



# wwPDB EM Validation Summary Report ⓘ

Nov 12, 2025 – 02:39 AM JST

PDB ID : 8ZSQ / pdb\_00008zsq  
EMDB ID : EMD-60424  
Title : Respirasome closed state 1 bound by metformin (SC-MetC1)  
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.  
Deposited on : 2024-06-05  
Resolution : 2.86 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](mailto: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>.

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

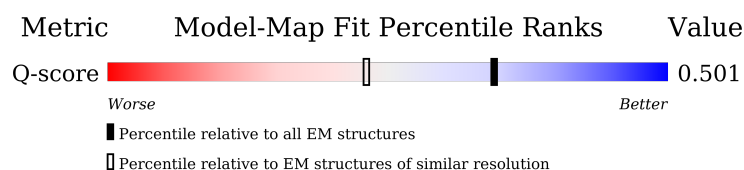
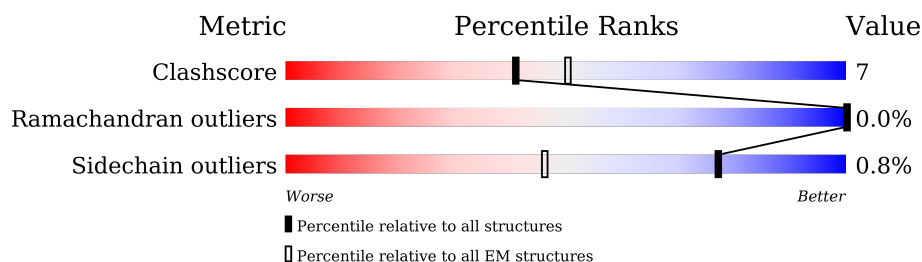
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.46

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.86 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.









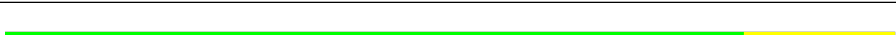
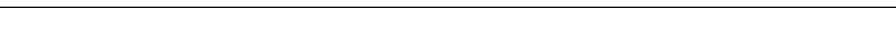
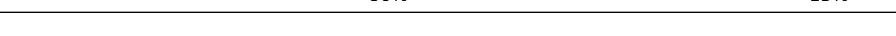
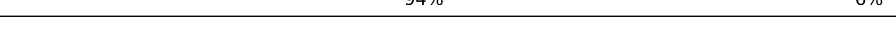
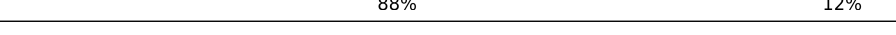
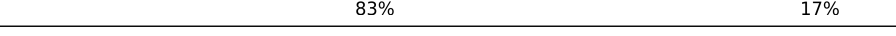













Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12017 ( 2.36 - 3.36 )

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  $\geq 3$ , 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	 78%21%
6	6C	70	 87%13%
7	7A	57	 84%16%
8	7B	50	 88%12%
9	7C	47	 74%23%
10	8B	43	 86%14%
11	A1	70	 83%17%
12	A2	85	 86%13%
13	A3	83	 94%6%
14	A5	112	 88%12%
15	A6	114	 83%17%
16	A7	112	 74%12%13%
17	A8	171	 85%15%
18	A9	341	 84%16%
19	AB	87	 70%18%11%
19	AC	87	 86%13%
20	AK	321	 85%15%
21	AL	140	 90%10%
22	AM	144	 89%10%
23	AN	142	 83%17%
24	B1	56	 80%20%
25	B2	67	 82%18%
26	B3	80	 85%15%
27	B4	128	 92%8%
28	B5	138	 90%10%


























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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	174	
34	BL	99	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
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	 82% 17% .
51	QE	274	 57% 15% 28%
51	QK	274	 22% 5% 73%
51	Qe	274	 61% 11% 28%
52	QF	67	 87% 13%
52	Qf	67	 82% 13% .
53	QG	101	 88% 12%
53	Qg	101	 87% 12% .
54	QH	79	 80% 19% .
54	Qh	79	 87% 13%
55	QI	62	 90% 8% .
55	Qi	62	 89% 8% .
56	QJ	52	 81% 13% 6%
56	Qj	52	 83% 13% ..
57	S1	689	 79% 21%
58	S2	430	 78% 22%
59	S3	208	 86% 14%
60	S4	124	 85% 15% .
61	S5	105	 92% 8%
62	S6	96	 91% 9%
63	S7	156	 79% 19% .
64	S8	176	 80% 20%
65	V1	431	 78% 22%
66	V2	217	 86% 13% .
67	V3	42	 74% 26%

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	303	-	-	X	-

## 2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 117589 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	341	Total	C	N	O	S	0	0
			2743	1777	480	477	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	321	Total	C	N	O	S	0	0
			2601	1655	444	492	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
			1173	755	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	103	Total	C	N	O	S	0	0
			882	577	156	148	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	318	Total	C	N	O	S	0	0
			2508	1678	385	424	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	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- 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	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- 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
			3147	1971	557	611	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 c1, heme protein, mitochondrial.

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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	S2	430	Total	C	N	O	S	0	0
			3459	2212	594	629	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
			3316	2092	592	612	20		

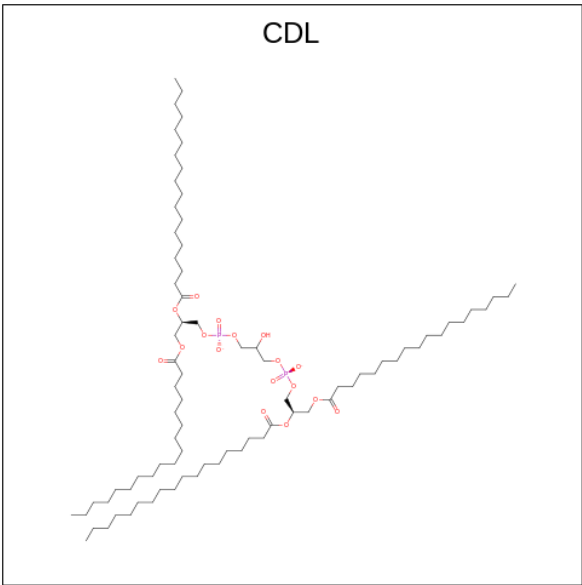
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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 NADH:ubiquinone oxidoreductase subunit V3.

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	7A	1	Total	C	O	P	0
			91	72	17	2	
68	A7	1	Total	C	O	P	0
			51	32	17	2	
68	A8	1	Total	C	O	P	0
			83	64	17	2	
68	AK	1	Total	C	O	P	0
			68	49	17	2	
68	AL	1	Total	C	O	P	0
			94	75	17	2	
68	B4	1	Total	C	O	P	0
			80	61	17	2	
68	B5	1	Total	C	O	P	0
			100	81	17	2	
68	C3	1	Total	C	O	P	0
			87	68	17	2	
68	C3	1	Total	C	O	P	0
			83	64	17	2	
68	CB	1	Total	C	O	P	0
			100	81	17	2	
68	N1	1	Total	C	O	P	0
			78	59	17	2	
68	N4	1	Total	C	O	P	0
			62	43	17	2	
68	N5	1	Total	C	O	P	0
			89	70	17	2	

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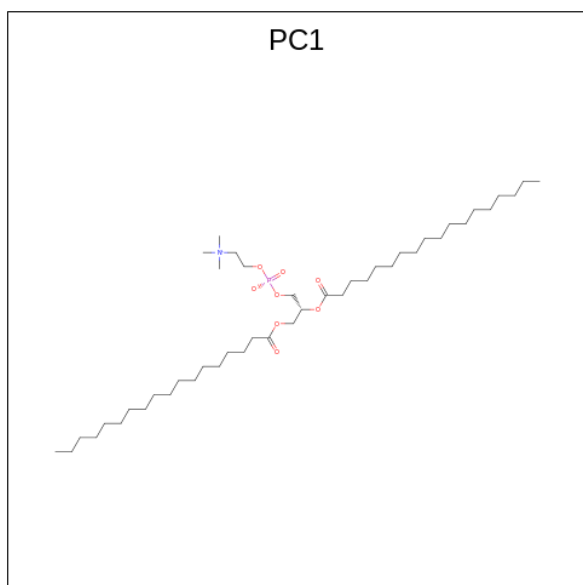
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Mol	Chain	Residues	Atoms				AltConf
68	N5	1	Total	C	O	P	0
			100	81	17	2	
68	QB	1	Total	C	O	P	0
			64	45	17	2	
68	QC	1	Total	C	O	P	0
			55	36	17	2	
68	QD	1	Total	C	O	P	0
			64	45	17	2	
68	QH	1	Total	C	O	P	0
			61	42	17	2	
68	QH	1	Total	C	O	P	0
			64	45	17	2	
68	Qb	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

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: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).

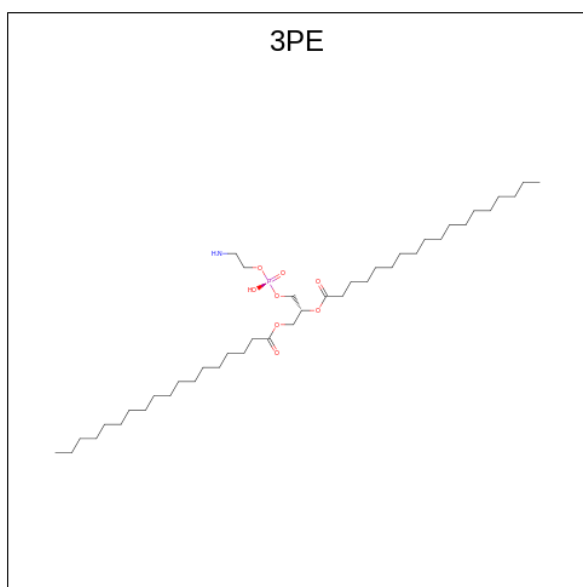


Mol	Chain	Residues	Atoms					AltConf
70	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	C1	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			50	40	1	8	1	
70	C3	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	C3	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C3	1	Total	C	N	O	P	0
			43	33	1	8	1	
70	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	N3	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
			48	38	1	8	1	
70	Qc	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	

- Molecule 71 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<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).

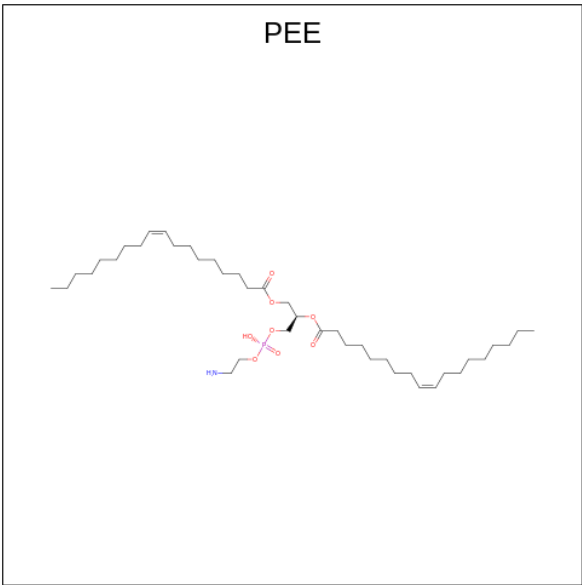


- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
72	7A	1	Total	C	N	O	P	0
			43	33	1	8	1	
72	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
72	C1	1	Total	C	N	O	P	0
			39	29	1	8	1	
72	C1	1	Total	C	N	O	P	0
			46	36	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	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	QE	1	Total	C	N	O	P	0
			44	34	1	8	1	
72	QJ	1	Total	C	N	O	P	0
			34	24	1	8	1	
72	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	
72	Qj	1	Total	C	N	O	P	0
			29	19	1	8	1	
72	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 73 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



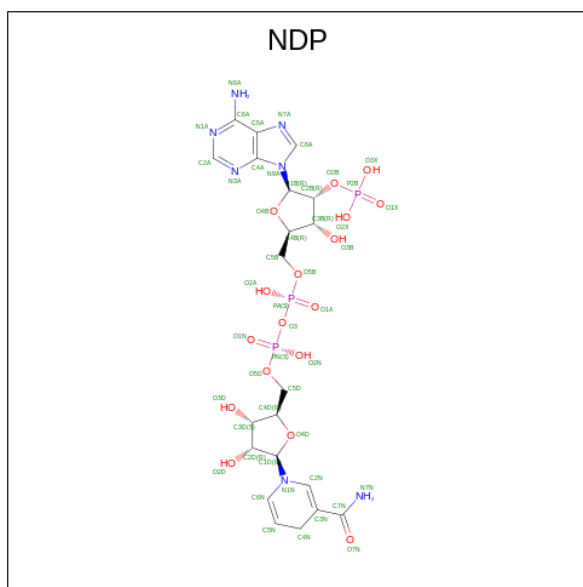
Mol	Chain	Residues	Atoms					AltConf
73	7C	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	
73	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
73	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
73	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
73	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
73	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	QB	1	Total	C	N	O	P	0
			34	24	1	8	1	
73	QC	1	Total	C	N	O	P	0
			40	30	1	8	1	
73	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
73	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
73	Qe	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	Qe	1	Total	C	N	O	P	0
			24	14	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
73	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
73	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

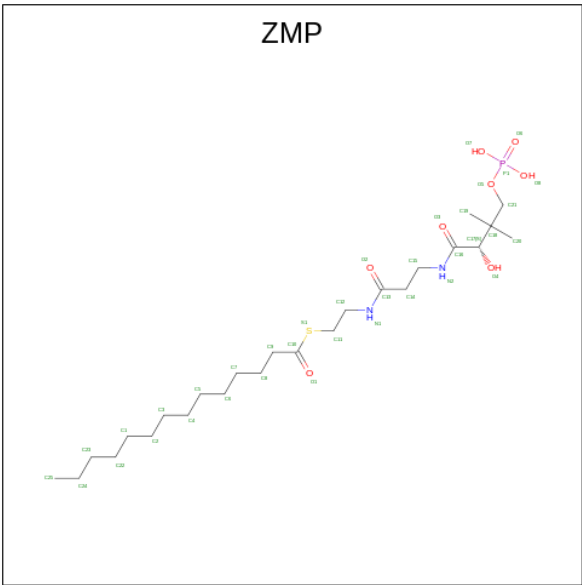
- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
74	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

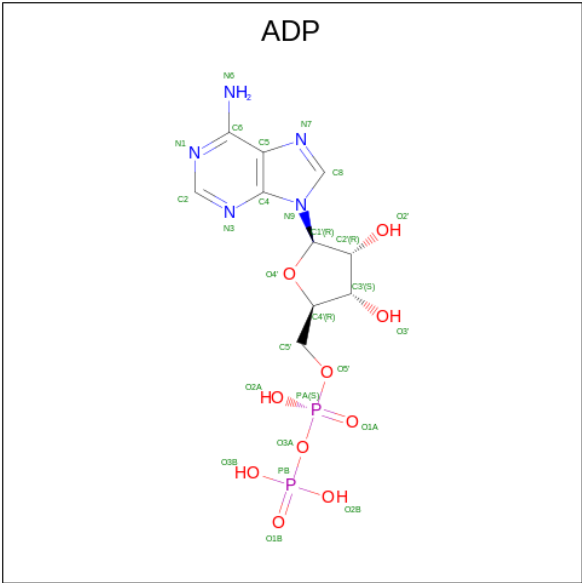
- Molecule 75 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula:  $C_{25}H_{49}N_2O_8PS$ ) (labeled as "Ligand of Interest" by depositor).





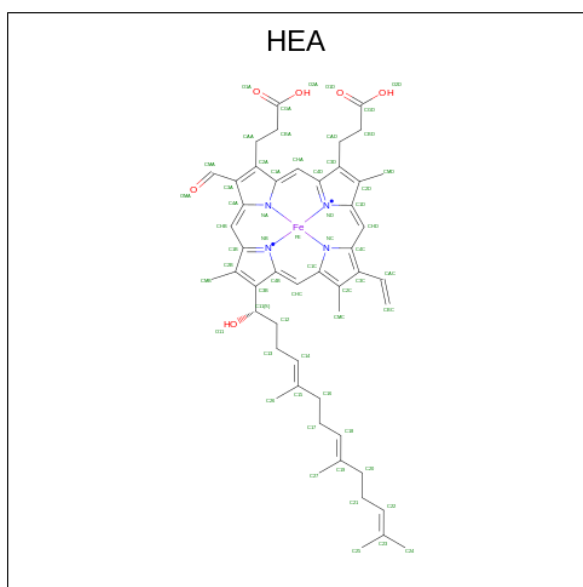
Mol	Chain	Residues	Atoms						AltConf
75	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
75	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 76 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 77 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

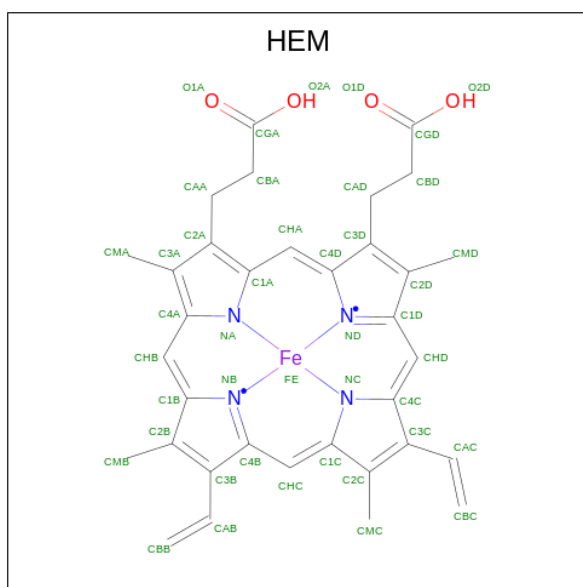
- Molecule 78 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

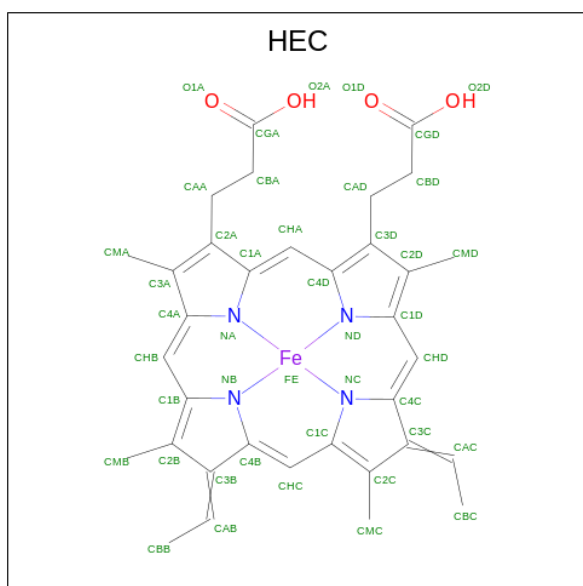
Mol	Chain	Residues	Atoms		AltConf
79	C1	1	Total	Mg	0
			1	1	
79	S1	1	Total	Mg	0
			1	1	

- Molecule 80 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



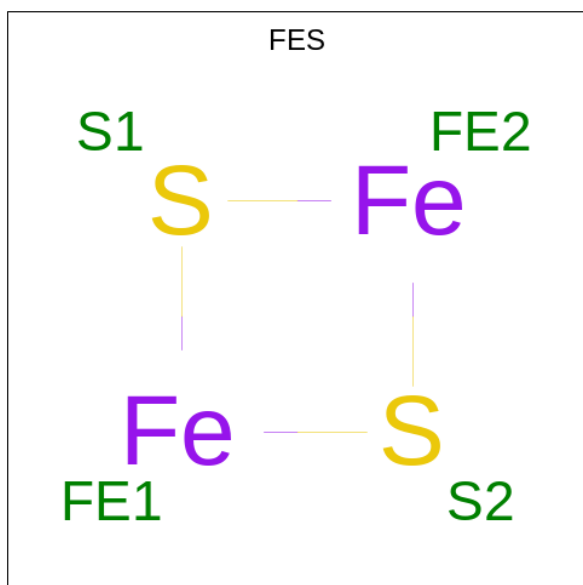
Mol	Chain	Residues	Atoms					AltConf
80	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0

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



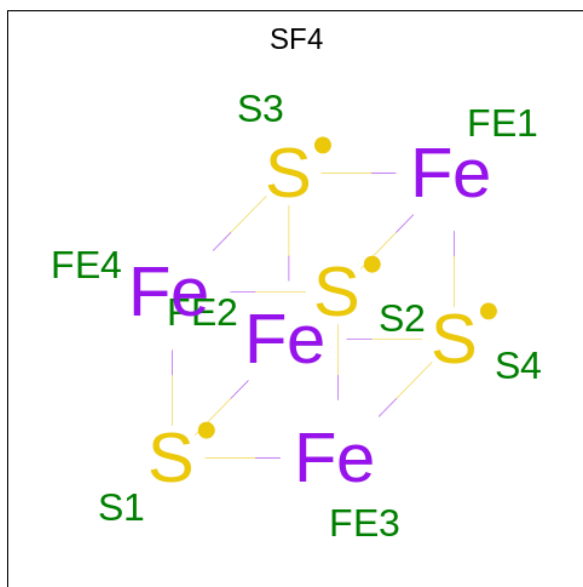
Mol	Chain	Residues	Atoms					AltConf
81	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
81	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 82 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



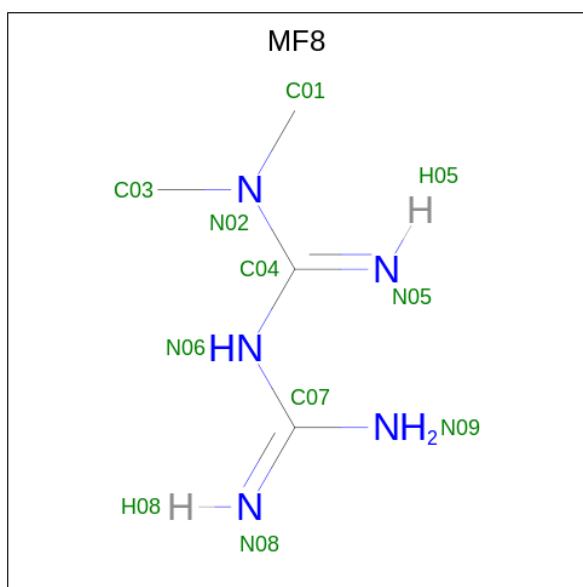
Mol	Chain	Residues	Atoms			AltConf
82	QE	1	Total	Fe	S	0
			4	2	2	
82	Qe	1	Total	Fe	S	0
			4	2	2	
82	S1	1	Total	Fe	S	0
			4	2	2	
82	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 83 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



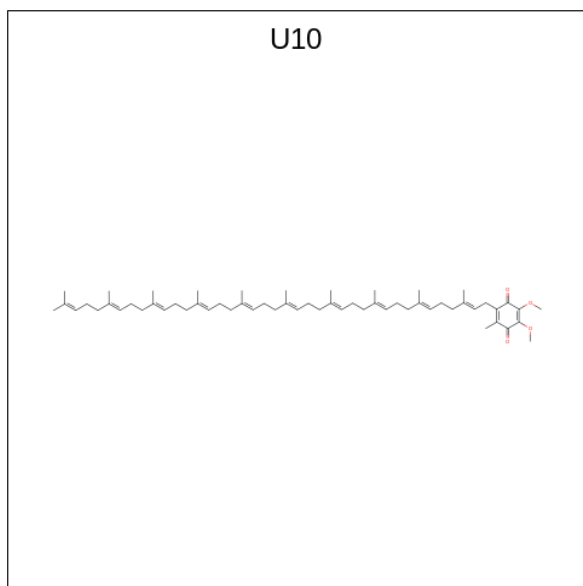
Mol	Chain	Residues	Atoms			AltConf
83	S1	1	Total	Fe	S	0
			8	4	4	
83	S1	1	Total	Fe	S	0
			8	4	4	
83	S7	1	Total	Fe	S	0
			8	4	4	
83	S8	1	Total	Fe	S	0
			8	4	4	
83	S8	1	Total	Fe	S	0
			8	4	4	
83	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 84 is Metformin (CCD ID: MF8) (formula:  $C_4H_{11}N_5$ ) (labeled as "Ligand of Interest" by depositor).



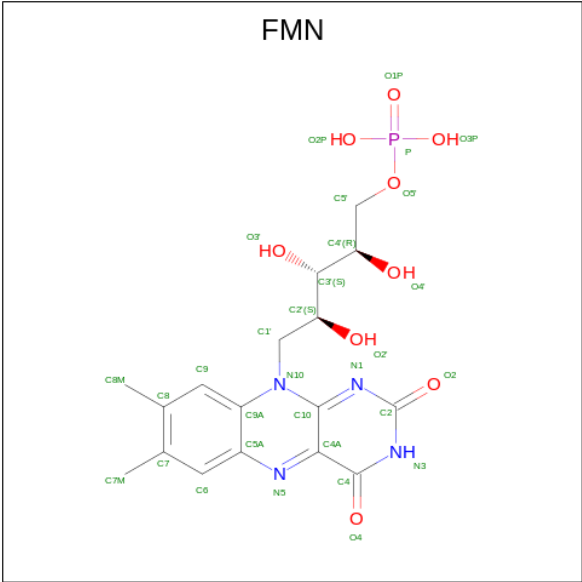
Mol	Chain	Residues	Atoms			AltConf
84	S2	1	Total	C	N	0
			9	4	5	

- Molecule 85 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
85	S7	1	Total	C	O	0
			63	59	4	

- Molecule 86 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).

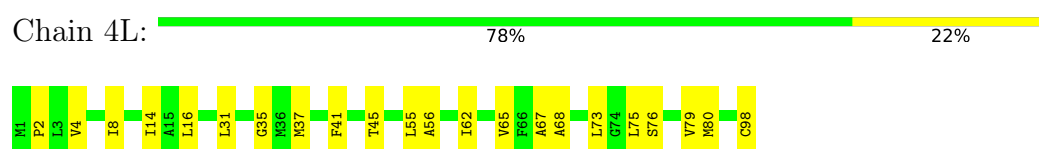


Mol	Chain	Residues	Atoms					AltConf
86	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

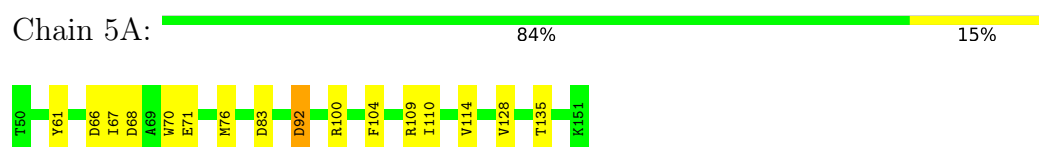
### 3 Residue-property plots [i](#)

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.

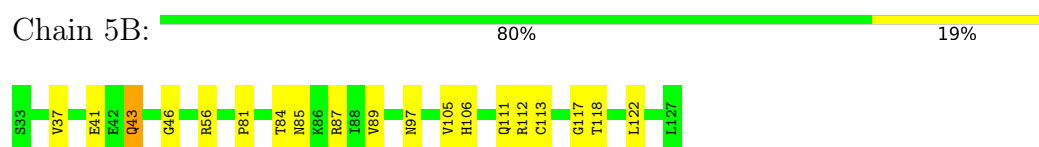
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



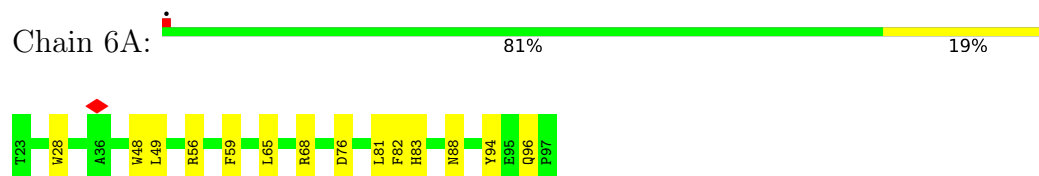
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial



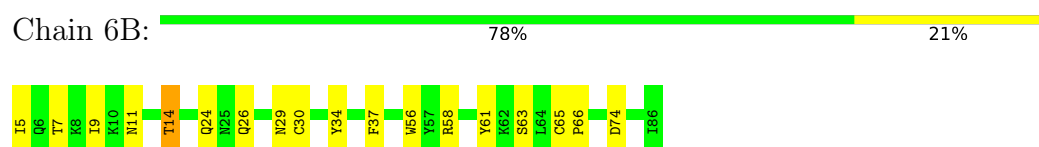
- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 4: Cytochrome c oxidase subunit



- Molecule 5: Cytochrome c oxidase subunit

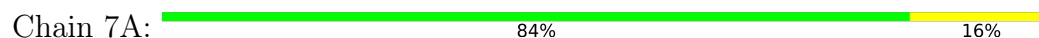


- Molecule 6: Cytochrome c oxidase subunit 6C

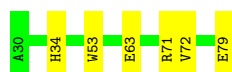




- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



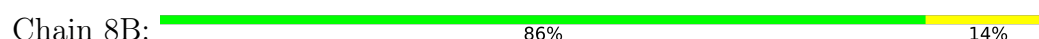
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



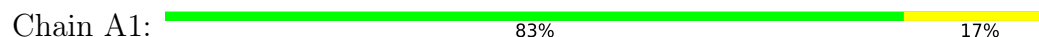
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



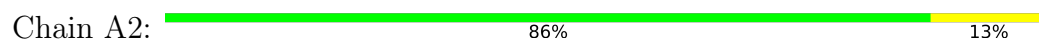
- Molecule 10: Cytochrome c oxidase subunit 8



- 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

Chain A3:  94% 6%




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

Chain A5:  88% 12%



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

Chain A6:  83% 17%



- Molecule 16: Complex I-B14.5a

Chain A7:  74% 12% 13%




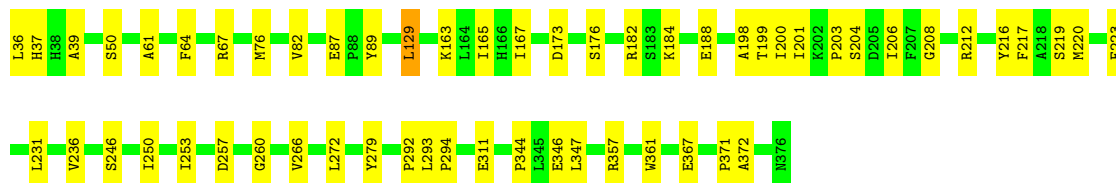
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:  85% 15%



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

Chain A9:  84% 16%



- Molecule 19: Acyl carrier protein

Chain AB:  70% 18% 11%





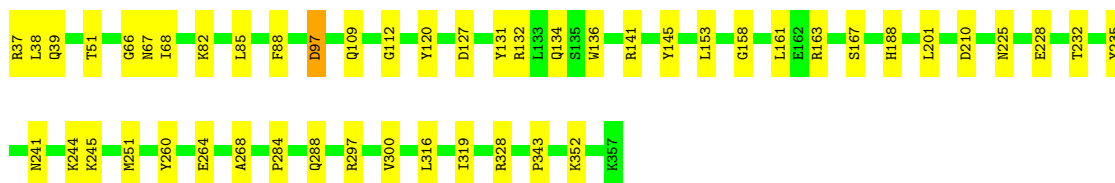
- Molecule 19: Acyl carrier protein

Chain AC: 86% 13%



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

Chain AK: 85% 15%



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

Chain AL: 90% 10%



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

Chain AM: 89% 10%



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

Chain AN: 83% 17%




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

Chain B1: 80% 20%




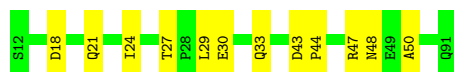
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:  82% 18%



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

Chain B3:  85% 15%



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

Chain B4:  92% 8%



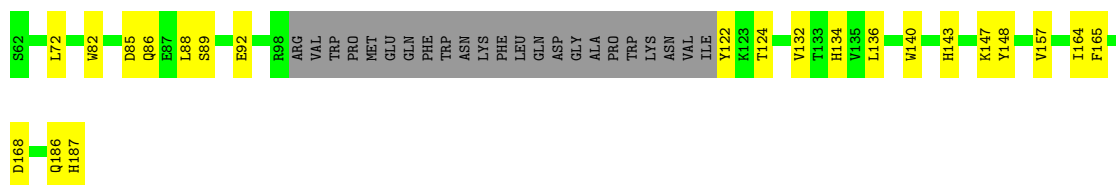
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:  90% 10%




- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:  64% 17% 18%



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

Chain B7:  81% 19%



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

Chain B8:  91% 9%




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

Chain B9:  87% 13%



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

Chain BK:  86% 14%




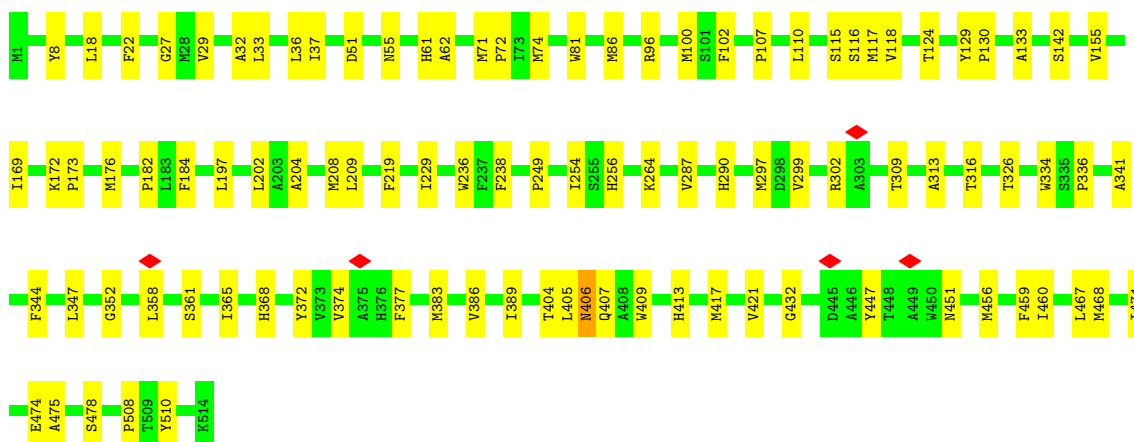
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:  89% 11%



- Molecule 35: Cytochrome c oxidase subunit 1

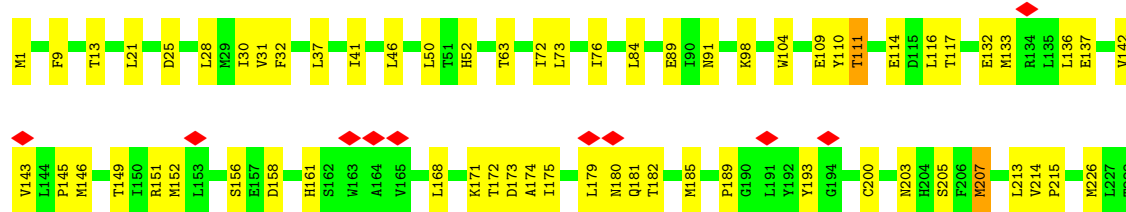
Chain C1:  81% 19%



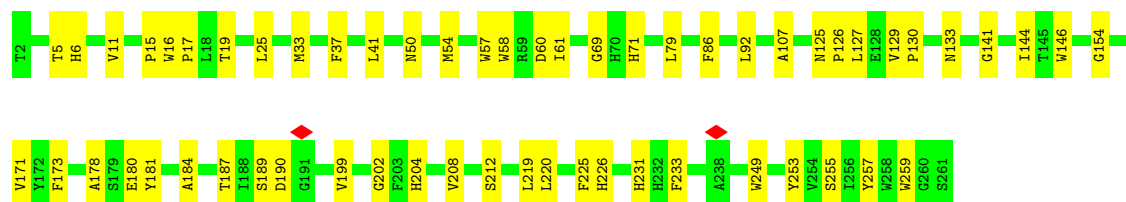
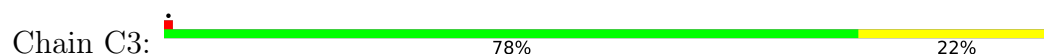
- Molecule 36: Cytochrome c oxidase subunit 2

Chain C2:  72% 27%

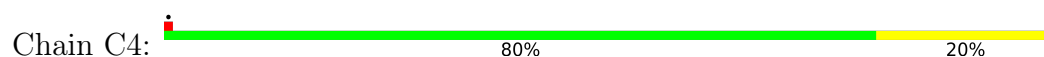




• Molecule 37: Cytochrome c oxidase subunit 3



• Molecule 38: Cytochrome c oxidase subunit 4



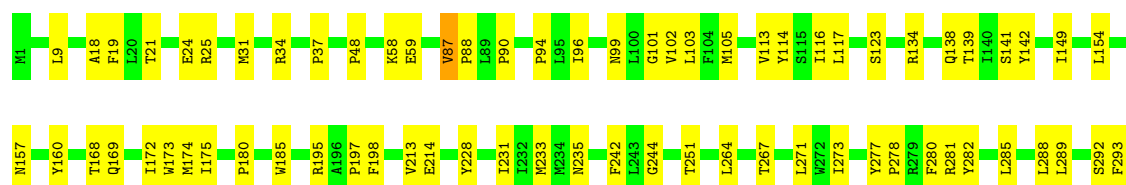
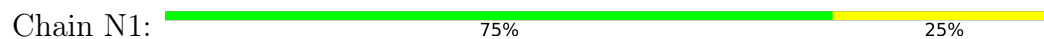
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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



• Molecule 41: NADH-ubiquinone oxidoreductase chain 1





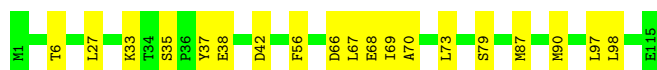
• Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2: 81% 19%



• Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3: 83% 17%



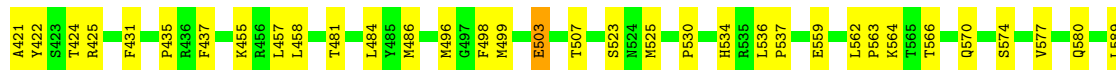
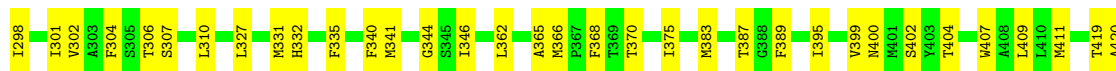
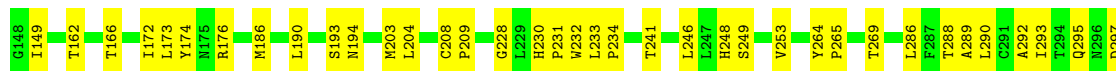
• Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 82% 17%



• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 76% 24%





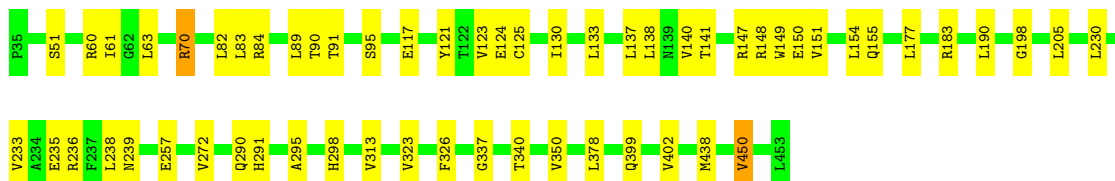
- Molecule 46: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 80% 20%



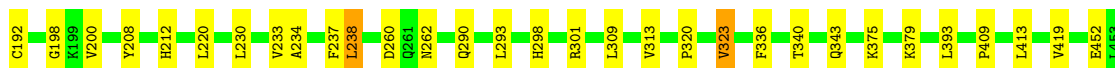
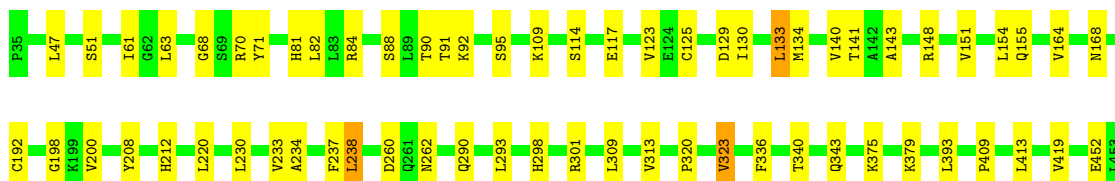
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain QA: 86% 13%



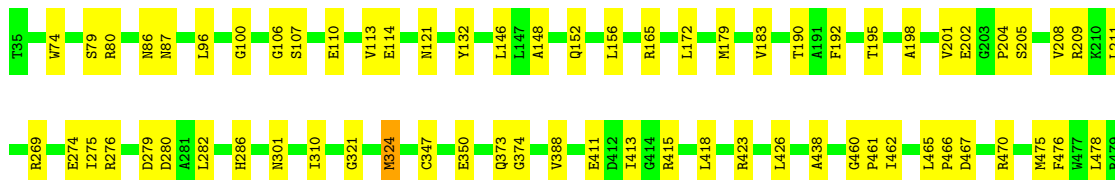
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Qa: 85% 15%



