



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 07:01 PM EST

PDB ID : 7TGH
EMDB ID : EMD-25882
Title : Cryo-EM structure of respiratory super-complex CI+III2 from Tetrahymena thermophila
Authors : Zhou, L.; Maldonado, M.; Padavannil, A.; Guo, F.; Letts, J.A.
Deposited on : 2022-01-07
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

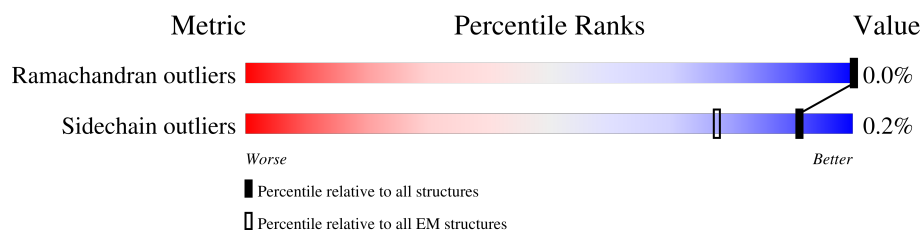
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.60 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.



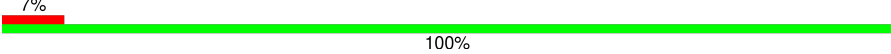





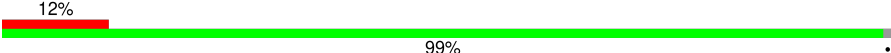
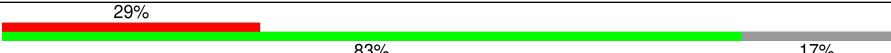
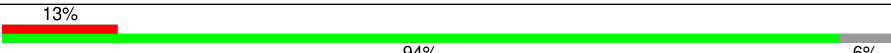
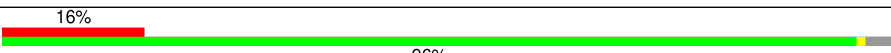
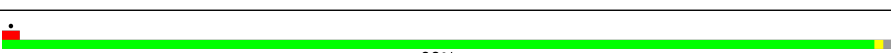
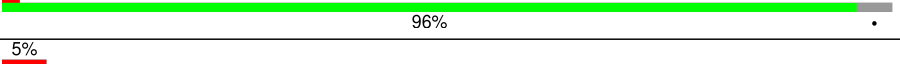
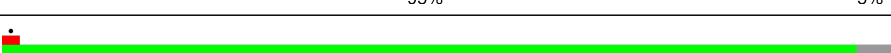
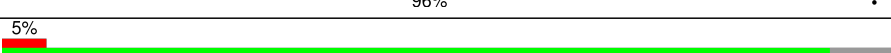
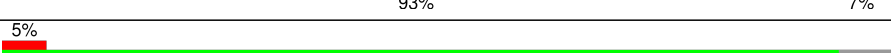
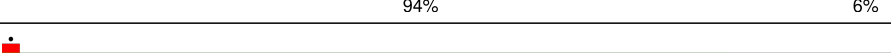
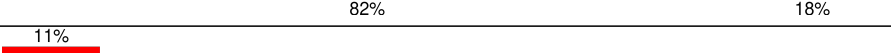
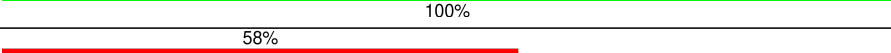
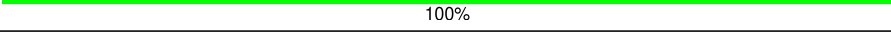
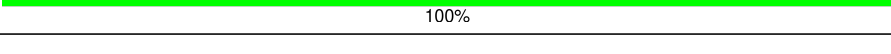
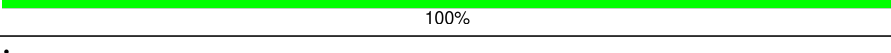
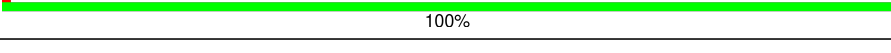

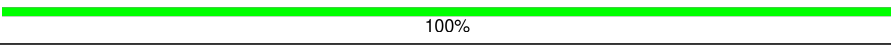
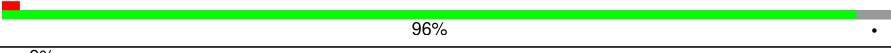
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	284	100%
2	1B	59	100%
3	2	360	99%
4	2B	178	100%
5	3	121	99%
6	3A	482	94%6%
6	3a	482	94%6%
7	3B	513	93%7%
7	3b	513	93%7%

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Mol	Chain	Length	Quality of chain
8	3C	426	
8	3c	426	
9	3D	319	
9	3d	319	
10	3E	269	
10	3e	269	
11	3F	90	
11	3f	90	
12	3G	328	
12	3g	328	
13	3H	130	
13	3h	130	
14	3I	119	
14	3i	119	
15	3J	62	
15	3j	62	
16	3M	19	
17	3l	24	
18	3m	17	
19	4	505	
20	4L	116	
21	5	750	
22	5B	100	
23	6	255	
24	A2	103	

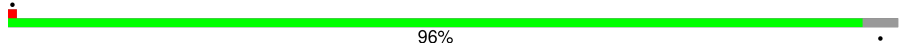
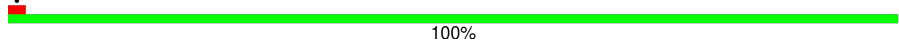
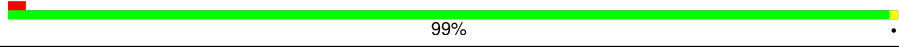
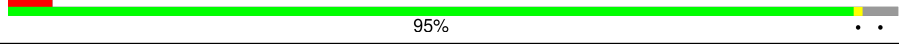

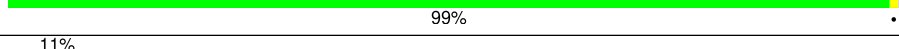
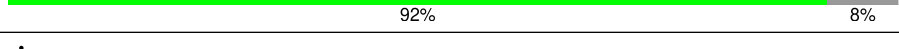
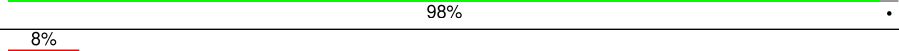
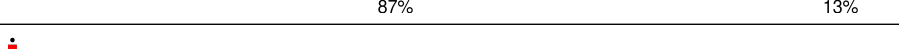
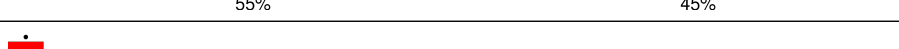
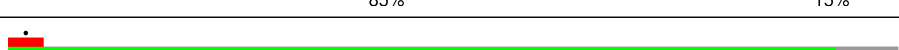
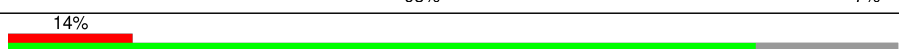
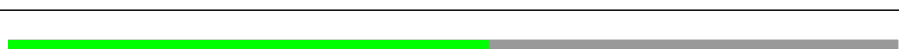

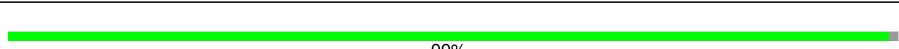



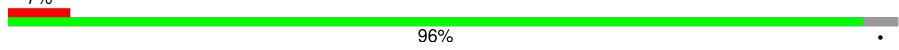
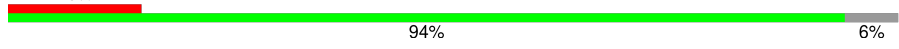
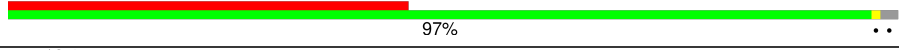
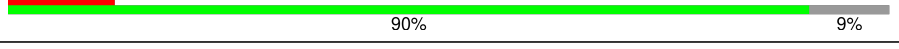

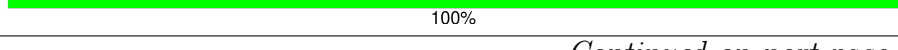

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Mol	Chain	Length	Quality of chain
25	A5	206	
26	A6	172	
27	A7	282	
28	A9	362	
29	AB	138	
30	AC	133	
31	AL	194	
32	AM	175	
33	B7	120	
34	B8	207	
35	BL	188	
36	C	209	
37	C1	257	
38	C2	233	
39	C3	346	
40	TD	73	
41	J1	317	
42	FX	172	
43	T2	333	
44	T1	516	
45	A1	94	
46	X1	150	
47	T6	144	
48	T5	205	
49	R	124	

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Mol	Chain	Length	Quality of chain
50	S1	718	
51	S2	442	
52	S3	198	
53	S4	185	
54	S6	132	
55	S7	162	
56	S8	236	
57	B9	189	
58	TX	166	
59	A8	238	
60	TB	113	
61	V1	474	
62	V2	274	
63	B6	129	
64	BM	214	
65	C4	102	
66	AN	231	
67	B4	108	
68	T4	212	
69	T8	135	
70	B2	126	
71	T3	311	
72	P1	251	
73	B3	83	
74	TA	102	

