



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:40 PM UTC

PDB ID : 8ZOU / pdb_00008zou
EMDB ID : EMD-60319
Title : Respirasome open state 2 in presence of metformin (SC-MetO2)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-05-29
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

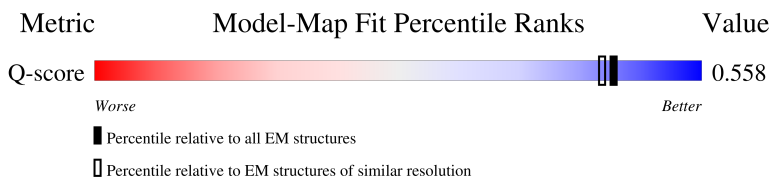
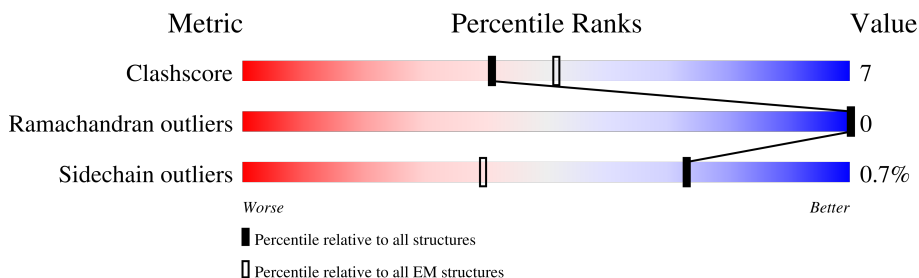
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.01 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.



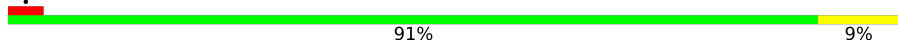
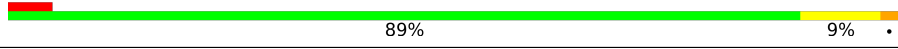
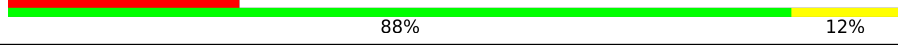
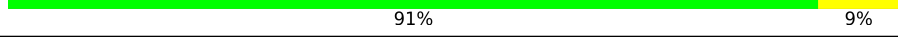
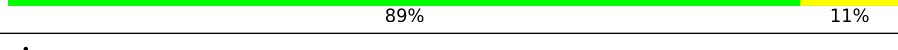
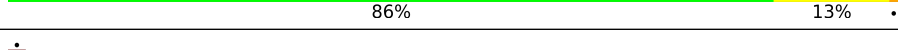
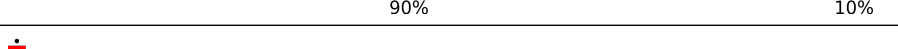
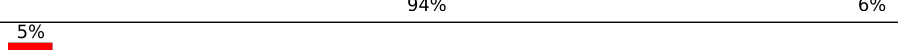
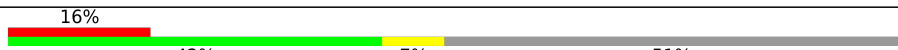
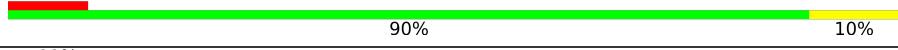
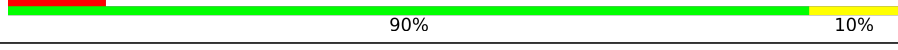
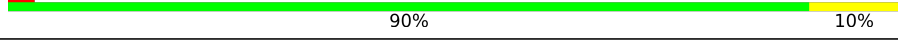
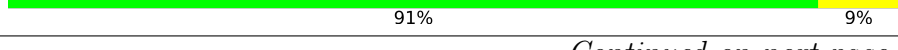
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13882 (2.51 - 3.51)

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	4L	98	
2	5A	102	
3	5B	95	
4	6A	75	

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Mol	Chain	Length	Quality of chain
5	6B	82	
6	6C	70	
7	7A	57	
8	7B	50	
9	7C	47	
10	8B	43	
11	A1	70	
12	A2	85	
13	A3	83	
14	A5	112	
15	A6	114	
16	A7	112	
17	A8	171	
18	A9	341	
19	AB	156	
19	AC	156	
20	AK	320	
21	AL	140	
22	AM	144	
23	AN	142	
24	B1	56	
25	B2	67	
26	B3	80	
27	B4	128	
28	B5	138	

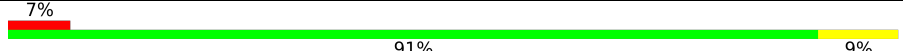
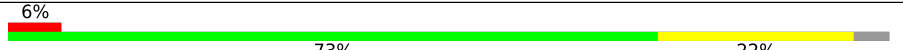
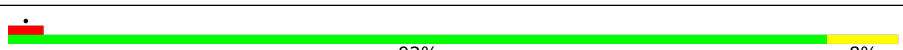
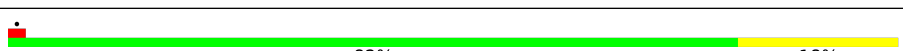
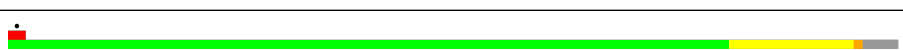
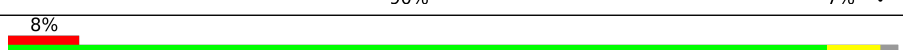
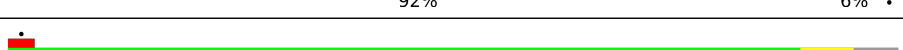
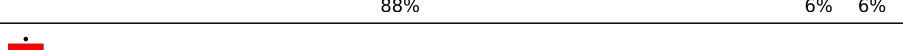
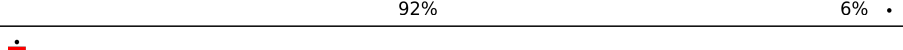
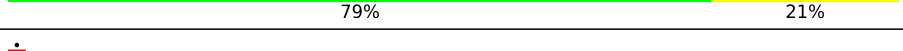
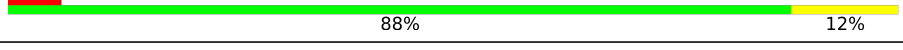
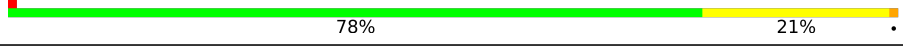
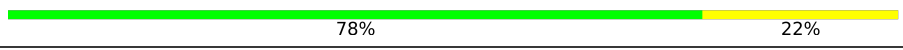
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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	176	
34	BL	102	
35	C1	514	
36	C2	228	
37	C3	261	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	114	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

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Mol	Chain	Length	Quality of chain
50	Qd	241	
51	QE	274	
51	QK	274	
51	Qe	274	
52	QF	67	
52	Qf	67	
53	QG	101	
53	Qg	101	
54	QH	81	
54	Qh	81	
55	QI	63	
55	Qi	63	
56	QJ	52	
56	Qj	52	
57	S1	689	
58	S2	430	
59	S3	208	
60	S4	124	
61	S5	105	
62	S6	96	
63	S7	156	
64	S8	176	
65	V1	431	
66	V2	217	
67	V3	42	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
82	FES	QE	303	-	-	X	-
82	FES	Qe	301	-	-	X	-
84	SF4	S8	302	-	-	X	-

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 118456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	102	Total	C	N	O	S	0	0
			825	528	139	156	2		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	95	Total	C	N	O	S	0	0
			724	449	128	141	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6A	75	Total	C	N	O	S	0	0
			620	401	118	100	1		

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6B	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6C	70	Total	C	N	O	S	0	0
			574	375	101	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7A	57	Total	C	N	O	S	0	0
			447	287	76	81	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7B	50	Total	C	N	O	S	0	0
			392	254	66	71	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7C	47	Total	C	N	O	S	0	0
			387	257	65	63	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8B	43	Total	C	N	O	0	0
			338	222	57	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 16 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	335	Total	C	N	O	S	0	0
			2684	1737	470	468	9		

- Molecule 19 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
19	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AM	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AN	142	Total	C	N	O	S	0	0
			1172	754	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B3	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B4	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 29 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	104	Total	C	N	O	S	0	0
			890	583	157	149	1		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C1	514	Total	C	N	O	S	0	0
			4024	2692	625	675	32		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C2	228	Total	C	N	O	S	0	0
			1833	1193	282	340	18		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C3	260	Total	C	N	O	S	0	0
			2103	1403	337	353	10		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C4	138	Total	C	N	O	S	0	0
			1153	751	188	210	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N1	308	Total	C	N	O	S	0	0
			2436	1634	374	407	21		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	N3	97	Total	C	N	O	S	0	0
			779	531	113	130	5		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N6	164	Total	C	N	O	S	0	0
			1243	835	178	219	11		

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	QA	419	Total	C	N	O	S	0	0
			3143	1969	557	609	8		
47	Qa	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QB	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
48	Qb	433	Total	C	N	O	S	0	0
			3367	2103	592	653	19		

- Molecule 49 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QC	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
49	Qc	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 50 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	QD	241	Total	C	N	O	S	0	0
			1921	1225	330	350	16		
50	Qd	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QE	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		
51	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		
51	Qe	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	QF	67	Total	C	N	O	S	0	0
			552	336	100	111	5		
52	Qf	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	QG	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
53	Qg	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	QH	78	Total	C	N	O	S	0	0
			662	432	121	107	2		
54	Qh	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 55 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	QI	62	Total	C	N	O	0	0
			507	331	90	86		
55	Qi	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	QJ	49	Total	C	N	O	S	0	0
			405	269	71	63	2		
56	Qj	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 57 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 58 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	S2	425	Total	C	N	O	S	0	0
			3423	2190	589	620	24		

- Molecule 59 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S3	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S5	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	V1	431	Total	C	N	O	S	0	0
			3312	2090	591	611	20		

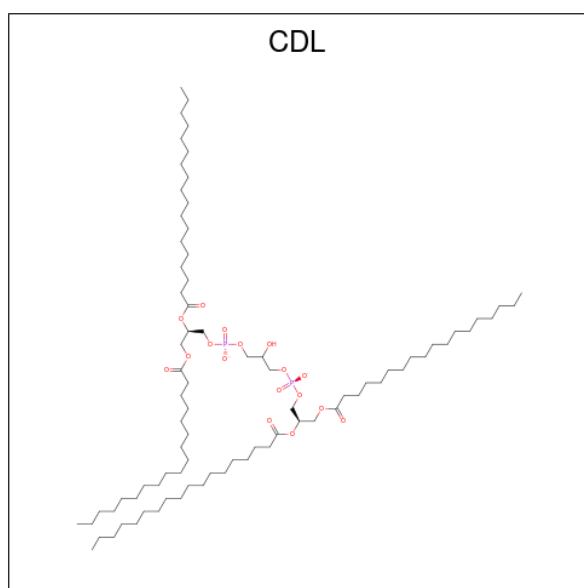
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 67 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 68 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
68	4L	1	Total	C	O	P	0
			92	73	17	2	
68	A7	1	Total	C	O	P	0
			94	75	17	2	
68	A8	1	Total	C	O	P	0
			83	64	17	2	
68	AL	1	Total	C	O	P	0
			94	75	17	2	
68	AL	1	Total	C	O	P	0
			82	63	17	2	
68	AL	1	Total	C	O	P	0
			80	61	17	2	
68	AN	1	Total	C	O	P	0
			81	62	17	2	
68	AN	1	Total	C	O	P	0
			66	47	17	2	
68	B4	1	Total	C	O	P	0
			62	43	17	2	
68	B5	1	Total	C	O	P	0
			96	77	17	2	
68	C1	1	Total	C	O	P	0
			77	58	17	2	
68	N2	1	Total	C	O	P	0
			68	49	17	2	
68	N4	1	Total	C	O	P	0
			100	81	17	2	
68	N5	1	Total	C	O	P	0
			89	70	17	2	
68	N5	1	Total	C	O	P	0
			100	81	17	2	
68	QB	1	Total	C	O	P	0
			64	45	17	2	
68	QC	1	Total	C	O	P	0
			90	71	17	2	
68	QC	1	Total	C	O	P	0
			55	36	17	2	
68	QD	1	Total	C	O	P	0
			64	45	17	2	
68	Qb	1	Total	C	O	P	0
			64	45	17	2	
68	Qc	1	Total	C	O	P	0
			61	42	17	2	
68	Qc	1	Total	C	O	P	0
			64	45	17	2	

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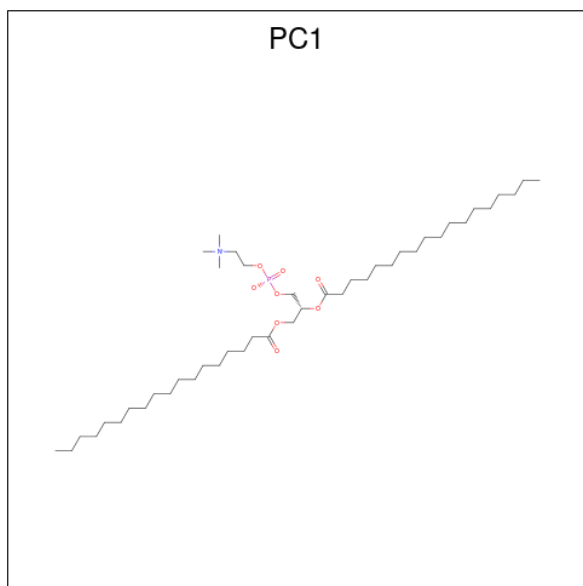
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Mol	Chain	Residues	Atoms				AltConf
68	Qh	1	Total	C	O	P	0
			100	81	17	2	
68	Qj	1	Total	C	O	P	0
			96	77	17	2	

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
69	5B	1	Total	Zn	0
			1	1	
69	S6	1	Total	Zn	0
			1	1	

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



Mol	Chain	Residues	Atoms					AltConf
70	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	7A	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	7C	1	Total	C	N	O	P	0
			42	32	1	8	1	
70	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	

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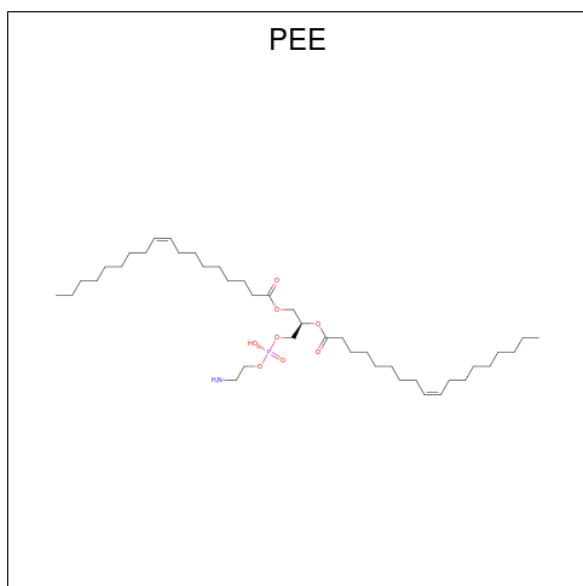
Mol	Chain	Residues	Atoms					AltConf
70	B7	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	B8	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	C1	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	C1	1	Total	C	N	O	P	0
			50	40	1	8	1	
70	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	C3	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	C4	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N4	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N5	1	Total	C	N	O	P	0
			31	21	1	8	1	
70	N6	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	QB	1	Total	C	N	O	P	0
			32	22	1	8	1	
70	QI	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	QJ	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qb	1	Total	C	N	O	P	0
			38	28	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
70	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qd	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qh	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	S8	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 71 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



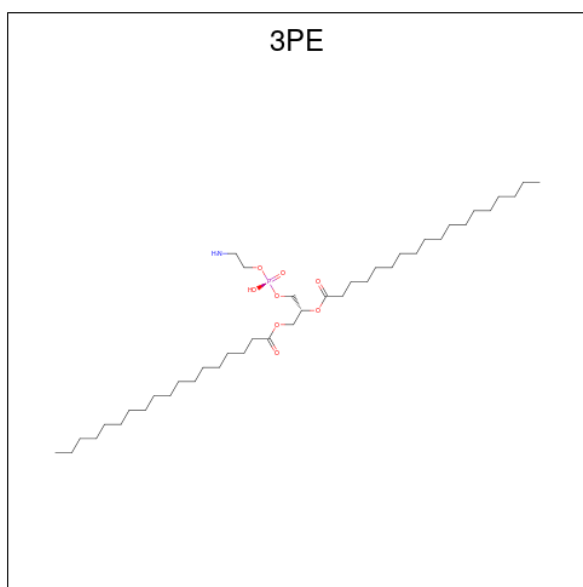
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	6A	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	8B	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	A3	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	A7	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	AL	1	Total	C	N	O	P	0
			36	26	1	8	1	
71	AL	1	Total	C	N	O	P	0
			40	30	1	8	1	

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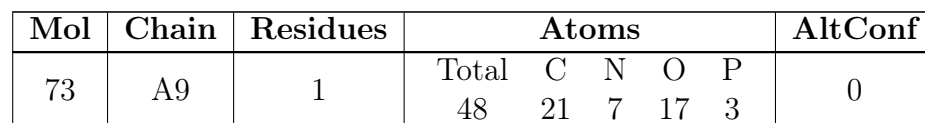
Mol	Chain	Residues	Atoms					AltConf
71	AN	1	Total 51	C 41	N 1	O 8	P 1	0
71	BL	1	Total 51	C 41	N 1	O 8	P 1	0
71	C1	1	Total 33	C 23	N 1	O 8	P 1	0
71	C3	1	Total 51	C 41	N 1	O 8	P 1	0
71	C3	1	Total 51	C 41	N 1	O 8	P 1	0
71	CB	1	Total 37	C 27	N 1	O 8	P 1	0
71	N5	1	Total 46	C 36	N 1	O 8	P 1	0
71	N5	1	Total 51	C 41	N 1	O 8	P 1	0
71	N5	1	Total 44	C 34	N 1	O 8	P 1	0
71	QC	1	Total 40	C 30	N 1	O 8	P 1	0
71	QC	1	Total 35	C 25	N 1	O 8	P 1	0
71	QC	1	Total 43	C 33	N 1	O 8	P 1	0
71	QE	1	Total 47	C 37	N 1	O 8	P 1	0
71	QH	1	Total 51	C 41	N 1	O 8	P 1	0
71	Qb	1	Total 51	C 41	N 1	O 8	P 1	0
71	Qc	1	Total 42	C 32	N 1	O 8	P 1	0
71	Qc	1	Total 48	C 38	N 1	O 8	P 1	0
71	Qe	1	Total 50	C 40	N 1	O 8	P 1	0
71	Qh	1	Total 51	C 41	N 1	O 8	P 1	0
71	S8	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).

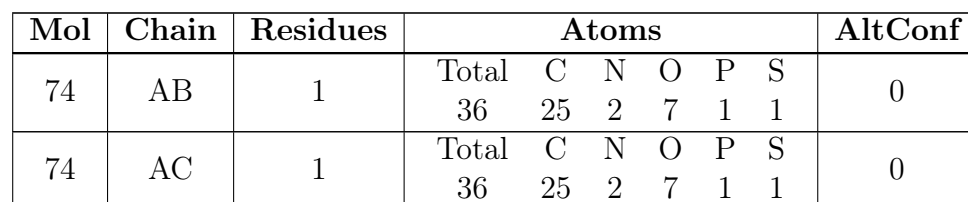


Mol	Chain	Residues	Atoms					AltConf
72	7B	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	Qc	1	Total	C	N	O	P	0
			44	34	1	8	1	
72	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	

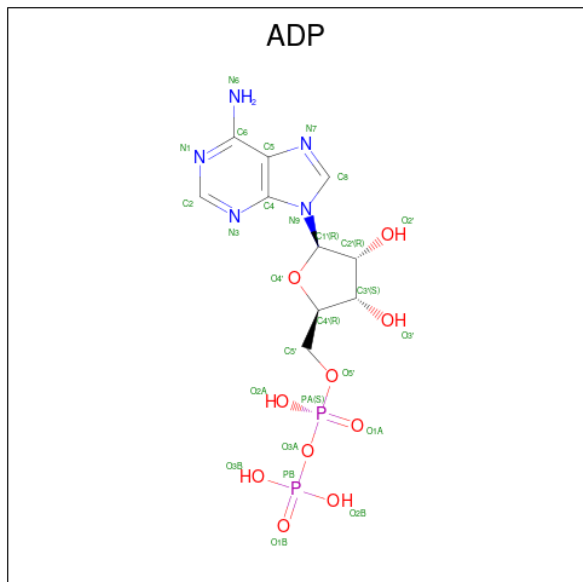
- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



- Molecule 74 is S-[2-($\{N-[(2S)-2\text{-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl} \}-\text{beta-alanyl}\}$)amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).

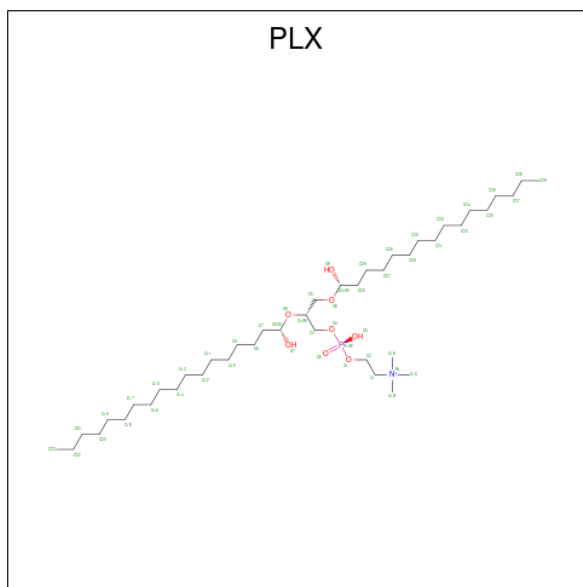


- Molecule 75 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



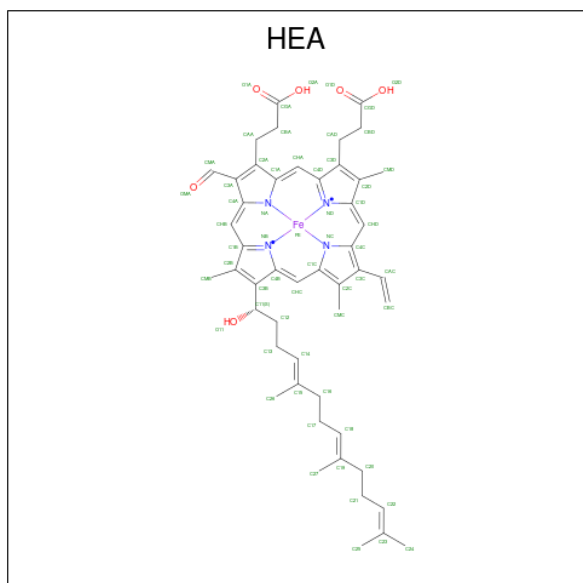
Mol	Chain	Residues	Atoms					AltConf
75	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 76 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
76	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
76	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	BL	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	C2	1	Total	C	N	O	P	0
			39	29	1	8	1	
76	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	QE	1	Total	C	N	O	P	0
			46	36	1	8	1	
76	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 77 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



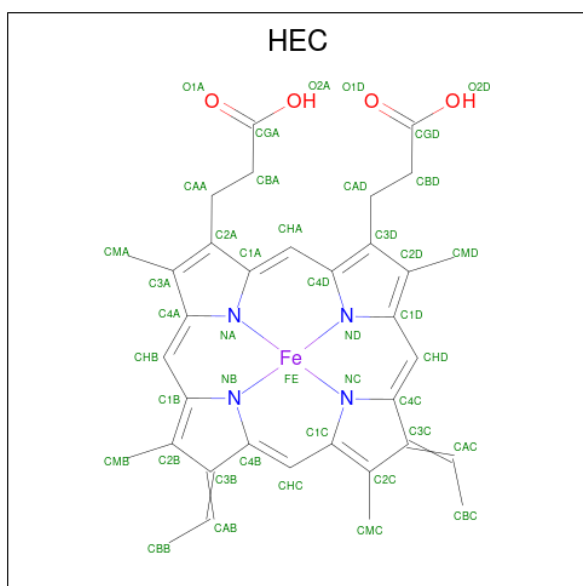
Mol	Chain	Residues	Atoms					AltConf
77	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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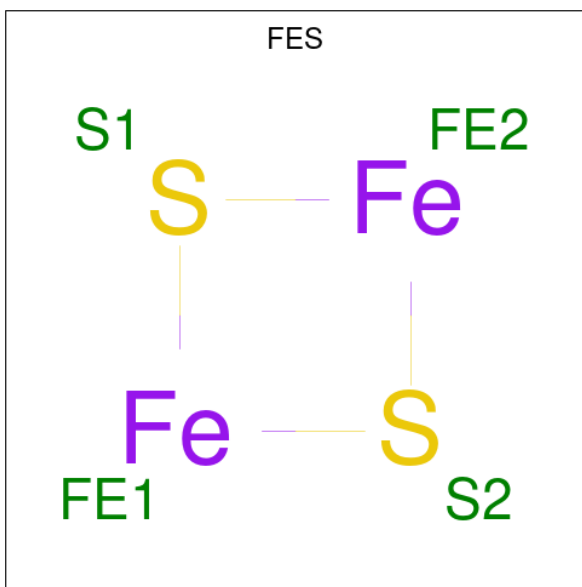
Mol	Chain	Residues	Atoms					AltConf
80	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 81 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



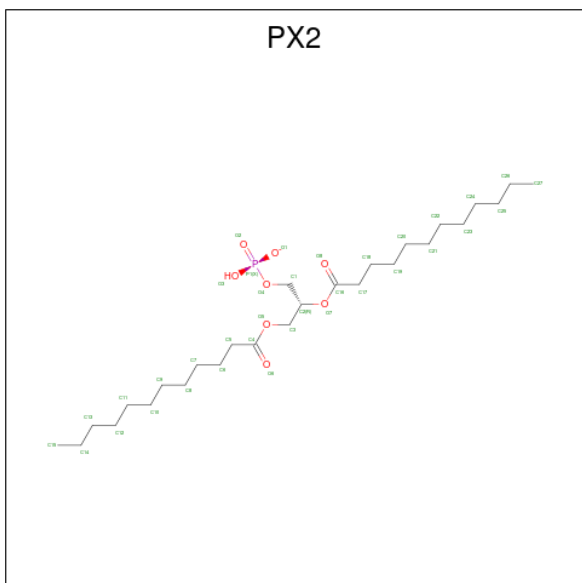
Mol	Chain	Residues	Atoms					AltConf
81	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



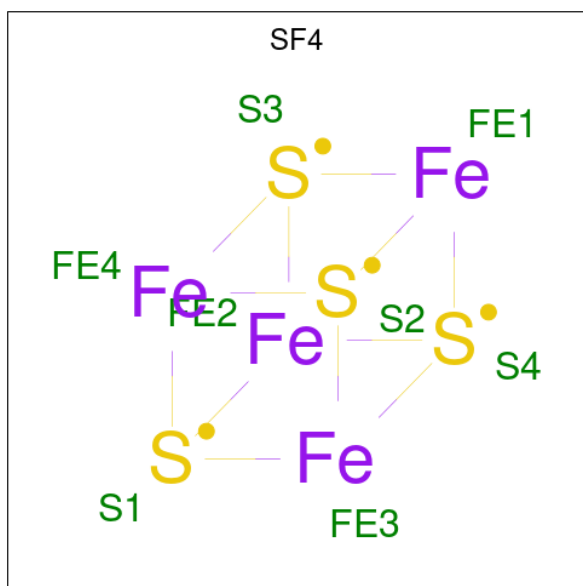
Mol	Chain	Residues	Atoms			AltConf
82	QE	1	Total 4	Fe 2	S 2	0
82	Qe	1	Total 4	Fe 2	S 2	0
82	S1	1	Total 4	Fe 2	S 2	0
82	V2	1	Total 4	Fe 2	S 2	0

- Molecule 83 is 1,2-DILAULOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



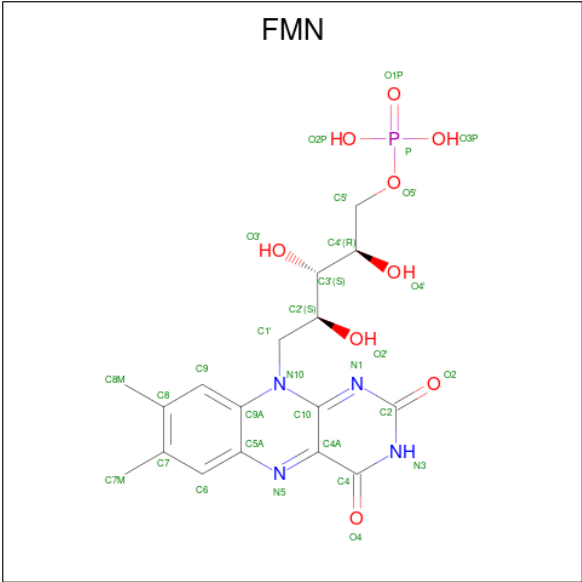
Mol	Chain	Residues	Atoms				AltConf
83	QH	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 84 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
84	S1	1	Total	Fe	S	0
			8	4	4	
84	S1	1	Total	Fe	S	0
			8	4	4	
84	S7	1	Total	Fe	S	0
			8	4	4	
84	S8	1	Total	Fe	S	0
			8	4	4	
84	S8	1	Total	Fe	S	0
			8	4	4	
84	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 85 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
85	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots [i](#)

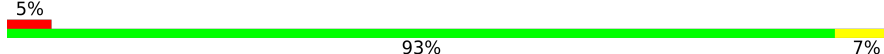
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:  85% 15%



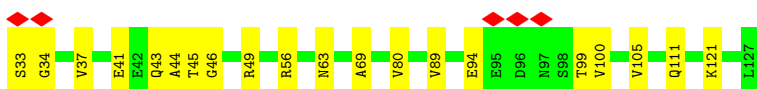
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 5A:  5% 93% 7%



- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 5B:  5% 79% 21%



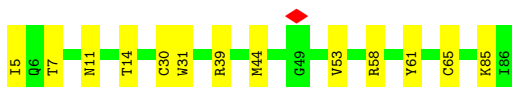
- Molecule 4: Cytochrome c oxidase subunit

Chain 6A:  7% 83% 17%

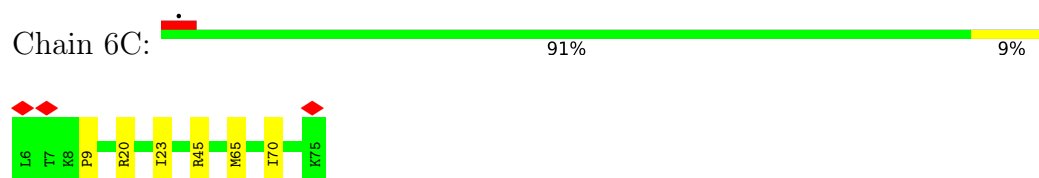


- Molecule 5: Cytochrome c oxidase subunit

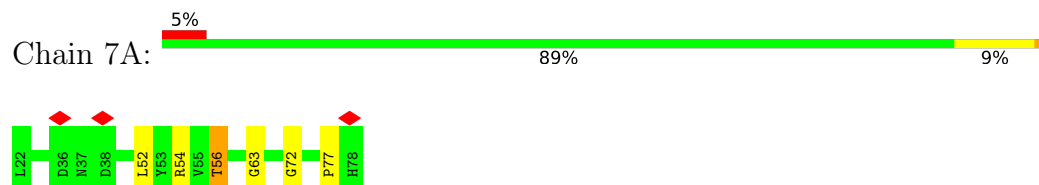
Chain 6B:  84% 16%



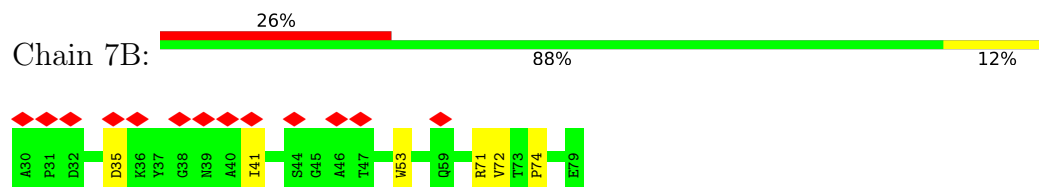
- Molecule 6: Cytochrome c oxidase subunit 6C



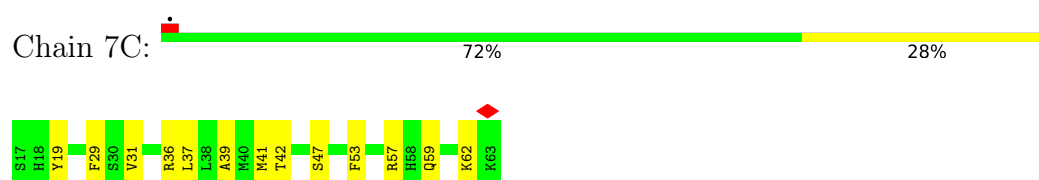
- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



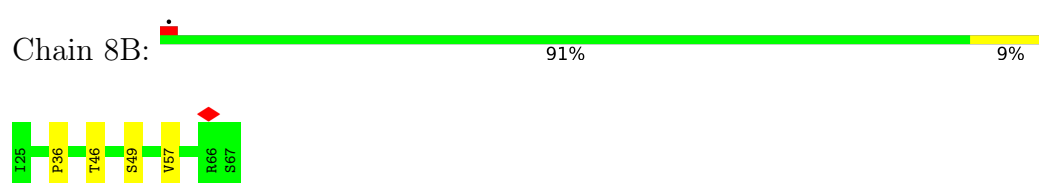
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



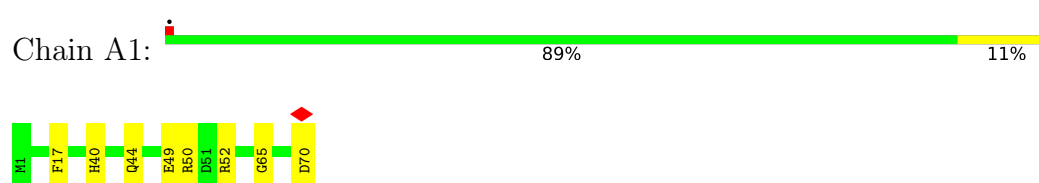
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



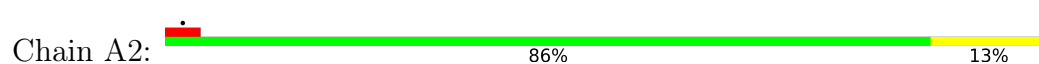
- Molecule 10: Cytochrome c oxidase subunit 8



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

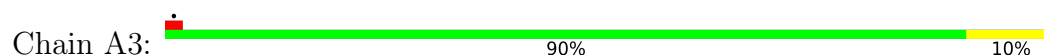


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2





- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



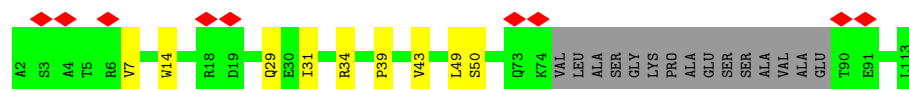
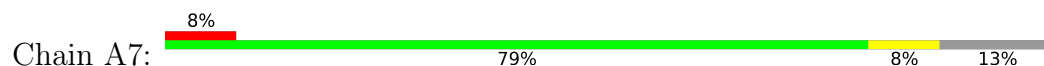
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



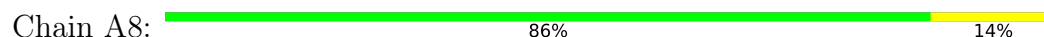
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



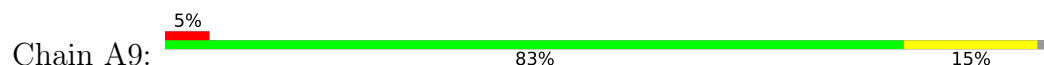
- Molecule 16: Complex I-B14.5a

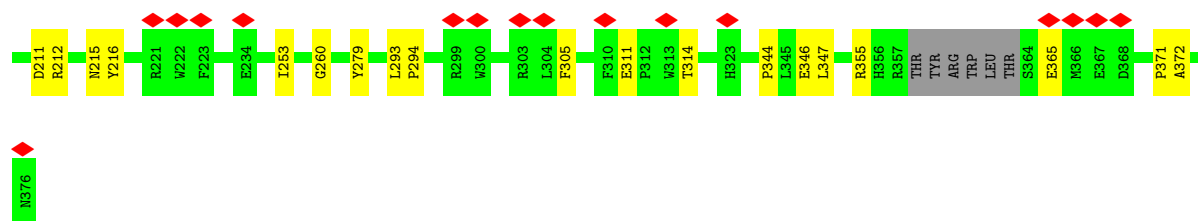


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

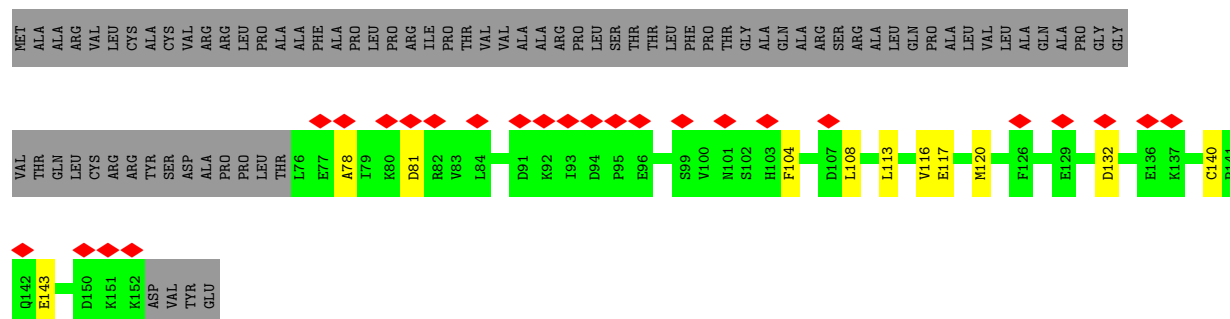
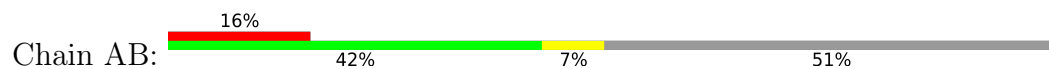


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

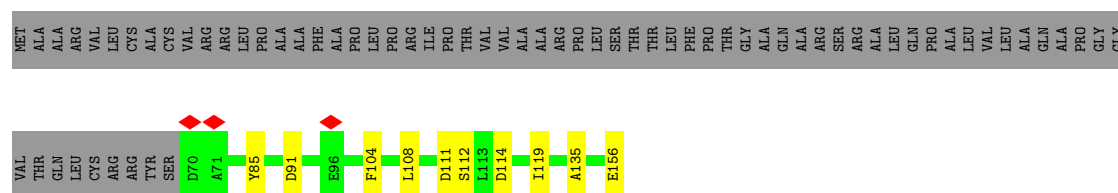




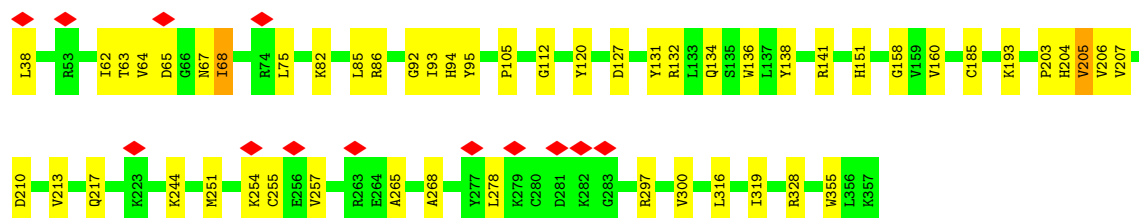
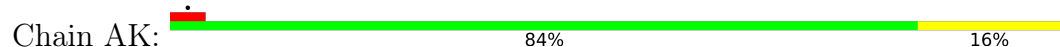
- Molecule 19: Acyl carrier protein



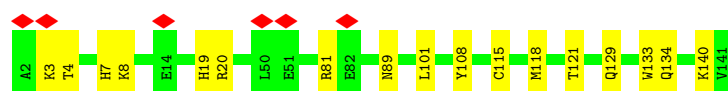
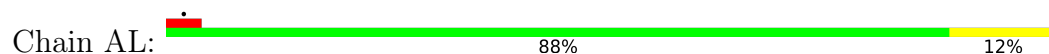
- Molecule 19: Acyl carrier protein



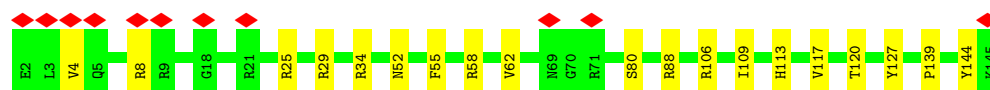
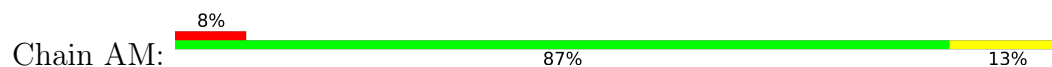
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



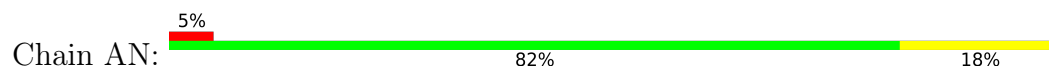
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



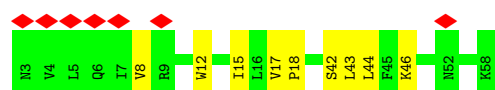
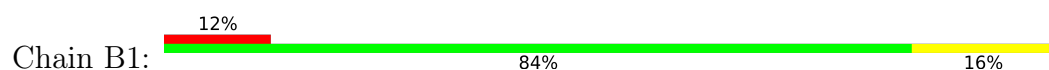
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



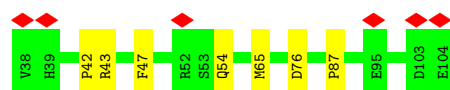
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



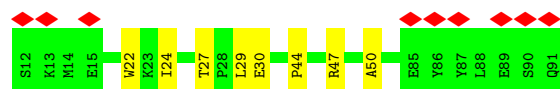
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



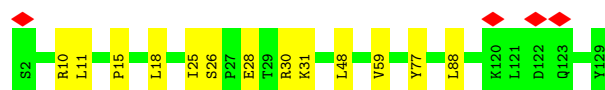
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

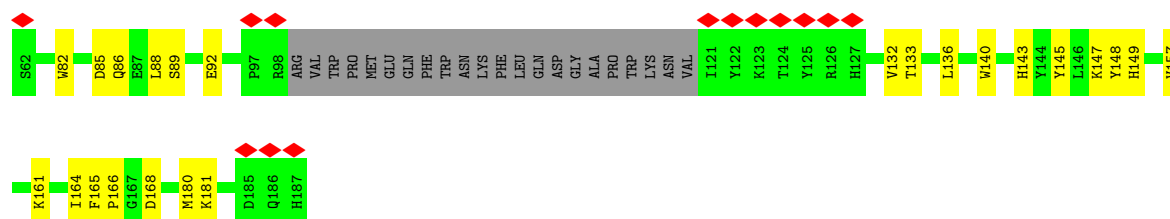


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

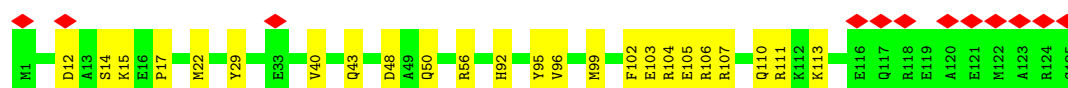
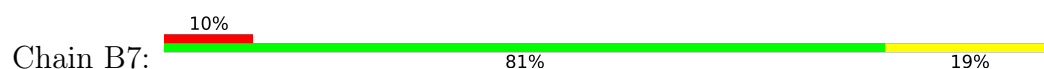




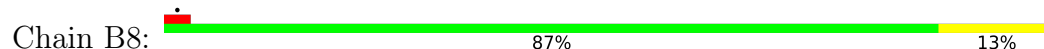
- Molecule 29: Complex I-B17



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



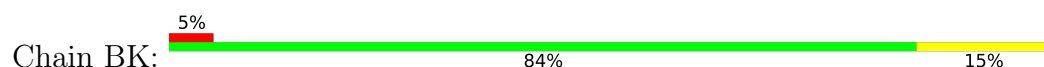
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



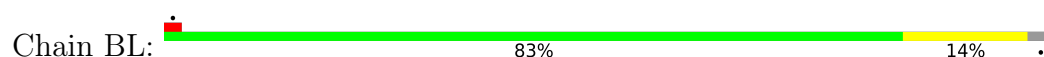
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

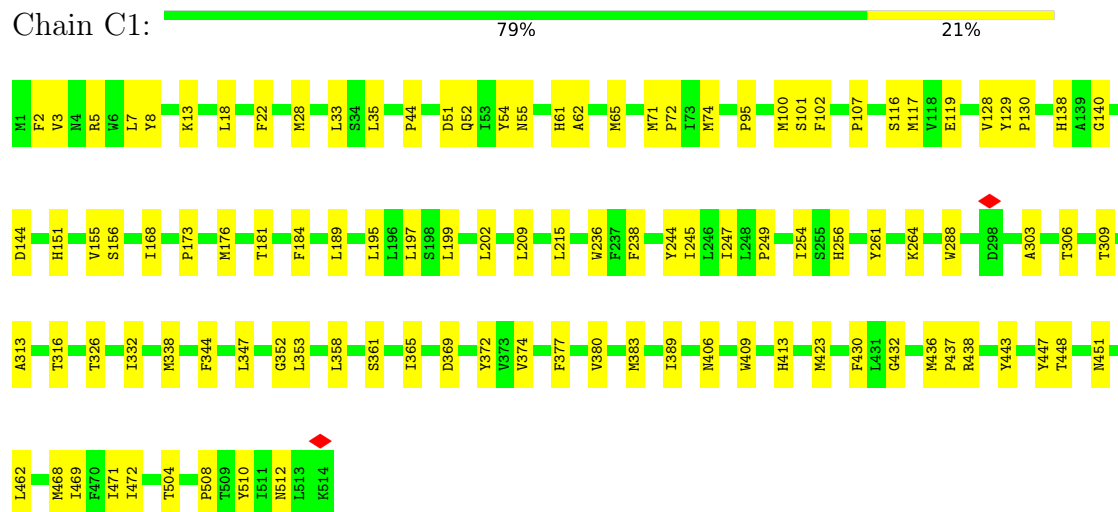


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

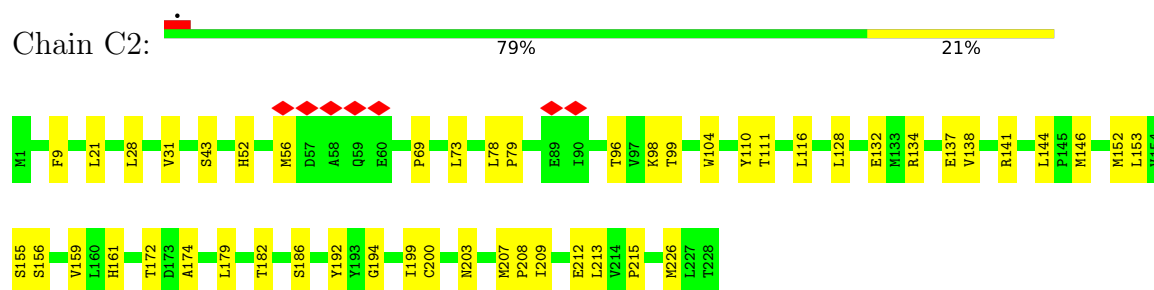




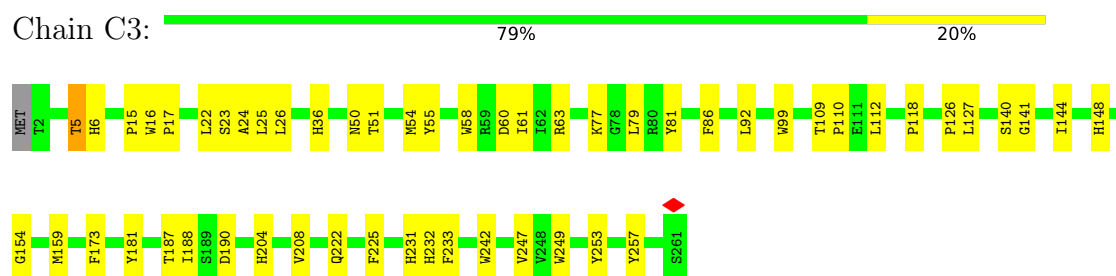
• Molecule 35: Cytochrome c oxidase subunit 1



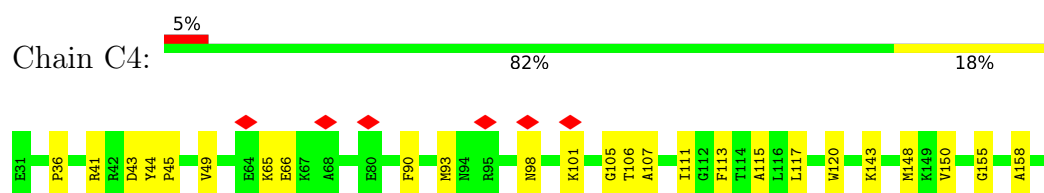
• Molecule 36: Cytochrome c oxidase subunit 2



• Molecule 37: Cytochrome c oxidase subunit 3

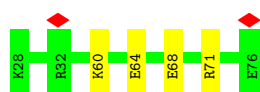


• Molecule 38: Cytochrome c oxidase subunit 4



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain CA:  92% 8%



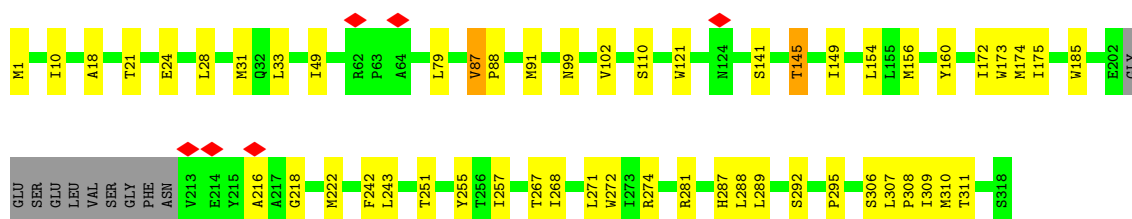
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB:  91% 9%



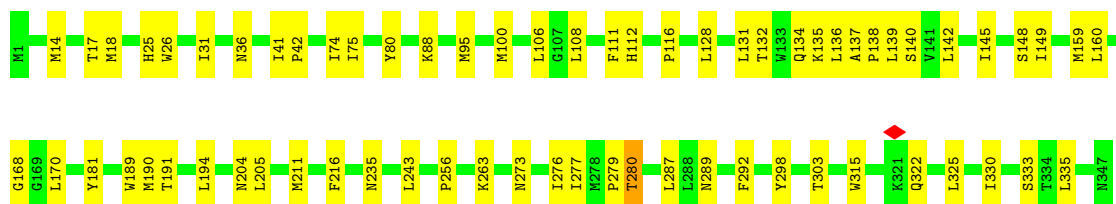
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain N1:  80% 16% ..