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

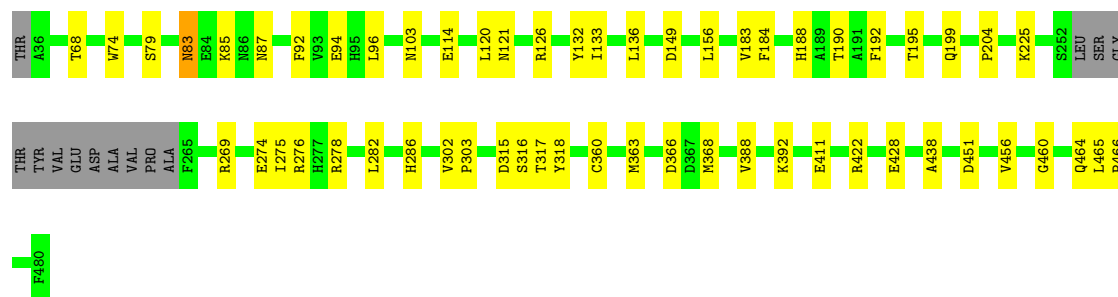
Chain QB: 85% 15%



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

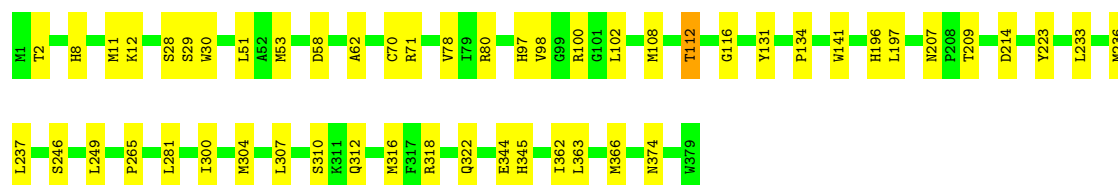
Chain Qb: 84% 13%





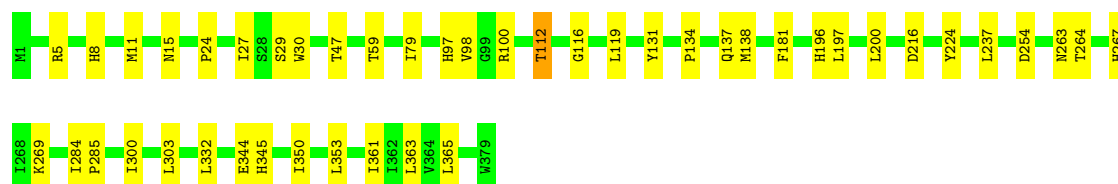
- Molecule 49: Cytochrome b

Chain QC: 86% 13%



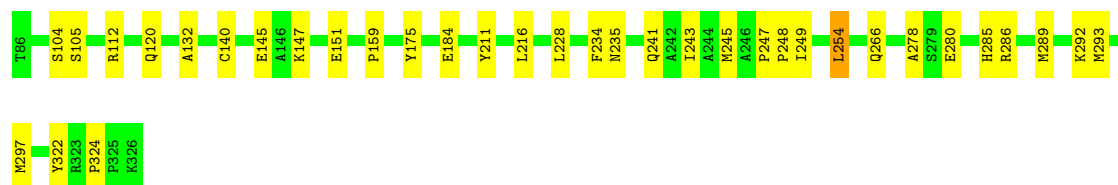
- Molecule 49: Cytochrome b

Chain Qc: 88% 12%



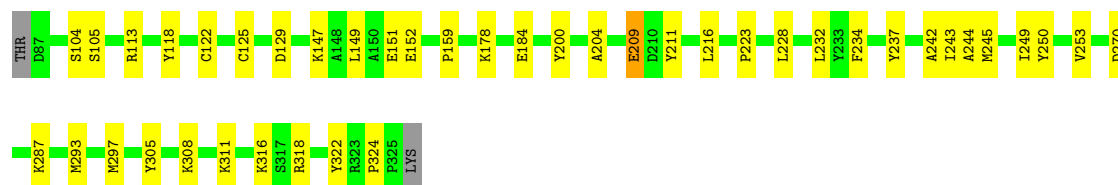
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

Chain QD: 85% 14%



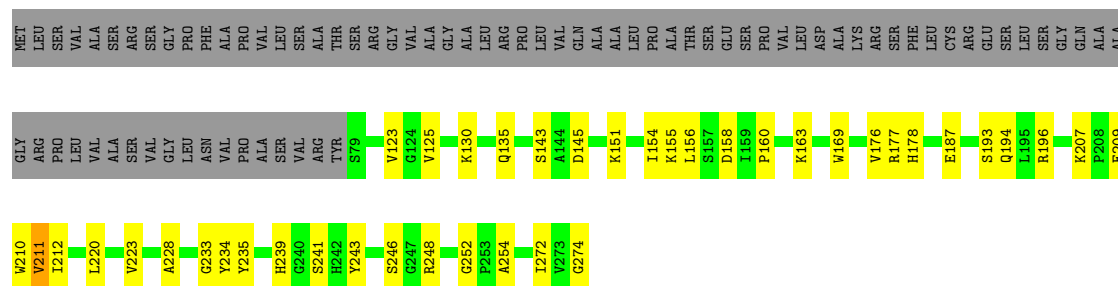
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

Chain Qd: 82% 17%



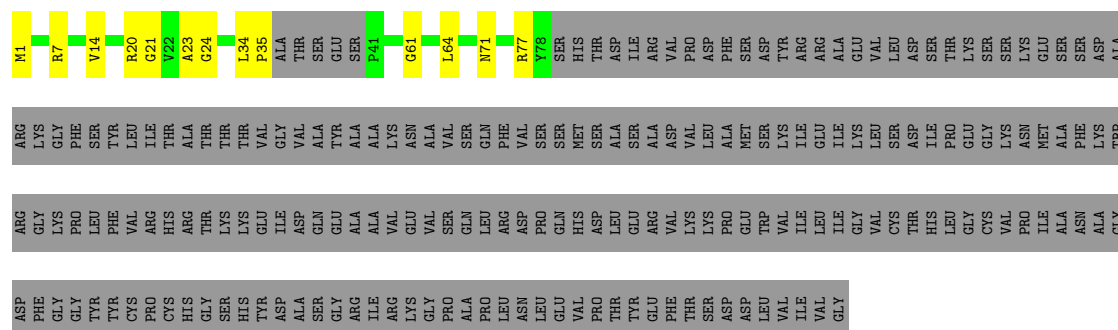
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain QE:  57% 15% 28%



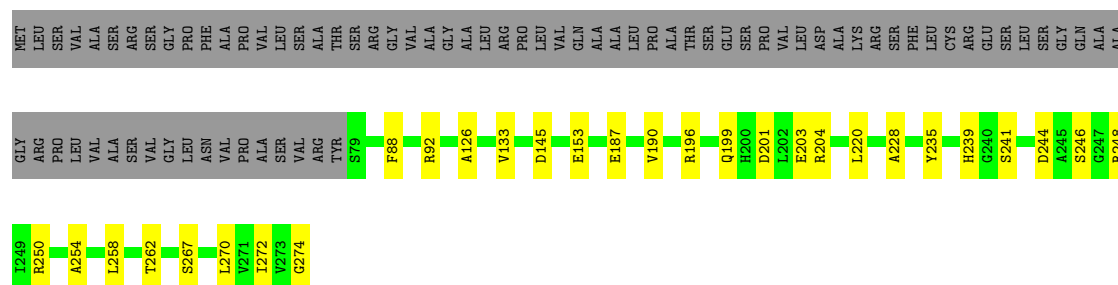
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain QK:  22% 5% 73%




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

Chain Qe:  61% 11% 28%




- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain QF:  87% 13%



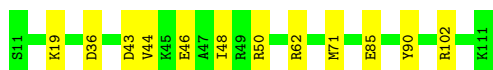
- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain Qf:  82% 13%



- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG: 88% 12%



- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg: 87% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH: 80% 19%



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh: 87% 13%



- Molecule 55: Complex III subunit 9

Chain QI: 90% 8%



- Molecule 55: Complex III subunit 9

Chain Qi: 89% 8%



- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain QJ: 81% 13% 6%



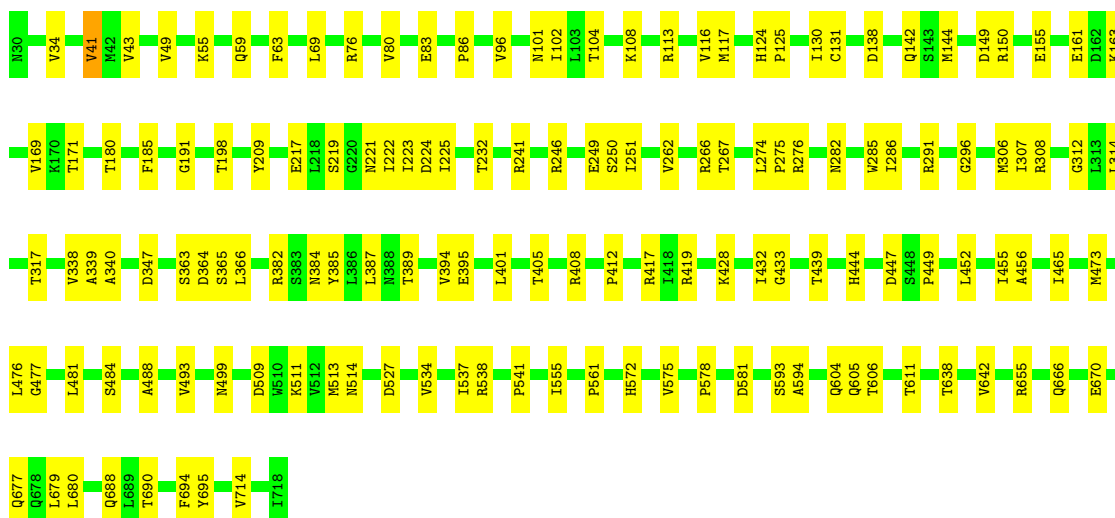
- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain Qj: 83% 13% ..



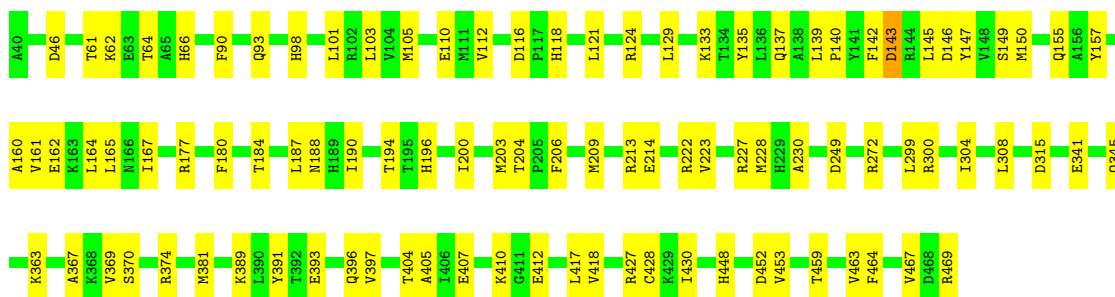
- Molecule 57: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 79% 21%



- Molecule 58: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain S2: 78% 22%




- Molecule 59: Complex I-30kD

Chain S3: 86% 14%



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

Chain S4:  85% 15%



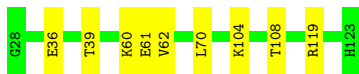
- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:  92% 8%



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

Chain S6:  91% 9%

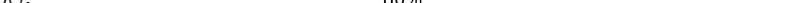


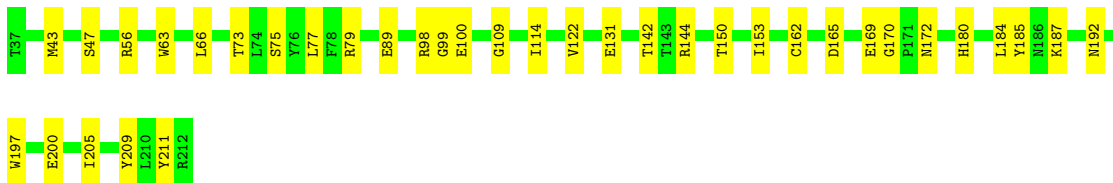
- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:  79% 19% .




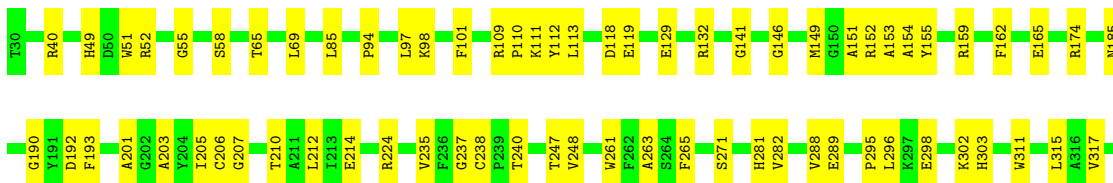
- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

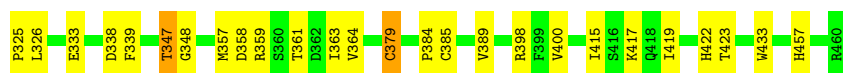
Chain S8:  80% 20%



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

Chain V1:  78% 22%





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

Chain V2: 86% 13%



- Molecule 67: NADH:ubiquinone oxidoreductase subunit V3

Chain V3: 74% 26%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	320129	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	46.884	Depositor
Minimum map value	-34.576	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.006	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: PEE, HEC, PC1, ZN, HEA, 2MR, MG, 3PE, SF4, ADP, CDL, HEM, U10, MF8, ZMP, FMN, PLX, NDP, CU, FES

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	0.15	0/759	0.29	0/1029
2	5A	0.09	0/843	0.23	0/1145
3	5B	0.12	0/739	0.30	0/1002
4	6A	0.10	0/648	0.23	0/888
5	6B	0.11	0/704	0.26	0/951
6	6C	0.10	0/587	0.25	0/781
7	7A	0.11	0/457	0.23	0/620
8	7B	0.10	0/405	0.26	0/555
9	7C	0.11	0/400	0.22	0/536
10	8B	0.11	0/349	0.23	0/477
11	A1	0.14	0/577	0.32	0/777
12	A2	0.10	0/697	0.25	0/938
13	A3	0.10	0/664	0.23	0/912
14	A5	0.13	0/929	0.23	0/1258
15	A6	0.14	0/991	0.29	0/1335
16	A7	0.12	0/798	0.26	0/1079
17	A8	0.11	0/1436	0.25	0/1938
18	A9	0.14	0/2820	0.27	0/3823
19	AB	0.10	0/633	0.23	0/851
19	AC	0.13	0/714	0.23	0/965
20	AK	0.12	0/2661	0.27	0/3602
21	AL	0.12	0/1042	0.21	0/1411
22	AM	0.10	0/1245	0.23	0/1694
23	AN	0.14	0/1204	0.27	0/1624
24	B1	0.13	0/491	0.28	0/663
25	B2	0.12	0/610	0.23	0/836
26	B3	0.12	0/660	0.25	0/892
27	B4	0.14	0/1092	0.26	0/1481
28	B5	0.15	0/1184	0.28	0/1603
29	B6	0.15	0/910	0.33	0/1237
30	B7	0.12	0/1092	0.25	0/1459



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	B8	0.13	0/1371	0.26	0/1875
32	B9	0.14	0/1590	0.27	0/2155
33	BK	0.13	0/1489	0.25	0/2008
34	BL	0.13	0/851	0.27	0/1155
35	C1	0.14	0/4164	0.28	0/5689
36	C2	0.12	0/1880	0.28	0/2564
37	C3	0.13	0/2186	0.26	0/2991
38	C4	0.12	0/1187	0.26	0/1606
39	CA	0.10	0/430	0.19	0/581
40	CB	0.13	0/1031	0.26	0/1394
41	N1	0.18	0/2581	0.35	0/3529
42	N2	0.17	0/2773	0.33	0/3768
43	N3	0.16	0/938	0.28	0/1281
44	N4	0.17	0/3723	0.31	0/5078
45	N5	0.16	0/4914	0.34	0/6683
46	N6	0.14	0/1364	0.31	0/1850
47	QA	0.15	0/3200	0.29	0/4333
47	Qa	0.15	0/3200	0.29	0/4333
48	QB	0.15	0/3531	0.30	0/4793
48	Qb	0.14	0/3436	0.27	0/4659
49	QC	0.17	0/3123	0.31	0/4269
49	Qc	0.17	0/3123	0.32	0/4269
50	QD	0.15	0/1979	0.26	0/2684
50	Qd	0.15	0/1962	0.27	0/2663
51	QE	0.12	0/1550	0.25	0/2098
51	QK	0.11	0/528	0.27	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	0.25	0/714
53	QG	0.14	0/913	0.25	0/1223
53	Qg	0.14	0/913	0.27	0/1223
54	QH	0.14	0/684	0.30	0/926
54	Qh	0.14	0/688	0.28	0/931
55	QI	0.11	0/520	0.20	0/701
55	Qi	0.16	0/506	0.27	0/683
56	QJ	0.10	0/420	0.22	0/576
56	Qj	0.14	0/437	0.31	0/598
57	S1	0.15	0/5378	0.32	2/7287 (0.0%)
58	S2	0.18	0/3538	0.31	0/4796
59	S3	0.15	0/1789	0.29	0/2436
60	S4	0.14	0/1030	0.27	0/1391
61	S5	0.11	0/889	0.23	0/1190
62	S6	0.13	0/755	0.29	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
63	S7	0.17	0/1279	0.30	0/1730
64	S8	0.16	0/1443	0.29	0/1952
65	V1	0.15	0/3391	0.31	0/4583
66	V2	0.14	0/1711	0.30	0/2328
67	V3	0.11	0/365	0.27	0/493
All	All	0.14	0/115736	0.29	2/157010 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	S1	364	ASP	CA-C-N	-5.03	114.77	122.21
57	S1	364	ASP	C-N-CA	-5.03	114.77	122.21

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	23	0
2	5A	825	0	823	12	0
3	5B	724	0	705	15	0
4	6A	620	0	589	16	0
5	6B	684	0	649	12	0
6	6C	574	0	590	7	0
7	7A	447	0	443	13	0
8	7B	392	0	372	4	0
9	7C	387	0	385	13	0
10	8B	338	0	342	6	0
11	A1	562	0	557	9	0
12	A2	686	0	699	8	0
13	A3	643	0	642	5	0
14	A5	910	0	950	8	0
15	A6	967	0	972	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A7	780	0	808	9	0
17	A8	1398	0	1372	20	0
18	A9	2743	0	2762	33	0
19	AB	624	0	625	10	0
19	AC	702	0	694	9	0
20	AK	2601	0	2566	28	0
21	AL	1021	0	1025	13	0
22	AM	1204	0	1162	15	0
23	AN	1173	0	1166	20	0
24	B1	479	0	486	8	0
25	B2	584	0	529	10	0
26	B3	641	0	620	8	0
27	B4	1062	0	1072	7	0
28	B5	1151	0	1164	13	0
29	B6	882	0	899	20	0
30	B7	1068	0	1043	22	0
31	B8	1315	0	1208	11	0
32	B9	1534	0	1470	21	0
33	BK	1456	0	1426	23	0
34	BL	828	0	788	8	0
35	C1	4024	0	4005	82	0
36	C2	1833	0	1843	45	0
37	C3	2103	0	2034	50	0
38	C4	1153	0	1130	20	0
39	CA	417	0	422	4	0
40	CB	1000	0	994	13	0
41	N1	2508	0	2607	60	0
42	N2	2710	0	2874	46	0
43	N3	914	0	951	18	0
44	N4	3631	0	3839	55	0
45	N5	4785	0	4933	98	0
46	N6	1329	0	1326	31	0
47	QA	3147	0	3129	40	0
47	Qa	3147	0	3129	40	0
48	QB	3459	0	3350	45	0
48	Qb	3367	0	3262	34	0
49	QC	3025	0	3090	38	0
49	Qc	3025	0	3090	35	0
50	QD	1921	0	1867	26	0
50	Qd	1904	0	1849	32	0
51	QE	1517	0	1500	33	0
51	QK	520	0	554	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Qe	1517	0	1500	21	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	6	0
53	QG	893	0	888	8	0
53	Qg	893	0	888	10	0
54	QH	662	0	660	12	0
54	Qh	666	0	663	9	0
55	QI	507	0	509	5	0
55	Qi	493	0	491	5	0
56	QJ	405	0	405	6	0
56	Qj	421	0	418	5	0
57	S1	5290	0	5321	92	0
58	S2	3459	0	3396	68	0
59	S3	1738	0	1693	18	0
60	S4	1007	0	1008	17	0
61	S5	867	0	871	9	0
62	S6	741	0	701	7	0
63	S7	1248	0	1254	31	0
64	S8	1412	0	1363	30	0
65	V1	3316	0	3272	56	0
66	V2	1671	0	1673	20	0
67	V3	355	0	329	10	0
68	4L	92	0	137	8	0
68	7A	91	0	132	6	0
68	A7	51	0	46	1	0
68	A8	83	0	113	7	0
68	AK	68	0	80	3	0
68	AL	94	0	138	7	0
68	B4	80	0	107	4	0
68	B5	100	0	156	6	0
68	C3	170	0	240	7	0
68	CB	100	0	156	4	0
68	N1	78	0	103	4	0
68	N4	62	0	68	2	0
68	N5	189	0	284	15	0
68	QB	64	0	72	3	0
68	QC	55	0	54	2	0
68	QD	64	0	72	1	0
68	QH	125	0	138	7	0
68	Qb	64	0	72	2	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	11	0
70	C1	183	0	274	14	0
70	C3	190	0	291	13	0
70	N1	48	0	73	3	0
70	N3	54	0	88	1	0
70	QB	51	0	79	2	0
70	Qb	48	0	73	2	0
70	Qc	54	0	88	4	0
70	Qh	54	0	88	1	0
71	6C	43	0	67	1	0
71	AL	47	0	75	2	0
71	AM	51	0	83	6	0
71	B1	52	0	88	1	0
71	CB	52	0	88	3	0
71	N4	49	0	79	4	0
71	N6	52	0	88	1	0
71	QI	52	0	88	2	0
71	Qi	46	0	73	5	0
71	S7	52	0	88	6	0
72	7A	43	0	60	6	0
72	B8	32	0	38	0	0
72	C1	85	0	124	1	0
72	CA	51	0	82	1	0
72	CB	46	0	69	1	0
72	N5	46	0	69	1	0
72	QE	44	0	65	1	0
72	QJ	34	0	42	1	0
72	Qc	48	0	73	2	0
72	Qj	29	0	32	0	0
72	S7	51	0	82	2	0
73	7C	51	0	82	5	0
73	A9	39	0	52	4	0
73	N1	31	0	36	0	0
73	N3	51	0	82	4	0
73	N4	49	0	75	5	0
73	N5	137	0	205	4	0
73	QB	34	0	42	1	0
73	QC	40	0	54	1	0
73	QE	47	0	71	2	0
73	Qc	42	0	61	1	0
73	Qe	75	0	104	8	0
73	S2	48	0	73	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	S8	51	0	82	7	0
74	A9	48	0	26	1	0
75	AB	36	0	47	2	0
75	AC	36	0	47	4	0
76	AK	27	0	12	3	0
77	C1	120	0	108	18	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	7	0
81	QD	43	0	30	2	0
81	Qd	43	0	32	4	0
82	QE	4	0	0	2	0
82	Qe	4	0	0	2	0
82	S1	4	0	0	0	0
82	V2	4	0	0	0	0
83	S1	16	0	0	1	0
83	S7	8	0	0	1	0
83	S8	16	0	0	1	0
83	V1	8	0	0	0	0
84	S2	9	0	0	0	0
85	S7	63	0	90	6	0
86	V1	31	0	19	1	0
All	All	117589	0	118918	1583	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 1583 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	1.73	0.88
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.62	0.81
49:QC:98:VAL:HG22	80:QC:402:HEM:HBC2	1.64	0.80
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.64	0.80
68:4L:201:CDL:H521	46:N6:88:THR:HG23	1.65	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	5A	100/102 (98%)	100 (100%)	0	0	100	100
3	5B	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
4	6A	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
5	6B	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	6C	68/70 (97%)	68 (100%)	0	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100
8	7B	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
9	7C	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
10	8B	41/43 (95%)	41 (100%)	0	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%)	108 (96%)	3 (3%)	1 (1%)	14	29
16	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
17	A8	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
18	A9	339/341 (99%)	331 (98%)	8 (2%)	0	100	100
19	AB	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
19	AC	85/87 (98%)	85 (100%)	0	0	100	100
20	AK	319/321 (99%)	310 (97%)	9 (3%)	0	100	100
21	AL	138/140 (99%)	138 (100%)	0	0	100	100
22	AM	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
23	AN	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
26	B3	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
29	B6	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
30	B7	123/125 (98%)	118 (96%)	5 (4%)	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	172/174 (99%)	171 (99%)	1 (1%)	0	100	100
34	BL	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
35	C1	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
36	C2	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
37	C3	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
38	C4	136/138 (99%)	131 (96%)	5 (4%)	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	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
42	N2	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
43	N3	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
44	N4	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
45	N5	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
46	N6	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
47	QA	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
47	Qa	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
48	QB	444/446 (100%)	431 (97%)	13 (3%)	0	100	100
48	Qb	429/446 (96%)	424 (99%)	5 (1%)	0	100	100
49	QC	377/379 (100%)	374 (99%)	3 (1%)	0	100	100
49	Qc	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
50	QD	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/241 (98%)	233 (98%)	4 (2%)	0	100	100
51	QE	194/274 (71%)	189 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	QK	69/274 (25%)	69 (100%)	0	0	100	100
51	Qe	194/274 (71%)	189 (97%)	5 (3%)	0	100	100
52	QF	65/67 (97%)	64 (98%)	1 (2%)	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	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
54	Qh	77/79 (98%)	77 (100%)	0	0	100	100
55	QI	60/62 (97%)	60 (100%)	0	0	100	100
55	Qi	58/62 (94%)	58 (100%)	0	0	100	100
56	QJ	47/52 (90%)	46 (98%)	1 (2%)	0	100	100
56	Qj	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
57	S1	687/689 (100%)	663 (96%)	24 (4%)	0	100	100
58	S2	427/430 (99%)	413 (97%)	14 (3%)	0	100	100
59	S3	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
60	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
61	S5	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
62	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
63	S7	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
64	S8	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
65	V1	429/431 (100%)	411 (96%)	18 (4%)	0	100	100
66	V2	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
67	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13972/14569 (96%)	13630 (98%)	341 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	A6	49	ARG

### 5.3.2 Protein sidechains [i](#)

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%)	88 (99%)	1 (1%)	70	85
3	5B	80/80 (100%)	78 (98%)	2 (2%)	42	68
4	6A	66/66 (100%)	66 (100%)	0	100	100
5	6B	73/73 (100%)	72 (99%)	1 (1%)	62	82
6	6C	57/57 (100%)	57 (100%)	0	100	100
7	7A	48/48 (100%)	48 (100%)	0	100	100
8	7B	39/39 (100%)	38 (97%)	1 (3%)	41	67
9	7C	40/40 (100%)	39 (98%)	1 (2%)	42	68
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%)	65	83
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	98 (99%)	1 (1%)	73	87
15	A6	107/107 (100%)	107 (100%)	0	100	100
16	A7	87/97 (90%)	83 (95%)	4 (5%)	23	44
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	295/295 (100%)	292 (99%)	3 (1%)	73	87
19	AB	71/80 (89%)	71 (100%)	0	100	100
19	AC	80/80 (100%)	79 (99%)	1 (1%)	65	83
20	AK	284/284 (100%)	281 (99%)	3 (1%)	70	85
21	AL	101/101 (100%)	100 (99%)	1 (1%)	73	87
22	AM	130/130 (100%)	128 (98%)	2 (2%)	60	81
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	B6	98/119 (82%)	98 (100%)	0	100	100
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	155/155 (100%)	155 (100%)	0	100	100
34	BL	91/91 (100%)	91 (100%)	0	100	100
35	C1	425/425 (100%)	423 (100%)	2 (0%)	86	94
36	C2	212/212 (100%)	205 (97%)	7 (3%)	33	59
37	C3	224/224 (100%)	223 (100%)	1 (0%)	89	95
38	C4	123/123 (100%)	122 (99%)	1 (1%)	79	90
39	CA	45/45 (100%)	45 (100%)	0	100	100
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	275/275 (100%)	272 (99%)	3 (1%)	70	85
42	N2	311/311 (100%)	311 (100%)	0	100	100
43	N3	100/100 (100%)	99 (99%)	1 (1%)	73	87
44	N4	410/410 (100%)	408 (100%)	2 (0%)	86	94
45	N5	537/537 (100%)	534 (99%)	3 (1%)	84	92
46	N6	140/140 (100%)	139 (99%)	1 (1%)	81	91
47	QA	330/330 (100%)	328 (99%)	2 (1%)	84	92
47	Qa	330/330 (100%)	323 (98%)	7 (2%)	48	72
48	QB	372/372 (100%)	370 (100%)	2 (0%)	86	94
48	Qb	362/372 (97%)	360 (99%)	2 (1%)	84	92
49	QC	332/332 (100%)	327 (98%)	5 (2%)	60	81
49	Qc	332/332 (100%)	329 (99%)	3 (1%)	75	88
50	QD	206/206 (100%)	205 (100%)	1 (0%)	86	94
50	Qd	204/206 (99%)	203 (100%)	1 (0%)	86	94
51	QE	166/225 (74%)	165 (99%)	1 (1%)	84	92
51	QK	55/225 (24%)	54 (98%)	1 (2%)	54	76
51	Qe	166/225 (74%)	166 (100%)	0	100	100
52	QF	64/64 (100%)	63 (98%)	1 (2%)	58	79
52	Qf	61/64 (95%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	QG	93/93 (100%)	93 (100%)	0	100	100
53	Qg	93/93 (100%)	92 (99%)	1 (1%)	70	85
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	70 (100%)	0	100	100
55	QI	50/50 (100%)	49 (98%)	1 (2%)	50	73
55	Qi	49/50 (98%)	48 (98%)	1 (2%)	50	73
56	QJ	40/42 (95%)	40 (100%)	0	100	100
56	Qj	41/42 (98%)	40 (98%)	1 (2%)	44	69
57	S1	579/579 (100%)	576 (100%)	3 (0%)	86	94
58	S2	370/370 (100%)	367 (99%)	3 (1%)	79	90
59	S3	190/190 (100%)	188 (99%)	2 (1%)	70	85
60	S4	112/112 (100%)	110 (98%)	2 (2%)	54	76
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%)	60	81
64	S8	151/151 (100%)	150 (99%)	1 (1%)	81	91
65	V1	344/344 (100%)	338 (98%)	6 (2%)	56	78
66	V2	183/183 (100%)	181 (99%)	2 (1%)	70	85
67	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12184/12531 (97%)	12090 (99%)	94 (1%)	77	90

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	Qa	129	ASP
55	Qi	18	THR
47	Qa	168	ASN
48	Qb	92	PHE
57	S1	690	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
59	S3	196	HIS

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Mol	Chain	Res	Type
62	S6	74	GLN
44	N4	213	HIS
43	N3	26	GLN
65	V1	303	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	2MR	S2	124	58	10,12,13	2.45	3 (30%)	5,13,15	1.01	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	S2	124	2MR	CZ-NE	5.20	1.45	1.34
58	S2	124	2MR	CZ-NH2	5.07	1.44	1.33
58	S2	124	2MR	CQ1-NH1	-2.03	1.42	1.46

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	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 7 are monoatomic - leaving 99 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	$\# Z  > 2$
72	3PE	C1	609	-	45,45,50	0.32	0	48,50,55	0.28	0
83	SF4	S1	802	57	0,12,12	-	-	-		
81	HEC	Qd	401	50	32,50,50	2.03	5 (15%)	24,82,82	2.25	13 (54%)
83	SF4	S1	801	57	0,12,12	-	-	-		
70	PC1	Qh	101	-	53,53,53	0.30	0	59,61,61	0.26	0
82	FES	V2	301	66	0,4,4	-	-	-		
73	PEE	N5	702	-	39,39,50	1.49	5 (12%)	41,44,55	1.22	2 (4%)
68	CDL	7A	102	-	90,90,99	0.31	0	96,102,111	0.28	0
86	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.41	0
77	HEA	C1	601	35	57,67,67	2.01	18 (31%)	61,103,103	2.68	29 (47%)
80	HEM	Qc	402	49	41,50,50	1.20	3 (7%)	45,82,82	1.69	8 (17%)
70	PC1	C1	608	-	53,53,53	0.29	0	59,61,61	0.32	0
70	PC1	C3	302	-	48,48,53	0.31	0	54,56,61	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
71	PLX	B1	101	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	1 (1%)
73	PEE	S2	501	-	47,47,50	1.35	5 (10%)	50,52,55	1.20	4 (8%)
72	3PE	Qj	101	-	28,28,50	0.39	0	31,33,55	0.36	0
68	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.27	0
68	CDL	QH	101	-	60,60,99	0.38	0	66,72,111	0.32	0
72	3PE	7A	101	-	42,42,50	0.33	0	45,47,55	0.28	0
72	3PE	C1	607	-	38,38,50	0.35	0	41,43,55	0.37	0
70	PC1	QB	503	-	50,50,53	0.30	0	56,58,61	0.36	0
70	PC1	C3	306	-	42,42,53	0.32	0	48,50,61	0.29	0
72	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.28	0
74	NDP	A9	401	-	45,52,52	0.54	0	53,80,80	0.53	1 (1%)
68	CDL	B4	201	-	79,79,99	0.33	0	85,91,111	0.32	0
68	CDL	QC	404	-	54,54,99	0.40	0	60,66,111	0.36	0
81	HEC	QD	401	50	32,50,50	1.99	4 (12%)	24,82,82	2.41	15 (62%)
73	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.20	3 (5%)
70	PC1	C1	610	-	49,49,53	0.30	0	55,57,61	0.35	0
82	FES	QE	303	51	0,4,4	-	-	-	-	-
73	PEE	N5	705	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	3 (5%)
68	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.33	0
68	CDL	N4	503	-	61,61,99	0.37	0	67,73,111	0.35	0
75	ZMP	AB	201	19	29,35,36	0.69	1 (3%)	34,42,45	0.77	1 (2%)
76	ADP	AK	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
73	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.18	3 (6%)
70	PC1	N3	202	-	53,53,53	0.30	0	59,61,61	0.29	0
71	PLX	CB	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.88	1 (1%)
73	PEE	QB	502	-	33,33,50	1.41	4 (12%)	36,38,55	1.14	2 (5%)
68	CDL	C3	305	-	82,82,99	0.32	0	88,94,111	0.27	0
73	PEE	QE	301	-	46,46,50	1.36	5 (10%)	49,51,55	1.24	5 (10%)
83	SF4	V1	501	65	0,12,12	-	-	-	-	-
73	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	3 (5%)
68	CDL	B5	201	-	99,99,99	0.31	0	105,111,111	0.37	0
70	PC1	C1	606	-	45,45,53	0.31	0	51,53,61	0.31	0
73	PEE	A9	402	-	38,38,50	1.48	5 (13%)	41,43,55	1.23	3 (7%)
70	PC1	C3	303	-	53,53,53	0.31	0	59,61,61	0.43	0
73	PEE	Qe	302	-	23,23,50	1.42	3 (13%)	26,28,55	1.34	3 (11%)
72	3PE	QE	302	-	43,43,50	0.32	0	46,48,55	0.31	0
72	3PE	CB	202	-	45,45,50	0.32	0	48,50,55	0.29	0
80	HEM	QC	402	49	41,50,50	1.23	3 (7%)	45,82,82	1.70	8 (17%)
75	ZMP	AC	201	19	29,35,36	0.65	1 (3%)	34,42,45	0.78	1 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
68	CDL	QB	501	-	63,63,99	0.37	0	69,75,111	0.38	0
68	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.30	0
72	3PE	S7	204	-	50,50,50	0.32	0	53,55,55	0.37	0
73	PEE	N4	501	-	48,48,50	1.34	5 (10%)	51,53,55	1.23	2 (3%)
73	PEE	QC	403	-	39,39,50	1.31	4 (10%)	42,44,55	1.19	3 (7%)
68	CDL	CB	203	-	99,99,99	0.30	0	105,111,111	0.27	0
71	PLX	6C	101	-	42,42,51	1.17	4 (9%)	46,50,59	0.85	1 (2%)
84	MF8	S2	502	-	7,8,8	1.06	0	7,10,10	1.40	1 (14%)
70	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.31	0
70	PC1	Qb	502	-	47,47,53	0.31	0	53,55,61	0.36	0
73	PEE	Qc	401	-	41,41,50	1.28	4 (9%)	44,46,55	1.17	3 (6%)
70	PC1	C1	605	-	32,32,53	0.36	0	38,40,61	0.35	0
71	PLX	AL	202	-	46,46,51	1.16	5 (10%)	50,54,59	0.87	1 (2%)
70	PC1	C3	301	-	43,43,53	0.31	0	49,51,61	0.30	0
71	PLX	AM	201	-	50,50,51	1.12	4 (8%)	54,58,59	0.85	1 (1%)
83	SF4	S7	202	63	0,12,12	-	-	-	-	-
73	PEE	N1	403	-	30,30,50	1.28	3 (10%)	33,35,55	1.15	2 (6%)
68	CDL	A7	201	-	50,50,99	0.40	0	56,62,111	0.33	0
72	3PE	Qc	404	-	47,47,50	0.31	0	50,52,55	0.29	0
70	PC1	Qc	405	-	53,53,53	0.29	0	59,61,61	0.33	0
72	3PE	N5	706	-	45,45,50	0.33	0	48,50,55	0.29	0
73	PEE	Qe	301	-	50,50,50	1.32	5 (10%)	53,55,55	1.19	3 (5%)
80	HEM	Qc	403	49	41,50,50	1.23	3 (7%)	45,82,82	1.69	8 (17%)
68	CDL	C3	304	-	86,86,99	0.32	0	92,98,111	0.28	0
68	CDL	AK	402	-	67,67,99	0.36	0	73,79,111	0.38	0
71	PLX	N4	502	-	48,48,51	1.13	4 (8%)	52,56,59	0.91	2 (3%)
71	PLX	N6	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
70	PC1	N1	402	-	47,47,53	0.31	0	53,55,61	0.30	0
68	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.35	0
68	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.31	0
82	FES	Qe	303	51	0,4,4	-	-	-	-	-
71	PLX	Qi	301	-	45,45,51	1.18	6 (13%)	49,53,59	0.82	1 (2%)
68	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.36	0
71	PLX	QI	301	-	51,51,51	1.11	4 (7%)	55,59,59	0.87	1 (1%)
85	U10	S7	201	-	63,63,63	2.17	21 (33%)	76,79,79	1.68	21 (27%)
80	HEM	QC	401	49	41,50,50	1.20	4 (9%)	45,82,82	1.74	9 (20%)
68	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.31	0
83	SF4	S8	301	64	0,12,12	-	-	-	-	-
68	CDL	QD	402	-	63,63,99	0.37	0	69,75,111	0.39	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
82	FES	S1	803	57	0,4,4	-	-	-		
68	CDL	QH	102	-	63,63,99	0.37	0	69,75,111	0.35	0
72	3PE	QJ	101	-	33,33,50	0.37	0	36,38,55	0.34	0
72	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.34	0
77	HEA	C1	602	35	57,67,67	2.04	18 (31%)	61,103,103	2.64	26 (42%)
83	SF4	S8	302	64	0,12,12	-	-	-		
73	PEE	7C	101	-	50,50,50	1.33	5 (10%)	53,55,55	1.16	4 (7%)
71	PLX	S7	203	-	51,51,51	1.11	3 (5%)	55,59,59	0.88	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	3PE	C1	609	-	-	15/49/49/54	-
83	SF4	S1	802	57	-	-	0/6/5/5
81	HEC	Qd	401	50	-	5/10/54/54	-
83	SF4	S1	801	57	-	-	0/6/5/5
70	PC1	Qh	101	-	-	5/57/57/57	-
82	FES	V2	301	66	-	-	0/1/1/1
73	PEE	N5	702	-	-	20/43/43/54	-
68	CDL	7A	102	-	-	18/101/101/110	-
86	FMN	V1	502	-	-	0/18/18/18	0/3/3/3
77	HEA	C1	601	35	-	10/32/76/76	-
80	HEM	Qc	402	49	-	7/12/54/54	-
70	PC1	C1	608	-	-	14/57/57/57	-
70	PC1	C3	302	-	-	16/52/52/57	-
71	PLX	B1	101	-	-	18/55/55/55	-
73	PEE	S2	501	-	-	30/51/51/54	-
72	3PE	Qj	101	-	-	7/32/32/54	-
68	CDL	N5	704	-	-	19/110/110/110	-
68	CDL	QH	101	-	-	11/71/71/110	-
72	3PE	7A	101	-	-	13/46/46/54	-
72	3PE	C1	607	-	-	13/42/42/54	-
70	PC1	QB	503	-	-	8/54/54/57	-
70	PC1	C3	306	-	-	8/46/46/57	-
72	3PE	CA	101	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	NDP	A9	401	-	-	6/30/77/77	0/5/5/5
68	CDL	B4	201	-	-	21/90/90/110	-
68	CDL	QC	404	-	-	19/65/65/110	-
81	HEC	QD	401	50	-	2/10/54/54	-
73	PEE	S8	303	-	-	24/54/54/54	-
70	PC1	C1	610	-	-	7/53/53/57	-
82	FES	QE	303	51	-	-	0/1/1/1
73	PEE	N5	705	-	-	27/54/54/54	-
68	CDL	A8	301	-	-	20/93/93/110	-
68	CDL	N4	503	-	-	22/72/72/110	-
75	ZMP	AB	201	19	-	8/40/42/43	-
76	ADP	AK	401	-	-	4/12/32/32	0/3/3/3
73	PEE	N5	701	-	-	26/49/49/54	-
70	PC1	N3	202	-	-	15/57/57/57	-
71	PLX	CB	201	-	-	26/55/55/55	-
73	PEE	QB	502	-	-	22/37/37/54	-
68	CDL	C3	305	-	-	11/93/93/110	-
73	PEE	QE	301	-	-	24/50/50/54	-
83	SF4	V1	501	65	-	-	0/6/5/5
73	PEE	N3	201	-	-	26/54/54/54	-
68	CDL	B5	201	-	-	17/110/110/110	-
70	PC1	C1	606	-	-	7/49/49/57	-
73	PEE	A9	402	-	-	20/42/42/54	-
70	PC1	C3	303	-	-	14/57/57/57	-
73	PEE	Qe	302	-	-	9/27/27/54	-
72	3PE	QE	302	-	-	7/47/47/54	-
72	3PE	CB	202	-	-	12/49/49/54	-
80	HEM	QC	402	49	-	4/12/54/54	-
75	ZMP	AC	201	19	-	19/40/42/43	-
68	CDL	QB	501	-	-	15/74/74/110	-
68	CDL	N1	401	-	-	14/88/88/110	-
72	3PE	S7	204	-	-	12/54/54/54	-
73	PEE	N4	501	-	-	24/52/52/54	-
73	PEE	QC	403	-	-	14/43/43/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	CDL	CB	203	-	-	25/110/110/110	-
71	PLX	6C	101	-	-	16/46/46/55	-
84	MF8	S2	502	-	-	5/8/8/8	-
70	PC1	6A	101	-	-	10/48/48/57	-
70	PC1	Qb	502	-	-	12/51/51/57	-
73	PEE	Qc	401	-	-	27/45/45/54	-
70	PC1	C1	605	-	-	8/36/36/57	-
71	PLX	AL	202	-	-	19/50/50/55	-
70	PC1	C3	301	-	-	12/47/47/57	-
71	PLX	AM	201	-	-	20/54/54/55	-
83	SF4	S7	202	63	-	-	0/6/5/5
73	PEE	N1	403	-	-	22/34/34/54	-
68	CDL	A7	201	-	-	12/61/61/110	-
72	3PE	Qc	404	-	-	10/51/51/54	-
70	PC1	Qc	405	-	-	11/57/57/57	-
72	3PE	N5	706	-	-	12/49/49/54	-
73	PEE	Qe	301	-	-	28/54/54/54	-
80	HEM	Qc	403	49	-	9/12/54/54	-
68	CDL	C3	304	-	-	13/97/97/110	-
68	CDL	AK	402	-	-	18/78/78/110	-
71	PLX	N4	502	-	-	17/52/52/55	-
71	PLX	N6	201	-	-	22/55/55/55	-
70	PC1	N1	402	-	-	14/51/51/57	-
68	CDL	Qb	501	-	-	18/74/74/110	-
68	CDL	AL	201	-	-	25/104/104/110	-
82	FES	Qe	303	51	-	-	0/1/1/1
71	PLX	Qi	301	-	-	24/49/49/55	-
68	CDL	4L	201	-	-	22/102/102/110	-
71	PLX	QI	301	-	-	15/55/55/55	-
85	U10	S7	201	-	-	22/63/87/87	0/1/1/1
80	HEM	QC	401	49	-	7/12/54/54	-
68	CDL	N5	703	-	-	23/99/99/110	-
83	SF4	S8	301	64	-	-	0/6/5/5
68	CDL	QD	402	-	-	17/74/74/110	-
82	FES	S1	803	57	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	CDL	QH	102	-	-	21/74/74/110	-
72	3PE	QJ	101	-	-	10/37/37/54	-
72	3PE	B8	201	-	-	8/35/35/54	-
77	HEA	C1	602	35	-	12/32/76/76	-
83	SF4	S8	302	64	-	-	0/6/5/5
73	PEE	7C	101	-	-	16/54/54/54	-
71	PLX	S7	203	-	-	22/55/55/55	-

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	S7	201	U10	C6-C1	10.34	1.54	1.35
81	Qd	401	HEC	C3C-C2C	-6.55	1.33	1.40
81	QD	401	HEC	C3C-C2C	-6.22	1.34	1.40
81	QD	401	HEC	C2B-C3B	-6.06	1.34	1.40
81	Qd	401	HEC	C2B-C3B	-5.84	1.34	1.40

The worst 5 of 205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	601	HEA	CAD-CBD-CGD	-7.00	98.54	113.60
77	C1	602	HEA	CAD-CBD-CGD	-6.96	98.63	113.60
77	C1	601	HEA	C3D-C4D-ND	6.30	116.46	110.36
77	C1	602	HEA	C2D-C1D-ND	5.64	116.52	109.84
77	C1	602	HEA	C1D-C2D-C3D	-5.62	101.05	106.96

There are no chirality outliers.

