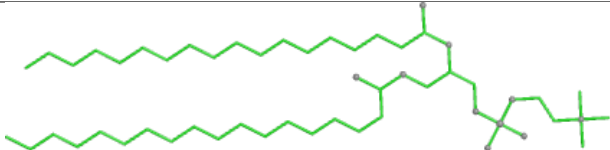
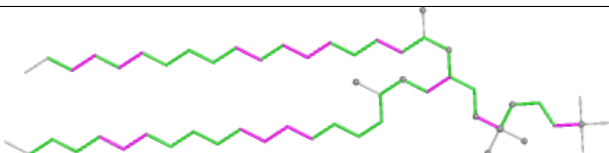
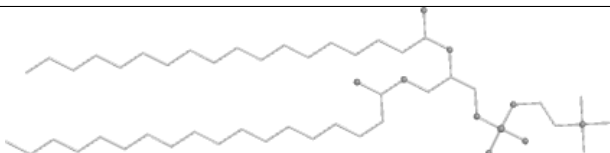
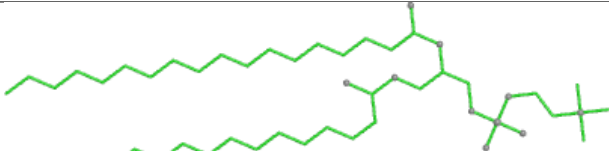
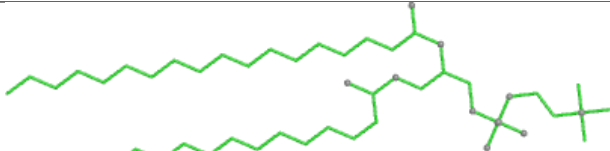
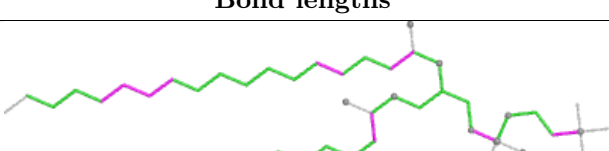
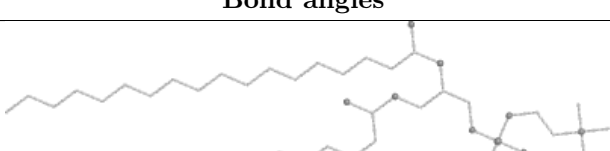
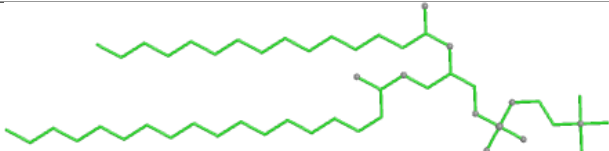
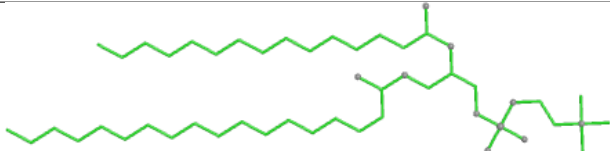
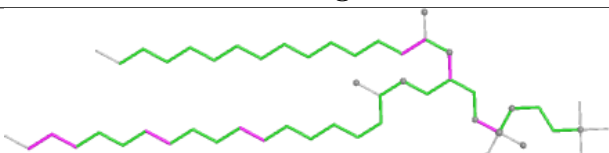
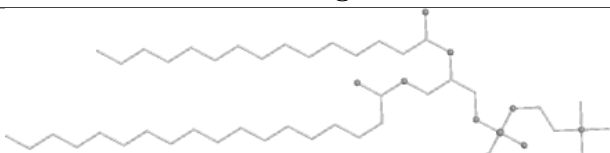




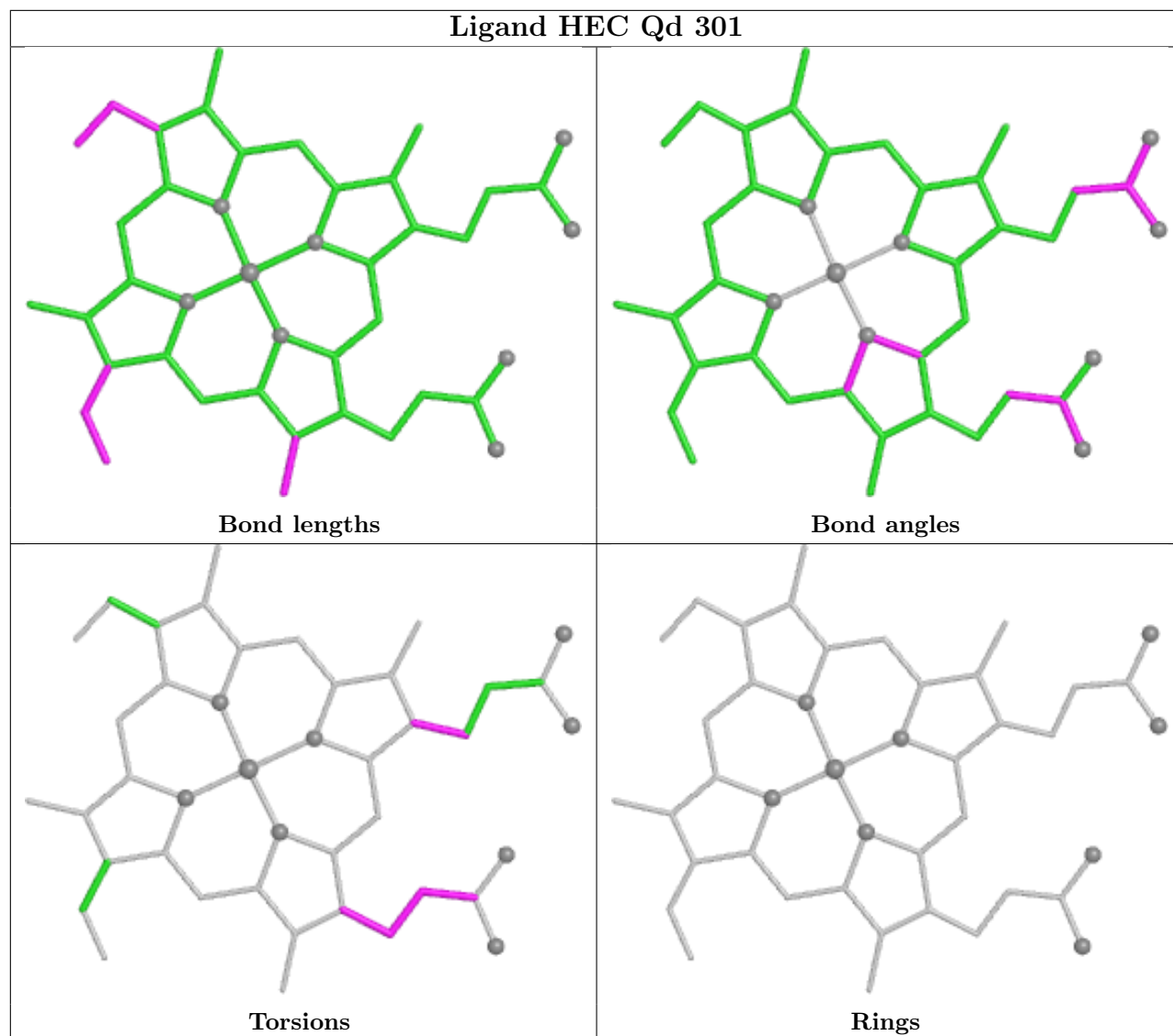




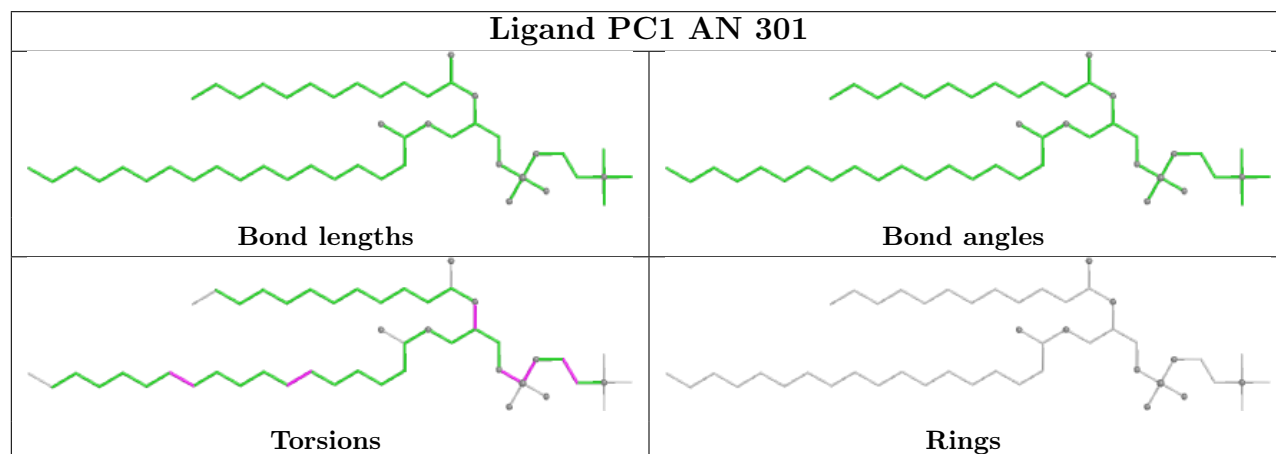


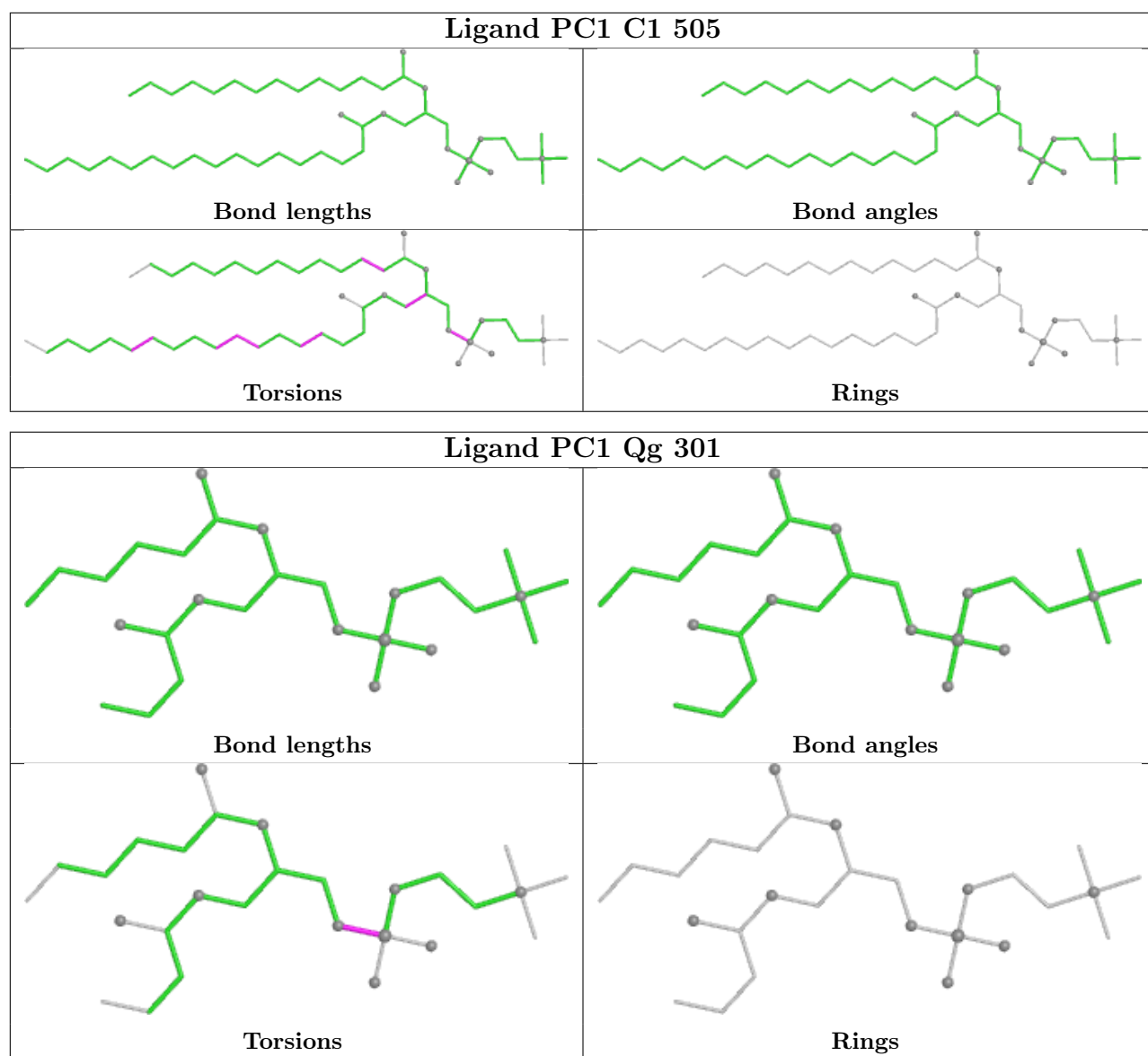
Ligand PC1 B5 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 N1 702	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 C3 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