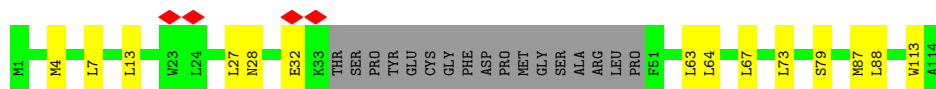
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2:  81% 19%



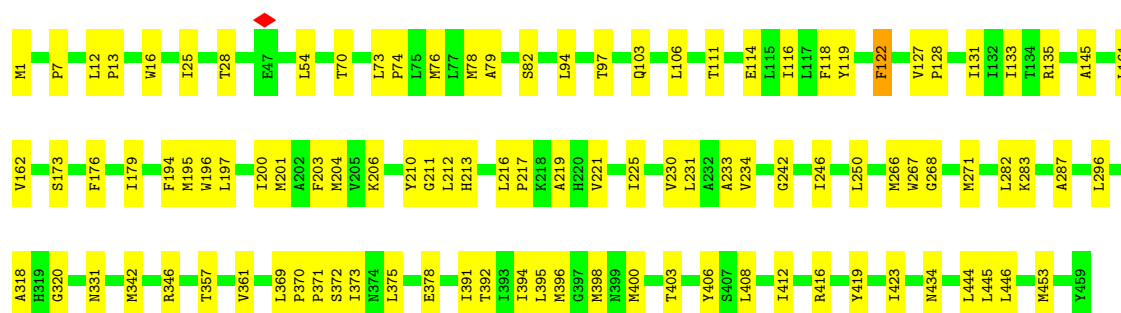
- Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3:  73% 12% 15%



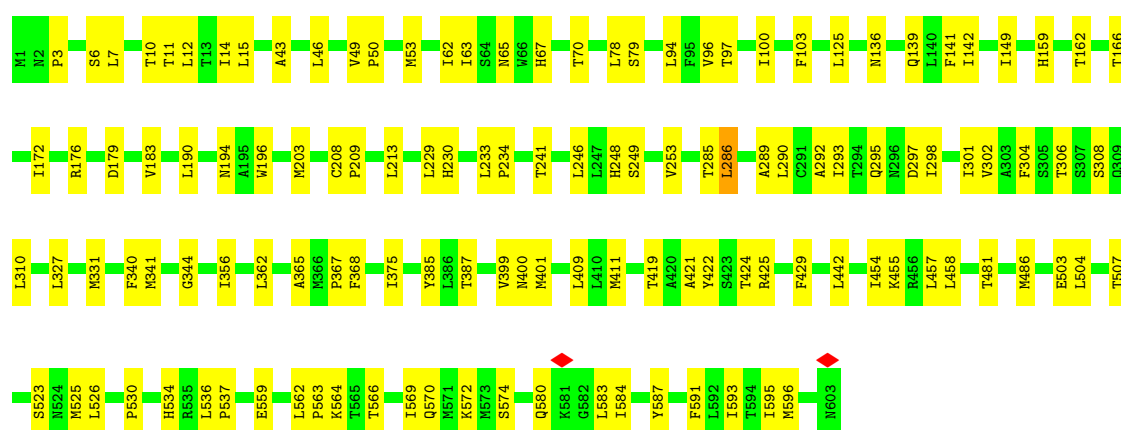
- Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4:  78% 22%



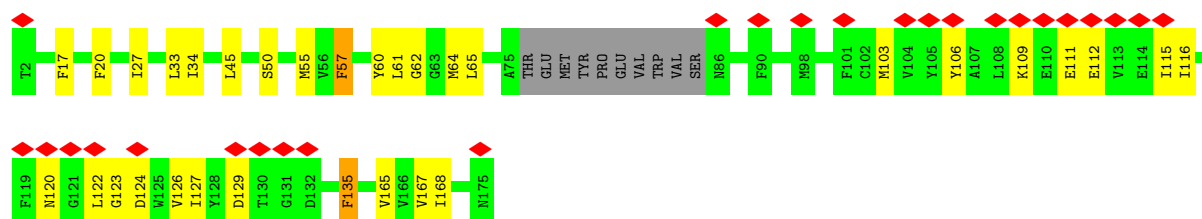
• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 79% 21%



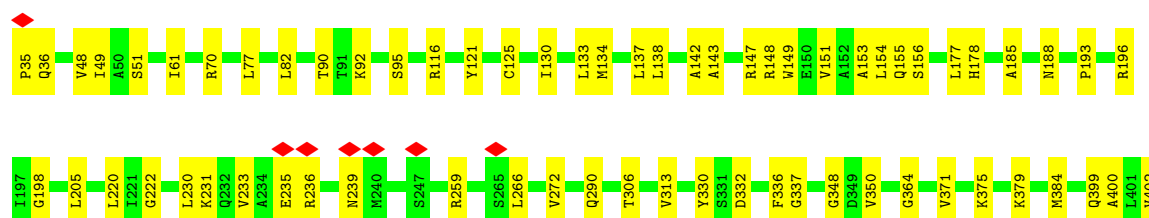
• Molecule 46: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 15% 76% 17% • 6%



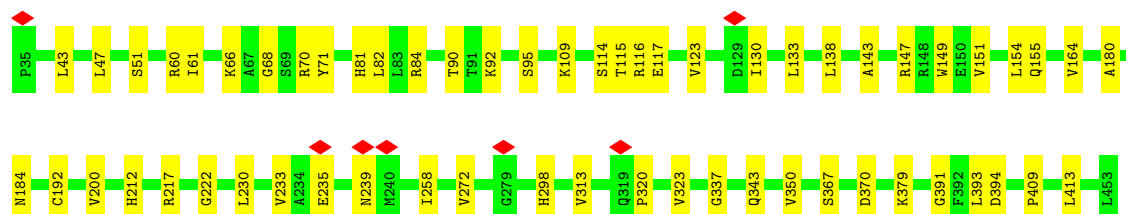
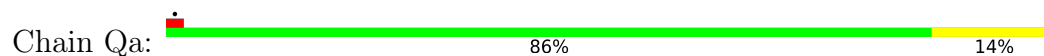
• Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain QA: 83% 17%

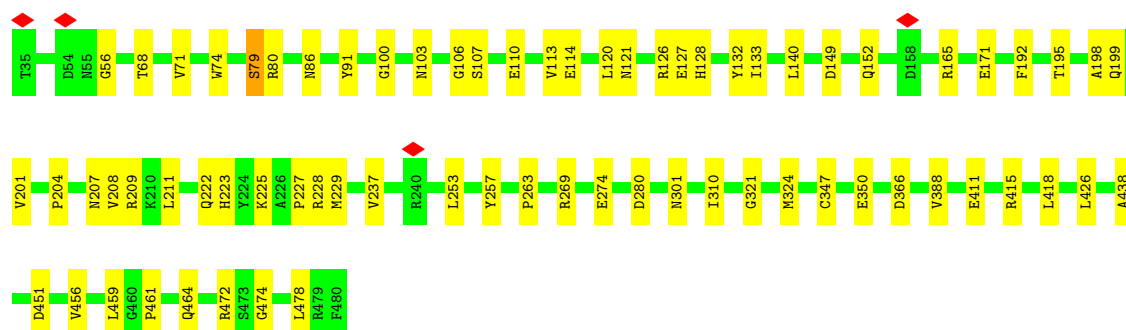
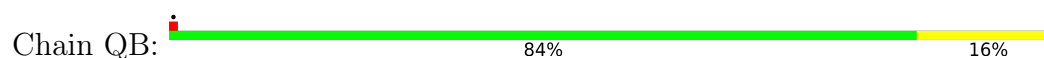




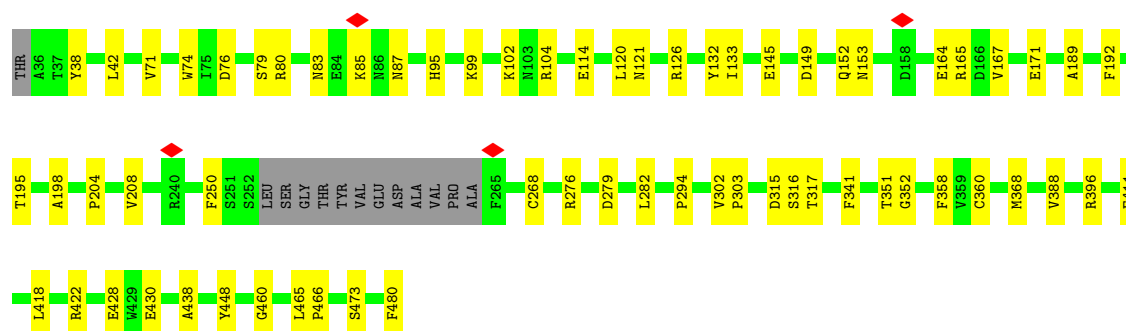
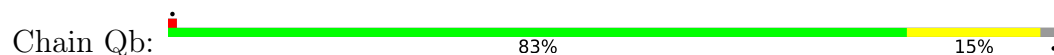
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial



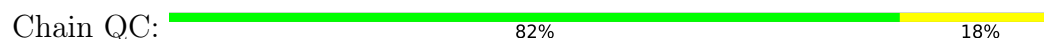
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

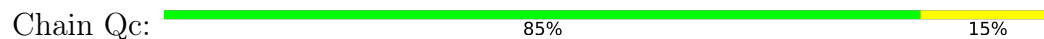


- Molecule 49: Cytochrome b

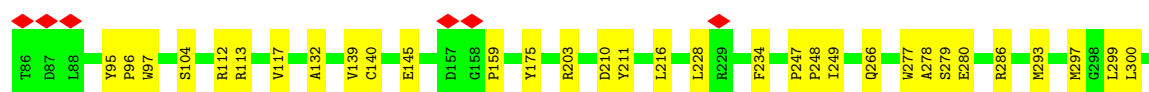
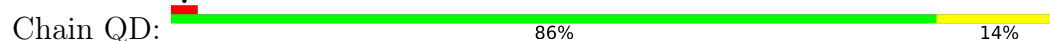




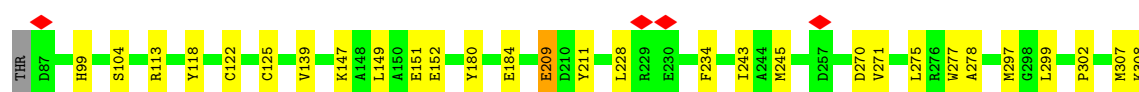
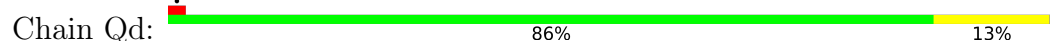
• Molecule 49: Cytochrome b



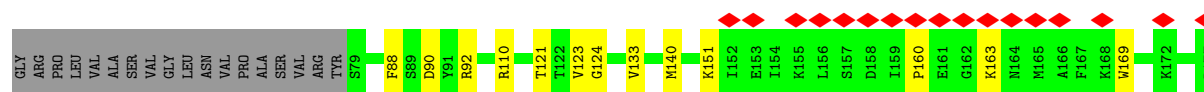
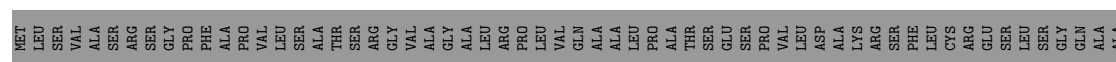
• Molecule 50: Cytochrome c domain-containing protein

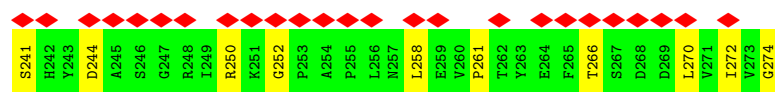


• Molecule 50: Cytochrome c domain-containing protein



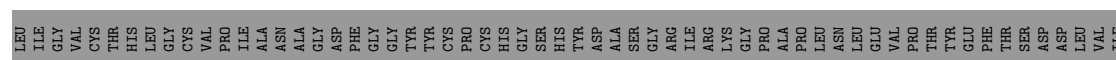
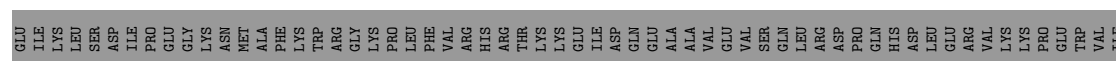
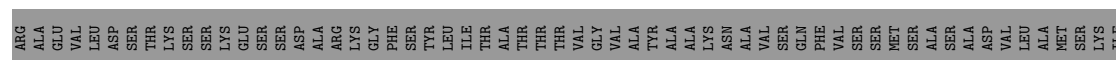
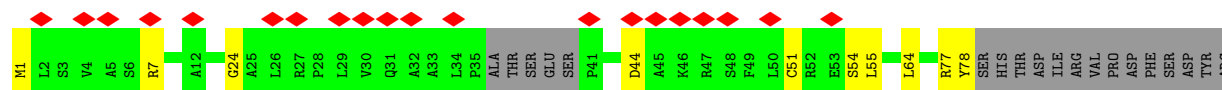
• Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial





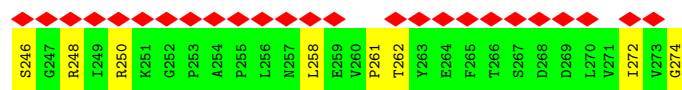
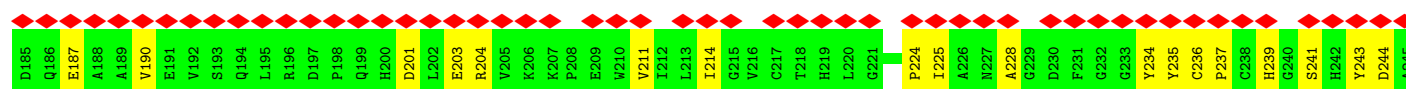
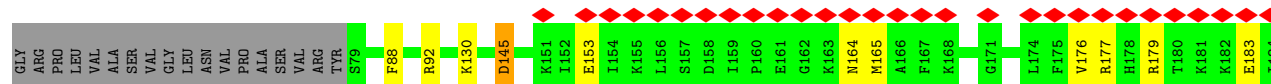
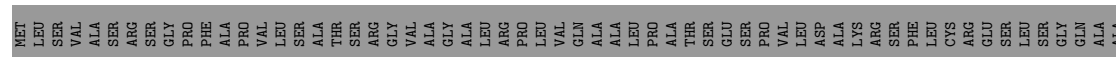
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain QK: 7% 23% 73%



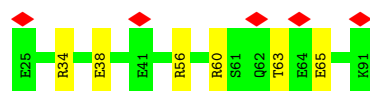
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Qe: 39% 58% 13% 28%



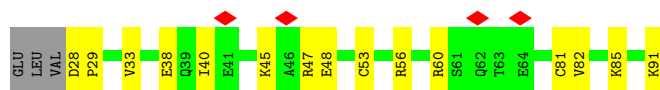
- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain QF: 7% 91% 9%



- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain Qf: 6% 73% 22%



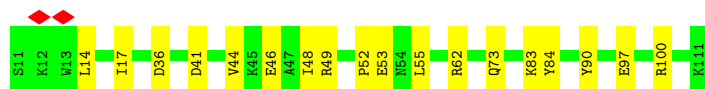
- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG: 92% 8%



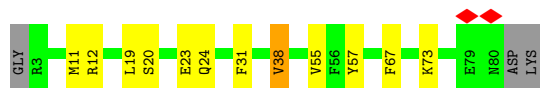
- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg: 82% 18%



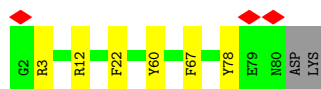
- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH: 81% 14% ..



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh: 90% 7% .



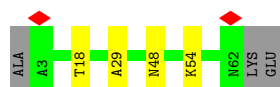
- Molecule 55: Complex III subunit 9

Chain QI: 8% 92% 6% .

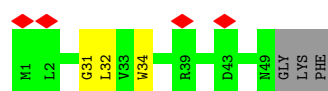
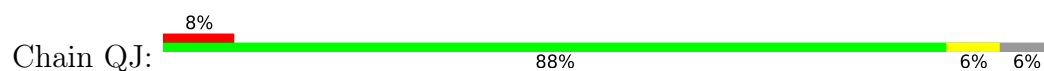


- Molecule 55: Complex III subunit 9

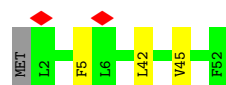
Chain Qi: 89% 6% 5%



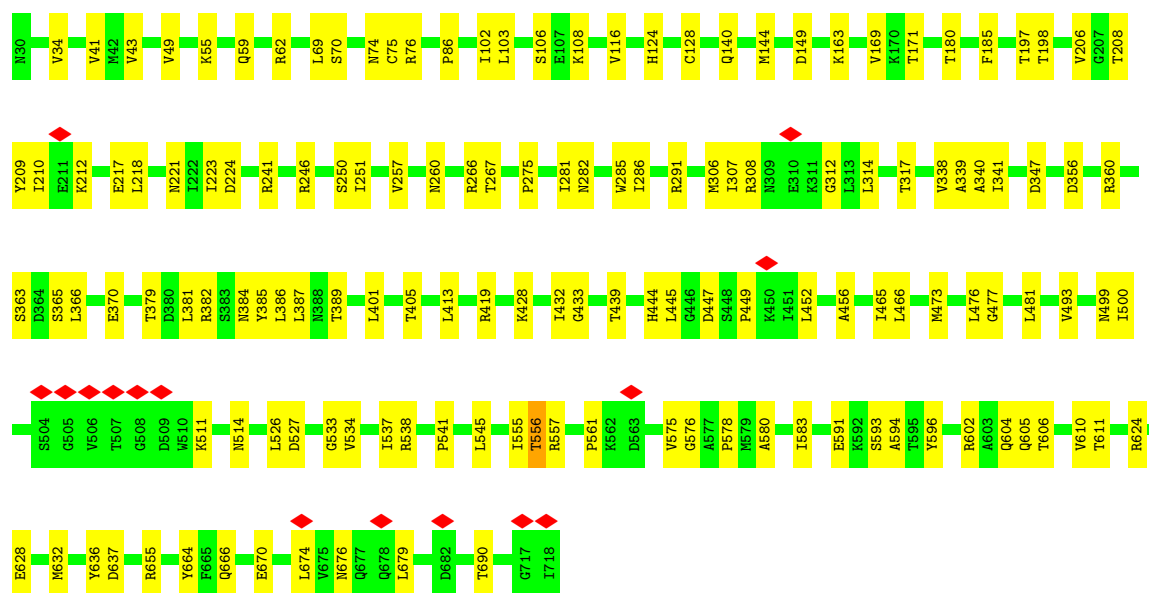
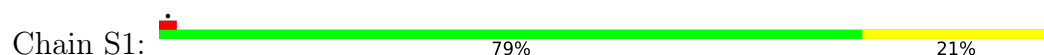
- Molecule 56: Cytochrome b-c1 complex subunit 10



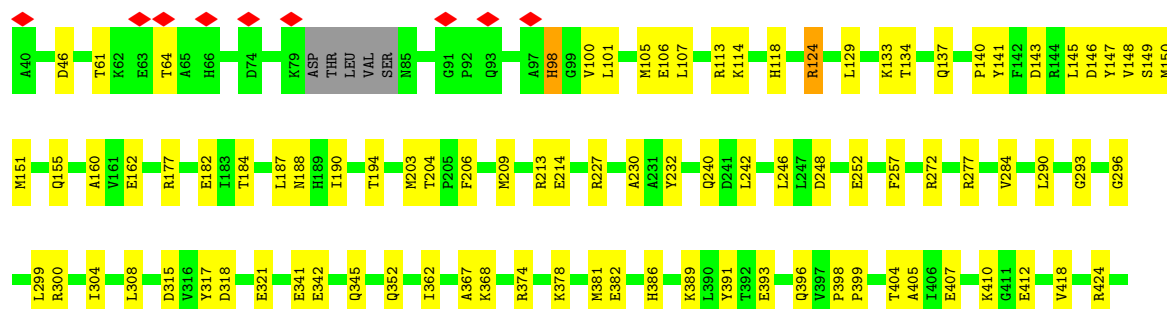
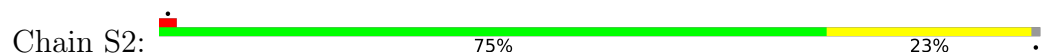
- Molecule 56: Cytochrome b-c1 complex subunit 10



- Molecule 57: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



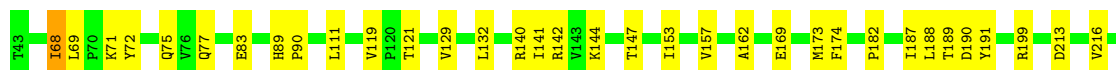
- Molecule 58: Complex I-49kD





- Molecule 59: Complex I-30kD

Chain S3: 82% 17%



- Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4: 6% 86% 14%



- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5: 5% 89% 11%



- Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6: 6% 88% 12%



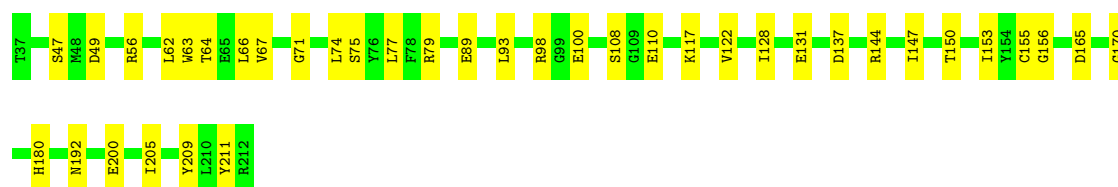
- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7: 78% 21%



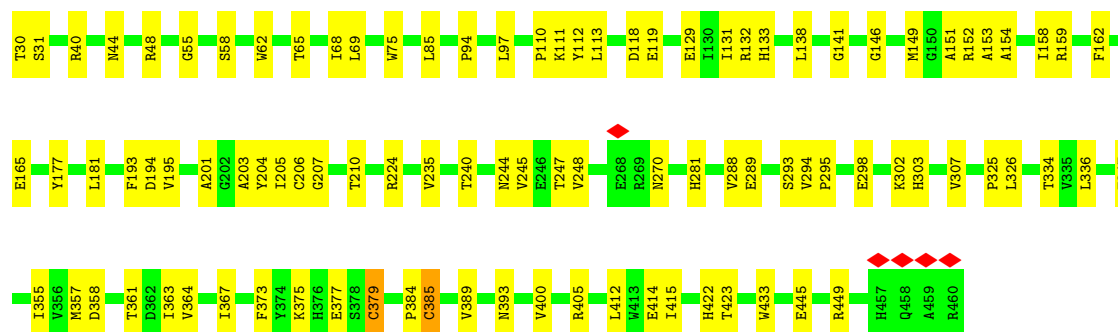
- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8: 78% 22%



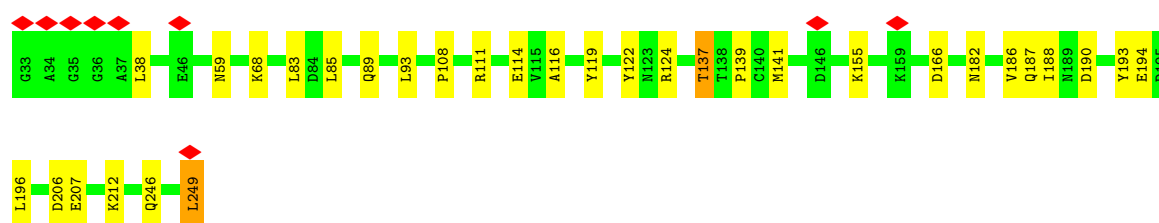
- Molecule 65: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1: 77% 22%



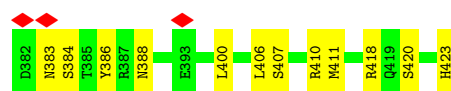
- Molecule 66: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 85% 14%



- Molecule 67: Complex I-9kD

Chain V3: 7% 71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250490	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 ($e^-/\text{\AA}^2$)	51.9	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	47.821	Depositor
Minimum map value	-24.261	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.078	Depositor
Recommended contour level	6	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	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: ADP, PX2, NDP, FMN, ZMP, MG, CU, HEC, FES, SF4, ZN, 2MR, PLX, CDL, PEE, HEA, HEM, 3PE, PC1

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	4L	0.16	0/759	0.26	0/1029
2	5A	0.11	0/843	0.23	0/1145
3	5B	0.14	0/739	0.30	0/1002
4	6A	0.12	0/648	0.27	0/888
5	6B	0.13	0/704	0.23	0/951
6	6C	0.12	0/587	0.22	0/781
7	7A	0.12	0/457	0.25	0/620
8	7B	0.11	0/405	0.24	0/555
9	7C	0.14	0/400	0.23	0/536
10	8B	0.14	0/349	0.26	0/477
11	A1	0.14	0/577	0.28	0/777
12	A2	0.10	0/697	0.25	0/938
13	A3	0.12	0/664	0.25	0/912
14	A5	0.13	0/929	0.21	0/1258
15	A6	0.13	0/991	0.26	0/1335
16	A7	0.12	0/798	0.23	0/1079
17	A8	0.13	0/1436	0.23	0/1938
18	A9	0.12	0/2757	0.25	0/3734
19	AB	0.08	0/633	0.21	0/851
19	AC	0.13	0/714	0.23	0/965
20	AK	0.15	0/2650	0.36	2/3588 (0.1%)
21	AL	0.13	0/1042	0.21	0/1411
22	AM	0.12	0/1245	0.23	0/1694
23	AN	0.14	0/1203	0.26	0/1622
24	B1	0.14	0/491	0.28	0/663
25	B2	0.13	0/610	0.26	0/836
26	B3	0.13	0/660	0.25	0/892
27	B4	0.14	0/1092	0.25	0/1481
28	B5	0.16	0/1184	0.27	0/1603
29	B6	0.15	0/918	0.31	0/1248
30	B7	0.12	0/1092	0.23	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.13	0/1371	0.25	0/1875
32	B9	0.14	0/1590	0.27	0/2155
33	BK	0.15	0/1489	0.24	0/2008
34	BL	0.15	0/851	0.29	0/1155
35	C1	0.19	0/4164	0.31	0/5689
36	C2	0.16	0/1880	0.27	0/2564
37	C3	0.16	0/2186	0.26	0/2991
38	C4	0.13	0/1187	0.23	0/1606
39	CA	0.12	0/430	0.22	0/581
40	CB	0.15	0/1031	0.25	0/1394
41	N1	0.17	0/2507	0.32	0/3428
42	N2	0.19	0/2773	0.33	0/3768
43	N3	0.15	0/797	0.26	0/1087
44	N4	0.19	0/3723	0.32	0/5078
45	N5	0.17	0/4914	0.34	0/6683
46	N6	0.15	0/1273	0.31	0/1722
47	QA	0.15	0/3196	0.27	0/4328
47	Qa	0.14	0/3200	0.26	0/4333
48	QB	0.15	0/3531	0.29	0/4793
48	Qb	0.14	0/3436	0.27	0/4659
49	QC	0.17	0/3123	0.30	0/4269
49	Qc	0.17	0/3123	0.30	0/4269
50	QD	0.14	0/1979	0.25	0/2684
50	Qd	0.14	0/1962	0.26	0/2663
51	QE	0.12	0/1550	0.25	0/2098
51	QK	0.11	0/528	0.26	0/716
51	Qe	0.12	0/1550	0.27	0/2098
52	QF	0.11	0/558	0.22	0/747
52	Qf	0.13	0/534	0.24	0/714
53	QG	0.14	0/913	0.24	0/1223
53	Qg	0.14	0/913	0.25	0/1223
54	QH	0.14	0/684	0.29	0/926
54	Qh	0.14	0/688	0.27	0/931
55	QI	0.11	0/520	0.18	0/701
55	Qi	0.15	0/506	0.24	0/683
56	QJ	0.10	0/420	0.24	0/576
56	Qj	0.14	0/437	0.28	0/598
57	S1	0.15	0/5378	0.29	0/7287
58	S2	0.18	0/3501	0.30	0/4743
59	S3	0.15	0/1789	0.27	0/2436
60	S4	0.15	0/1030	0.28	0/1391
61	S5	0.13	0/889	0.23	0/1190
62	S6	0.13	0/755	0.26	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	S7	0.17	0/1279	0.28	0/1730
64	S8	0.17	0/1443	0.26	0/1952
65	V1	0.14	0/3387	0.29	0/4578
66	V2	0.12	0/1711	0.28	0/2328
67	V3	0.10	0/365	0.25	0/493
All	All	0.15	0/115318	0.28	2/156430 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AK	204	HIS	CA-C-N	-6.18	114.45	123.10
20	AK	204	HIS	C-N-CA	-6.18	114.45	123.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	13	0
2	5A	825	0	823	5	0
3	5B	724	0	705	12	0
4	6A	620	0	589	13	0
5	6B	684	0	649	9	0
6	6C	574	0	590	4	0
7	7A	447	0	443	5	0
8	7B	392	0	372	7	0
9	7C	387	0	385	13	0
10	8B	338	0	342	4	0
11	A1	562	0	557	6	0
12	A2	686	0	699	8	0
13	A3	643	0	642	6	0
14	A5	910	0	950	5	0
15	A6	967	0	972	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A7	780	0	808	7	0
17	A8	1398	0	1372	20	0
18	A9	2684	0	2704	31	0
19	AB	624	0	625	8	0
19	AC	702	0	694	8	0
20	AK	2590	0	2553	31	0
21	AL	1021	0	1025	13	0
22	AM	1204	0	1162	12	0
23	AN	1172	0	1162	23	0
24	B1	479	0	486	6	0
25	B2	584	0	529	6	0
26	B3	641	0	620	6	0
27	B4	1062	0	1072	9	0
28	B5	1151	0	1164	13	0
29	B6	890	0	910	23	0
30	B7	1068	0	1043	19	0
31	B8	1315	0	1208	14	0
32	B9	1534	0	1470	17	0
33	BK	1456	0	1426	22	0
34	BL	828	0	788	10	0
35	C1	4024	0	4005	80	0
36	C2	1833	0	1843	31	0
37	C3	2103	0	2034	48	0
38	C4	1153	0	1130	21	0
39	CA	417	0	422	2	0
40	CB	1000	0	994	11	0
41	N1	2436	0	2543	39	0
42	N2	2710	0	2874	54	0
43	N3	779	0	829	12	0
44	N4	3631	0	3839	70	0
45	N5	4785	0	4933	95	0
46	N6	1243	0	1248	26	0
47	QA	3143	0	3125	42	0
47	Qa	3147	0	3129	38	0
48	QB	3459	0	3350	46	0
48	Qb	3367	0	3262	38	0
49	QC	3025	0	3090	55	0
49	Qc	3025	0	3090	51	0
50	QD	1921	0	1867	23	0
50	Qd	1904	0	1849	24	0
51	QE	1517	0	1500	33	0
51	QK	520	0	554	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Qe	1517	0	1500	24	0
52	QF	552	0	536	4	0
52	Qf	528	0	510	9	0
53	QG	893	0	888	5	0
53	Qg	893	0	888	11	0
54	QH	662	0	660	12	0
54	Qh	666	0	663	6	0
55	QI	507	0	509	3	0
55	Qi	493	0	491	4	0
56	QJ	405	0	405	3	0
56	Qj	421	0	418	2	0
57	S1	5290	0	5321	91	0
58	S2	3423	0	3359	71	0
59	S3	1738	0	1693	25	0
60	S4	1007	0	1008	11	0
61	S5	867	0	871	16	0
62	S6	741	0	701	10	0
63	S7	1248	0	1254	24	0
64	S8	1412	0	1363	32	0
65	V1	3312	0	3266	58	0
66	V2	1671	0	1673	19	0
67	V3	355	0	329	9	0
68	4L	92	0	137	3	0
68	A7	94	0	141	5	0
68	A8	83	0	113	7	0
68	AL	256	0	359	14	0
68	AN	147	0	188	10	0
68	B4	62	0	68	3	0
68	B5	96	0	145	7	0
68	C1	77	0	98	5	0
68	N2	68	0	80	1	0
68	N4	100	0	156	10	0
68	N5	189	0	284	12	0
68	QB	64	0	72	10	0
68	QC	145	0	187	4	0
68	QD	64	0	72	2	0
68	Qb	64	0	72	4	0
68	Qc	125	0	138	8	0
68	Qh	100	0	156	2	0
68	Qj	96	0	145	4	0
69	5B	1	0	0	0	0
69	S6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	6A	45	0	64	13	0
70	7A	54	0	88	2	0
70	7C	42	0	58	6	0
70	B5	54	0	88	0	0
70	B7	54	0	88	1	0
70	B8	54	0	88	1	0
70	C1	144	0	219	16	0
70	C3	100	0	154	7	0
70	C4	54	0	88	1	0
70	N1	54	0	88	7	0
70	N3	54	0	88	3	0
70	N4	54	0	88	11	0
70	N5	31	0	36	2	0
70	N6	54	0	88	8	0
70	QB	83	0	117	16	0
70	QI	54	0	88	3	0
70	QJ	54	0	88	4	0
70	Qb	38	0	50	5	0
70	Qc	198	0	310	13	0
70	Qd	54	0	88	3	0
70	Qh	54	0	88	5	0
70	S8	45	0	67	10	0
71	6A	102	0	164	6	0
71	8B	42	0	61	3	0
71	A3	51	0	82	4	0
71	A7	28	0	30	1	0
71	AL	76	0	103	0	0
71	AN	51	0	82	5	0
71	BL	51	0	82	1	0
71	C1	33	0	40	3	0
71	C3	102	0	164	7	0
71	CB	37	0	51	3	0
71	N5	141	0	213	16	0
71	QC	118	0	161	12	0
71	QE	47	0	71	4	0
71	QH	51	0	82	4	0
71	Qb	51	0	82	1	0
71	Qc	90	0	134	6	0
71	Qe	50	0	77	3	0
71	Qh	51	0	82	3	0
71	S8	51	0	82	1	0
72	7B	51	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	C1	51	0	82	4	0
72	CA	51	0	82	4	0
72	CB	46	0	69	0	0
72	Qc	92	0	138	3	0
73	A9	48	0	26	2	0
74	AB	36	0	47	2	0
74	AC	36	0	47	5	0
75	AK	27	0	12	3	0
76	AL	47	0	75	4	0
76	AM	52	0	88	3	0
76	B1	52	0	88	1	0
76	BL	52	0	88	6	0
76	C2	39	0	56	4	0
76	CB	52	0	88	4	0
76	N3	52	0	88	3	0
76	QE	46	0	73	3	0
76	QI	52	0	88	5	0
76	S7	52	0	88	9	0
77	C1	120	0	108	19	0
78	C1	1	0	0	0	0
78	C2	2	0	0	0	0
79	C1	1	0	0	0	0
79	S1	1	0	0	0	0
80	QC	86	0	60	8	0
80	Qc	86	0	60	10	0
81	QD	43	0	30	1	0
81	Qd	43	0	32	3	0
82	QE	4	0	0	2	0
82	Qe	4	0	0	2	0
82	S1	4	0	0	1	0
82	V2	4	0	0	0	0
83	QH	36	0	52	1	0
84	S1	16	0	0	1	0
84	S7	8	0	0	0	0
84	S8	16	0	0	2	0
84	V1	8	0	0	0	0
85	V1	31	0	19	2	0
All	All	118456	0	120593	1656	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 7.

The worst 5 of 1656 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)
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.66	0.95
49:Qc:98:VAL:HG22	80:Qc:405:HEM:HBC2	1.61	0.82
49:QC:97:HIS:HE1	80:QC:402:HEM:ND	1.81	0.79
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.65	0.79
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.66	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	5A	100/102 (98%)	100 (100%)	0	0	100	100
3	5B	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
4	6A	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
5	6B	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	6C	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100
8	7B	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
9	7C	45/47 (96%)	45 (100%)	0	0	100	100
10	8B	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	A1	68/70 (97%)	68 (100%)	0	0	100	100
12	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
13	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
14	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
15	A6	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
16	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	A8	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
18	A9	331/341 (97%)	322 (97%)	9 (3%)	0	100	100
19	AB	75/156 (48%)	75 (100%)	0	0	100	100
19	AC	85/156 (54%)	85 (100%)	0	0	100	100
20	AK	318/320 (99%)	302 (95%)	16 (5%)	0	100	100
21	AL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
22	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
23	AN	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100
25	B2	65/67 (97%)	65 (100%)	0	0	100	100
26	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
29	B6	100/126 (79%)	97 (97%)	3 (3%)	0	100	100
30	B7	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
31	B8	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
32	B9	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
33	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
34	BL	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
35	C1	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
36	C2	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
37	C3	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
38	C4	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
39	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	304/318 (96%)	290 (95%)	14 (5%)	0	100	100
42	N2	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
43	N3	93/114 (82%)	90 (97%)	3 (3%)	0	100	100
44	N4	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
45	N5	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
46	N6	160/174 (92%)	145 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	QA	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
47	Qa	417/419 (100%)	413 (99%)	4 (1%)	0	100	100
48	QB	444/446 (100%)	432 (97%)	12 (3%)	0	100	100
48	Qb	429/446 (96%)	422 (98%)	7 (2%)	0	100	100
49	QC	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
49	Qc	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
50	QD	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/241 (98%)	230 (97%)	7 (3%)	0	100	100
51	QE	194/274 (71%)	190 (98%)	4 (2%)	0	100	100
51	QK	69/274 (25%)	69 (100%)	0	0	100	100
51	Qe	194/274 (71%)	188 (97%)	6 (3%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	62 (100%)	0	0	100	100
53	QG	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
53	Qg	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
54	QH	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
54	Qh	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
55	QI	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/63 (92%)	58 (100%)	0	0	100	100
56	QJ	47/52 (90%)	47 (100%)	0	0	100	100
56	Qj	49/52 (94%)	47 (96%)	2 (4%)	0	100	100
57	S1	687/689 (100%)	663 (96%)	24 (4%)	0	100	100
58	S2	420/430 (98%)	396 (94%)	24 (6%)	0	100	100
59	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
60	S4	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
61	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
62	S6	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
63	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
64	S8	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
65	V1	429/431 (100%)	407 (95%)	22 (5%)	0	100	100
66	V2	215/217 (99%)	207 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13913/14717 (94%)	13526 (97%)	387 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	89 (100%)	0	100	100
3	5B	80/80 (100%)	77 (96%)	3 (4%)	29	62
4	6A	66/66 (100%)	66 (100%)	0	100	100
5	6B	73/73 (100%)	73 (100%)	0	100	100
6	6C	57/57 (100%)	57 (100%)	0	100	100
7	7A	48/48 (100%)	47 (98%)	1 (2%)	47	74
8	7B	39/39 (100%)	39 (100%)	0	100	100
9	7C	40/40 (100%)	40 (100%)	0	100	100
10	8B	37/37 (100%)	37 (100%)	0	100	100
11	A1	58/58 (100%)	58 (100%)	0	100	100
12	A2	76/76 (100%)	75 (99%)	1 (1%)	61	80
13	A3	69/69 (100%)	68 (99%)	1 (1%)	59	79
14	A5	99/99 (100%)	99 (100%)	0	100	100
15	A6	107/107 (100%)	106 (99%)	1 (1%)	70	84
16	A7	87/97 (90%)	84 (97%)	3 (3%)	32	64
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	289/295 (98%)	287 (99%)	2 (1%)	76	85
19	AB	71/132 (54%)	71 (100%)	0	100	100
19	AC	80/132 (61%)	79 (99%)	1 (1%)	61	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AK	283/283 (100%)	278 (98%)	5 (2%)	51	76
21	AL	101/101 (100%)	100 (99%)	1 (1%)	68	83
22	AM	130/130 (100%)	129 (99%)	1 (1%)	73	85
23	AN	123/123 (100%)	123 (100%)	0	100	100
24	B1	53/53 (100%)	53 (100%)	0	100	100
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	62/62 (100%)	62 (100%)	0	100	100
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	99/119 (83%)	98 (99%)	1 (1%)	68	83
30	B7	112/112 (100%)	112 (100%)	0	100	100
31	B8	141/141 (100%)	141 (100%)	0	100	100
32	B9	159/159 (100%)	159 (100%)	0	100	100
33	BK	155/156 (99%)	155 (100%)	0	100	100
34	BL	91/94 (97%)	90 (99%)	1 (1%)	65	82
35	C1	425/425 (100%)	423 (100%)	2 (0%)	81	88
36	C2	212/212 (100%)	208 (98%)	4 (2%)	50	75
37	C3	224/225 (100%)	222 (99%)	2 (1%)	70	84
38	C4	123/123 (100%)	123 (100%)	0	100	100
39	CA	45/45 (100%)	45 (100%)	0	100	100
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	267/275 (97%)	262 (98%)	5 (2%)	50	75
42	N2	311/311 (100%)	310 (100%)	1 (0%)	86	90
43	N3	85/99 (86%)	84 (99%)	1 (1%)	63	81
44	N4	410/410 (100%)	409 (100%)	1 (0%)	87	91
45	N5	537/537 (100%)	534 (99%)	3 (1%)	78	87
46	N6	130/140 (93%)	127 (98%)	3 (2%)	44	72
47	QA	329/330 (100%)	329 (100%)	0	100	100
47	Qa	330/330 (100%)	330 (100%)	0	100	100
48	QB	372/372 (100%)	370 (100%)	2 (0%)	81	88
48	Qb	362/372 (97%)	360 (99%)	2 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	QC	332/332 (100%)	331 (100%)	1 (0%)	86	90
49	Qc	332/332 (100%)	330 (99%)	2 (1%)	78	87
50	QD	206/206 (100%)	206 (100%)	0	100	100
50	Qd	204/206 (99%)	203 (100%)	1 (0%)	81	88
51	QE	166/225 (74%)	165 (99%)	1 (1%)	78	87
51	QK	55/225 (24%)	53 (96%)	2 (4%)	31	64
51	Qe	166/225 (74%)	165 (99%)	1 (1%)	78	87
52	QF	64/64 (100%)	64 (100%)	0	100	100
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	93 (100%)	0	100	100
53	Qg	93/93 (100%)	92 (99%)	1 (1%)	65	82
54	QH	70/72 (97%)	69 (99%)	1 (1%)	59	79
54	Qh	70/72 (97%)	70 (100%)	0	100	100
55	QI	50/51 (98%)	50 (100%)	0	100	100
55	Qi	49/51 (96%)	49 (100%)	0	100	100
56	QJ	40/42 (95%)	40 (100%)	0	100	100
56	Qj	41/42 (98%)	41 (100%)	0	100	100
57	S1	579/579 (100%)	575 (99%)	4 (1%)	76	85
58	S2	365/370 (99%)	358 (98%)	7 (2%)	50	75
59	S3	190/190 (100%)	188 (99%)	2 (1%)	65	82
60	S4	112/112 (100%)	108 (96%)	4 (4%)	31	64
61	S5	93/93 (100%)	93 (100%)	0	100	100
62	S6	79/79 (100%)	79 (100%)	0	100	100
63	S7	132/132 (100%)	130 (98%)	2 (2%)	57	79
64	S8	151/151 (100%)	151 (100%)	0	100	100
65	V1	343/344 (100%)	336 (98%)	7 (2%)	48	75
66	V2	183/183 (100%)	181 (99%)	2 (1%)	65	82
67	V3	41/41 (100%)	40 (98%)	1 (2%)	43	72
All	All	12138/12644 (96%)	12051 (99%)	87 (1%)	73	85

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	Qg	83	LYS
60	S4	53	ILE
57	S1	636	TYR
58	S2	204	THR
63	S7	67	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 267 such sidechains are listed below:

Mol	Chain	Res	Type
57	S1	498	GLN
58	S2	153	ASN
66	V2	153	GLN
37	C3	204	HIS
37	C3	133	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
58	2MR	S2	124	58	10,12,13	2.50	2 (20%)	5,13,15	1.07	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
58	2MR	S2	124	58	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	S2	124	2MR	CZ-NH2	5.29	1.44	1.33
58	S2	124	2MR	CZ-NE	5.23	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	S2	124	2MR	NE-CD-CG-CB
58	S2	124	2MR	CA-CB-CG-CD
58	S2	124	2MR	CG-CD-NE-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	S2	124	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 127 ligands modelled in this entry, 7 are monoatomic - leaving 120 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
80	HEM	QC	402	49	50,50,50	1.32	6 (12%)	67,82,82	1.59	13 (19%)
70	PC1	N6	201	-	53,53,53	0.30	0	59,61,61	0.41	0
71	PEE	Qc	403	-	41,41,50	1.30	4 (9%)	44,46,55	1.18	2 (4%)
84	SF4	S8	302	64	0,12,12	-	-	-	-	-
70	PC1	Qc	407	-	53,53,53	0.29	0	59,61,61	0.31	0
70	PC1	C3	304	-	50,50,53	0.30	0	56,58,61	0.30	0
70	PC1	Qd	402	-	53,53,53	0.28	0	59,61,61	0.31	0
76	PLX	N3	201	-	51,51,51	1.14	4 (7%)	53,59,59	0.89	1 (1%)
82	FES	V2	301	66	0,4,4	-	-	-	-	-
85	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.39	0
70	PC1	QB	503	-	31,31,53	0.37	0	37,39,61	0.37	0
70	PC1	N5	705	-	30,30,53	0.37	0	36,38,61	0.42	0
71	PEE	Qh	101	-	50,50,50	1.35	5 (10%)	53,55,55	1.17	5 (9%)
70	PC1	B5	202	-	53,53,53	0.29	0	59,61,61	0.29	0
68	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.31	0
70	PC1	C1	606	-	45,45,53	0.31	0	51,53,61	0.38	0
68	CDL	AN	201	-	80,80,99	0.33	0	86,92,111	0.34	0
71	PEE	AN	202	-	50,50,50	1.35	5 (10%)	53,55,55	1.17	5 (9%)
68	CDL	AL	204	-	79,79,99	0.33	0	85,91,111	0.41	1 (1%)
68	CDL	Qh	102	-	99,99,99	0.30	0	105,111,111	0.29	0
68	CDL	Qc	402	-	60,60,99	0.38	0	66,72,111	0.36	0
70	PC1	C3	301	-	48,48,53	0.31	0	54,56,61	0.35	0
68	CDL	N5	703	-	99,99,99	0.30	0	105,111,111	0.29	0
72	3PE	7B	101	-	50,50,50	0.30	0	53,55,55	0.33	0
71	PEE	Qe	302	-	49,49,50	1.35	5 (10%)	52,54,55	1.21	6 (11%)
75	ADP	AK	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
77	HEA	C1	603	35	67,67,67	2.27	26 (38%)	81,103,103	2.46	29 (35%)
76	PLX	CB	201	-	51,51,51	1.15	4 (7%)	53,59,59	0.86	1 (1%)
74	ZMP	AC	201	19	30,35,36	0.70	1 (3%)	34,42,45	0.74	0
84	SF4	V1	501	65	0,12,12	-	-	-	-	-
70	PC1	C1	610	-	49,49,53	0.31	0	55,57,61	0.33	0
82	FES	Qe	301	51	0,4,4	-	-	-	-	-
71	PEE	Qb	503	-	50,50,50	1.34	5 (10%)	53,55,55	1.11	4 (7%)
72	3PE	C1	601	-	50,50,50	0.30	0	53,55,55	0.30	0
71	PEE	N5	706	-	43,43,50	1.43	5 (11%)	46,48,55	1.20	3 (6%)
72	3PE	CA	101	-	50,50,50	0.30	0	53,55,55	0.40	0
83	PX2	QH	101	-	35,35,35	0.98	4 (11%)	38,40,40	1.05	2 (5%)
70	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.33	0
73	NDP	A9	401	-	51,52,52	0.33	0	71,80,80	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	PLX	AM	201	-	51,51,51	1.15	5 (9%)	53,59,59	0.87	1 (1%)
68	CDL	QD	402	-	63,63,99	0.37	0	69,75,111	0.31	0
68	CDL	Qb	502	-	63,63,99	0.37	0	69,75,111	0.42	0
68	CDL	N5	702	-	88,88,99	0.32	0	94,100,111	0.34	0
71	PEE	QC	403	-	39,39,50	1.33	4 (10%)	42,44,55	1.20	2 (4%)
80	HEM	QC	401	49	50,50,50	1.30	7 (14%)	67,82,82	1.59	11 (16%)
70	PC1	Qc	409	-	41,41,53	0.32	0	47,49,61	0.31	0
76	PLX	BL	202	-	51,51,51	1.15	6 (11%)	53,59,59	0.88	1 (1%)
68	CDL	Qj	101	-	95,95,99	0.31	0	101,107,111	0.37	0
76	PLX	B1	101	-	51,51,51	1.15	4 (7%)	53,59,59	0.91	1 (1%)
68	CDL	QC	407	-	54,54,99	0.39	0	60,66,111	0.37	0
70	PC1	QI	101	-	53,53,53	0.29	0	59,61,61	0.30	0
71	PEE	QE	302	-	46,46,50	1.39	5 (10%)	49,51,55	1.25	5 (10%)
70	PC1	C4	201	-	53,53,53	0.29	0	59,61,61	0.37	0
71	PEE	C1	609	-	32,32,50	1.42	4 (12%)	35,37,55	1.29	4 (11%)
76	PLX	C2	301	-	38,38,51	1.25	5 (13%)	40,46,59	0.88	1 (2%)
71	PEE	QC	404	-	34,34,50	1.43	5 (14%)	37,39,55	1.32	4 (10%)
71	PEE	AL	203	-	35,35,50	1.38	4 (11%)	38,40,55	1.09	3 (7%)
84	SF4	S8	301	64	0,12,12	-	-	-	-	-
71	PEE	N5	704	-	50,50,50	1.33	5 (10%)	53,55,55	1.18	6 (11%)
76	PLX	QE	301	-	45,45,51	1.20	6 (13%)	47,53,59	0.90	1 (2%)
70	PC1	Qc	410	-	47,47,53	0.31	0	53,55,61	0.34	0
81	HEC	QD	401	50	46,50,50	1.91	9 (19%)	58,82,82	1.85	7 (12%)
68	CDL	B4	201	-	61,61,99	0.37	0	67,73,111	0.37	0
70	PC1	Qh	103	-	53,53,53	0.28	0	59,61,61	0.28	0
68	CDL	AL	201	-	93,93,99	0.30	0	99,105,111	0.27	0
68	CDL	QC	406	-	89,89,99	0.32	0	95,101,111	0.35	0
82	FES	QE	303	51	0,4,4	-	-	-	-	-
70	PC1	7A	101	-	53,53,53	0.30	0	59,61,61	0.44	0
70	PC1	B7	201	-	53,53,53	0.29	0	59,61,61	0.32	0
84	SF4	S1	802	57	0,12,12	-	-	-	-	-
80	HEM	Qc	404	49	50,50,50	1.30	7 (14%)	67,82,82	1.58	10 (14%)
71	PEE	QC	405	-	42,42,50	1.44	5 (11%)	45,47,55	1.21	3 (6%)
74	ZMP	AB	201	19	30,35,36	0.70	1 (3%)	34,42,45	0.80	1 (2%)
70	PC1	C1	608	-	47,47,53	0.30	0	53,55,61	0.32	0
70	PC1	QJ	101	-	53,53,53	0.29	0	59,61,61	0.30	0
70	PC1	Qc	412	-	53,53,53	0.29	0	59,61,61	0.43	0
82	FES	S1	803	57	0,4,4	-	-	-	-	-
80	HEM	Qc	405	49	50,50,50	1.31	5 (10%)	67,82,82	1.58	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	CDL	4L	101	-	91,91,99	0.31	0	97,103,111	0.29	0
76	PLX	S7	302	-	51,51,51	1.14	5 (9%)	53,59,59	0.93	1 (1%)
70	PC1	B8	201	-	53,53,53	0.29	0	59,61,61	0.28	0
84	SF4	S1	801	57	0,12,12	-	-	-	-	-
71	PEE	BL	201	-	50,50,50	1.34	5 (10%)	53,55,55	1.19	4 (7%)
71	PEE	8B	101	-	41,41,50	1.31	5 (12%)	44,46,55	1.24	4 (9%)
70	PC1	S8	304	-	44,44,53	0.32	0	50,52,61	0.36	0
71	PEE	S8	303	-	50,50,50	1.33	5 (10%)	53,55,55	1.16	5 (9%)
70	PC1	QB	502	-	50,50,53	0.30	0	56,58,61	0.44	0
71	PEE	N5	701	-	45,45,50	1.40	5 (11%)	48,50,55	1.21	5 (10%)
77	HEA	C1	602	35	67,67,67	2.24	26 (38%)	81,103,103	2.43	27 (33%)
68	CDL	A7	201	-	93,93,99	0.30	0	99,105,111	0.31	0
71	PEE	C3	302	-	50,50,50	1.34	5 (10%)	53,55,55	1.11	4 (7%)
71	PEE	A7	202	-	27,27,50	1.36	3 (11%)	30,32,55	1.17	2 (6%)
71	PEE	AL	206	-	39,39,50	1.51	6 (15%)	42,44,55	1.30	5 (11%)
71	PEE	C3	303	-	50,50,50	1.35	6 (12%)	53,55,55	1.20	4 (7%)
70	PC1	N3	202	-	53,53,53	0.29	0	59,61,61	0.36	0
81	HEC	Qd	401	50	46,50,50	1.91	9 (19%)	58,82,82	1.82	6 (10%)
71	PEE	QH	102	-	50,50,50	1.35	5 (10%)	53,55,55	1.18	5 (9%)
72	3PE	Qc	406	-	47,47,50	0.31	0	50,52,55	0.38	0
72	3PE	CB	202	-	45,45,50	0.31	0	48,50,55	0.33	0
68	CDL	B5	201	-	95,95,99	0.30	0	101,107,111	0.34	0
68	CDL	AN	203	-	65,65,99	0.36	0	71,77,111	0.39	0
68	CDL	Qc	411	-	63,63,99	0.37	0	69,75,111	0.37	0
68	CDL	C1	607	-	76,76,99	0.33	0	82,88,111	0.32	0
68	CDL	QB	501	-	63,63,99	0.37	0	69,75,111	0.40	0
72	3PE	Qc	401	-	43,43,50	0.32	0	46,48,55	0.32	0
70	PC1	N4	502	-	53,53,53	0.29	0	59,61,61	0.33	0
68	CDL	AL	202	-	81,81,99	0.32	0	87,93,111	0.42	0
71	PEE	Qc	408	-	47,47,50	1.38	5 (10%)	50,52,55	1.17	6 (12%)
76	PLX	AL	205	-	46,46,51	1.19	5 (10%)	48,54,59	0.91	1 (2%)
71	PEE	CB	203	-	36,36,50	1.39	5 (13%)	39,41,55	1.20	4 (10%)
68	CDL	N4	501	-	99,99,99	0.30	0	105,111,111	0.28	0
71	PEE	6A	103	-	50,50,50	1.34	6 (12%)	53,55,55	1.16	4 (7%)
70	PC1	Qb	501	-	37,37,53	0.35	0	43,45,61	0.34	0
76	PLX	QI	102	-	51,51,51	1.14	6 (11%)	53,59,59	0.88	1 (1%)
70	PC1	N1	401	-	53,53,53	0.28	0	59,61,61	0.31	0
71	PEE	A3	201	-	50,50,50	1.34	5 (10%)	53,55,55	1.15	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	PEE	6A	102	-	50,50,50	1.35	5 (10%)	53,55,55	1.15	6 (11%)
70	PC1	7C	101	-	41,41,53	0.32	0	47,49,61	0.38	0
84	SF4	S7	301	63	0,12,12	-	-	-	-	-
68	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	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
80	HEM	QC	402	49	-	6/14/54/54	-
70	PC1	N6	201	-	-	23/57/57/57	-
71	PEE	Qc	403	-	-	21/45/45/54	-
84	SF4	S8	302	64	-	-	0/6/5/5
70	PC1	Qc	407	-	-	21/57/57/57	-
70	PC1	C3	304	-	-	11/54/54/57	-
70	PC1	Qd	402	-	-	12/57/57/57	-
76	PLX	N3	201	-	-	20/55/55/55	-
82	FES	V2	301	66	-	-	0/1/1/1
85	FMN	V1	502	-	-	5/18/18/18	0/3/3/3
70	PC1	QB	503	-	-	16/35/35/57	-
70	PC1	N5	705	-	-	10/34/34/57	-
71	PEE	Qh	101	-	-	33/54/54/54	-
70	PC1	B5	202	-	-	17/57/57/57	-
68	CDL	A8	301	-	-	23/93/93/110	-
70	PC1	C1	606	-	-	15/49/49/57	-
68	CDL	AN	201	-	-	24/91/91/110	-
71	PEE	AN	202	-	-	37/54/54/54	-
68	CDL	AL	204	-	-	24/90/90/110	-
68	CDL	Qh	102	-	-	27/110/110/110	-
68	CDL	Qc	402	-	-	16/71/71/110	-
70	PC1	C3	301	-	-	14/52/52/57	-
68	CDL	N5	703	-	-	24/110/110/110	-
72	3PE	7B	101	-	-	15/54/54/54	-
71	PEE	Qe	302	-	-	30/53/53/54	-
75	ADP	AK	401	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEA	C1	603	35	-	14/36/76/76	-
76	PLX	CB	201	-	-	25/55/55/55	-
74	ZMP	AC	201	19	-	19/40/42/43	-
84	SF4	V1	501	65	-	-	0/6/5/5
70	PC1	C1	610	-	-	10/53/53/57	-
82	FES	Qe	301	51	-	-	0/1/1/1
71	PEE	Qb	503	-	-	30/54/54/54	-
72	3PE	C1	601	-	-	9/54/54/54	-
71	PEE	N5	706	-	-	18/47/47/54	-
72	3PE	CA	101	-	-	11/54/54/54	-
83	PX2	QH	101	-	-	25/37/37/37	-
70	PC1	6A	101	-	-	13/48/48/57	-
73	NDP	A9	401	-	-	4/34/77/77	0/5/5/5
76	PLX	AM	201	-	-	14/55/55/55	-
68	CDL	QD	402	-	-	19/74/74/110	-
68	CDL	Qb	502	-	-	10/74/74/110	-
68	CDL	N5	702	-	-	26/99/99/110	-
71	PEE	QC	403	-	-	14/43/43/54	-
80	HEM	QC	401	49	-	7/14/54/54	-
70	PC1	Qc	409	-	-	10/45/45/57	-
76	PLX	BL	202	-	-	24/55/55/55	-
68	CDL	Qj	101	-	-	29/106/106/110	-
76	PLX	B1	101	-	-	16/55/55/55	-
68	CDL	QC	407	-	-	8/65/65/110	-
70	PC1	QI	101	-	-	17/57/57/57	-
71	PEE	QE	302	-	-	20/50/50/54	-
70	PC1	C4	201	-	-	15/57/57/57	-
71	PEE	C1	609	-	-	23/36/36/54	-
76	PLX	C2	301	-	-	17/42/42/55	-
71	PEE	QC	404	-	-	21/38/38/54	-
71	PEE	AL	203	-	-	24/39/39/54	-
84	SF4	S8	301	64	-	-	0/6/5/5
71	PEE	N5	704	-	-	25/54/54/54	-
76	PLX	QE	301	-	-	16/49/49/55	-
70	PC1	Qc	410	-	-	13/51/51/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	HEC	QD	401	50	-	8/14/54/54	-
68	CDL	B4	201	-	-	17/72/72/110	-
70	PC1	Qh	103	-	-	13/57/57/57	-
68	CDL	AL	201	-	-	20/104/104/110	-
68	CDL	QC	406	-	-	30/100/100/110	-
82	FES	QE	303	51	-	-	0/1/1/1
70	PC1	7A	101	-	-	22/57/57/57	-
70	PC1	B7	201	-	-	23/57/57/57	-
84	SF4	S1	802	57	-	-	0/6/5/5
80	HEM	Qc	404	49	-	7/14/54/54	-
71	PEE	QC	405	-	-	27/46/46/54	-
74	ZMP	AB	201	19	-	13/40/42/43	-
70	PC1	C1	608	-	-	14/51/51/57	-
70	PC1	QJ	101	-	-	10/57/57/57	-
70	PC1	Qc	412	-	-	13/57/57/57	-
82	FES	S1	803	57	-	-	0/1/1/1
80	HEM	Qc	405	49	-	11/14/54/54	-
68	CDL	4L	101	-	-	20/102/102/110	-
76	PLX	S7	302	-	-	20/55/55/55	-
70	PC1	B8	201	-	-	16/57/57/57	-
84	SF4	S1	801	57	-	-	0/6/5/5
71	PEE	BL	201	-	-	26/54/54/54	-
71	PEE	8B	101	-	-	23/45/45/54	-
70	PC1	S8	304	-	-	9/48/48/57	-
71	PEE	S8	303	-	-	22/54/54/54	-
70	PC1	QB	502	-	-	19/54/54/57	-
71	PEE	N5	701	-	-	18/49/49/54	-
77	HEA	C1	602	35	-	16/36/76/76	-
68	CDL	A7	201	-	-	26/104/104/110	-
71	PEE	C3	302	-	-	25/54/54/54	-
71	PEE	A7	202	-	-	10/31/31/54	-
71	PEE	AL	206	-	-	22/43/43/54	-
71	PEE	C3	303	-	-	23/54/54/54	-
70	PC1	N3	202	-	-	13/57/57/57	-
81	HEC	Qd	401	50	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PEE	QH	102	-	-	27/54/54/54	-
72	3PE	Qc	406	-	-	14/51/51/54	-
72	3PE	CB	202	-	-	11/49/49/54	-
68	CDL	B5	201	-	-	15/106/106/110	-
68	CDL	AN	203	-	-	27/76/76/110	-
68	CDL	Qc	411	-	-	15/74/74/110	-
68	CDL	C1	607	-	-	20/87/87/110	-
68	CDL	QB	501	-	-	23/74/74/110	-
72	3PE	Qc	401	-	-	11/47/47/54	-
70	PC1	N4	502	-	-	18/57/57/57	-
68	CDL	AL	202	-	-	20/92/92/110	-
71	PEE	Qc	408	-	-	24/51/51/54	-
76	PLX	AL	205	-	-	20/50/50/55	-
71	PEE	CB	203	-	-	26/40/40/54	-
68	CDL	N4	501	-	-	24/110/110/110	-
71	PEE	6A	103	-	-	29/54/54/54	-
70	PC1	Qb	501	-	-	11/41/41/57	-
76	PLX	QI	102	-	-	22/55/55/55	-
70	PC1	N1	401	-	-	20/57/57/57	-
71	PEE	A3	201	-	-	25/54/54/54	-
71	PEE	6A	102	-	-	28/54/54/54	-
70	PC1	7C	101	-	-	8/45/45/57	-
84	SF4	S7	301	63	-	-	0/6/5/5
68	CDL	N2	401	-	-	15/78/78/110	-

The worst 5 of 287 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	QD	401	HEC	CAC-C3C	7.15	1.58	1.35
81	Qd	401	HEC	CAC-C3C	7.14	1.58	1.35
81	Qd	401	HEC	CAB-C3B	6.78	1.57	1.35
81	QD	401	HEC	CAB-C3B	6.67	1.56	1.35
77	C1	603	HEA	FE-ND	5.05	2.10	1.94

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	QD	401	HEC	CBB-CAB-C3B	-8.80	109.84	127.43
81	Qd	401	HEC	CBB-CAB-C3B	-8.53	110.39	127.43
81	QD	401	HEC	CBC-CAC-C3C	-6.89	113.66	127.43
77	C1	603	HEA	CAD-CBD-CGD	-6.80	95.62	113.67
81	Qd	401	HEC	CBC-CAC-C3C	-6.67	114.10	127.43

There are no chirality outliers.

5 of 1990 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	4L	101	CDL	CA2-OA2-PA1-OA3
68	4L	101	CDL	CA2-OA2-PA1-OA4
68	4L	101	CDL	CA2-OA2-PA1-OA5
68	4L	101	CDL	CA3-OA5-PA1-OA2
68	4L	101	CDL	CB3-OB5-PB2-OB2

There are no ring outliers.

110 monomers are involved in 409 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	QC	402	HEM	6	0
70	N6	201	PC1	8	0
71	Qc	403	PEE	1	0
84	S8	302	SF4	2	0
70	Qc	407	PC1	4	0
70	C3	304	PC1	1	0
70	Qd	402	PC1	3	0
76	N3	201	PLX	3	0
85	V1	502	FMN	2	0
70	QB	503	PC1	6	0
70	N5	705	PC1	2	0
71	Qh	101	PEE	3	0
68	A8	301	CDL	7	0
68	AN	201	CDL	3	0
71	AN	202	PEE	5	0
68	AL	204	CDL	5	0
68	Qh	102	CDL	2	0
68	Qc	402	CDL	1	0
70	C3	301	PC1	6	0
68	N5	703	CDL	5	0
72	7B	101	3PE	5	0
71	Qe	302	PEE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	AK	401	ADP	3	0
77	C1	603	HEA	8	0
76	CB	201	PLX	4	0
74	AC	201	ZMP	5	0
70	C1	610	PC1	9	0
82	Qe	301	FES	2	0
71	Qb	503	PEE	1	0
72	C1	601	3PE	4	0
71	N5	706	PEE	1	0
72	CA	101	3PE	4	0
83	QH	101	PX2	1	0
70	6A	101	PC1	13	0
73	A9	401	NDP	2	0
76	AM	201	PLX	3	0
68	QD	402	CDL	2	0
68	Qb	502	CDL	4	0
68	N5	702	CDL	7	0
71	QC	403	PEE	5	0
80	QC	401	HEM	2	0
70	Qc	409	PC1	2	0
76	BL	202	PLX	6	0
68	Qj	101	CDL	4	0
76	B1	101	PLX	1	0
68	QC	407	CDL	2	0
70	QI	101	PC1	3	0
71	QE	302	PEE	4	0
70	C4	201	PC1	1	0
71	C1	609	PEE	3	0
76	C2	301	PLX	4	0
71	QC	404	PEE	1	0
71	N5	704	PEE	6	0
76	QE	301	PLX	3	0
70	Qc	410	PC1	4	0
81	QD	401	HEC	1	0
68	B4	201	CDL	3	0
70	Qh	103	PC1	5	0
68	AL	201	CDL	3	0
68	QC	406	CDL	2	0
82	QE	303	FES	2	0
70	7A	101	PC1	2	0
70	B7	201	PC1	1	0
84	S1	802	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	Qc	404	HEM	2	0
71	QC	405	PEE	6	0
74	AB	201	ZMP	2	0
70	C1	608	PC1	7	0
70	QJ	101	PC1	4	0
70	Qc	412	PC1	3	0
82	S1	803	FES	1	0
80	Qc	405	HEM	8	0
68	4L	101	CDL	3	0
76	S7	302	PLX	9	0
70	B8	201	PC1	1	0
71	BL	201	PEE	1	0
71	8B	101	PEE	3	0
70	S8	304	PC1	10	0
71	S8	303	PEE	1	0
70	QB	502	PC1	11	0
71	N5	701	PEE	9	0
77	C1	602	HEA	11	0
68	A7	201	CDL	5	0
71	C3	302	PEE	6	0
71	A7	202	PEE	1	0
71	C3	303	PEE	1	0
70	N3	202	PC1	3	0
81	Qd	401	HEC	3	0
71	QH	102	PEE	4	0
72	Qc	406	3PE	1	0
68	B5	201	CDL	7	0
68	AN	203	CDL	7	0
68	Qc	411	CDL	7	0
68	C1	607	CDL	5	0
68	QB	501	CDL	10	0
72	Qc	401	3PE	2	0
70	N4	502	PC1	11	0
68	AL	202	CDL	6	0
71	Qc	408	PEE	5	0
76	AL	205	PLX	4	0
71	CB	203	PEE	3	0
68	N4	501	CDL	10	0
71	6A	103	PEE	4	0
70	Qb	501	PC1	5	0
76	QI	102	PLX	5	0
70	N1	401	PC1	7	0

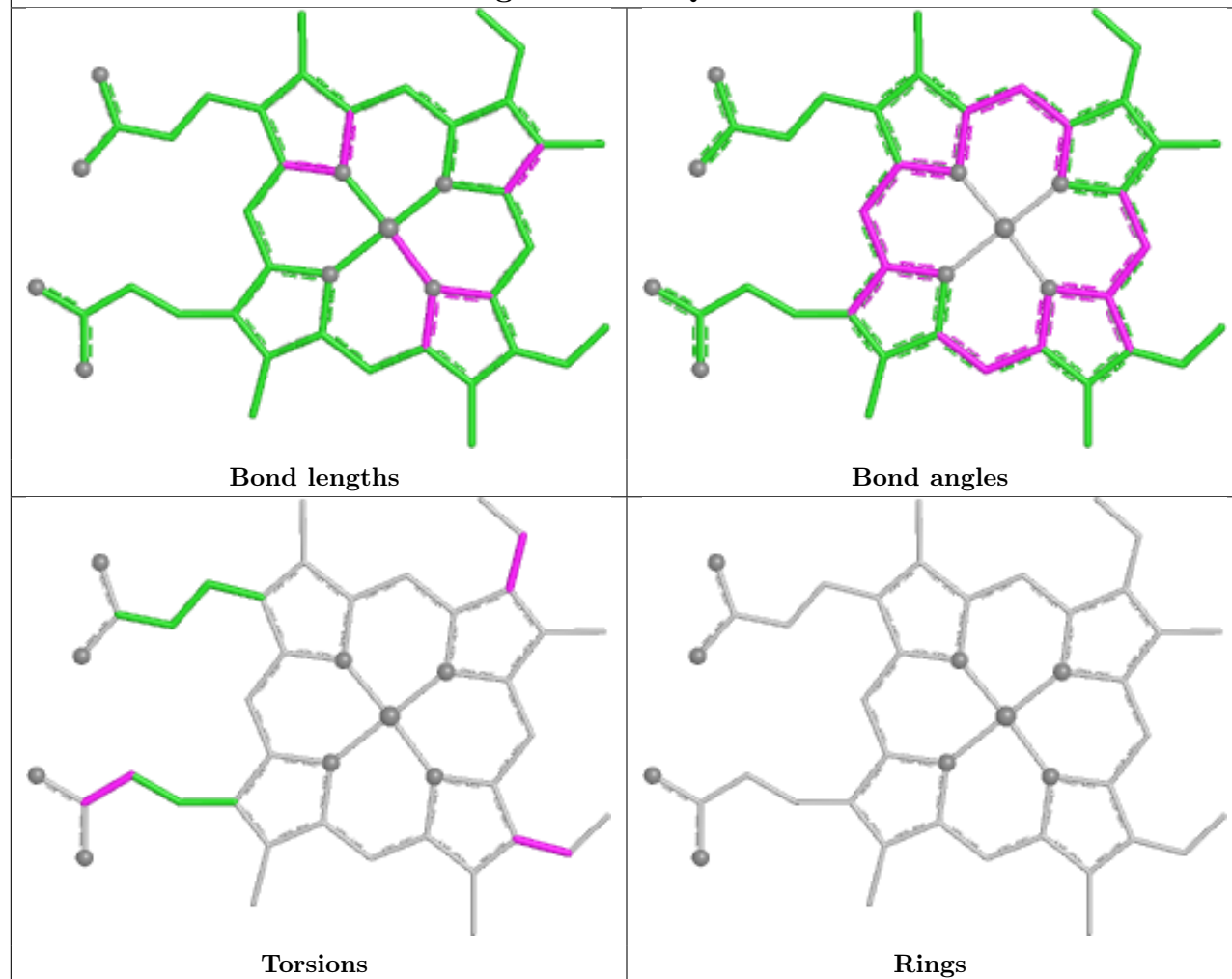
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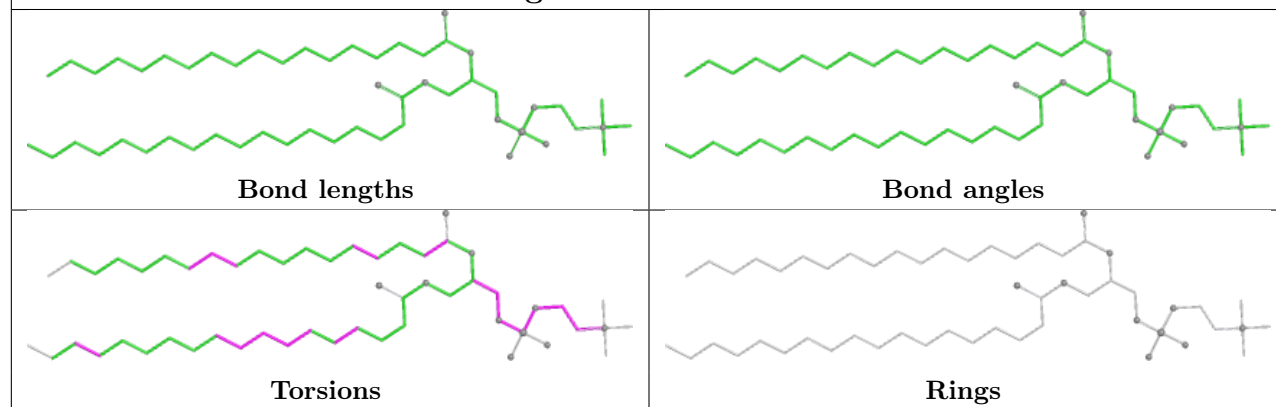
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	A3	201	PEE	4	0
71	6A	102	PEE	3	0
70	7C	101	PC1	6	0
68	N2	401	CDL	1	0

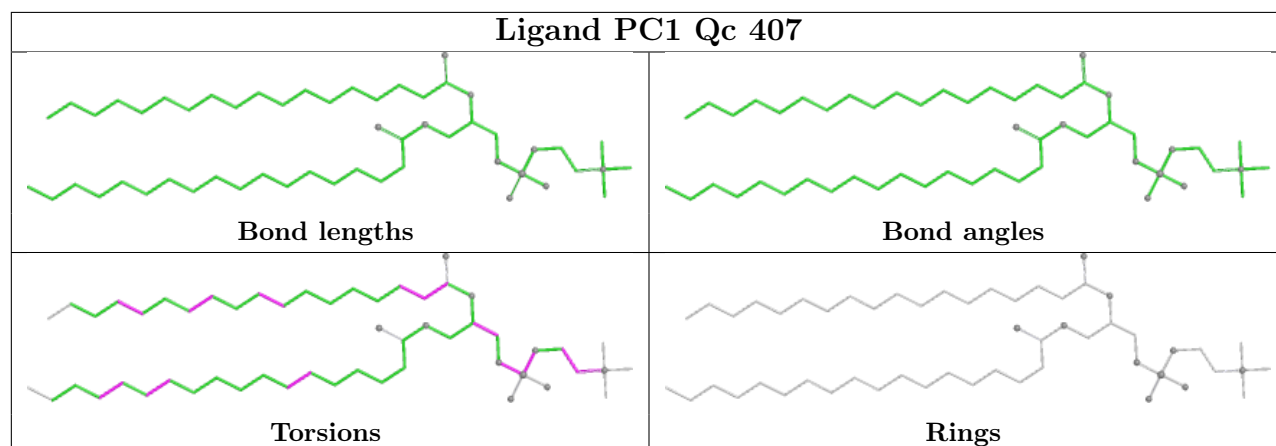
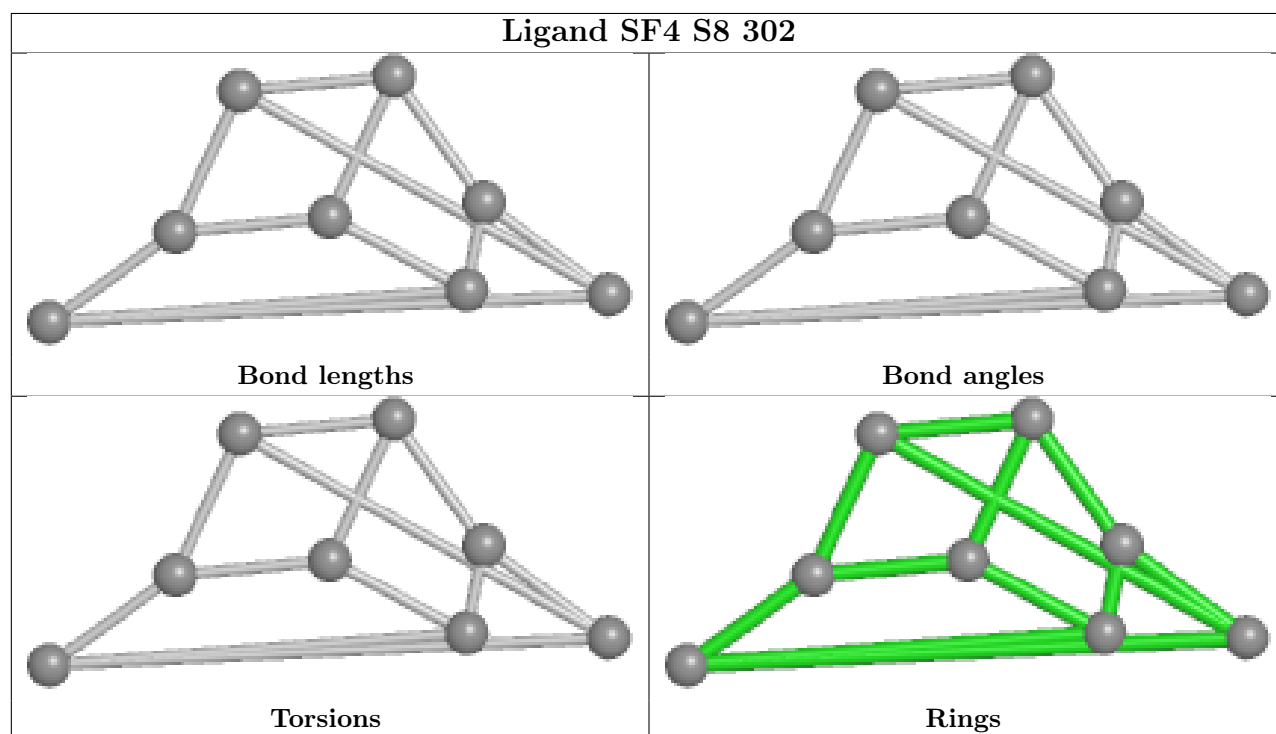
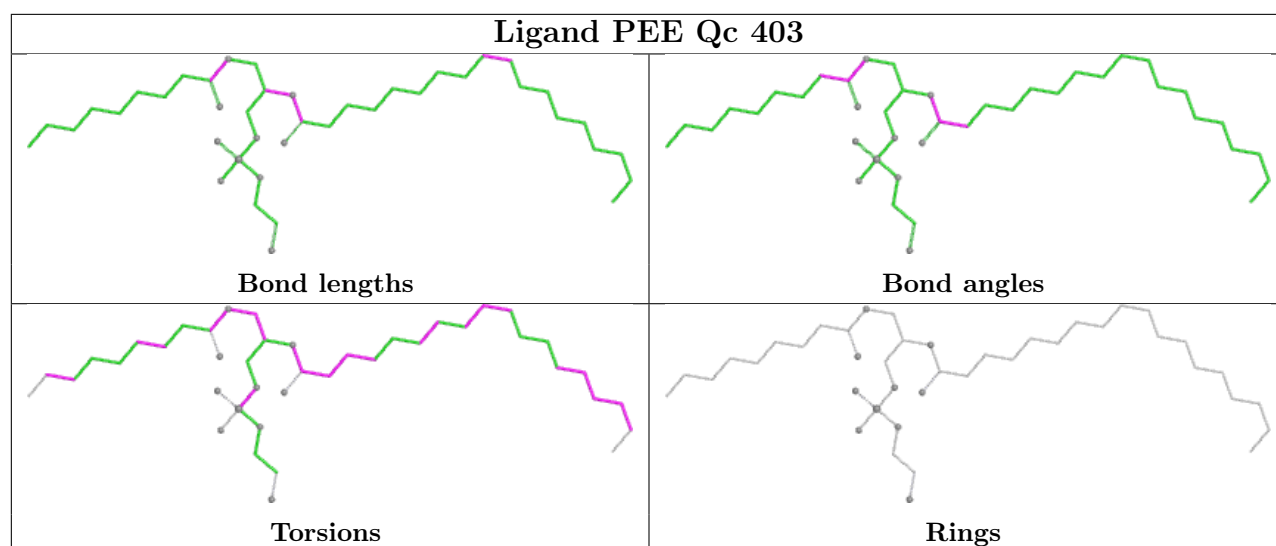
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

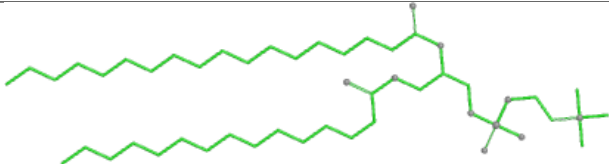
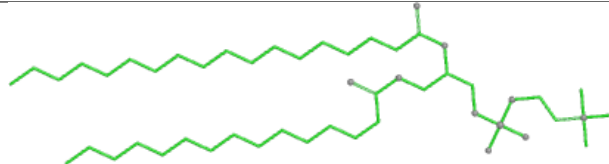
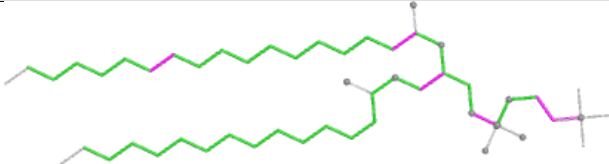
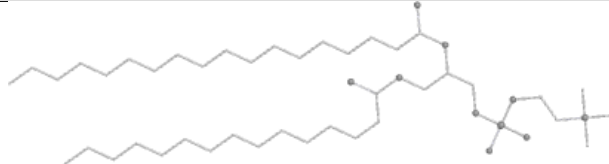
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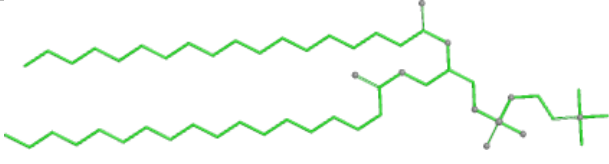
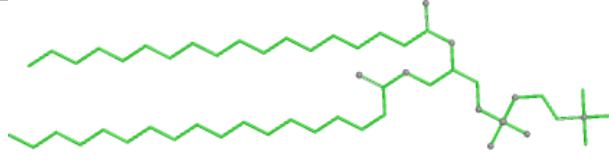
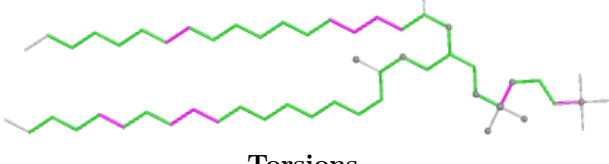
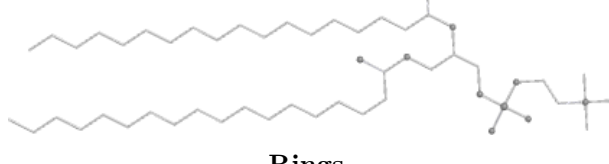


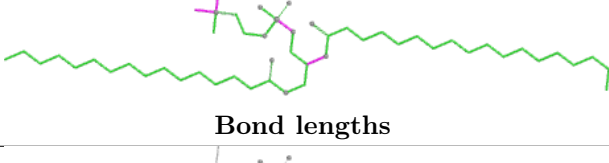
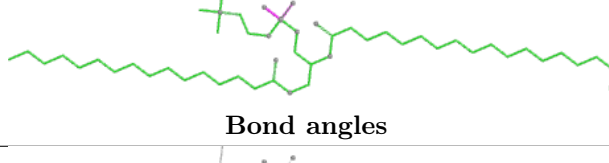
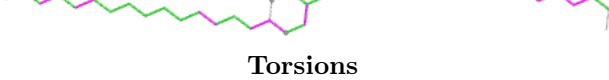
Ligand PC1 N6 201

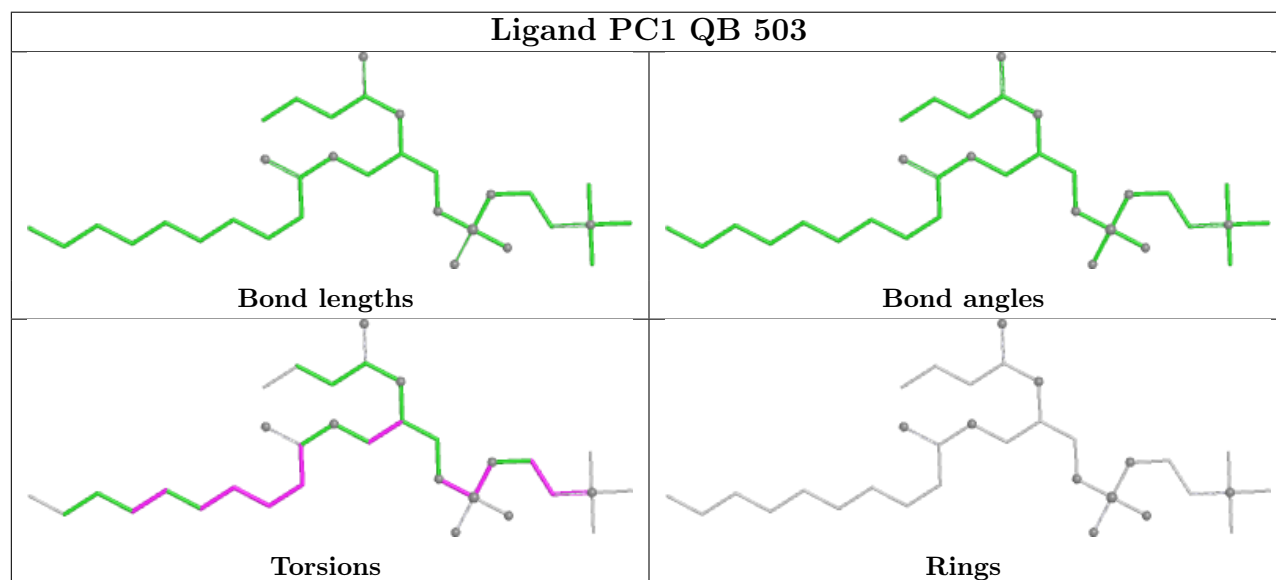
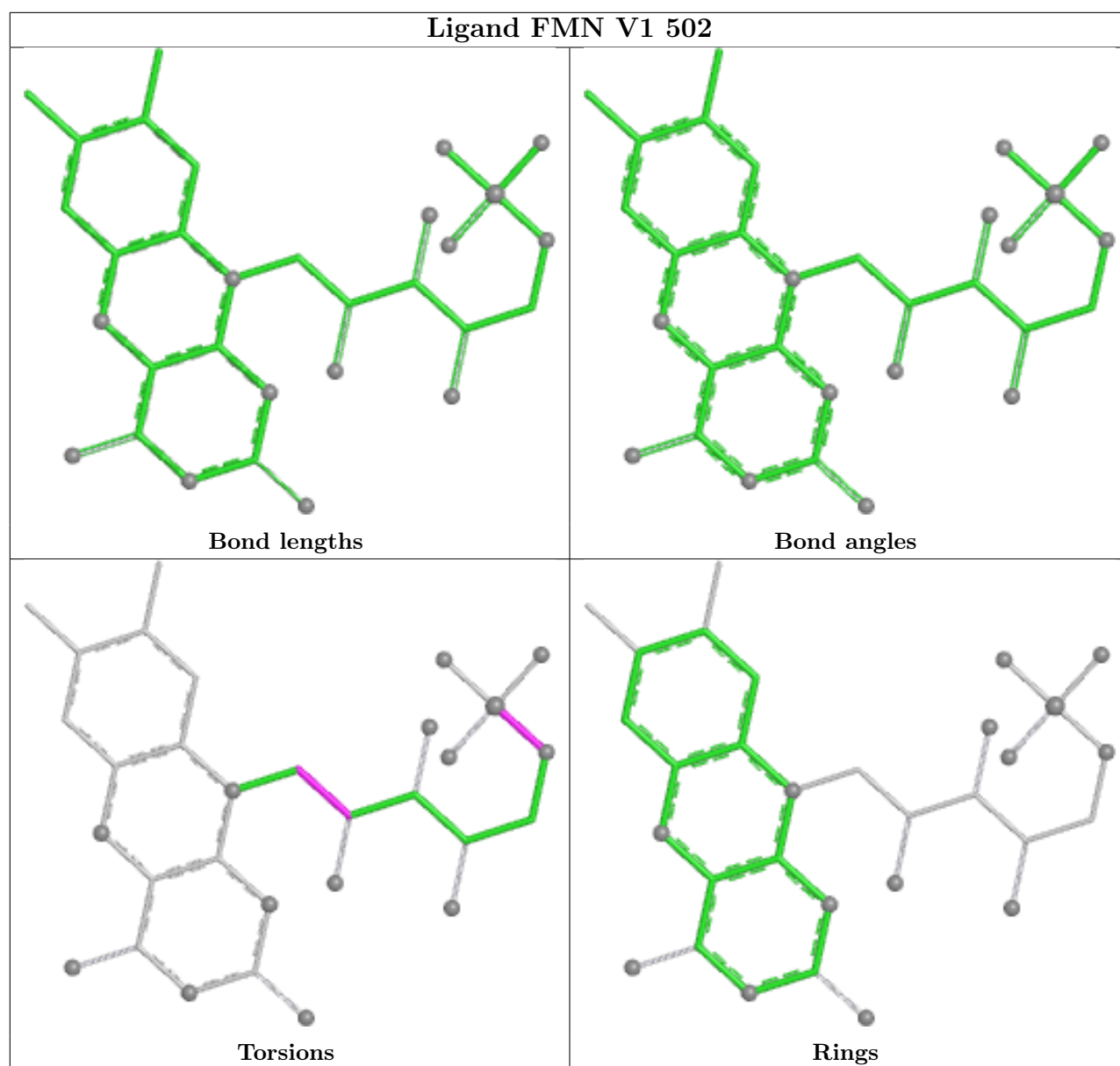


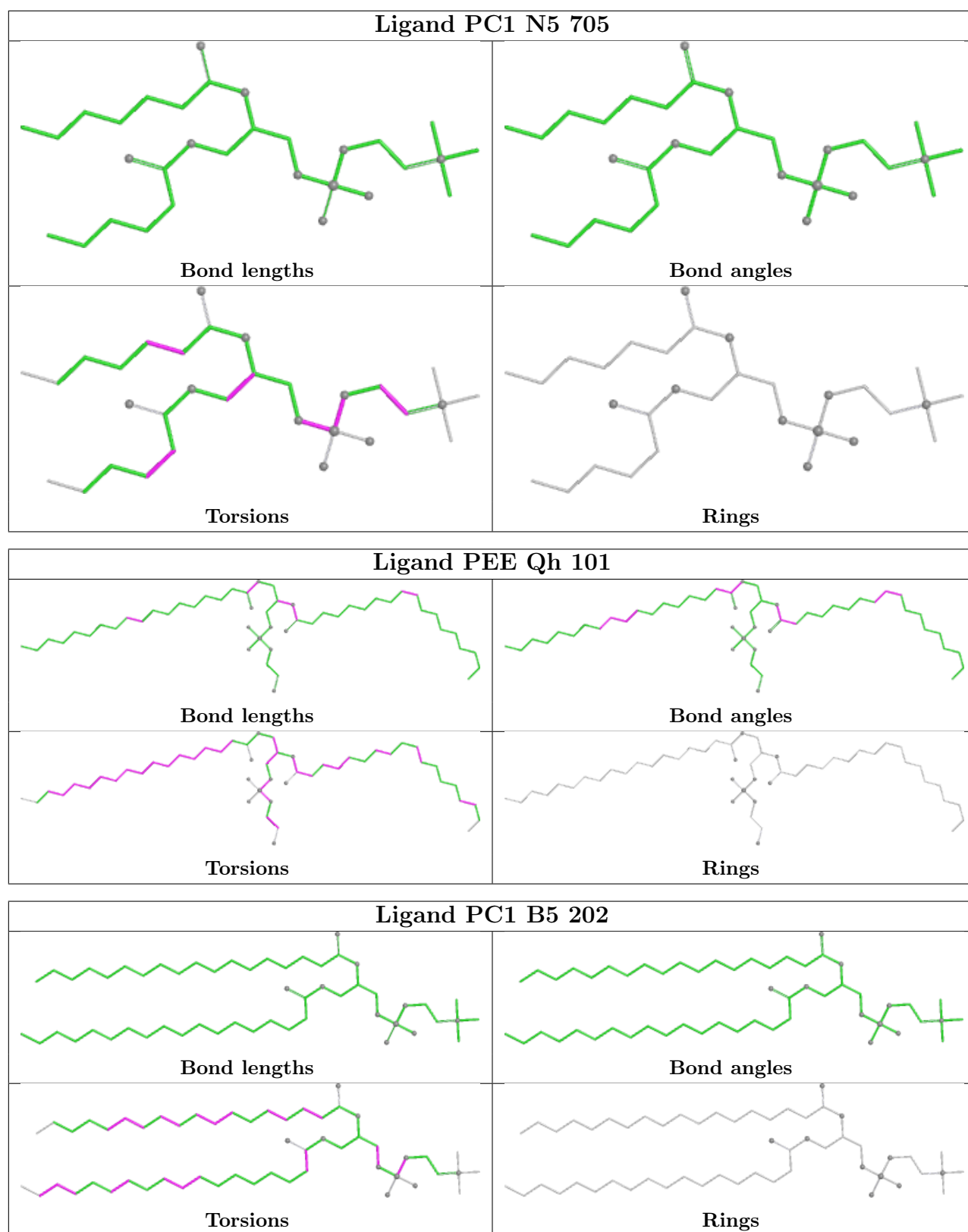


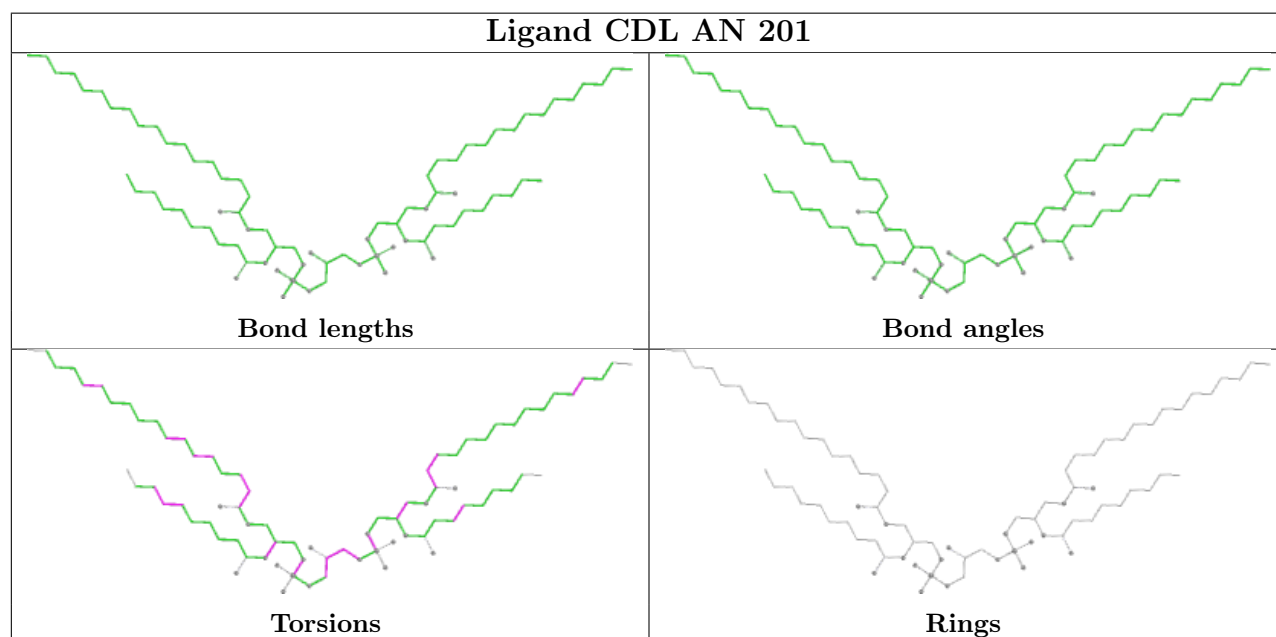
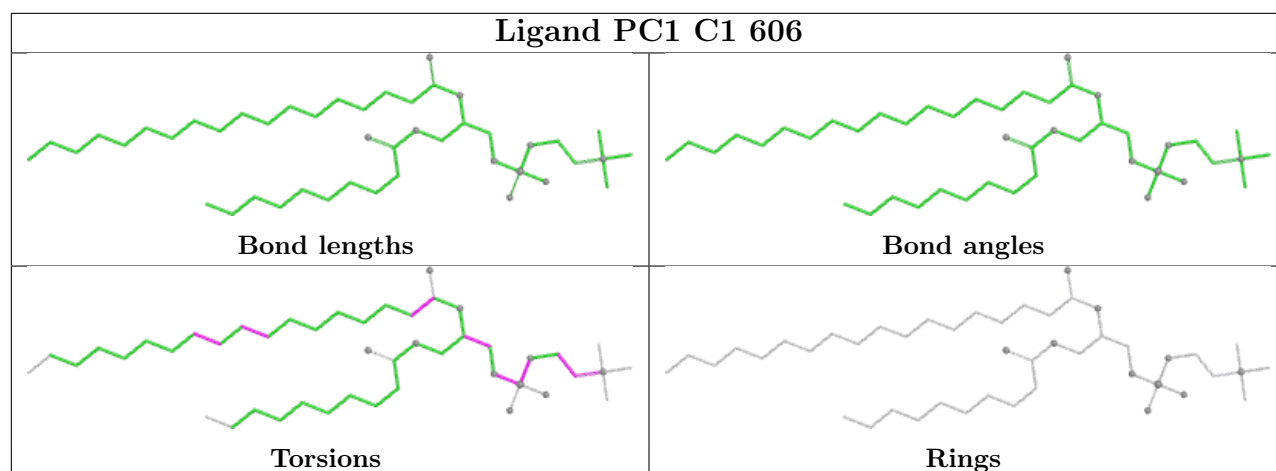
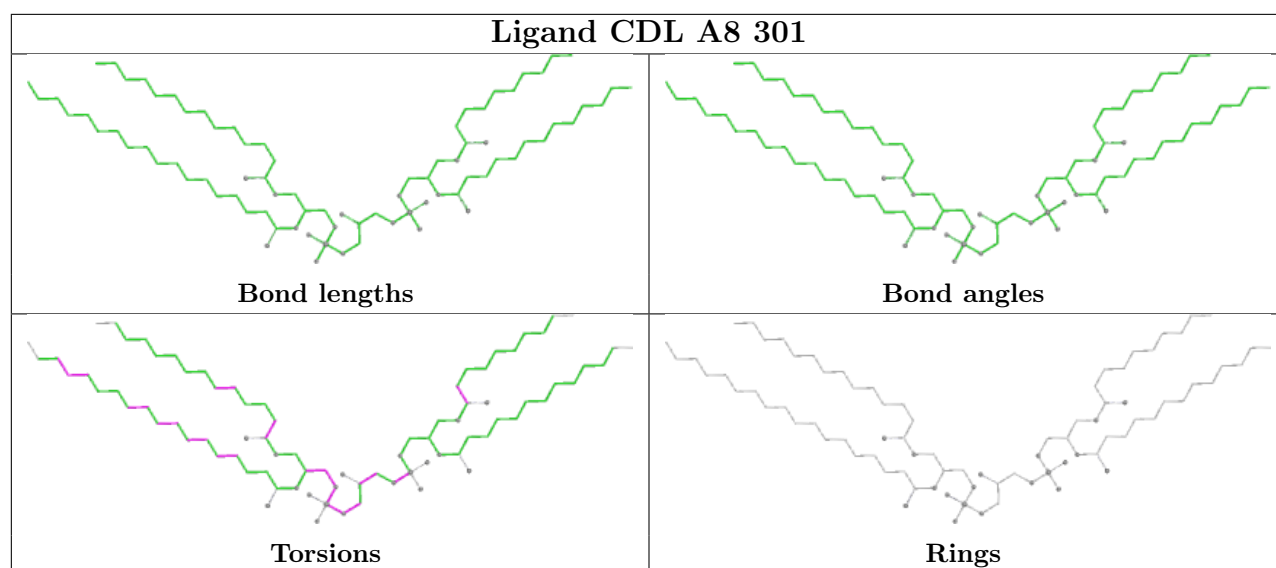
Ligand PC1 C3 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