5 of 1349 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	4L	201	CDL	CA2-OA2-PA1-OA3
68	4L	201	CDL	CB2-OB2-PB2-OB3
68	4L	201	CDL	CB2-OB2-PB2-OB4
68	4L	201	CDL	CB2-OB2-PB2-OB5
68	7A	102	CDL	CA2-OA2-PA1-OA3

There are no ring outliers.

86 monomers are involved in 277 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	C1	609	3PE	1	0
83	S1	802	SF4	1	0
81	Qd	401	HEC	4	0
70	Qh	101	PC1	1	0
73	N5	702	PEE	1	0
68	7A	102	CDL	6	0
86	V1	502	FMN	1	0
77	C1	601	HEA	8	0
70	C1	608	PC1	4	0
70	C3	302	PC1	4	0
71	B1	101	PLX	1	0
73	S2	501	PEE	4	0
68	N5	704	CDL	2	0
72	7A	101	3PE	6	0
70	QB	503	PC1	2	0
70	C3	306	PC1	2	0
72	CA	101	3PE	1	0
74	A9	401	NDP	1	0
68	B4	201	CDL	4	0
68	QC	404	CDL	2	0
81	QD	401	HEC	2	0
73	S8	303	PEE	7	0
70	C1	610	PC1	9	0
82	QE	303	FES	2	0
73	N5	705	PEE	1	0
68	A8	301	CDL	7	0
68	N4	503	CDL	2	0
75	AB	201	ZMP	2	0
76	AK	401	ADP	3	0
73	N5	701	PEE	2	0
70	N3	202	PC1	1	0
71	CB	201	PLX	3	0
73	QB	502	PEE	1	0
68	C3	305	CDL	4	0
73	QE	301	PEE	2	0
73	N3	201	PEE	4	0
68	B5	201	CDL	6	0
73	A9	402	PEE	4	0
70	C3	303	PC1	4	0
73	Qe	302	PEE	1	0
72	QE	302	3PE	1	0
72	CB	202	3PE	1	0
80	QC	402	HEM	6	0

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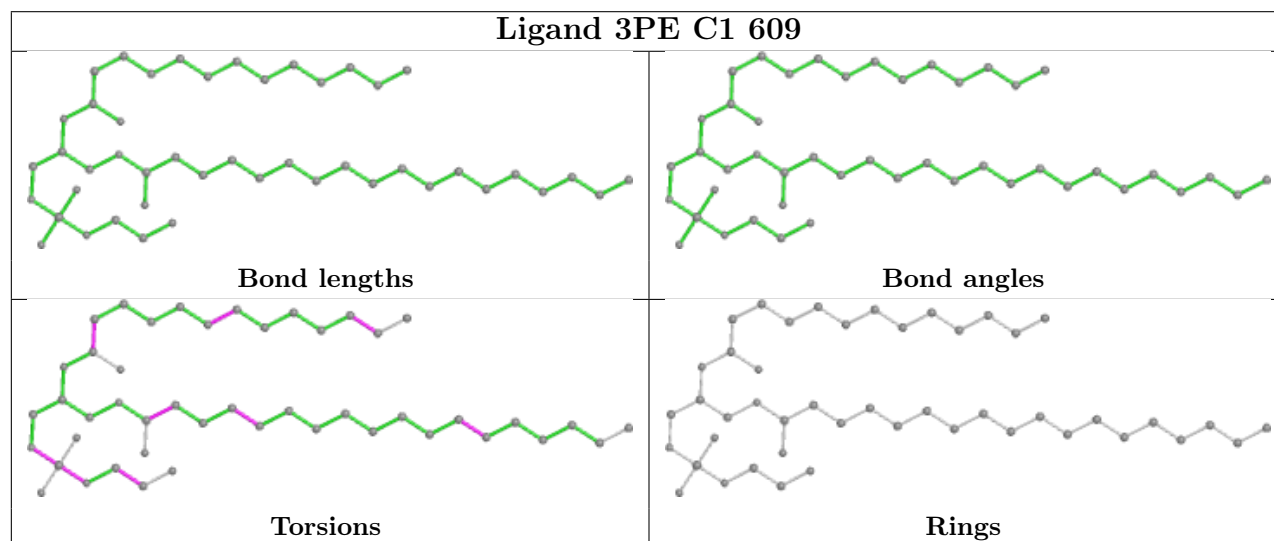
Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	AC	201	ZMP	4	0
68	QB	501	CDL	3	0
68	N1	401	CDL	4	0
72	S7	204	3PE	2	0
73	N4	501	PEE	5	0
73	QC	403	PEE	1	0
68	CB	203	CDL	4	0
71	6C	101	PLX	1	0
70	6A	101	PC1	11	0
70	Qb	502	PC1	2	0
73	Qc	401	PEE	1	0
70	C1	605	PC1	1	0
71	AL	202	PLX	2	0
70	C3	301	PC1	3	0
71	AM	201	PLX	6	0
83	S7	202	SF4	1	0
68	A7	201	CDL	1	0
72	Qc	404	3PE	2	0
70	Qc	405	PC1	4	0
72	N5	706	3PE	1	0
73	Qe	301	PEE	7	0
80	Qc	403	HEM	7	0
68	C3	304	CDL	4	0
68	AK	402	CDL	3	0
71	N4	502	PLX	4	0
71	N6	201	PLX	1	0
70	N1	402	PC1	3	0
68	Qb	501	CDL	2	0
68	AL	201	CDL	7	0
82	Qe	303	FES	2	0
71	Qi	301	PLX	5	0
68	4L	201	CDL	8	0
71	QI	301	PLX	2	0
85	S7	201	U10	6	0
80	QC	401	HEM	2	0
68	N5	703	CDL	13	0
68	QD	402	CDL	1	0
68	QH	102	CDL	7	0
72	QJ	101	3PE	1	0
77	C1	602	HEA	10	0
83	S8	302	SF4	1	0
73	7C	101	PEE	5	0

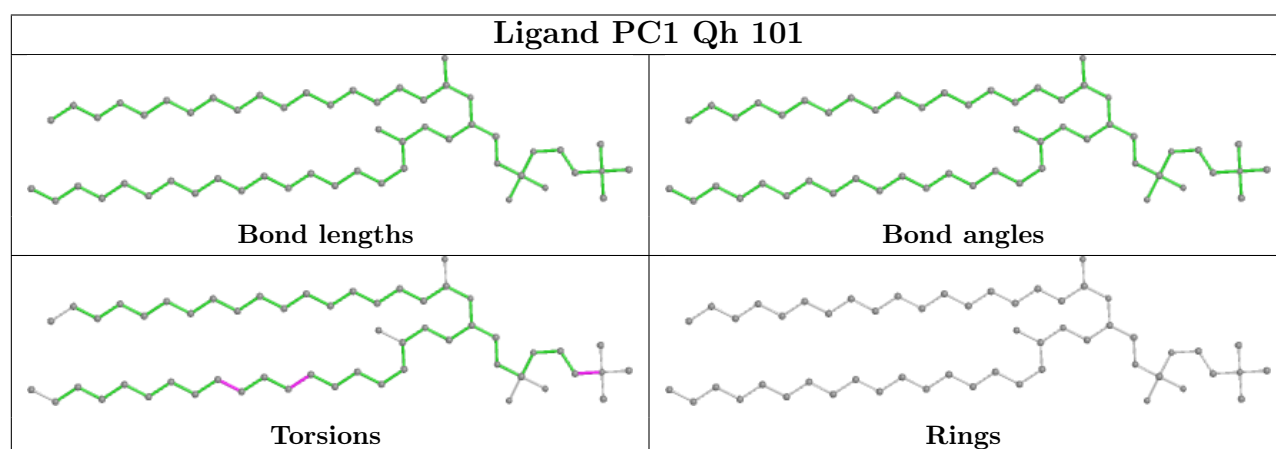
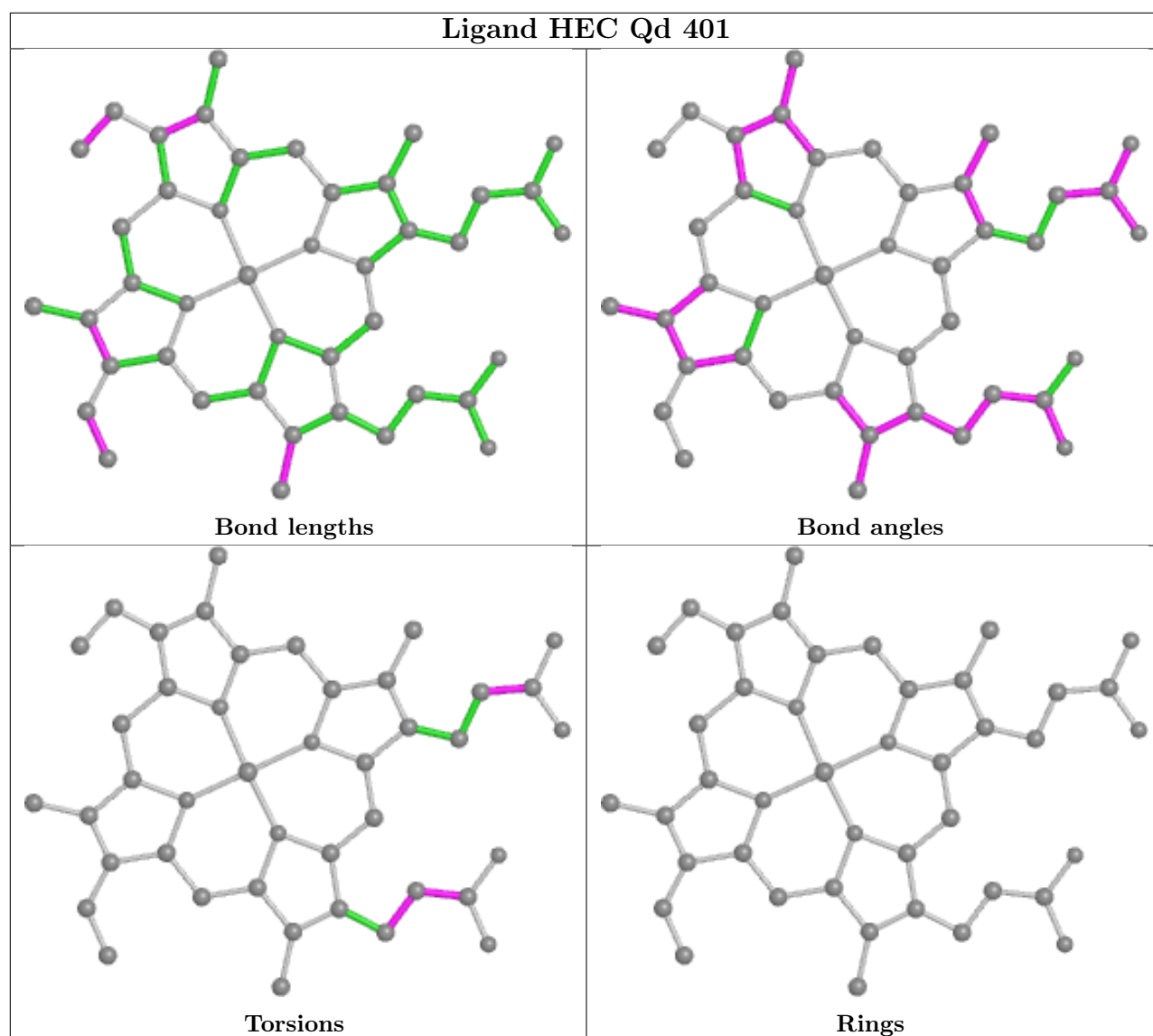
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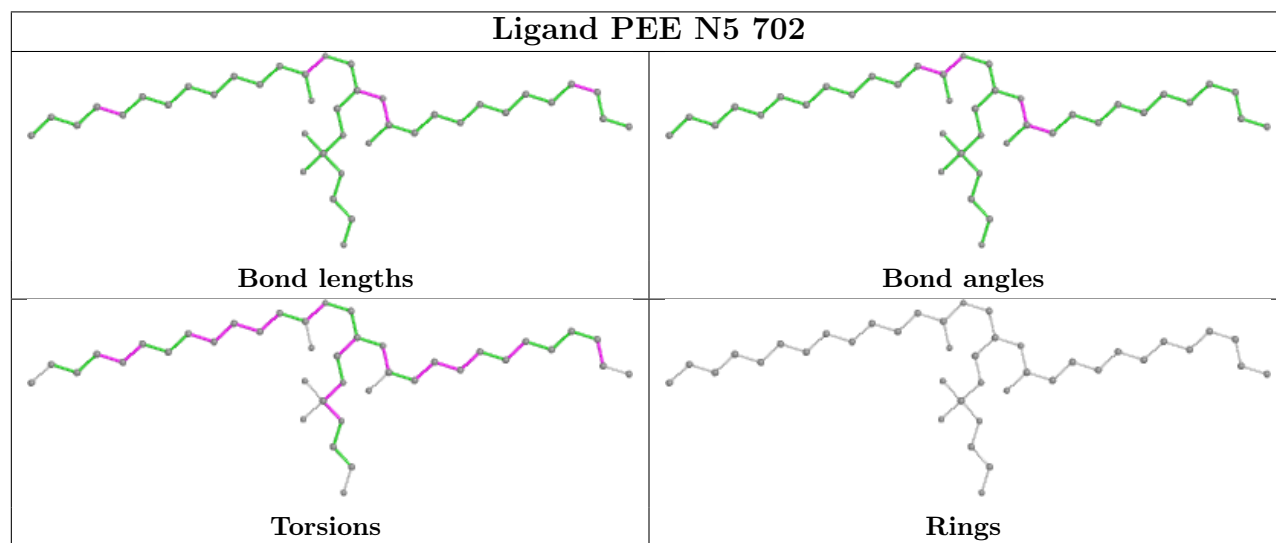
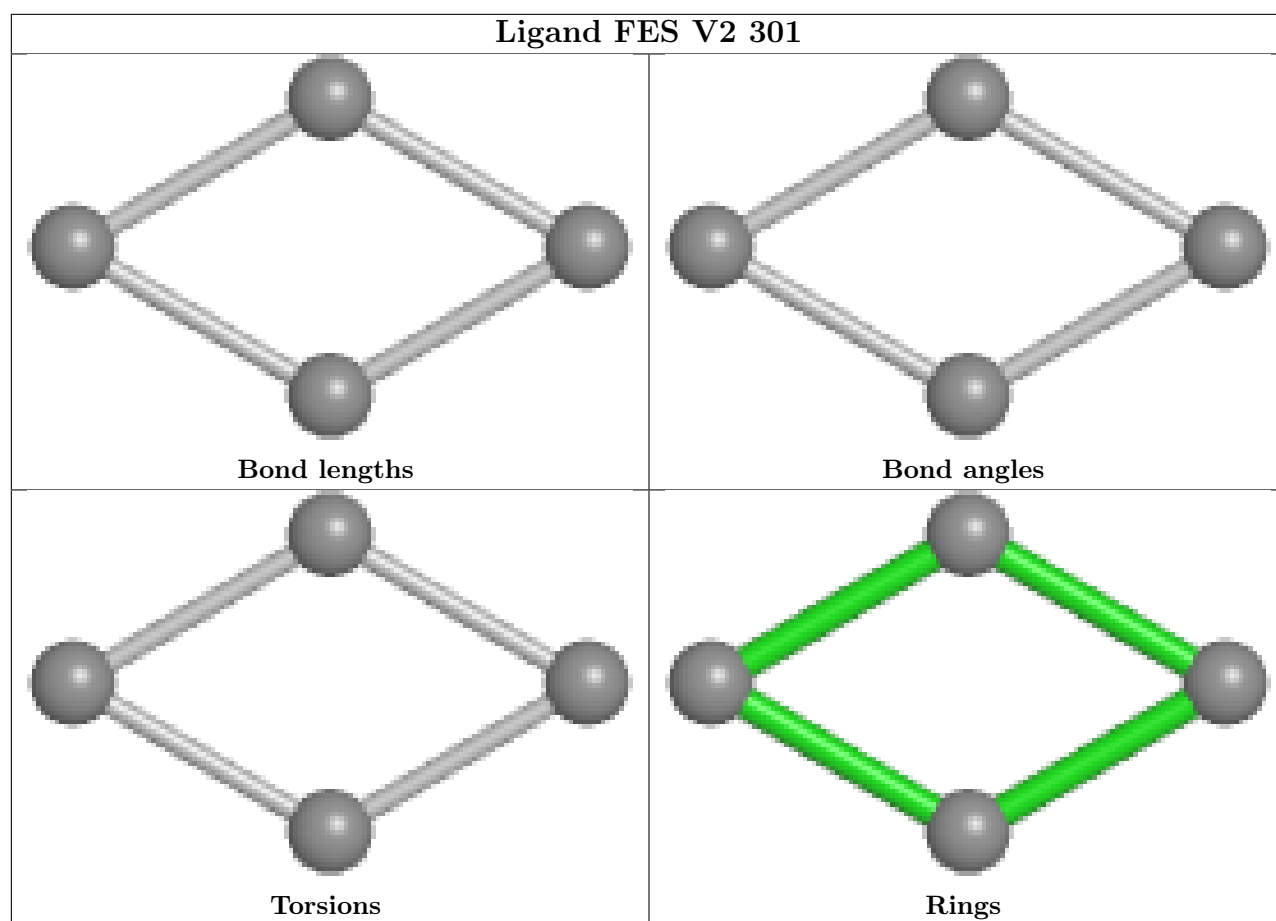
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	S7	203	PLX	6	0

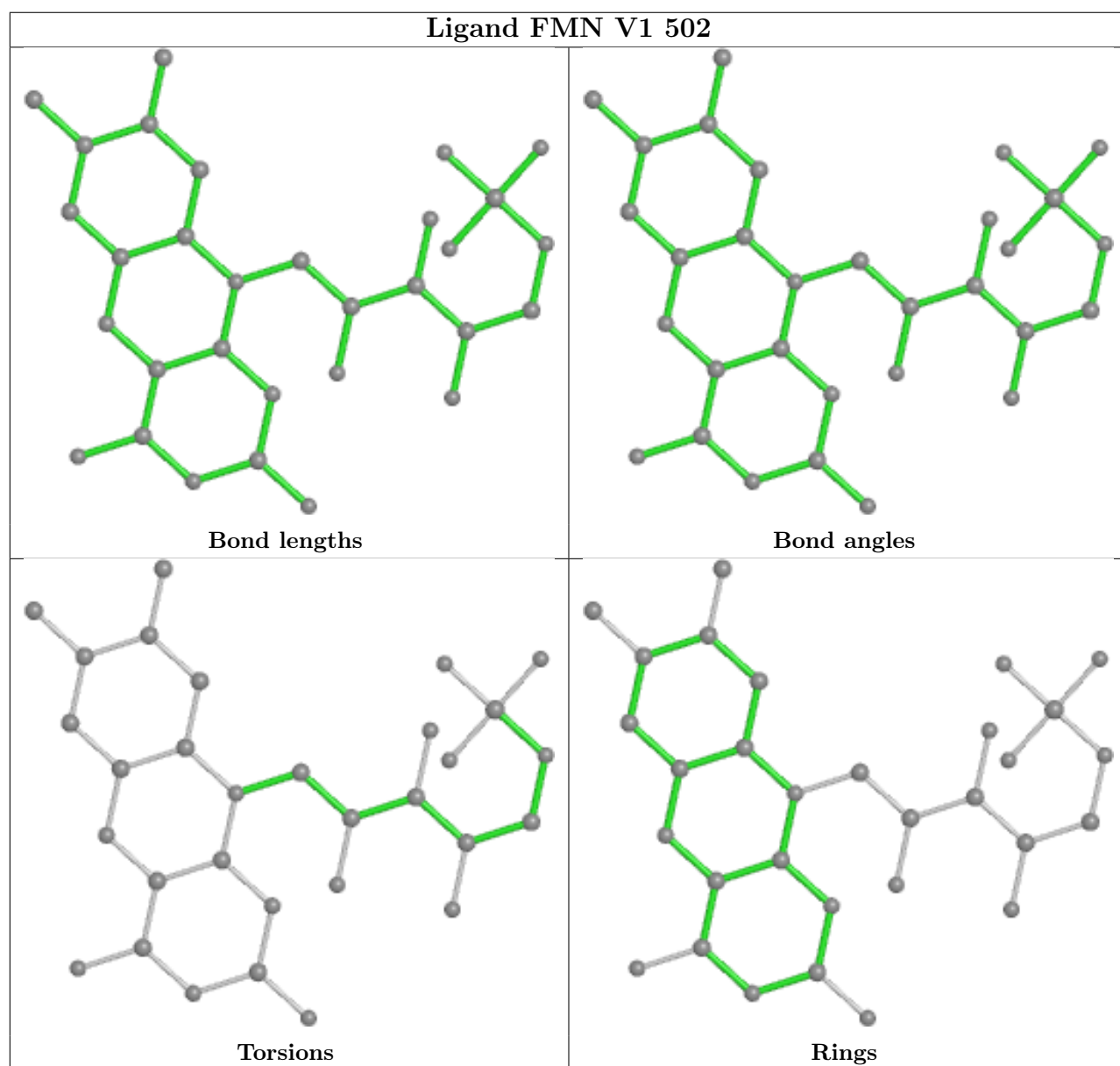
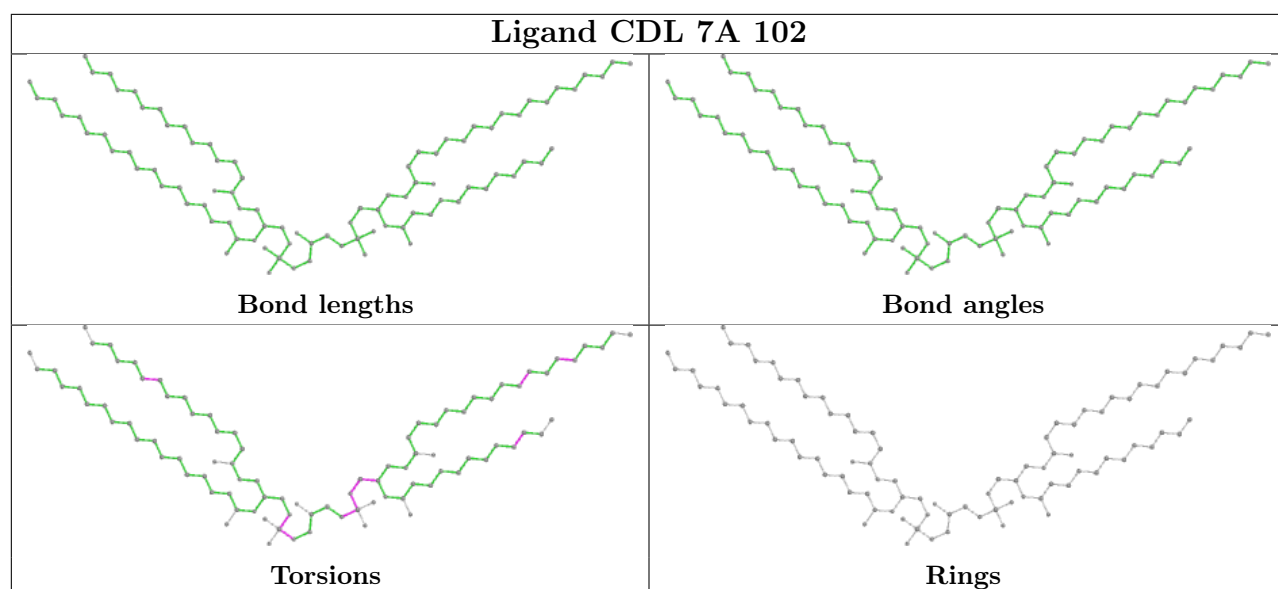
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



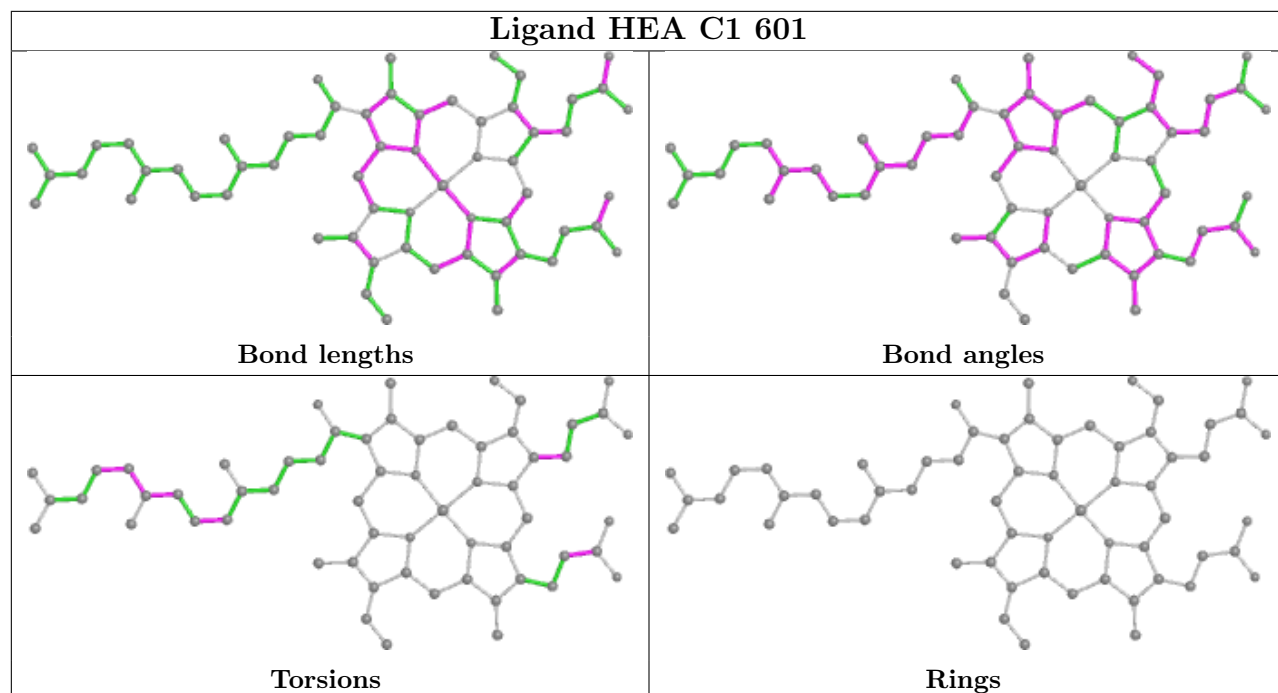




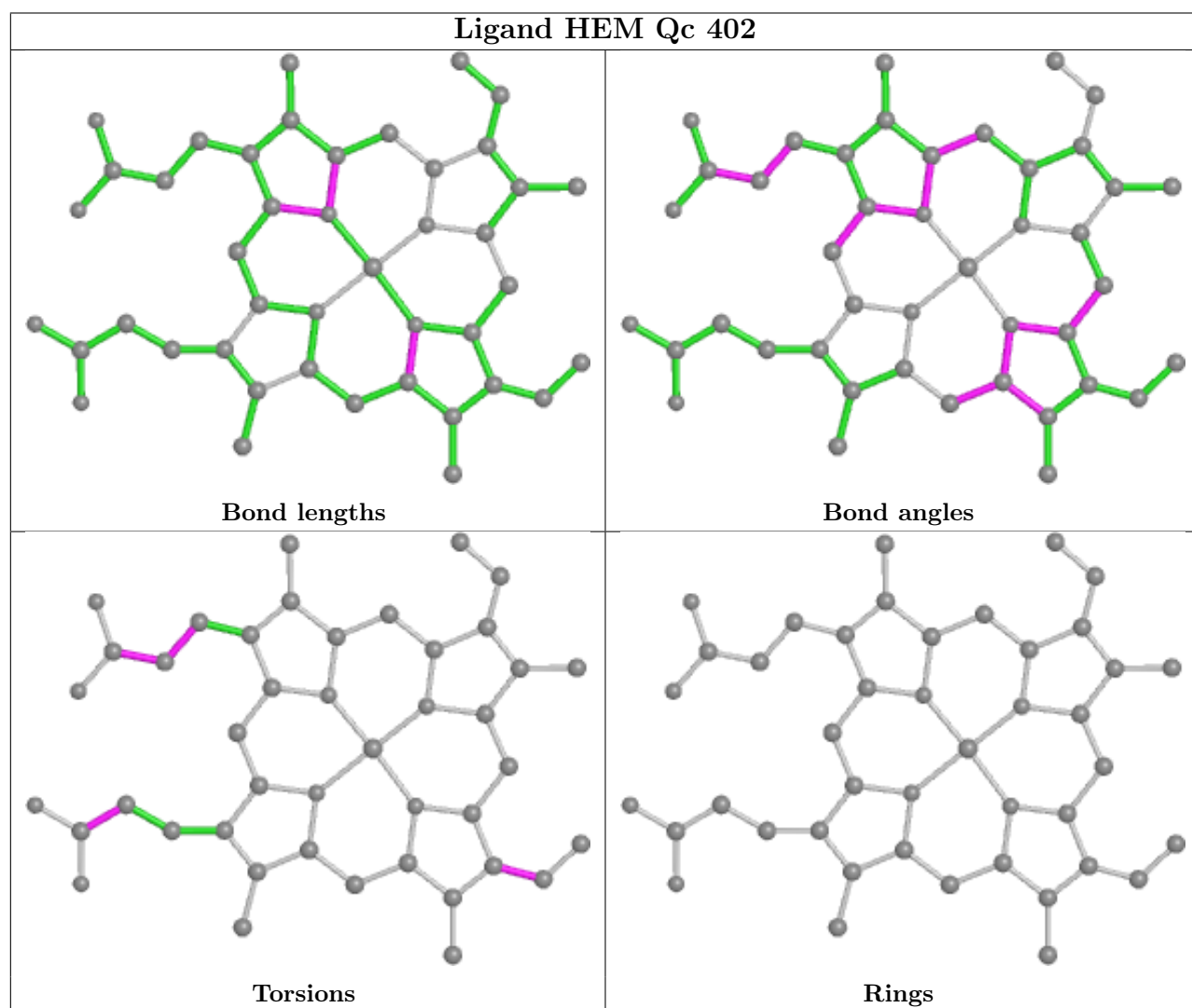


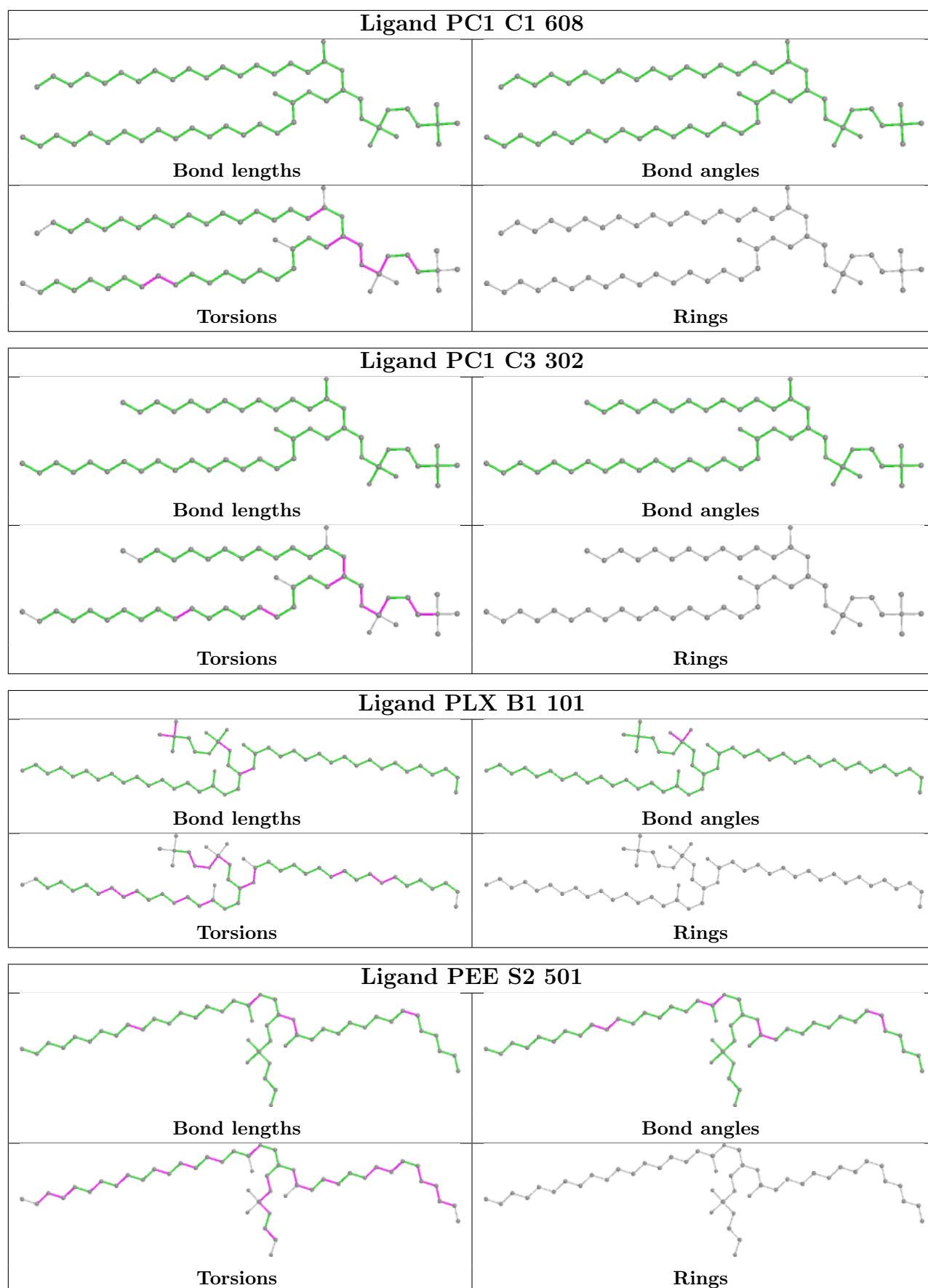


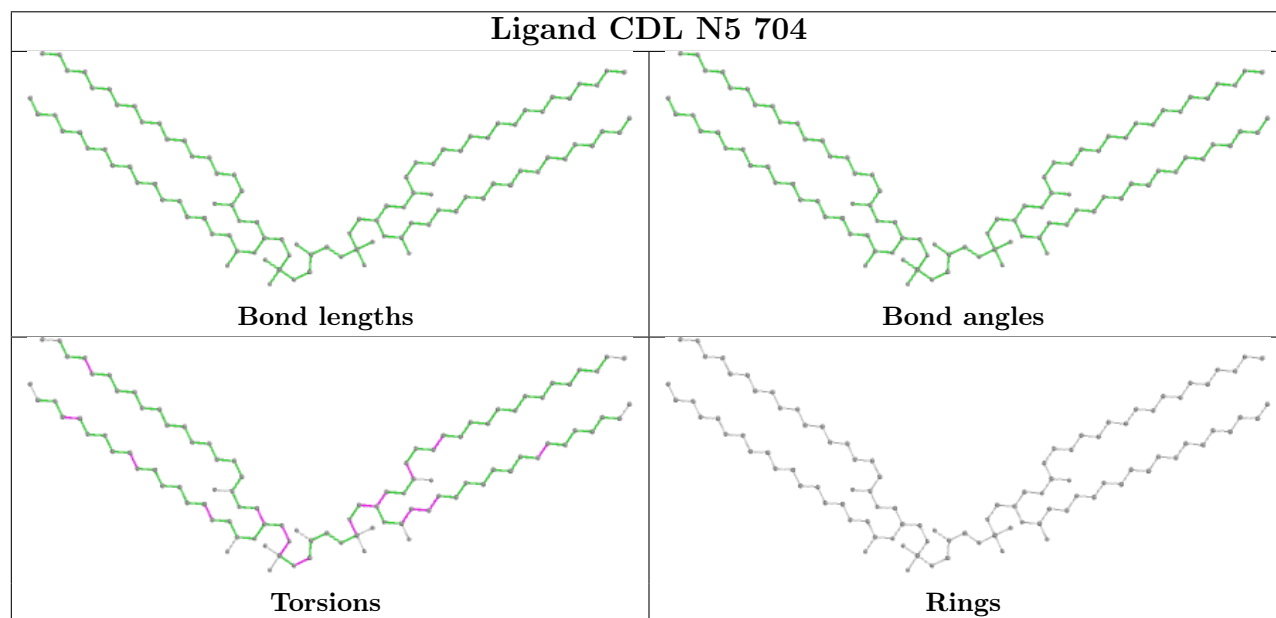
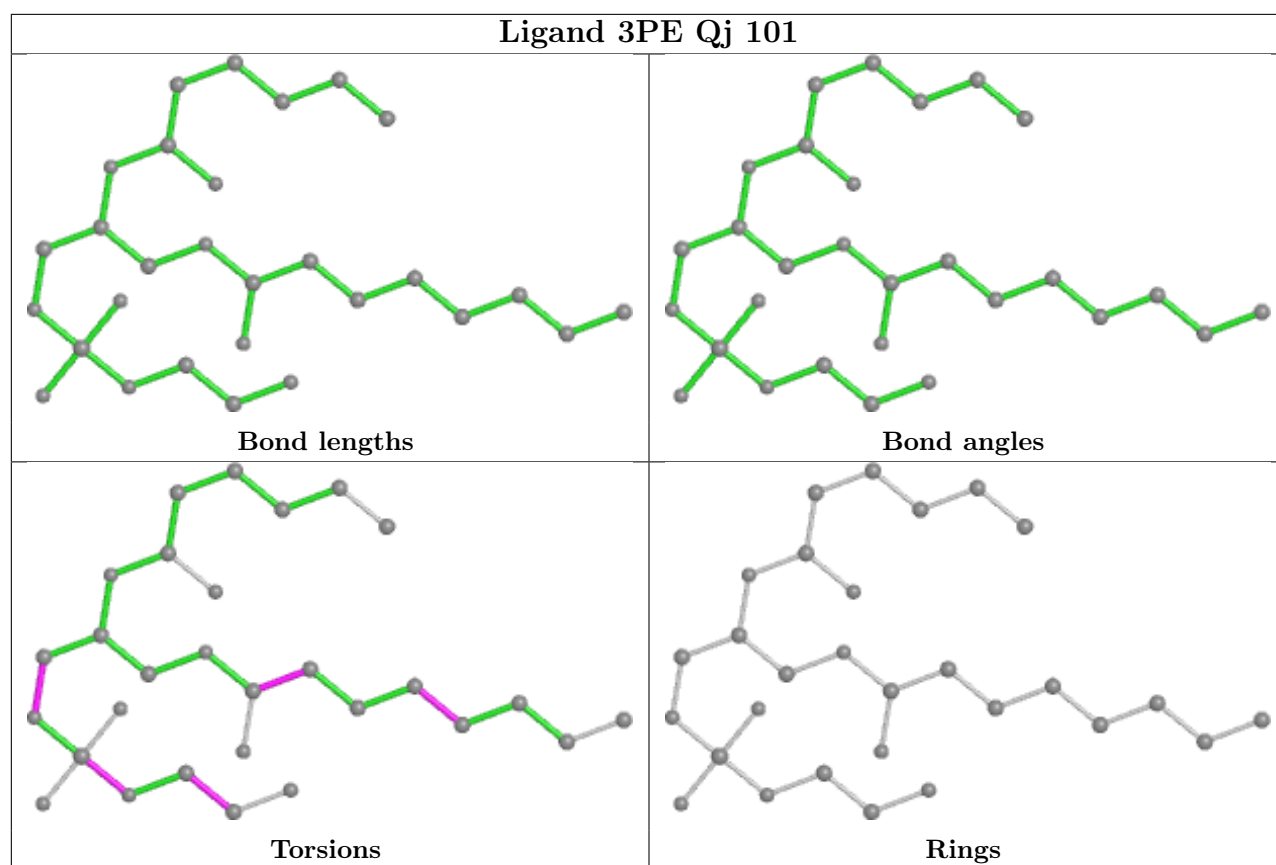
## Ligand HEA C1 601