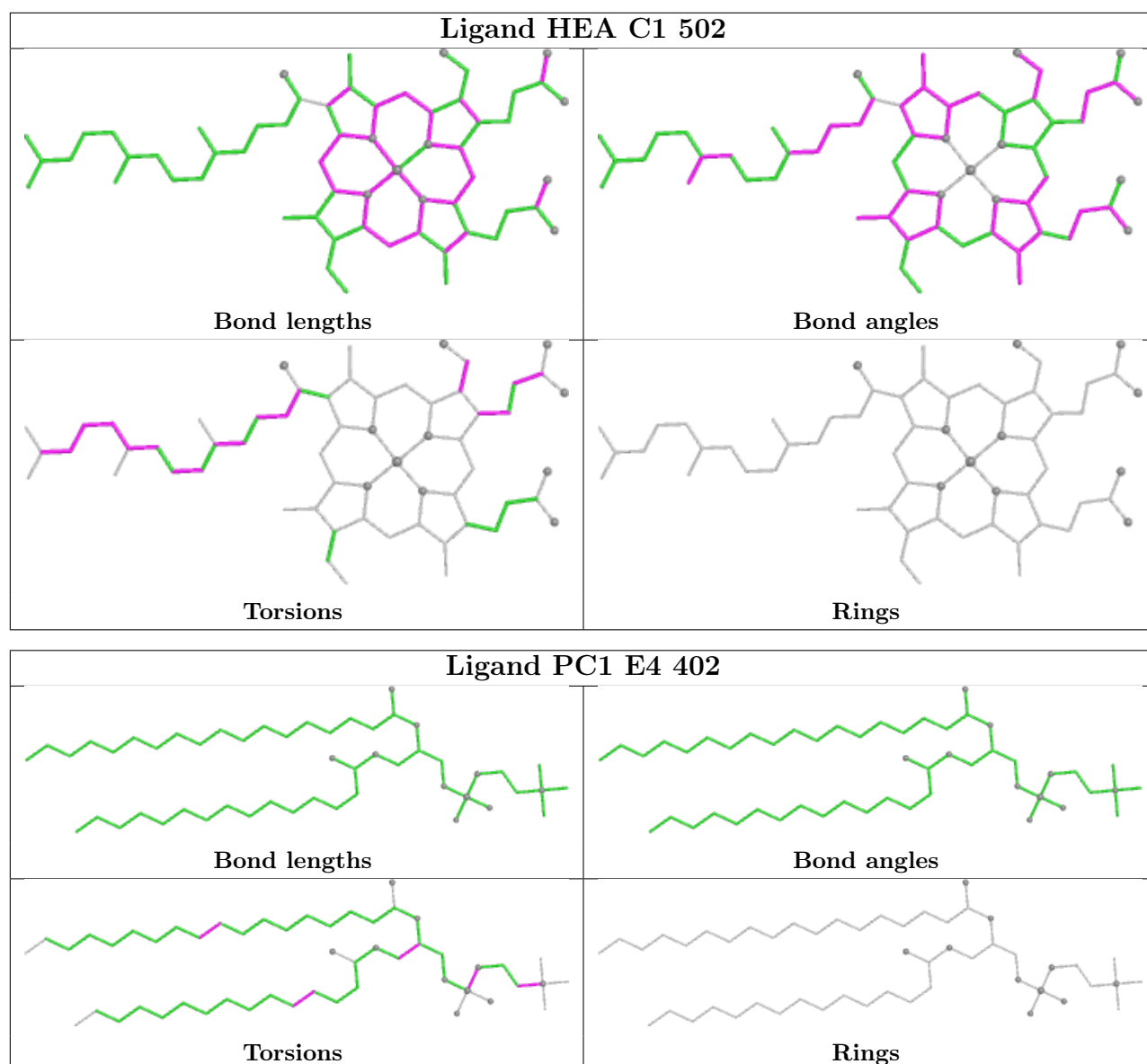
Ligand HEC Qd 301

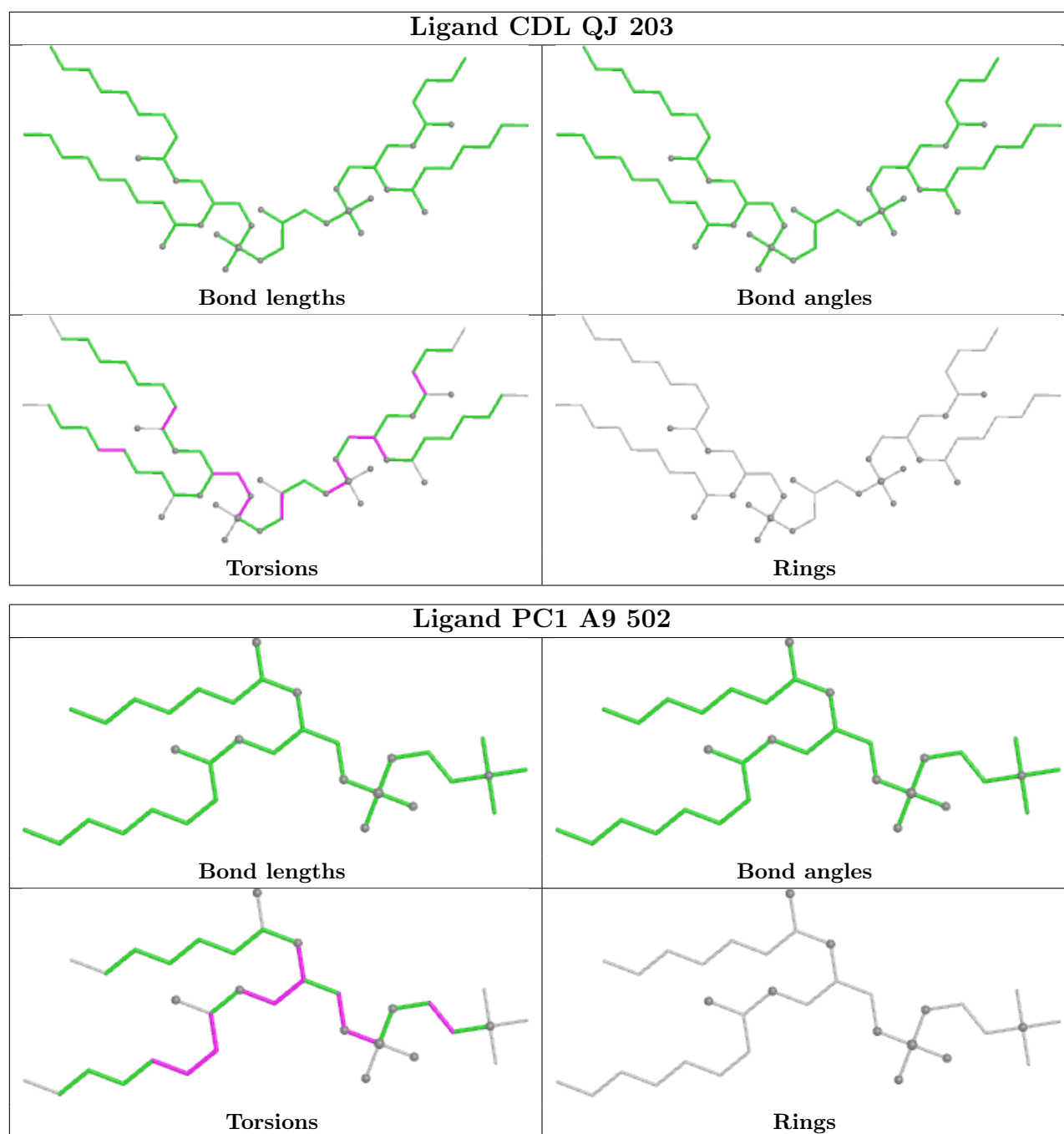


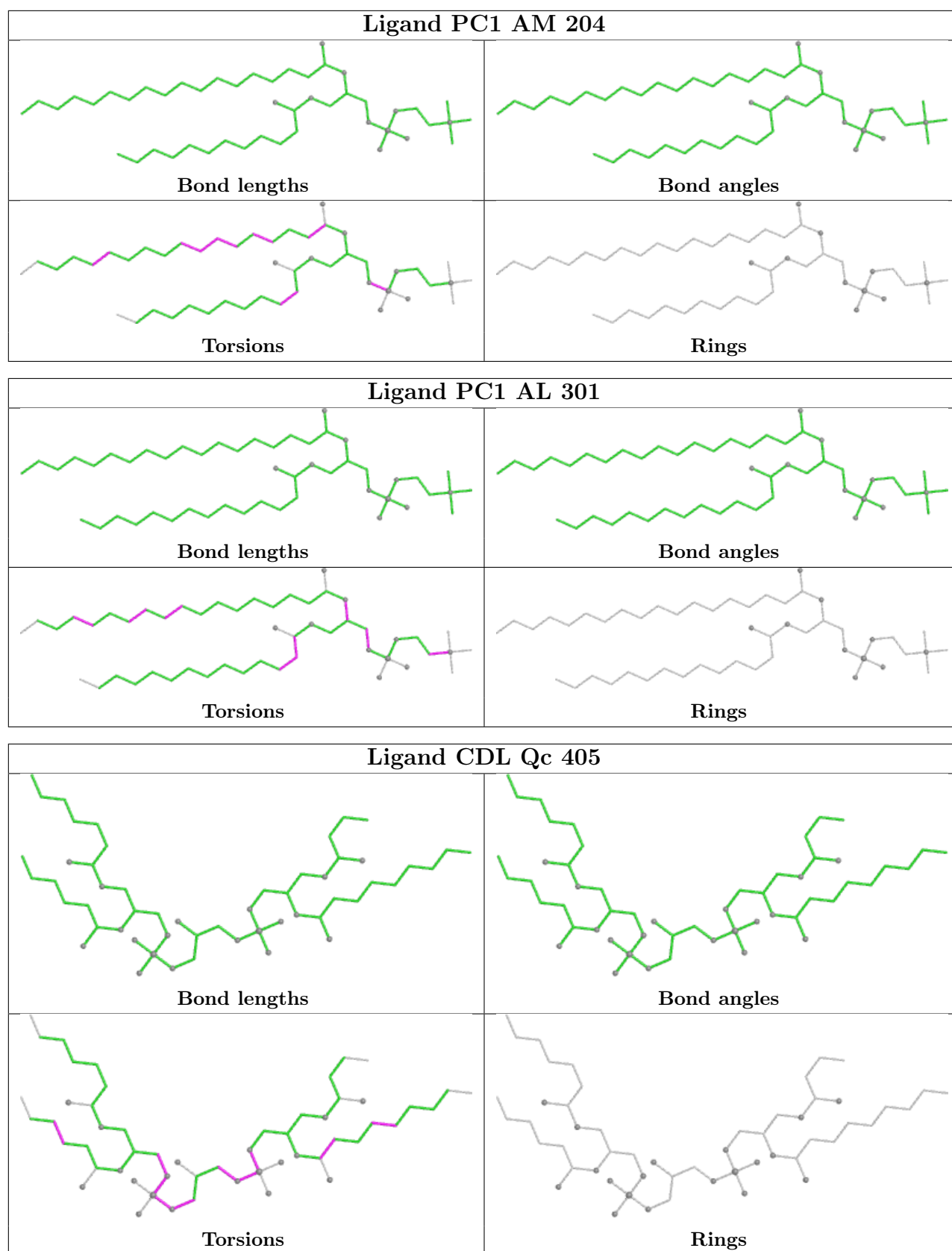