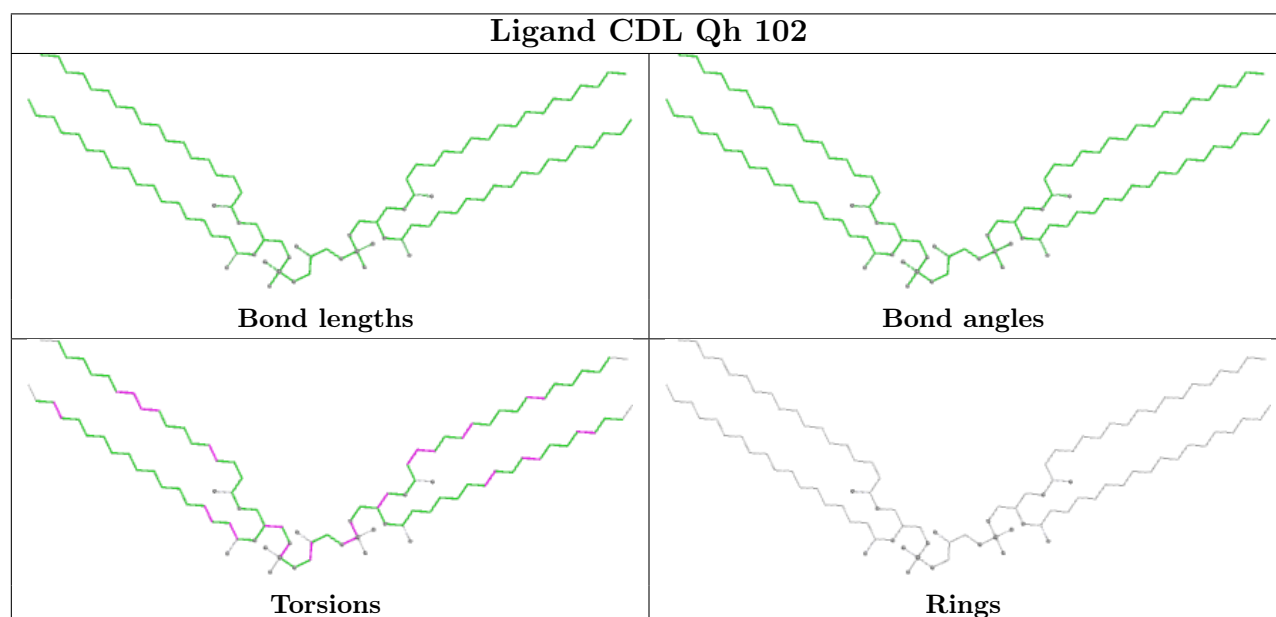
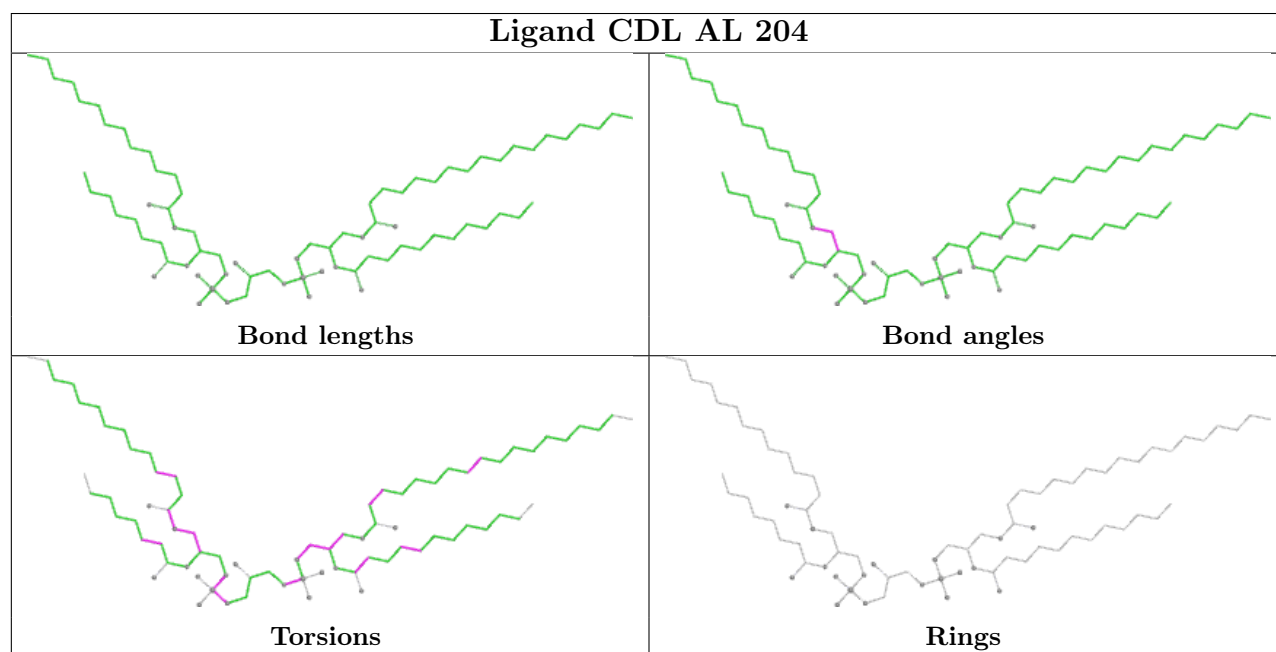
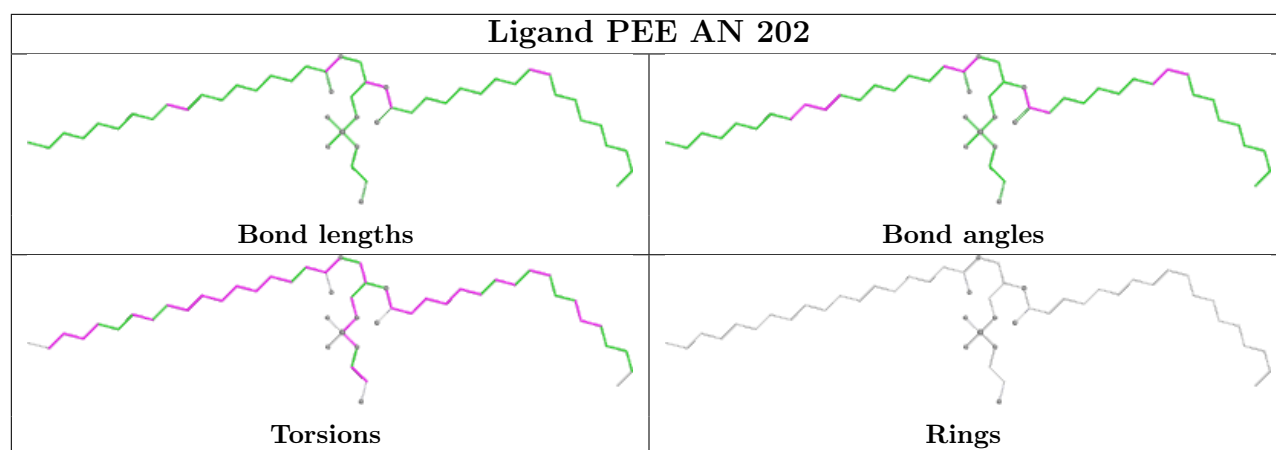
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Bond lengths	Bond angles
	
Torsions	Rings

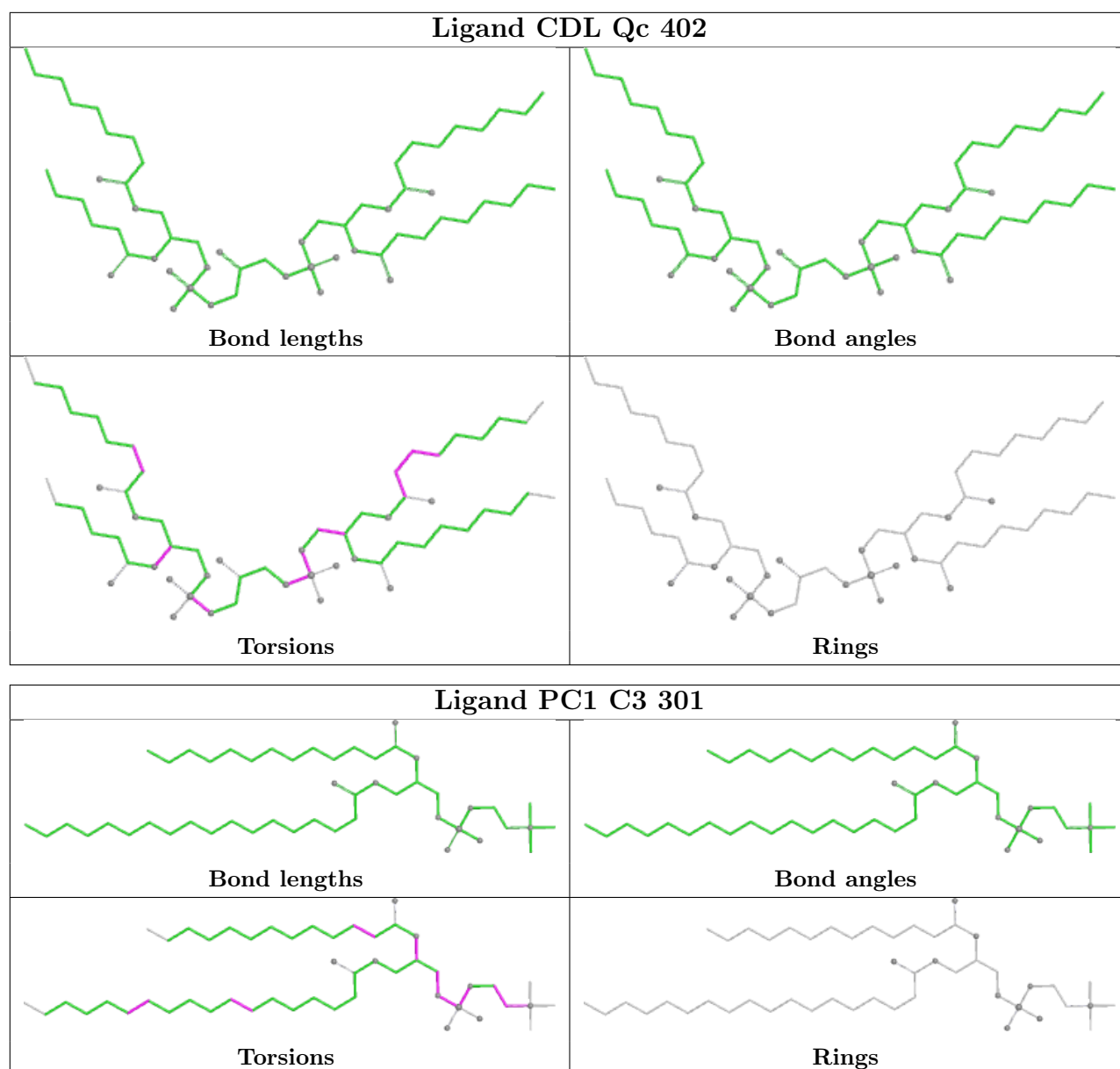
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Bond lengths	Bond angles
	
Torsions	Rings

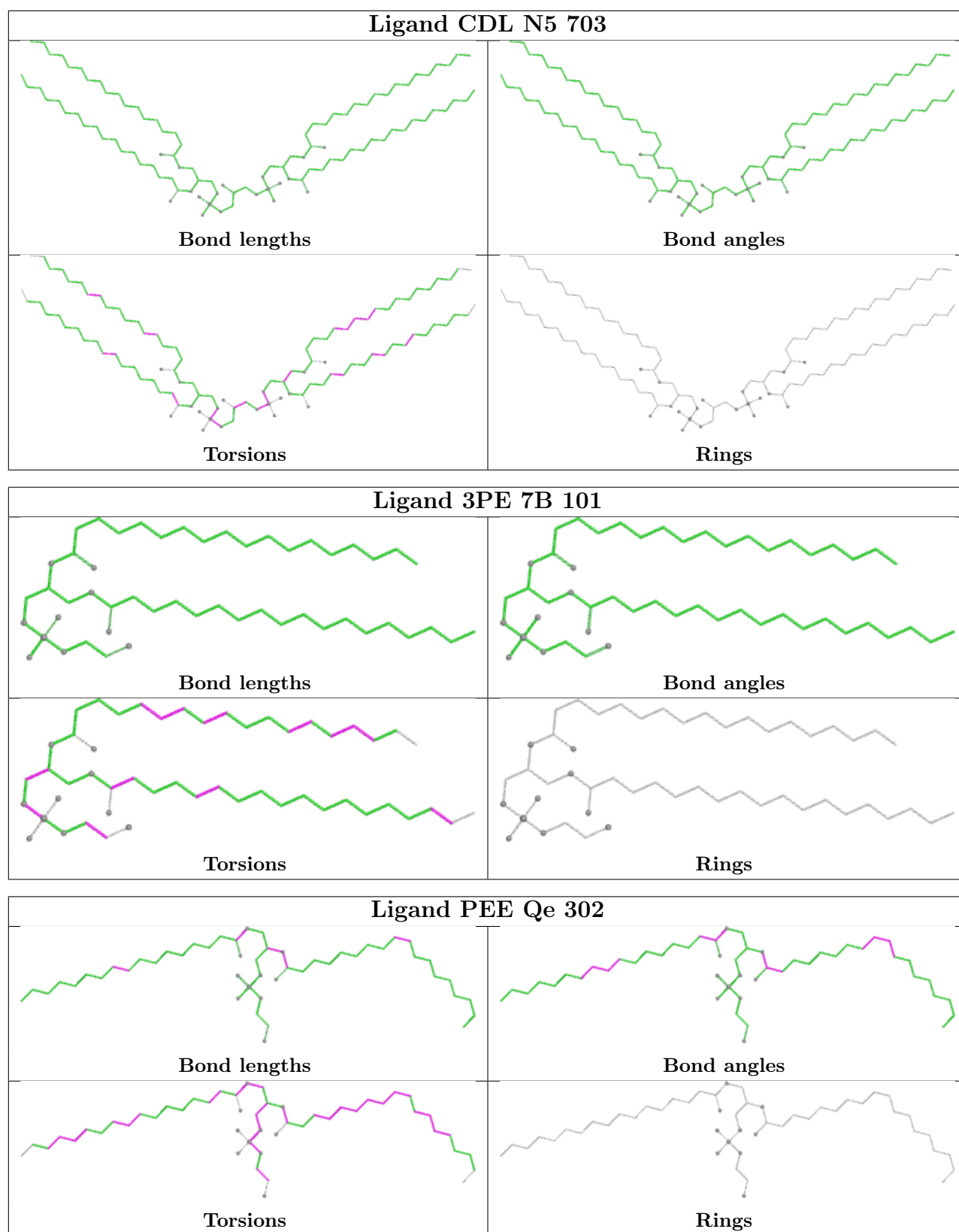


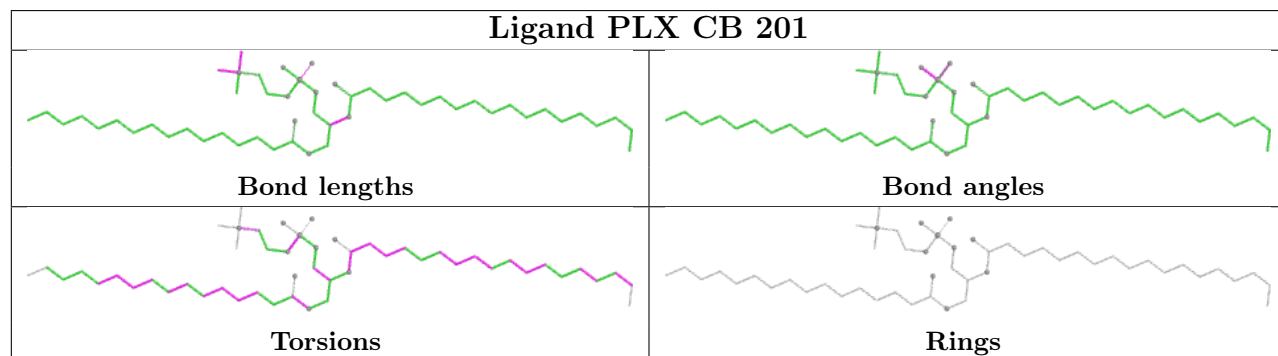
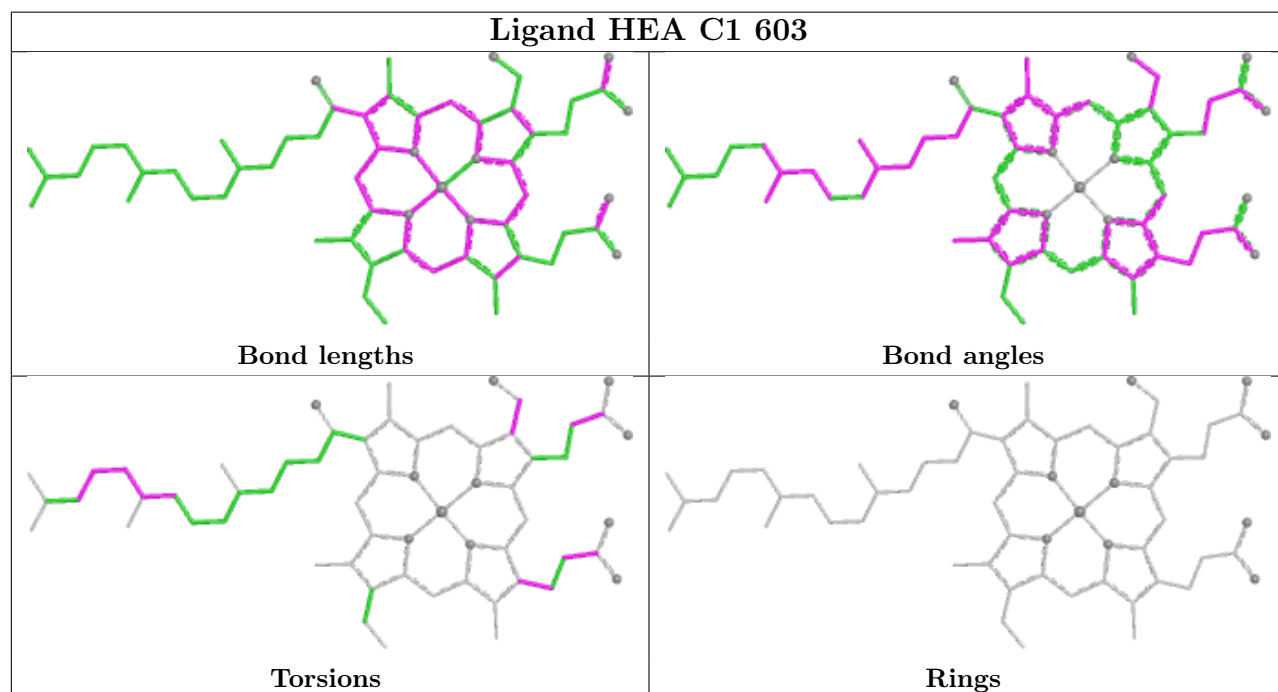
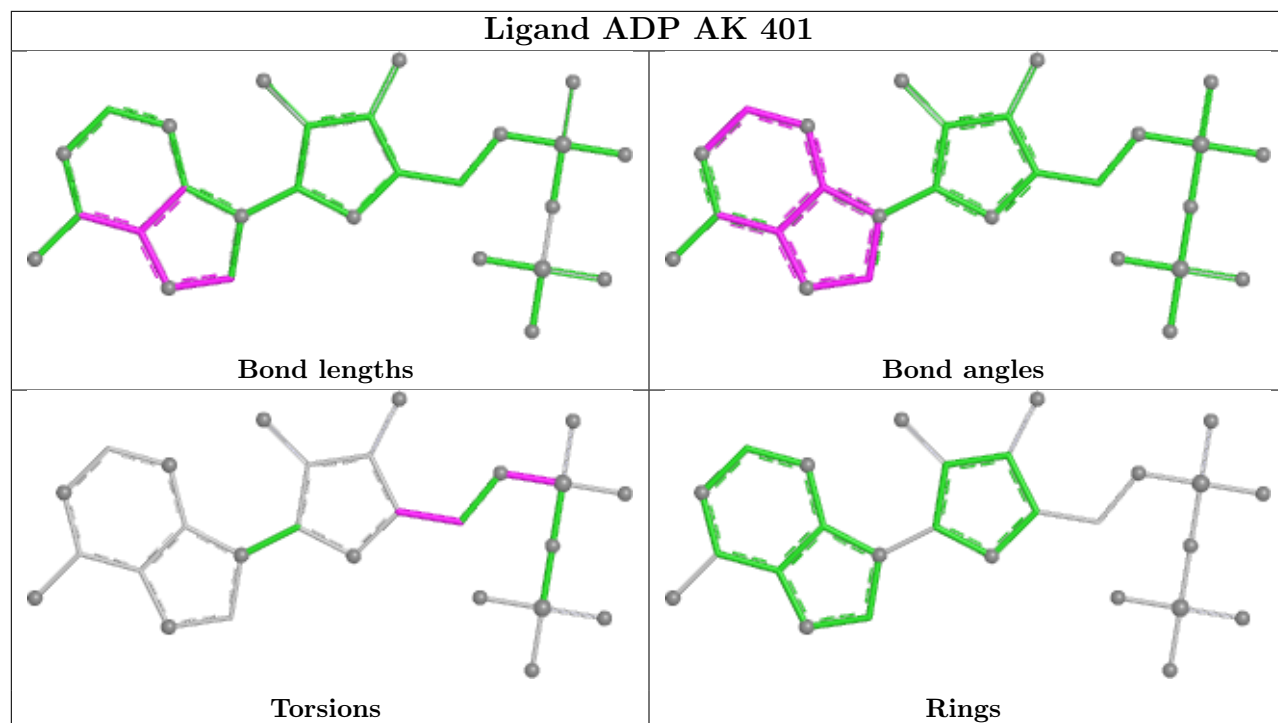


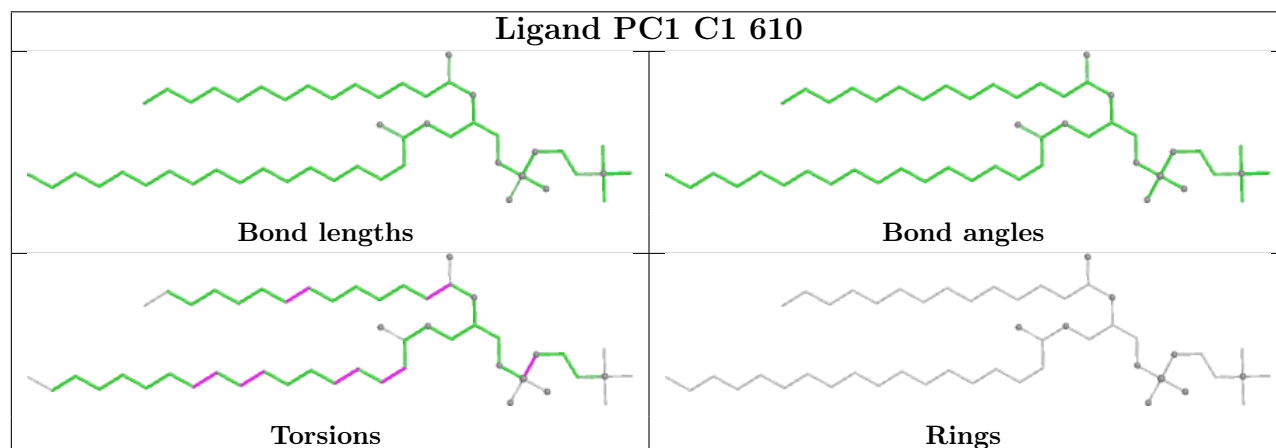
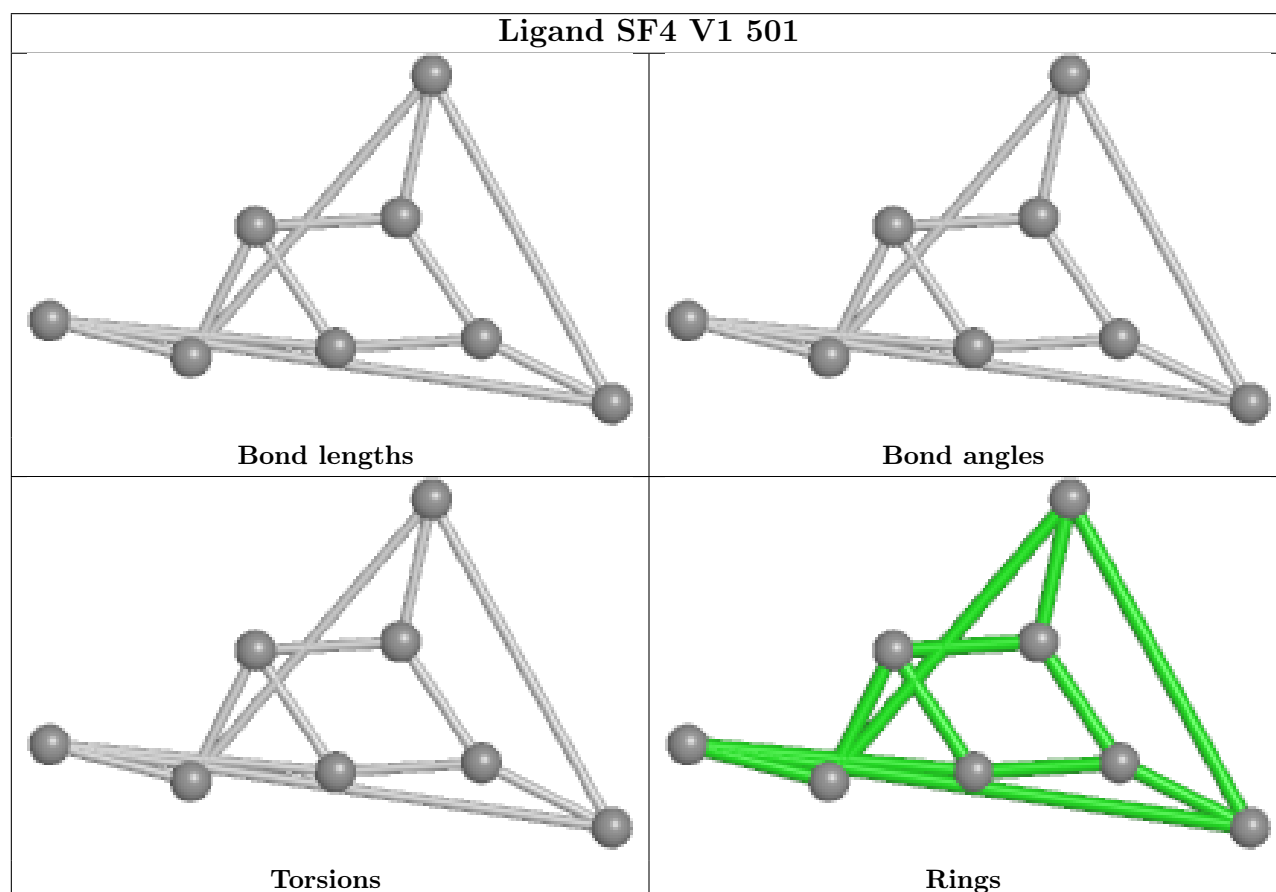
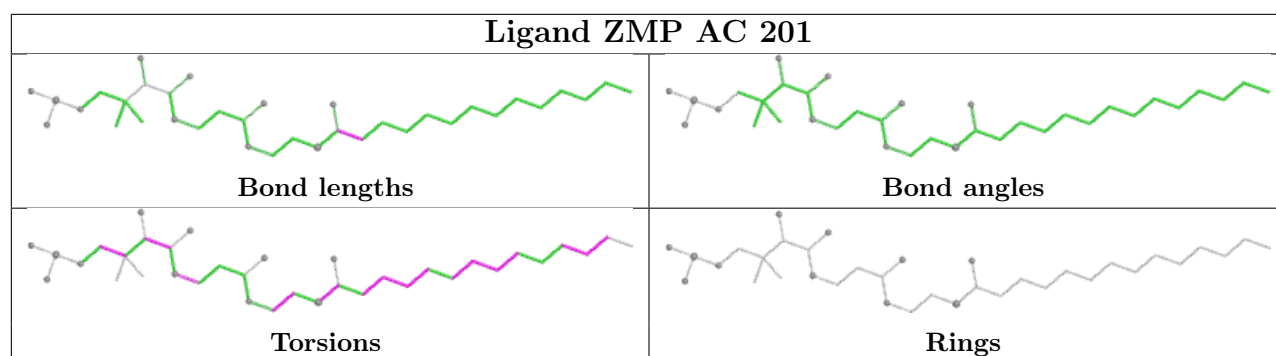


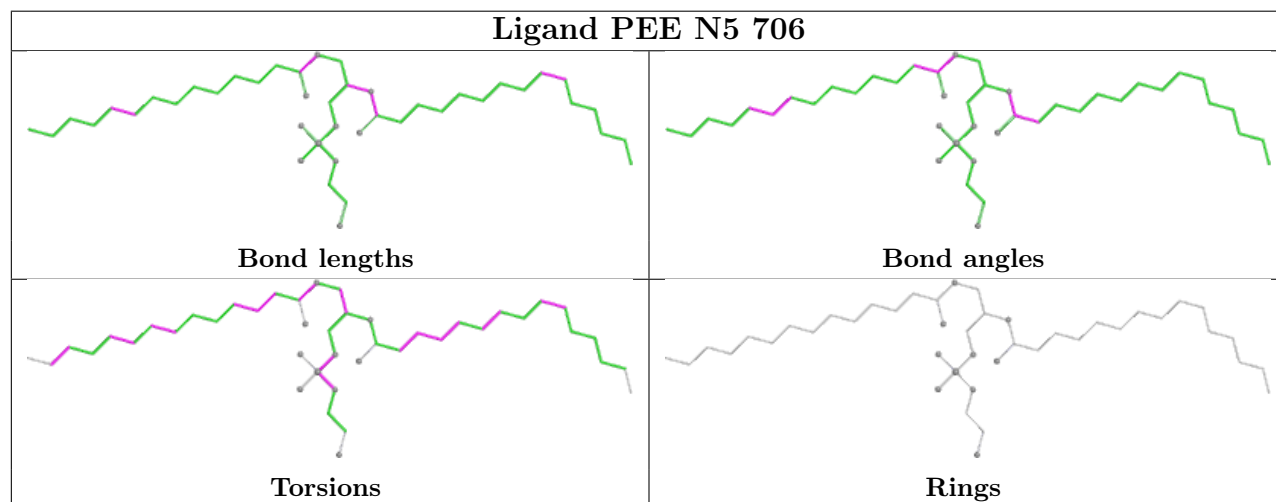
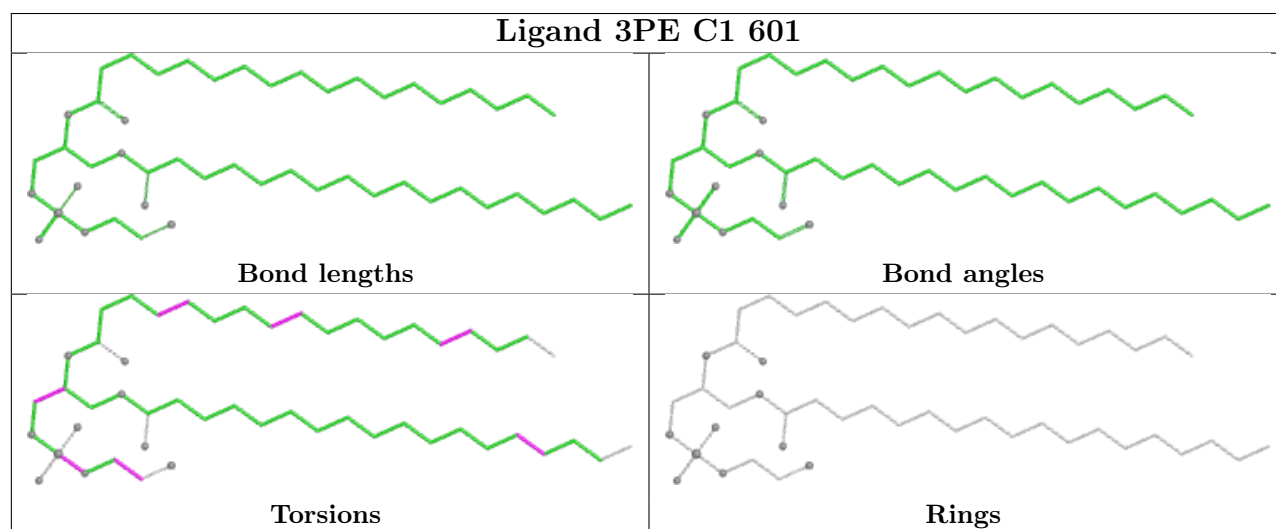
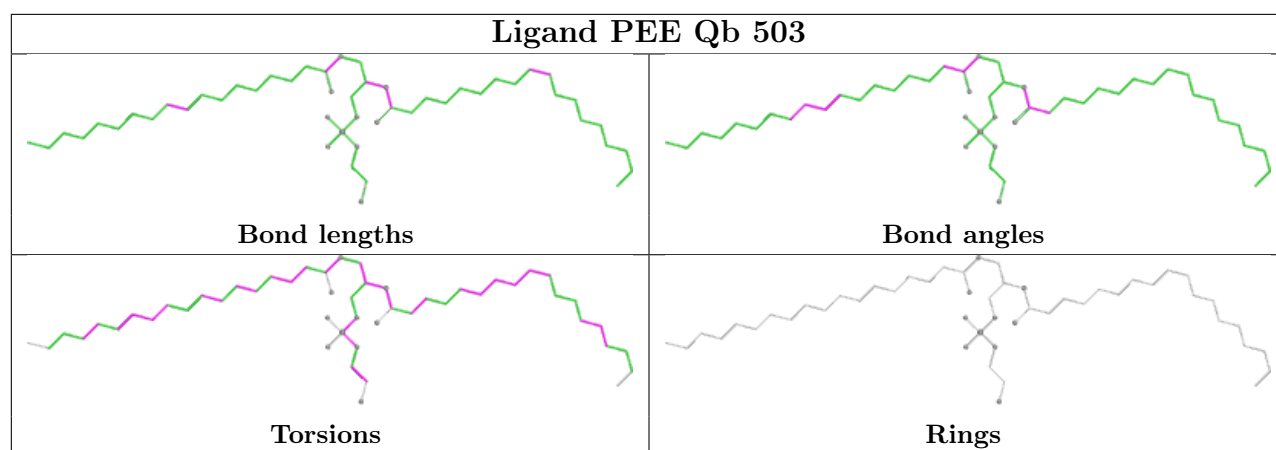


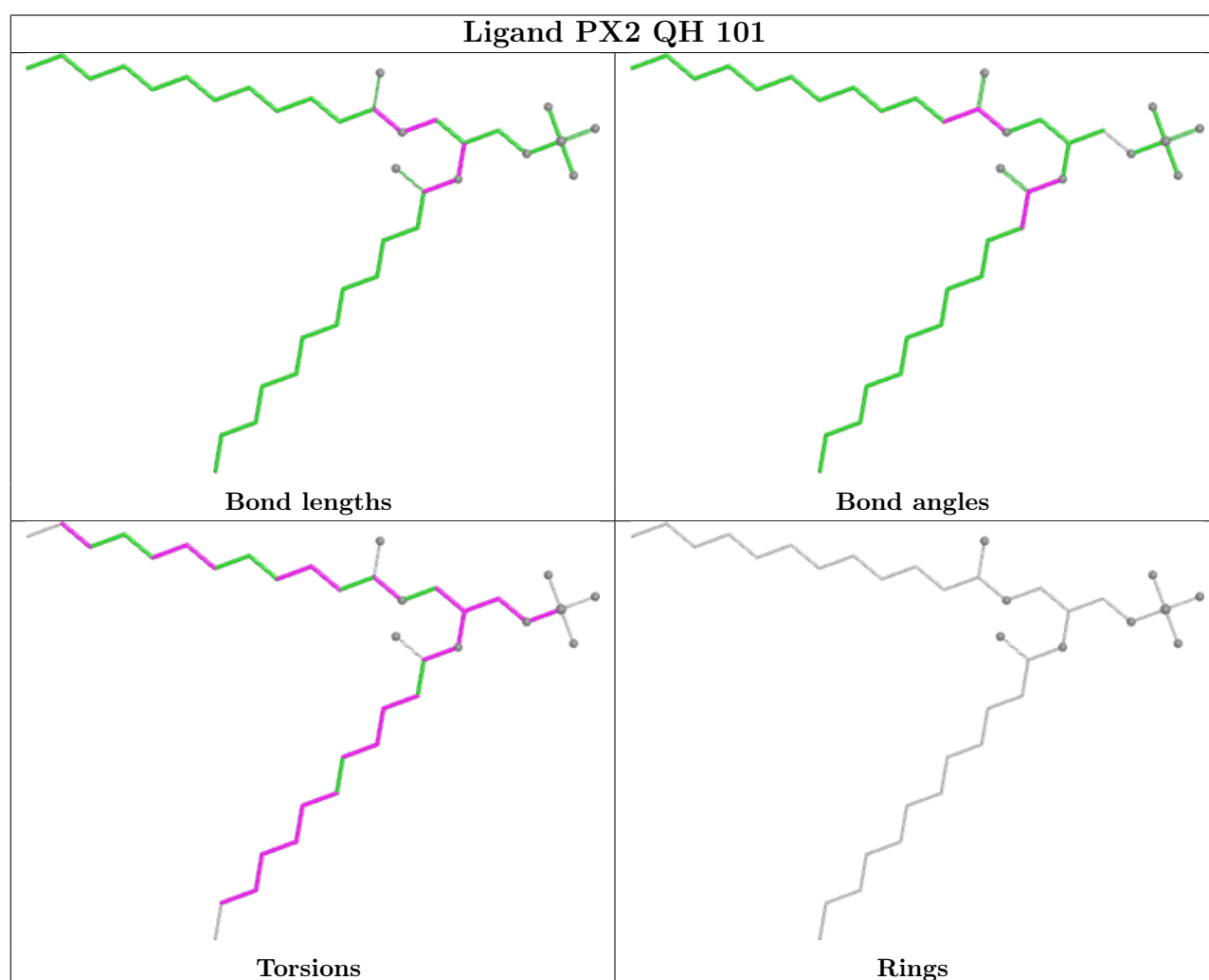
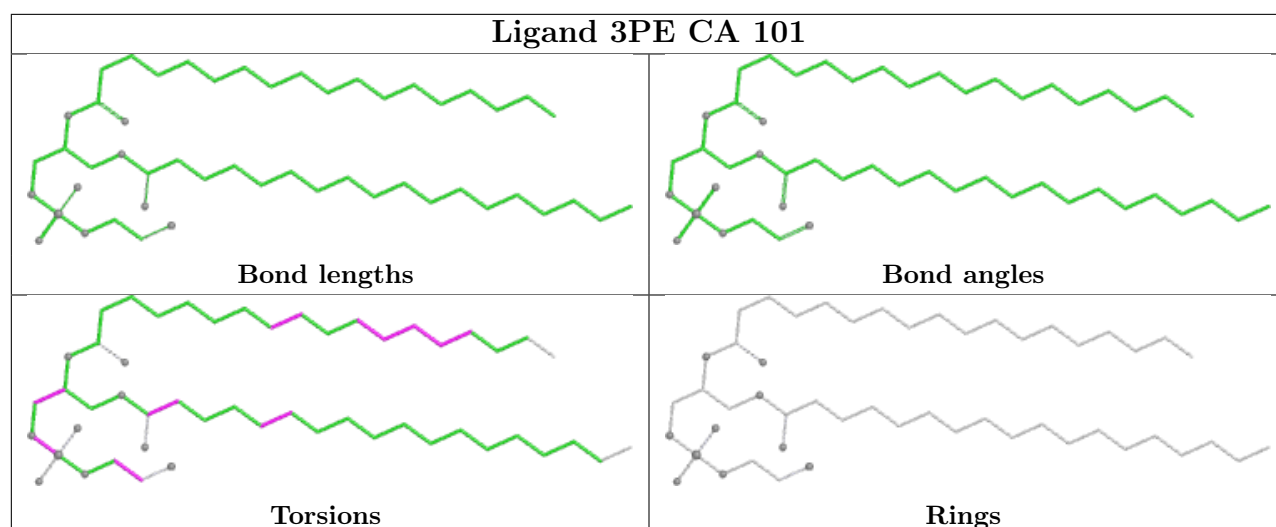