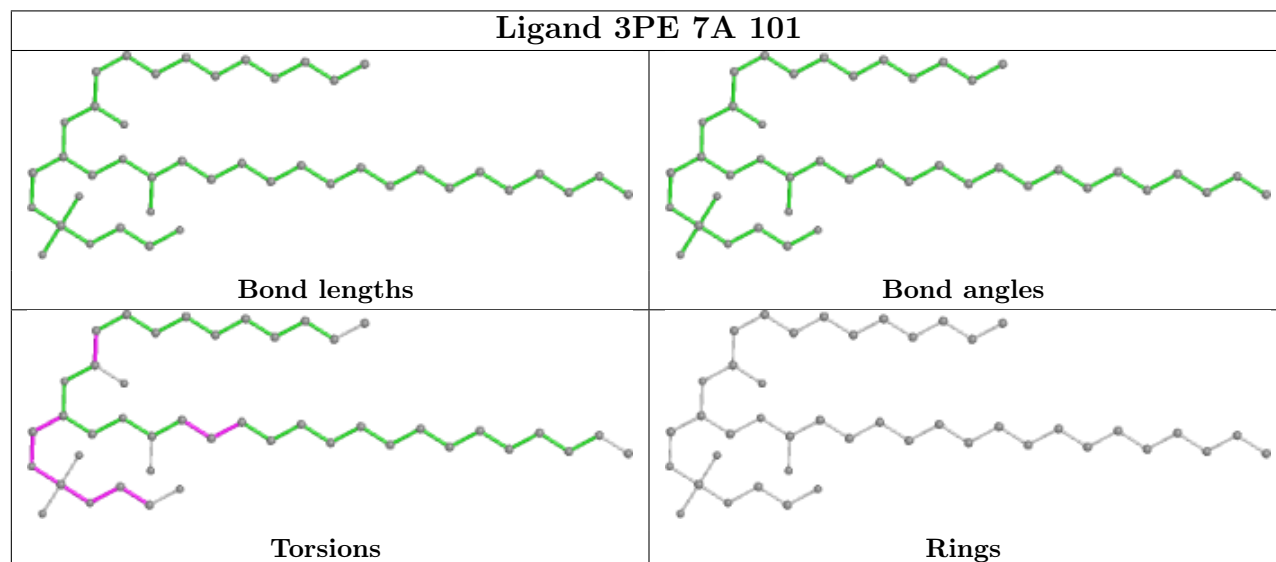
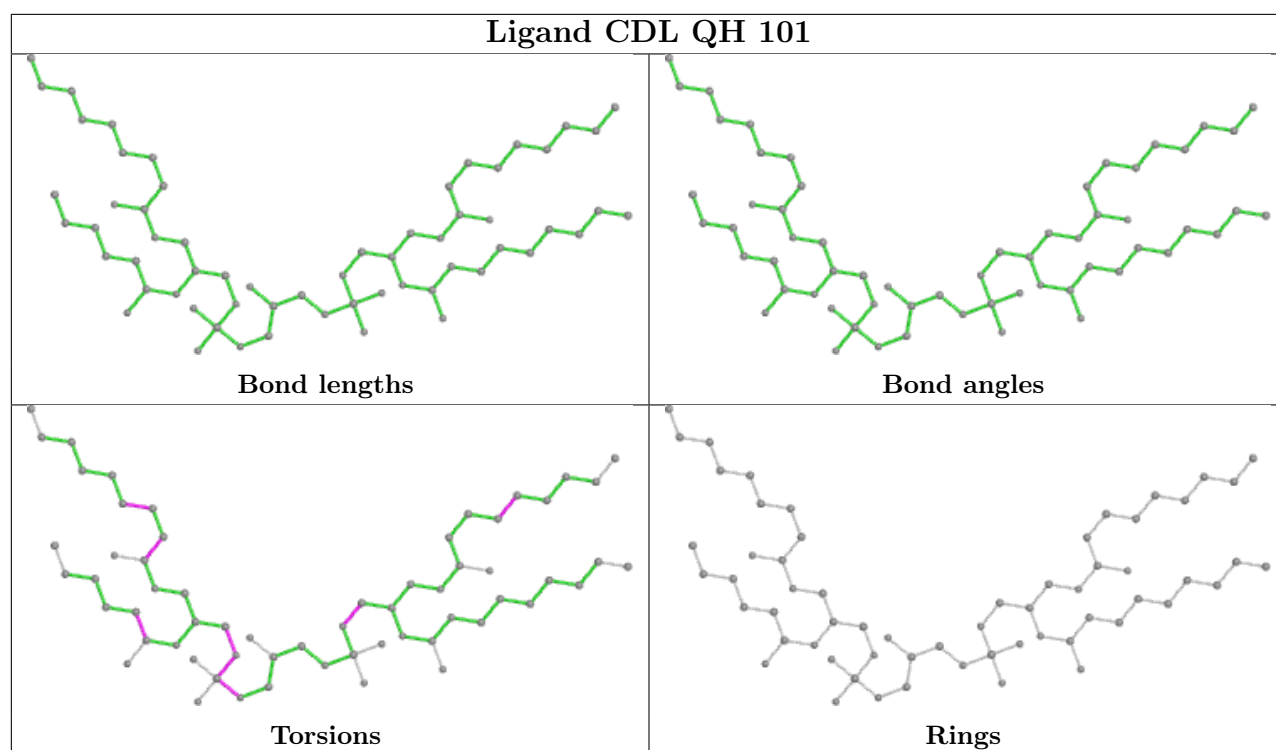


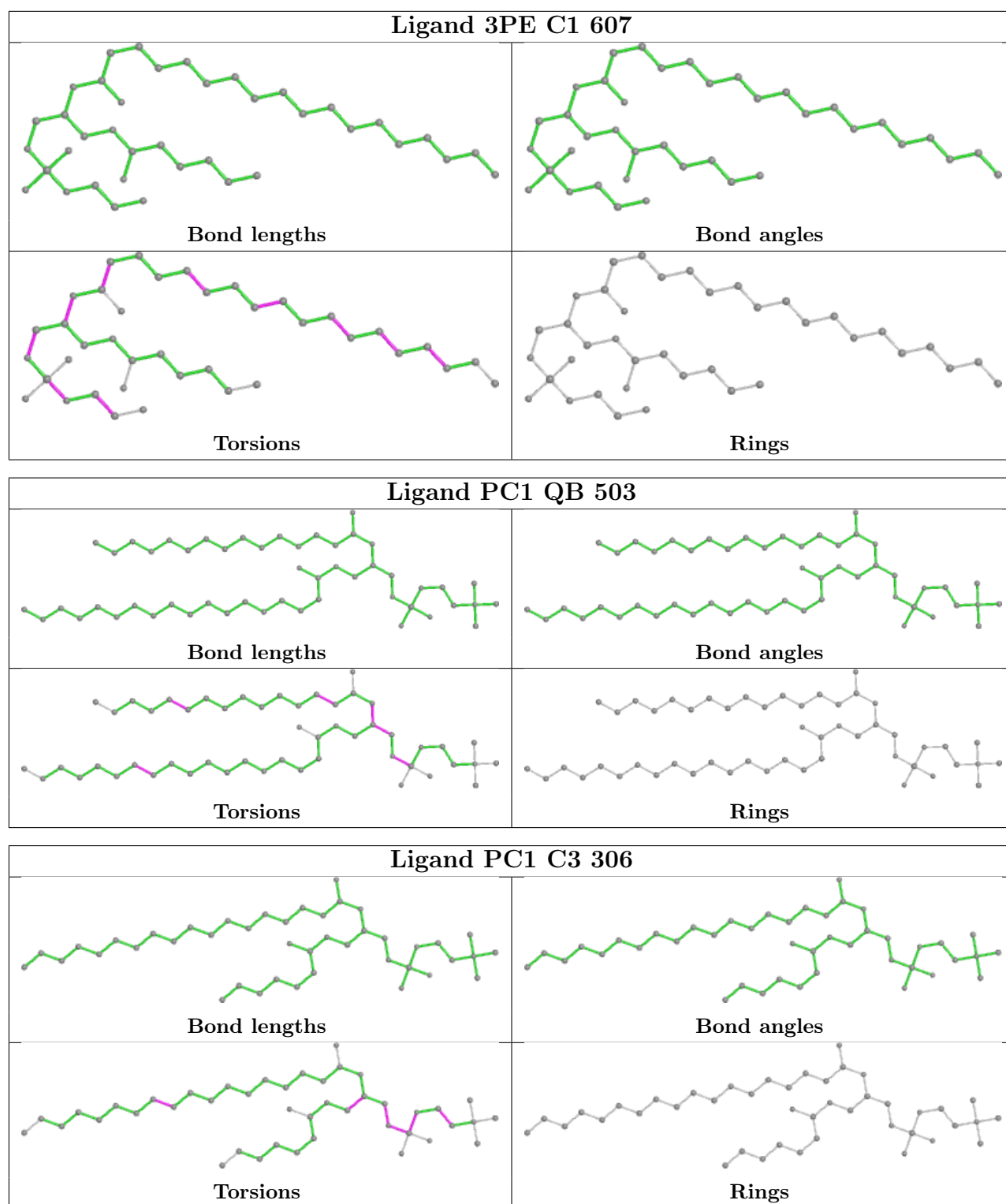
## Ligand HEM Qc 402

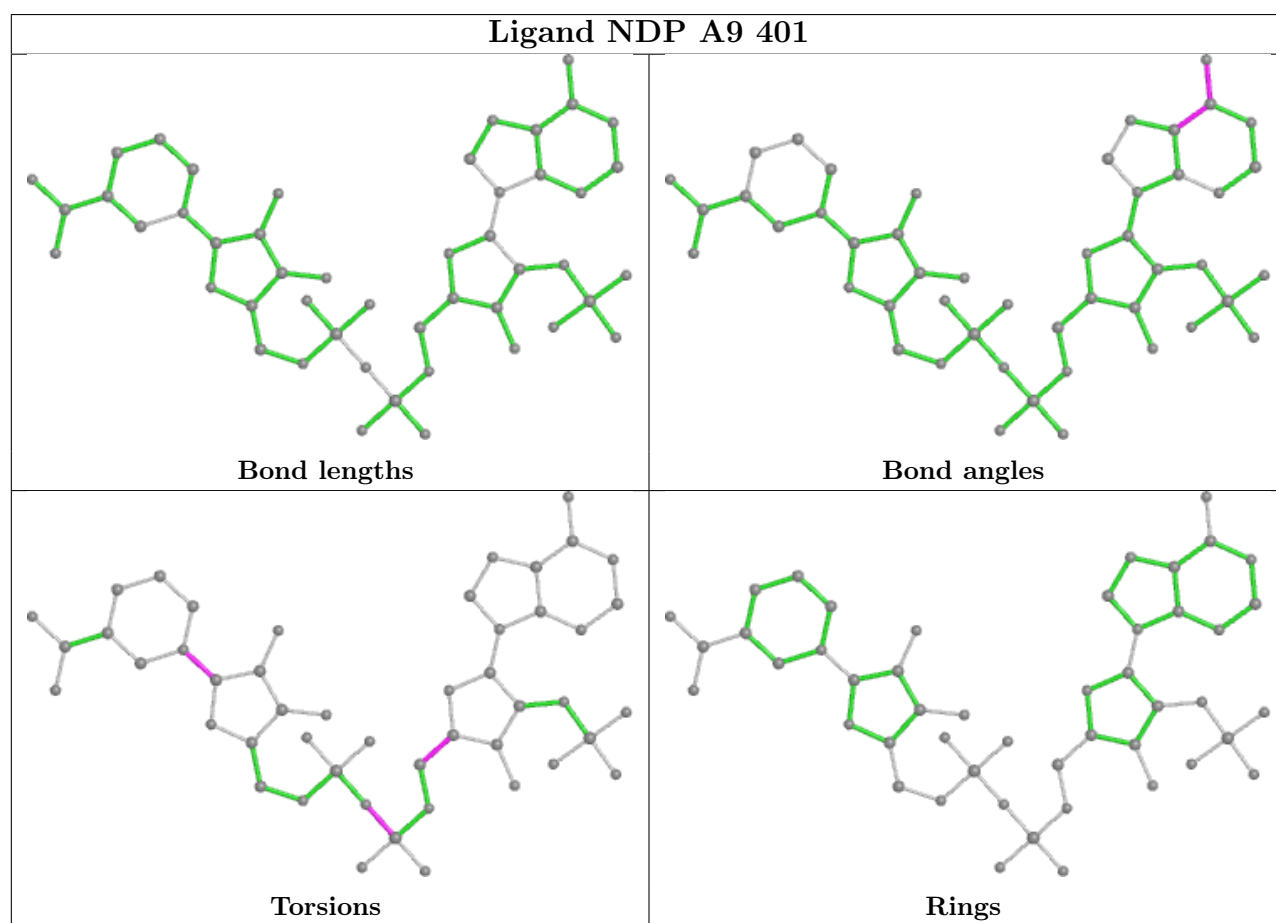
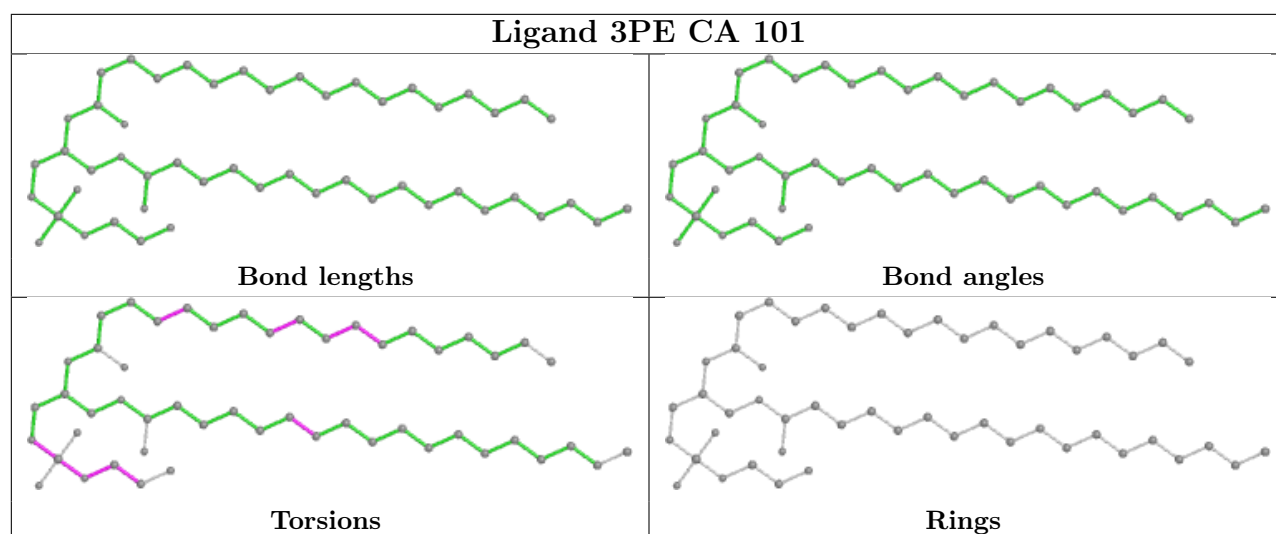




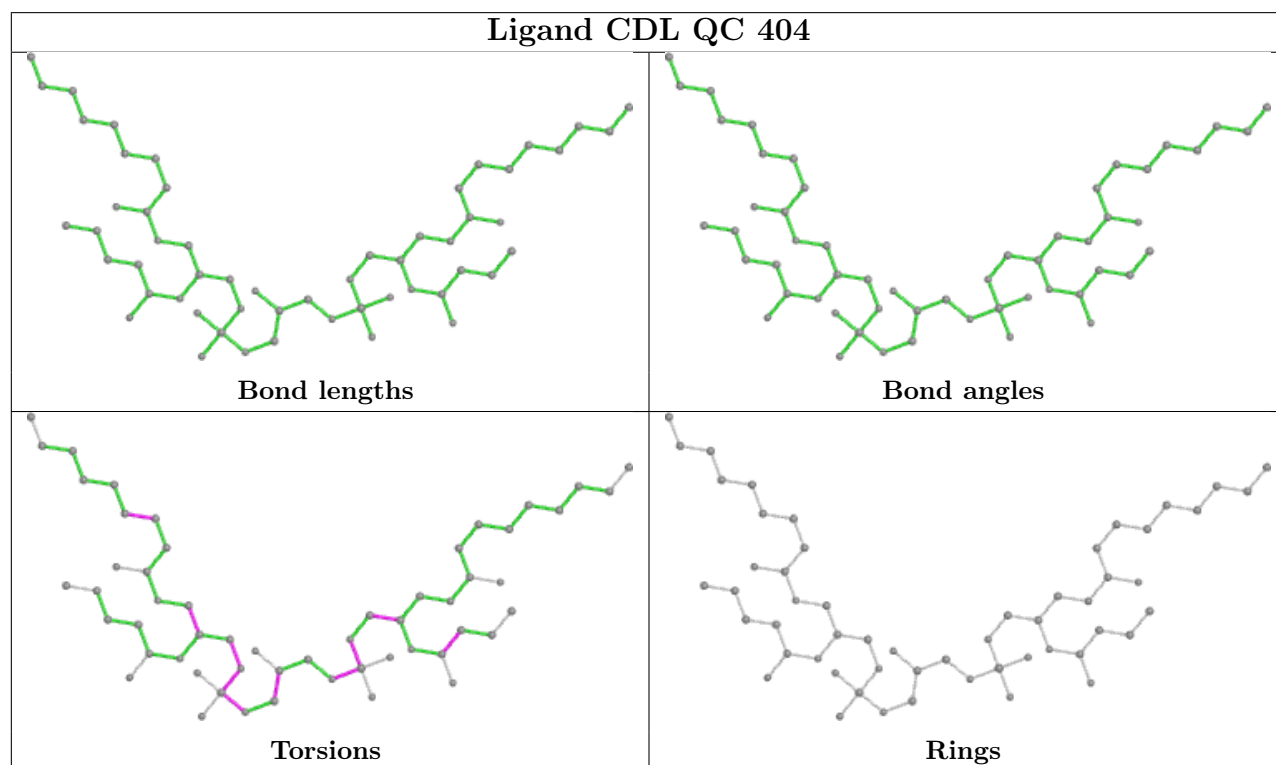
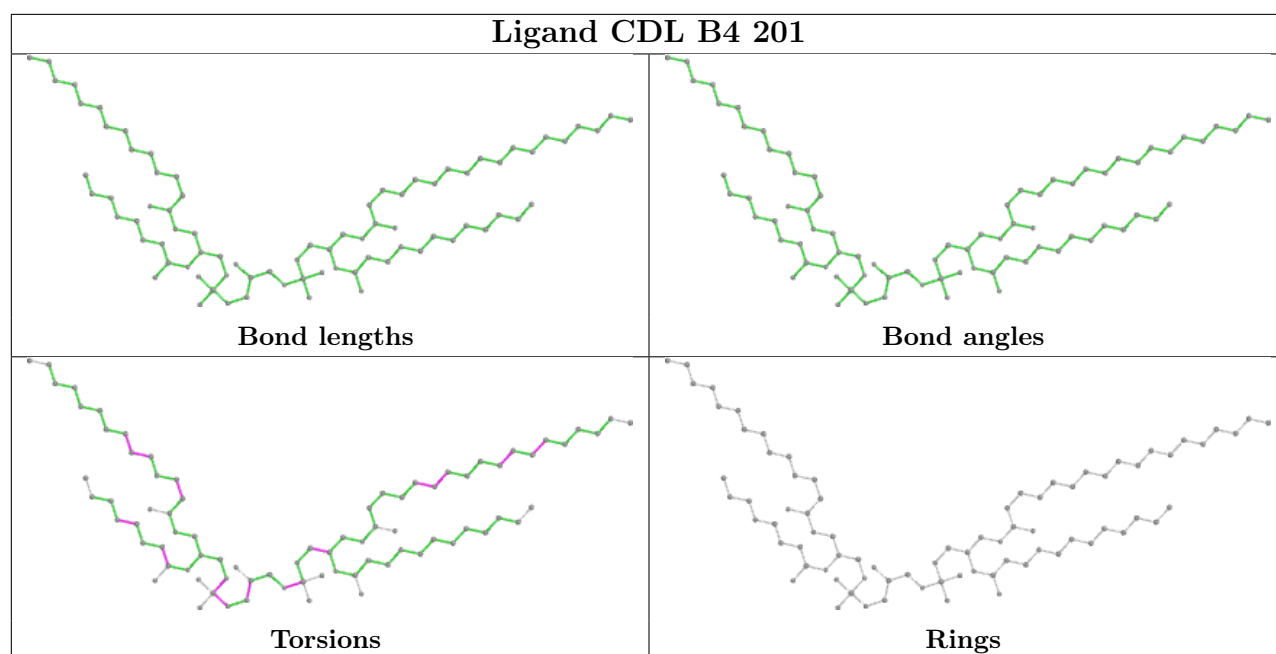




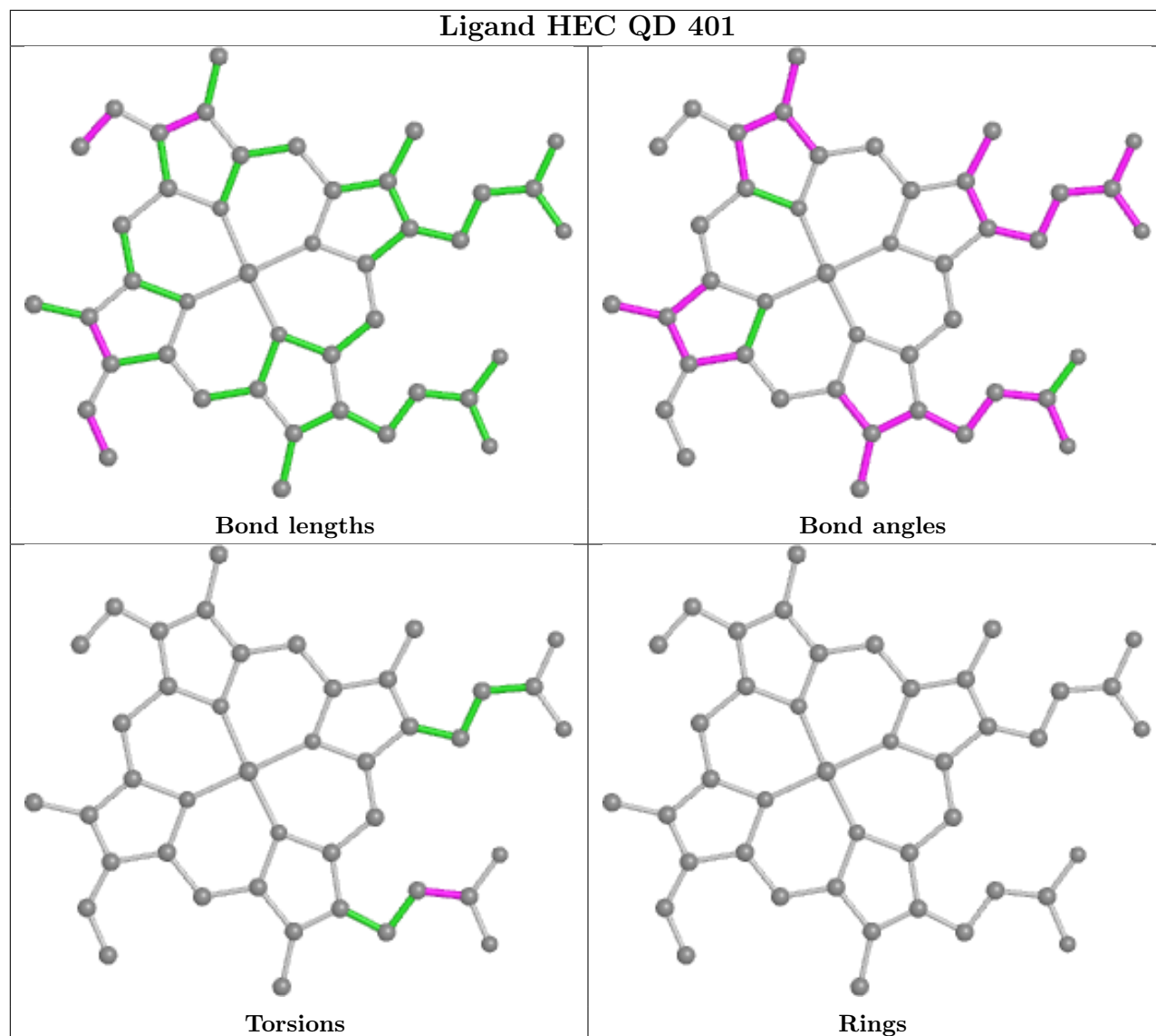




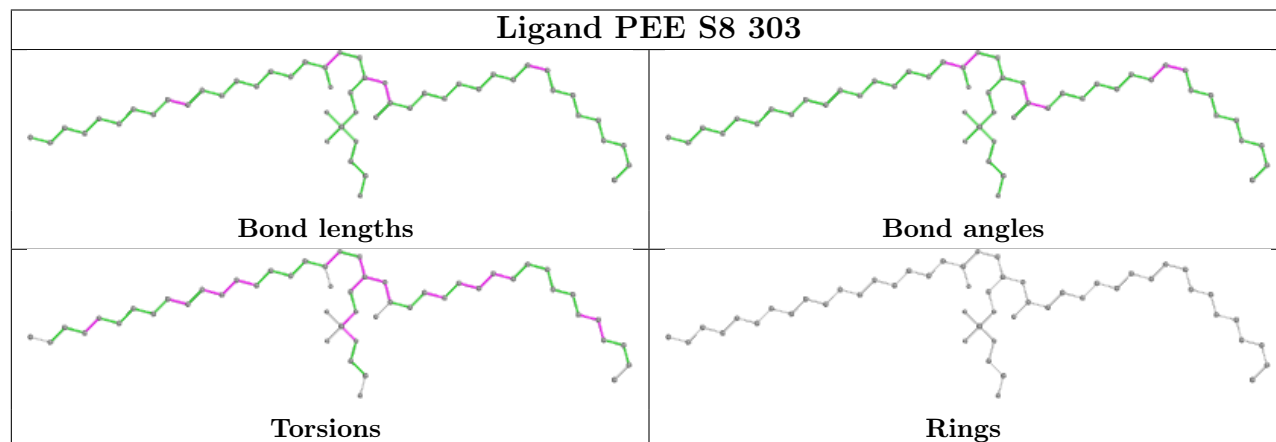


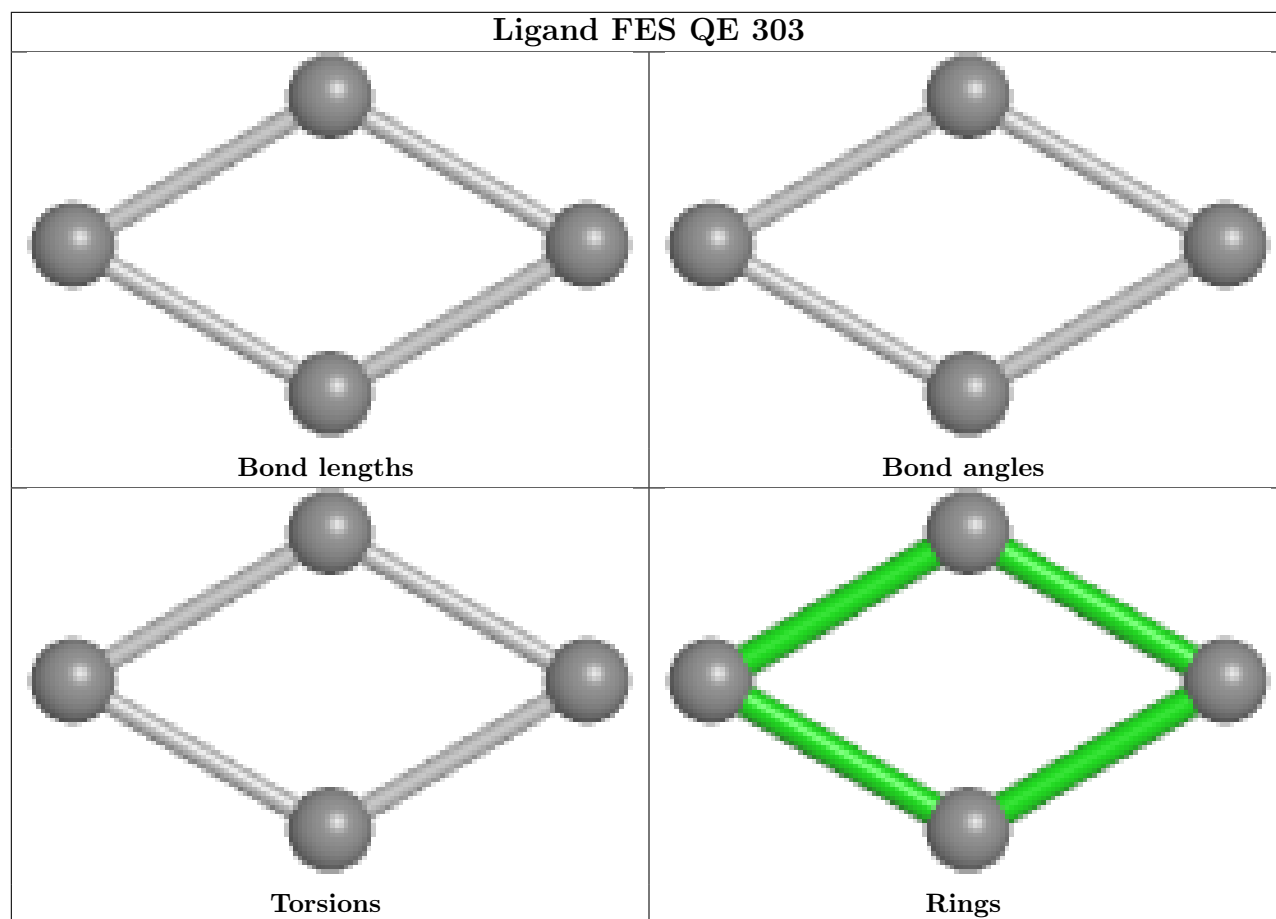
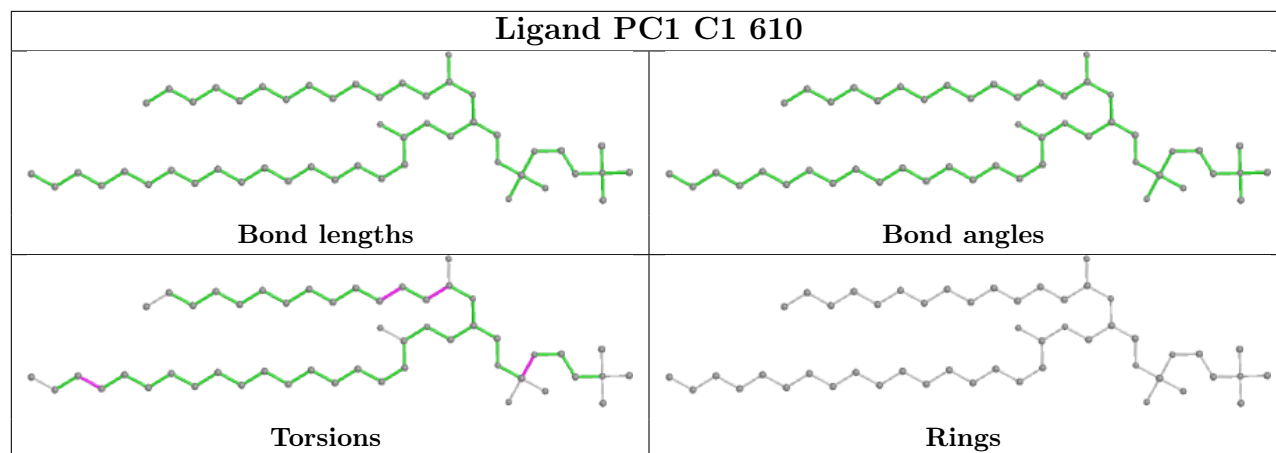


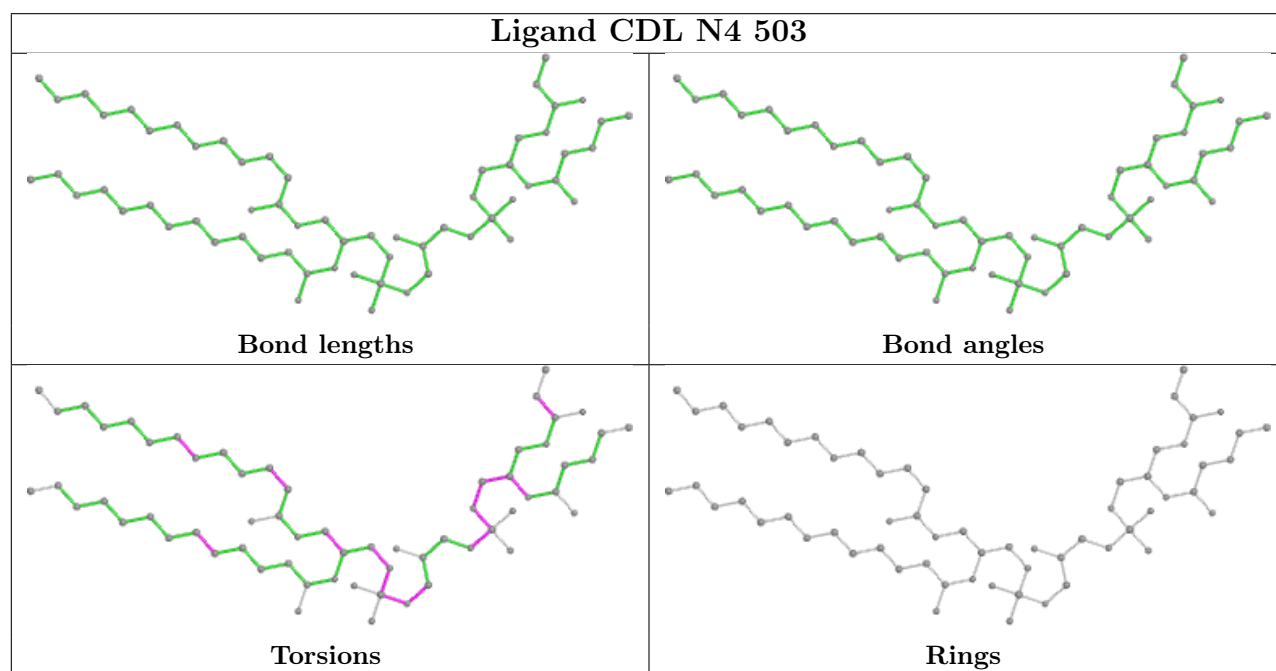
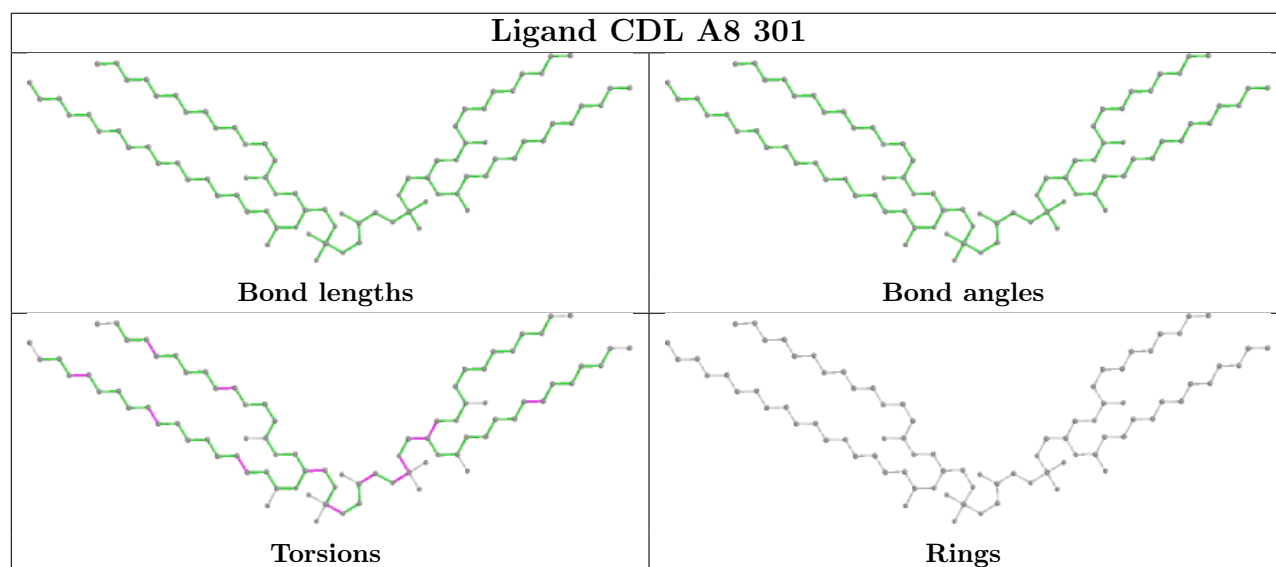
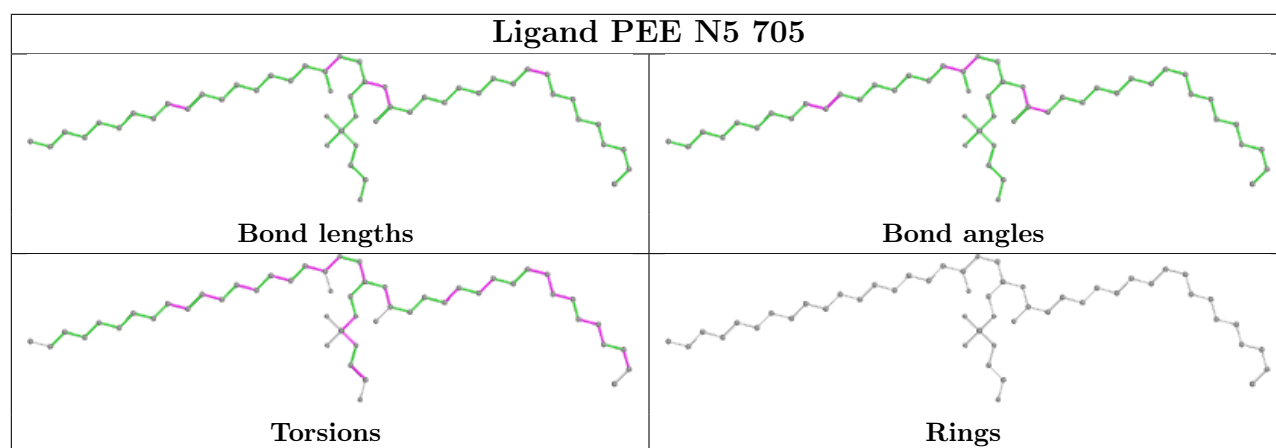
## Ligand HEC QD 401