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Mol	Chain	Length	Quality of chain
75	S5	94	
76	TC	93	
77	P2	189	
78	A3	135	
79	T9	135	
80	TE	71	
81	T7	143	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 153366 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	284	Total	C	N	O	S	0	0
			2313	1586	335	379	13		

- Molecule 2 is a protein called NADH dehydrogenase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	59	Total	C	N	O	S	0	0
			516	362	78	73	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1B	49	VAL	LEU	conflict	UNP Q09FB0
1B	56	THR	SER	conflict	UNP Q09FB0

- Molecule 3 is a protein called Ymf65.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	359	Total	C	N	O	S	0	0
			3065	2129	435	494	7		

- Molecule 4 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2B	178	Total	C	N	O	S	0	0
			1483	1015	215	248	5		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	120	Total	C	N	O	S	0	0
			1017	705	142	166	4		

- Molecule 6 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3A	453	Total	C	N	O	S	0	0
			3511	2210	598	697	6		
6	3a	451	Total	C	N	O	S	0	0
			3495	2199	595	695	6		

- Molecule 7 is a protein called Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3B	479	Total	C	N	O	S	0	0
			3826	2426	667	728	5		
7	3b	478	Total	C	N	O	S	0	0
			3815	2420	663	727	5		

- Molecule 8 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3C	426	Total	C	N	O	S	0	0
			3590	2417	541	610	22		
8	3c	426	Total	C	N	O	S	0	0
			3589	2417	541	609	22		

- Molecule 9 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3D	295	Total	C	N	O	S	0	0
			2488	1627	418	430	13		
9	3d	285	Total	C	N	O	S	0	0
			2403	1569	405	416	13		

- Molecule 10 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3E	230	Total	C	N	O	S	0	0
			1846	1178	325	334	9		
10	3e	104	Total	C	N	O	S	0	0
			882	567	162	152	1		

- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3F	89	Total	C	N	O	S	0	0
			703	439	125	130	9		
11	3f	75	Total	C	N	O	S	0	0
			597	374	105	109	9		

- Molecule 12 is a protein called UQCRB.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3G	307	Total	C	N	O	S	0	0
			2595	1676	450	463	6		
12	3g	317	Total	C	N	O	S	0	0
			2682	1738	464	474	6		

- Molecule 13 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3H	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
13	3h	124	Total	C	N	O	S	0	0
			1046	669	190	179	8		

- Molecule 14 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3I	114	Total	C	N	O	S	0	0
			971	651	161	158	1		
14	3i	111	Total	C	N	O	S	0	0
			948	638	157	152	1		

- Molecule 15 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3J	58	Total	C	N	O	S	0	0
			501	341	79	79	2		
15	3j	51	Total	C	N	O	S	0	0
			443	306	65	70	2		

- Molecule 16 is a protein called UNK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3M	19	Total	C	N	O	S	0	0
			150	94	27	27	2		

- Molecule 17 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	3l	24	Total	C	N	O	0	0
			124	74	24	26		

- Molecule 18 is a protein called UNK3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	3m	17	Total	C	N	O	0	0
			121	78	25	18		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	505	Total	C	N	O	S	0	0
			4170	2859	601	692	18		

- Molecule 20 is a protein called Ymf58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4L	116	Total	C	N	O	S	0	0
			957	648	142	163	4		

- Molecule 21 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	587	Total	C	N	O	S	0	0
			4844	3313	696	819	16		

- Molecule 22 is a protein called Ymf57.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5B	100	Total	C	N	O	S	0	0
			888	620	128	137	3		

- Molecule 23 is a protein called Ymf62.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	244	Total	C	N	O	S	0	0
			2076	1419	295	358	4		

- Molecule 24 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A2	92	Total	C	N	O	S	0	0
			765	486	136	141	2		

- Molecule 25 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A5	155	Total	C	N	O	S	0	0
			1307	838	219	244	6		

- Molecule 26 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A6	172	Total	C	N	O	S	0	0
			1421	903	253	257	8		

- Molecule 27 is a protein called NDUA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A7	281	Total	C	N	O	S	0	0
			2339	1473	412	452	2		

- Molecule 28 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A9	338	Total	C	N	O	S	0	0
			2718	1737	475	494	12		

- Molecule 29 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	AB	112	Total	C	N	O	0	0
			926	586	158	182		

- Molecule 30 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AC	98	Total	C	N	O	S	0	0
			806	513	134	158	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AL	193	Total	C	N	O	S	0	0
			1612	1019	303	285	5		

- Molecule 32 is a protein called NDUA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AM	160	Total	C	N	O	S	0	0
			1349	858	256	227	8		

- Molecule 33 is a protein called NDUB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B7	115	Total	C	N	O	S	0	0
			937	593	162	176	6		

- Molecule 34 is a protein called NDUB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B8	169	Total	C	N	O	S	0	0
			1408	904	238	260	6		

- Molecule 35 is a protein called NDUB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BL	175	Total	C	N	O	S	0	0
			1461	925	264	268	4		

- Molecule 36 is a protein called UNK4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C	209	Total	C	N	O	S	0	0
			1045	627	209	209			

- Molecule 37 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C1	229	Total	C	N	O	S	0	0
			1769	1110	304	350	5		

- Molecule 38 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C2	223	Total	C	N	O	S	0	0
			1624	1020	294	303	7		

- Molecule 39 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C3	346	Total	C	N	O	S	0	0
			2804	1766	481	549	8		

- Molecule 40 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	TD	71	Total	C	N	O	S	0	0
			608	399	108	101			

- Molecule 41 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	J1	262	Total	C	N	O	S	0	0
			2146	1361	396	386	3		

- Molecule 42 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	FX	146	Total	C	N	O	S	0	0
			1162	722	207	223	10		

- Molecule 43 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T2	271	Total	C	N	O	S	0	0
			2117	1347	362	407	1		

- Molecule 44 is a protein called Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T1	481	Total	C	N	O	S	0	0
			3884	2492	662	717	13		

- Molecule 45 is a protein called NDUA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	A1	92	Total	C	N	O	0	0
			799	526	138	135		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	X1	149	Total	C	N	O	0	0
			1227	800	213	214		

- Molecule 47 is a protein called NDUTT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	T6	109	Total	C	N	O	S	0	0
			903	562	161	174	6		

- Molecule 48 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T5	134	Total	C	N	O	S	0	0
			1088	699	193	194	2		

- Molecule 49 is a protein called UNK5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R	124	Total	C	N	O	S	0	0
			943	613	160	167	3		

- Molecule 50 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S1	687	Total	C	N	O	S	0	0
			5394	3404	933	1029	28		

- Molecule 51 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S2	442	Total	C	N	O	S	0	0
			3599	2291	624	660	24		

- Molecule 52 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S3	198	Total	C	N	O	S	0	0
			1681	1096	267	312	6		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S4	177	Total	C	N	O	S	0	0
			1463	928	257	269	9		

- Molecule 54 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S6	90	Total	C	N	O	S	0	0
			722	456	128	134	4		

- Molecule 55 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S7	162	Total	C	N	O	S	0	0
			1286	827	221	227	11		

- Molecule 56 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	S8	218	Total	C	N	O	S	0	0
			1812	1155	299	347	11		

- Molecule 57 is a protein called NDUB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B9	186	Total	C	N	O	S	0	0
			1579	1021	252	302	4		

- Molecule 58 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	TX	144	Total	C	N	O	S	0	0
			1206	767	205	227	7		

- Molecule 59 is a protein called NDUA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	A8	132	Total	C	N	O	S	0	0
			1075	676	180	208	11		

- Molecule 60 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	TB	96	Total	C	N	O		0	0
			801	515	139	147			

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	V1	442	Total	C	N	O	S	0	0
			3410	2146	600	640	24		

- Molecule 62 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	V2	231	Total	C	N	O	S	0	0
			1858	1173	318	357	10		

- Molecule 63 is a protein called NDUB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	B6	70	Total	C	N	O	S	0	0
			596	400	98	94	4		

- Molecule 64 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BM	145	Total	C	N	O	S	0	0
			1163	737	195	226	5		

- Molecule 65 is a protein called NDUC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	C4	101	Total	C	N	O	S	0	0
			842	548	138	149	7		

- Molecule 66 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AN	231	Total	C	N	O	S	0	0
			1879	1219	317	336	7		

- Molecule 67 is a protein called NDUB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	B4	108	Total	C	N	O	S	0	0
			898	601	138	157	2		

- Molecule 68 is a protein called NDUTT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	T4	170	Total	C	N	O	S	0	0
			1408	918	242	245	3		

- Molecule 69 is a protein called NDUTT8.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	T8	129	Total	C	N	O	S	0	0
			1064	691	189	184			

- Molecule 70 is a protein called NDUB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	B2	118	Total	C	N	O	S	0	0
			955	615	165	172	3		