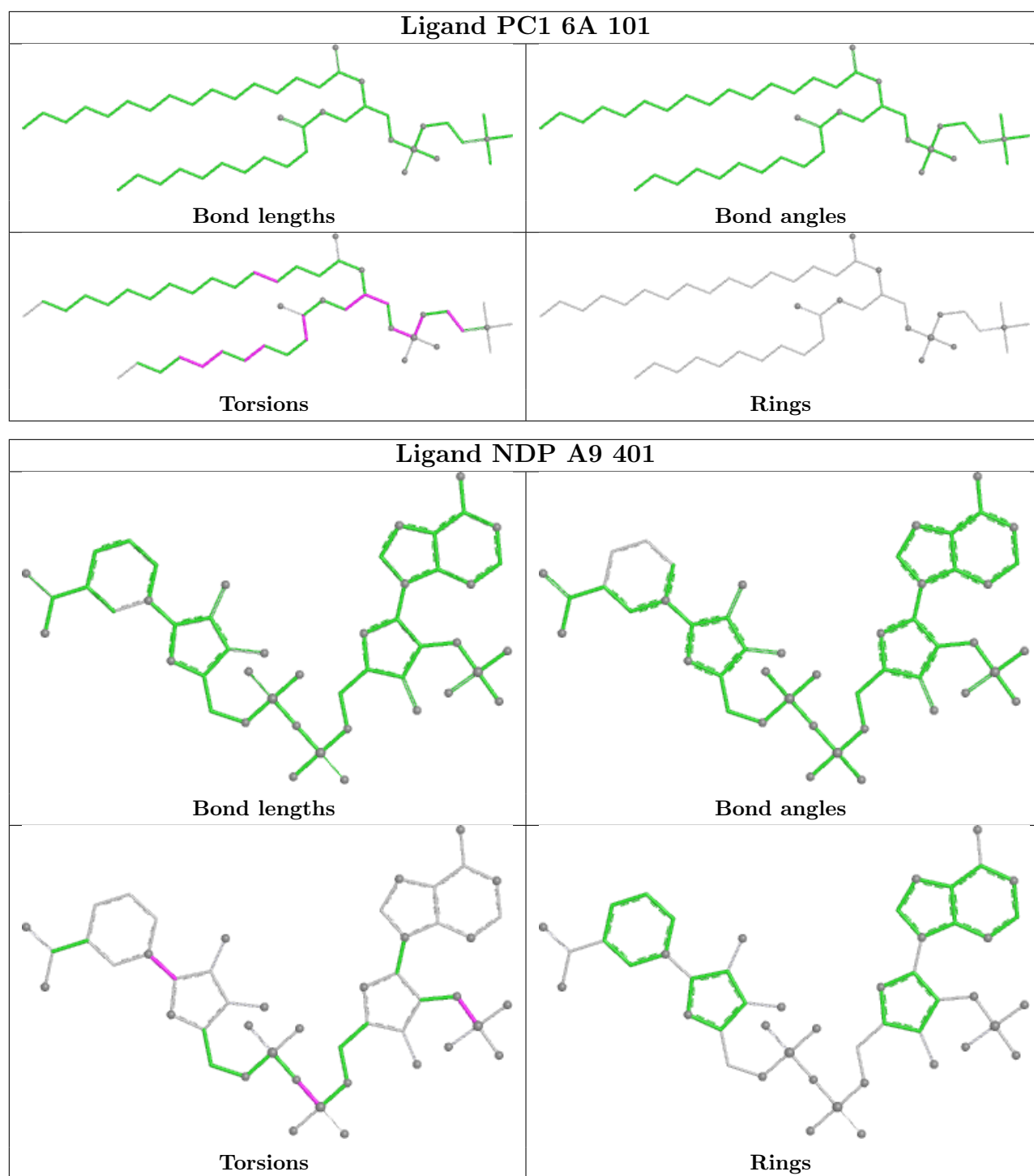


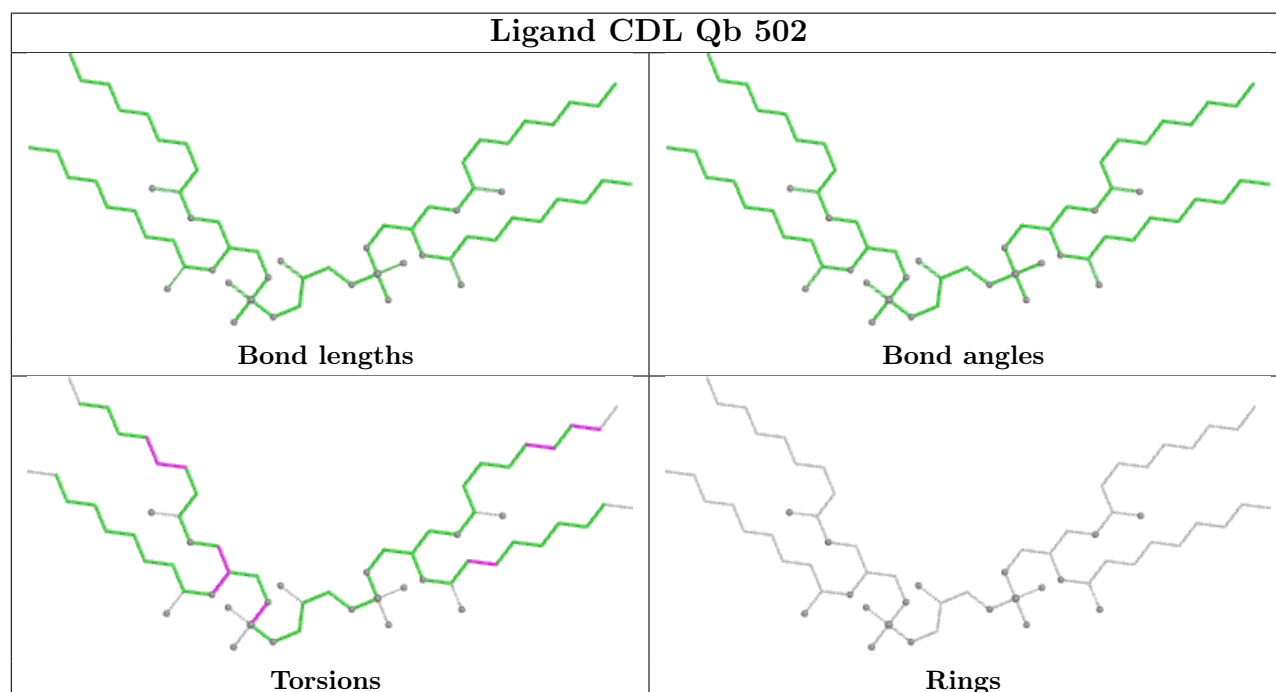
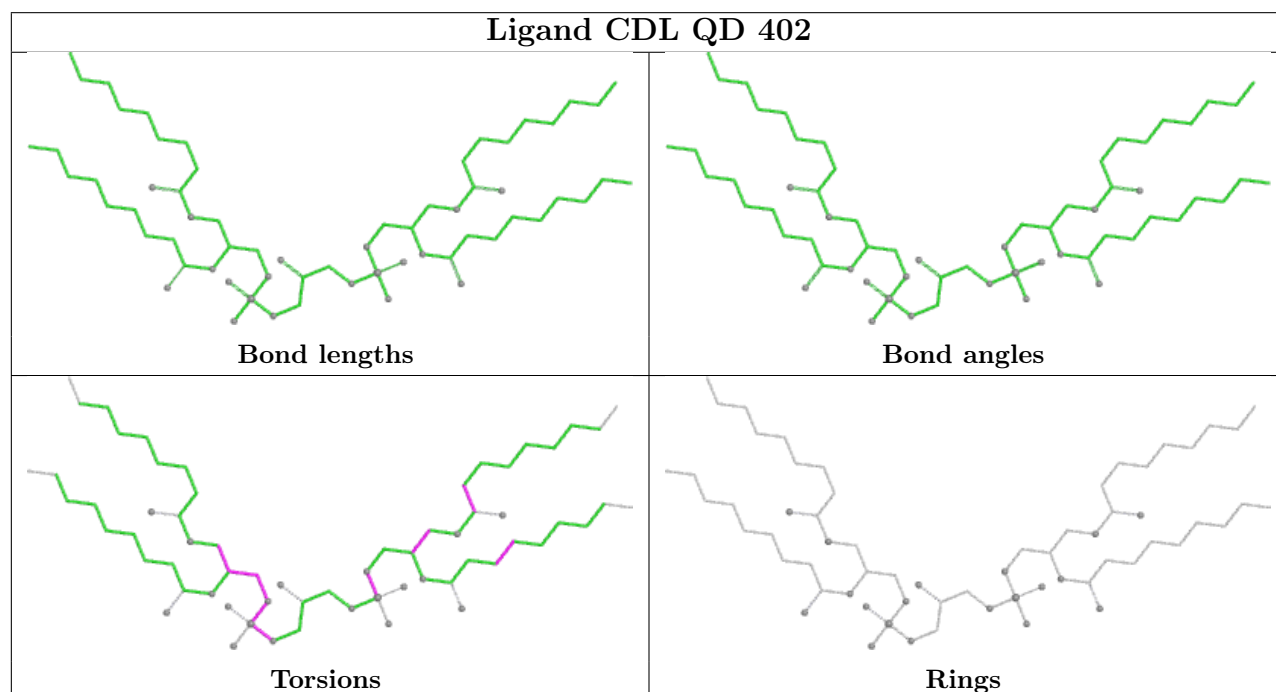
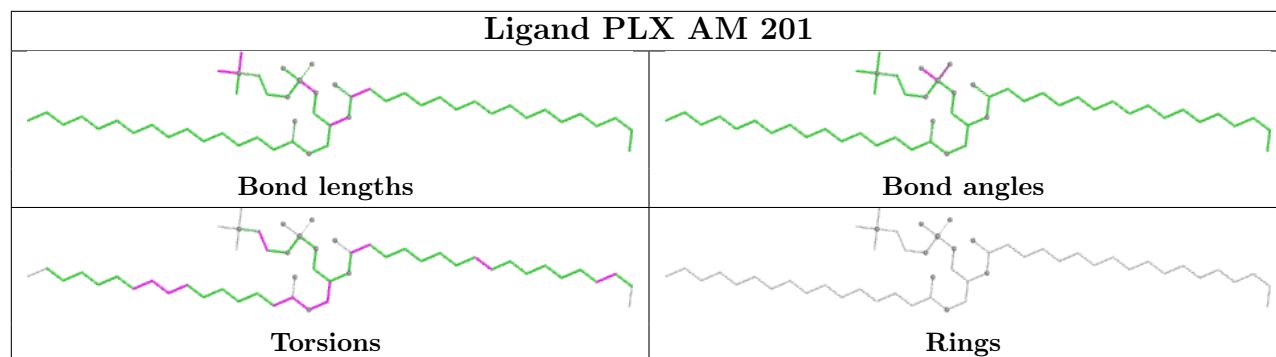


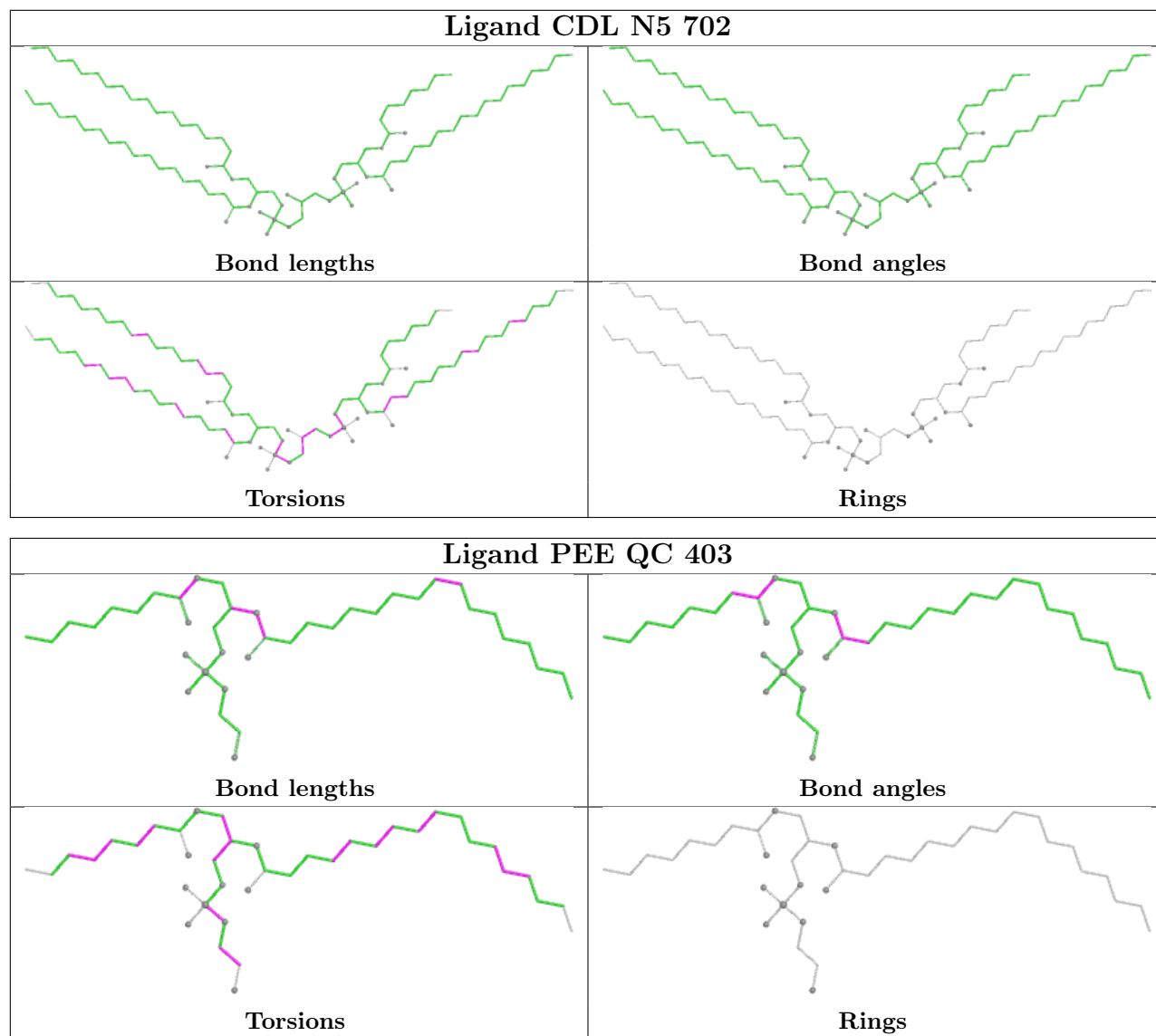




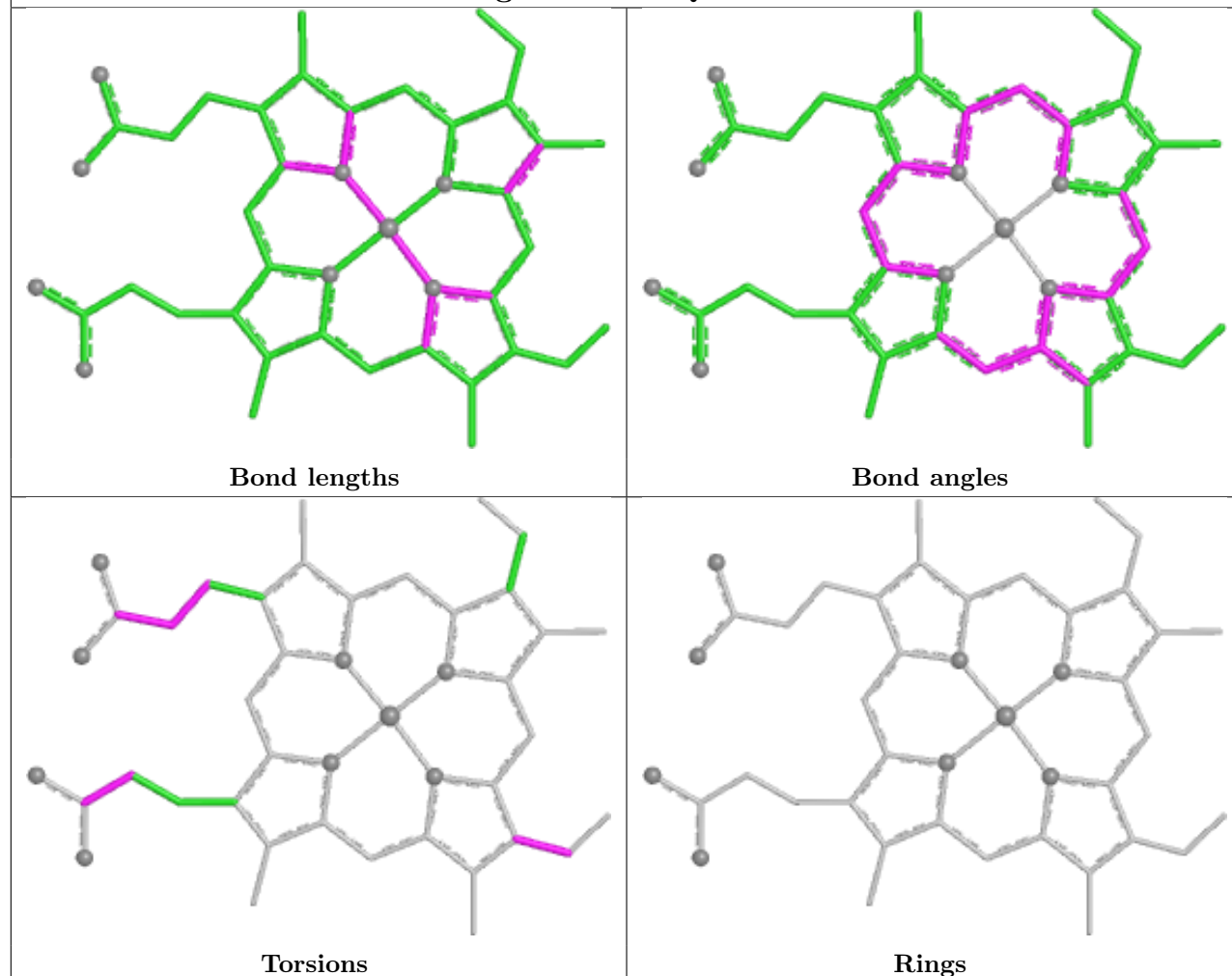




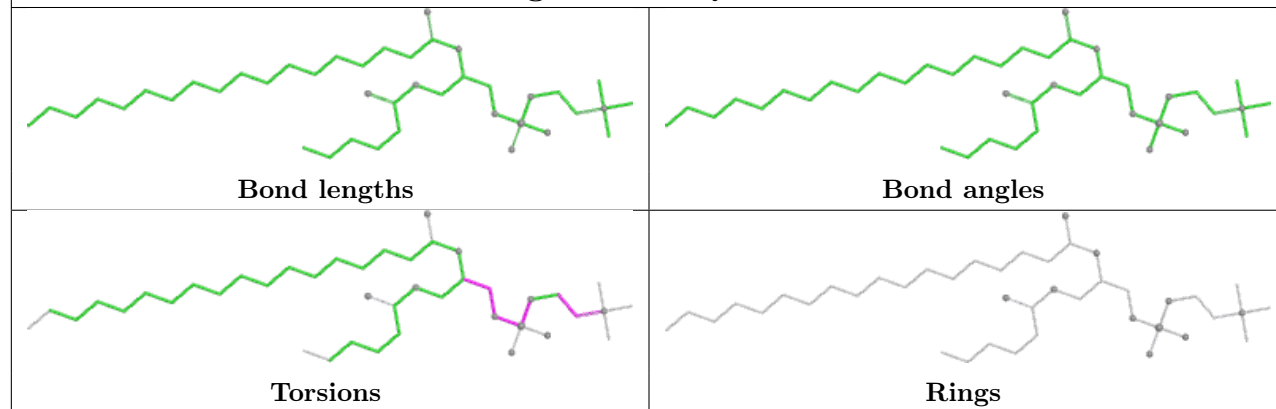


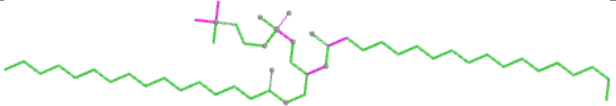
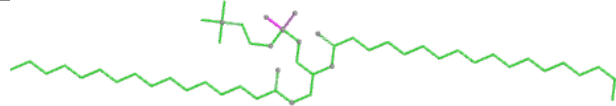
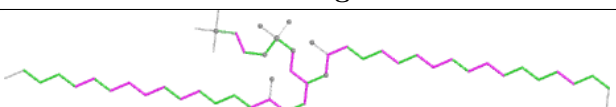
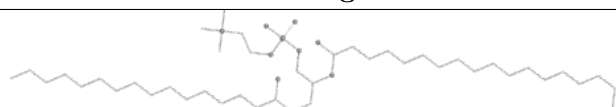


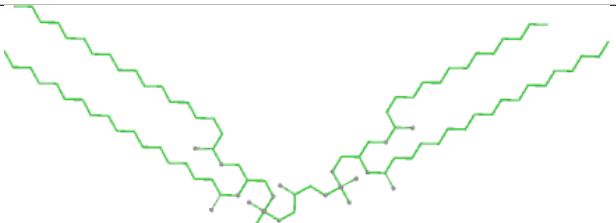
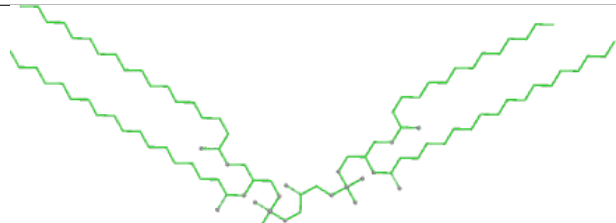
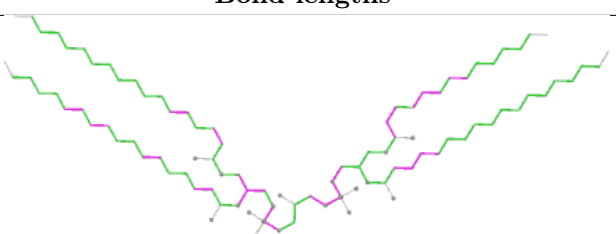
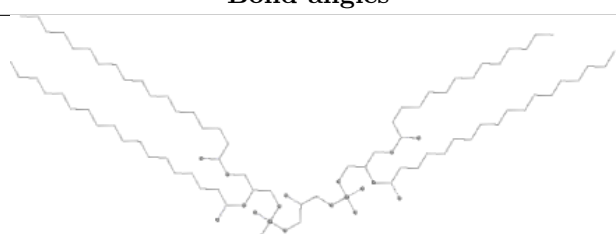
Ligand HEM QC 401

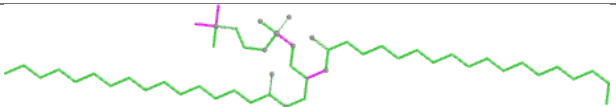
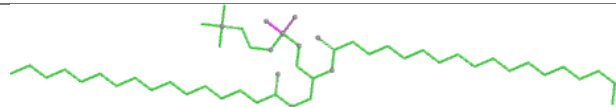
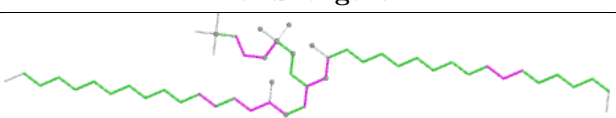
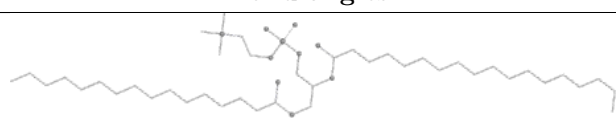


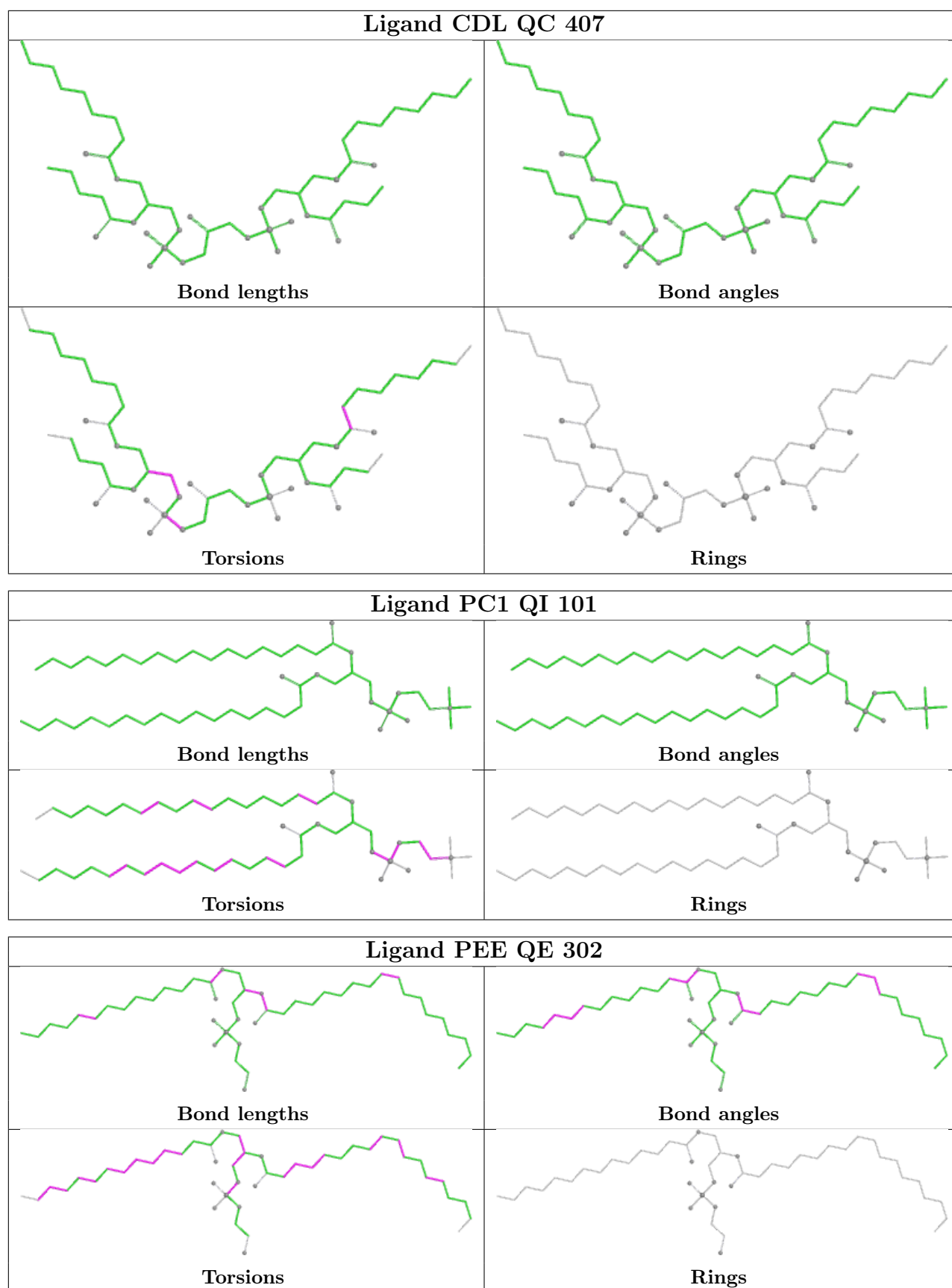
Ligand PC1 Qc 409

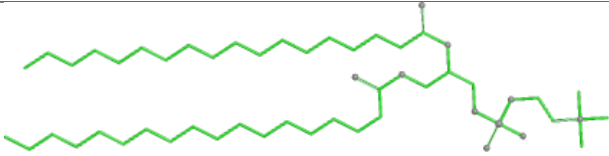
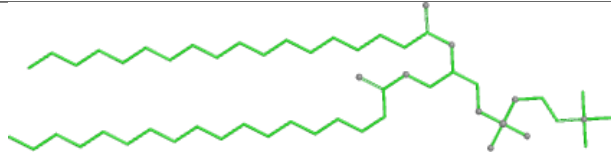
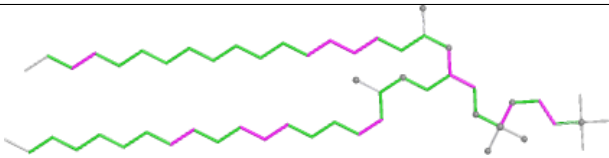
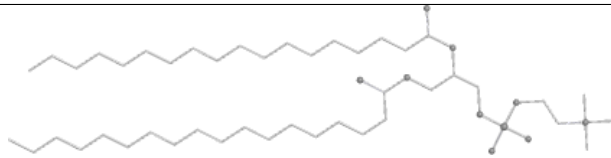


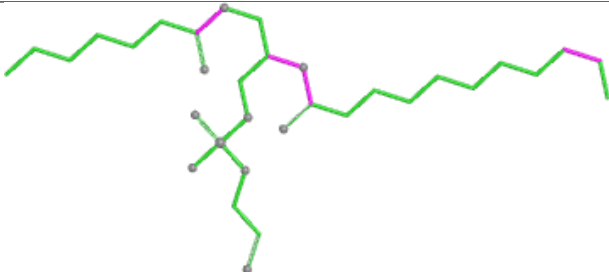
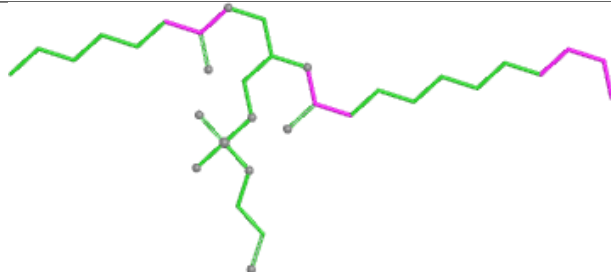
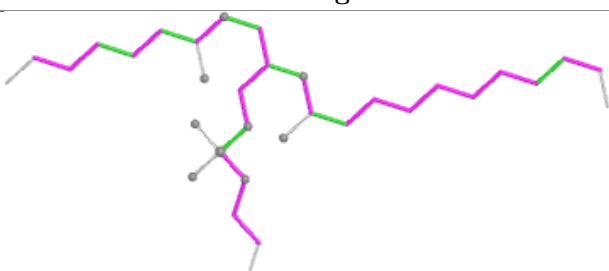
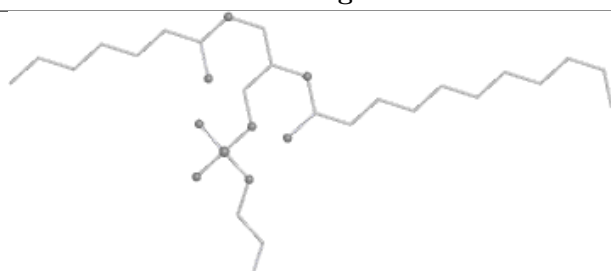
Ligand PLX BL 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

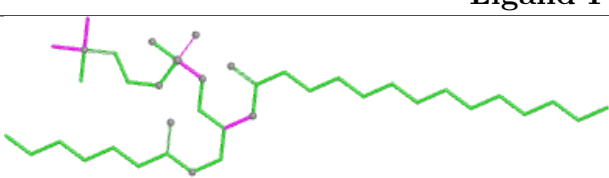
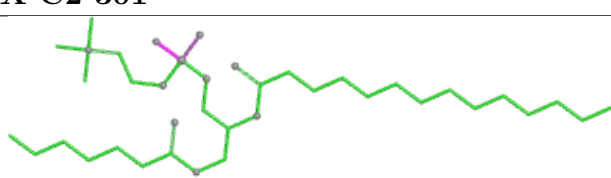
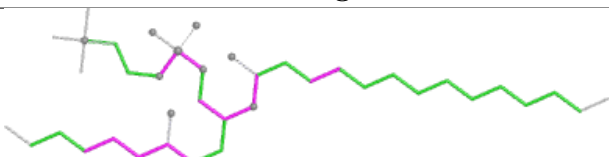
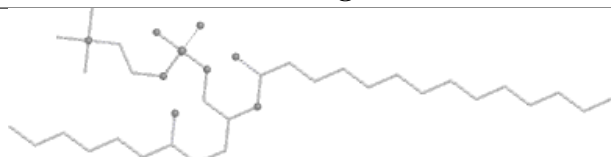
Ligand CDL Qj 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

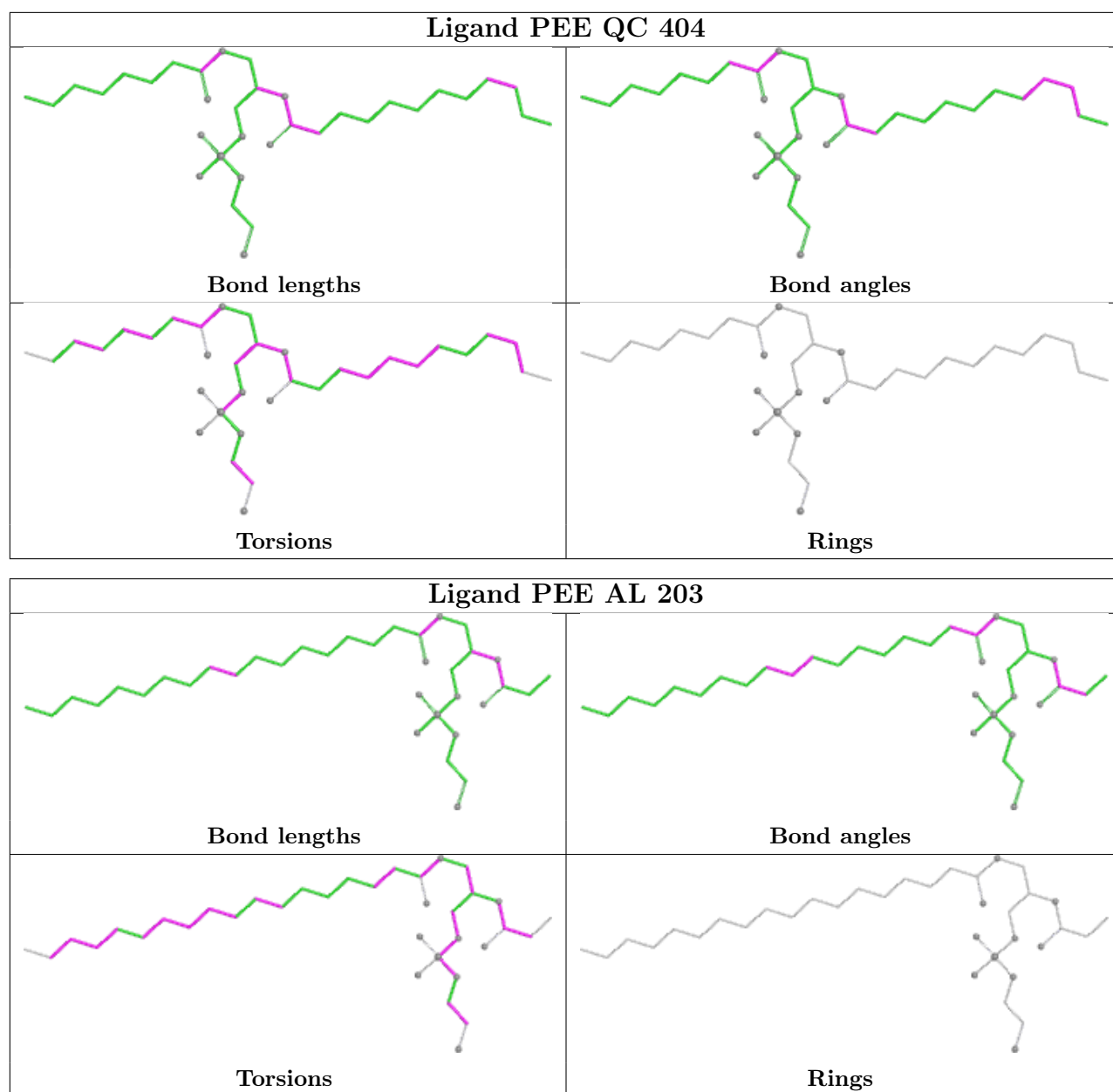
Ligand PLX B1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

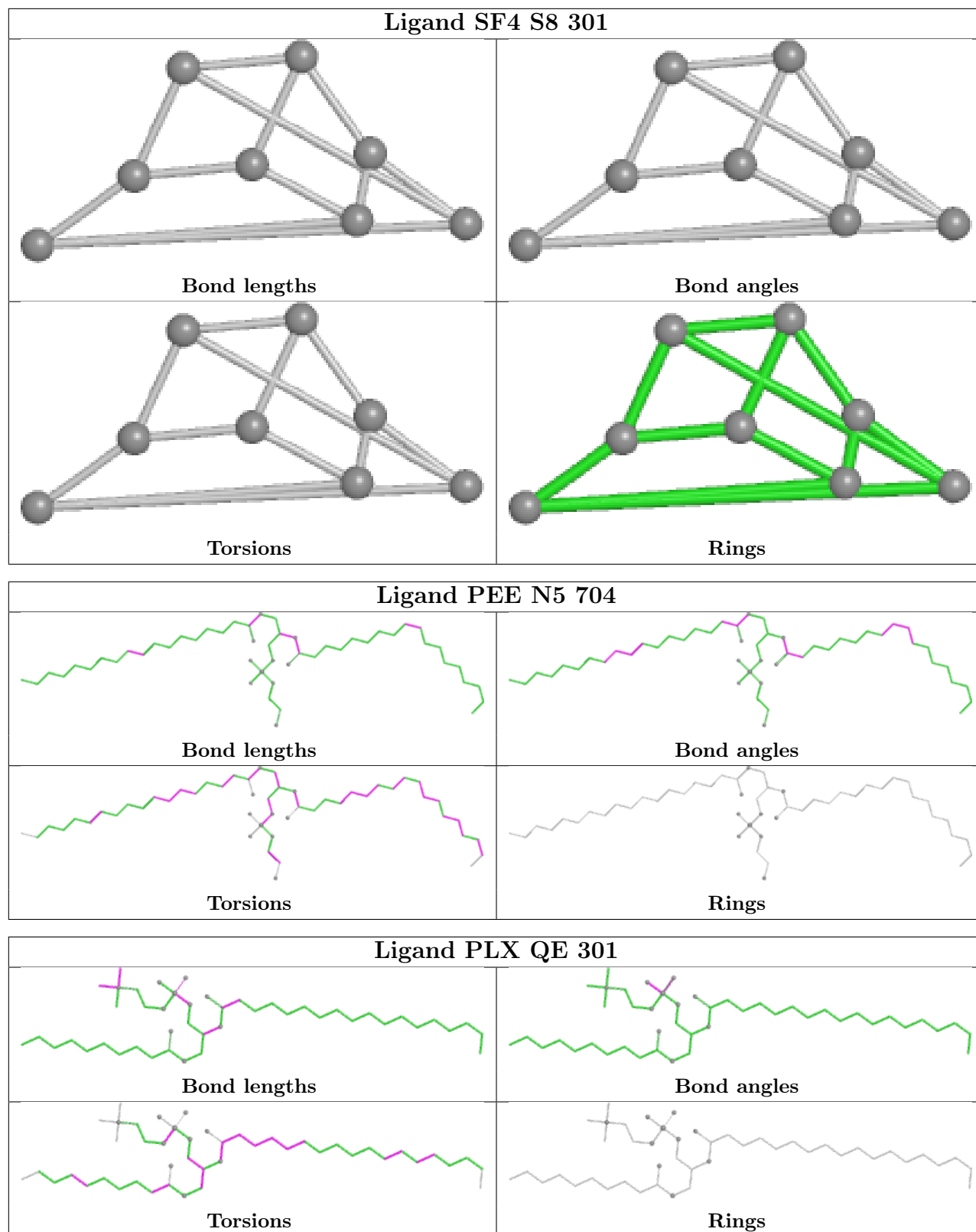


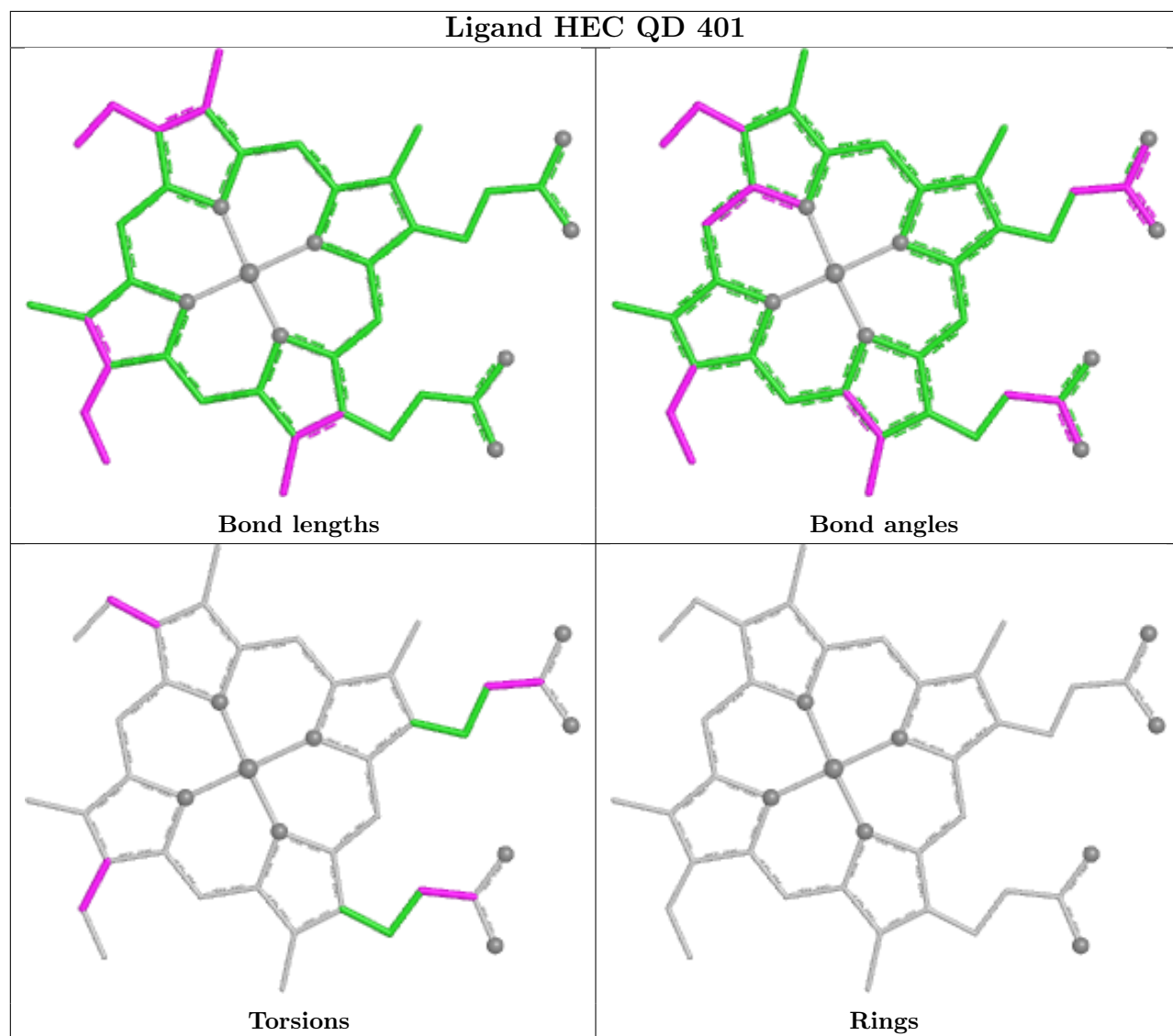
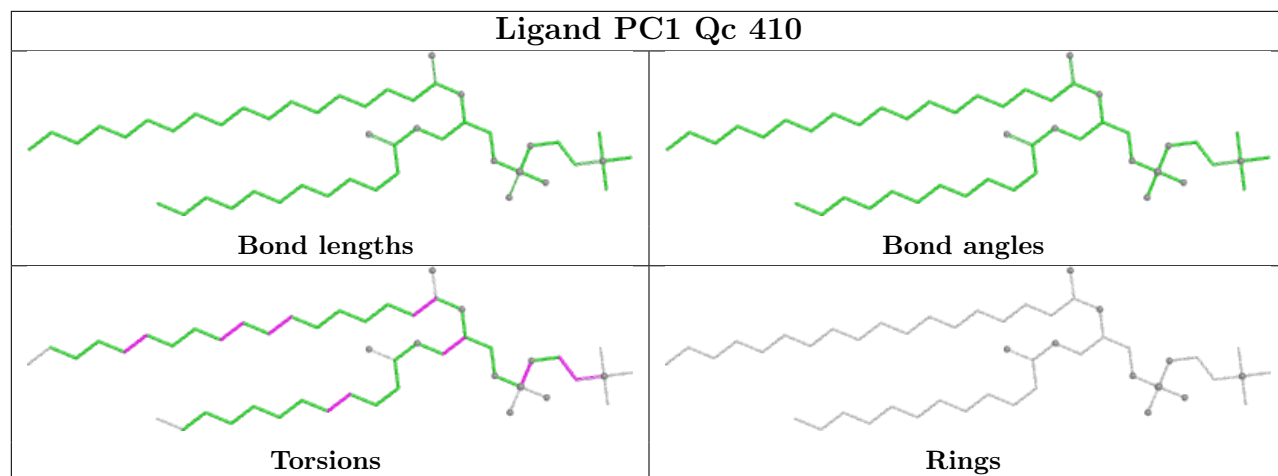
Ligand PC1 C4 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

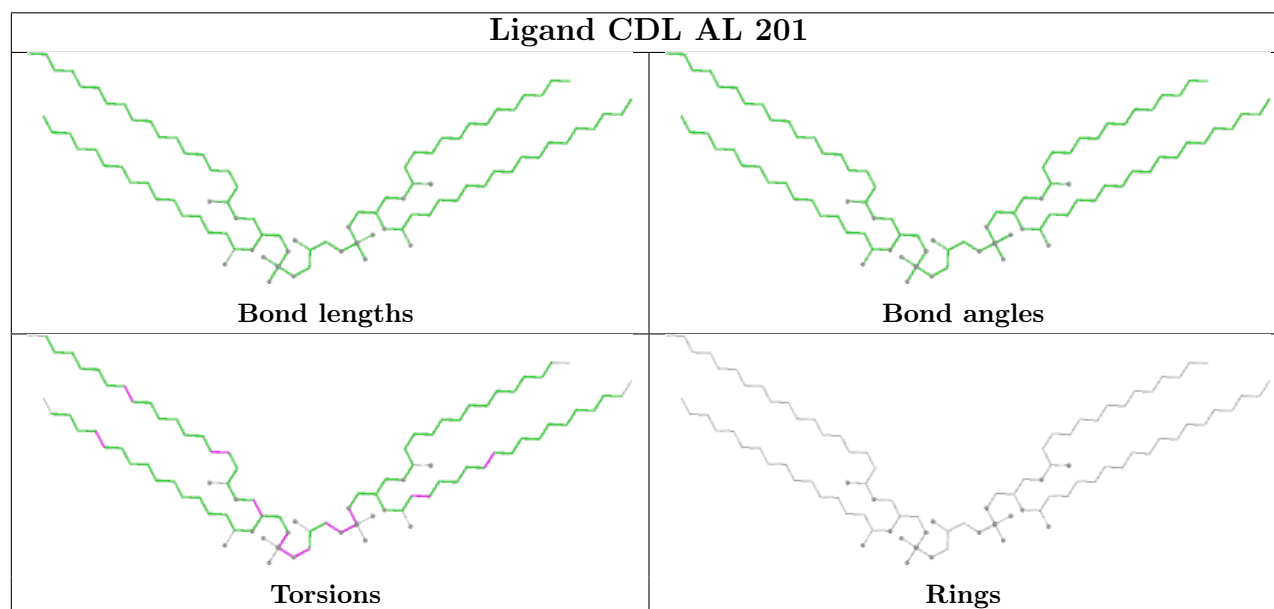
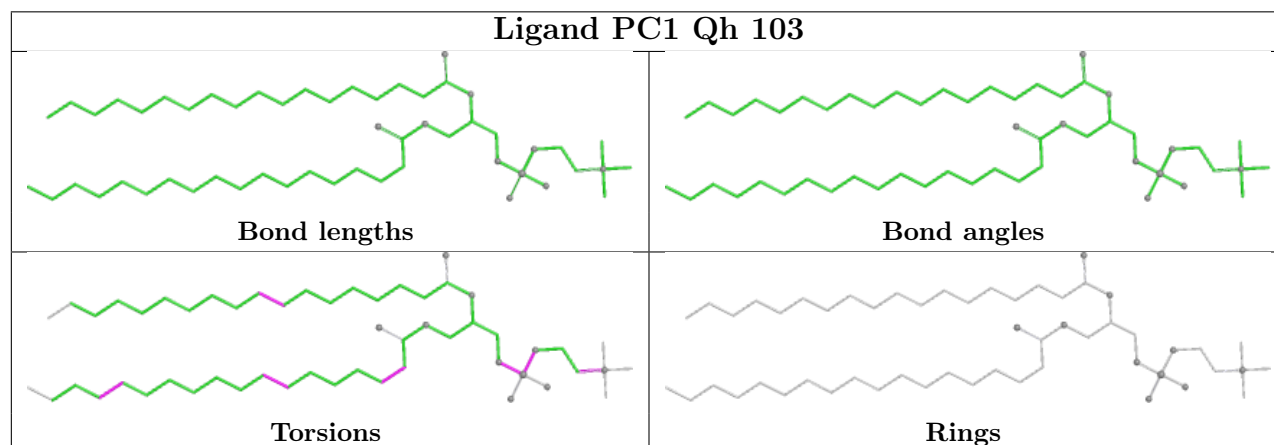
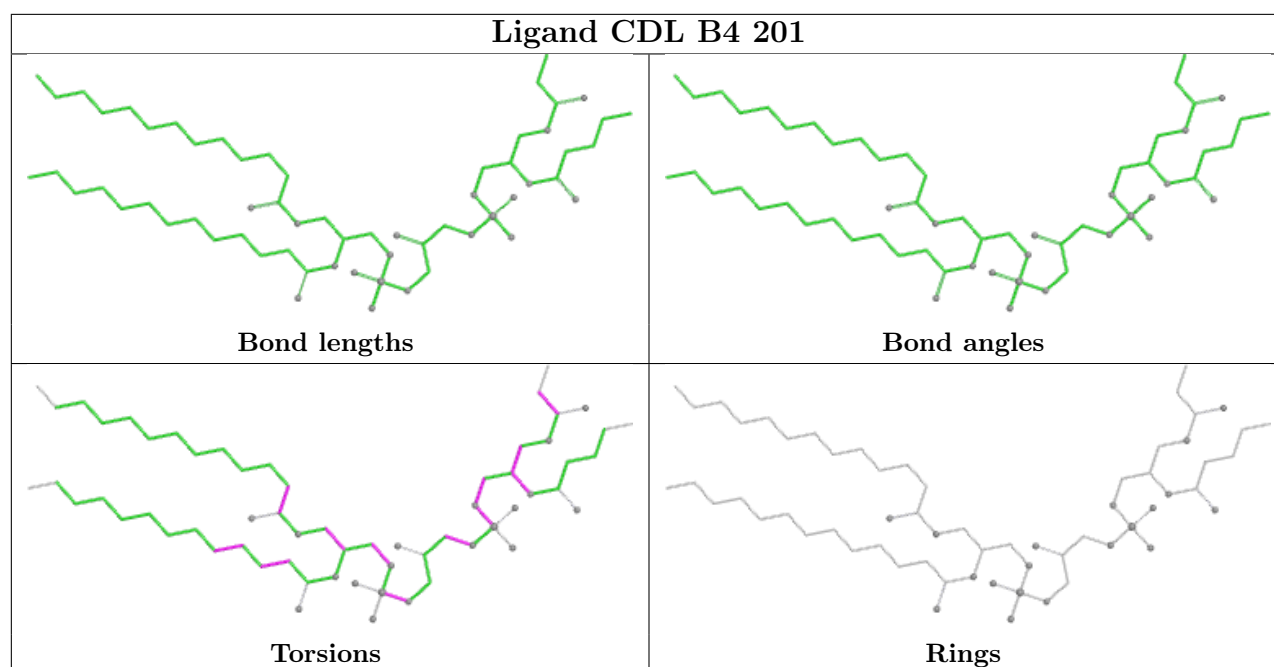
Ligand PEE C1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