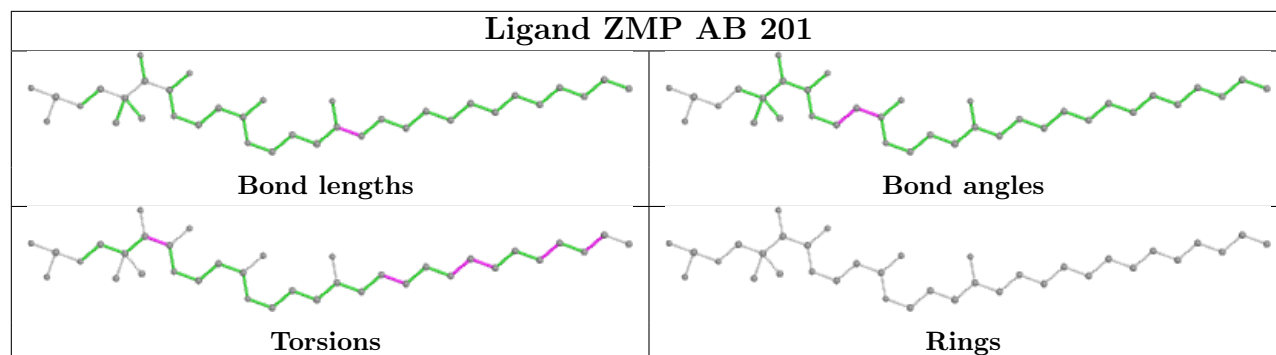
## Ligand PEE S8 303



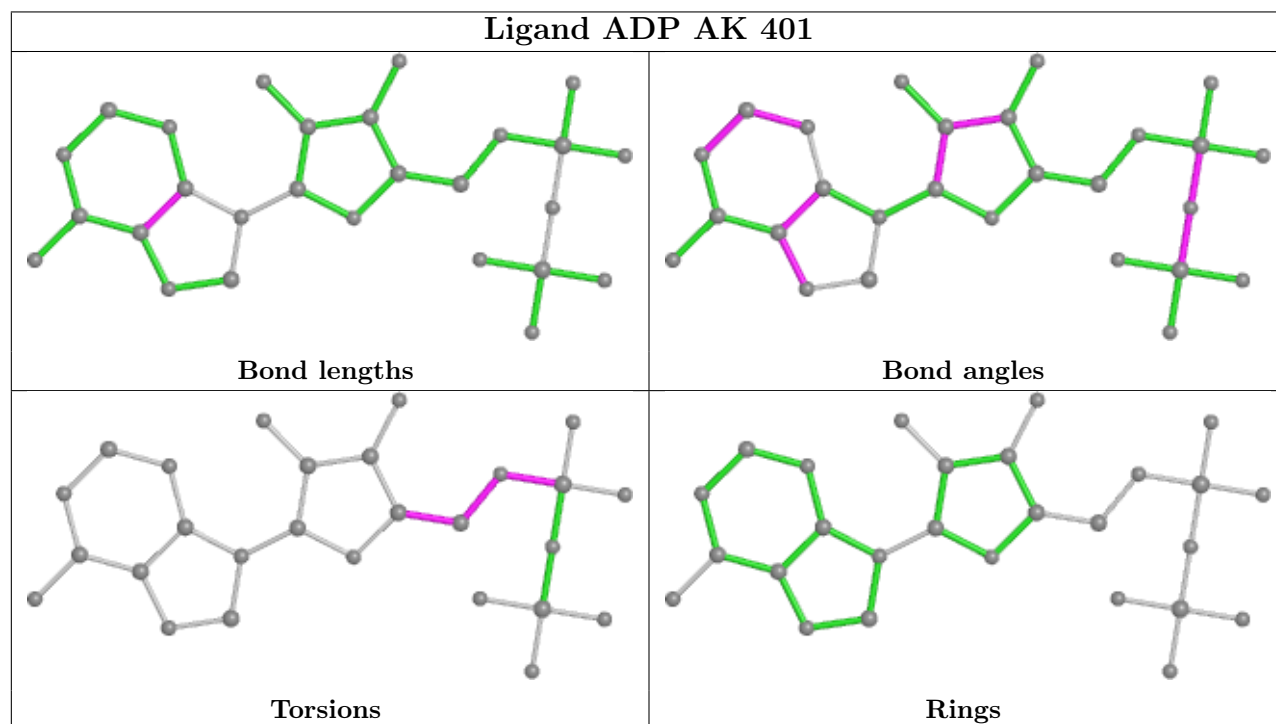




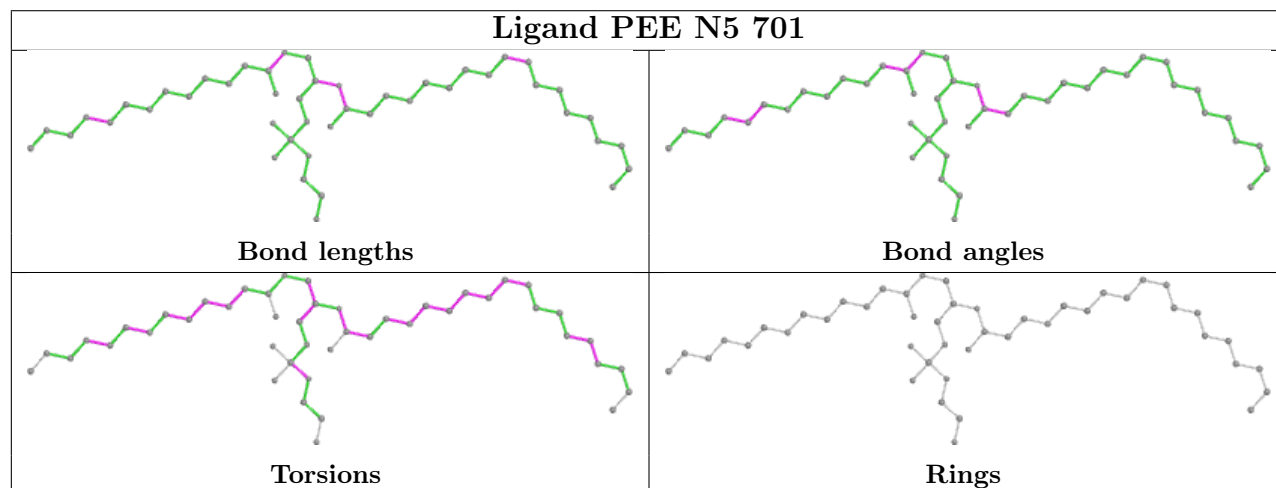
## Ligand ZMP AB 201

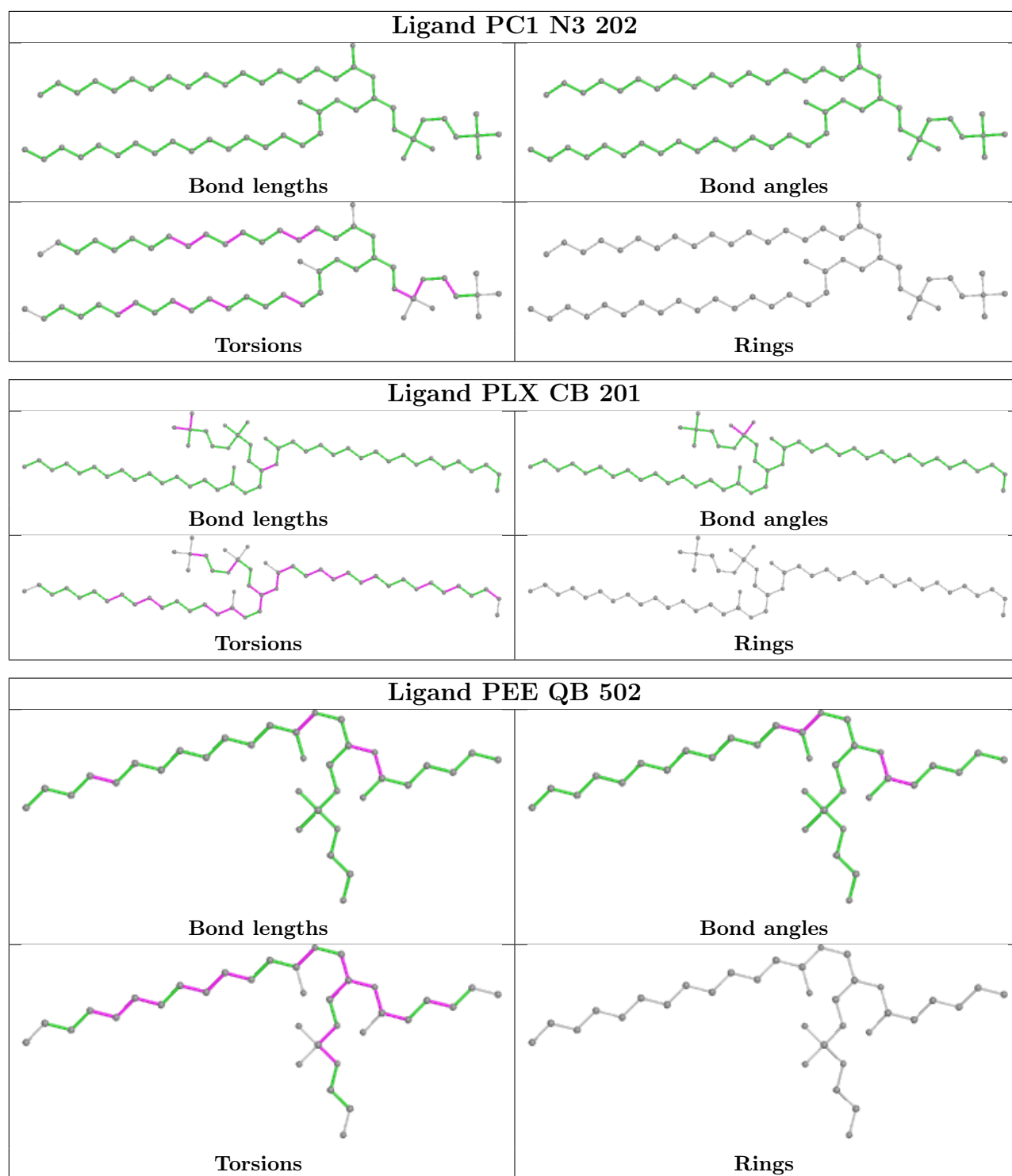


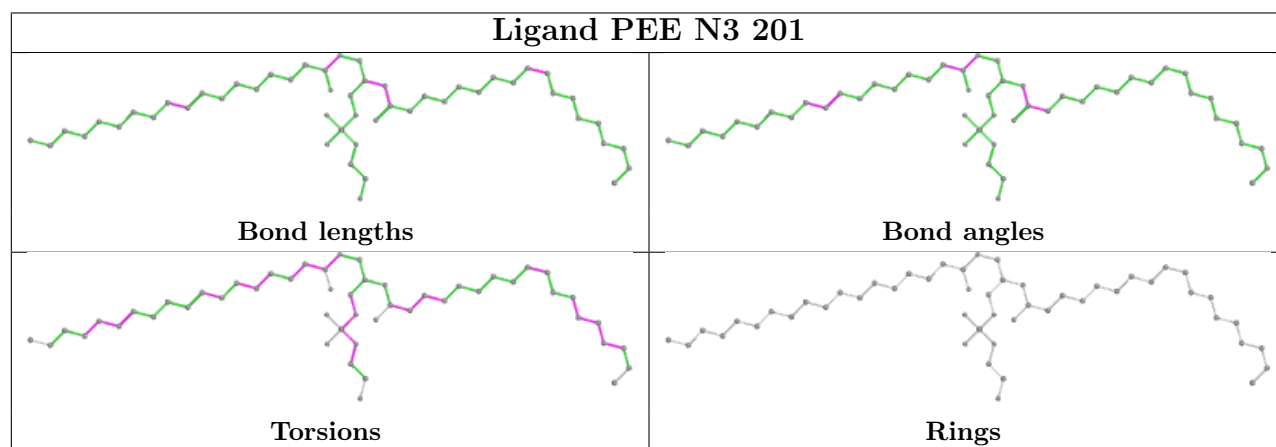
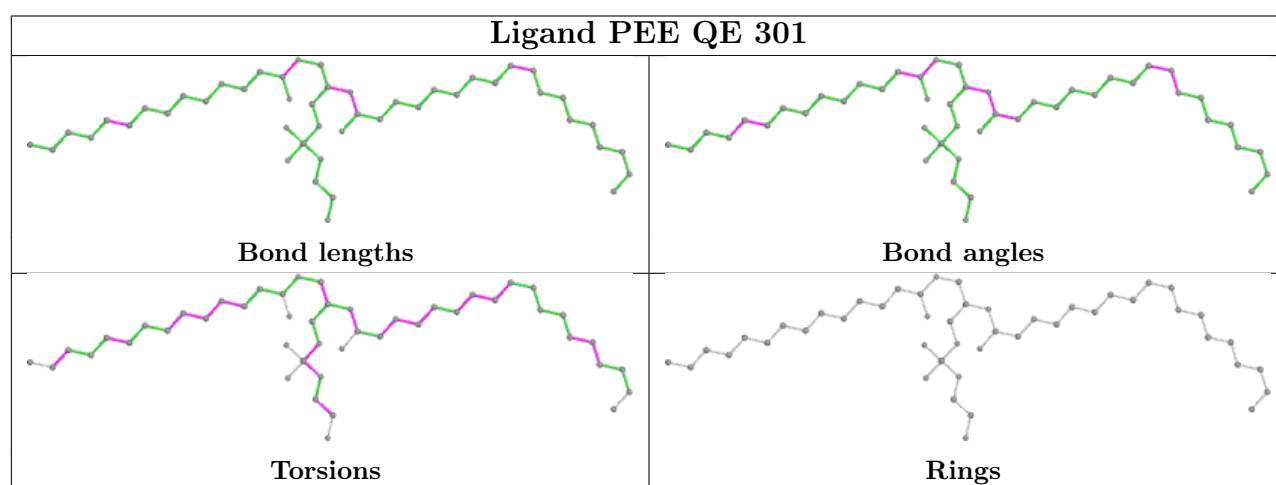
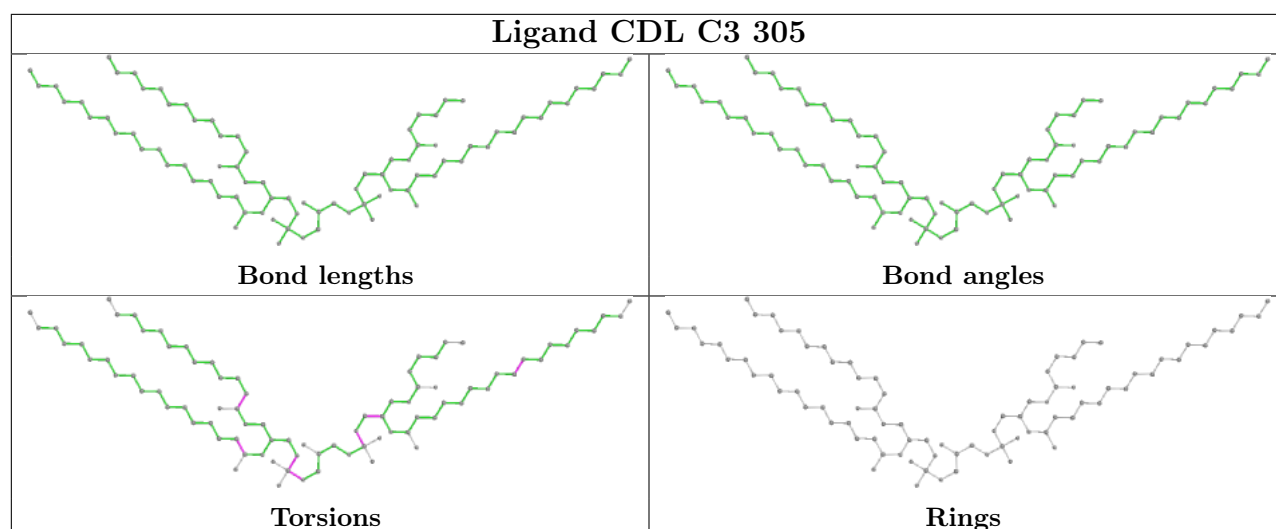
## Ligand ADP AK 401

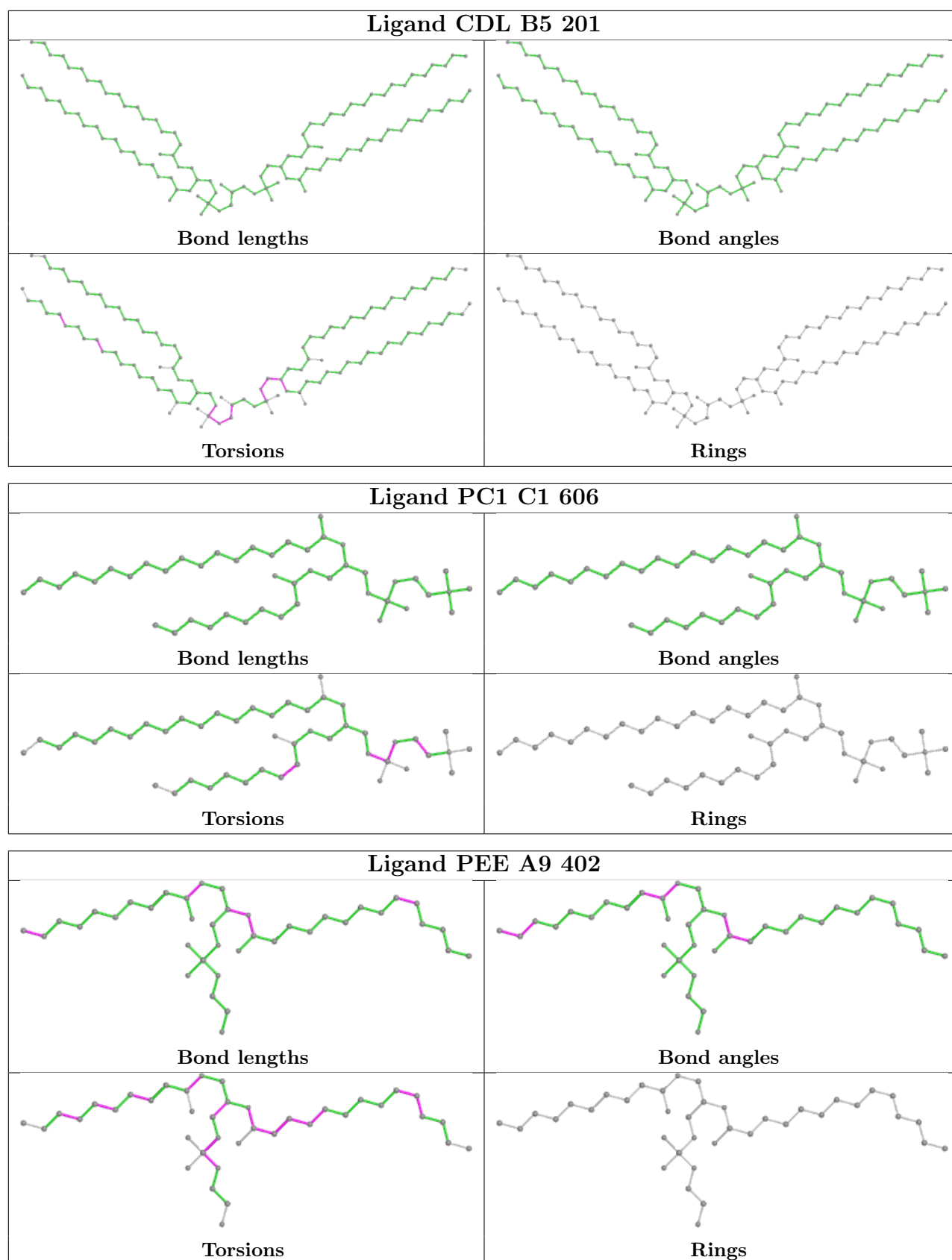


## Ligand PEE N5 701

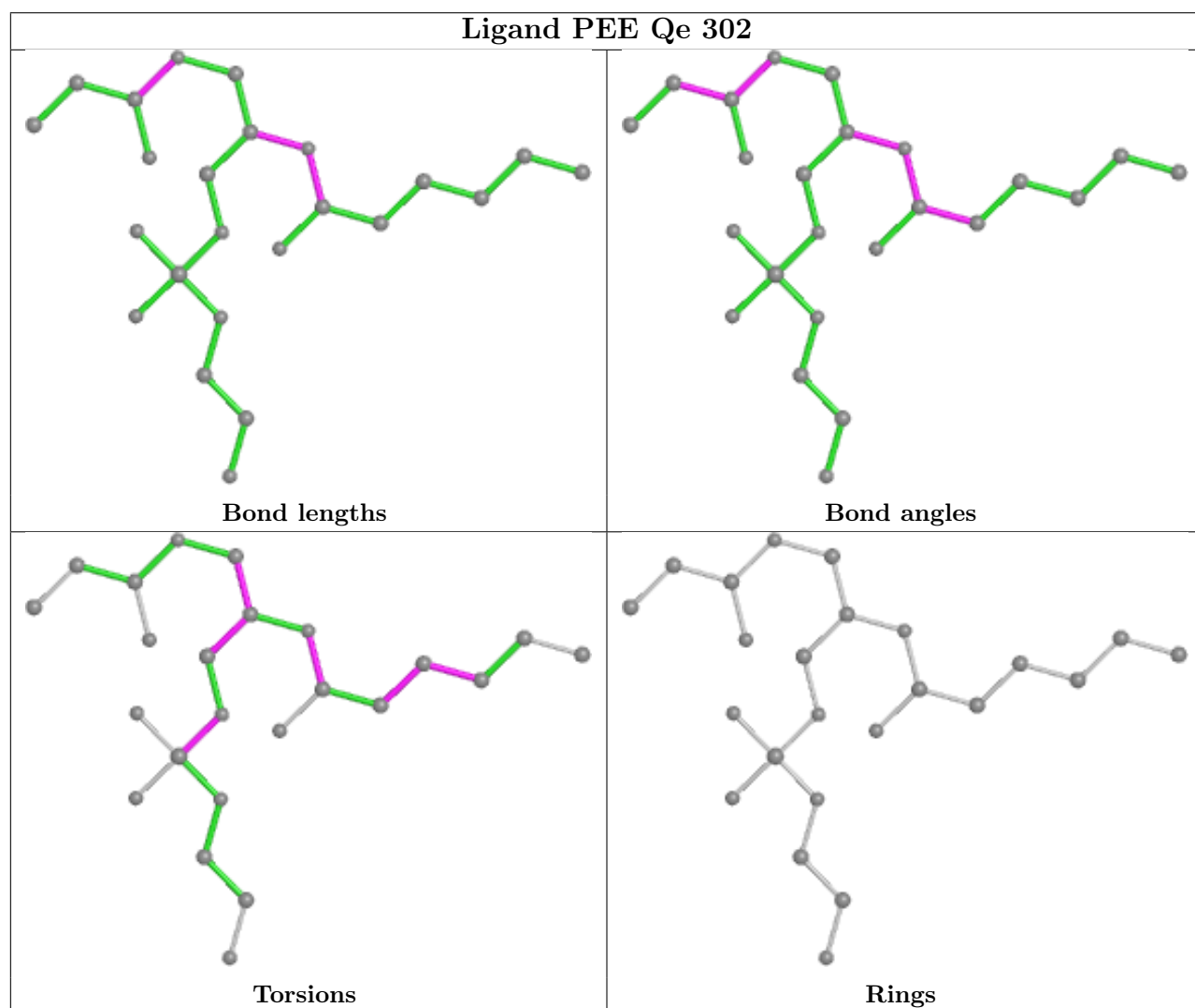
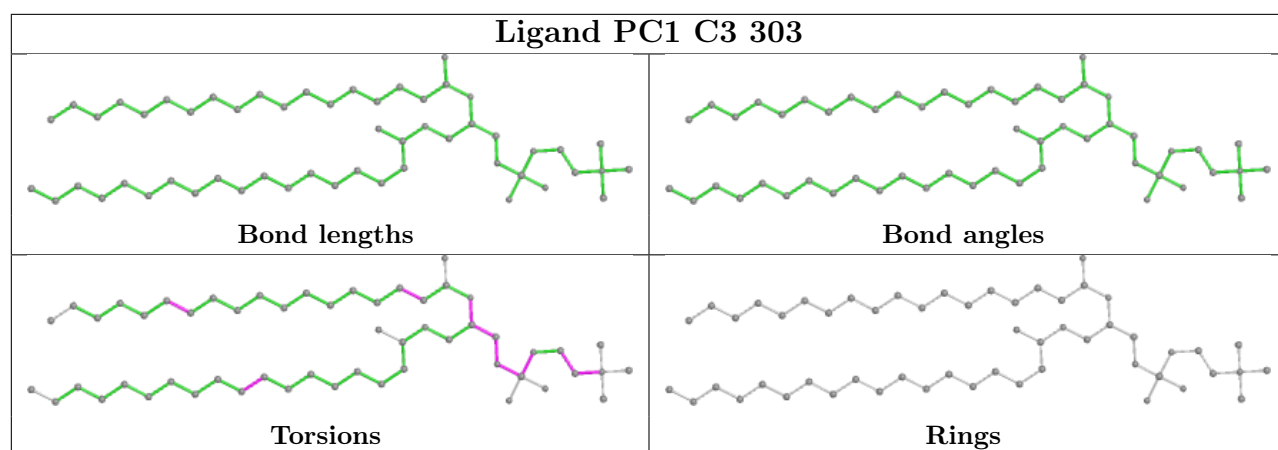


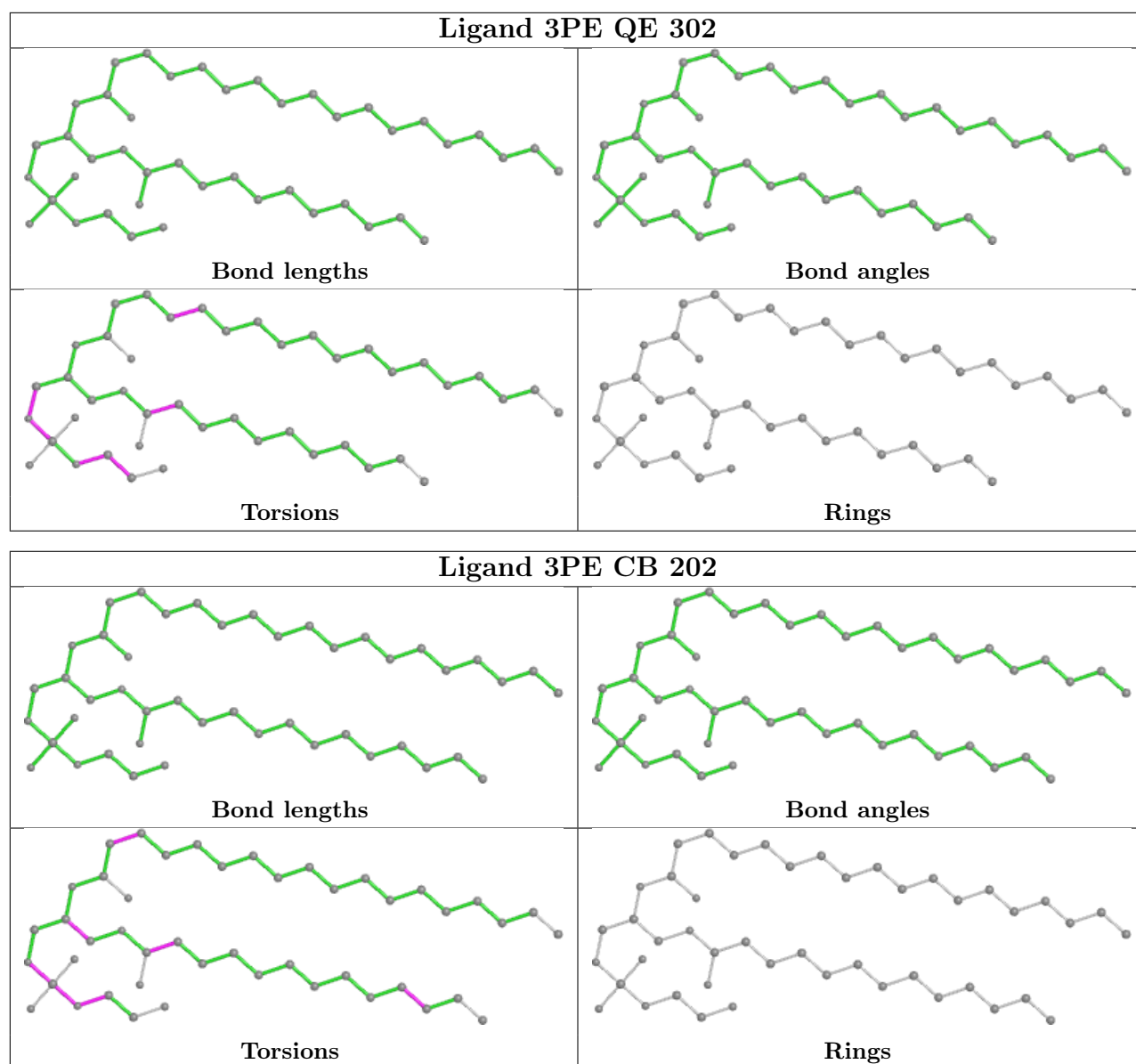


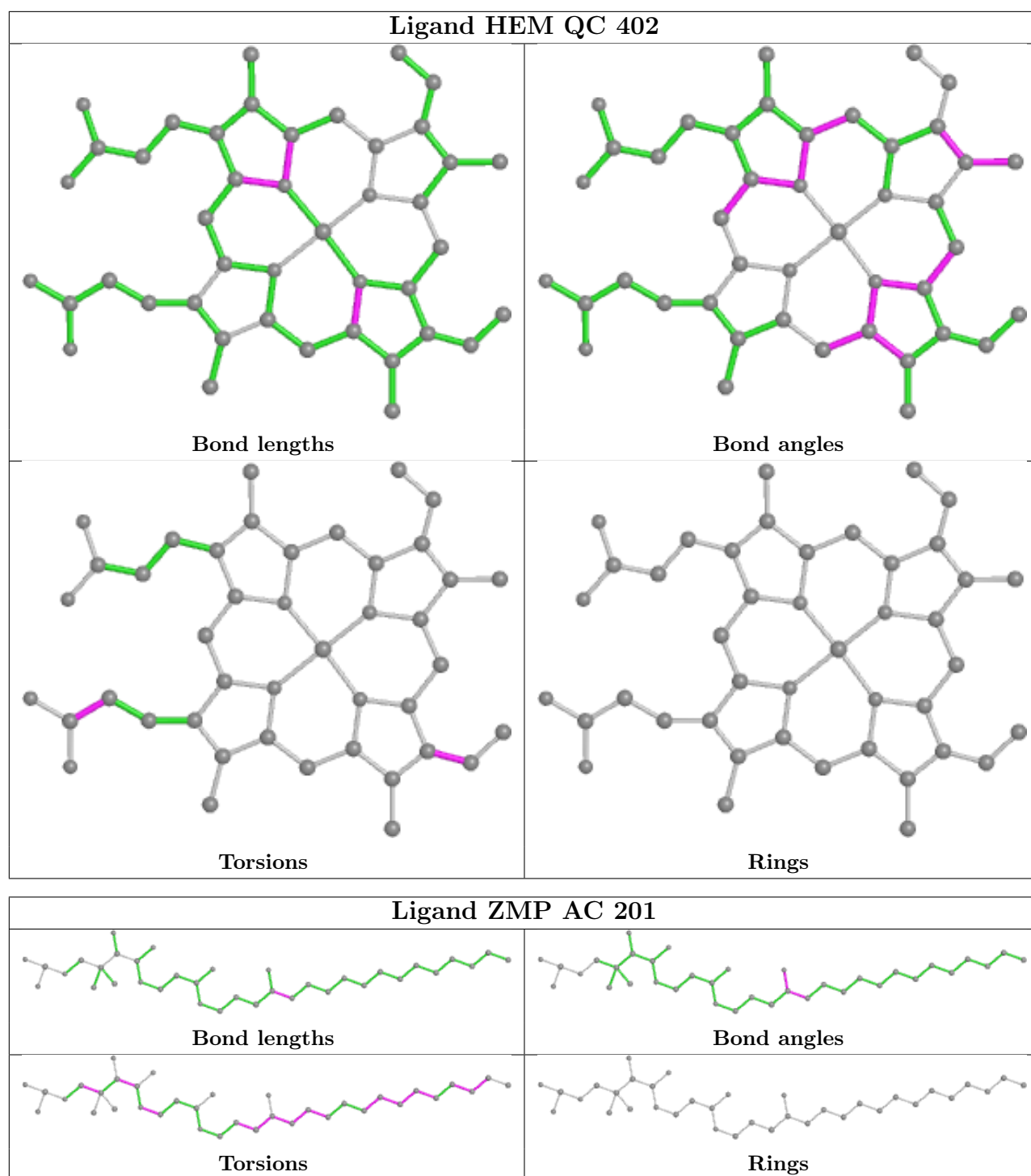


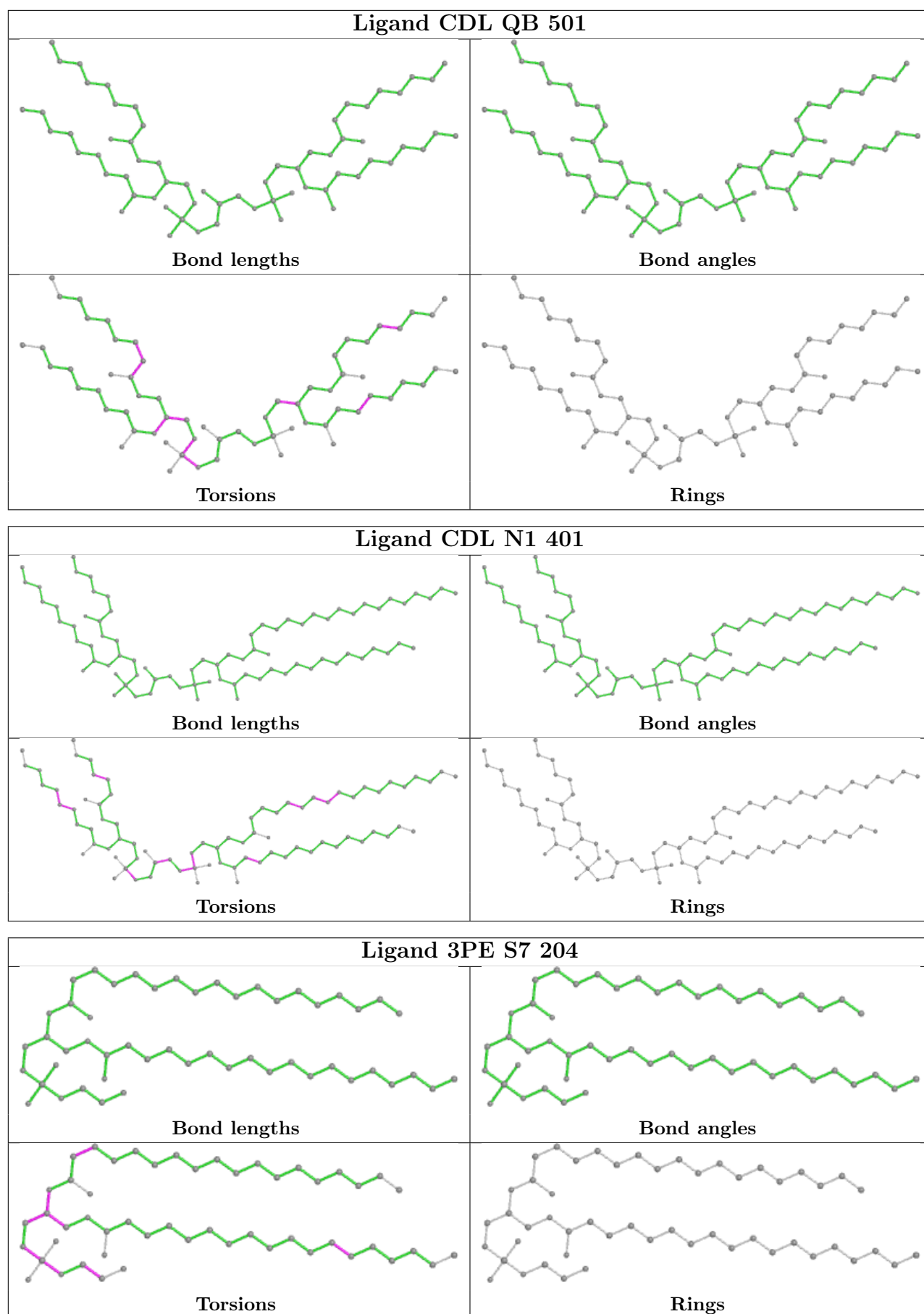


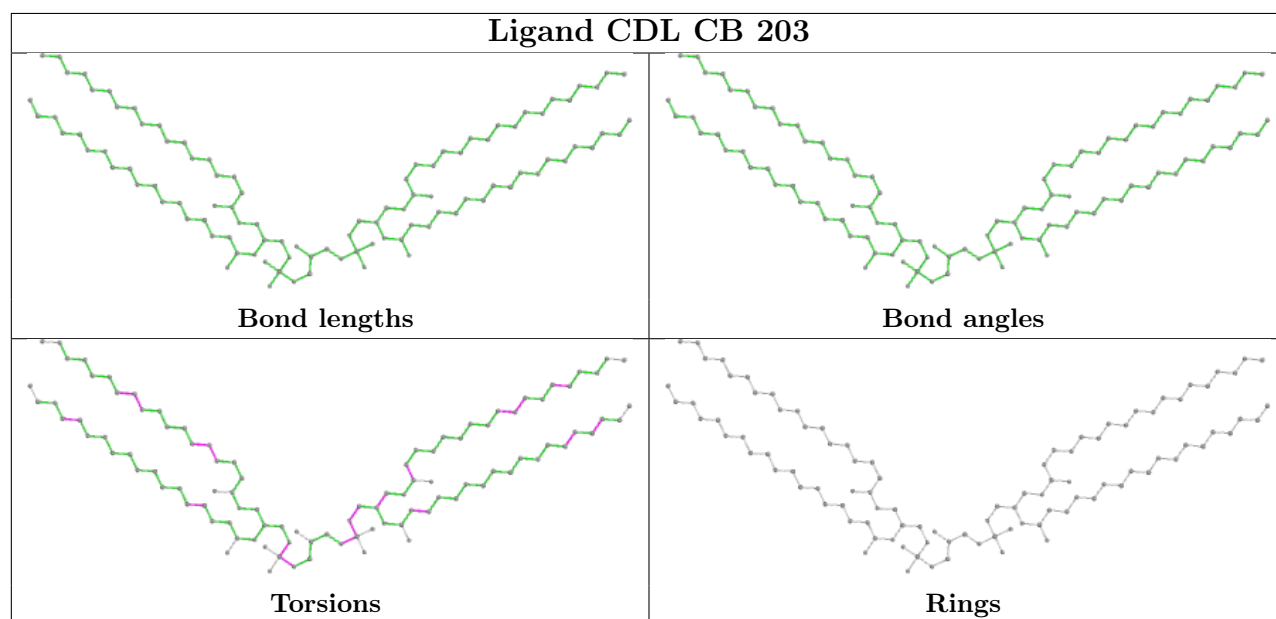
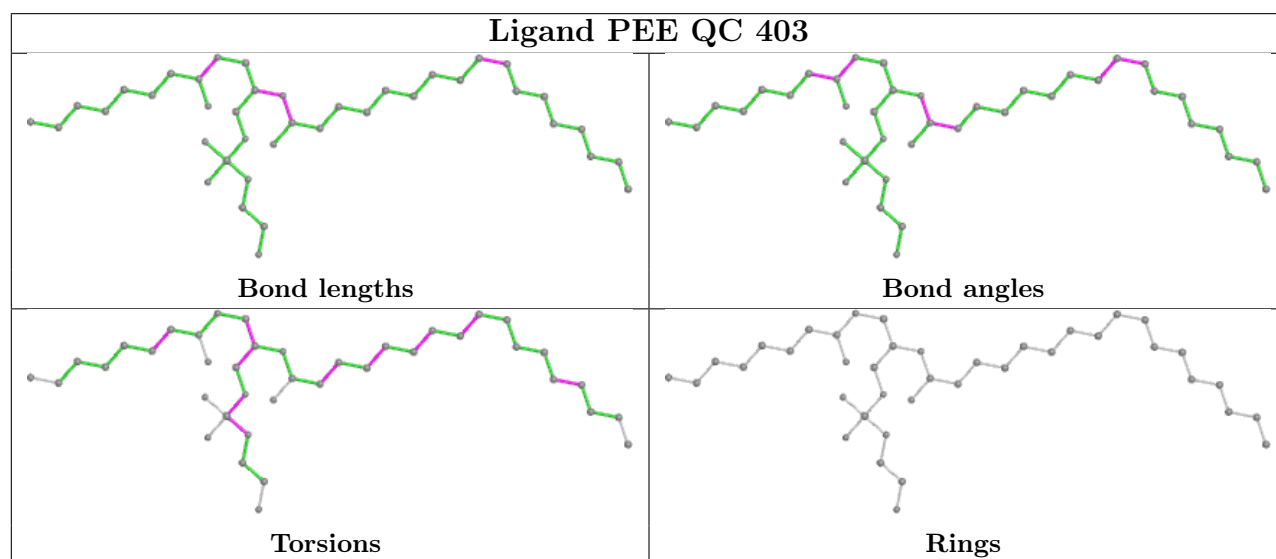
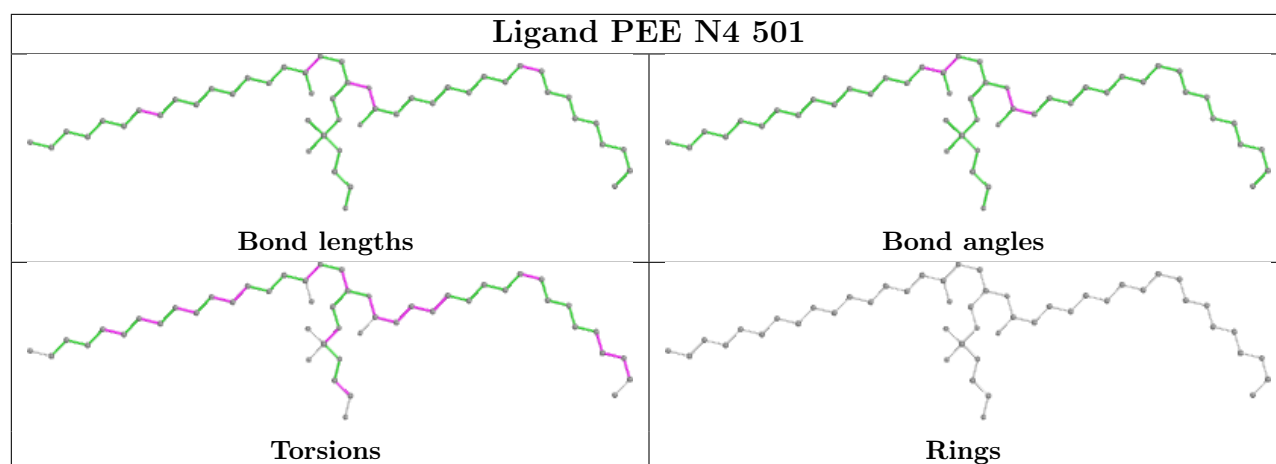