- Molecule 71 is a protein called NDUTT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	T3	305	Total	C	N	O	S	0	0
			2442	1555	426	455	6		

- Molecule 72 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	P1	228	Total	C	N	O	S	0	0
			1896	1235	320	336	5		

- Molecule 73 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	B3	68	Total	C	N	O	S	0	0
			594	392	104	97	1		

- Molecule 74 is a protein called NDUTT10.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	TA	102	Total	C	N	O	S	0	0
			854	553	141	155	5		

- Molecule 75 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	S5	85	Total	C	N	O	S	0	0
			693	440	118	129	6		

- Molecule 76 is a protein called NDUTT12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	TC	91	Total	C	N	O	S	0	0
			781	491	145	144	1		

- Molecule 77 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	P2	167	Total	C	N	O	S	0	0
			1414	926	225	258	5		

- Molecule 78 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	A3	127	Total	C	N	O	S	0	0
			1065	691	193	178	3		

- Molecule 79 is a protein called NDUTT9.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	T9	132	Total	C	N	O	S	0	0
			1066	670	185	201	10		

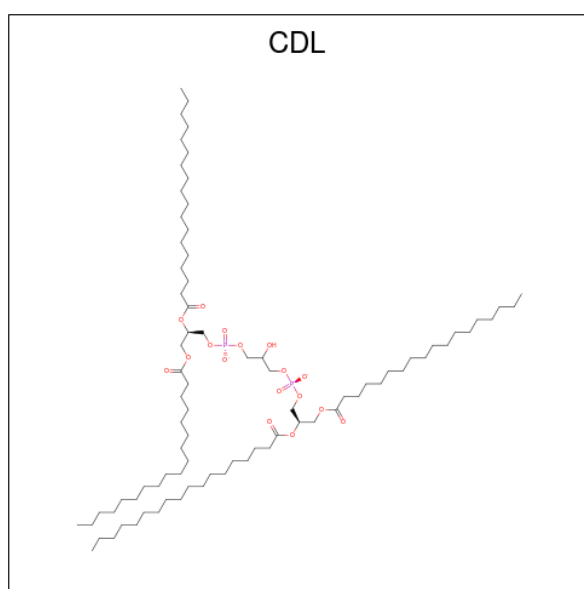
- Molecule 80 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	TE	49	Total	C	N	O	S	0	0
			413	277	63	71	2		

- Molecule 81 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	T7	142	Total	C	N	O	S	0	0
			1187	770	202	209	6		

- Molecule 82 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
82	1	1	Total	C	O	P	0
			50	31	17	2	
82	2B	1	Total	C	O	P	0
			53	34	17	2	
82	3	1	Total	C	O	P	0
			44	25	17	2	
82	3B	1	Total	C	O	P	0
			78	59	17	2	
82	3C	1	Total	C	O	P	0
			65	46	17	2	
82	3G	1	Total	C	O	P	0
			66	47	17	2	
82	3H	1	Total	C	O	P	0
			62	43	17	2	

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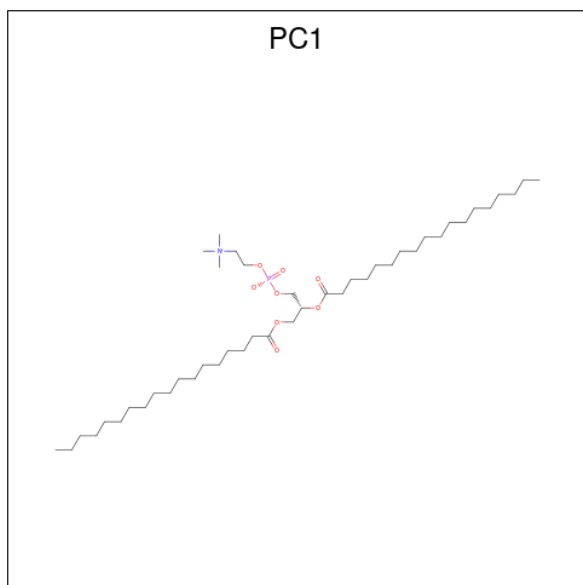
Mol	Chain	Residues	Atoms				AltConf
82	3H	1	Total	C	O	P	0
			66	47	17	2	
82	3I	1	Total	C	O	P	0
			71	52	17	2	
82	3I	1	Total	C	O	P	0
			37	18	17	2	
82	3b	1	Total	C	O	P	0
			68	49	17	2	
82	3c	1	Total	C	O	P	0
			64	45	17	2	
82	3c	1	Total	C	O	P	0
			56	37	17	2	
82	3i	1	Total	C	O	P	0
			71	52	17	2	
82	5	1	Total	C	O	P	0
			90	71	17	2	
82	5	1	Total	C	O	P	0
			96	77	17	2	
82	AL	1	Total	C	O	P	0
			53	34	17	2	
82	AM	1	Total	C	O	P	0
			62	43	17	2	
82	B8	1	Total	C	O	P	0
			45	26	17	2	
82	TD	1	Total	C	O	P	0
			66	47	17	2	
82	T1	1	Total	C	O	P	0
			55	36	17	2	
82	A1	1	Total	C	O	P	0
			53	34	17	2	
82	R	1	Total	C	O	P	0
			84	65	17	2	
82	BM	1	Total	C	O	P	0
			86	67	17	2	
82	C4	1	Total	C	O	P	0
			98	79	17	2	
82	AN	1	Total	C	O	P	0
			53	34	17	2	
82	B4	1	Total	C	O	P	0
			40	21	17	2	
82	P2	1	Total	C	O	P	0
			82	63	17	2	

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Mol	Chain	Residues	Atoms				AltConf
82	T7	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 83 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
83	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
83	3	1	Total	C	N	O	P	0
			31	21	1	8	1	
83	3C	1	Total	C	N	O	P	0
			46	36	1	8	1	
83	3C	1	Total	C	N	O	P	0
			44	34	1	8	1	
83	3C	1	Total	C	N	O	P	0
			29	19	1	8	1	
83	3E	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	3E	1	Total	C	N	O	P	0
			24	14	1	8	1	
83	3F	1	Total	C	N	O	P	0
			22	12	1	8	1	
83	3I	1	Total	C	N	O	P	0
			32	22	1	8	1	
83	3I	1	Total	C	N	O	P	0
			46	36	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
83	3J	1	Total	C	N	O	P	0
			37	27	1	8	1	
83	3b	1	Total	C	N	O	P	0
			30	20	1	8	1	
83	3c	1	Total	C	N	O	P	0
			31	21	1	8	1	
83	3c	1	Total	C	N	O	P	0
			38	28	1	8	1	
83	3e	1	Total	C	N	O	P	0
			50	40	1	8	1	
83	3g	1	Total	C	N	O	P	0
			33	23	1	8	1	
83	3j	1	Total	C	N	O	P	0
			36	26	1	8	1	
83	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	5	1	Total	C	N	O	P	0
			39	29	1	8	1	
83	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	6	1	Total	C	N	O	P	0
			39	29	1	8	1	
83	6	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	AM	1	Total	C	N	O	P	0
			30	20	1	8	1	
83	J1	1	Total	C	N	O	P	0
			40	30	1	8	1	
83	T1	1	Total	C	N	O	P	0
			26	16	1	8	1	
83	X1	1	Total	C	N	O	P	0
			49	39	1	8	1	
83	B6	1	Total	C	N	O	P	0
			52	42	1	8	1	
83	C4	1	Total	C	N	O	P	0
			32	22	1	8	1	
83	AN	1	Total	C	N	O	P	0
			36	26	1	8	1	
83	B2	1	Total	C	N	O	P	0
			48	38	1	8	1	
83	P1	1	Total	C	N	O	P	0
			40	30	1	8	1	

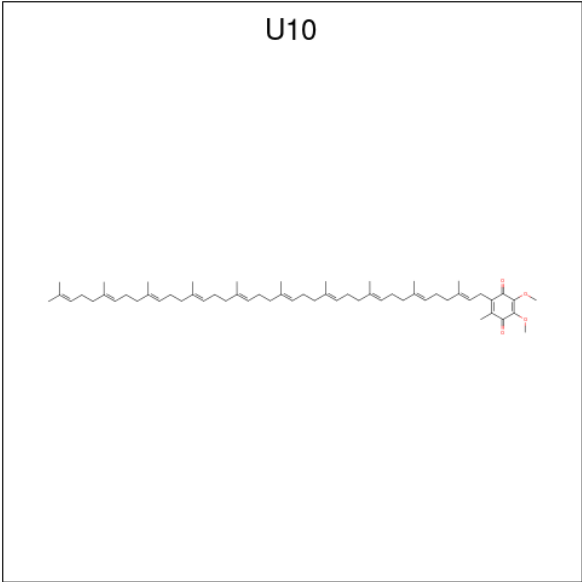
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Mol	Chain	Residues	Atoms				AltConf	
83	TC	1	Total	C	N	O	P	0
			42	32	1	8	1	