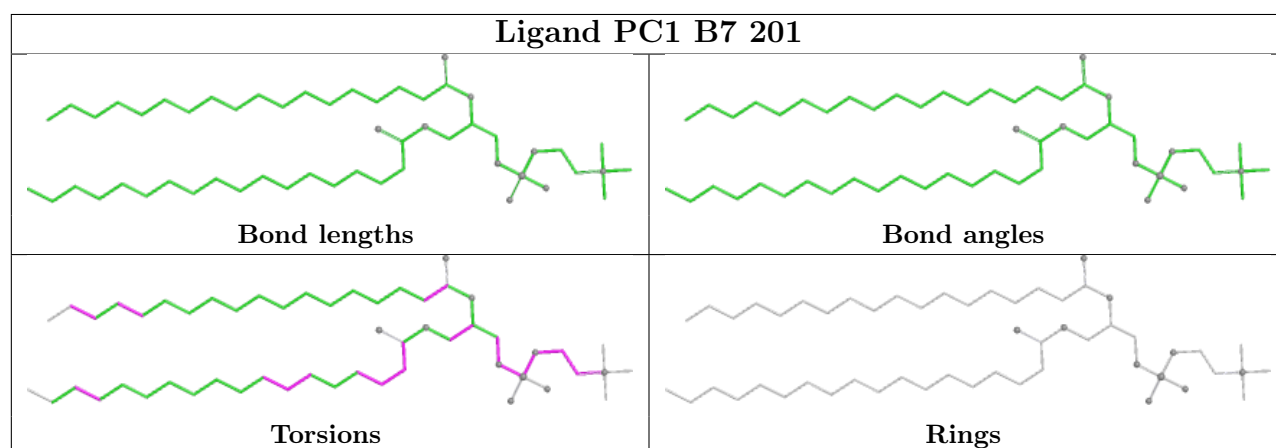
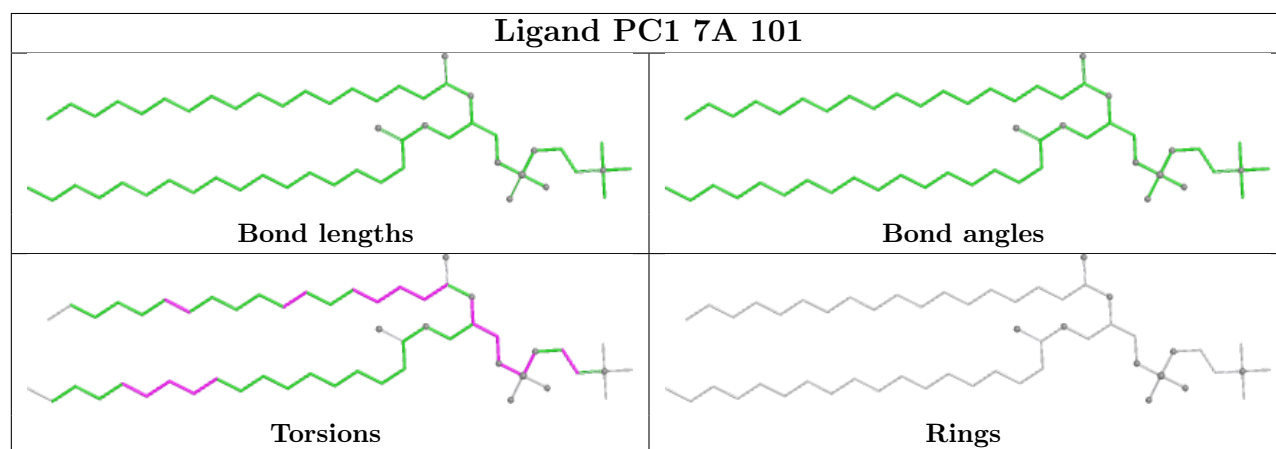
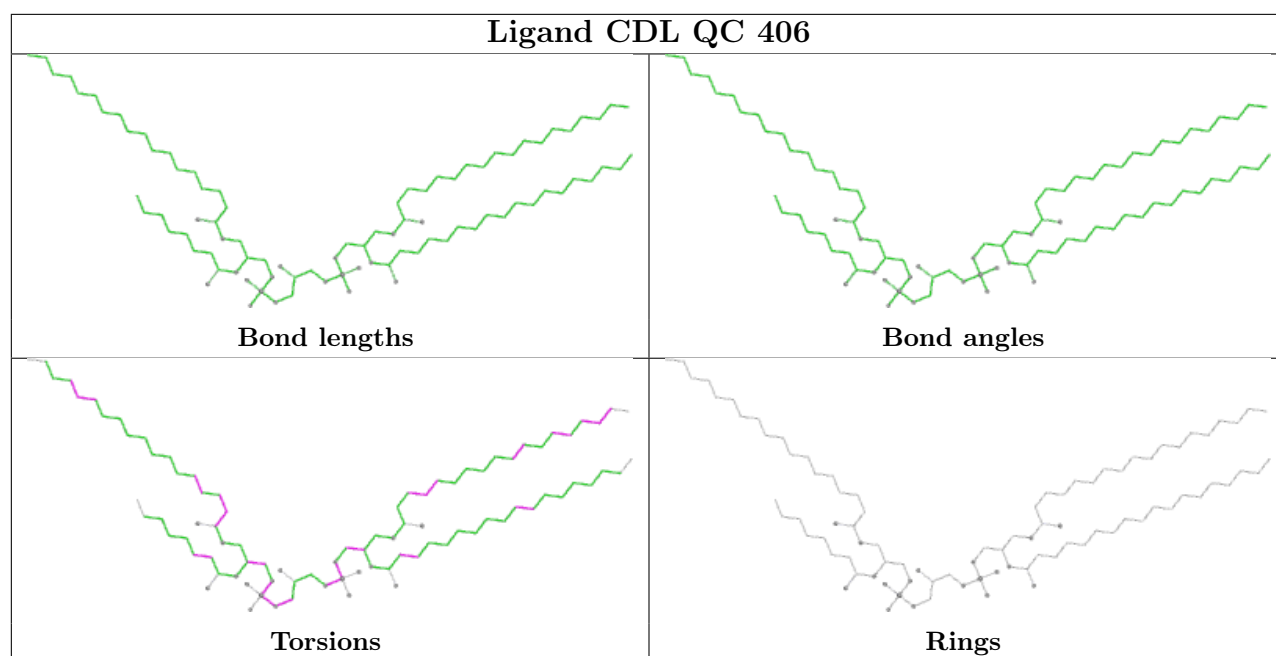
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Bond lengths	Bond angles
	
Torsions	Rings

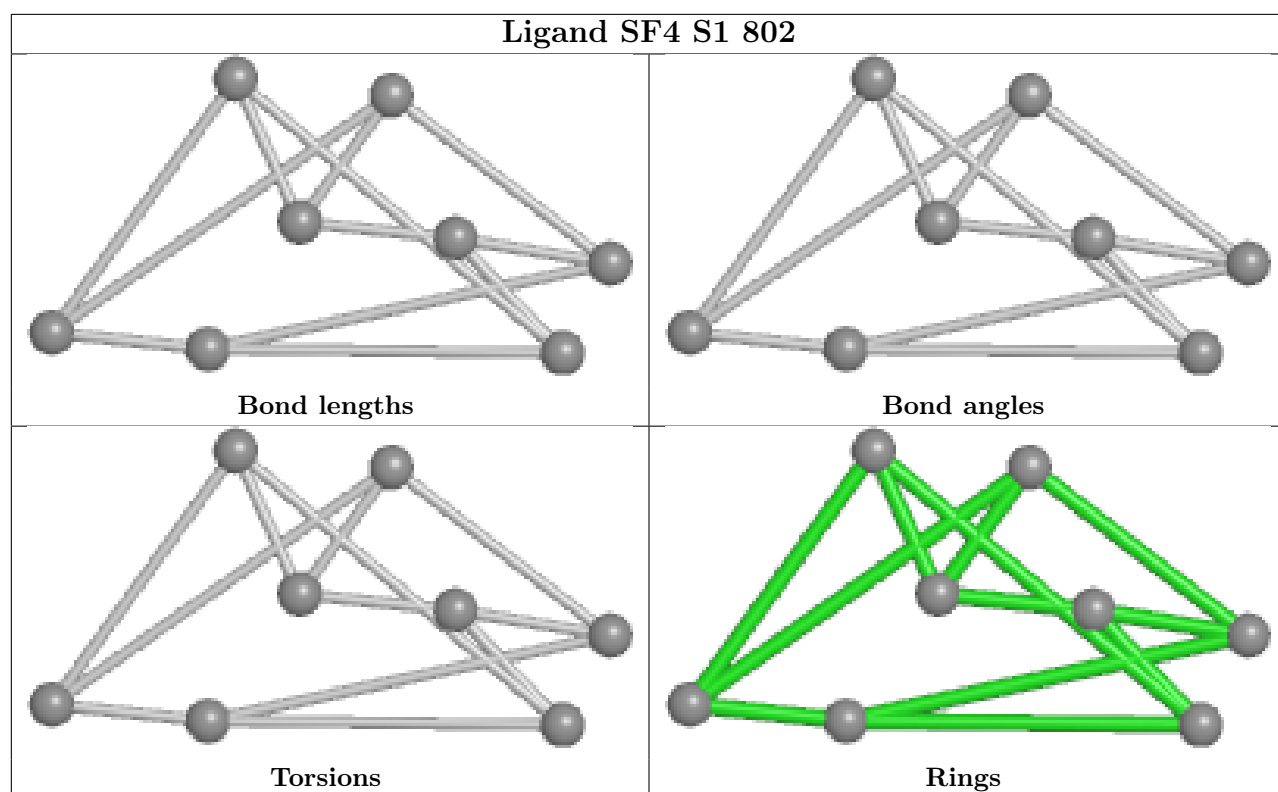




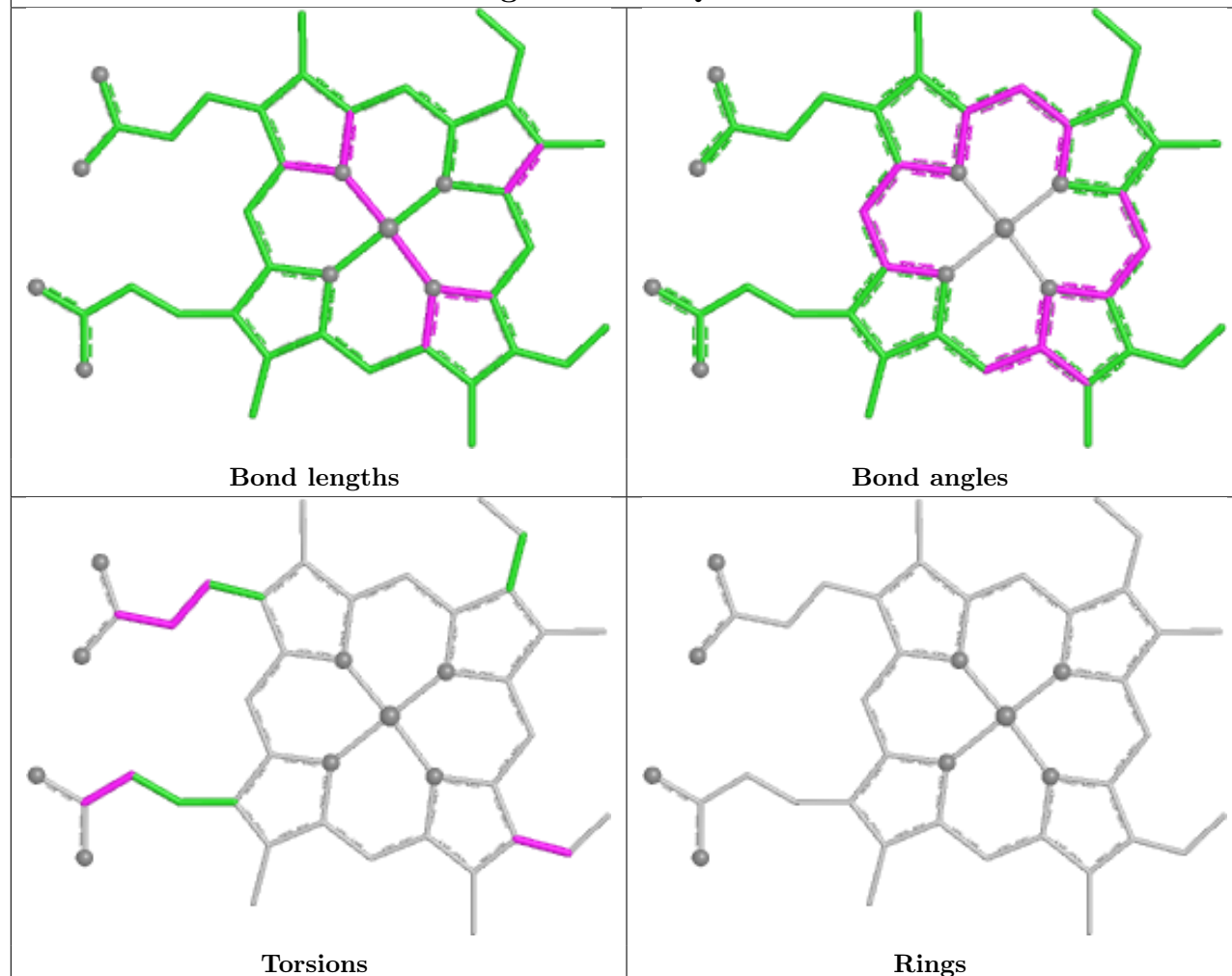




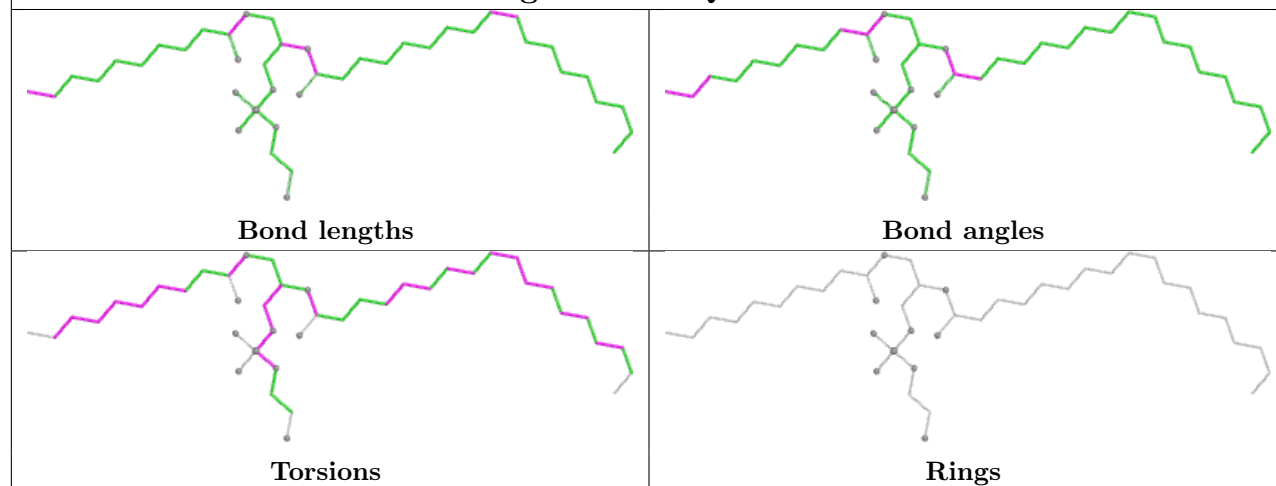


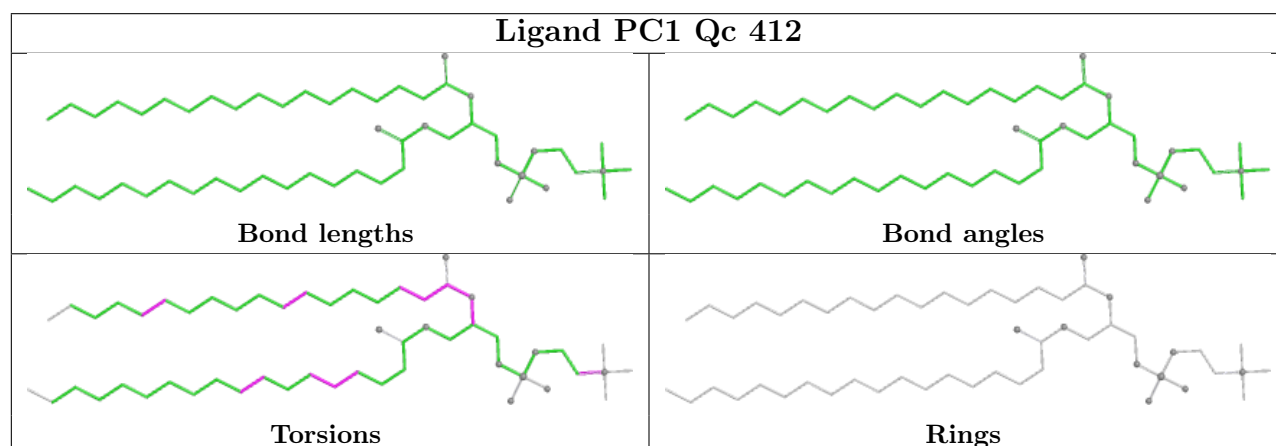
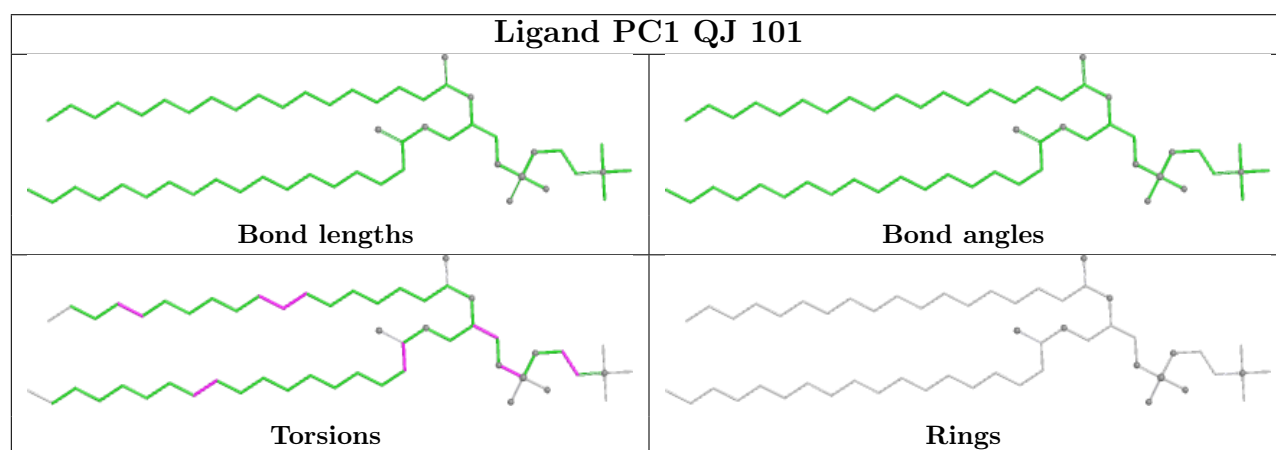
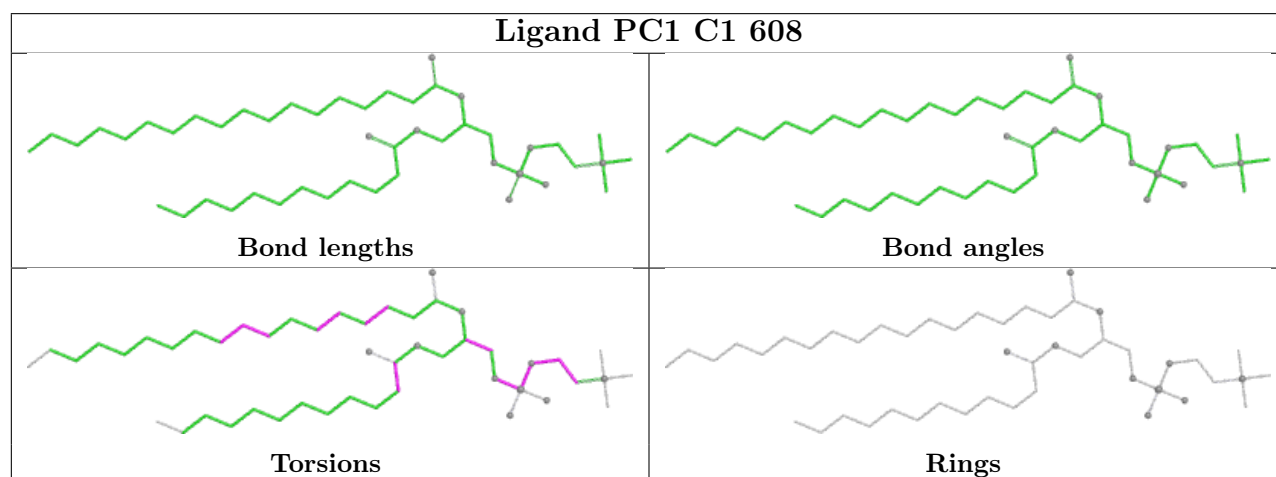
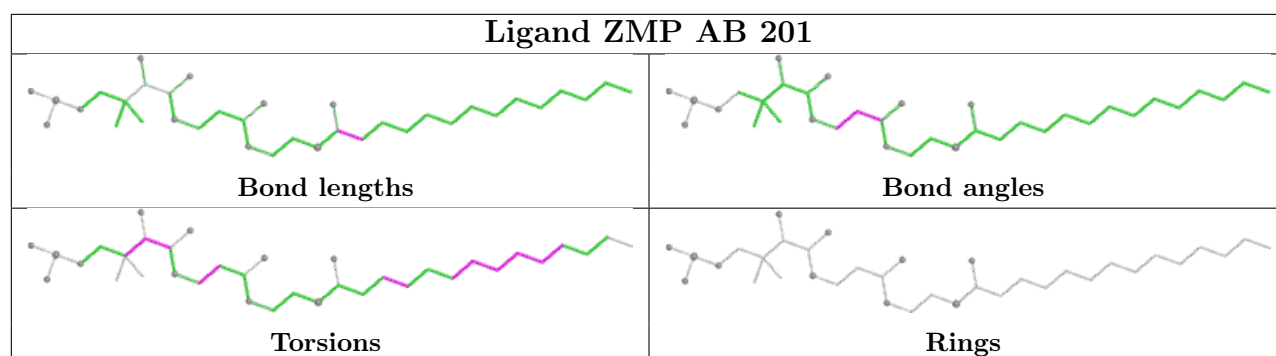


Ligand HEM Qc 404

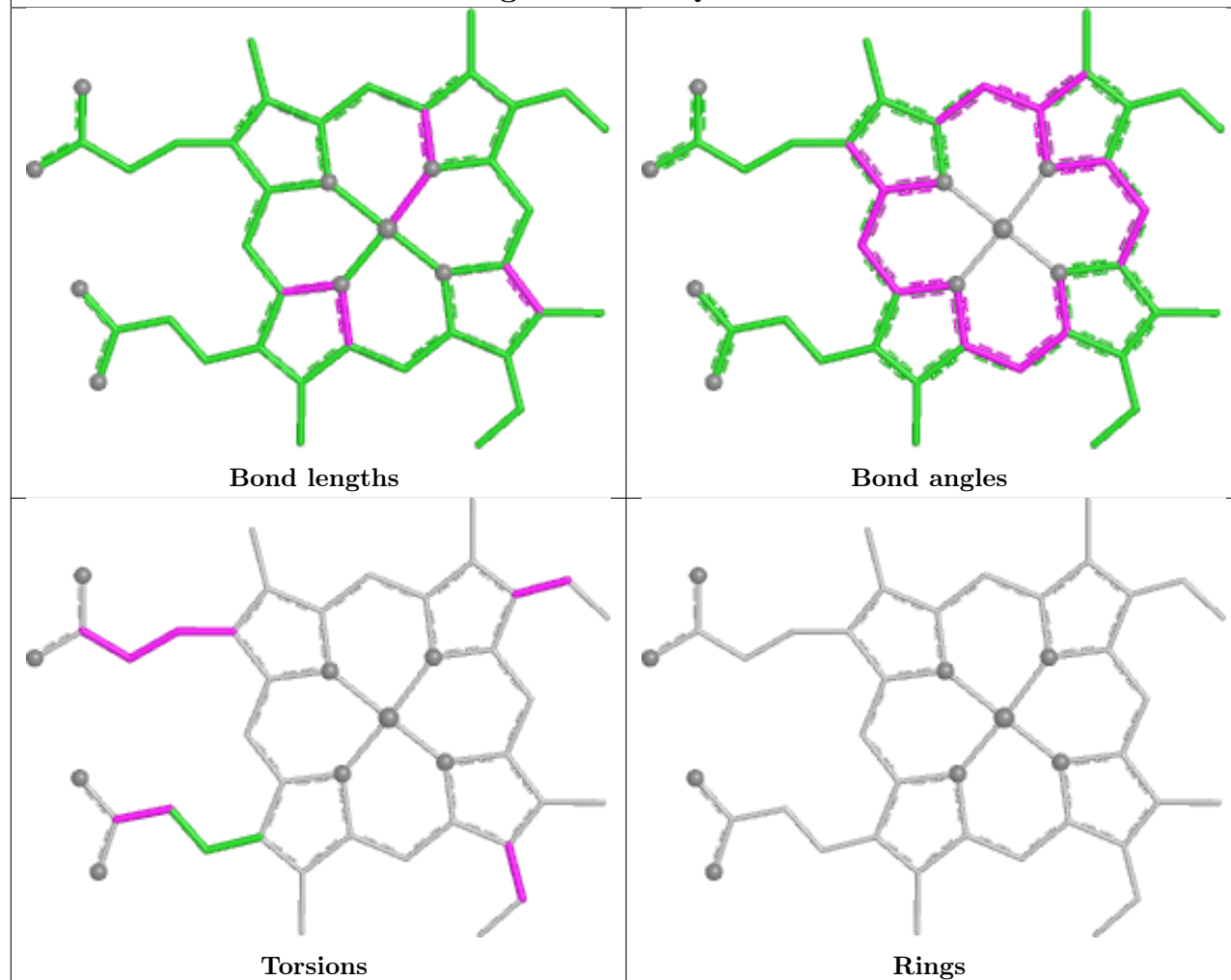


Ligand PEE QC 405

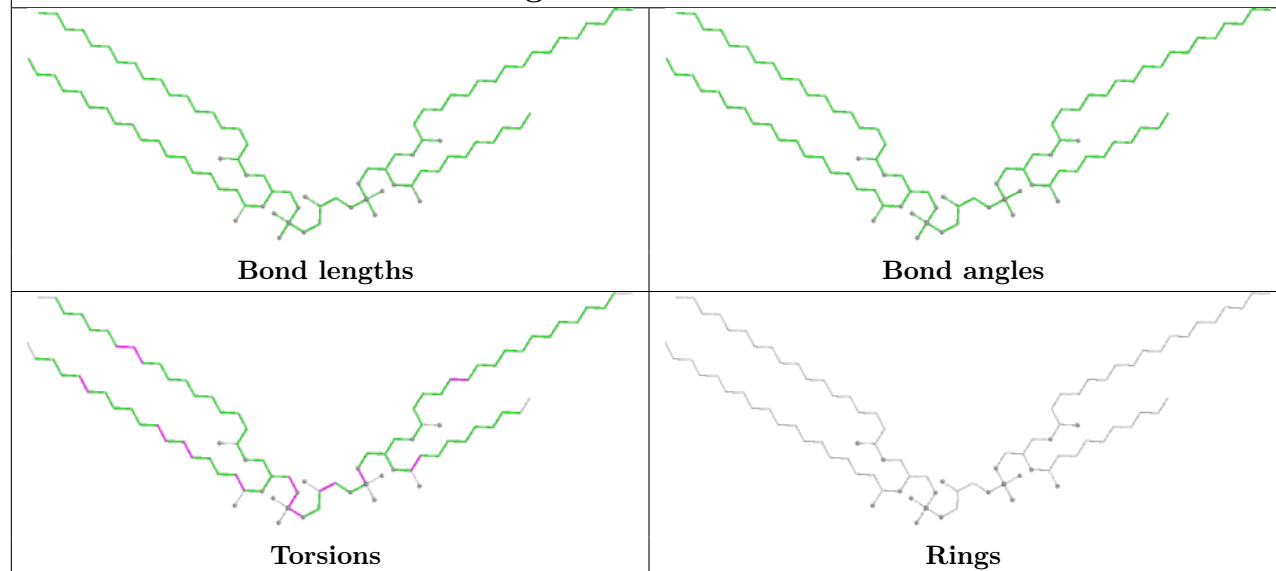


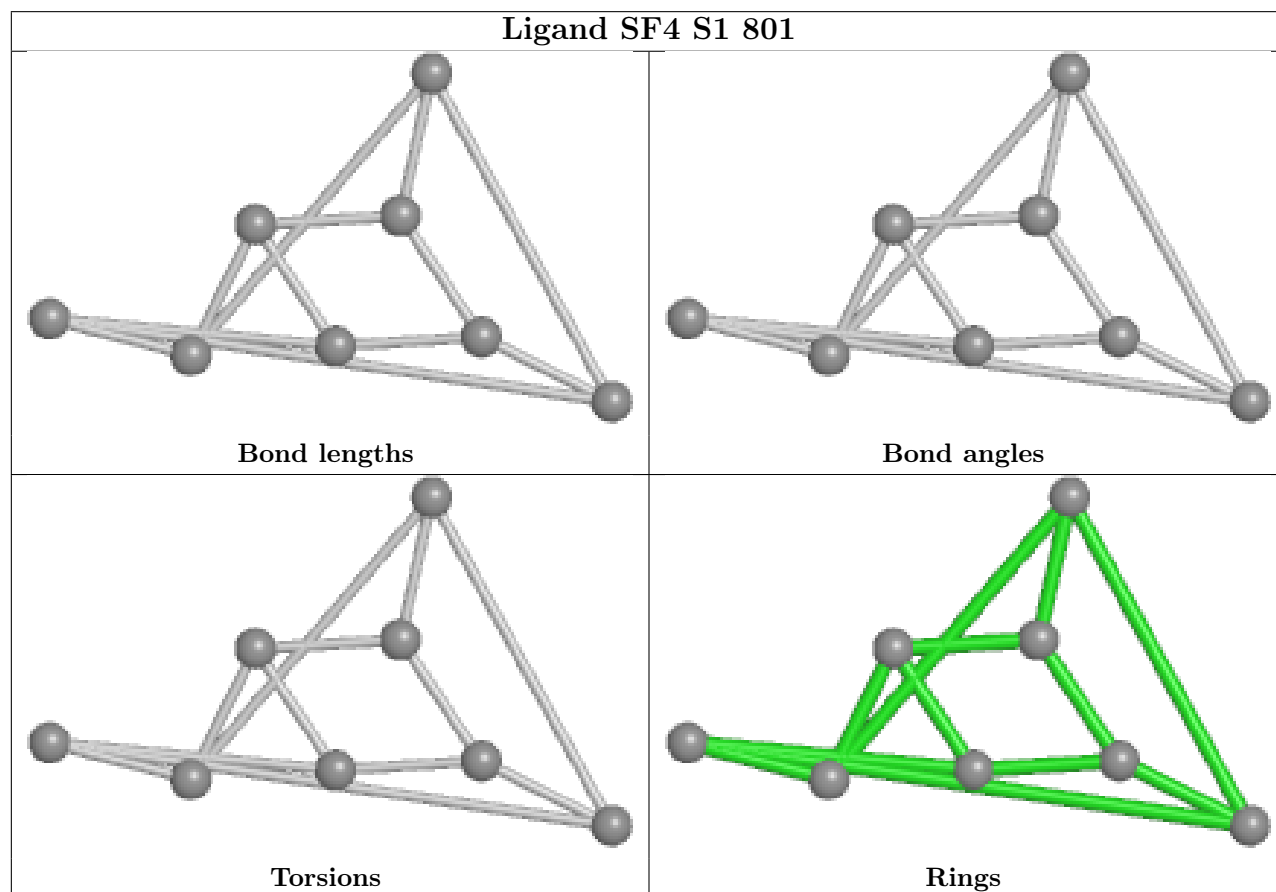
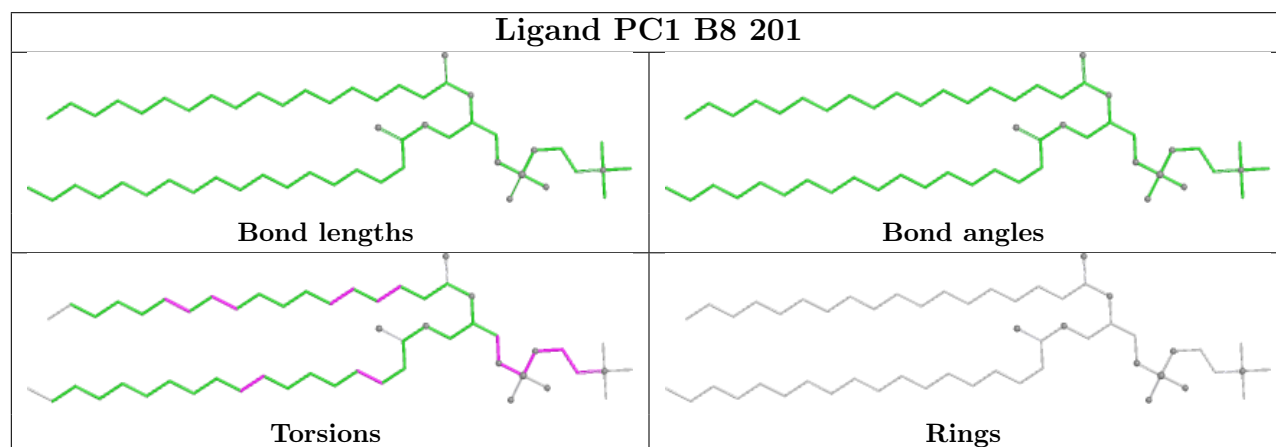
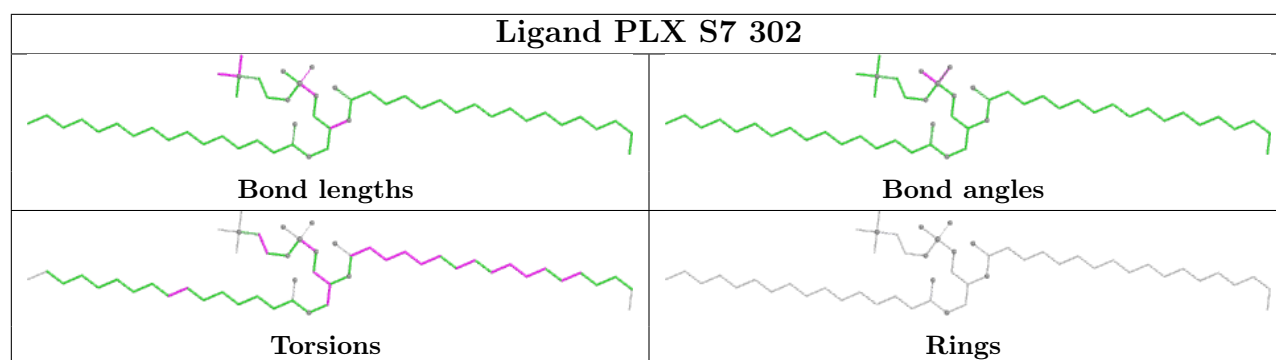


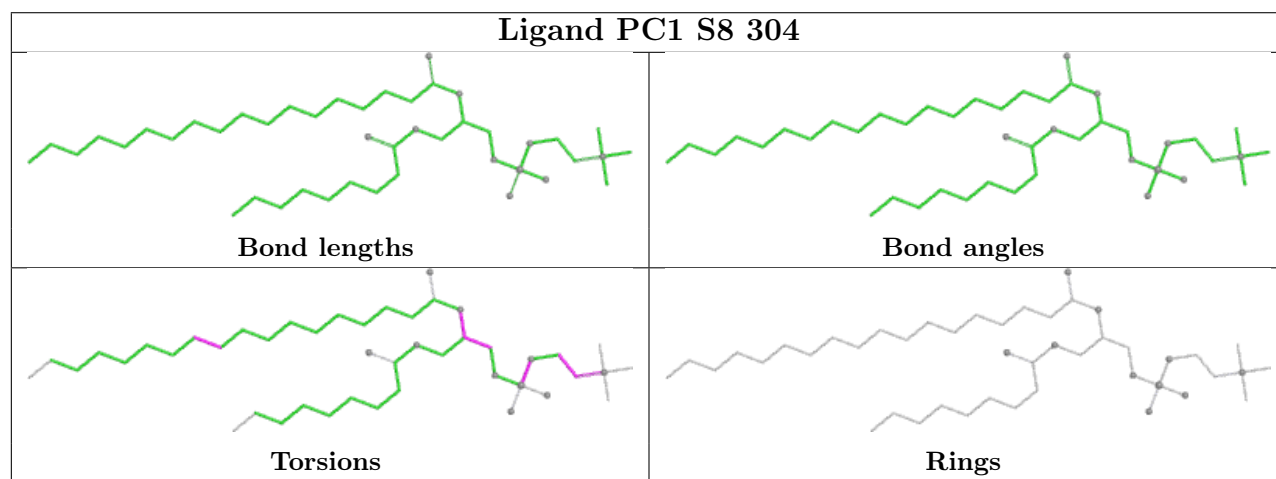
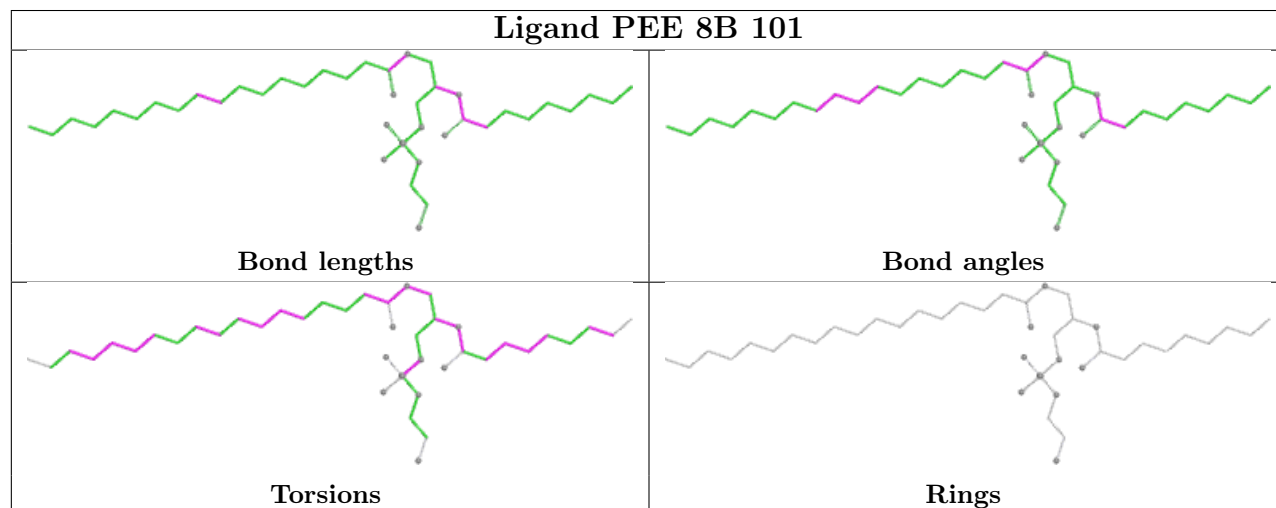
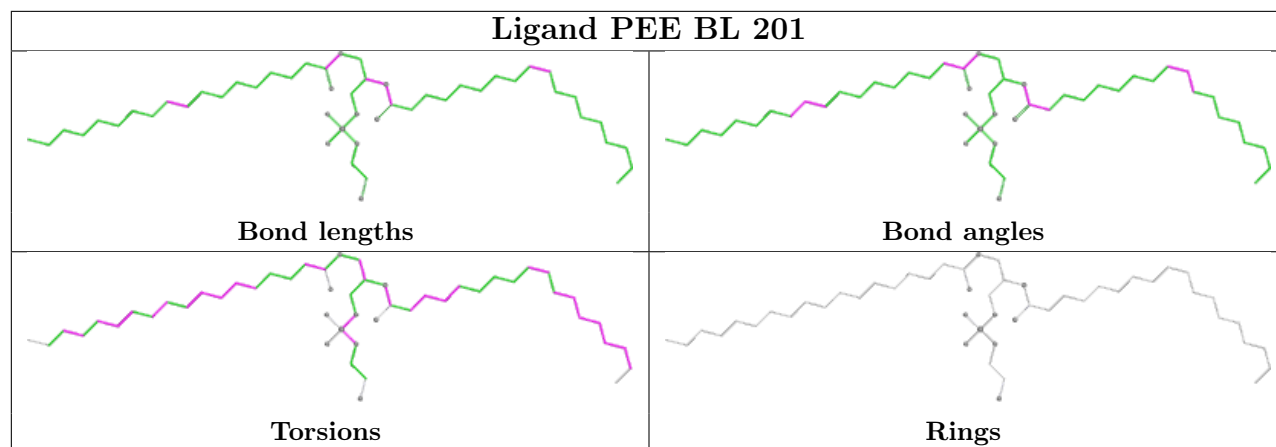
Ligand HEM Qc 405

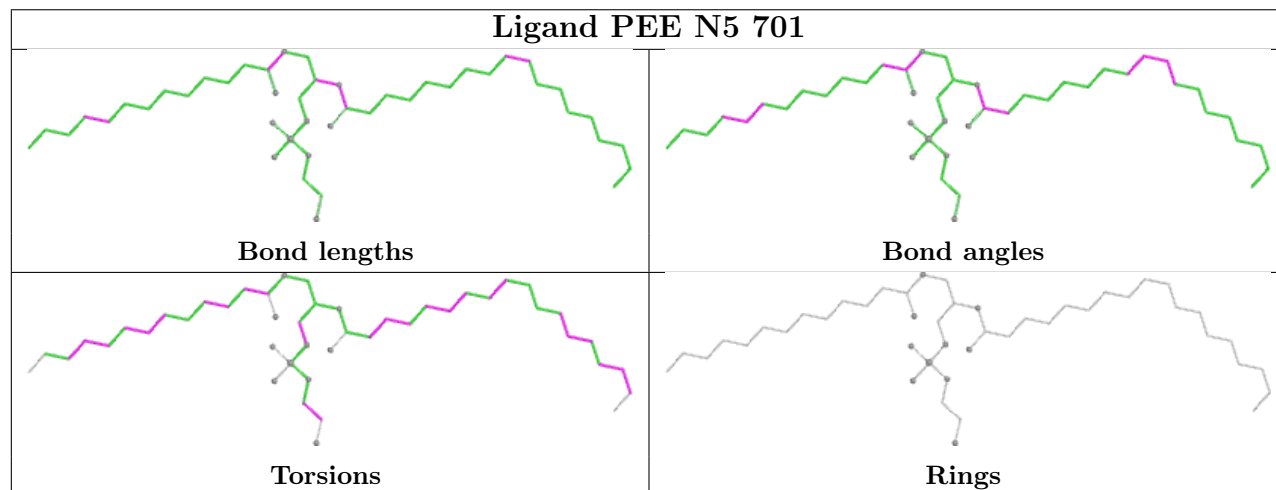
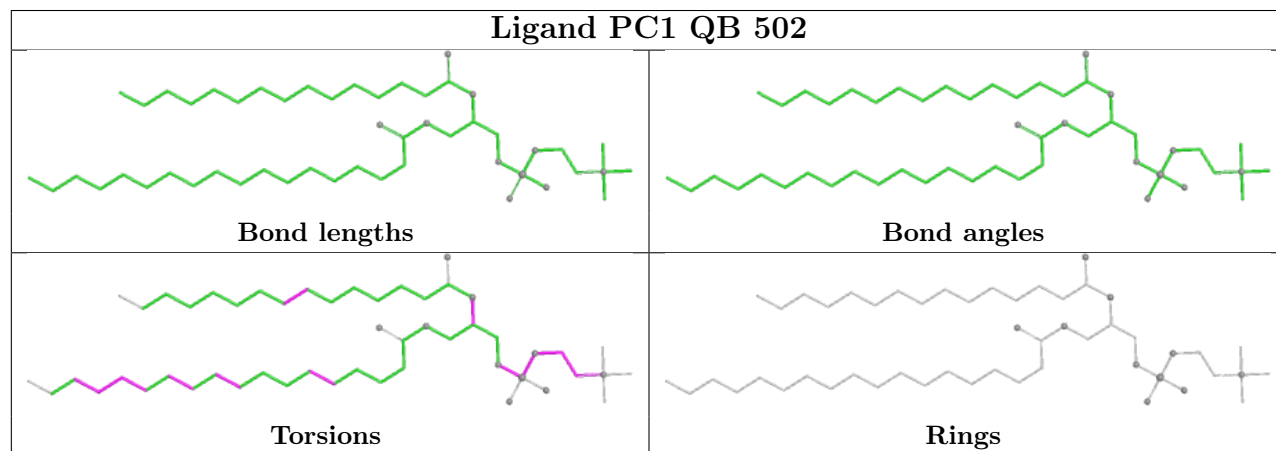
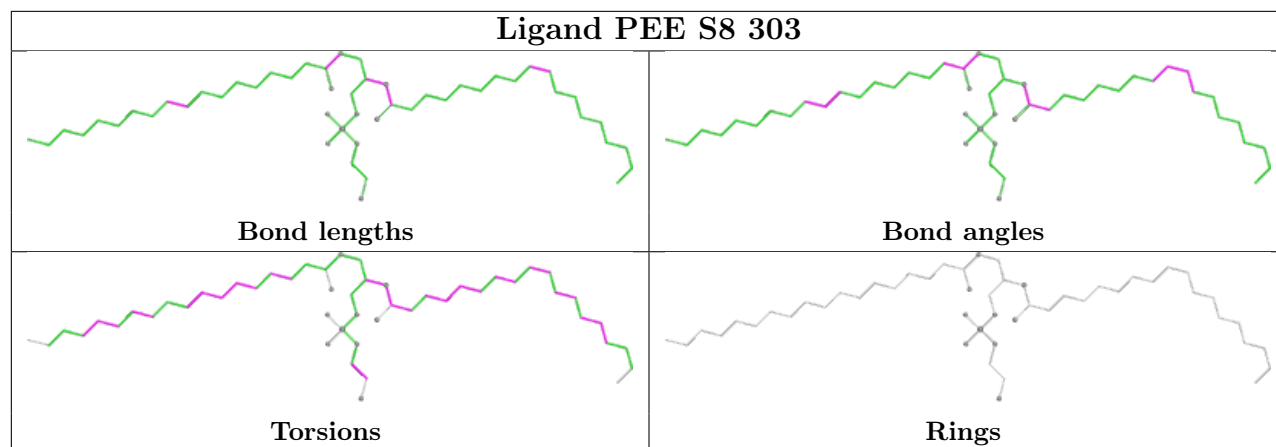


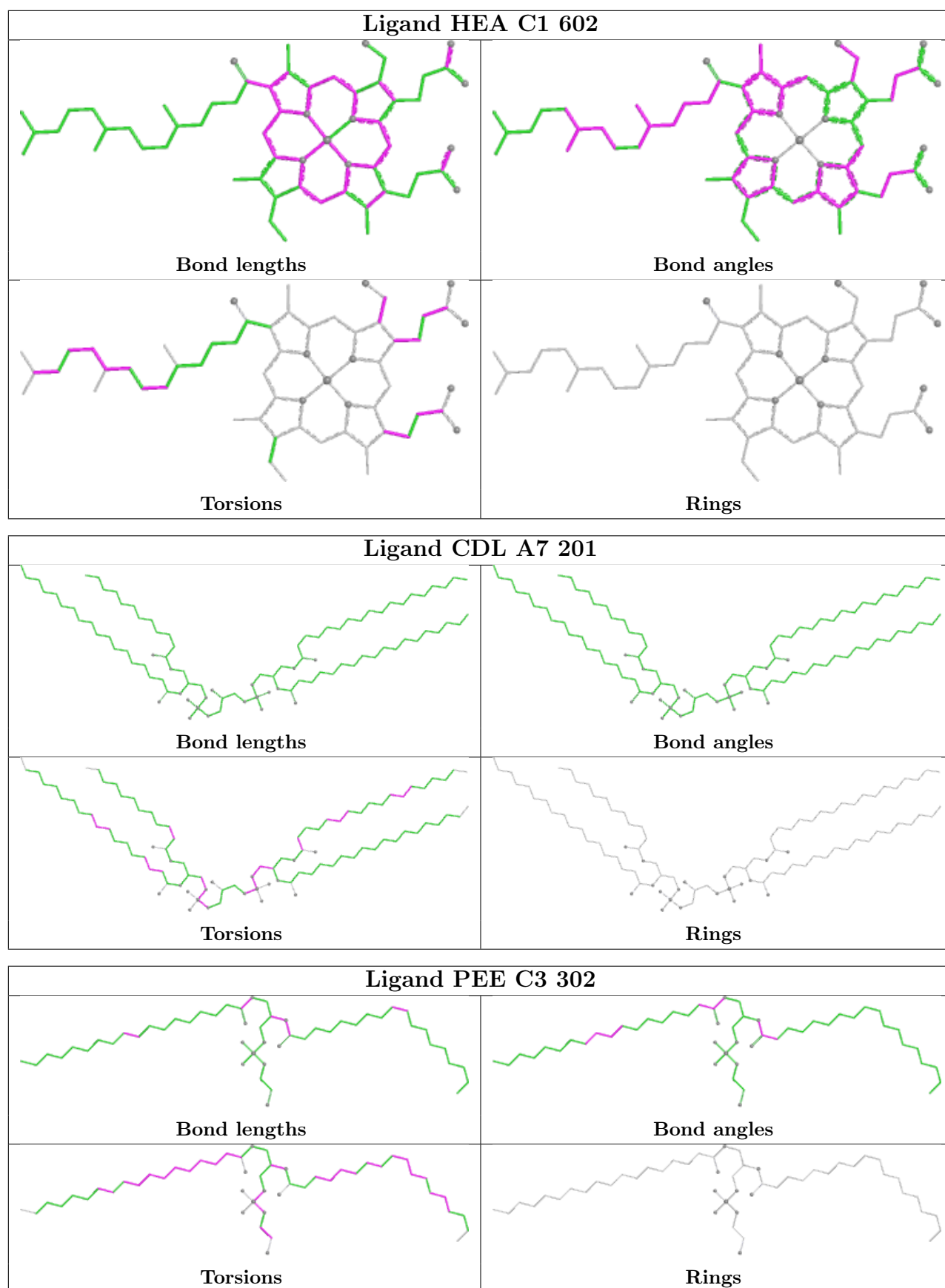
Ligand CDL 4L 101

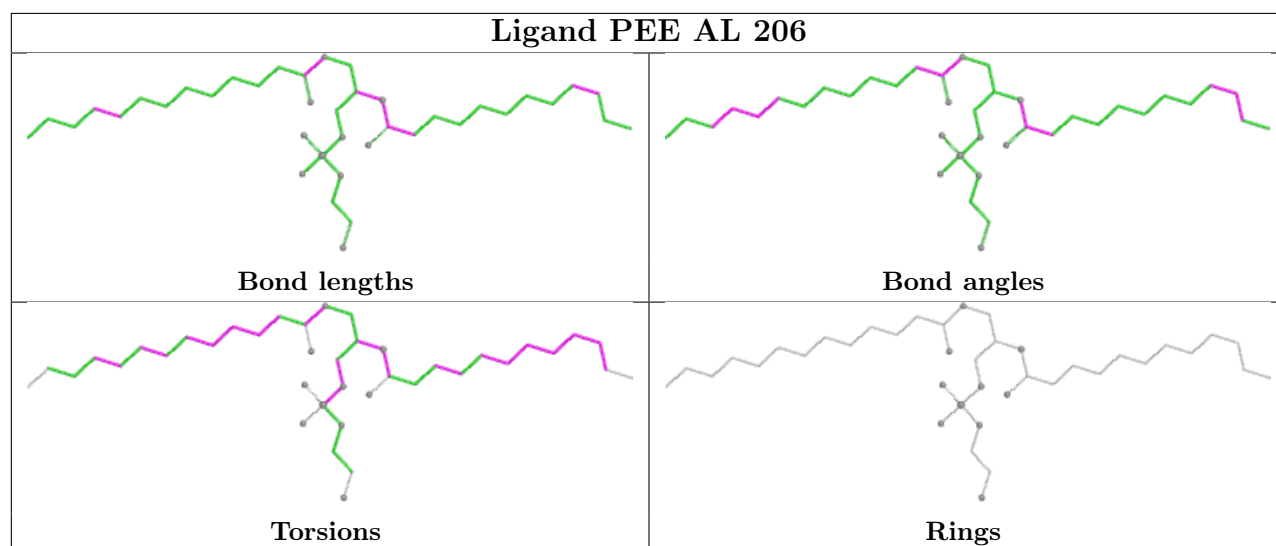
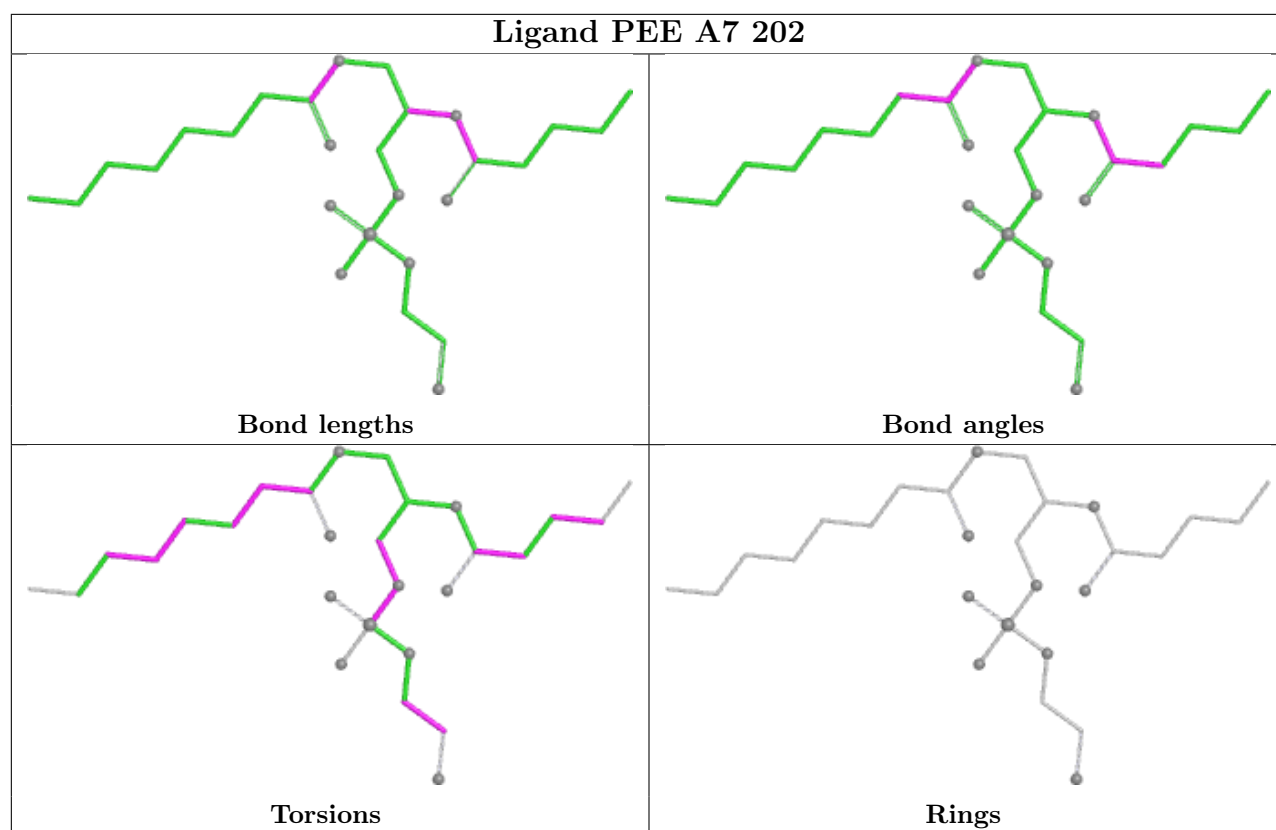