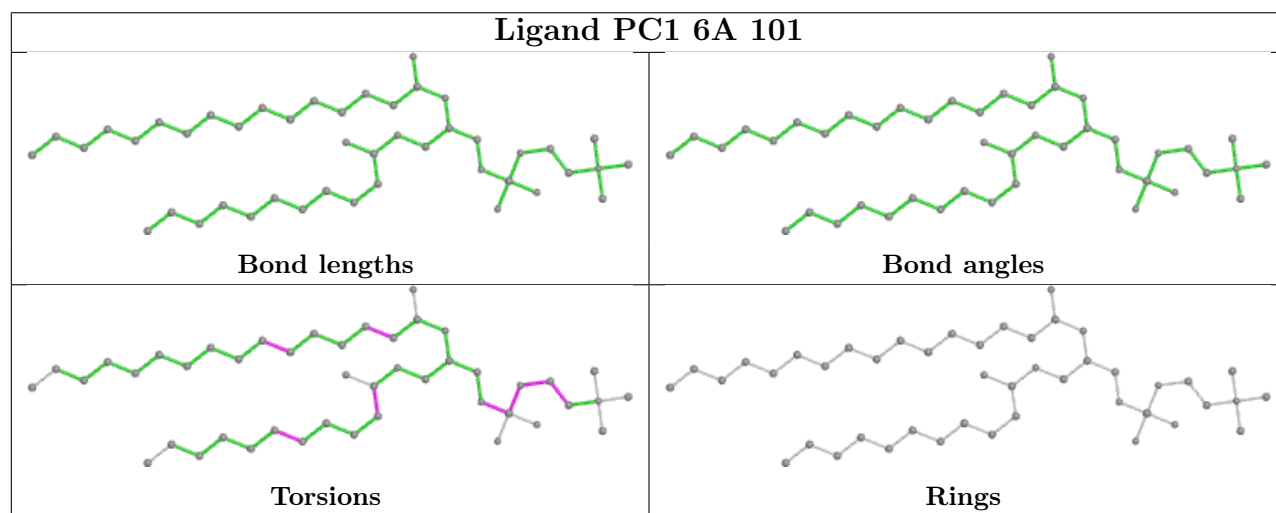
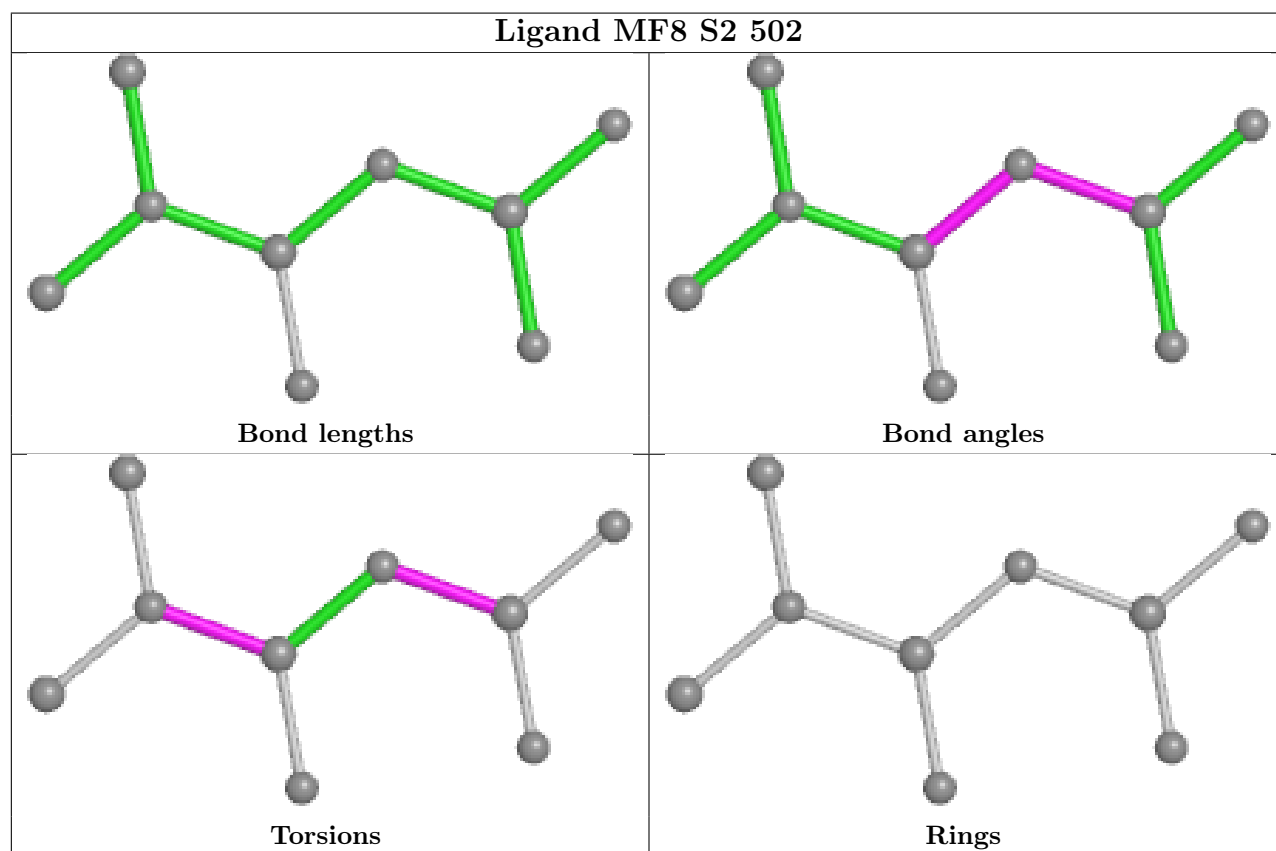
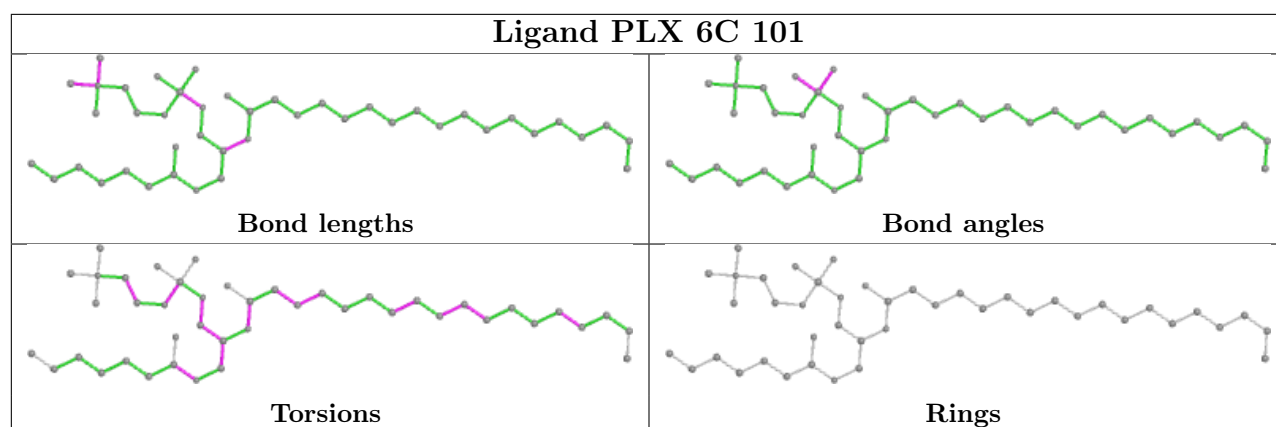


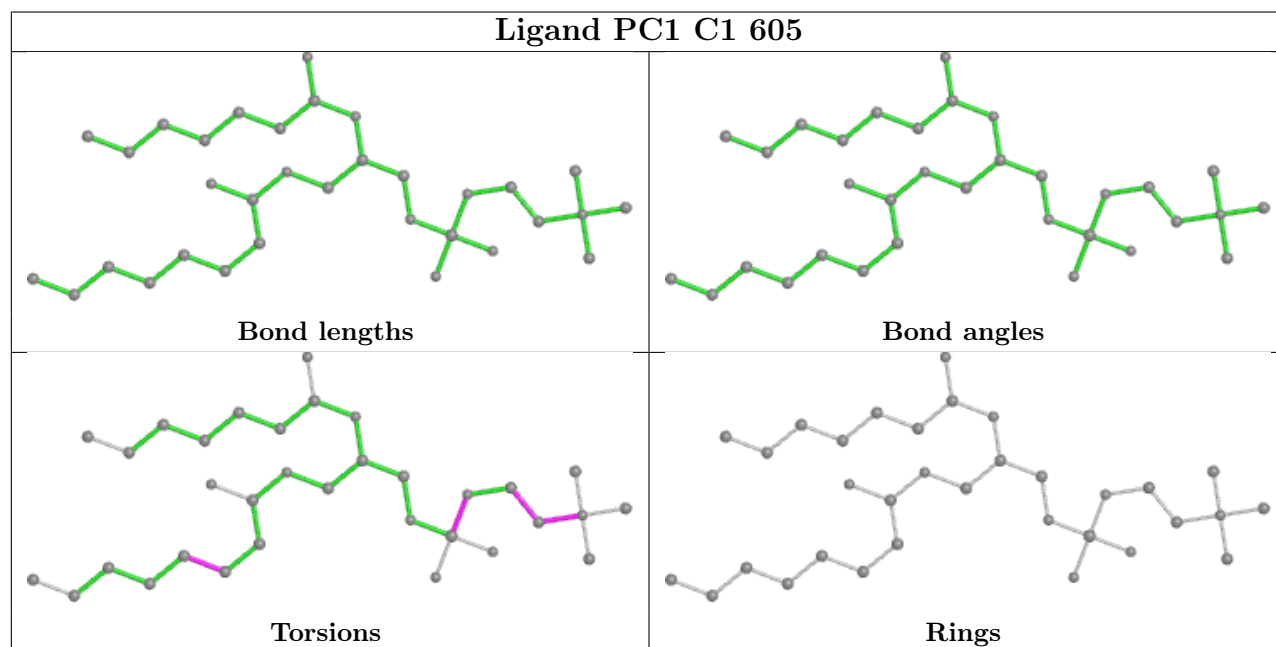
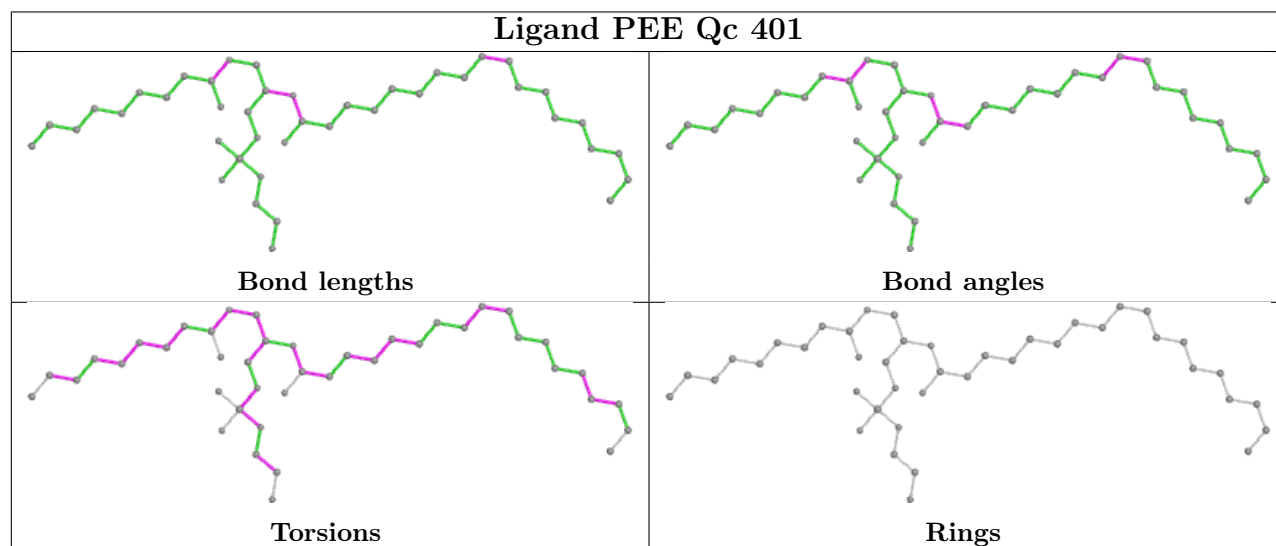
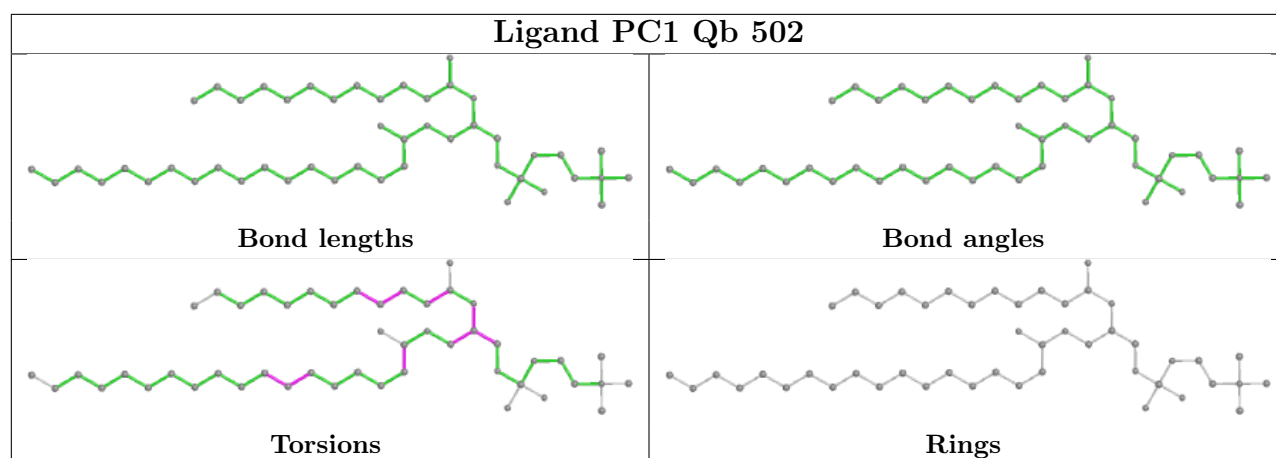


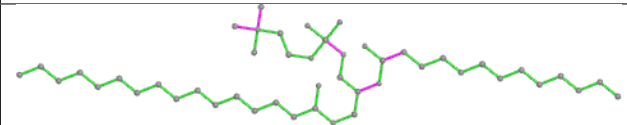
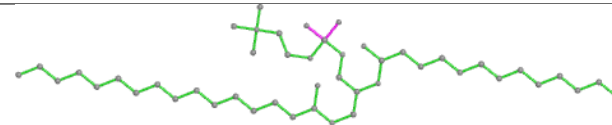
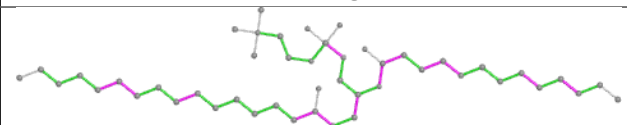
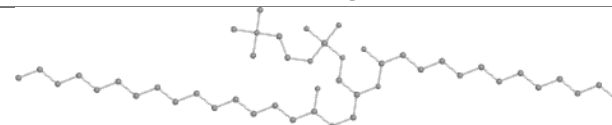


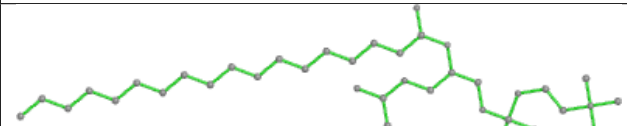
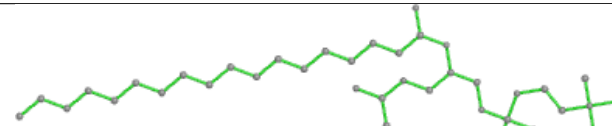
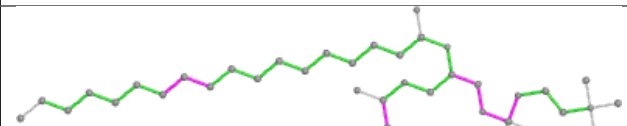
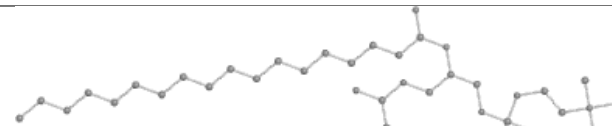


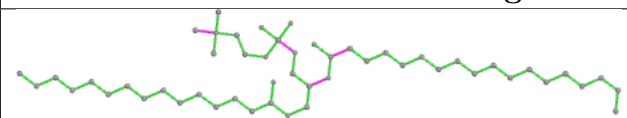
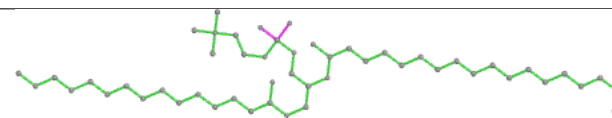
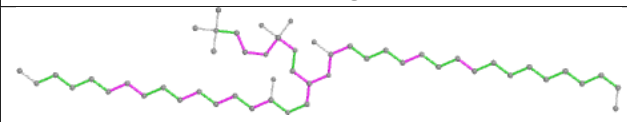
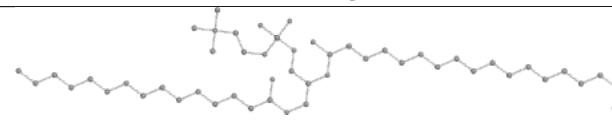




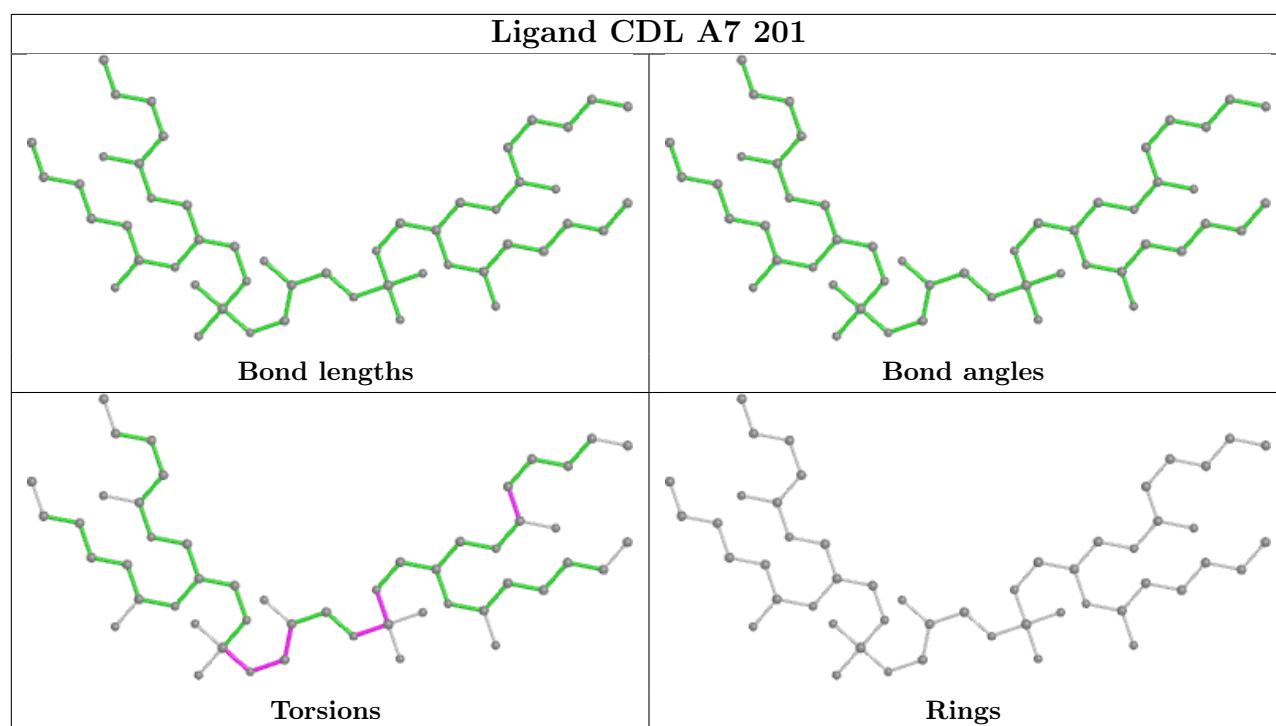
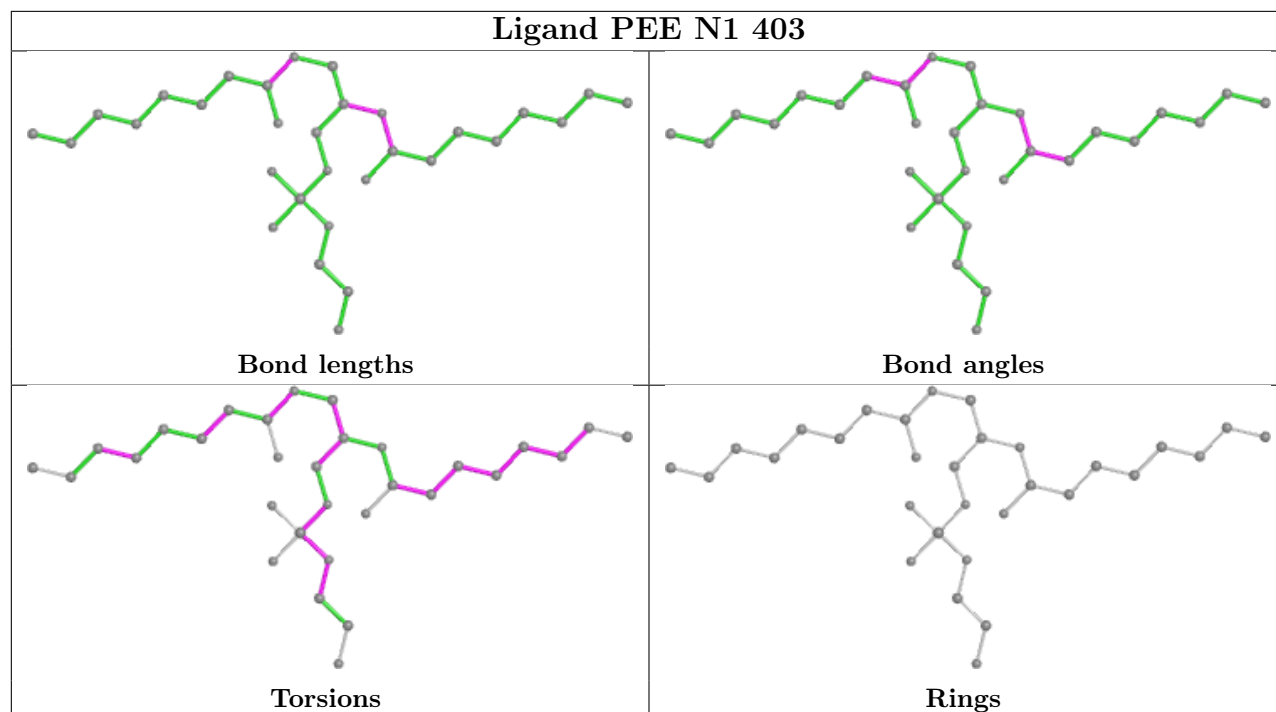


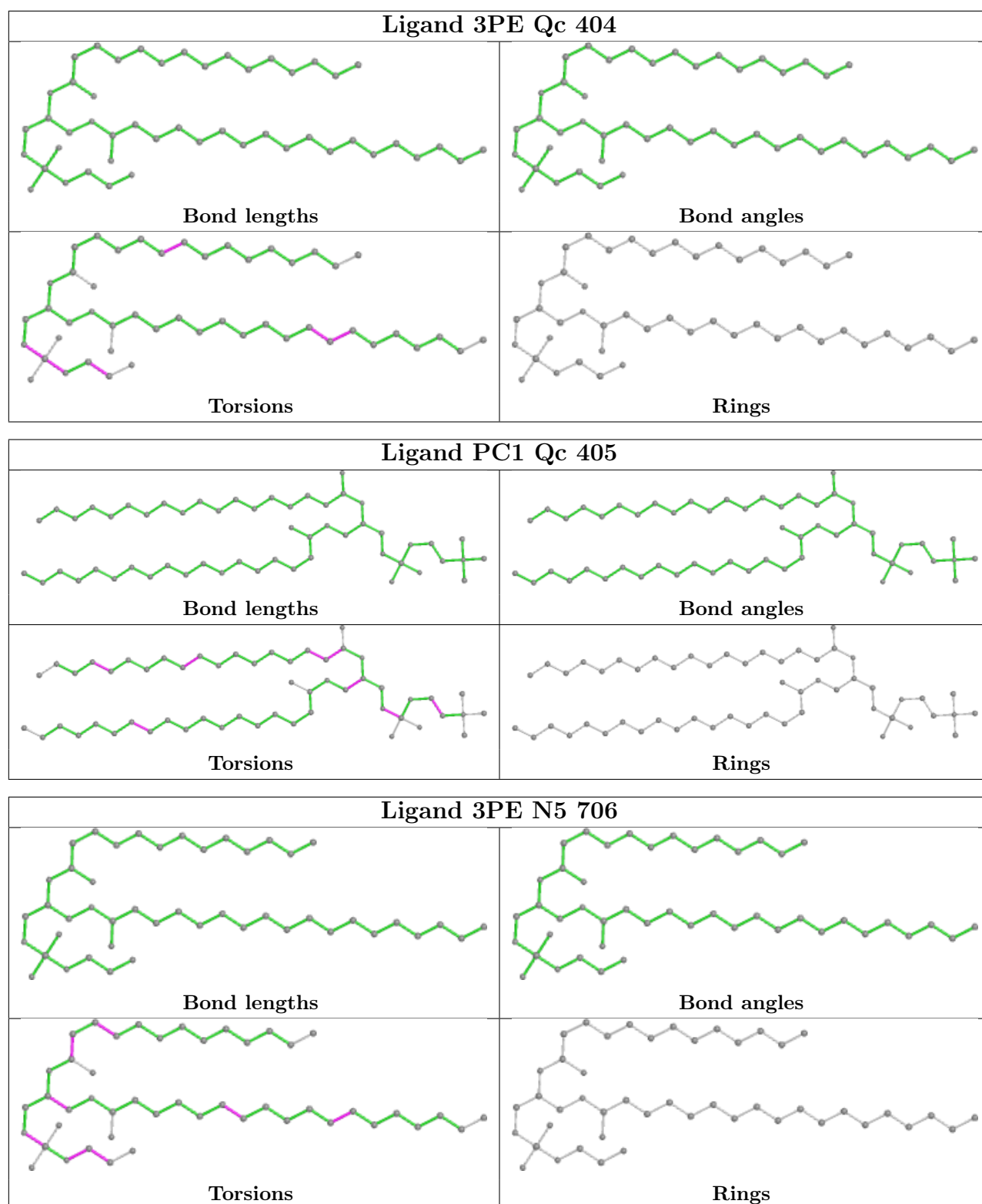
Ligand PLX AL 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

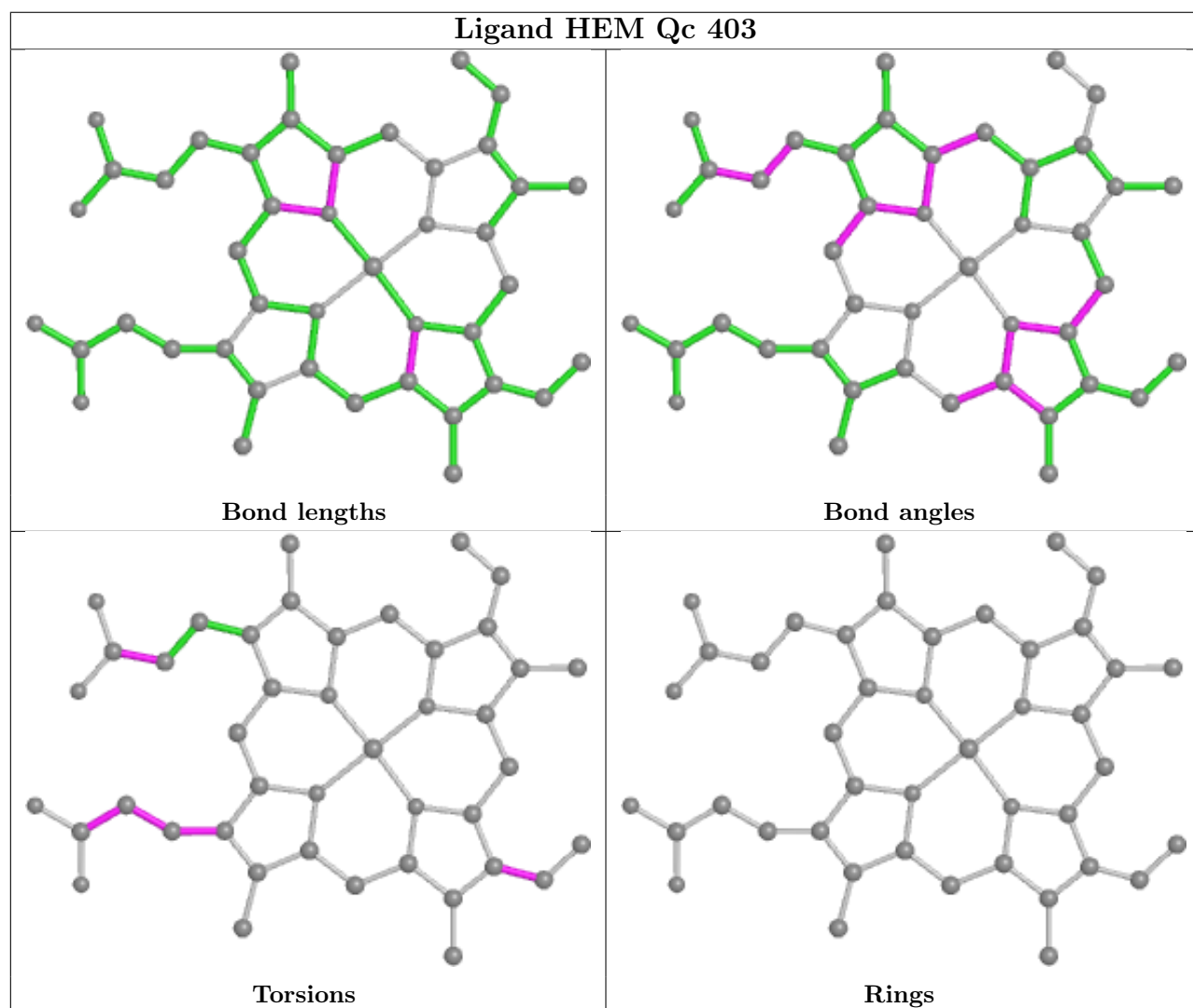
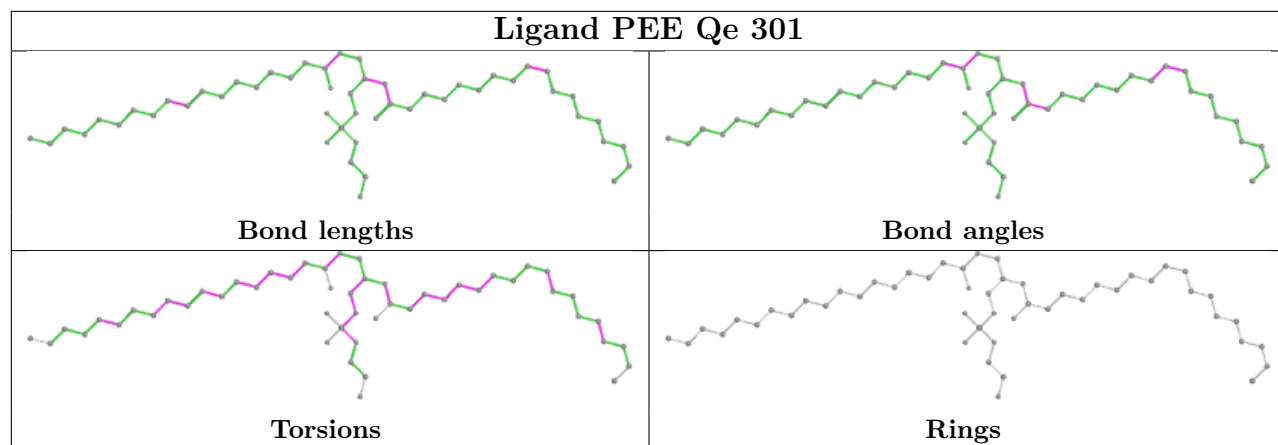
Ligand PC1 C3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

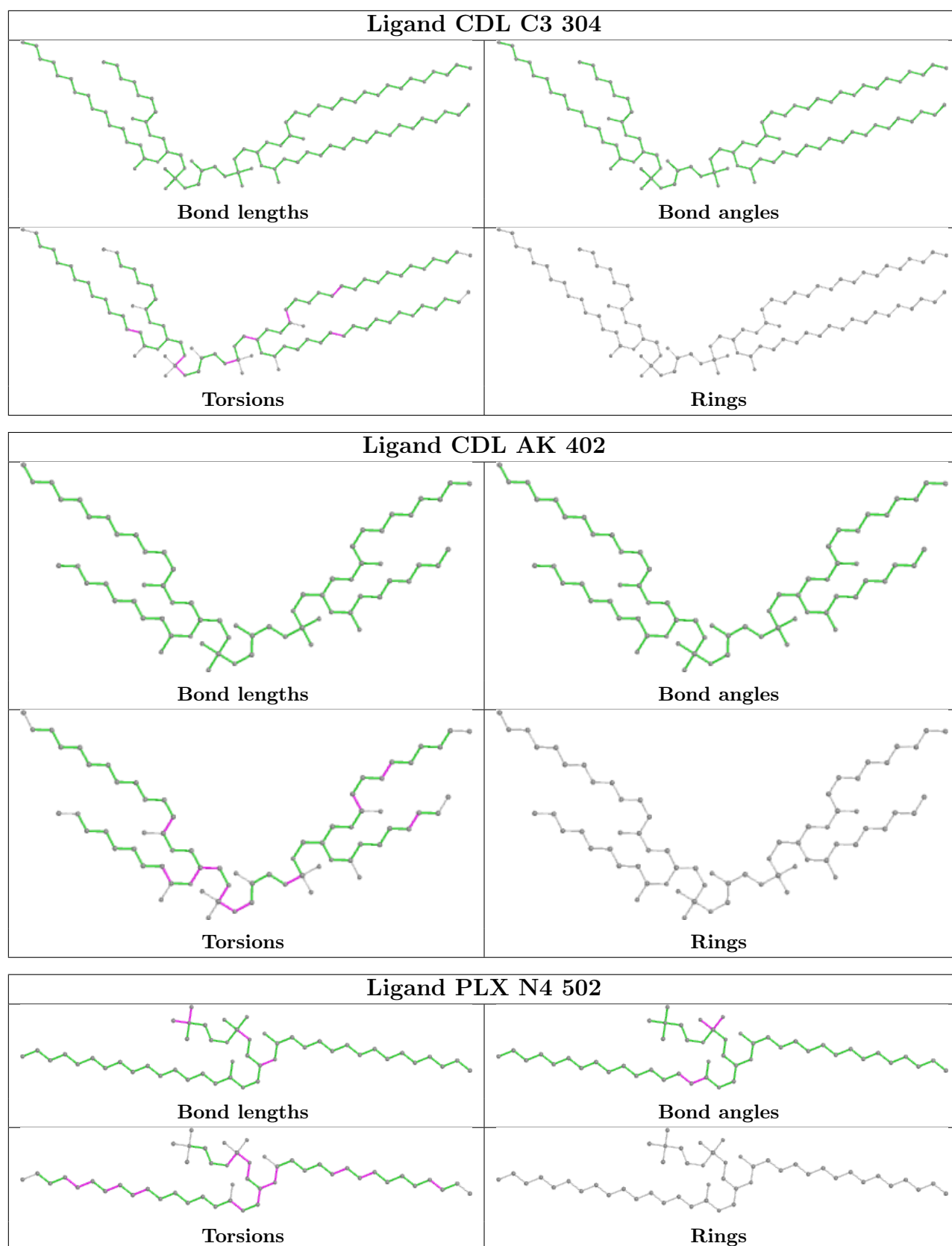
Ligand PLX AM 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