- # HEM

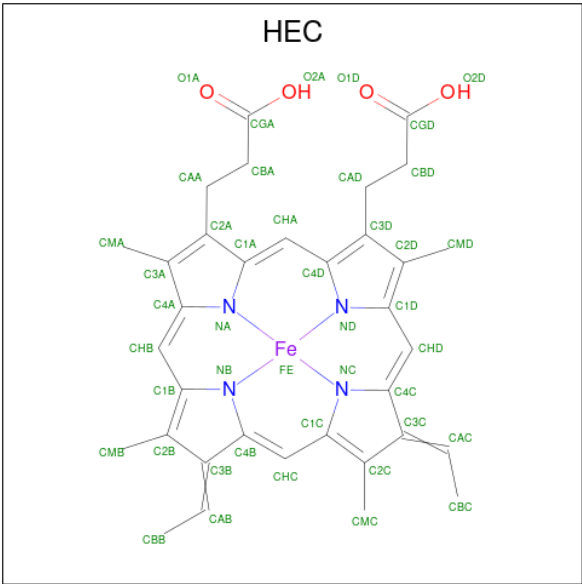
Mol	Chain	Residues	Atoms					AltConf
84	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	3c	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	3c	1	Total 43	C 34	Fe 1	N 4	O 4	0

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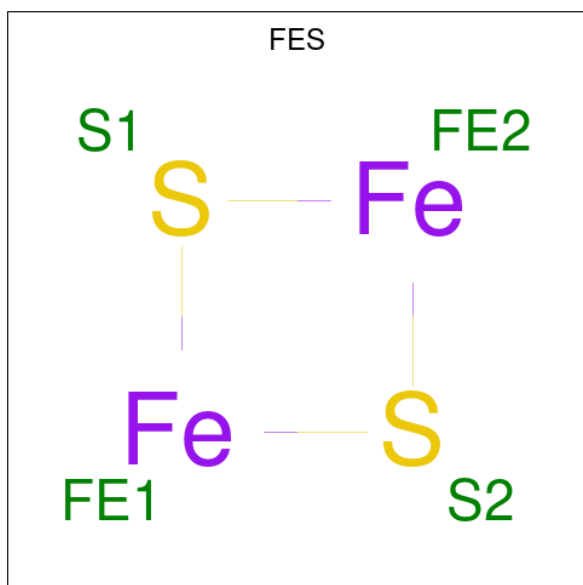
Mol	Chain	Residues	Atoms		AltConf
85	3C	1	Total	C	0
			26	26	
85	3H	1	Total	C	O
			29	25	4
85	5B	1	Total	C	O
			63	59	4

- Molecule 86 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



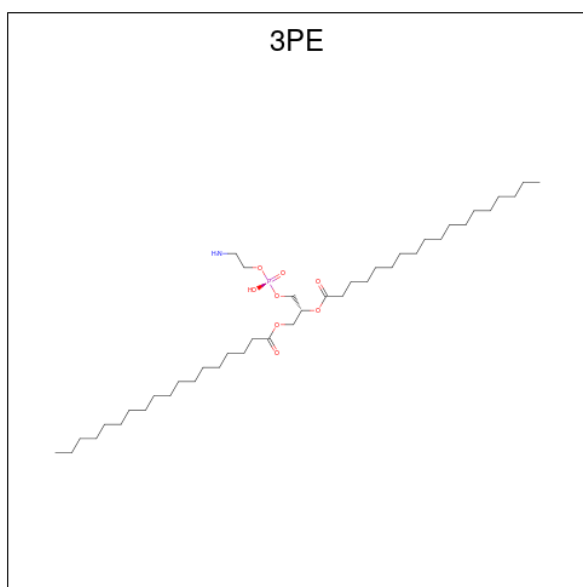
Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total 43	C 34	Fe 1	N 4	O 4	0
86	3d	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 87 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
87	3E	1	Total	Fe	S	0
			4	2	2	
87	FX	1	Total	Fe	S	0
			4	2	2	
87	S1	1	Total	Fe	S	0
			4	2	2	
87	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 88 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
88	3E	1	Total	C	N	O	P	0
			34	24	1	8	1	
88	3d	1	Total	C	N	O	P	0
			47	37	1	8	1	
88	4	1	Total	C	N	O	P	0
			47	37	1	8	1	
88	4	1	Total	C	N	O	P	0
			36	26	1	8	1	
88	5	1	Total	C	N	O	P	0
			37	27	1	8	1	
88	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
88	5B	1	Total	C	N	O	P	0
			24	14	1	8	1	
88	B8	1	Total	C	N	O	P	0
			36	26	1	8	1	
88	S8	1	Total	C	N	O	P	0
			41	31	1	8	1	
88	C4	1	Total	C	N	O	P	0
			51	41	1	8	1	
88	AN	1	Total	C	N	O	P	0
			45	35	1	8	1	
88	AN	1	Total	C	N	O	P	0
			35	25	1	8	1	
88	T4	1	Total	C	N	O	P	0
			25	15	1	8	1	
88	T8	1	Total	C	N	O	P	0
			39	29	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
88	P1	1	Total 47	C 37	N 1	O 8	P 1	0
88	TA	1	Total 26	C 16	N 1	O 8	P 1	0
88	A3	1	Total 45	C 35	N 1	O 8	P 1	0

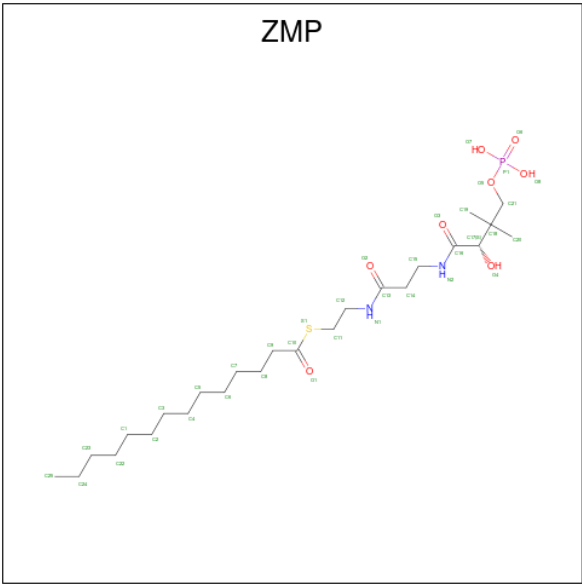
- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 89 | 3F | 1 | Total Zn
1 1 | 0 |
| 89 | A9 | 1 | Total Zn
1 1 | 0 |
| 89 | S6 | 1 | Total Zn
1 1 | 0 |

- # NDP

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

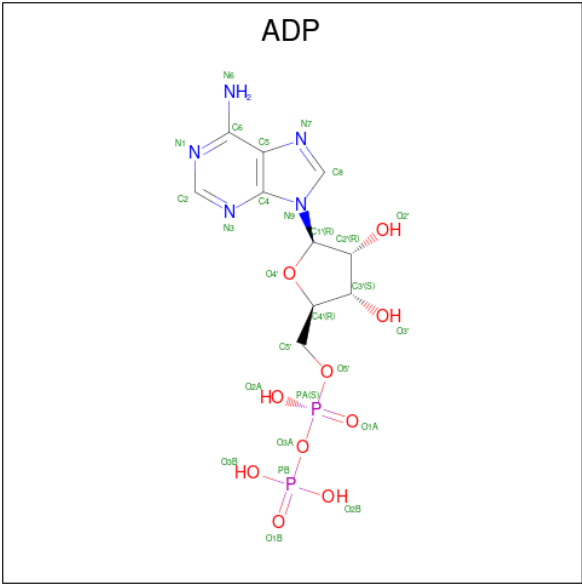
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lanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



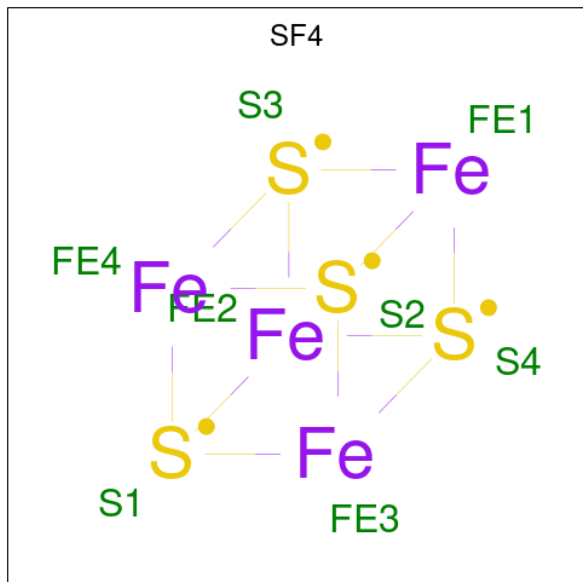
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	AB	1	34	23	2	7	1	0

- Molecule 92 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



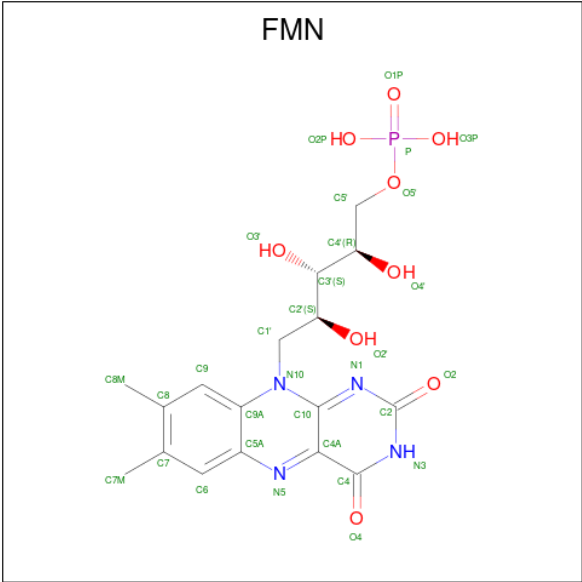
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	B8	1	27	10	5	10	2	0

- Molecule 93 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 94 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).