Ligand PC1 AN 301

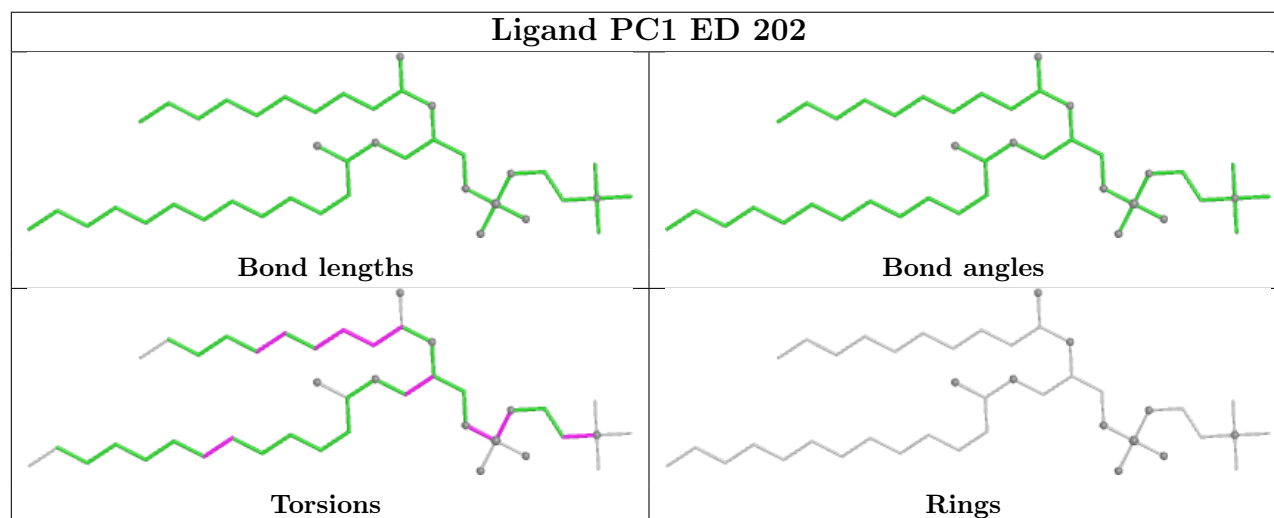
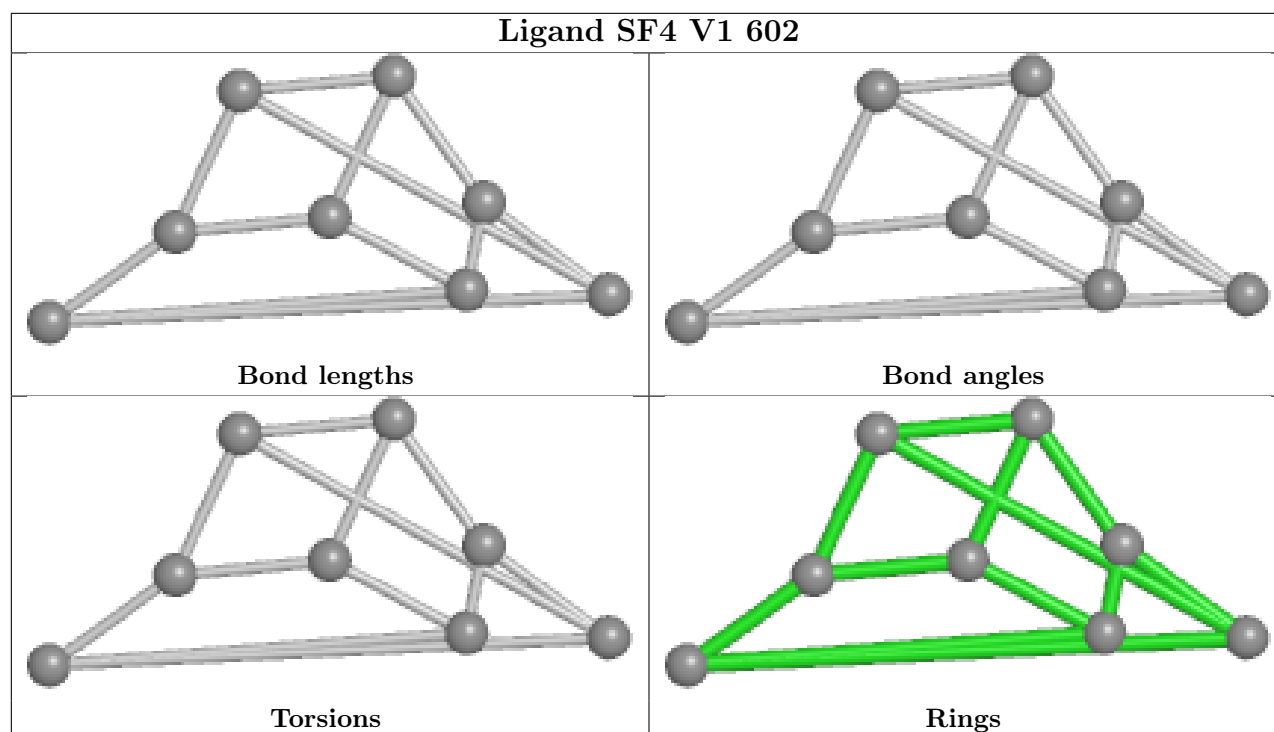
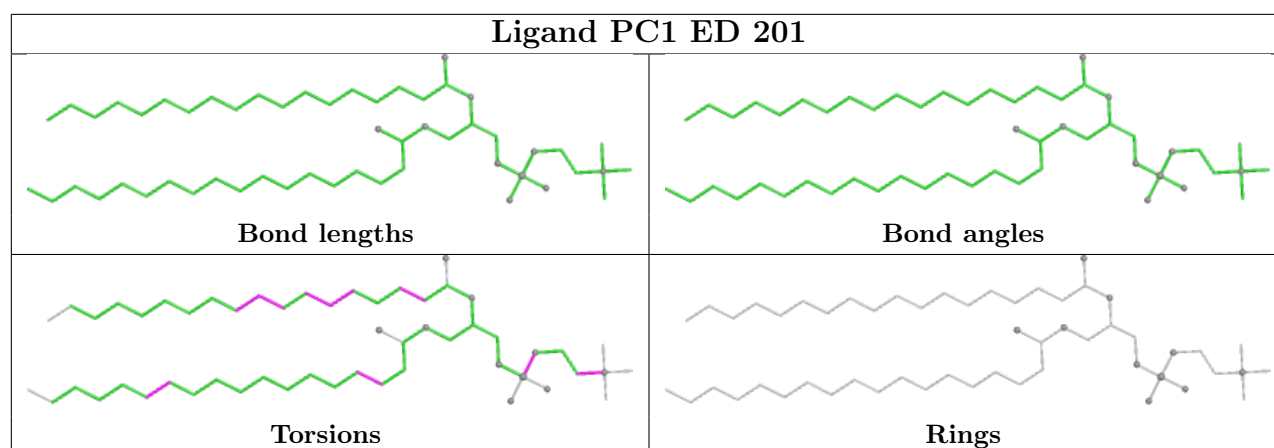