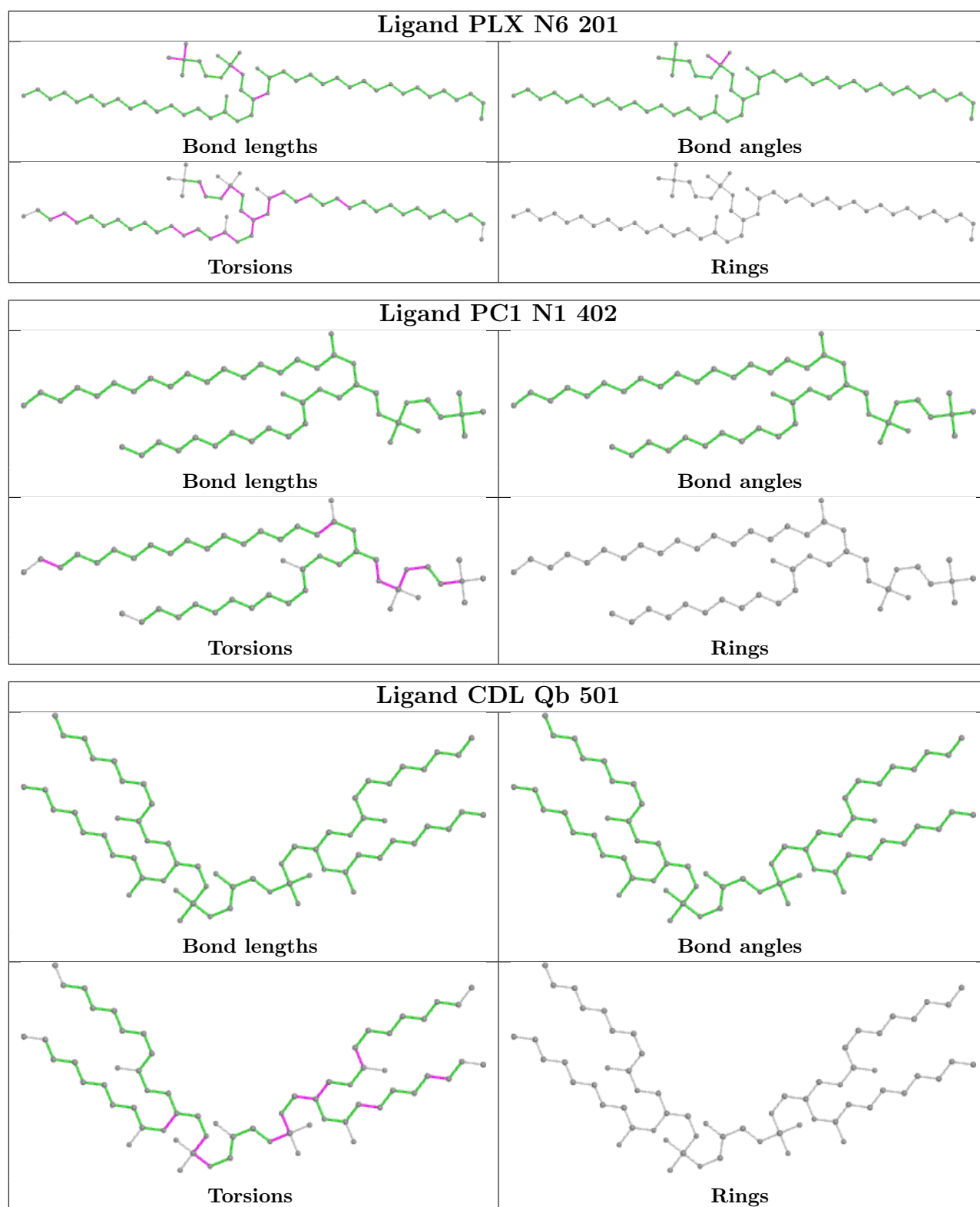


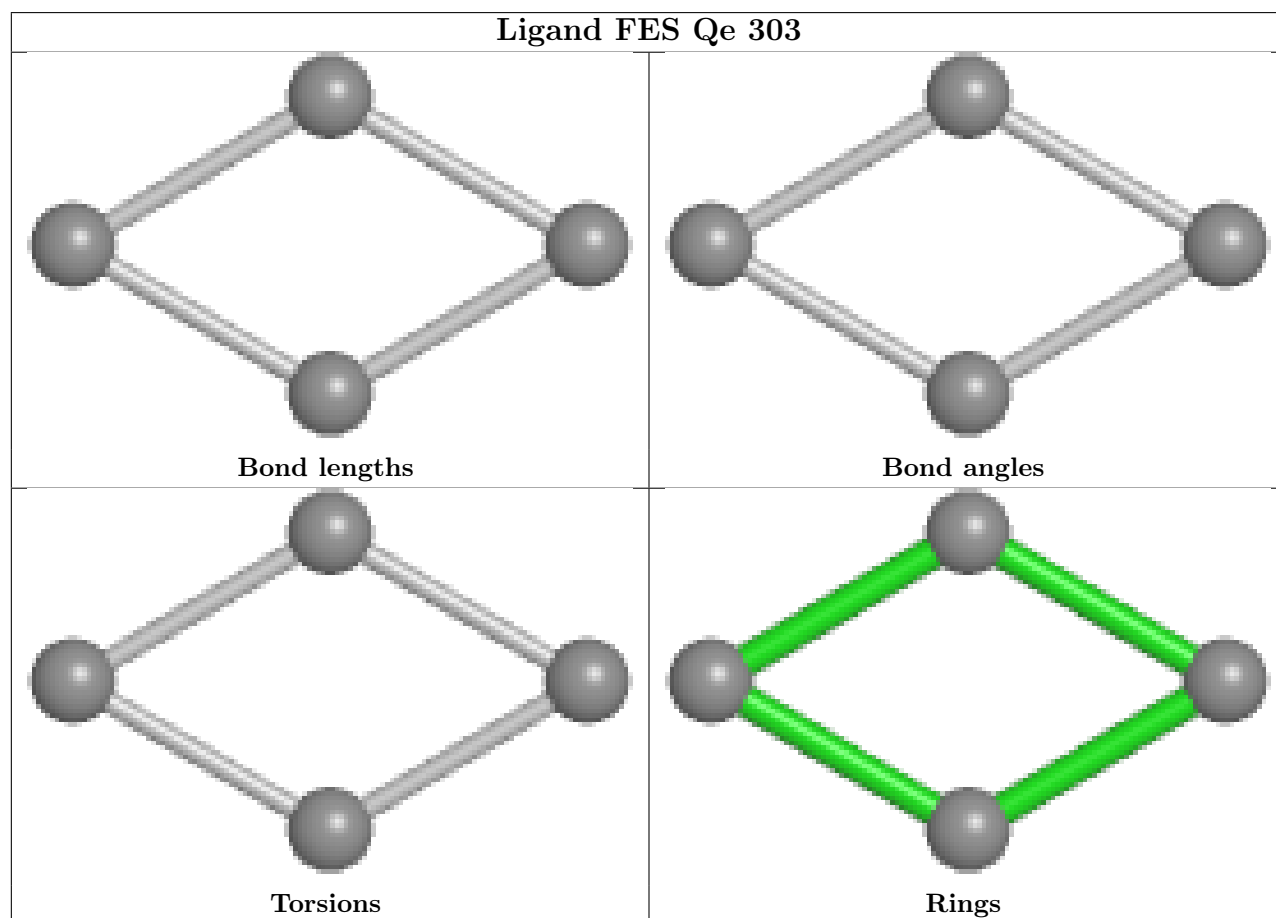
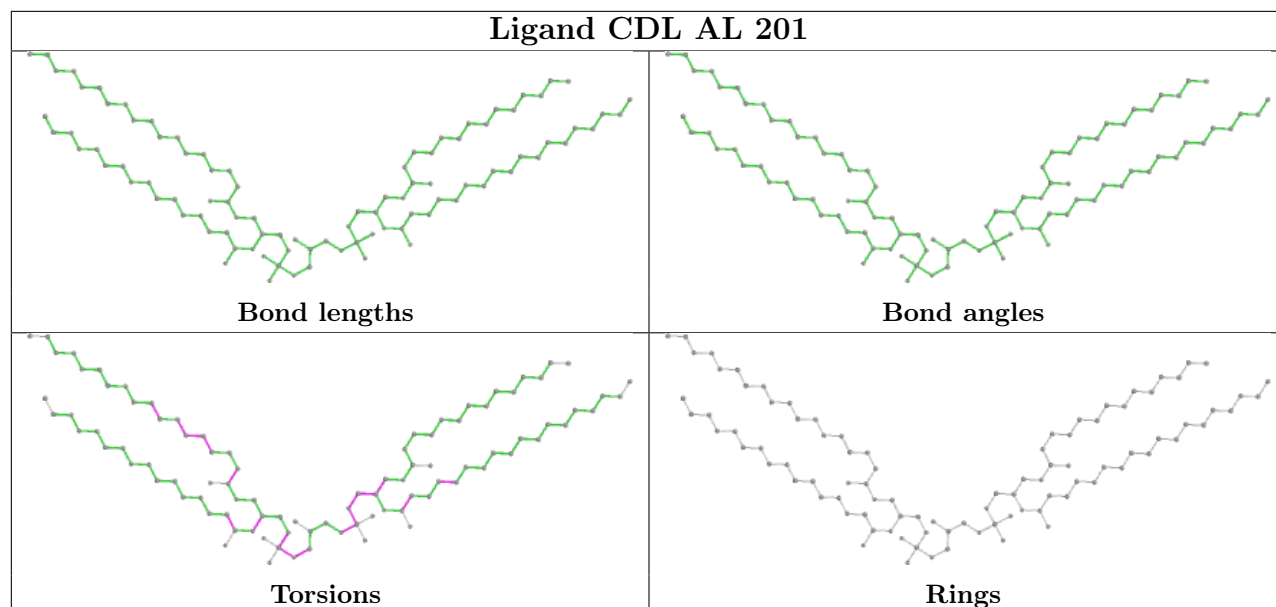


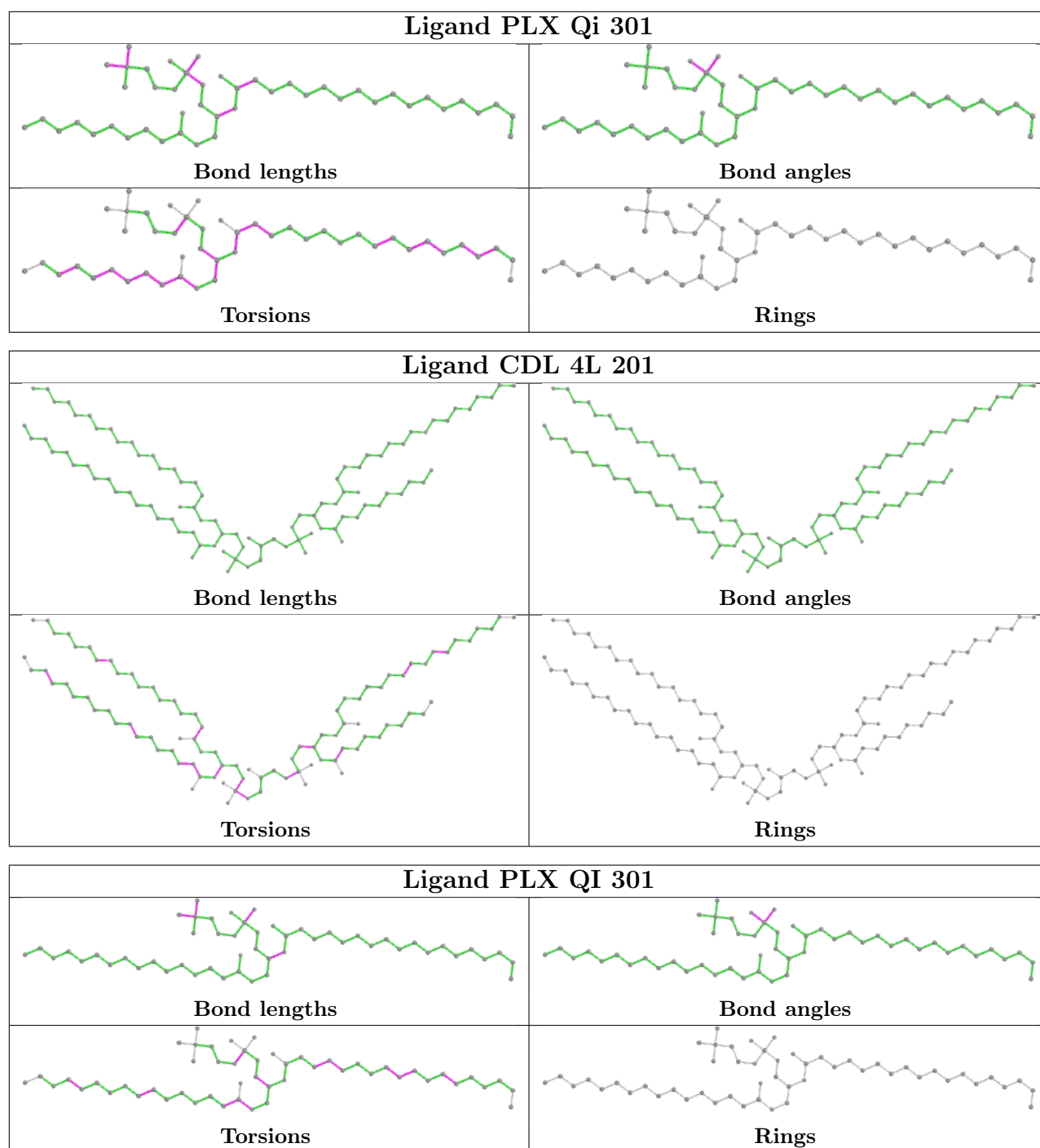


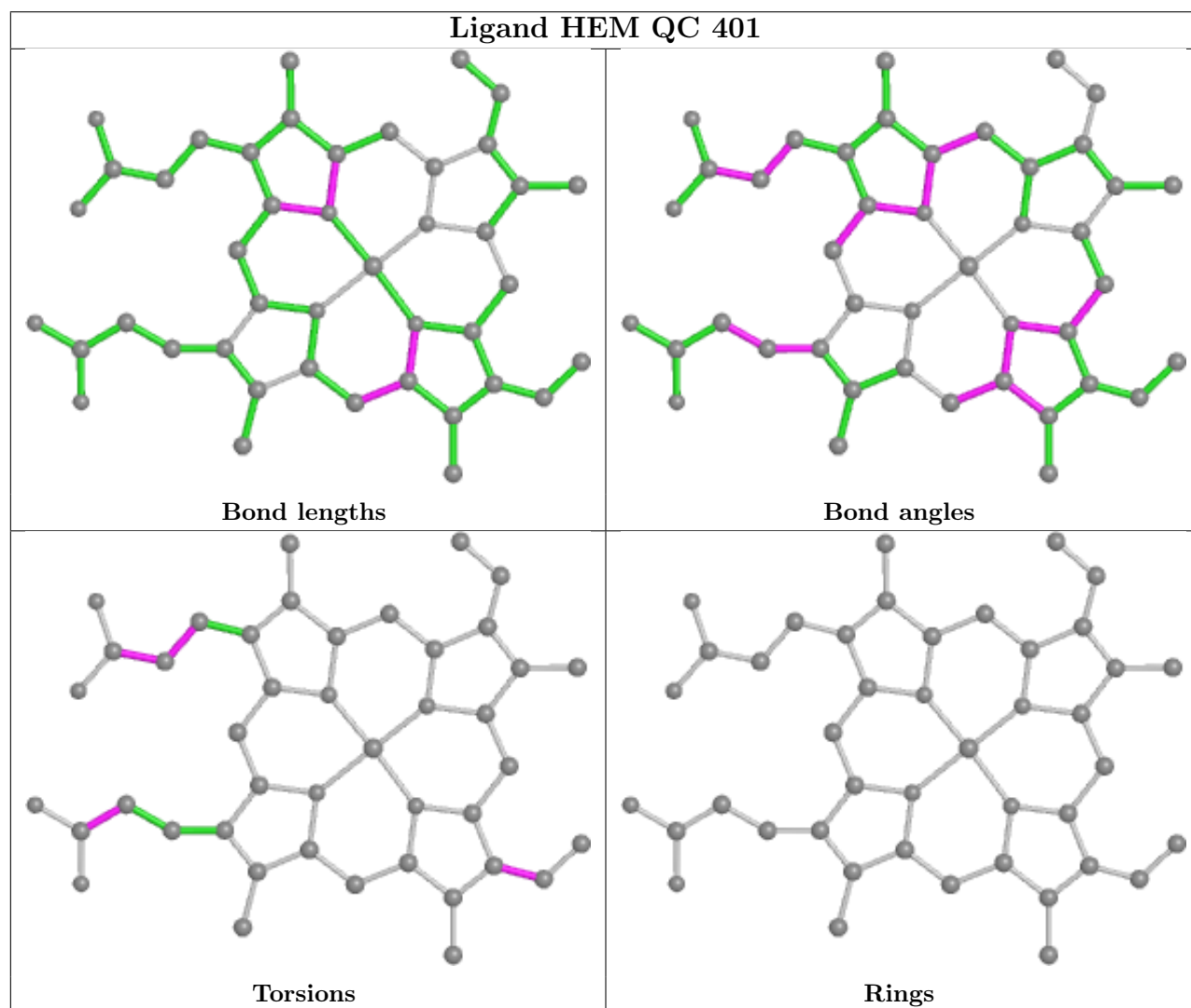
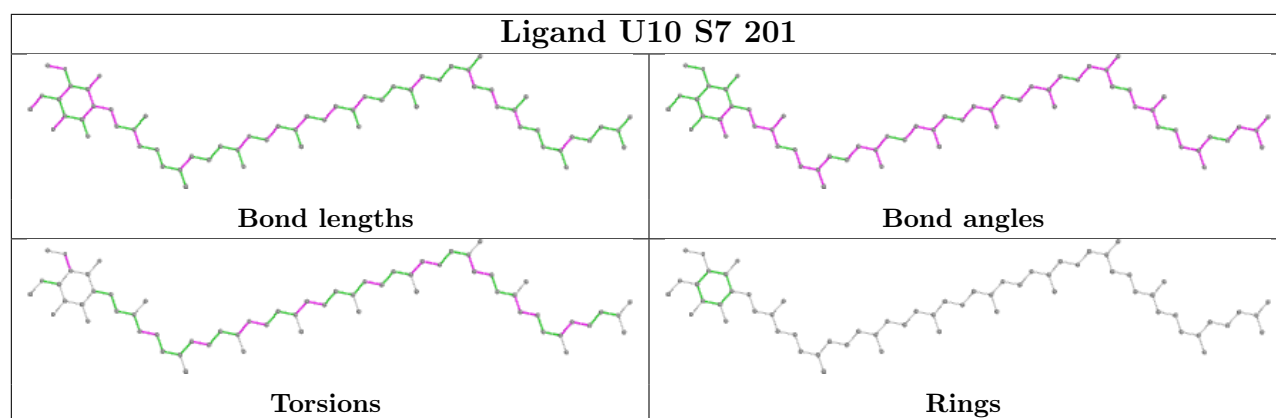




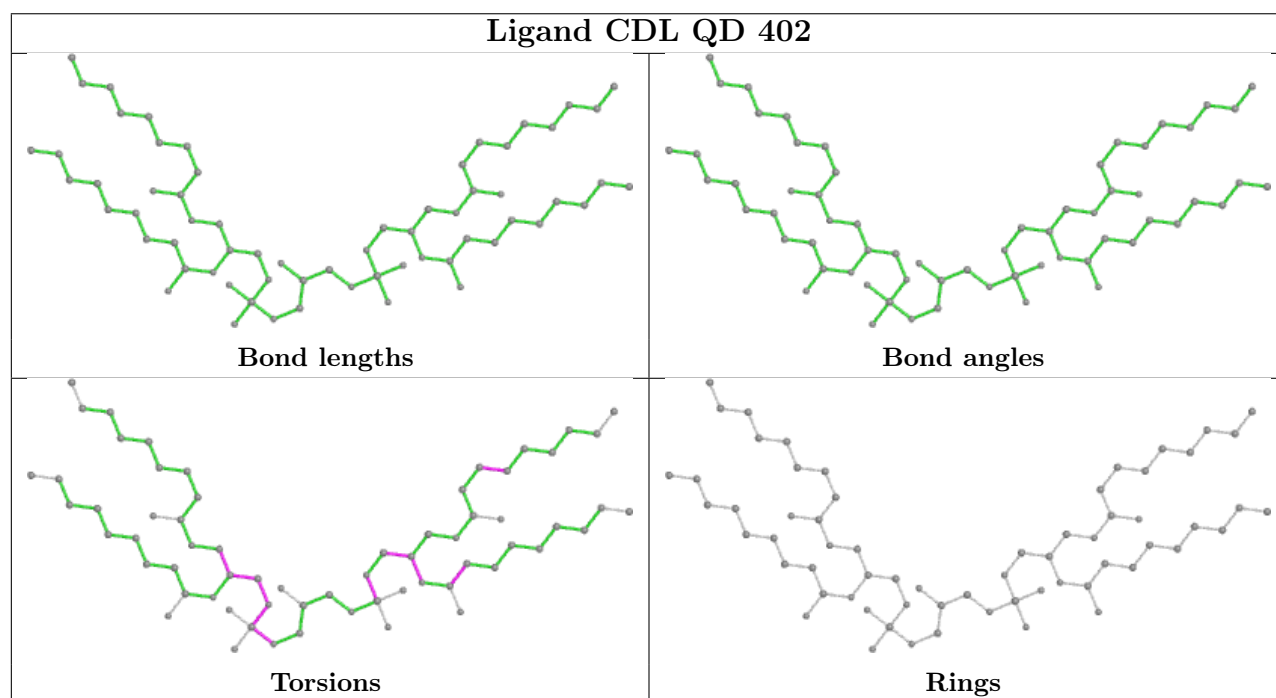
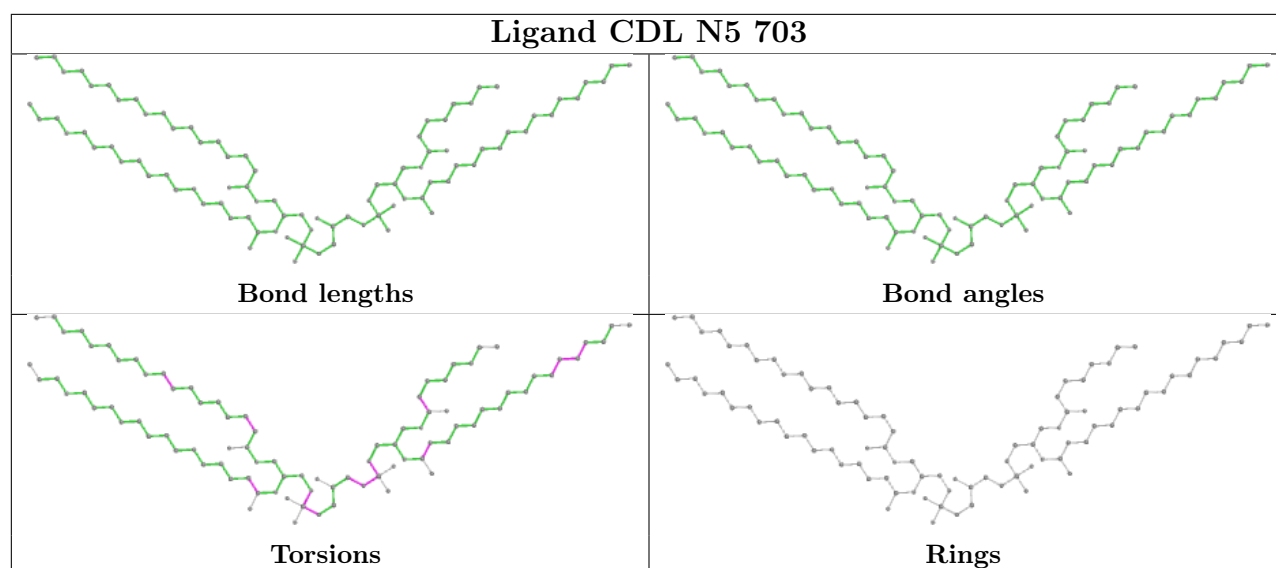


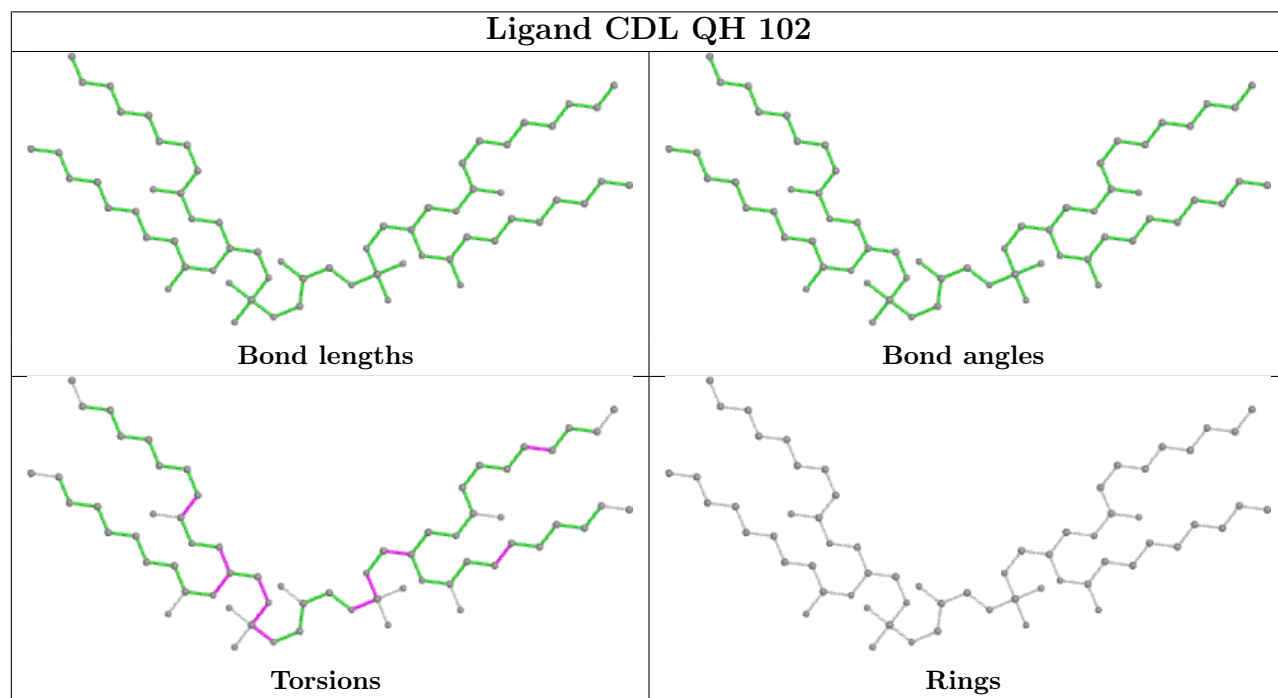
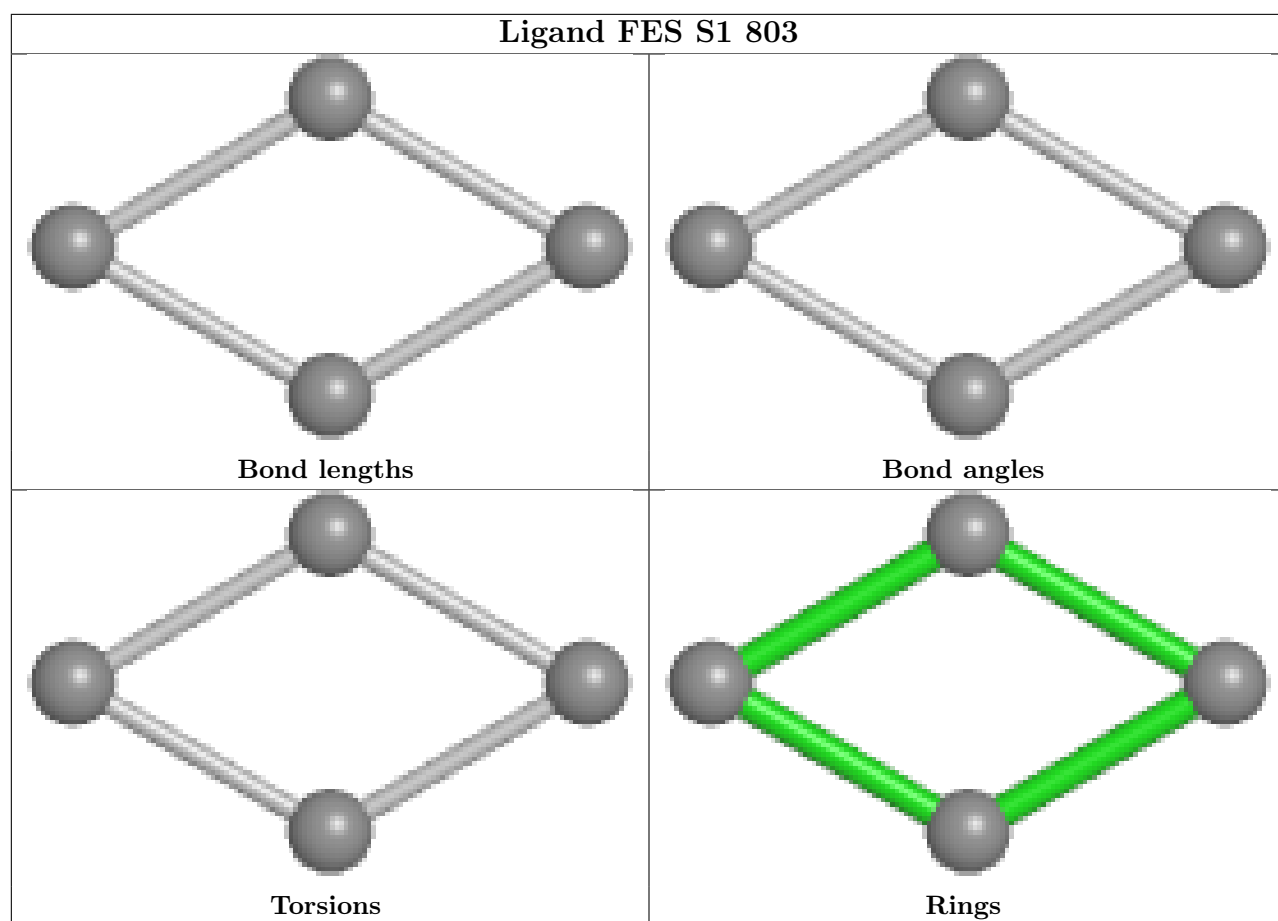


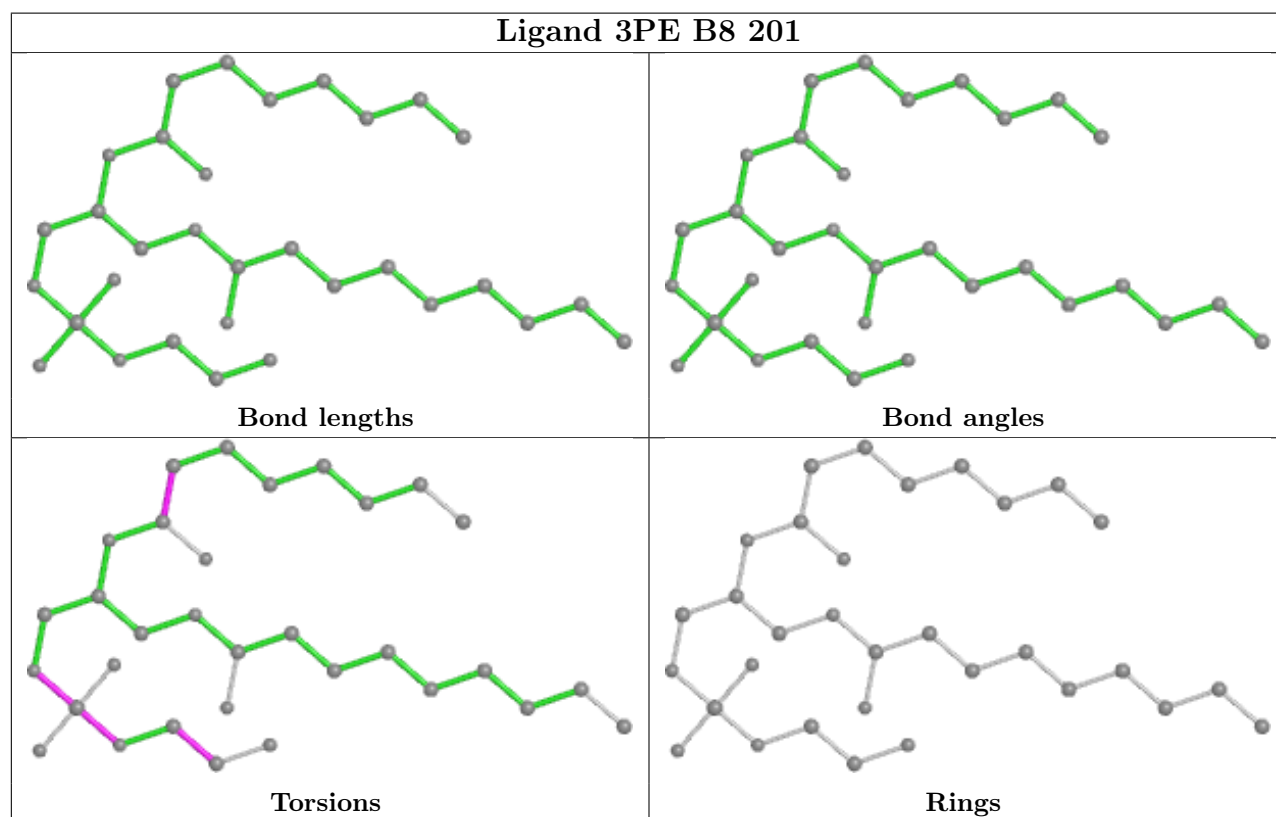
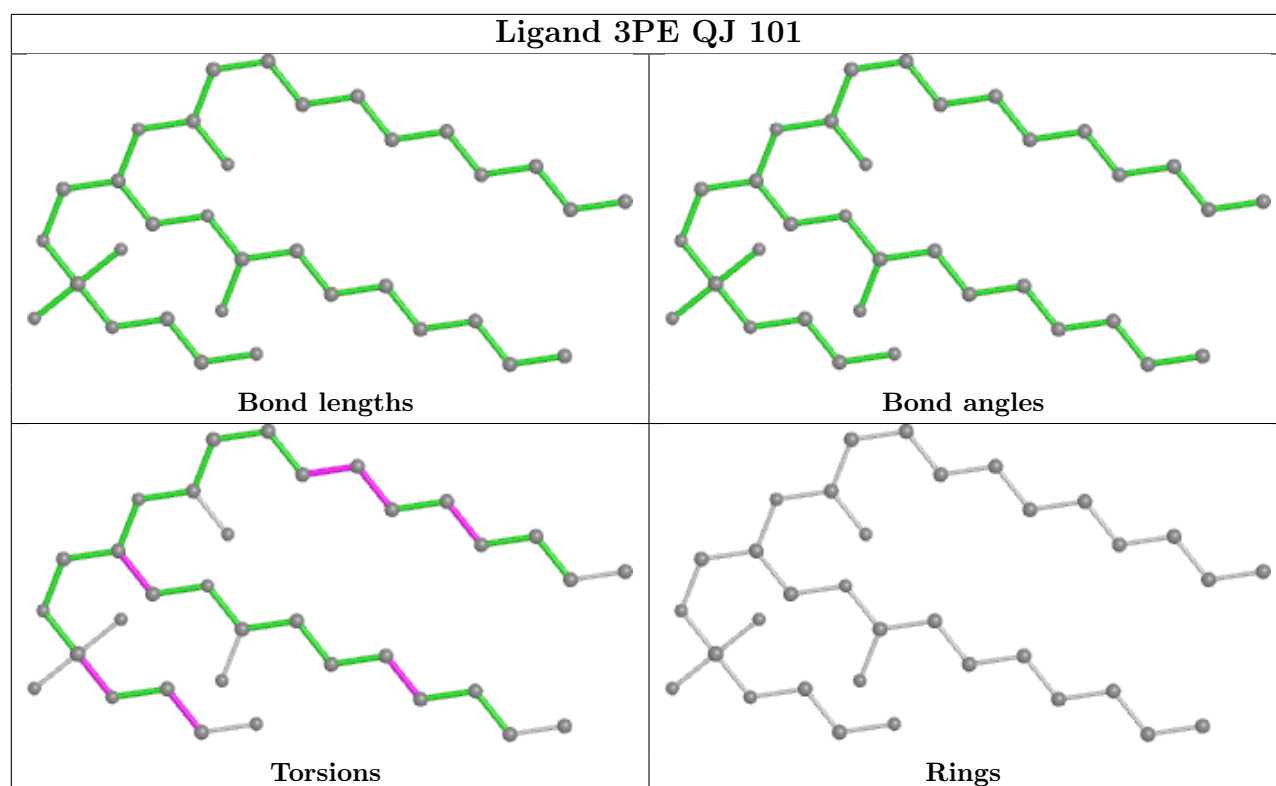


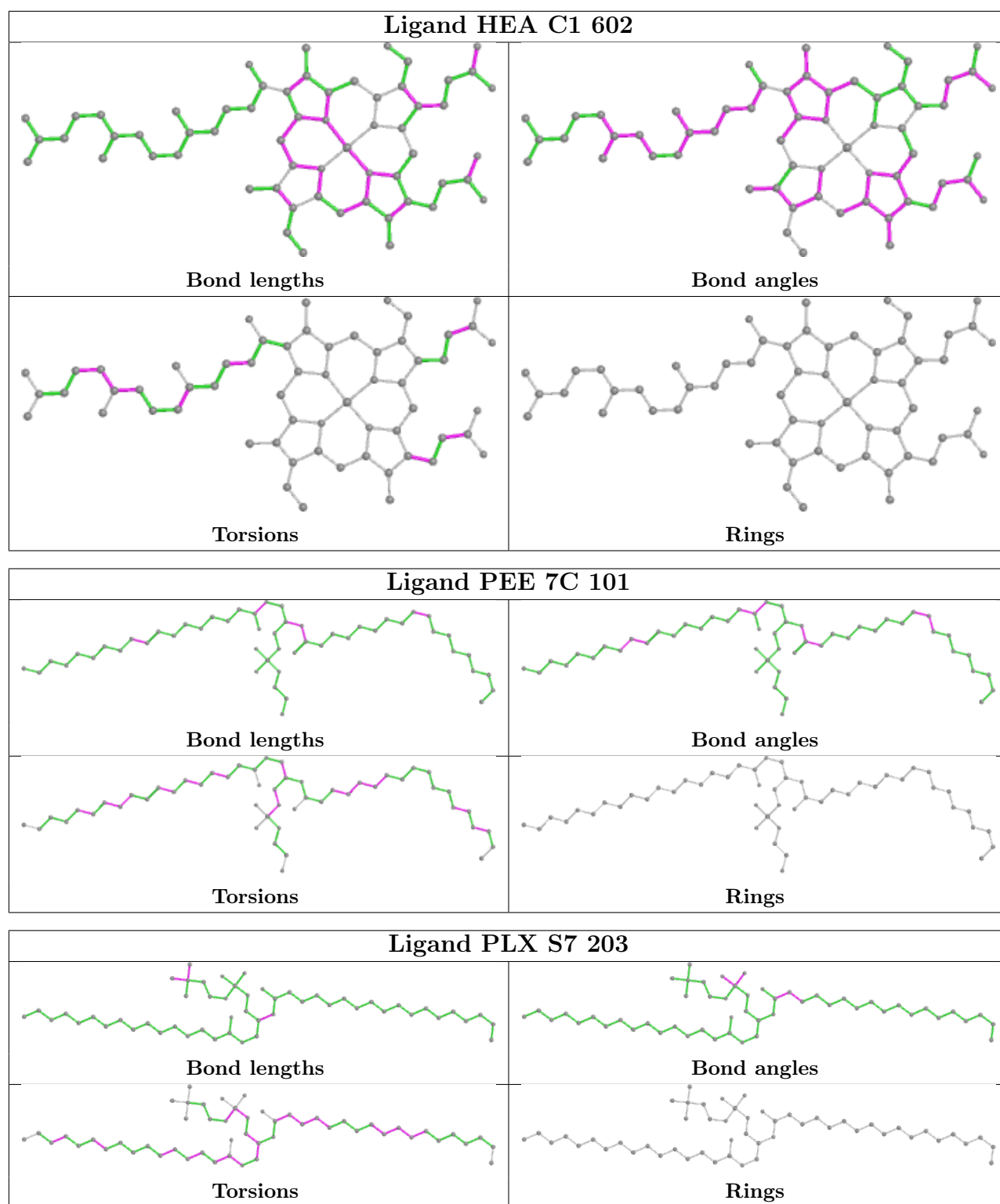












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

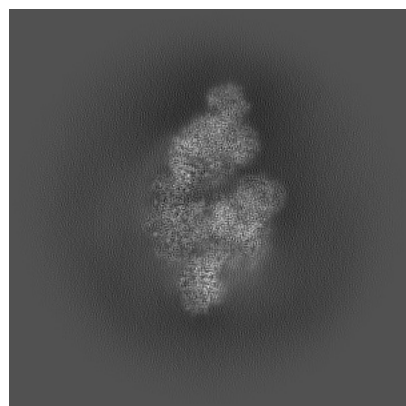
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60424. These allow visual inspection of the internal detail of the map and identification of artifacts.