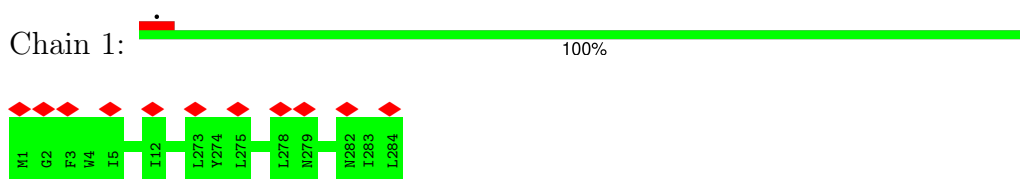


Mol	Chain	Residues	Atoms					AltConf
94	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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 1

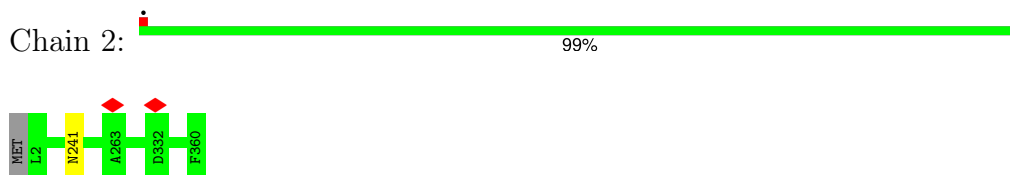


- Molecule 2: NADH dehydrogenase subunit 1



There are no outlier residues recorded for this chain.

- Molecule 3: Ymf65

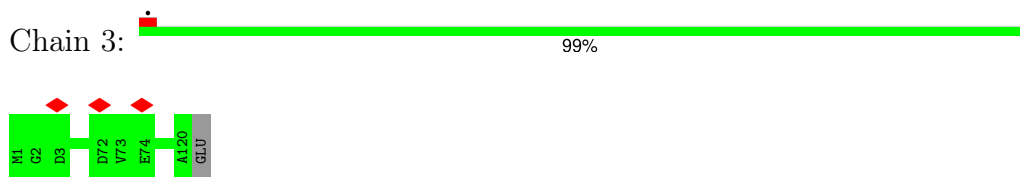


- Molecule 4: NADH dehydrogenase subunit 2



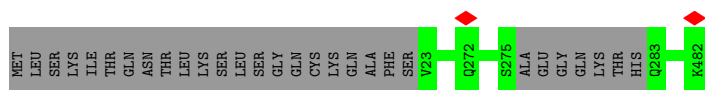
There are no outlier residues recorded for this chain.

- Molecule 5: NADH-ubiquinone oxidoreductase chain 3



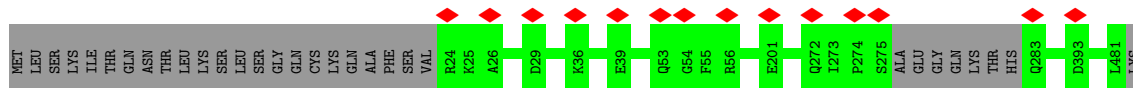
- Molecule 6: M16 family peptidase, putative





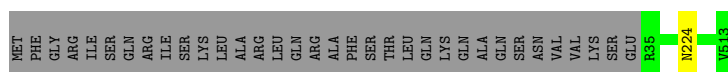
- Molecule 6: M16 family peptidase, putative

Chain 3a: 94% 6%



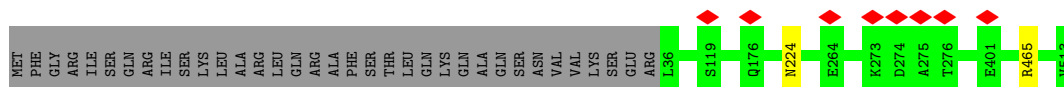
- Molecule 7: Peptidase M16 inactive domain protein

Chain 3B: 93% 7%



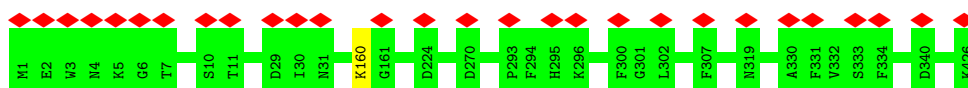
- Molecule 7: Peptidase M16 inactive domain protein

Chain 3b: 93% 7%



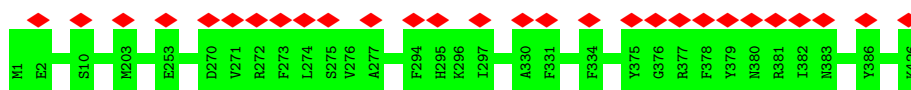
- Molecule 8: Apocytochrome b

Chain 3C: 7% 100%



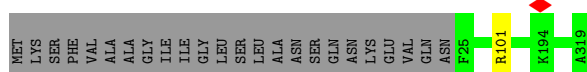
- Molecule 8: Apocytochrome b

Chain 3c: 7% 100%

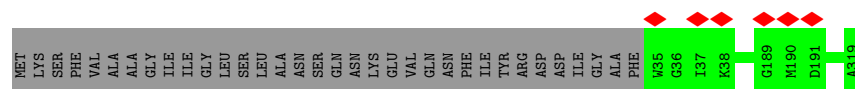
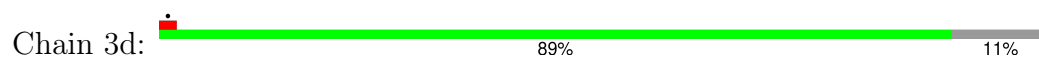


- Molecule 9: Cytochrome protein c1

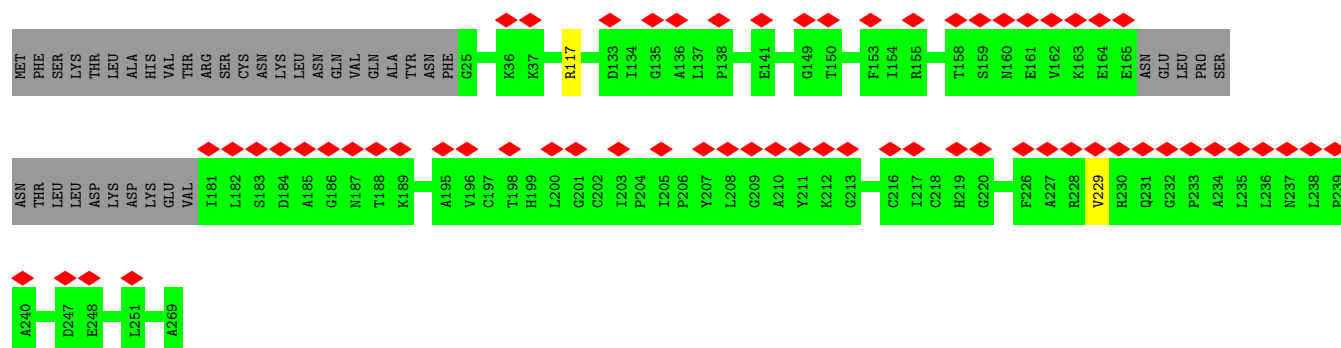
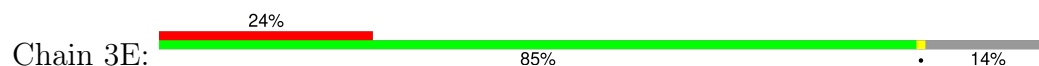
Chain 3D: 92% 8%