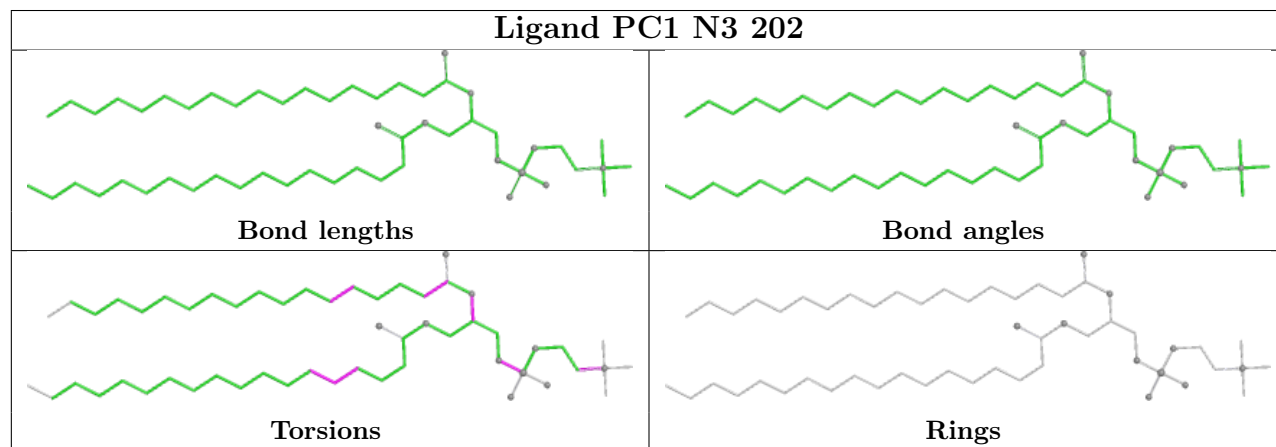
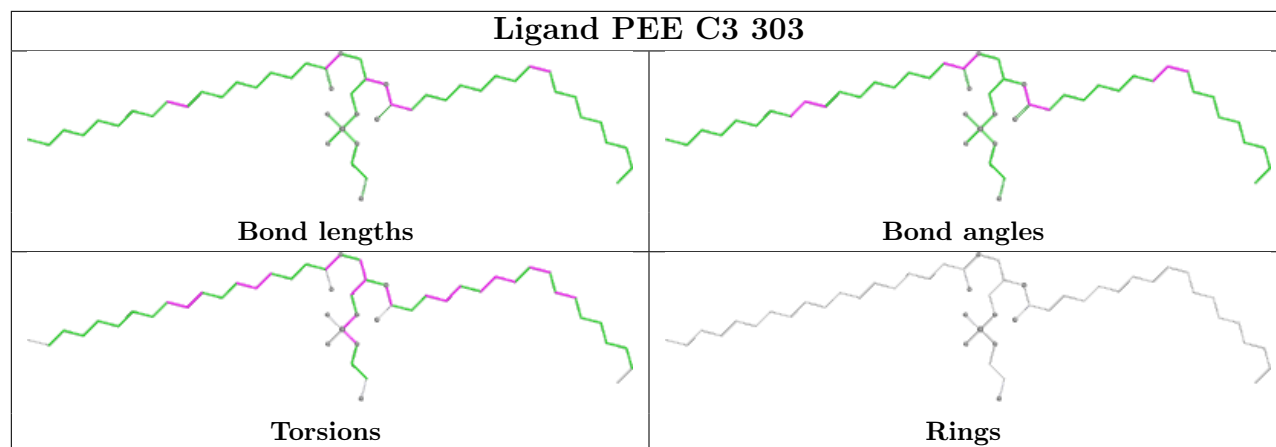




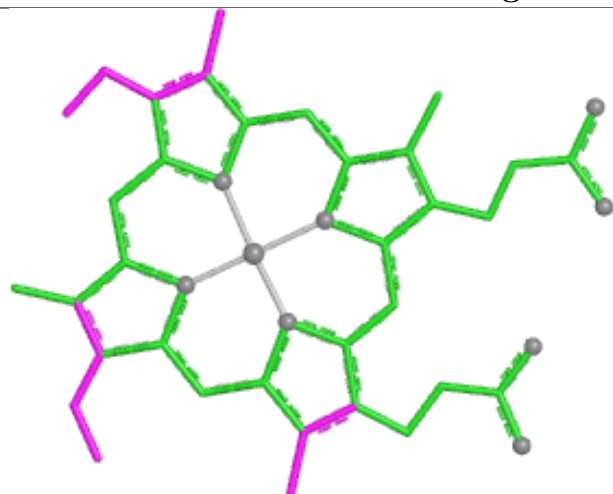




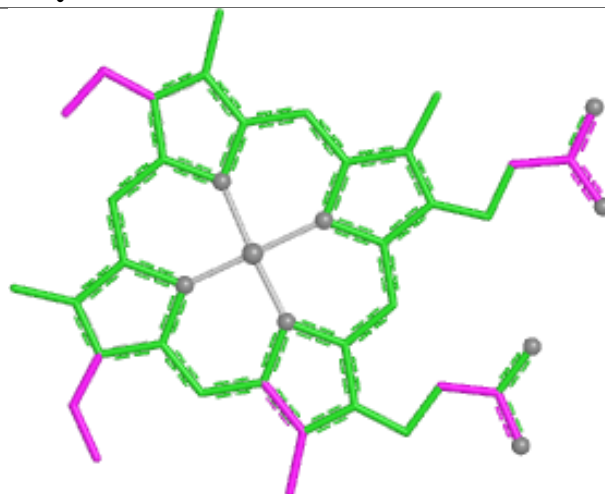




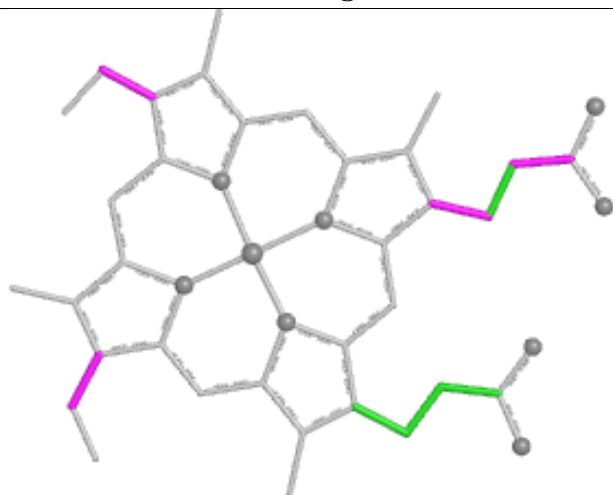
Ligand HEC Qd 401



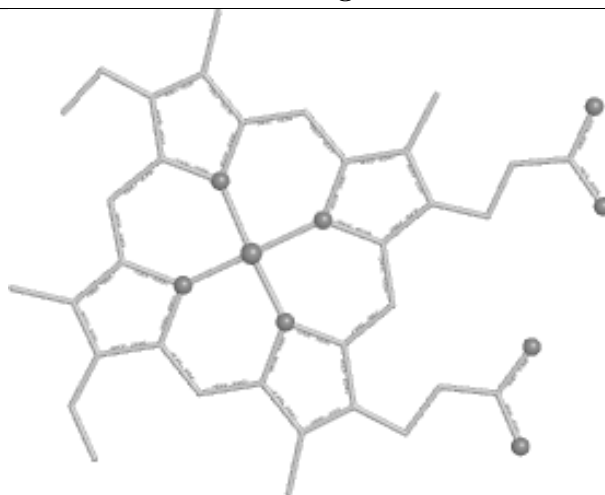
Bond lengths



Bond angles



Torsions

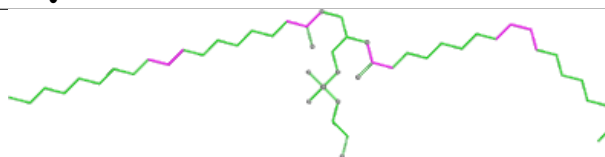


Rings

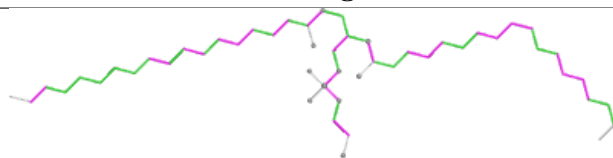
Ligand PEE QH 102



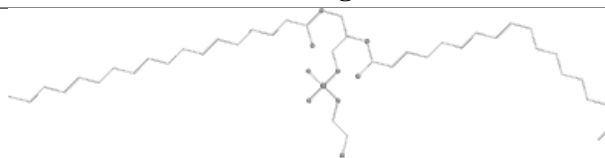
Bond lengths



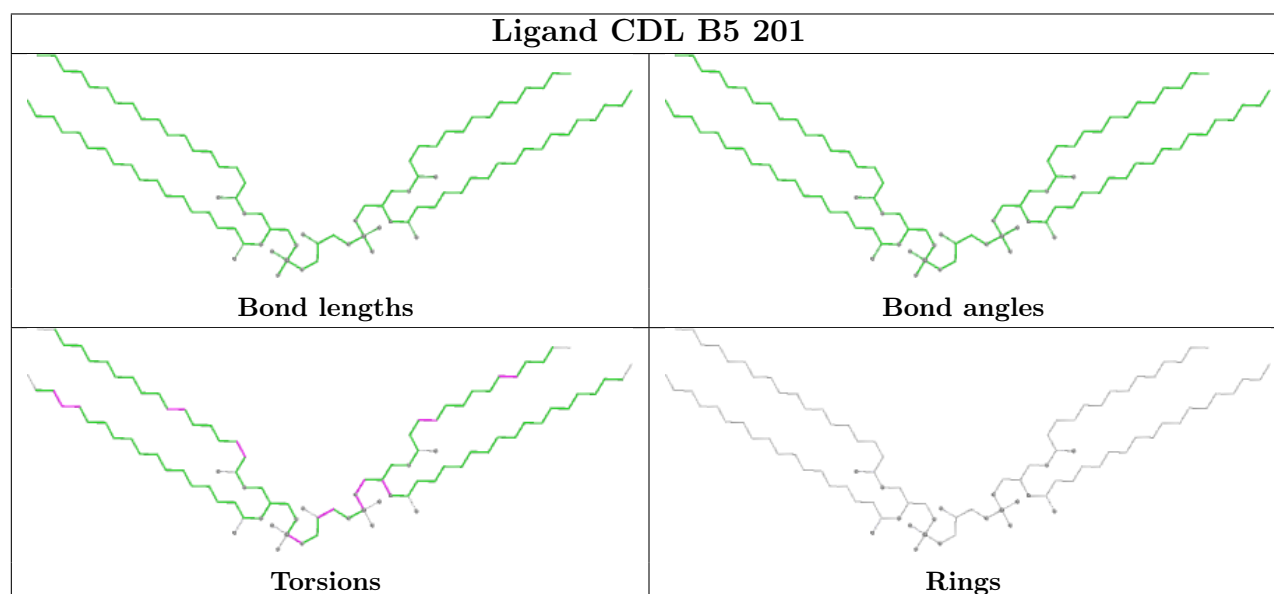
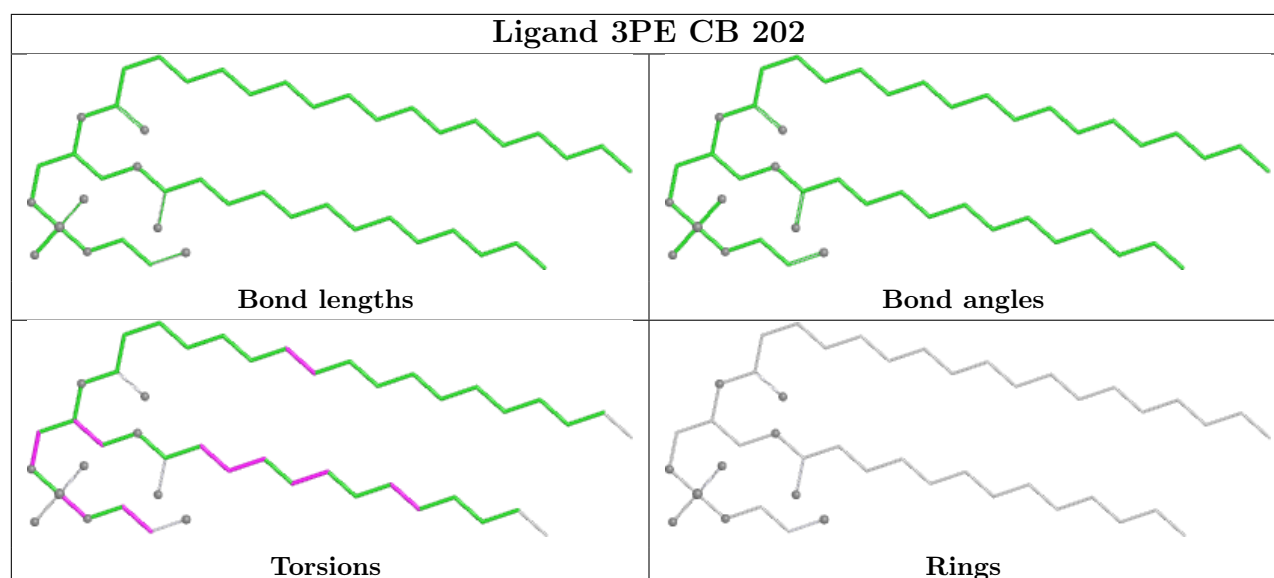
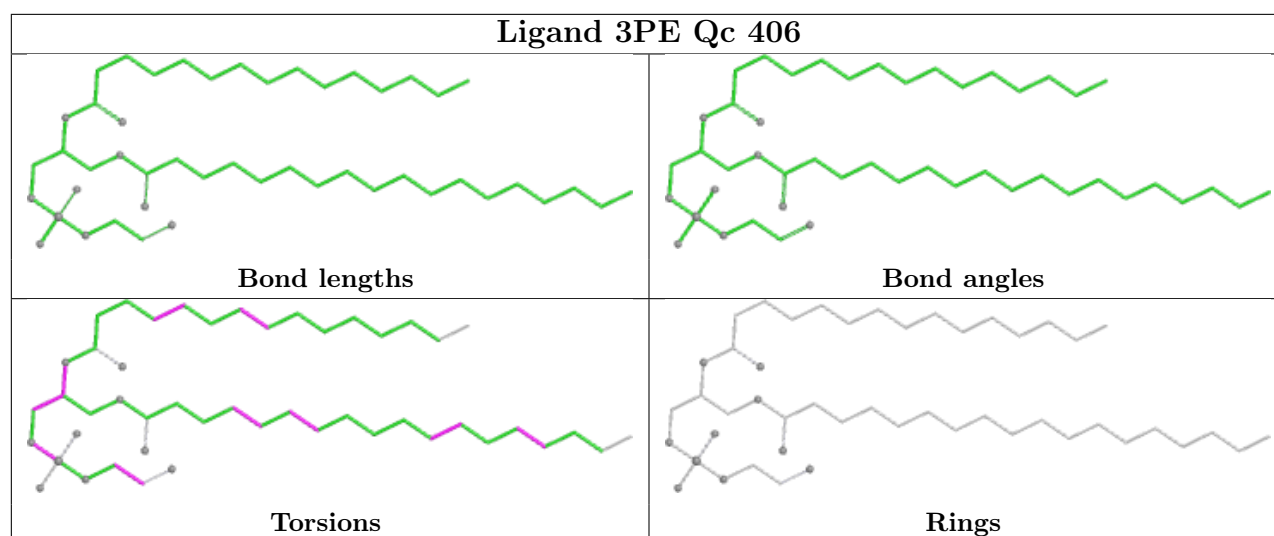
Bond angles

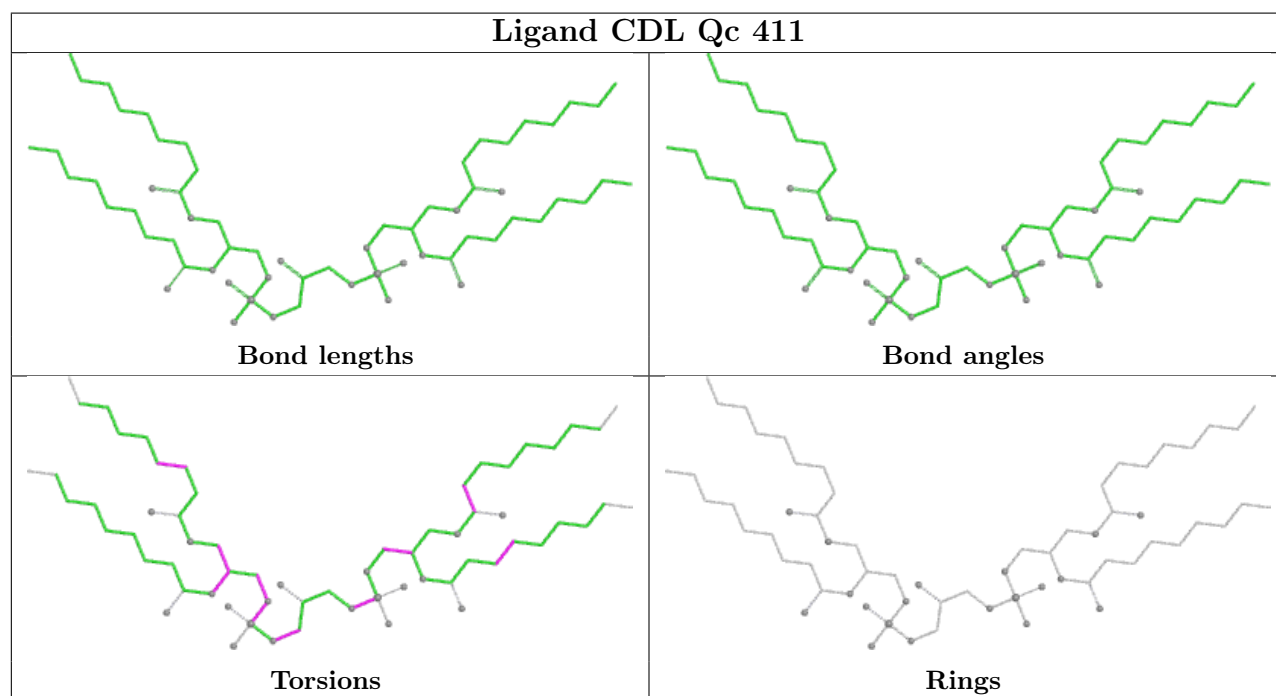
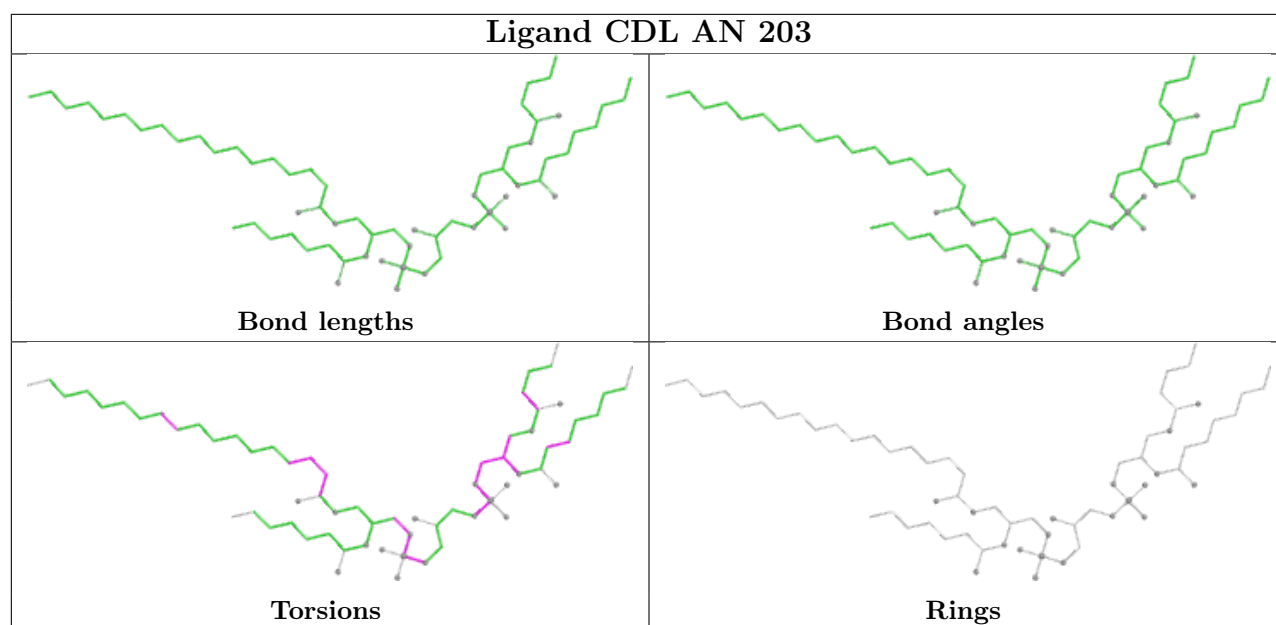


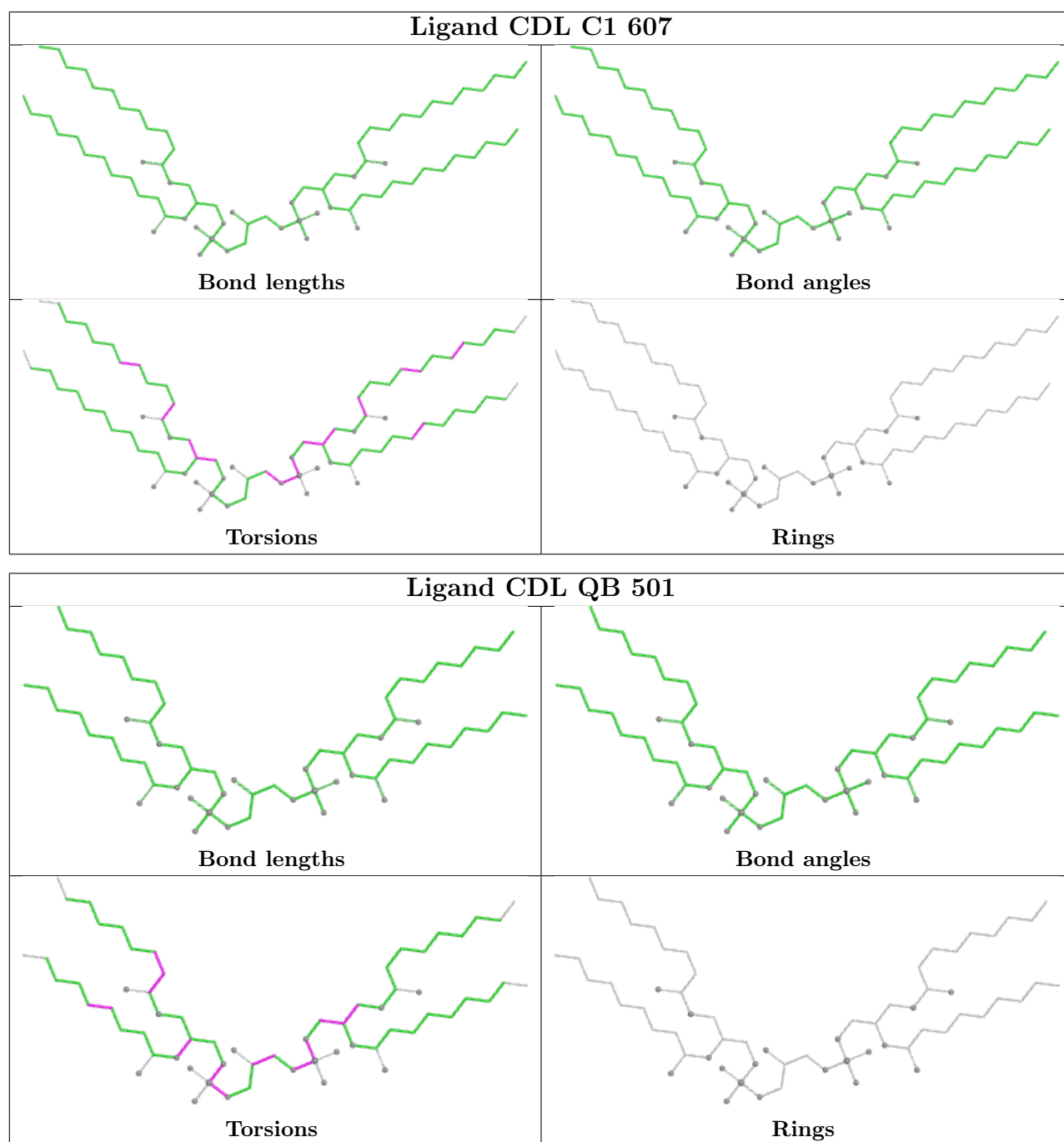
Torsions

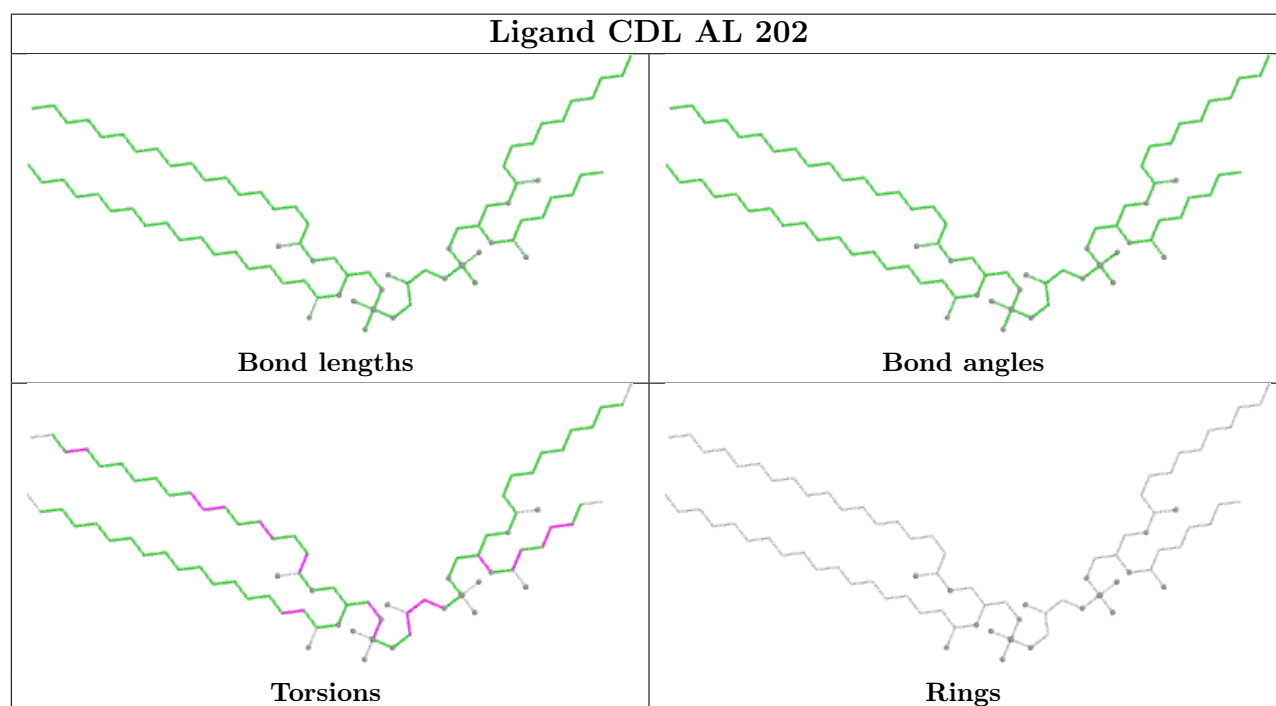
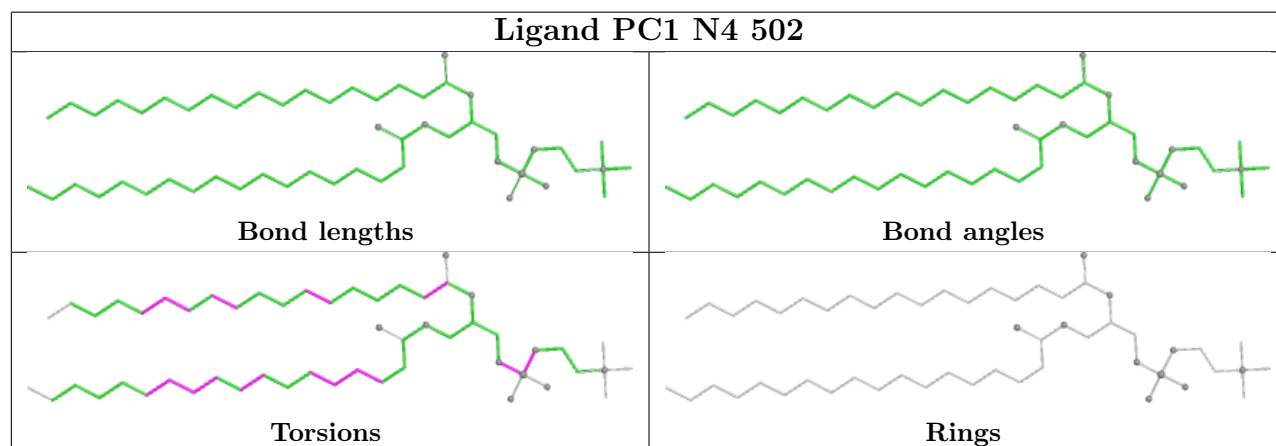
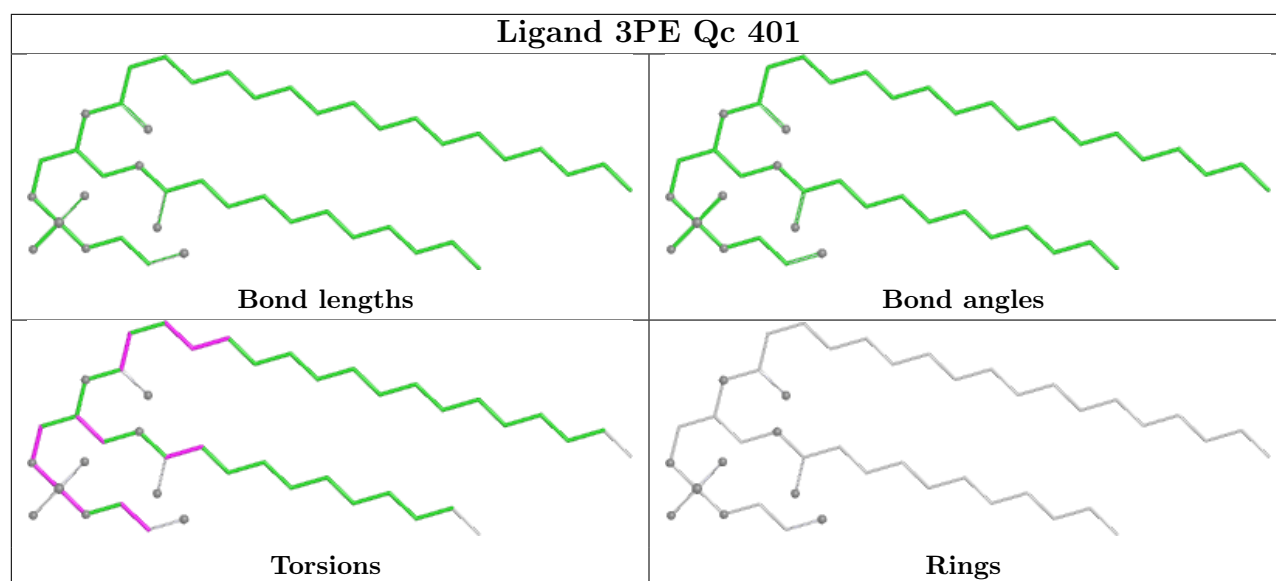


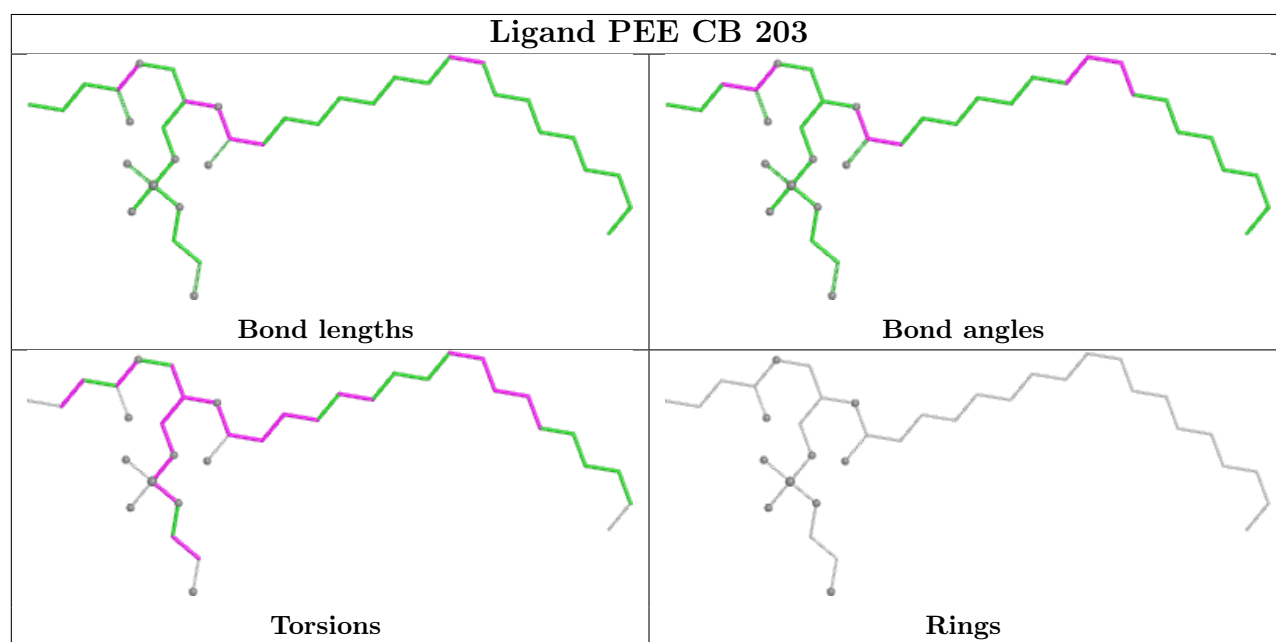
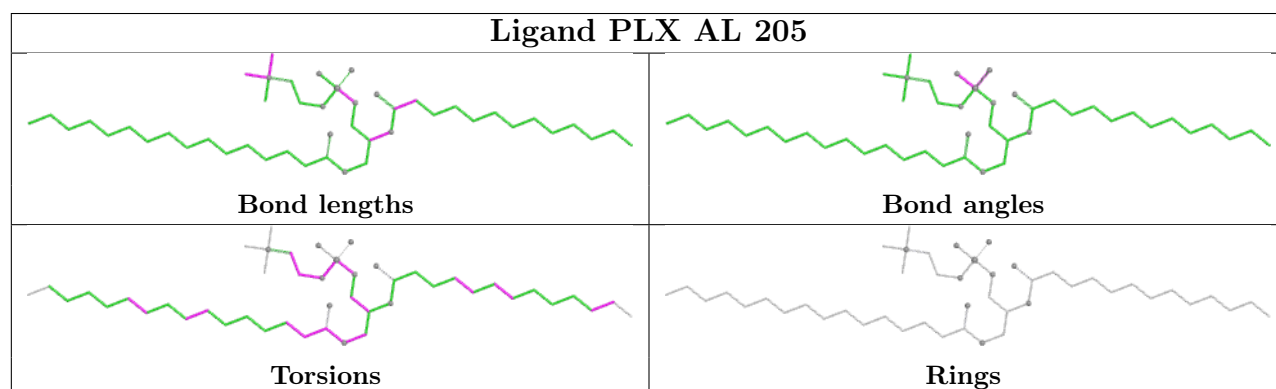
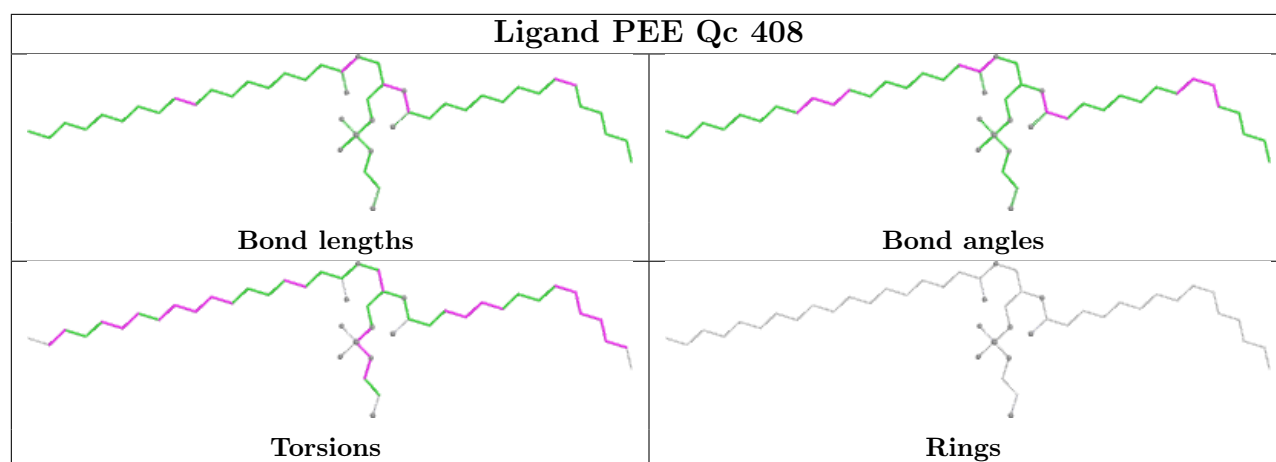
Rings

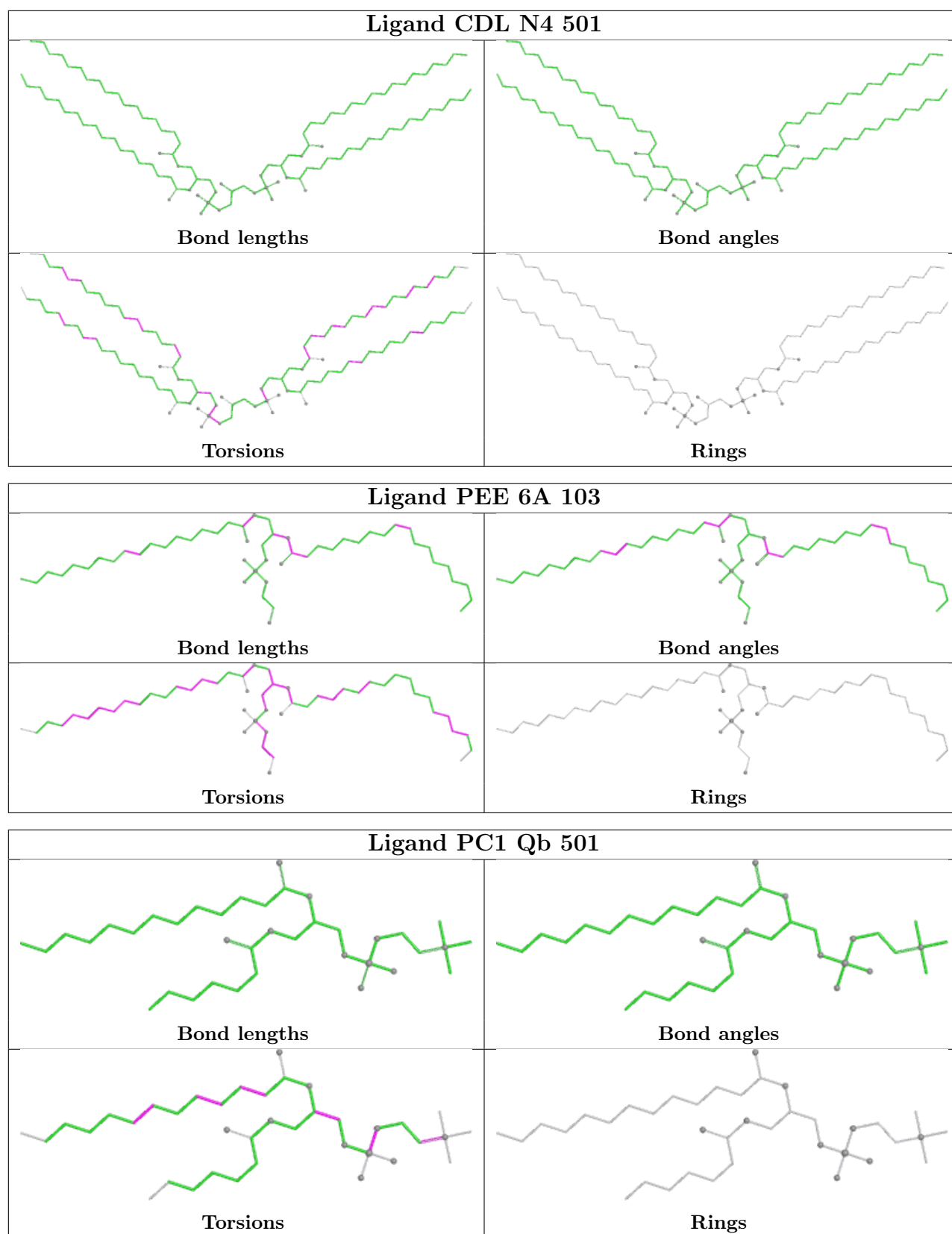


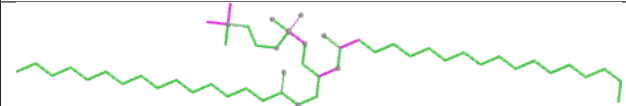
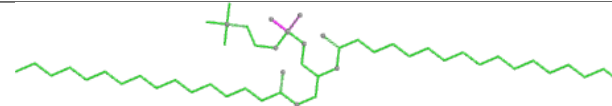
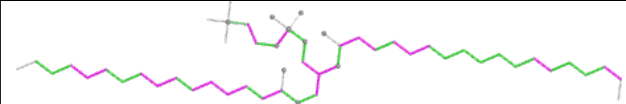
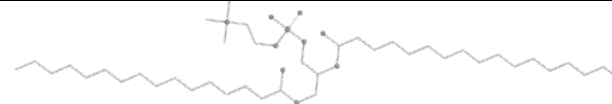


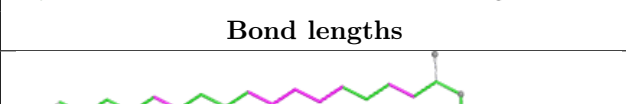
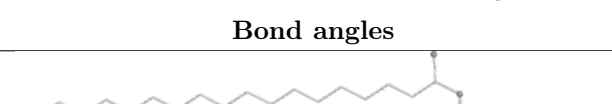


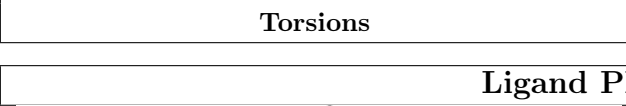
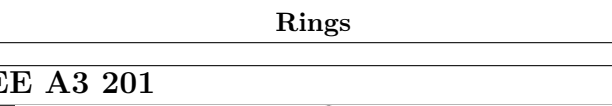




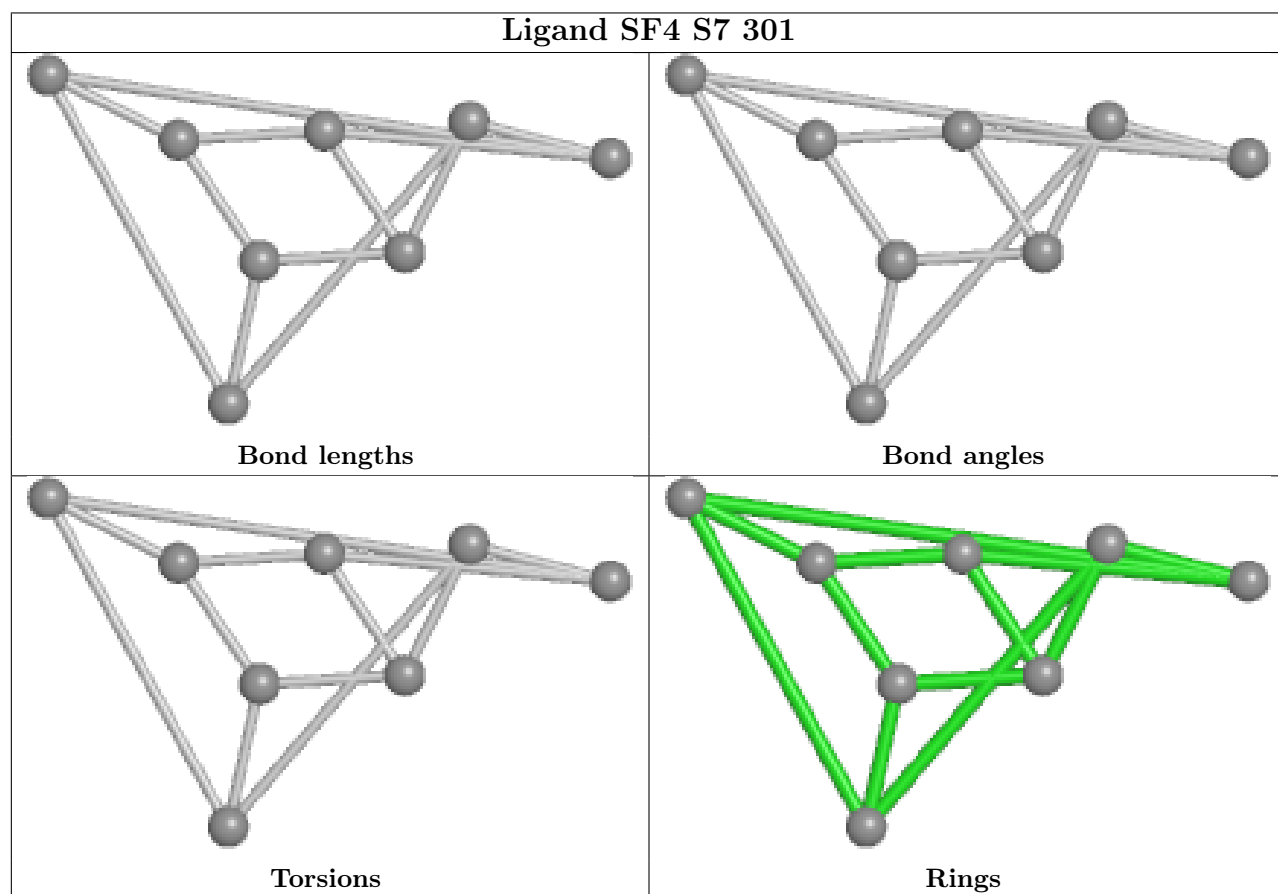
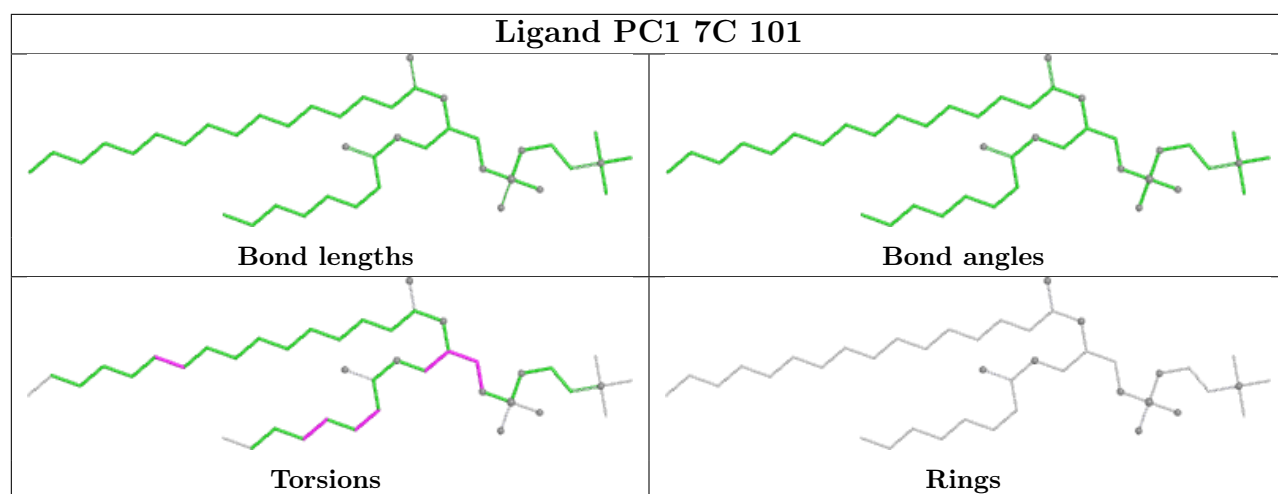


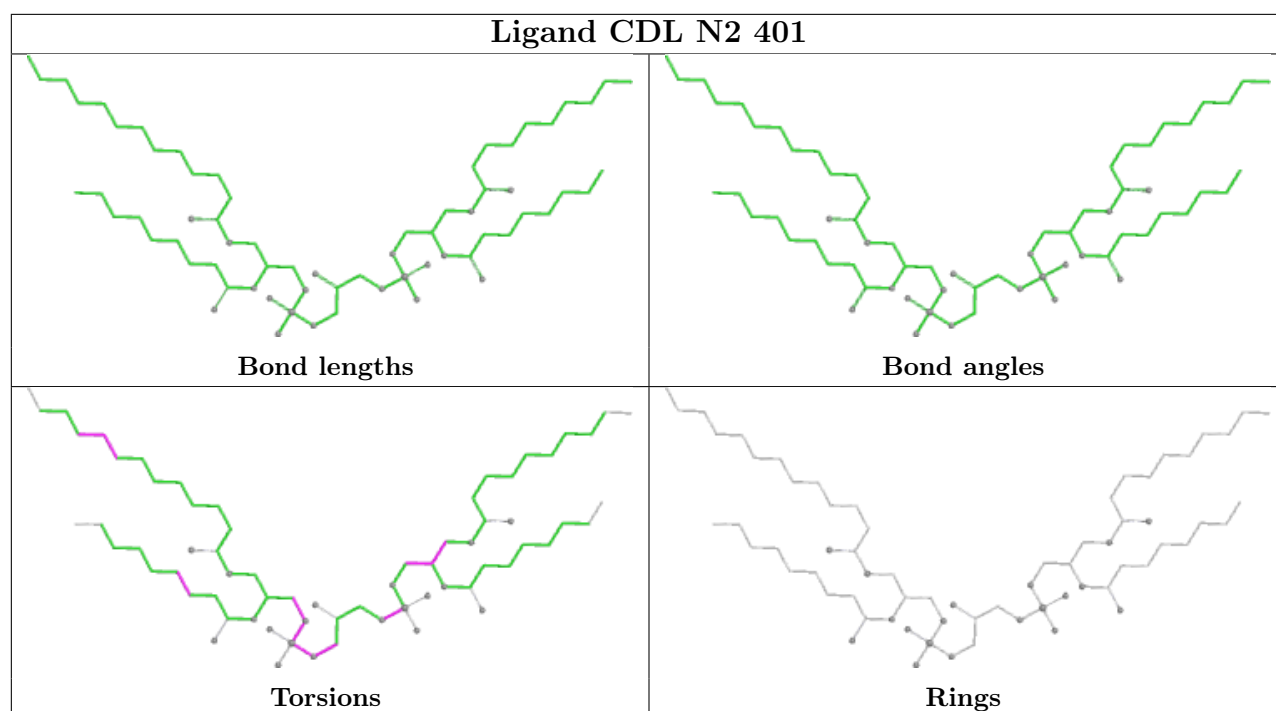
Ligand PLX QI 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 N1 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE A3 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE 6A 102	
	
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.