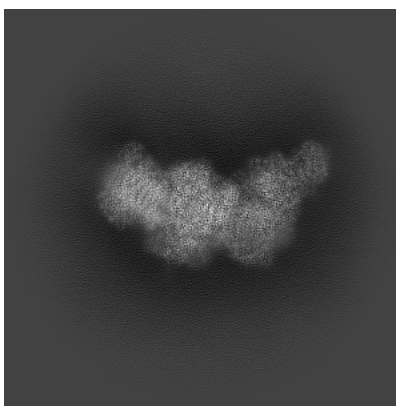
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

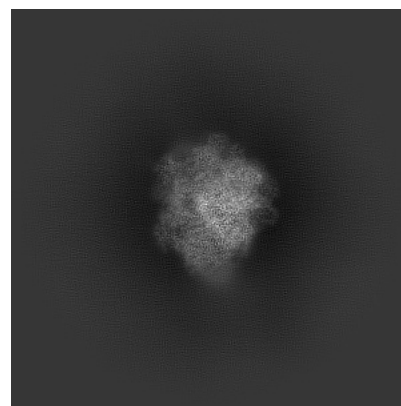
#### 6.1.1 Primary map



X

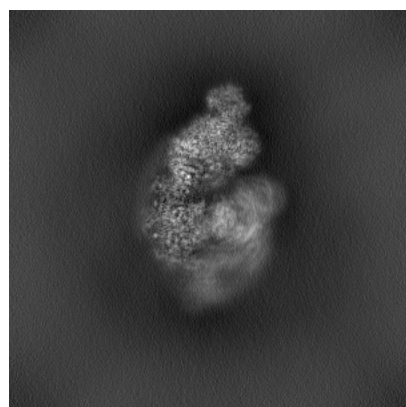


Y

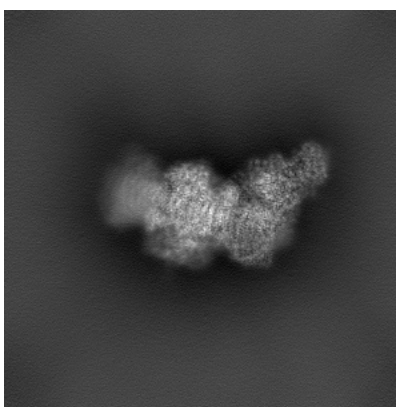


Z

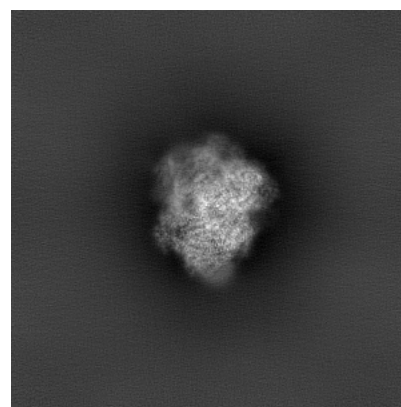
#### 6.1.2 Raw map



X



Y

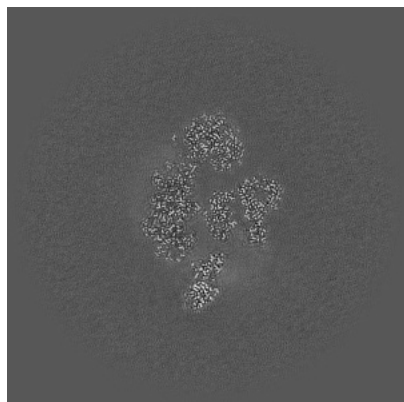


Z

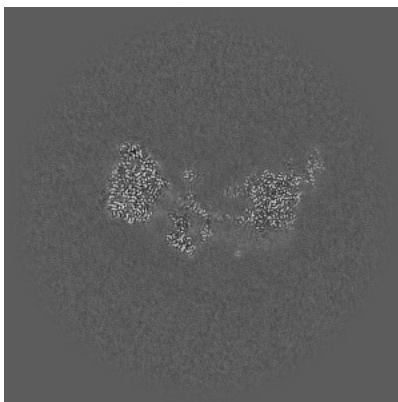
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

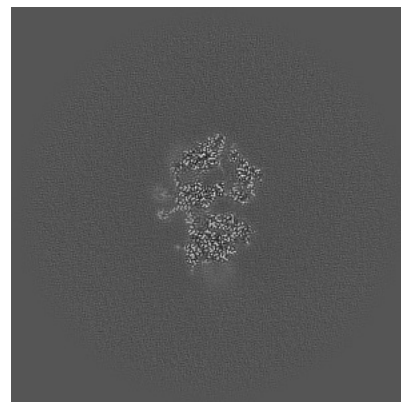
### 6.2.1 Primary map



X Index: 240

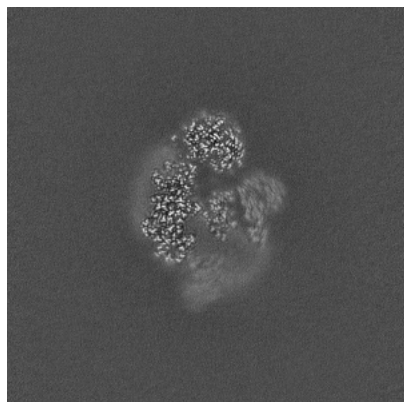


Y Index: 240

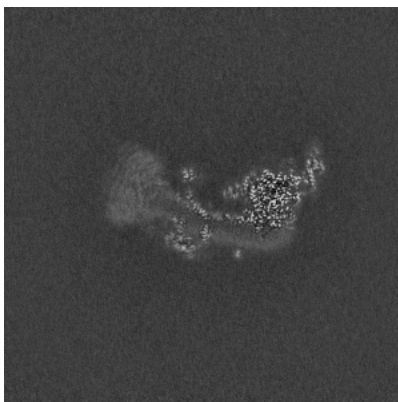


Z Index: 240

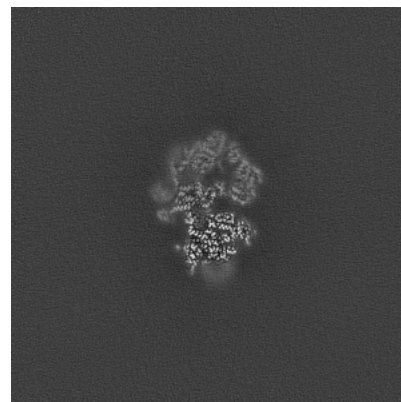
### 6.2.2 Raw map



X Index: 240



Y Index: 240

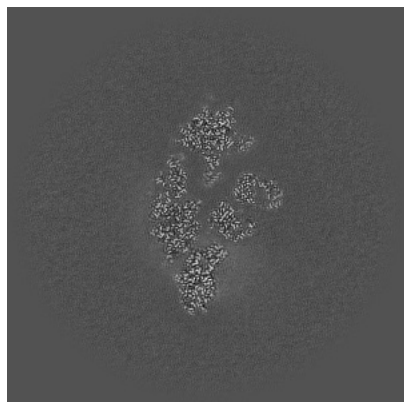


Z Index: 240

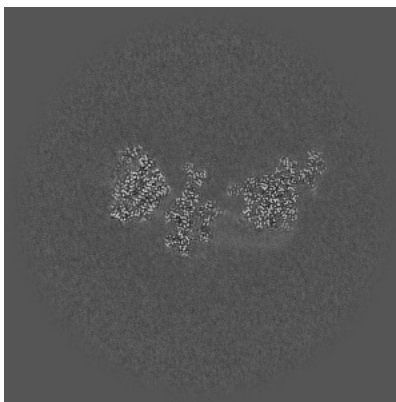
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

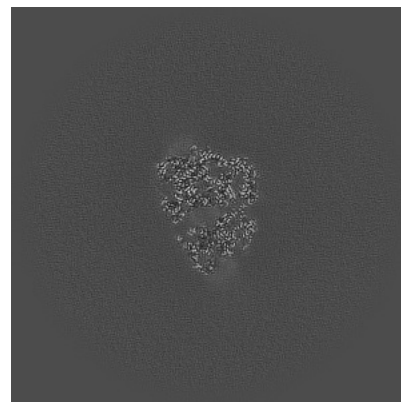
### 6.3.1 Primary map



X Index: 255

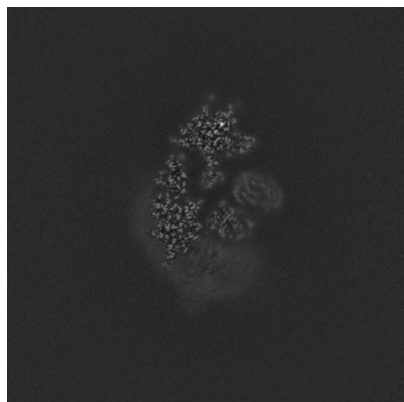


Y Index: 245

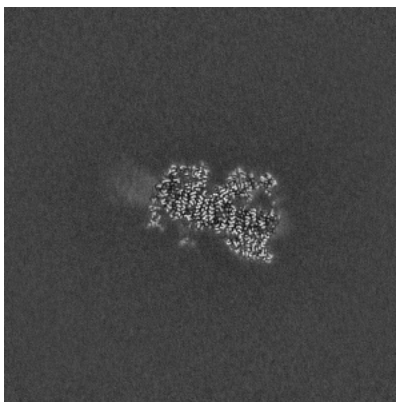


Z Index: 219

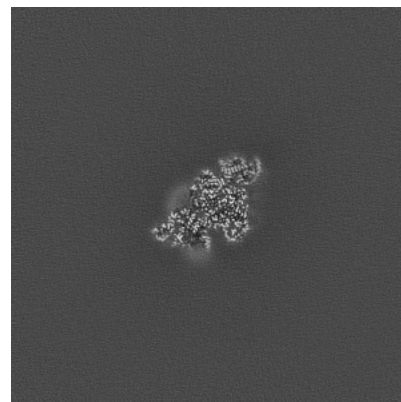
### 6.3.2 Raw map



X Index: 256



Y Index: 205



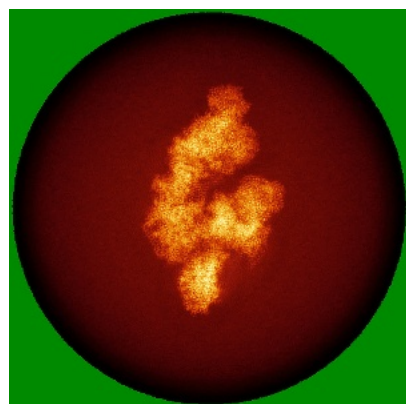
Z Index: 314

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

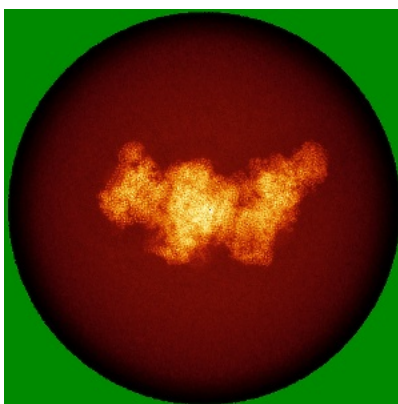


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

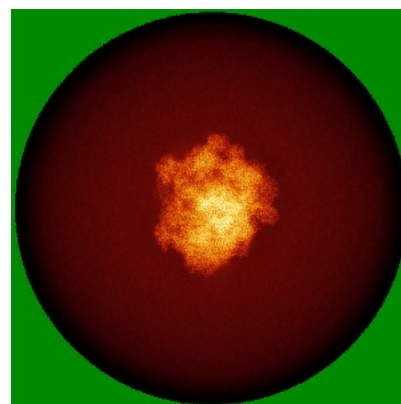
### 6.4.1 Primary map



X

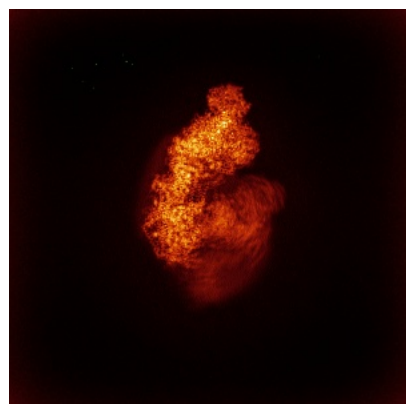


Y

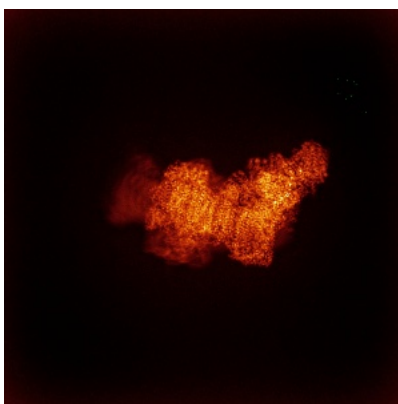


Z

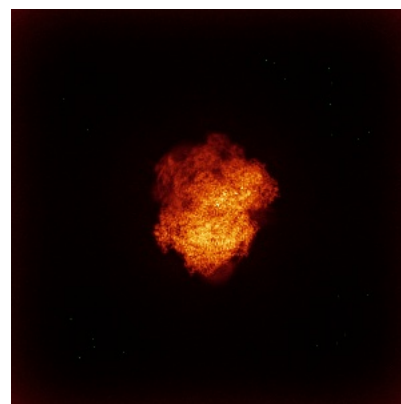
### 6.4.2 Raw map



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](#)

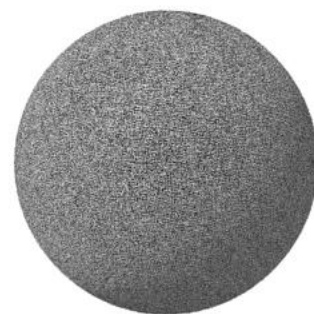
### 6.5.1 Primary map



X



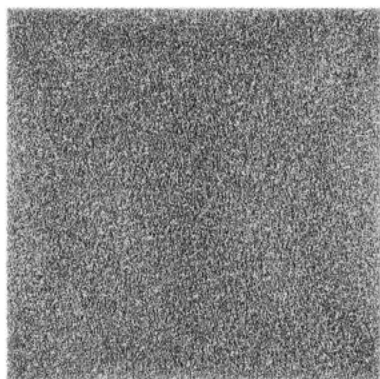
Y



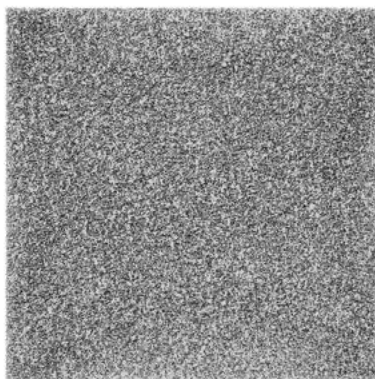
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

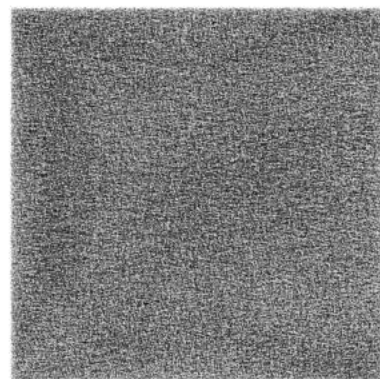
### 6.5.2 Raw map



X



Y



Z

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

## 6.6 Mask visualisation [i](#)

This section 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

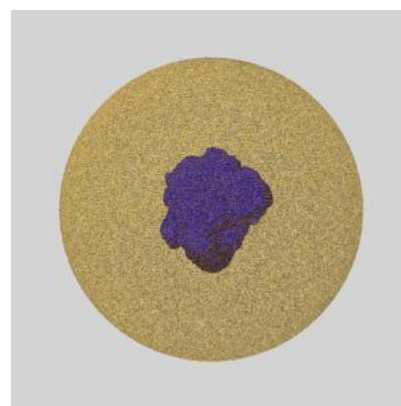
### 6.6.1 emd\_60424\_msk\_1.map [i](#)



X



Y

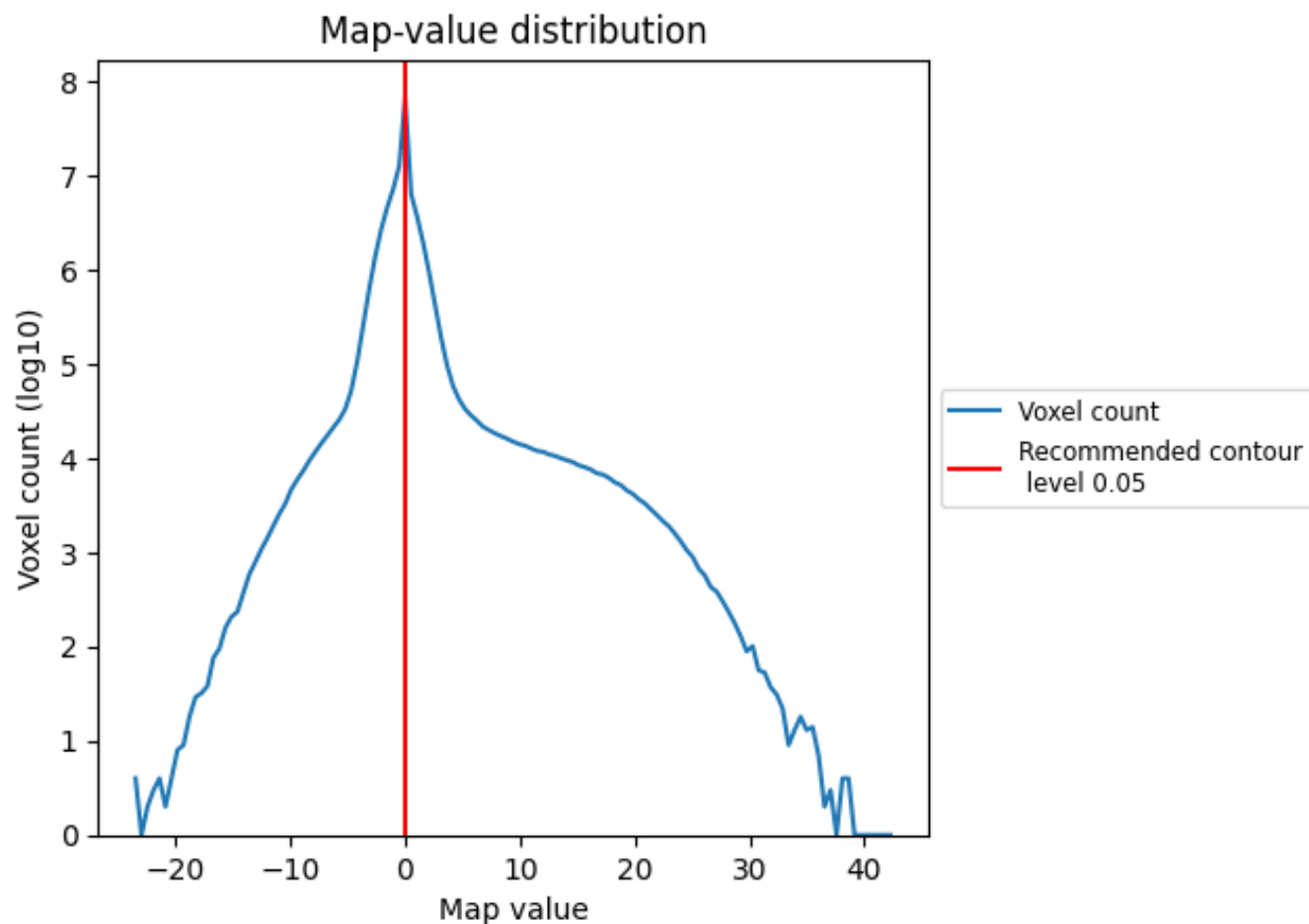


Z

## 7 Map analysis [i](#)

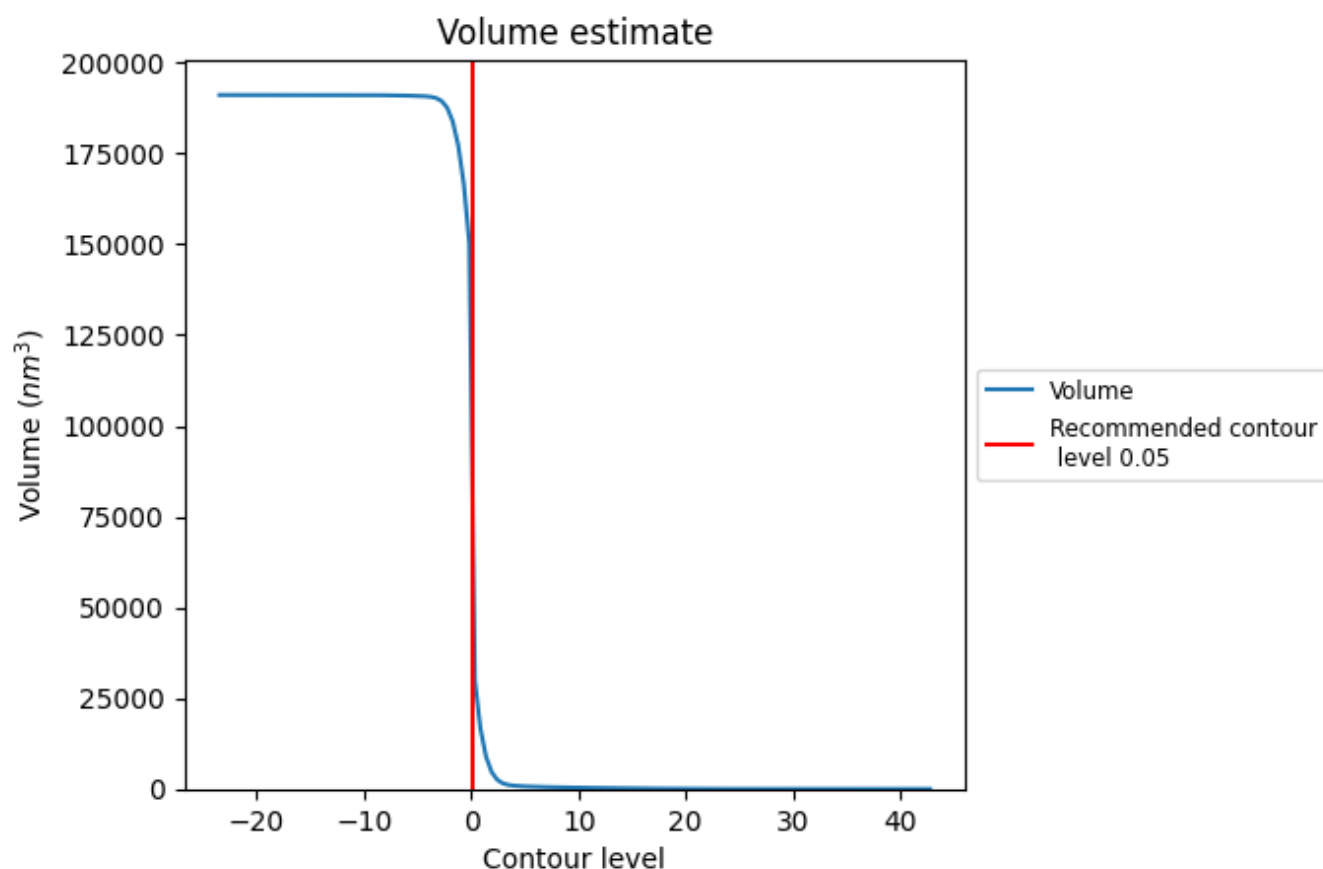
This section contains the results of statistical analysis of the map.

### 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.

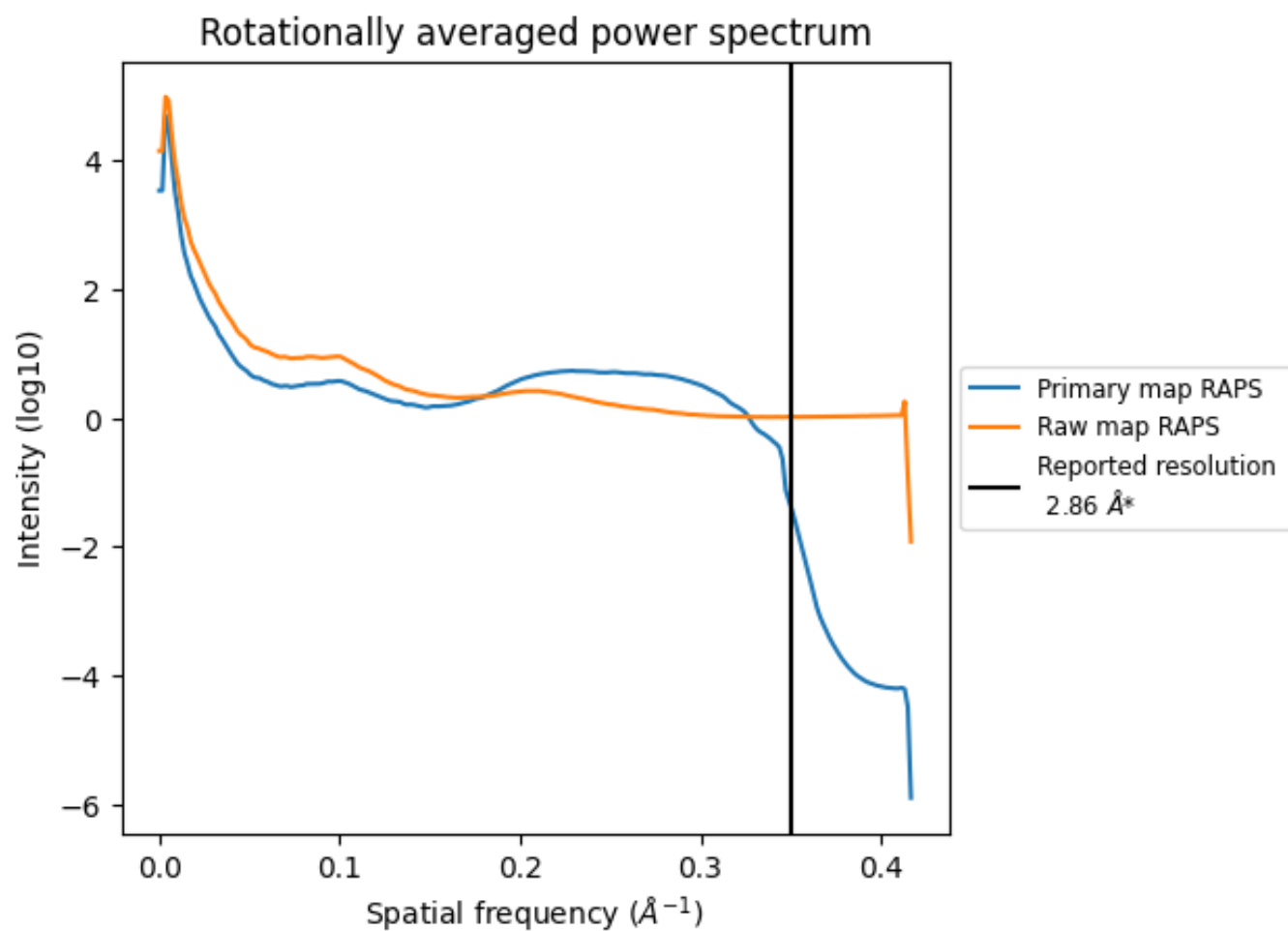
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97381  $\text{nm}^3$ ; this corresponds to an approximate mass of 87967 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 ⓘ

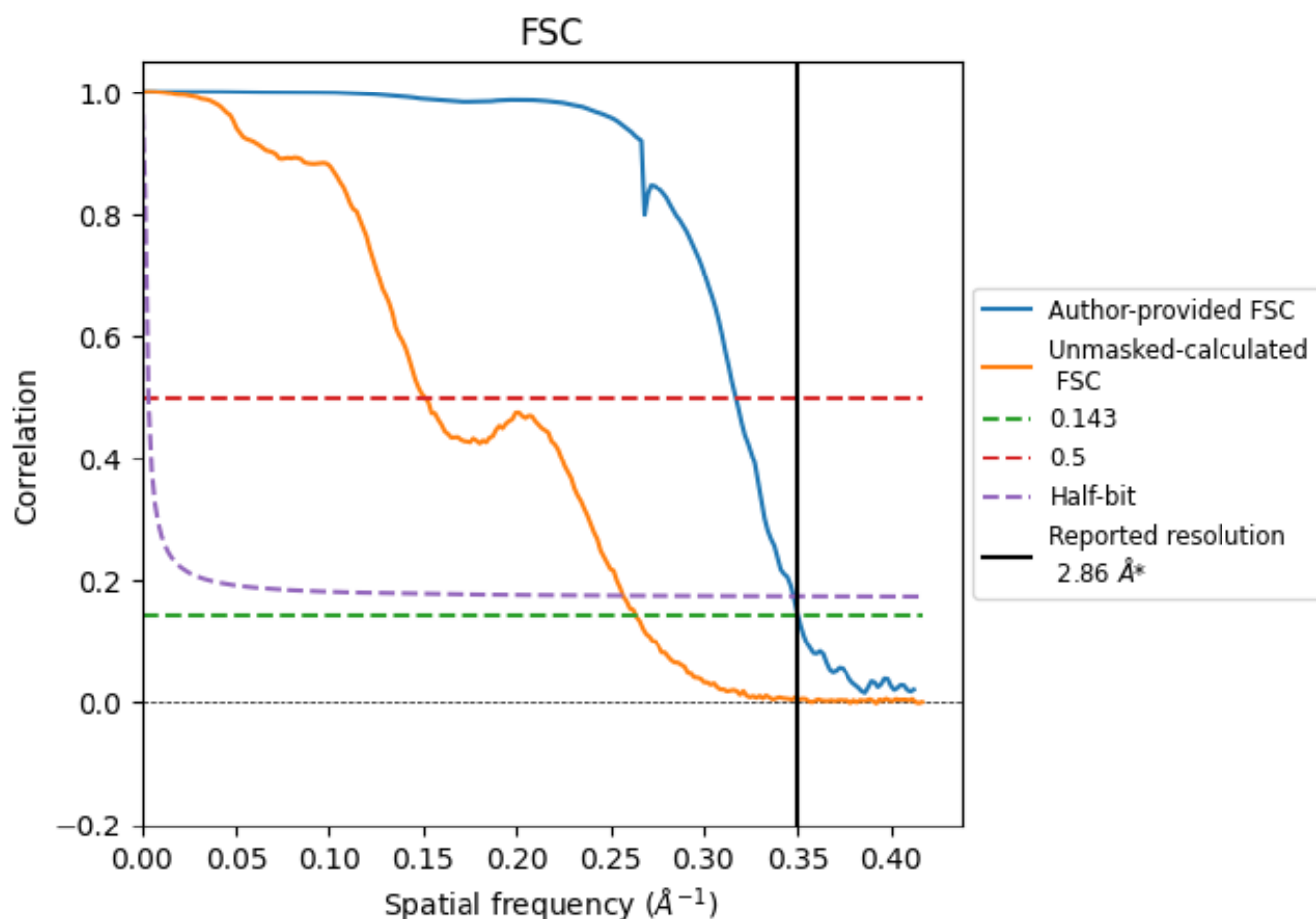


\*Reported resolution corresponds to spatial frequency of 0.350  $\text{\AA}^{-1}$

## 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 0.350  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.15	2.88
Unmasked-calculated*	3.80	6.63	3.89

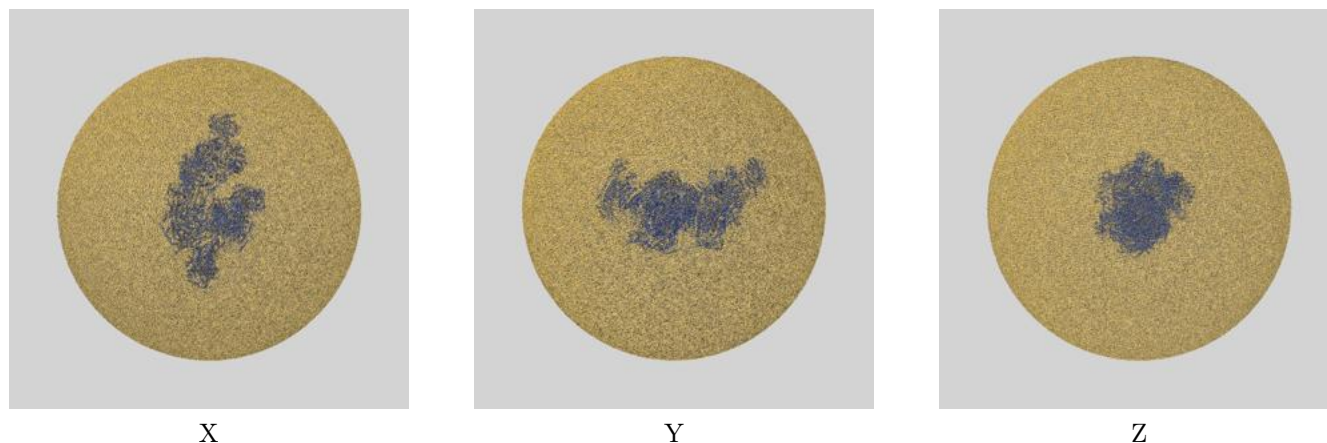
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.86 by more than 10 %



## 9 Map-model fit [i](#)

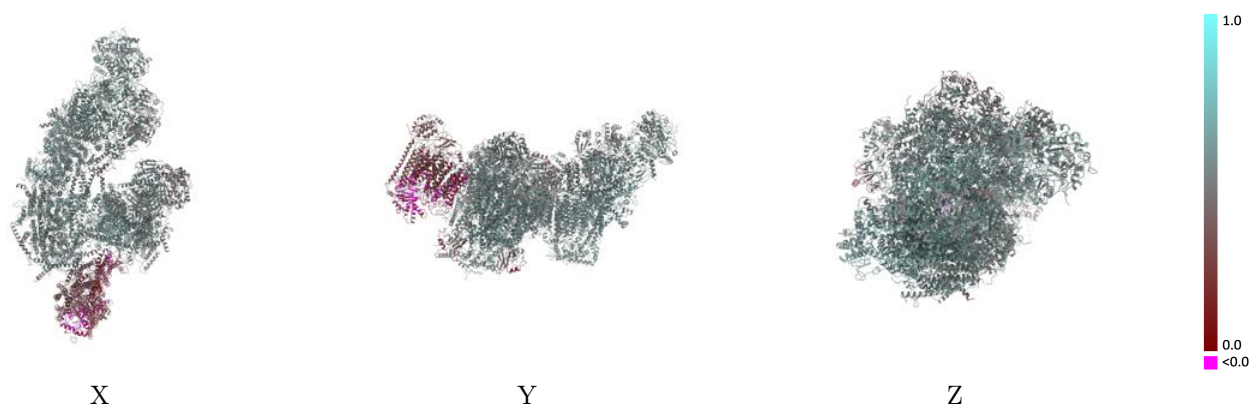
This section contains information regarding the fit between EMDB map EMD-60424 and PDB model 8ZSQ. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

### 9.1 Map-model overlay [i](#)



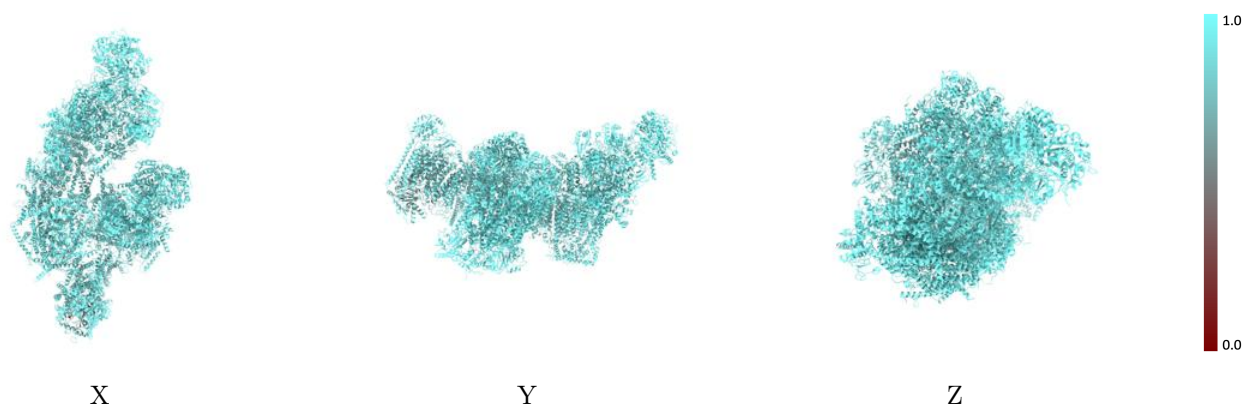
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



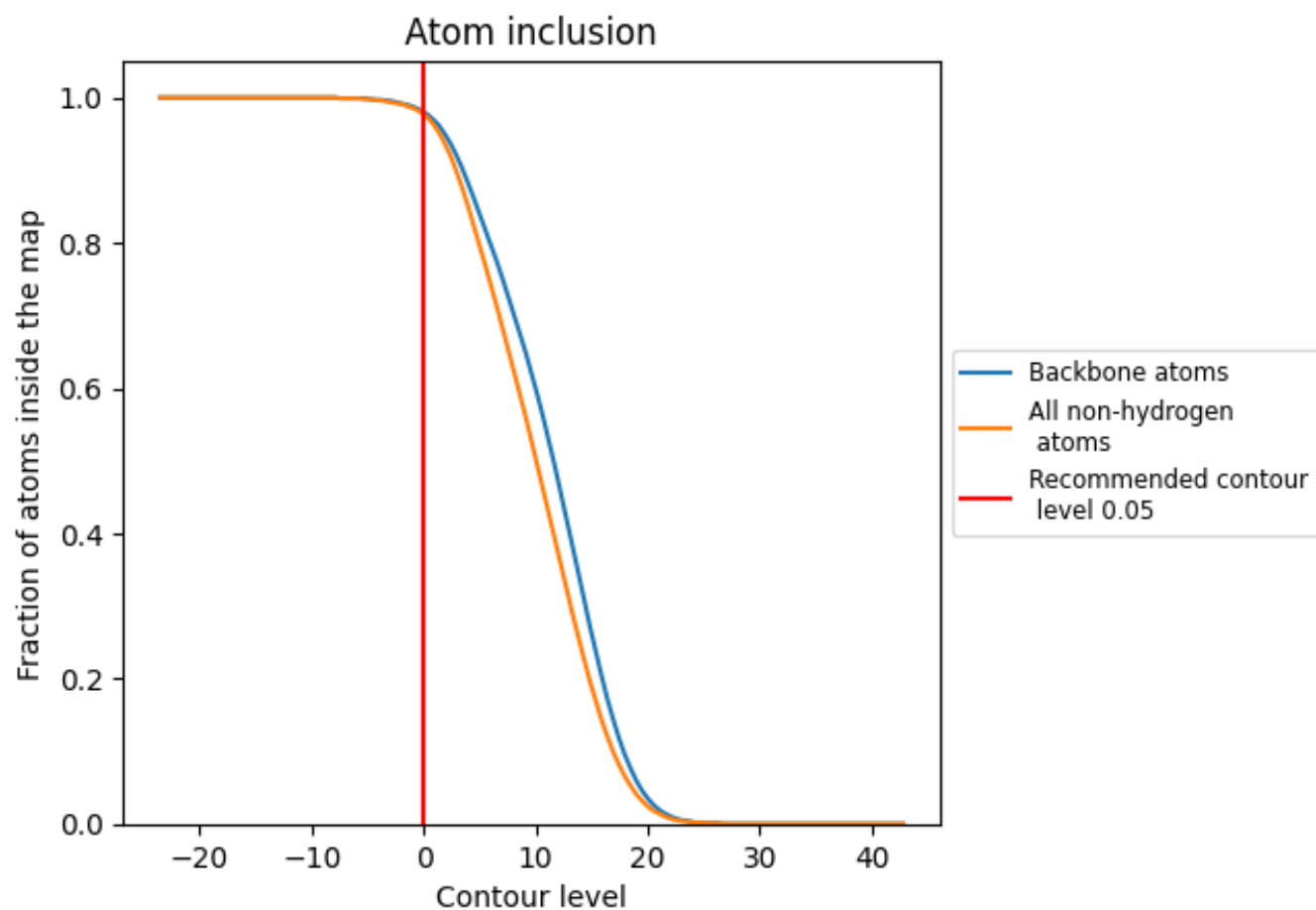
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.5010
4L	 0.9980	 0.5900
5A	 0.9340	 0.3250
5B	 0.9410	 0.2880
6A	 0.8750	 0.1680
6B	 0.8540	 0.1040
6C	 0.8800	 0.2080
7A	 0.9620	 0.3680
7B	 0.9370	 0.2730
7C	 0.9260	 0.3160
8B	 0.9460	 0.3220
A1	 0.9980	 0.5820
A2	 0.9900	 0.4670
A3	 1.0000	 0.5660
A5	 0.9910	 0.5260
A6	 0.9930	 0.5300
A7	 0.9990	 0.5370
A8	 0.9990	 0.5720
A9	 0.9970	 0.5550
AB	 0.9910	 0.4550
AC	 0.9840	 0.5280
AK	 0.9940	 0.5360
AL	 0.9990	 0.5640
AM	 0.9980	 0.5510
AN	 0.9970	 0.5710
B1	 0.9920	 0.5020
B2	 0.9950	 0.5290
B3	 0.9940	 0.4910
B4	 0.9960	 0.5560
B5	 0.9910	 0.5400
B6	 0.9930	 0.4920
B7	 0.9950	 0.5250
B8	 0.9950	 0.5680
B9	 0.9940	 0.5480
BK	 0.9820	 0.5200









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Chain	Atom inclusion	Q-score
BL	 0.9880	 0.5140
C1	 0.8590	 0.2160
C2	 0.7950	 0.1000
C3	 0.8800	 0.2140
C4	 0.9010	 0.2690
CA	 0.9960	 0.5340
CB	 0.9950	 0.5620
N1	 0.9940	 0.5840
N2	 0.9950	 0.5890
N3	 0.9990	 0.5810
N4	 0.9900	 0.5550
N5	 0.9920	 0.5520
N6	 0.9900	 0.5500
QA	 0.9880	 0.5170
QB	 0.9920	 0.5650
QC	 0.9960	 0.5870
QD	 0.9970	 0.5640
QE	 0.9890	 0.4590
QF	 0.9930	 0.4580
QG	 0.9840	 0.5110
QH	 0.9800	 0.5020
QI	 0.9840	 0.5180
QJ	 0.9880	 0.5250
QK	 0.9960	 0.5060
Qa	 0.9790	 0.5100
Qb	 0.9840	 0.5160
Qc	 0.9870	 0.5500
Qd	 0.9890	 0.5270
Qe	 0.9800	 0.4240
Qf	 0.9900	 0.5140
Qg	 0.9880	 0.5720
Qh	 0.9960	 0.5710
Qi	 0.9980	 0.5700
Qj	 0.9910	 0.5600
S1	 0.9880	 0.5210
S2	 0.9940	 0.5710
S3	 0.9950	 0.5640
S4	 0.9920	 0.5480
S5	 0.9970	 0.5620
S6	 0.9990	 0.5600
S7	 0.9940	 0.5760
S8	 0.9990	 0.5880

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Chain	Atom inclusion	Q-score
V1	 0.9920	 0.5350
V2	 0.9950	 0.5350
V3	 0.9970	 0.5290