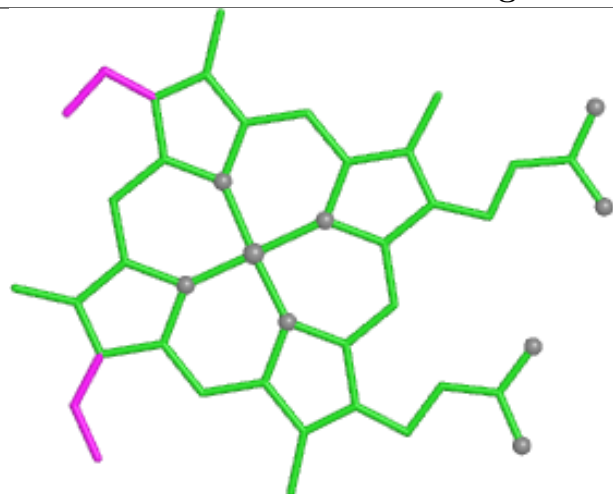




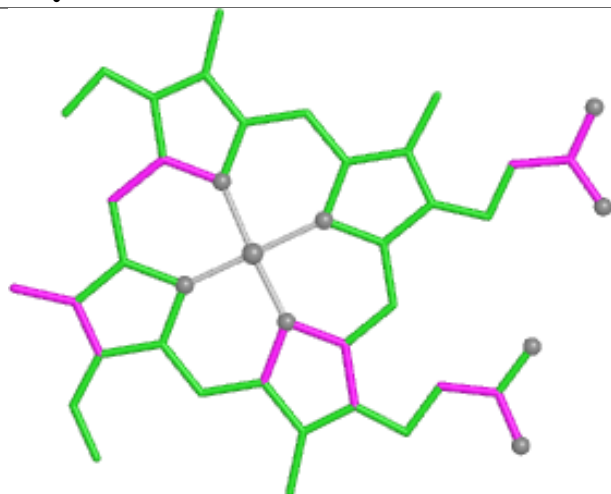




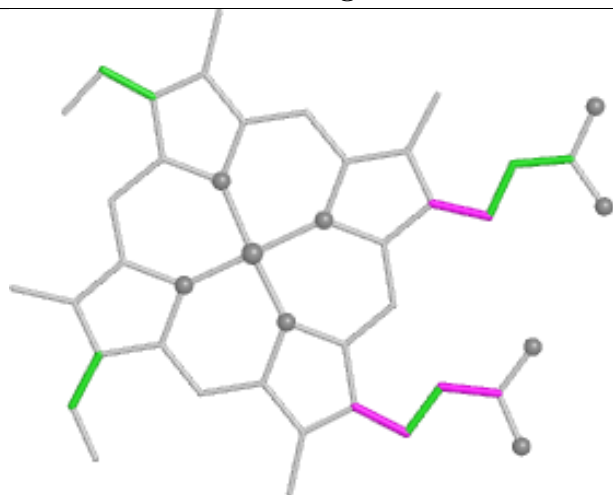
Ligand HEC QD 301



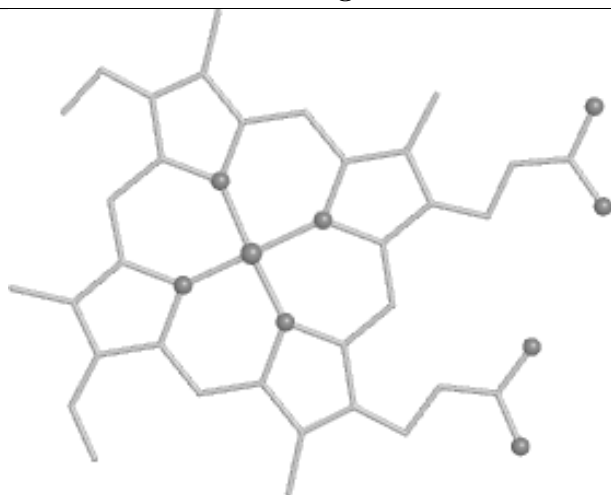
Bond lengths



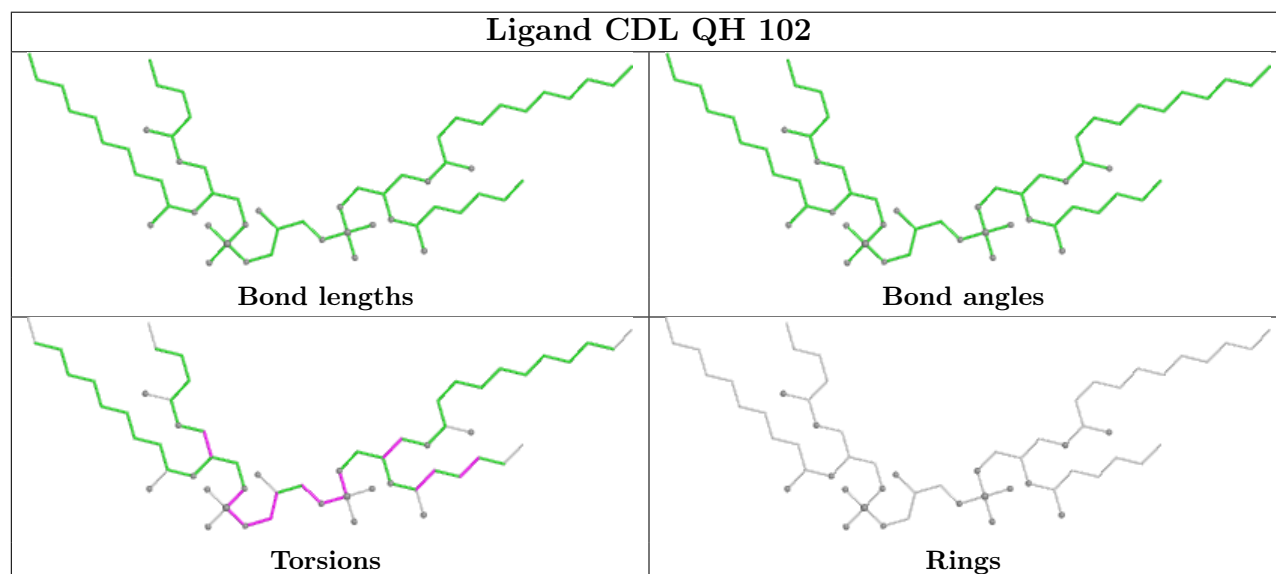
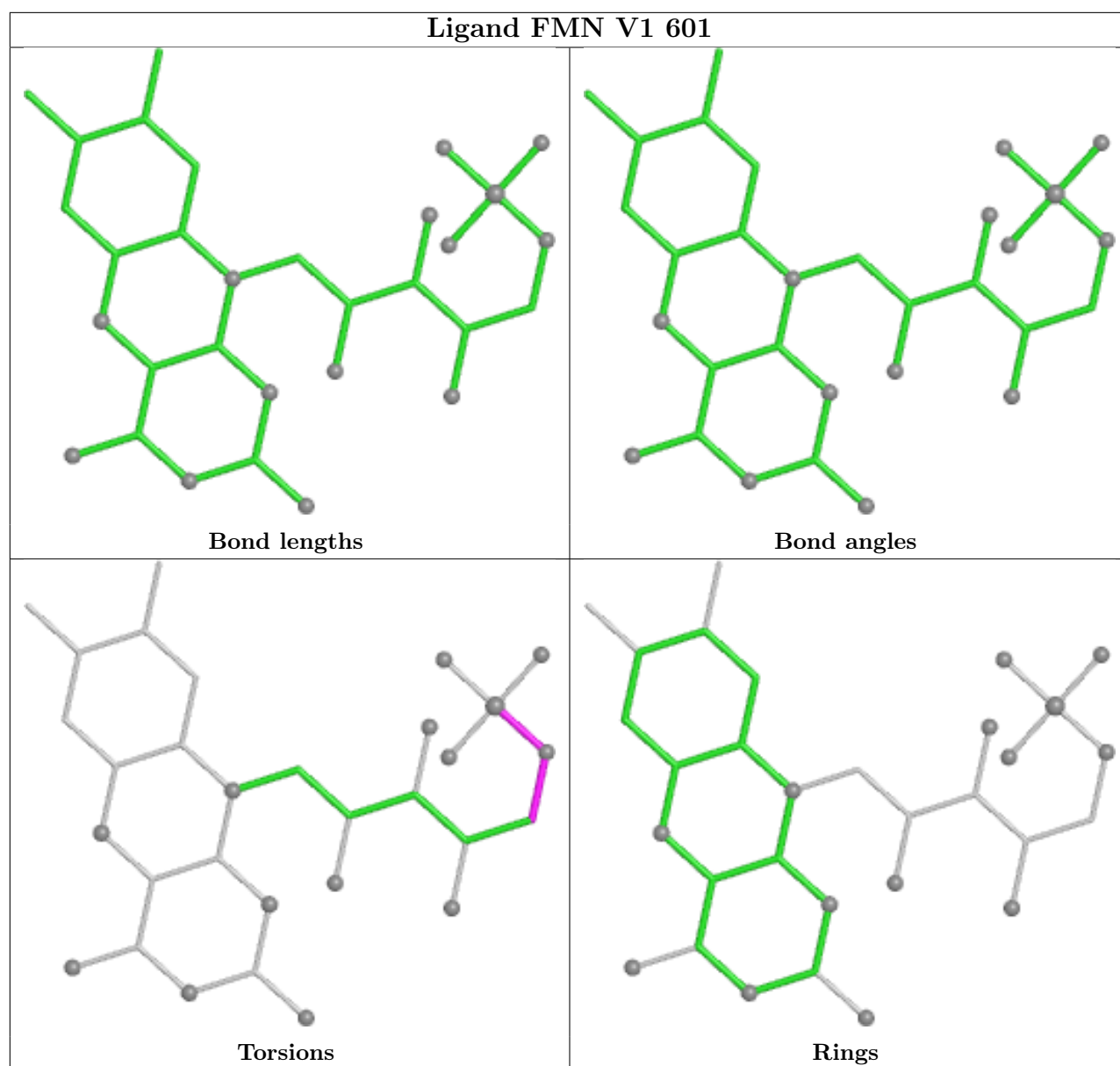
Bond angles

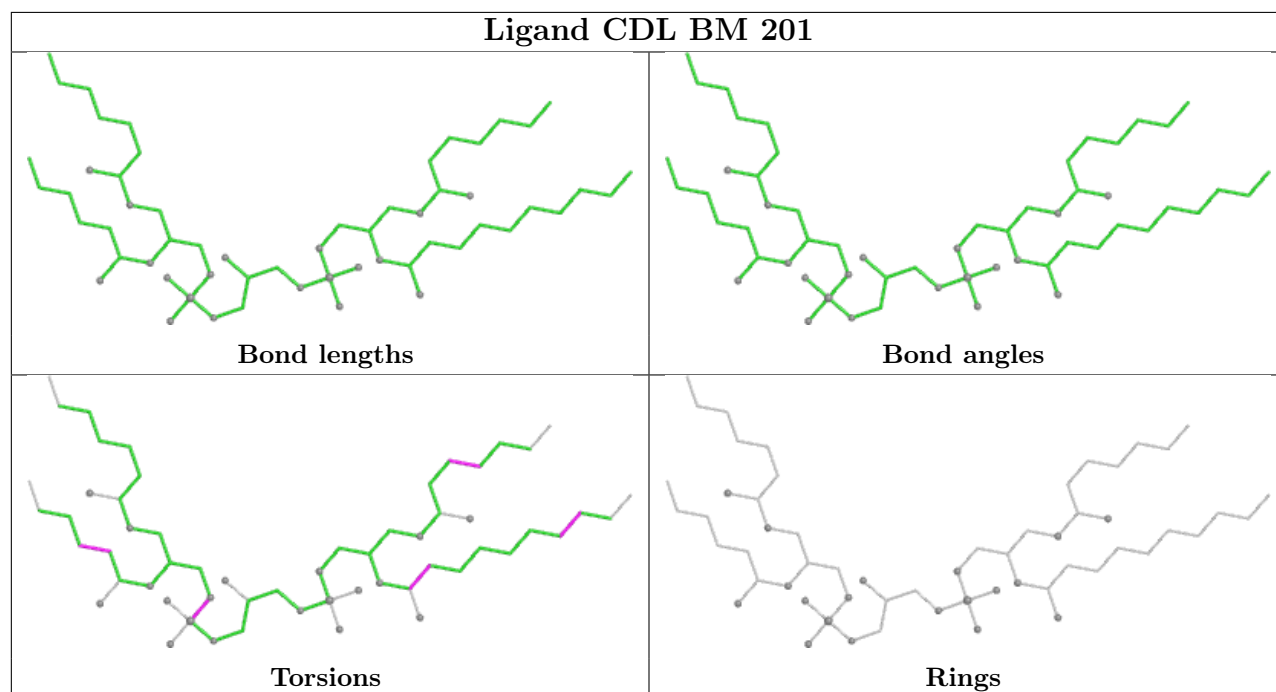
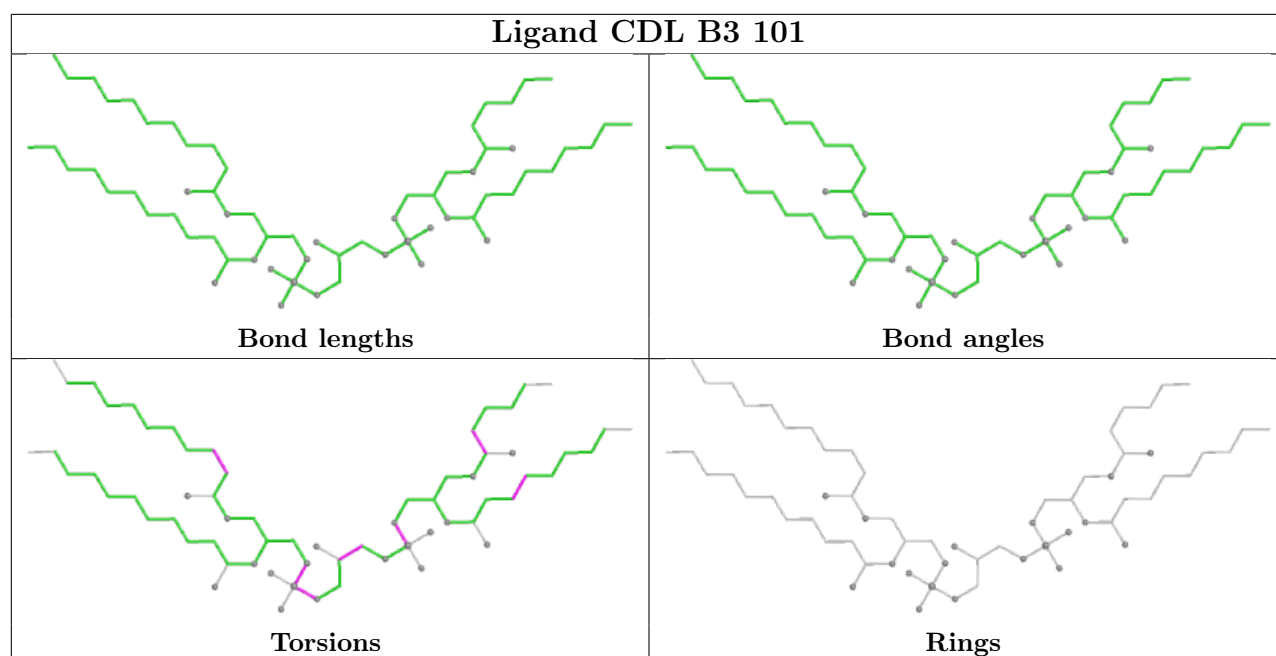