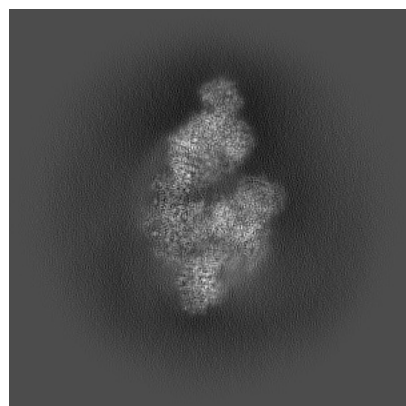
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60319. These allow visual inspection of the internal detail of the map and identification of artifacts.

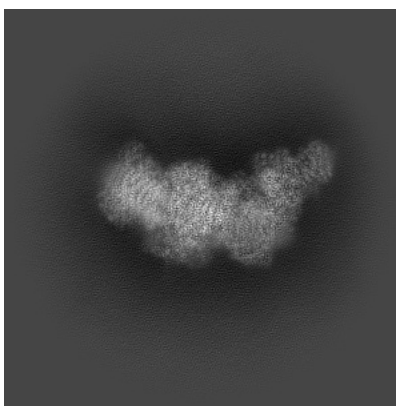
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

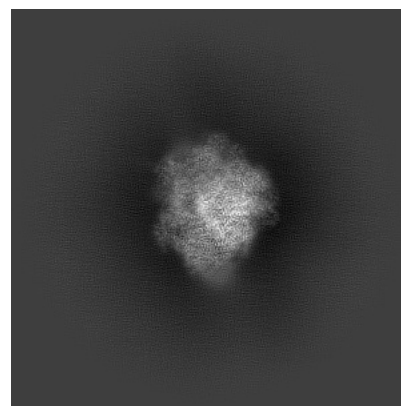
6.1.1 Primary map



X

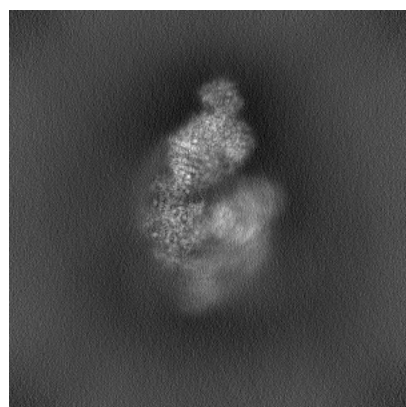


Y

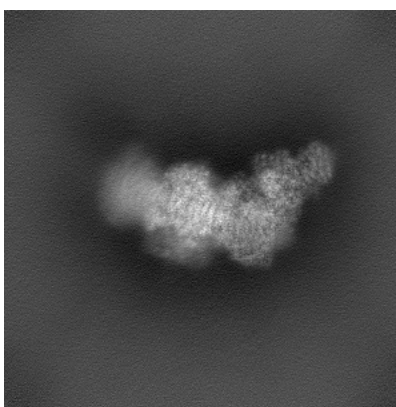


Z

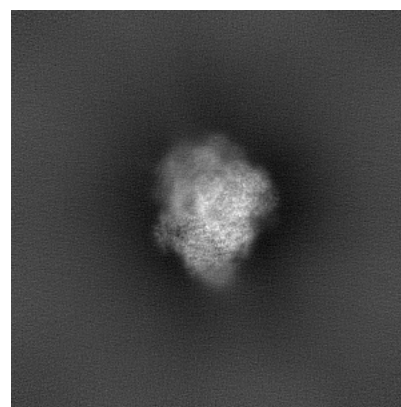
6.1.2 Raw map



X



Y

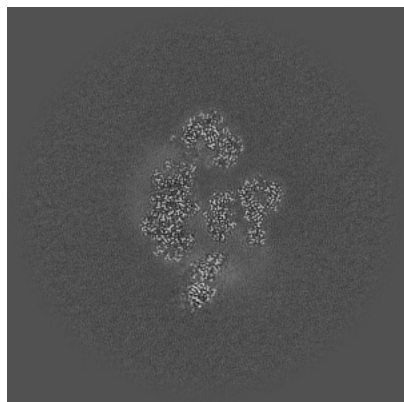


Z

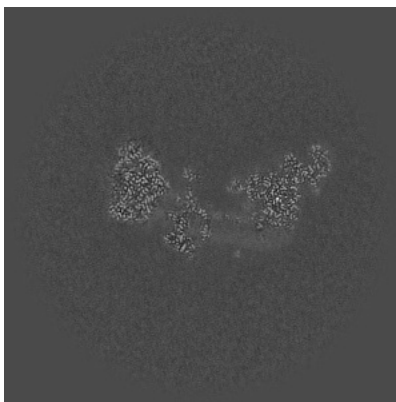
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

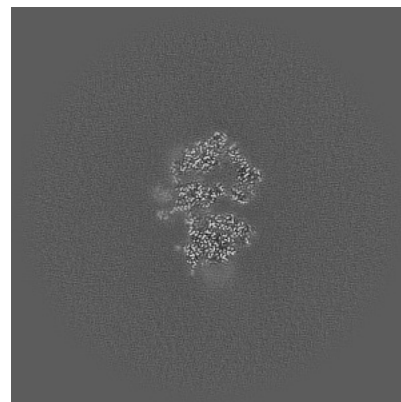
6.2.1 Primary map



X Index: 240

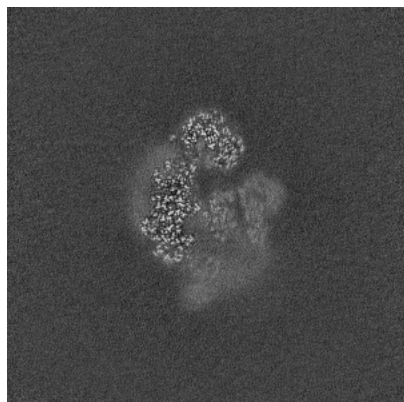


Y Index: 240

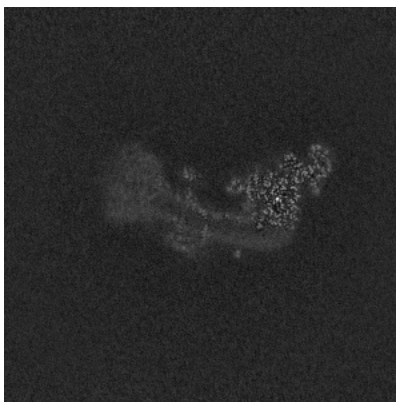


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

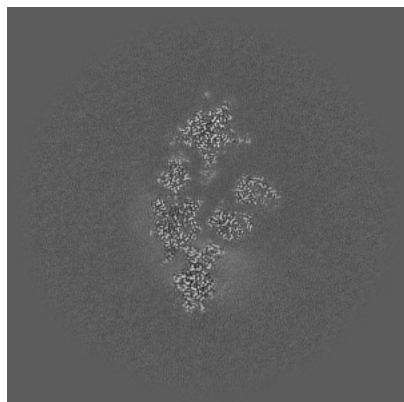


Z Index: 240

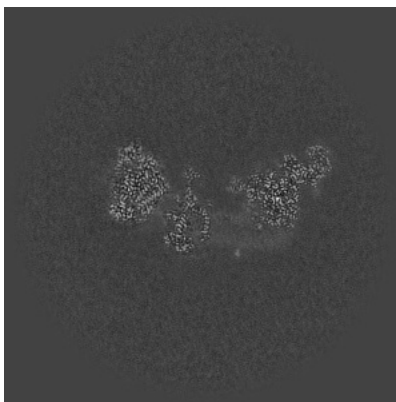
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

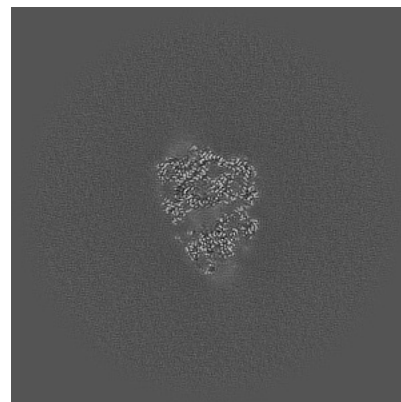
6.3.1 Primary map



X Index: 259

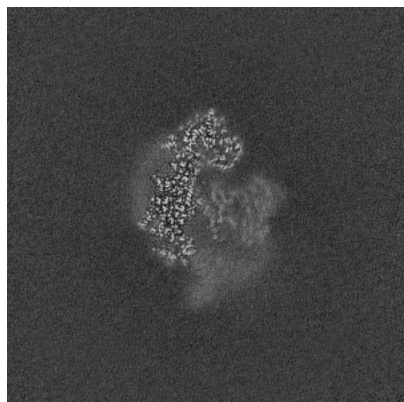


Y Index: 241

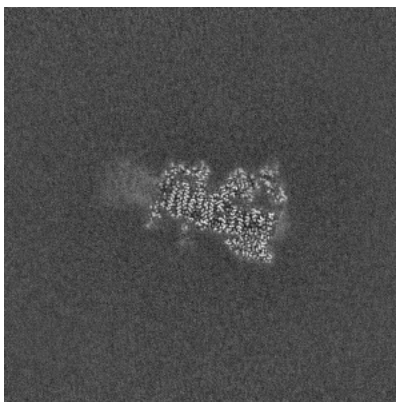


Z Index: 217

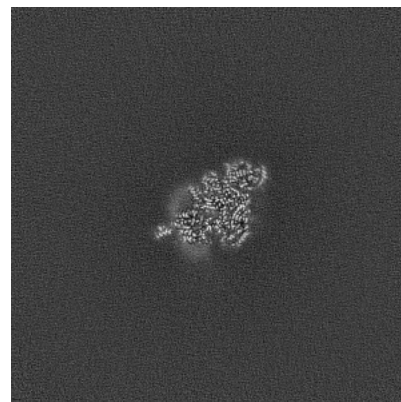
6.3.2 Raw map



X Index: 235



Y Index: 206

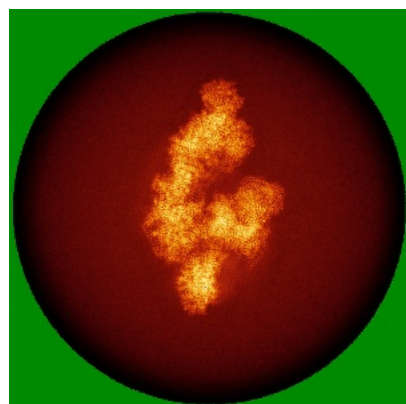


Z Index: 320

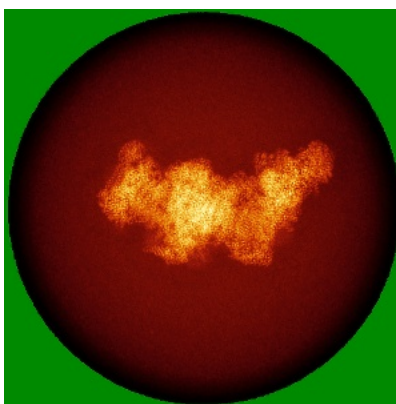
The images above show the largest variance slices of the map in three orthogonal directions.

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

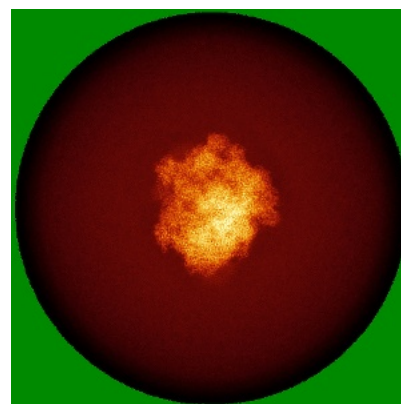
6.4.1 Primary map



X

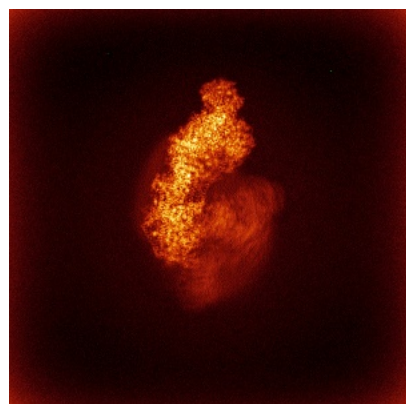


Y

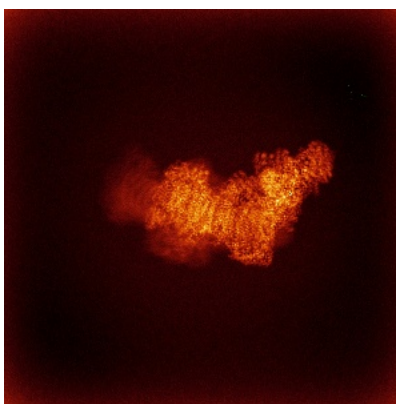


Z

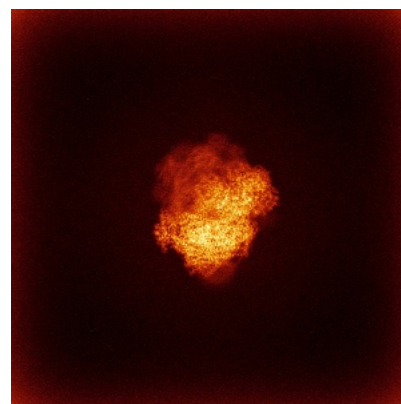
6.4.2 Raw map



X



Y



Z

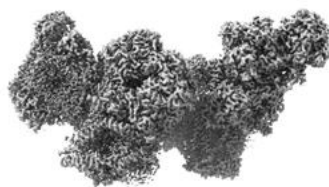
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

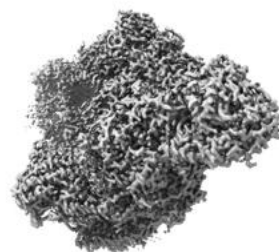
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

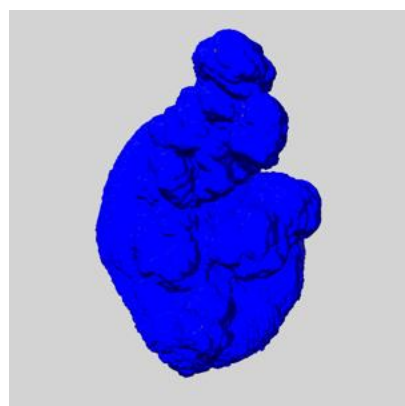
6.6 Mask visualisation [i](#)

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

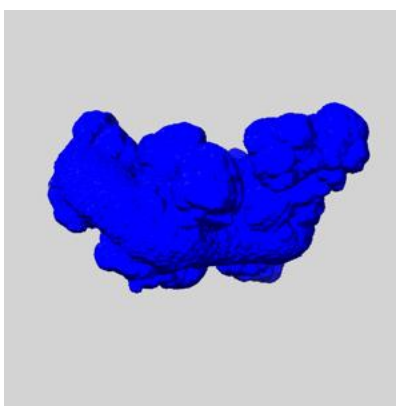
A mask typically either:

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

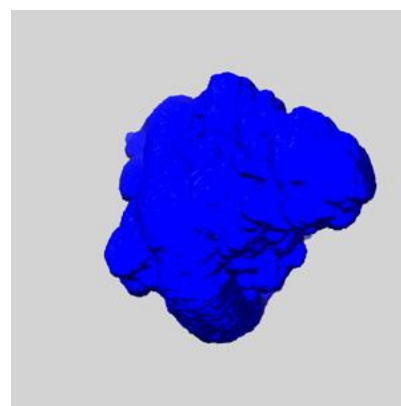
6.6.1 emd_60319_msk_1.map [i](#)



X



Y

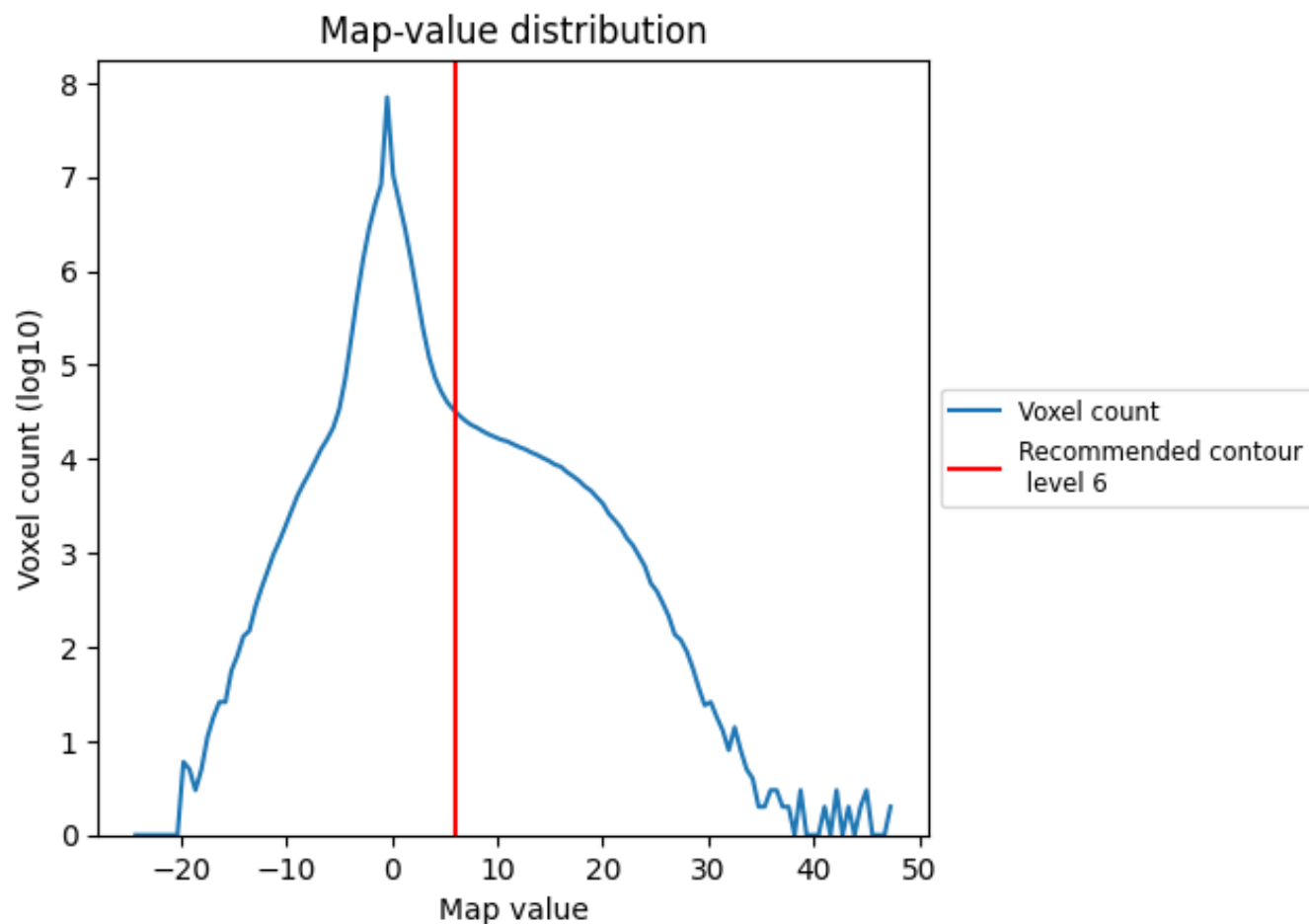


Z

7 Map analysis [i](#)

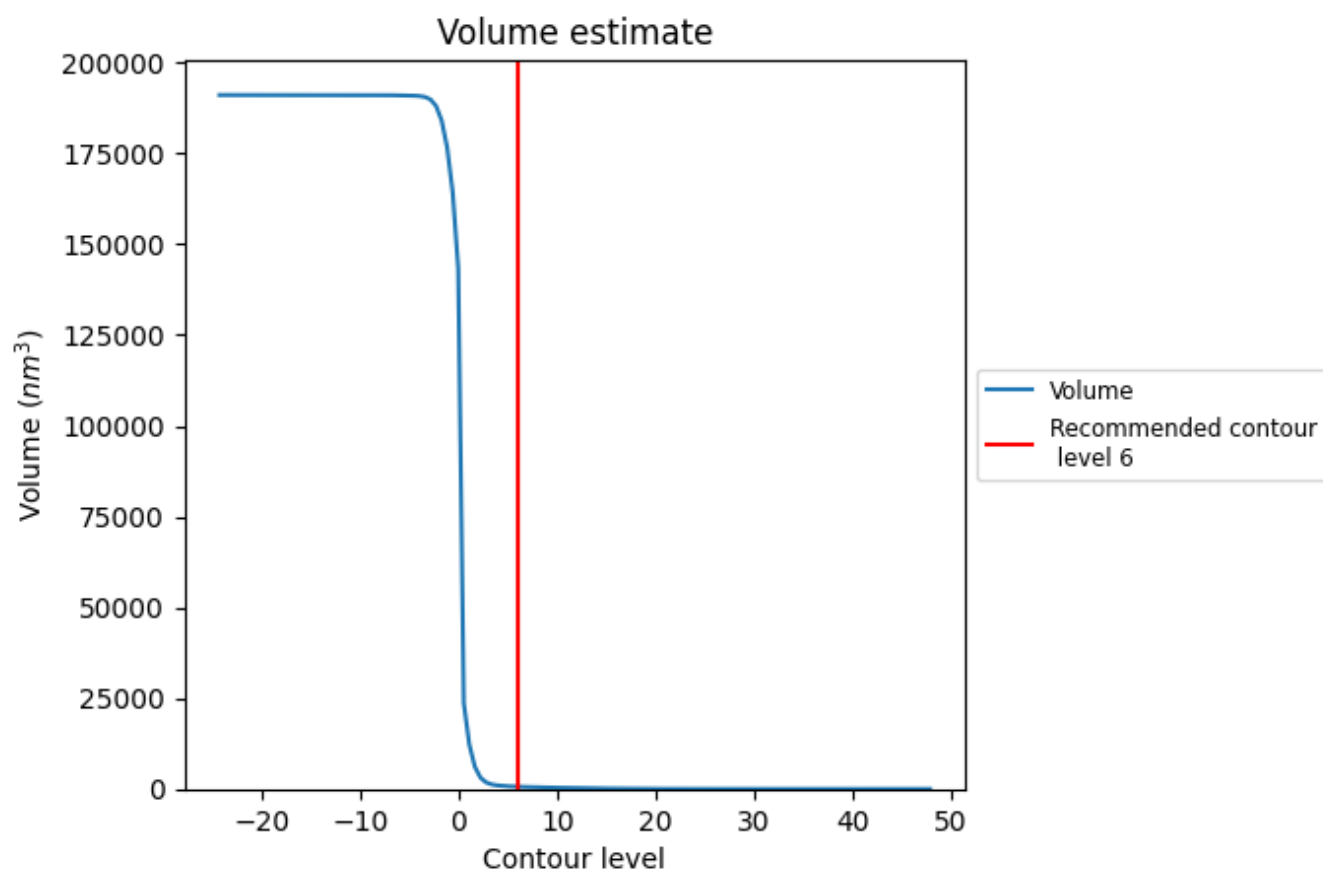
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

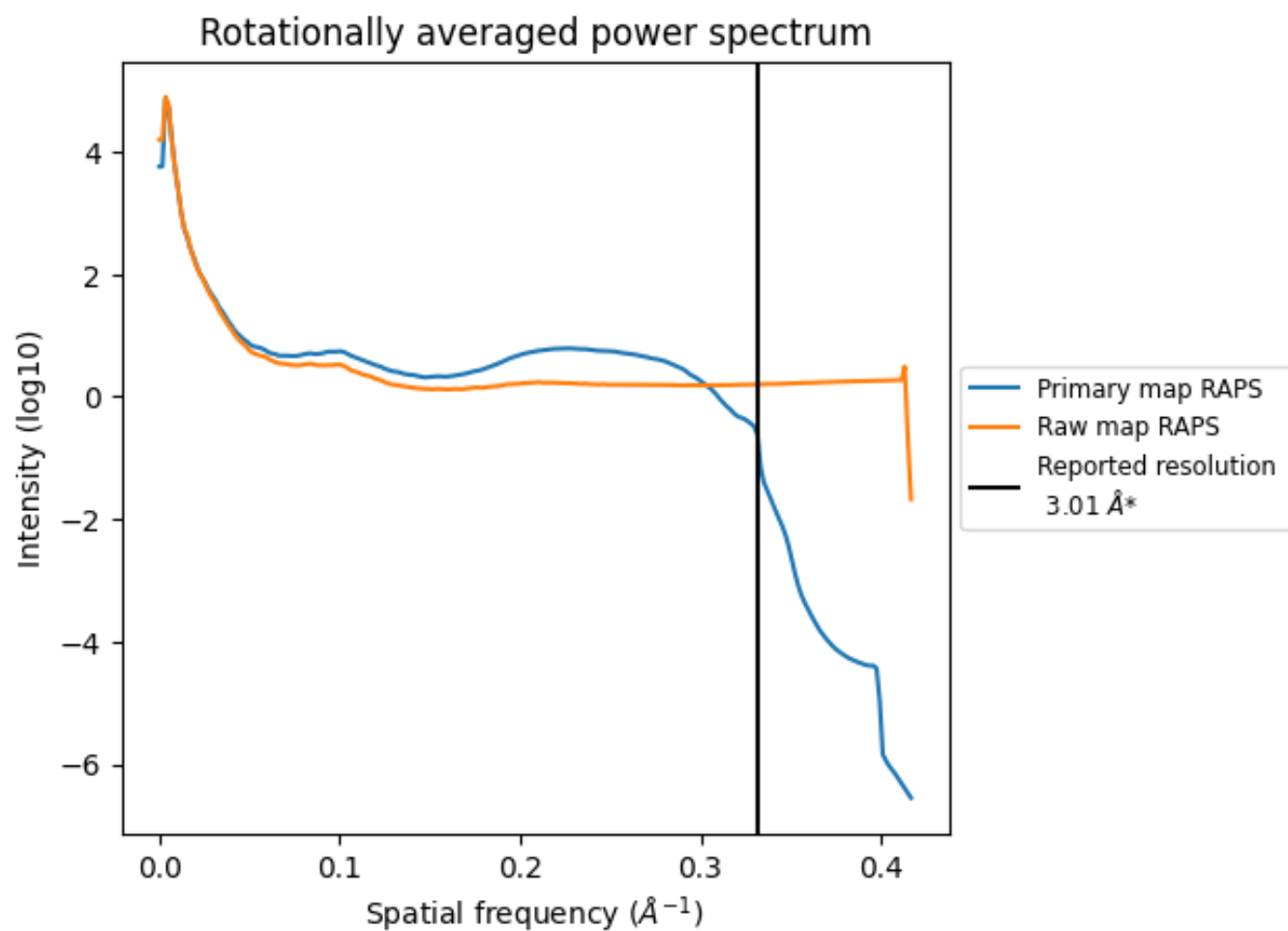
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 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 ⓘ

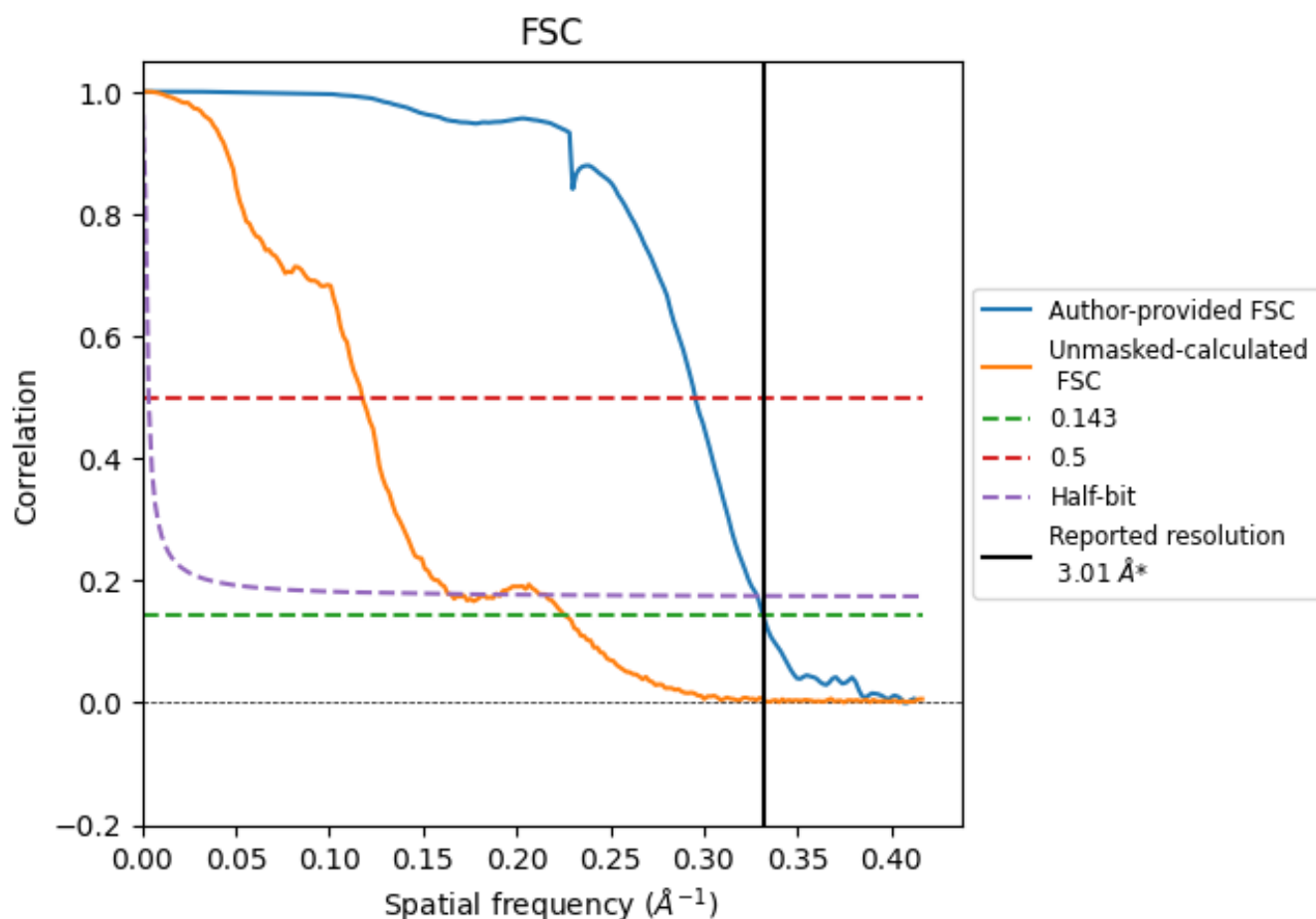


*Reported resolution corresponds to spatial frequency of $0.332 \text{ \AA}^{-1}$

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 0.332 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

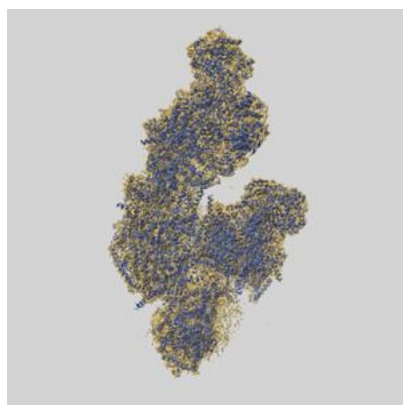
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.38	3.04
Unmasked-calculated*	4.43	8.50	6.09

*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 4.43 differs from the reported value 3.01 by more than 10 %

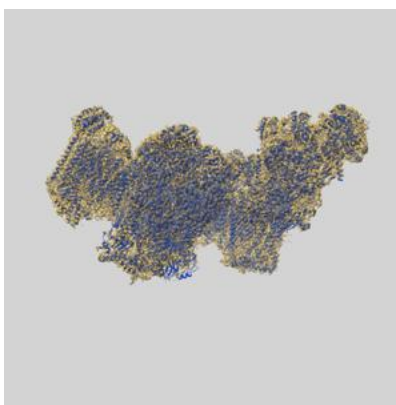
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60319 and PDB model 8ZOU. Per-residue inclusion information can be found in section [3](#) on page [32](#).

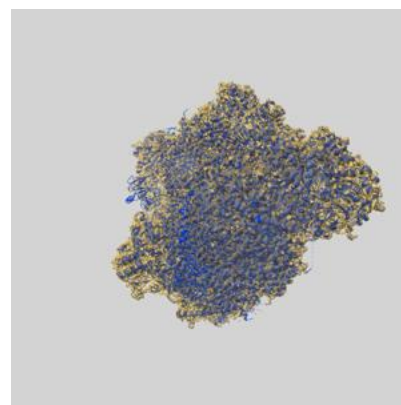
9.1 Map-model overlay [i](#)



X



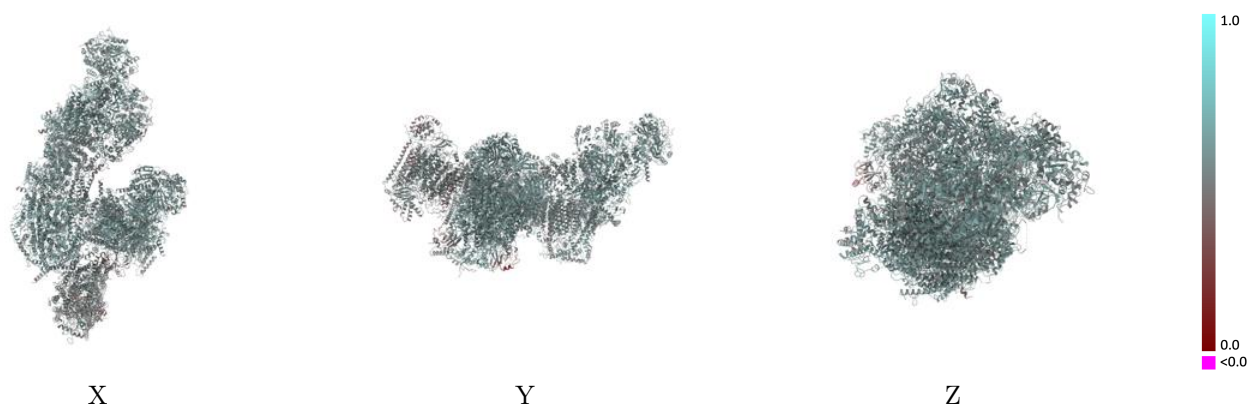
Y



Z

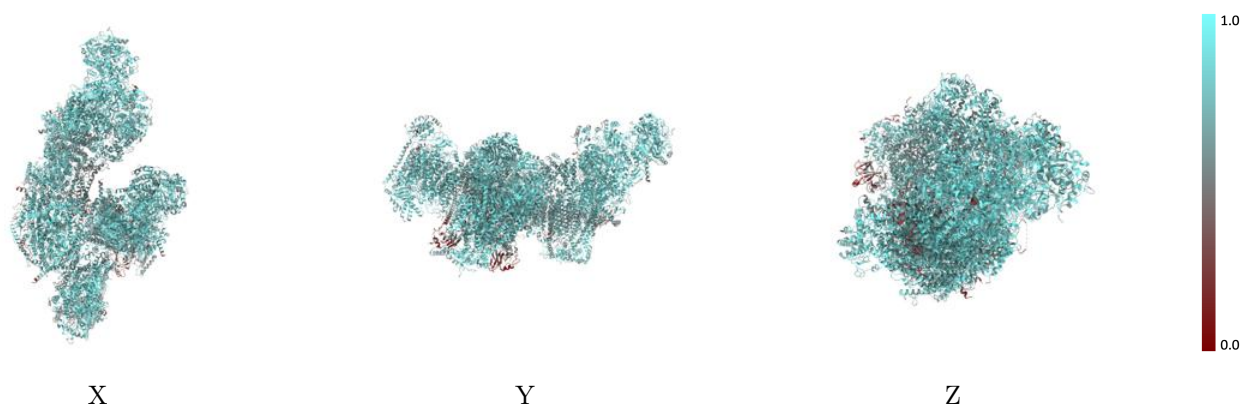
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



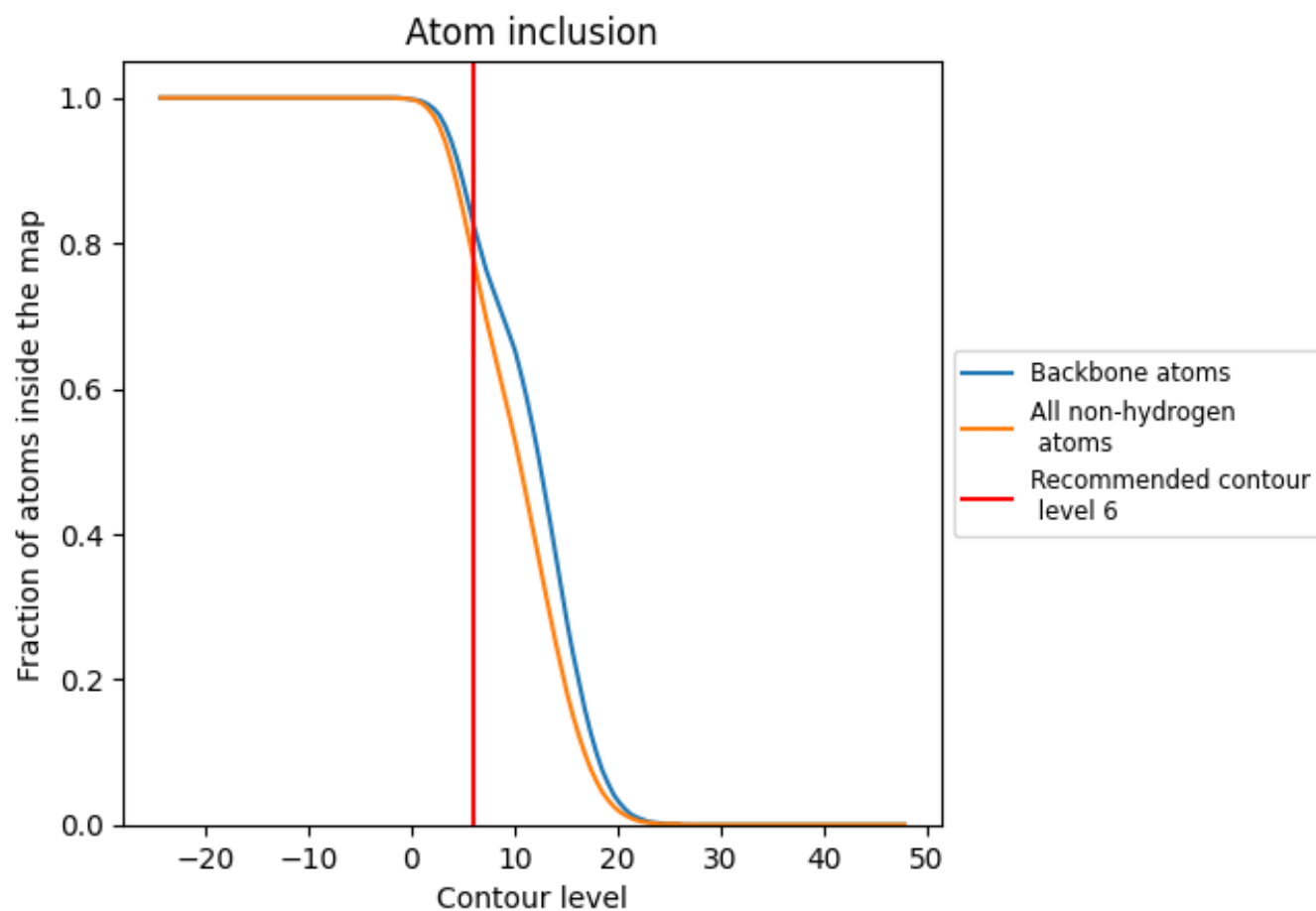
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.5580
4L	 0.7600	 0.5780
5A	 0.7180	 0.4680
5B	 0.7780	 0.4750
6A	 0.7540	 0.4710
6B	 0.8190	 0.4810
6C	 0.6900	 0.4820
7A	 0.6780	 0.4760
7B	 0.5560	 0.4770
7C	 0.8480	 0.5140
8B	 0.7590	 0.5000
A1	 0.8560	 0.5720
A2	 0.7060	 0.5380
A3	 0.8060	 0.5710
A5	 0.7730	 0.5540
A6	 0.7650	 0.5650
A7	 0.6750	 0.5590
A8	 0.8070	 0.5730
A9	 0.7650	 0.5610
AB	 0.5650	 0.4790
AC	 0.7990	 0.5800
AK	 0.7660	 0.5460
AL	 0.6430	 0.5600
AM	 0.7100	 0.5610
AN	 0.7160	 0.5620
B1	 0.7070	 0.5710
B2	 0.7750	 0.5790
B3	 0.7340	 0.5510
B4	 0.7520	 0.5770
B5	 0.8290	 0.5930
B6	 0.7290	 0.5540
B7	 0.7420	 0.5620
B8	 0.8050	 0.5840
B9	 0.8360	 0.5840
BK	 0.7910	 0.5740



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BL	 0.7700	 0.5760
C1	 0.8600	 0.5320
C2	 0.8090	 0.5070
C3	 0.8260	 0.5080
C4	 0.7290	 0.4770
CA	 0.7520	 0.5670
CB	 0.8180	 0.5890
N1	 0.8050	 0.5690
N2	 0.8550	 0.5840
N3	 0.7000	 0.5580
N4	 0.8670	 0.5920
N5	 0.8360	 0.5890
N6	 0.6730	 0.5230
QA	 0.8000	 0.5700
QB	 0.8040	 0.5710
QC	 0.8260	 0.5770
QD	 0.8050	 0.5730
QE	 0.4530	 0.4770
QF	 0.6500	 0.5050
QG	 0.7980	 0.5650
QH	 0.7490	 0.5640
QI	 0.7000	 0.5680
QJ	 0.6610	 0.5380
QK	 0.5450	 0.5320
Qa	 0.7830	 0.5680
Qb	 0.7920	 0.5730
Qc	 0.7970	 0.5740
Qd	 0.8270	 0.5800
Qe	 0.3810	 0.4410
Qf	 0.6530	 0.5160
Qg	 0.7810	 0.5610
Qh	 0.6700	 0.5610
Qi	 0.7980	 0.5730
Qj	 0.6660	 0.5400
S1	 0.8170	 0.5670
S2	 0.8560	 0.5860
S3	 0.8890	 0.5960
S4	 0.8120	 0.5780
S5	 0.7720	 0.5600
S6	 0.7820	 0.5680
S7	 0.8550	 0.5830
S8	 0.8830	 0.5940

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Chain	Atom inclusion	Q-score
V1	 0.7980	 0.5570
V2	 0.7490	 0.5470
V3	 0.7620	 0.5520