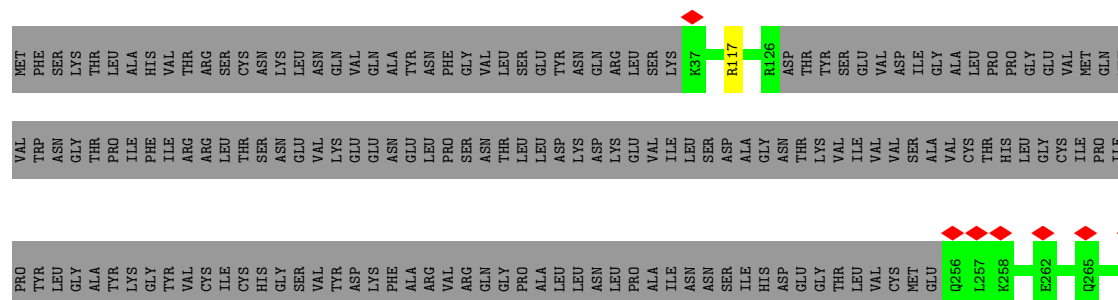
- Molecule 9: Cytochrome protein c1



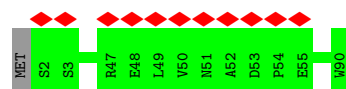
- Molecule 10: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



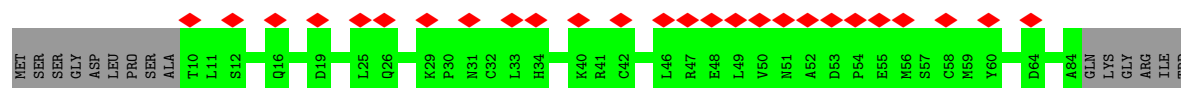
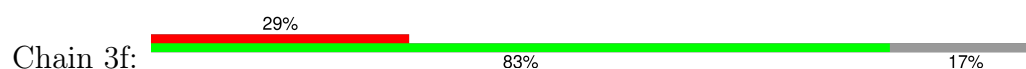
- Molecule 10: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



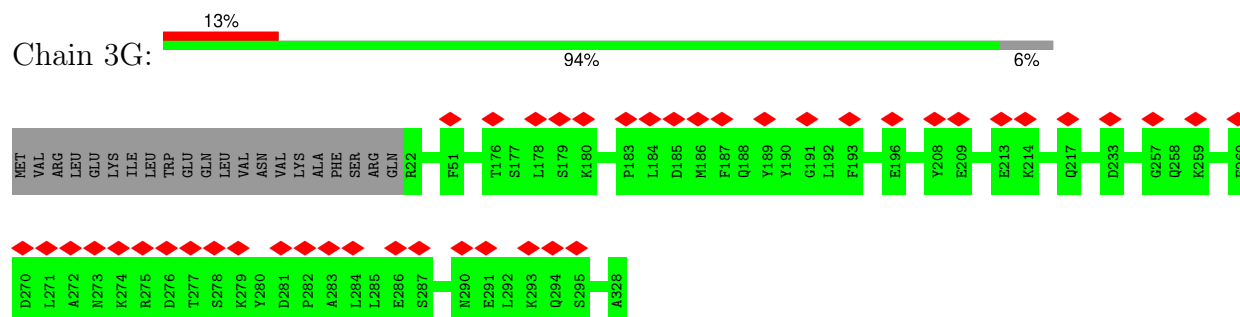
- Molecule 11: Ubiquinol-cytochrome C reductase hinge protein



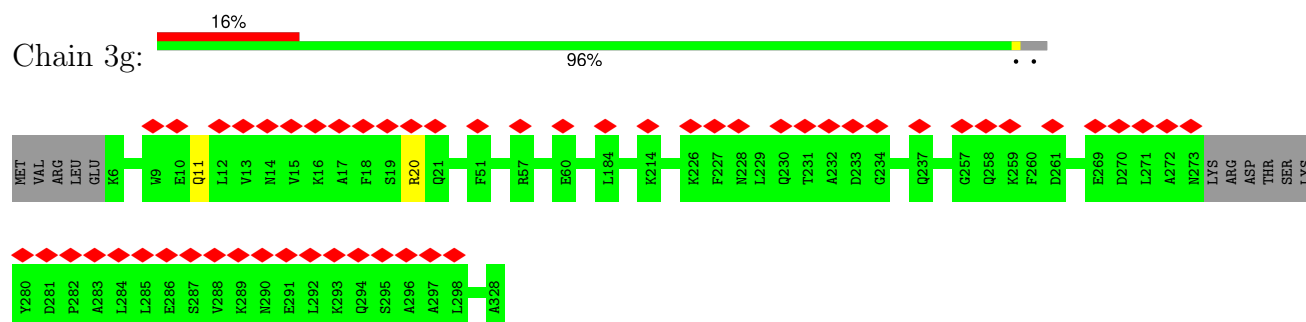
- Molecule 11: Ubiquinol-cytochrome C reductase hinge protein.



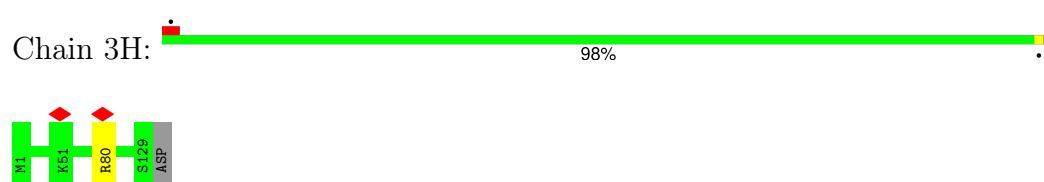
- Molecule 12: UQCRB



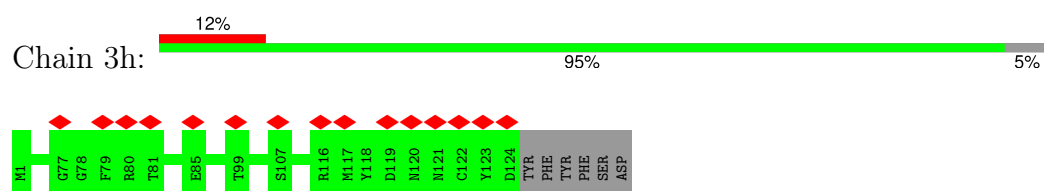
- Molecule 12: UQCRB



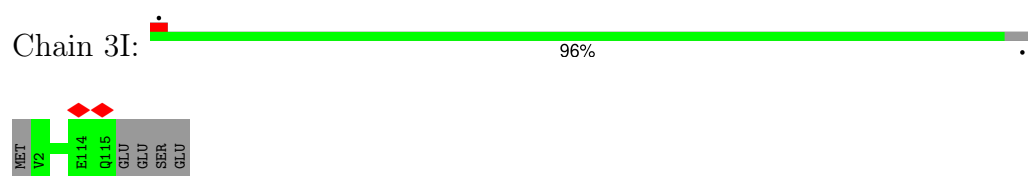
- Molecule 13: Transmembrane protein, putative



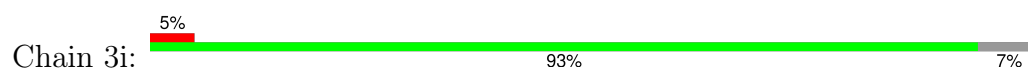
- Molecule 13: Transmembrane protein, putative

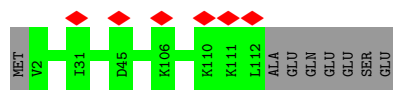


- Molecule 14: Transmembrane protein, putative

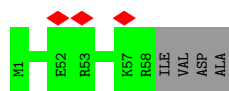


- Molecule 14: Transmembrane protein, putative

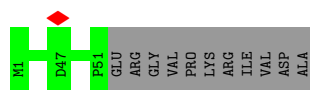
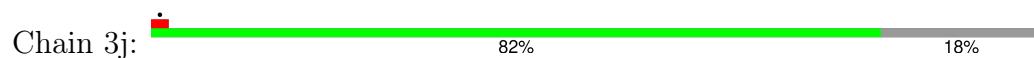




- Molecule 15: Transmembrane protein, putative



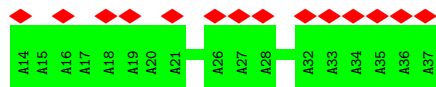
- Molecule 15: Transmembrane protein, putative



- Molecule 16: UNK1



- Molecule 17: UNK2

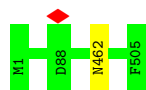


- Molecule 18: UNK3



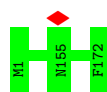
There are no outlier residues recorded for this chain.