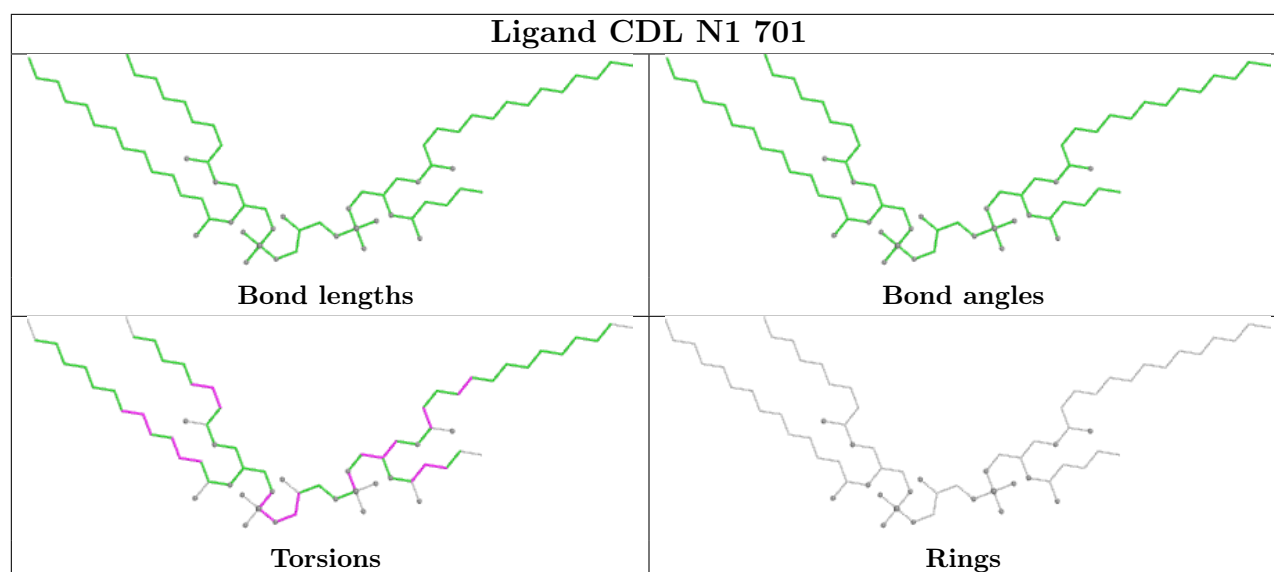
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

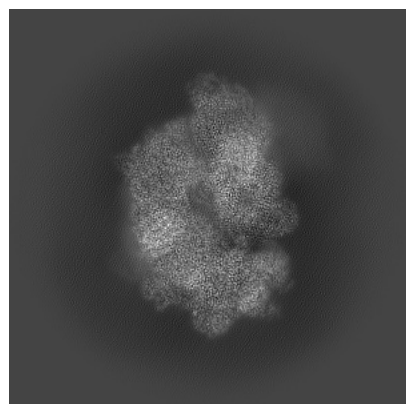
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35720. These allow visual inspection of the internal detail of the map and identification of artifacts.

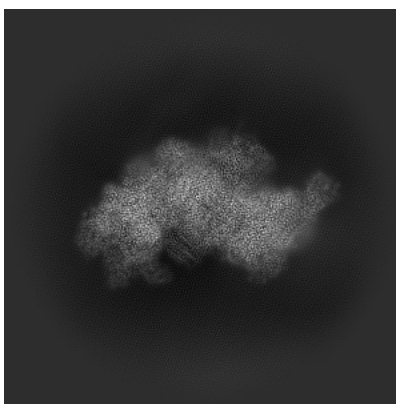
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

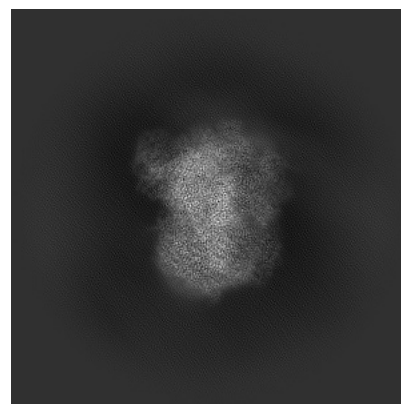
6.1.1 Primary map



X

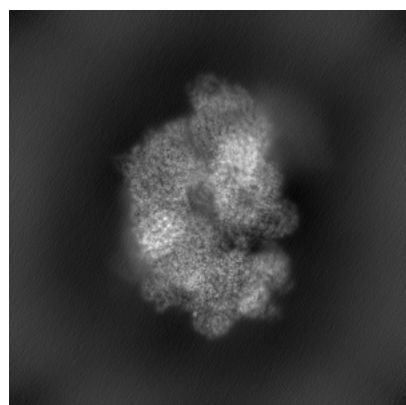


Y

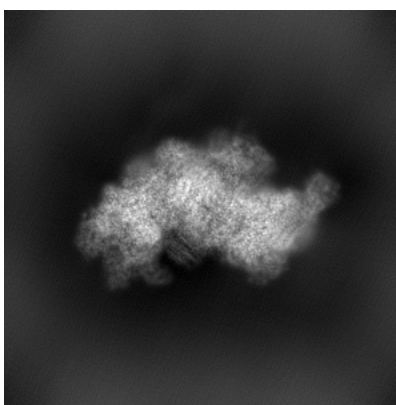


Z

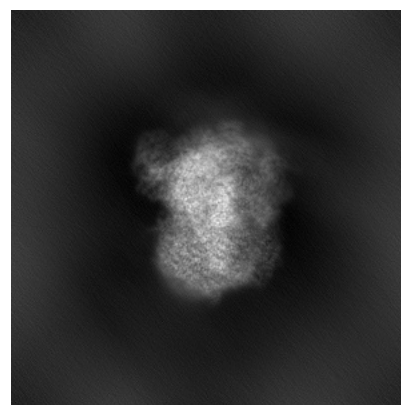
6.1.2 Raw map



X



Y

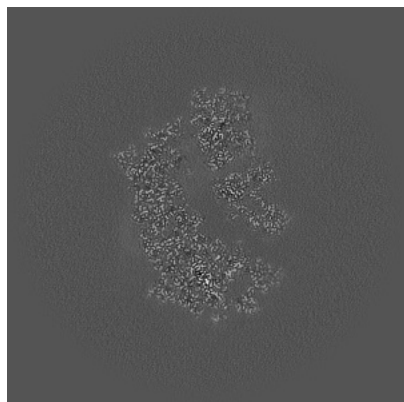


Z

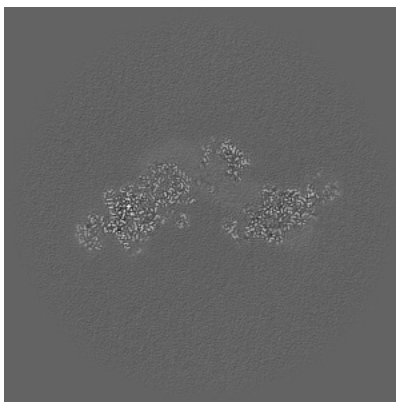
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

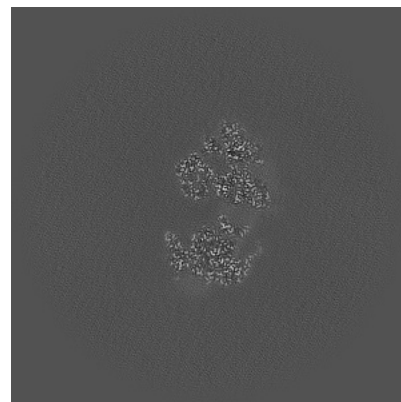
6.2.1 Primary map



X Index: 224

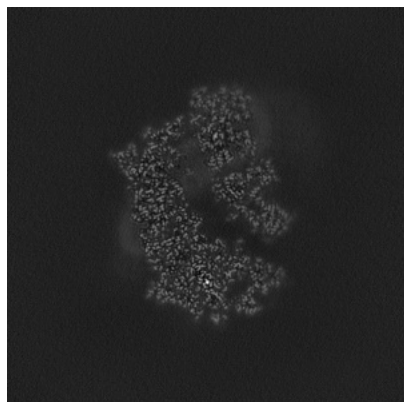


Y Index: 224

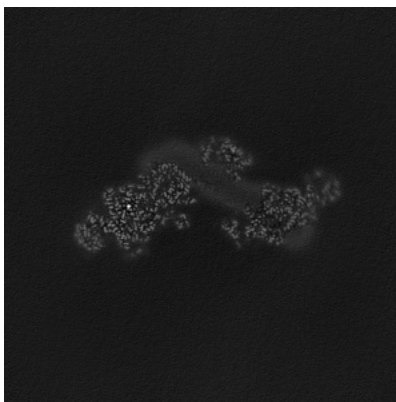


Z Index: 224

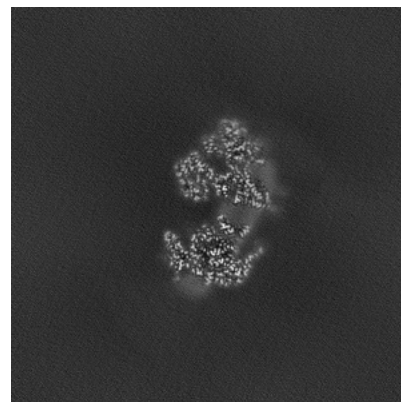
6.2.2 Raw map



X Index: 224



Y Index: 224

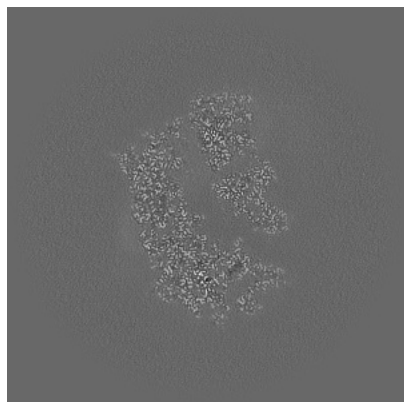


Z Index: 224

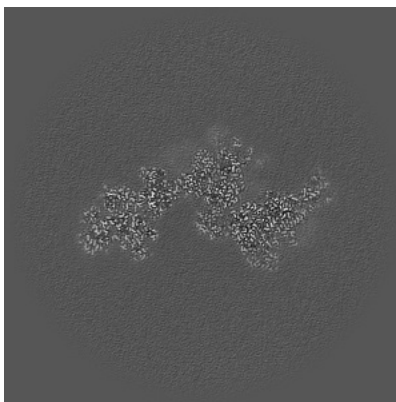
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

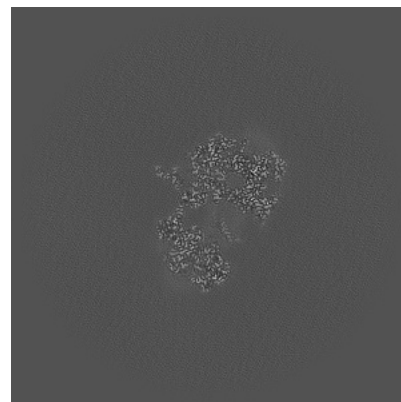
6.3.1 Primary map



X Index: 222

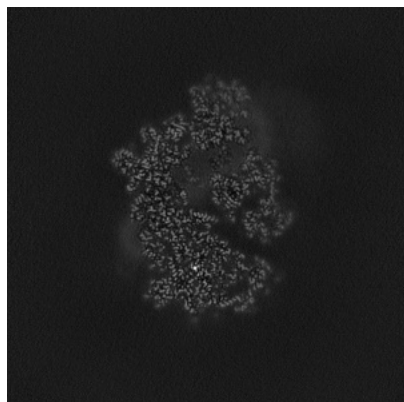


Y Index: 237

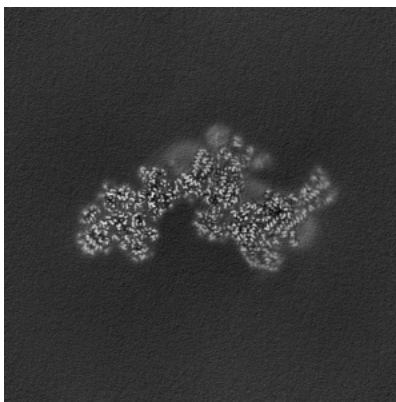


Z Index: 257

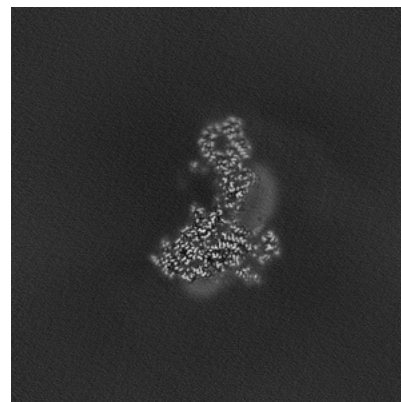
6.3.2 Raw map



X Index: 229



Y Index: 237

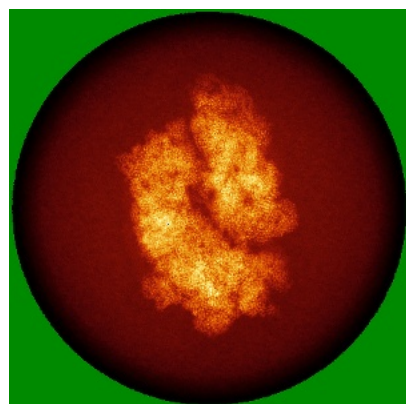


Z Index: 206

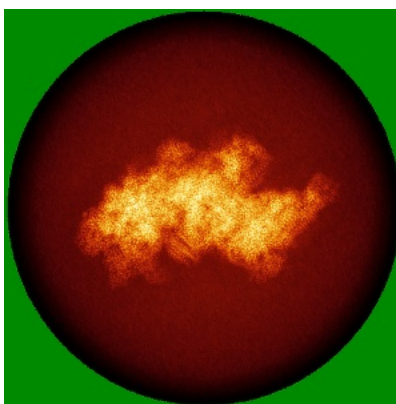
The images above show the largest variance slices of the map in three orthogonal directions.

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

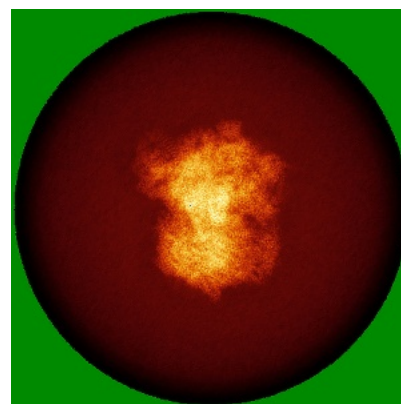
6.4.1 Primary map



X

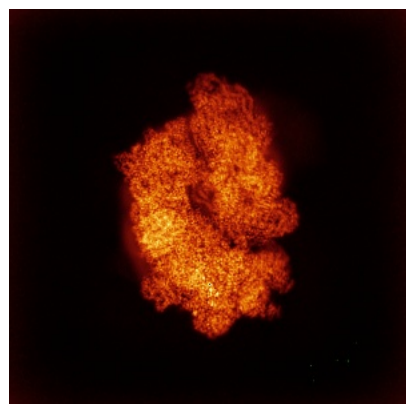


Y

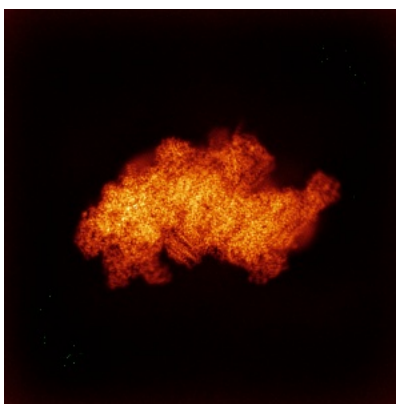


Z

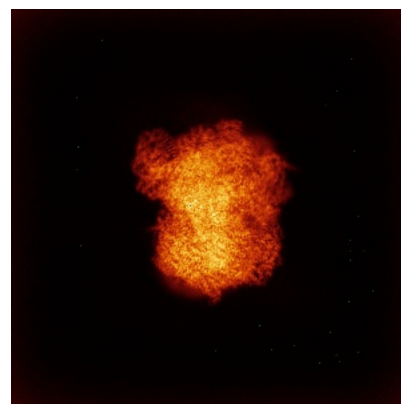
6.4.2 Raw map



X



Y

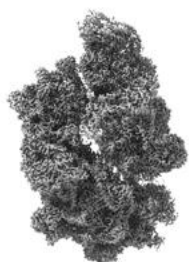


Z

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

6.5 Orthogonal surface views [i](#)

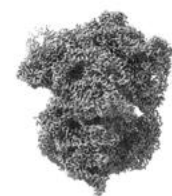
6.5.1 Primary map



X



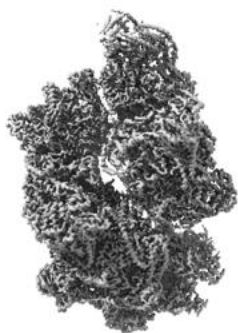
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

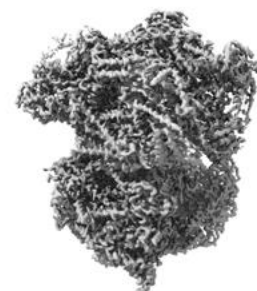
6.5.2 Raw map



X



Y



Z

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

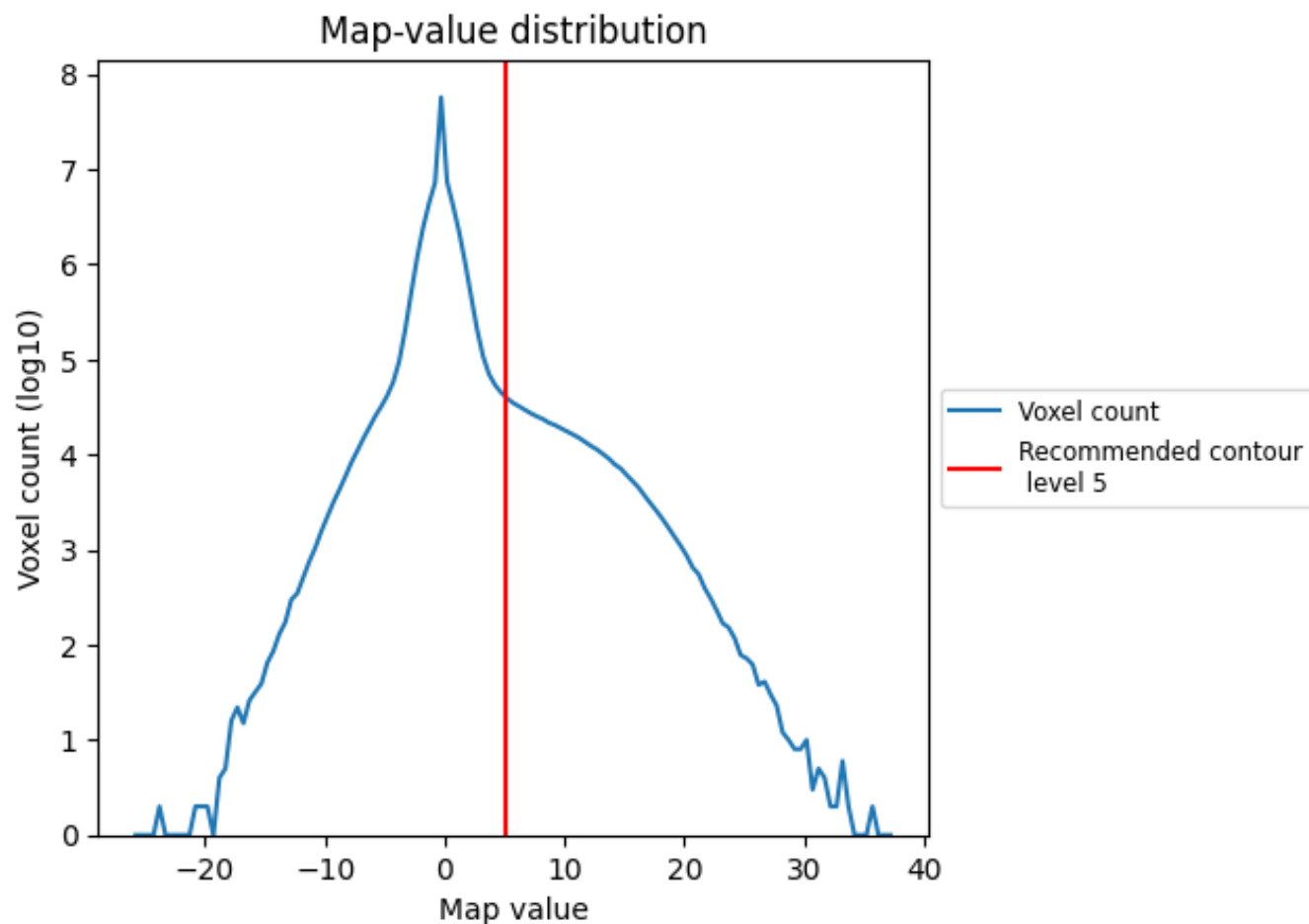
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