- Molecule 19: NADH-ubiquinone oxidoreductase chain 4

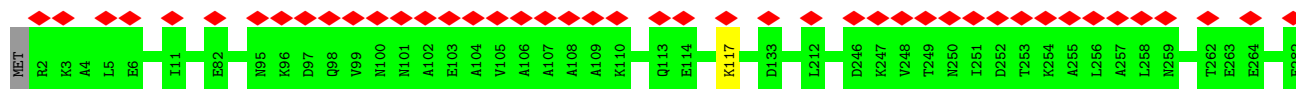


- Molecule 20: Ymf58

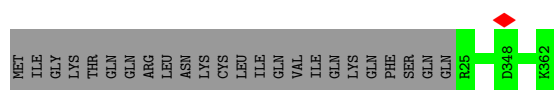




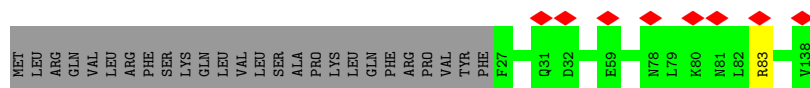
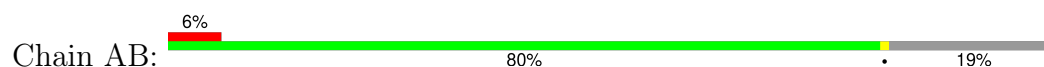
- Molecule 27: NDUA7



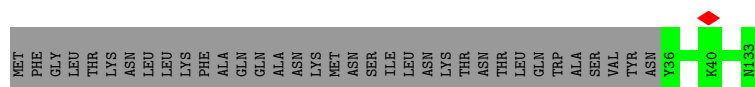
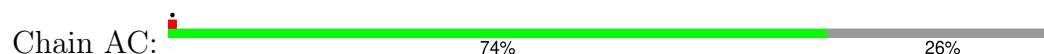
- Molecule 28: NAD-dependent epimerase/dehydratase family protein



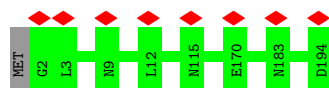
- Molecule 29: Acyl carrier protein



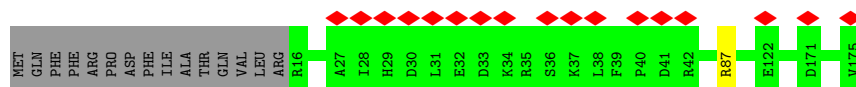
- Molecule 30: Acyl carrier protein



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

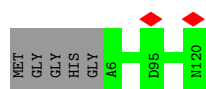


- Molecule 32: NDUA13




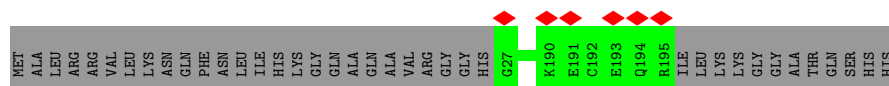
- Molecule 33: NDUB7

Chain B7:  96%



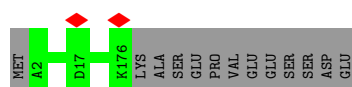
- Molecule 34: NDUB8

Chain B8:  82% 18%



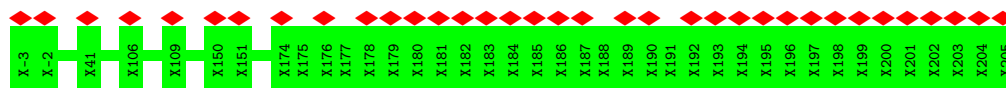
- Molecule 35: NDUB10

Chain BL:  93% 7%




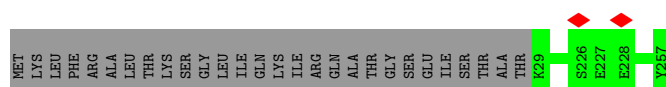
- Molecule 36: UNK4

Chain C:  17% 100%



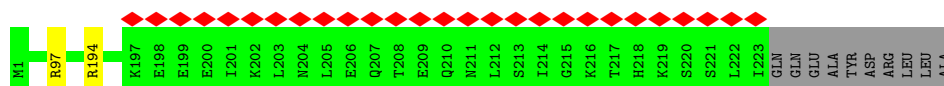
- Molecule 37: Gamma-carbonic anhydrase

Chain C1:  89% 11%



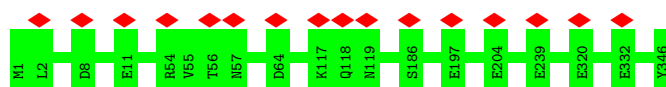
- Molecule 38: Gamma-carbonic anhydrase

Chain C2:  12% 95%

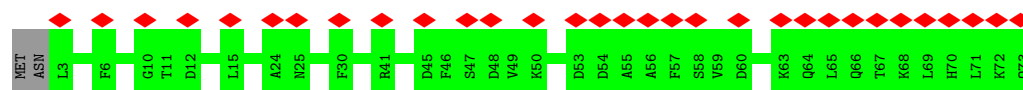
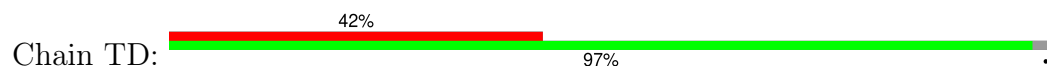


- Molecule 39: Transcription factor apfi protein, putative

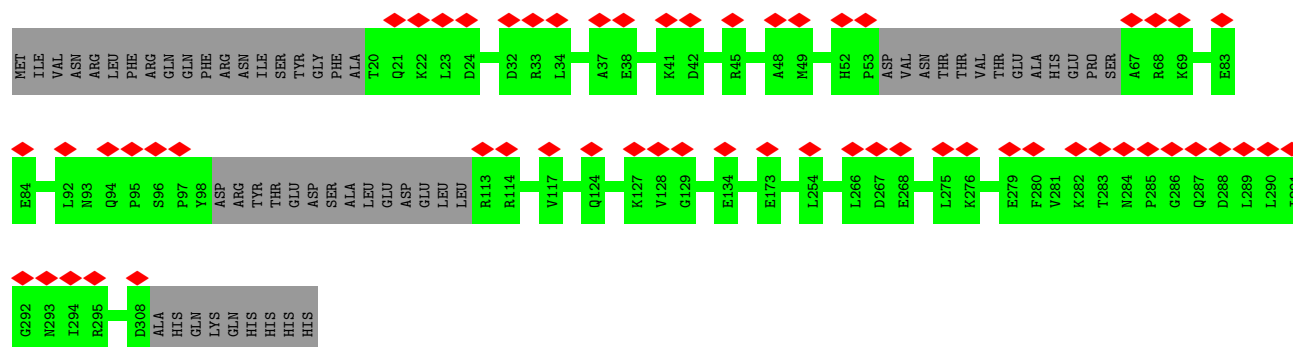
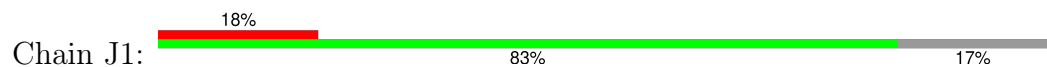
Chain C3:  5% 100%



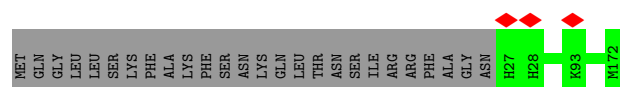
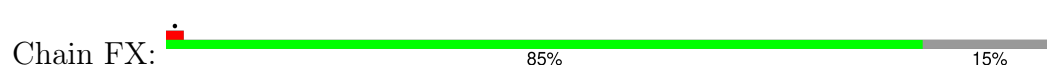
- Molecule 40: Transmembrane protein, putative



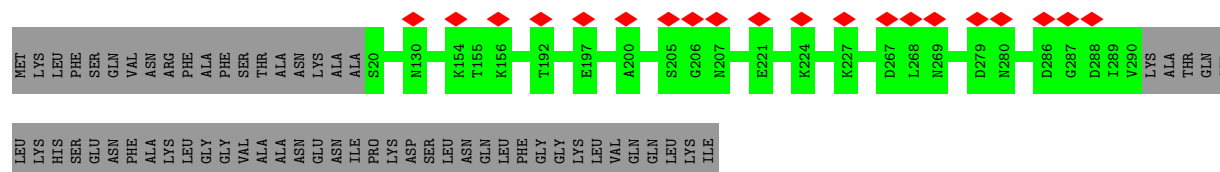
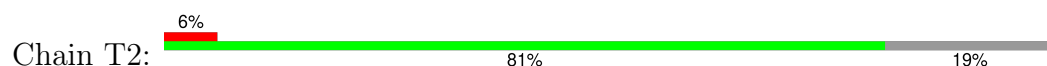
- Molecule 41: DnaJ domain protein



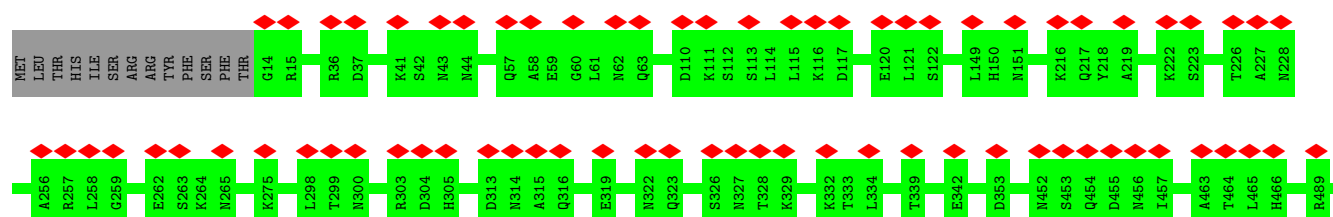
- Molecule 42: 2 iron, 2 sulfur cluster-binding protein