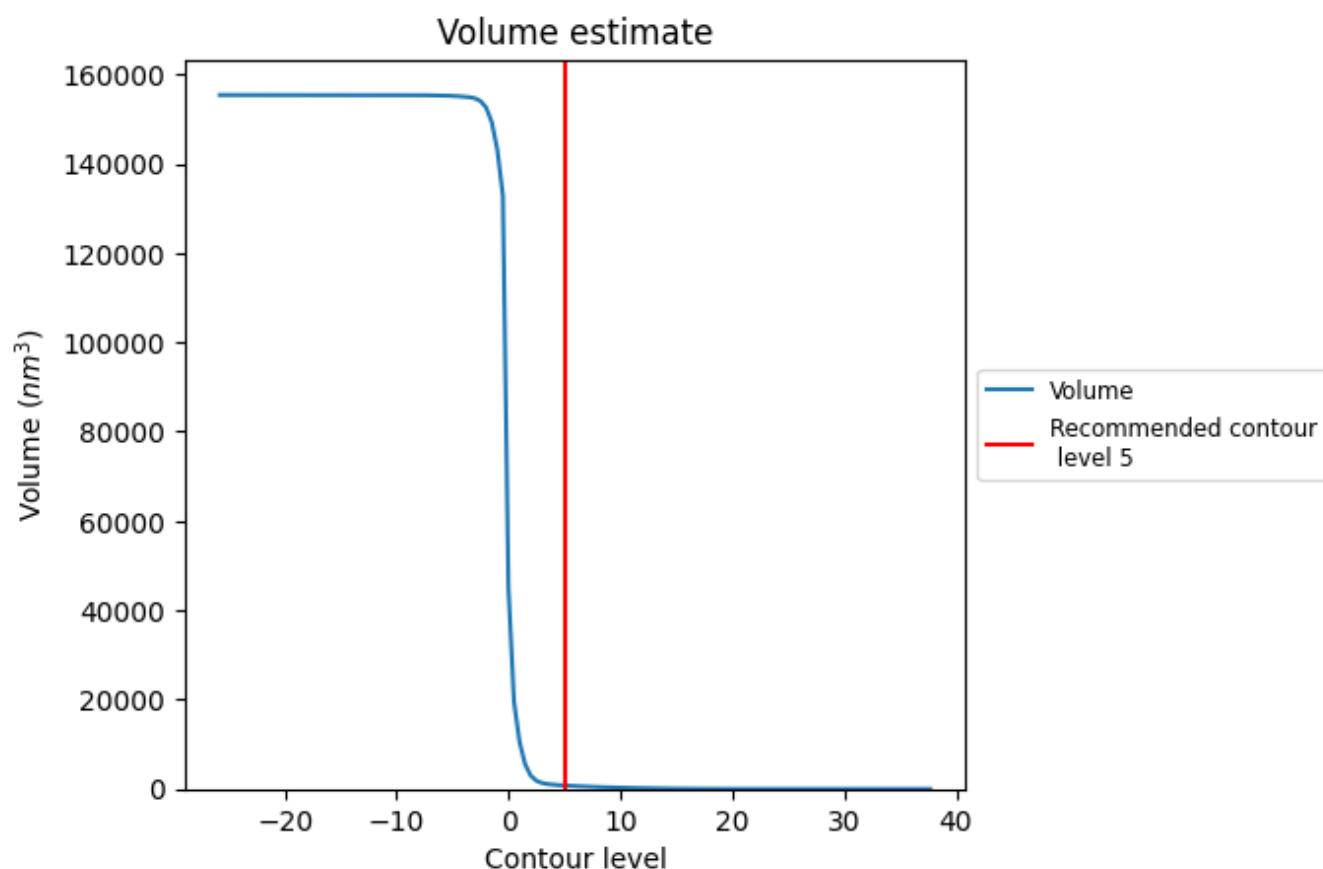
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

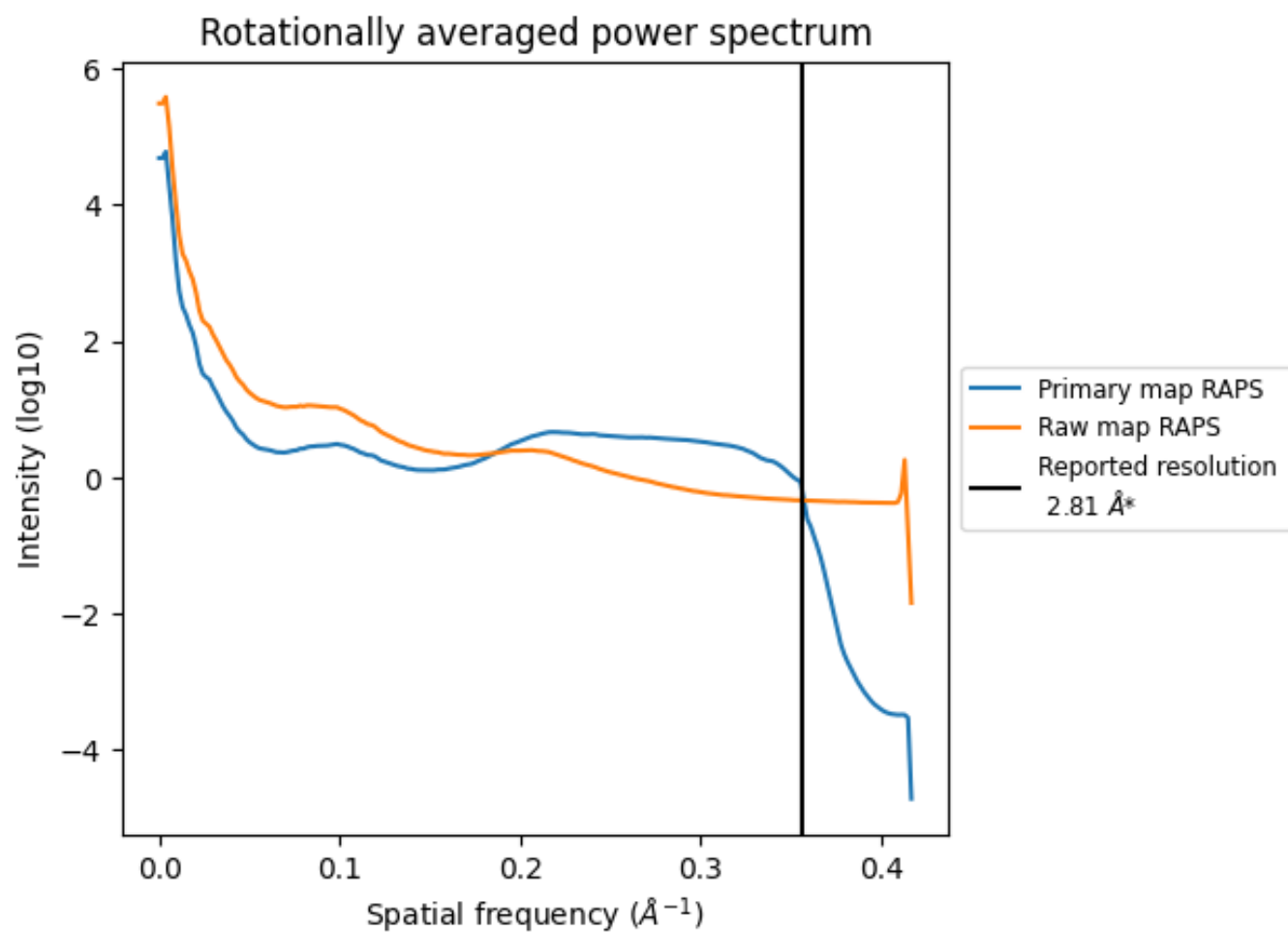
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

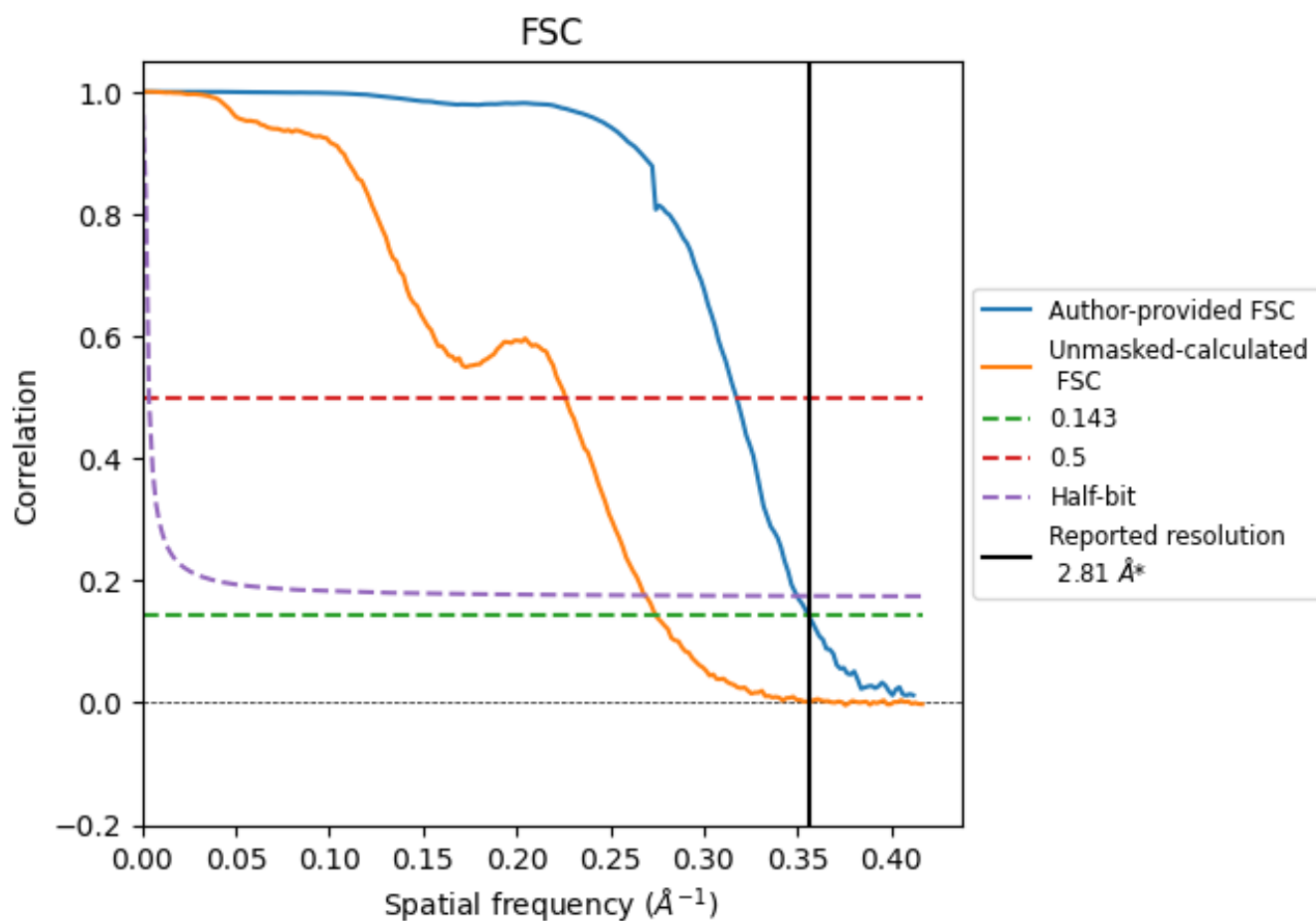


*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

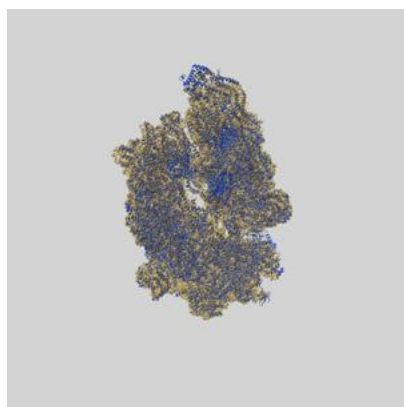
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.15	2.86
Unmasked-calculated*	3.64	4.42	3.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 2.81 by more than 10 %

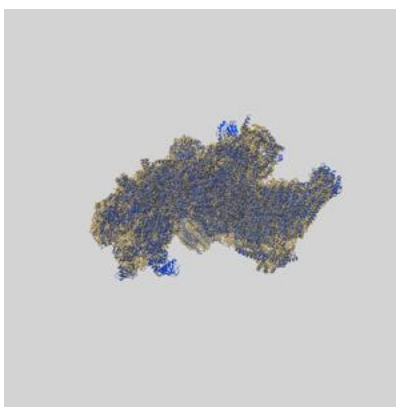
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35720 and PDB model 8IUF. Per-residue inclusion information can be found in [section 3](#) on [page 35](#).

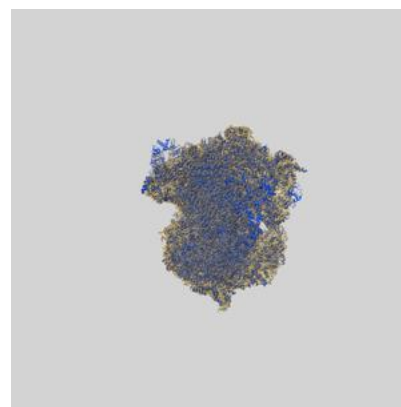
9.1 Map-model overlay [i](#)



X



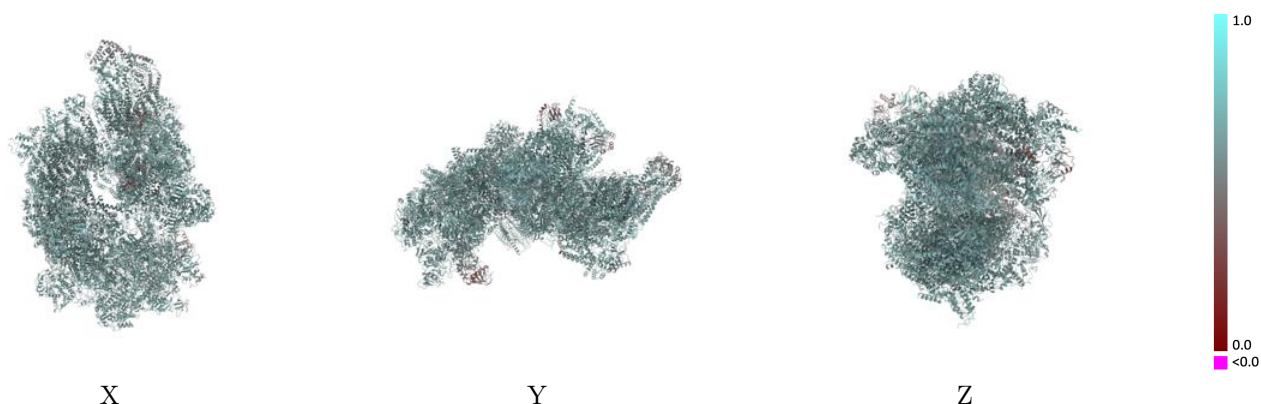
Y



Z

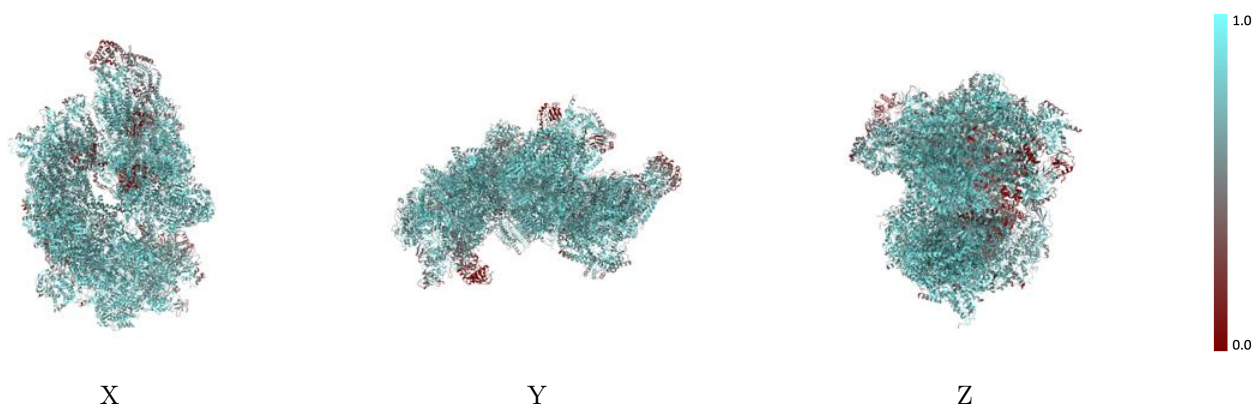
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



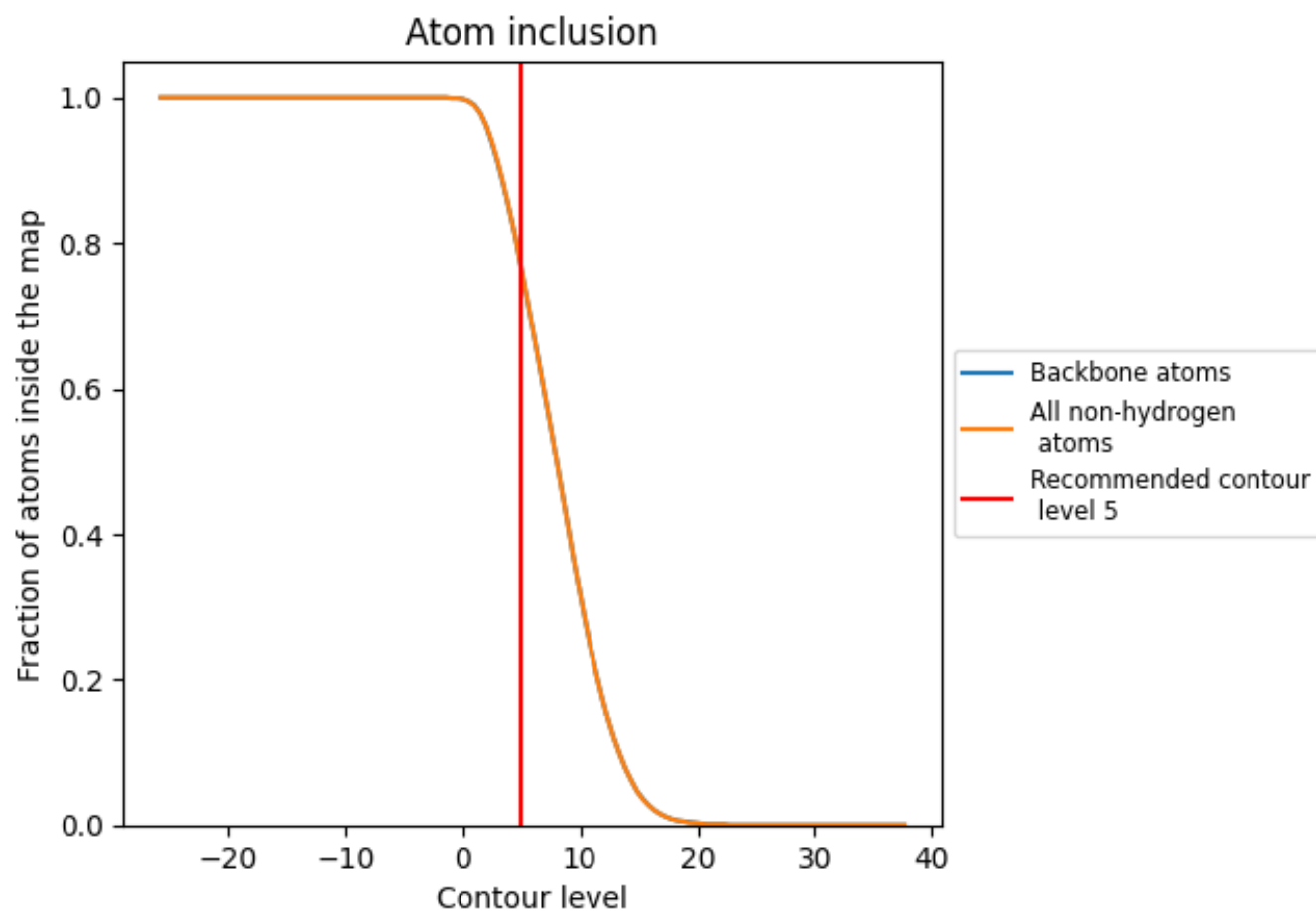
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.6150
1A	 0.8550	 0.6330
1B	 0.8450	 0.6320
2B	 0.8700	 0.6340
4A	 0.5880	 0.5830
4C	 0.6060	 0.5810
4D	 0.7000	 0.6030
4E	 0.4990	 0.5490
4F	 0.7000	 0.6000
4G	 0.6870	 0.5950
4H	 0.6790	 0.5990
4I	 0.8560	 0.6340
4J	 0.8180	 0.6340
4L	 0.8470	 0.6390
5B	 0.8410	 0.6250
5C	 0.8040	 0.6290
6A	 0.5940	 0.5900
6B	 0.6180	 0.5810
7A	 0.7190	 0.6040
7C	 0.8060	 0.6320
A	 0.7830	 0.5880
A1	 0.7270	 0.6080
A2	 0.7790	 0.6190
A3	 0.7690	 0.6180
A5	 0.7290	 0.6020
A6	 0.7320	 0.6040
A7	 0.8480	 0.6340
A8	 0.7610	 0.6100
A9	 0.8050	 0.6270
AB	 0.7370	 0.6110
AC	 0.7760	 0.6180
AL	 0.8060	 0.6260
AM	 0.7200	 0.6070
AN	 0.7820	 0.6210
B	 0.4830	 0.5890



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Chain	Atom inclusion	Q-score
B2	 0.8220	 0.6330
B3	 0.8270	 0.6210
B4	 0.8160	 0.6230
B5	 0.7880	 0.6140
B6	 0.8060	 0.6260
B7	 0.8000	 0.6190
B8	 0.8520	 0.6370
B9	 0.8490	 0.6380
BL	 0.8130	 0.6240
BM	 0.7830	 0.6260
C1	 0.8750	 0.6310
C2	 0.8730	 0.6370
C3	 0.7520	 0.6070
C4	 0.7590	 0.6160
DC	 0.8190	 0.6340
E1	 0.7540	 0.6050
E2	 0.6510	 0.5910
E3	 0.6600	 0.5970
E4	 0.7730	 0.6130
E5	 0.2040	 0.4480
E6	 0.7370	 0.6030
E7	 0.6880	 0.5990
E8	 0.7530	 0.6190
E9	 0.2920	 0.5490
EA	 0.8140	 0.6240
EB	 0.7810	 0.6150
EC	 0.6560	 0.5810
ED	 0.7470	 0.6080
FX	 0.8370	 0.6340
G1	 0.8310	 0.6310
G2	 0.7730	 0.6120
G3	 0.7790	 0.6130
N1	 0.8130	 0.6220
N2	 0.8780	 0.6340
N3	 0.8190	 0.6330
N4	 0.8440	 0.6260
N5	 0.8410	 0.6260
N6	 0.7910	 0.6220
QA	 0.8070	 0.6340
QB	 0.8080	 0.6280
QC	 0.8330	 0.6320
QD	 0.8120	 0.6290

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Chain	Atom inclusion	Q-score
QE	 0.4290	 0.5270
QF	 0.5600	 0.5730
QG	 0.8650	 0.6400
QH	 0.7660	 0.6270
QI	 0.7880	 0.6240
QJ	 0.6980	 0.6130
QK	 0.7810	 0.6290
Qa	 0.7860	 0.6220
Qb	 0.8110	 0.6290
Qc	 0.8130	 0.6280
Qd	 0.7880	 0.6210
Qe	 0.3790	 0.5130
Qf	 0.5530	 0.5610
Qg	 0.8430	 0.6350
Qh	 0.7750	 0.6260
Qi	 0.7550	 0.6070
Qj	 0.6260	 0.5940
Qk	 0.7470	 0.6280
S2	 0.8960	 0.6420
S3	 0.8590	 0.6340
S4	 0.8190	 0.6330
S5	 0.7280	 0.6060
S6	 0.8710	 0.6290
S7	 0.9050	 0.6400
S8	 0.8840	 0.6400
V1	 0.7860	 0.6110
V2	 0.7950	 0.6140