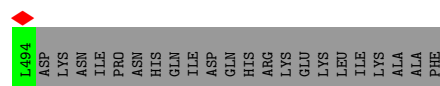


- Molecule 43: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

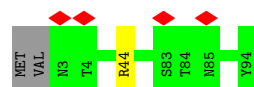


- Molecule 44: Lipid-A-disaccharide synthase

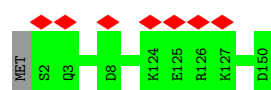




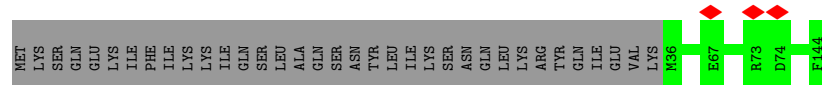
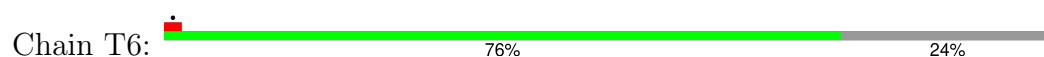
• Molecule 45: NDUA1



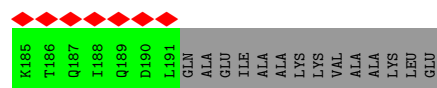
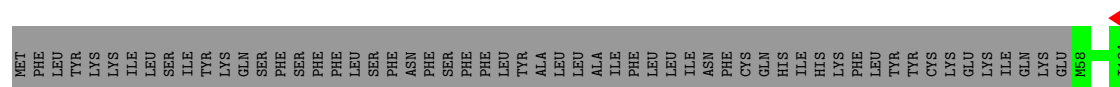
• Molecule 46: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit



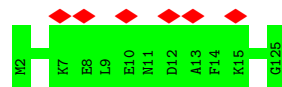
• Molecule 47: NDUTT6



• Molecule 48: Transmembrane protein, putative

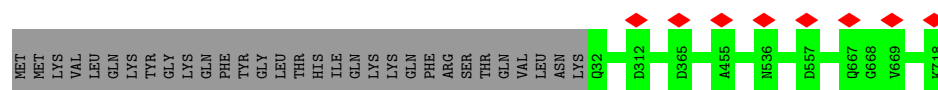


• Molecule 49: UNK5

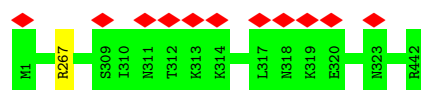


• Molecule 50: NADH-ubiquinone oxidoreductase 75 kDa subunit

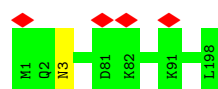




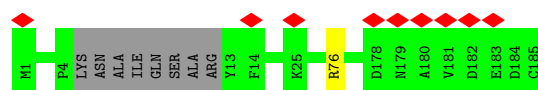
- Molecule 51: NADH dehydrogenase subunit 7



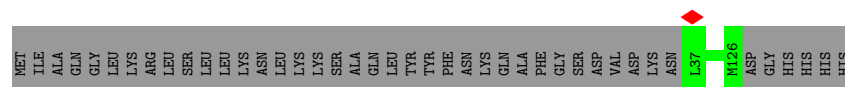
- Molecule 52: NADH dehydrogenase subunit 9



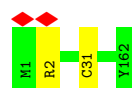
- Molecule 53: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



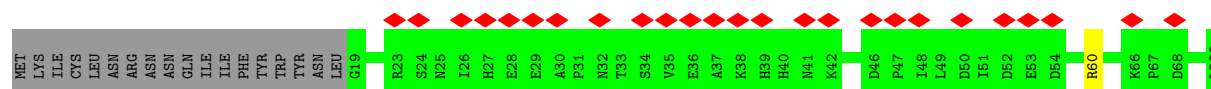
- Molecule 54: Zinc-finger protein



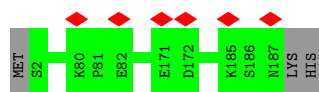
- Molecule 55: NADH dehydrogenase subunit 10



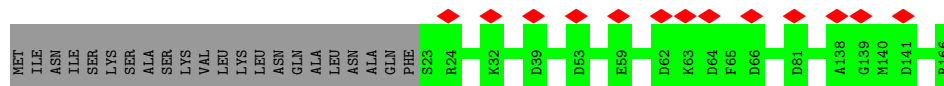
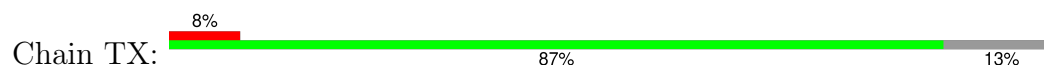
- Molecule 56: NADH-ubiquinone oxidoreductase 1, chain, putative



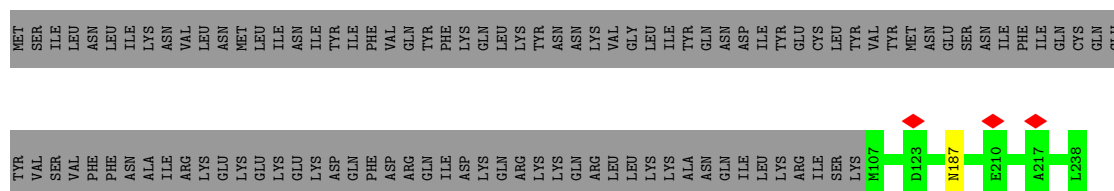
- Molecule 57: NDUB9



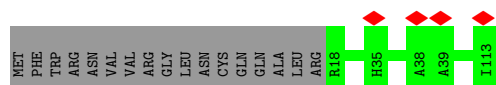
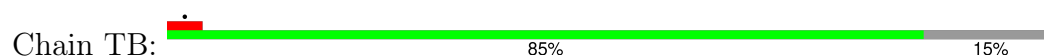
- Molecule 58: Thioredoxin



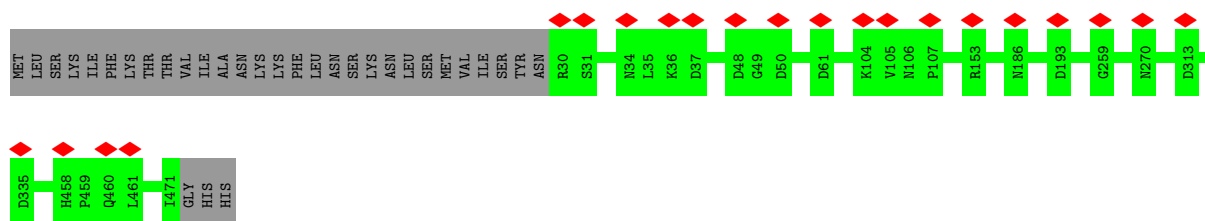
- Molecule 59: NDUA8



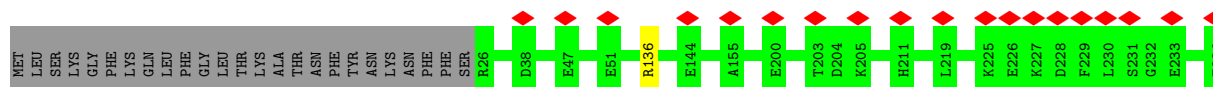
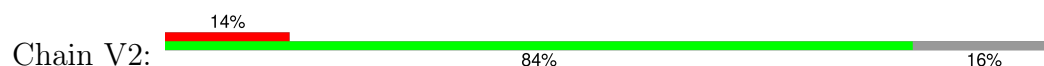
- Molecule 60: Transmembrane protein, putative

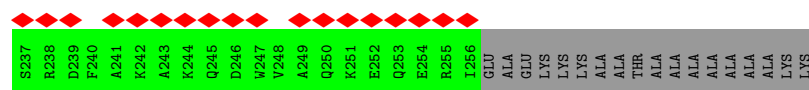


- Molecule 61: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



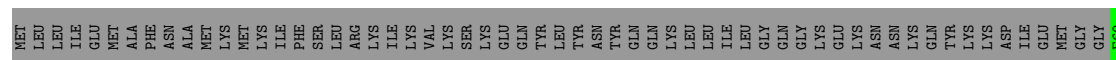
- Molecule 62: NADH-ubiquinone oxidoreductase 24 kDa subunit





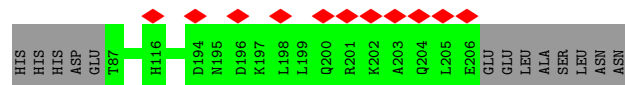
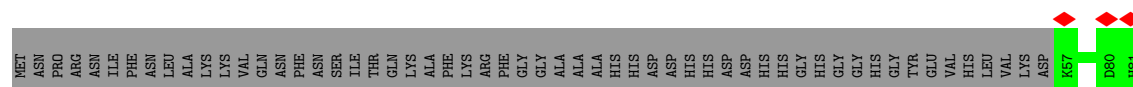
- Molecule 63: NDUB6

Chain B6: 54% 46%



- Molecule 64: Transmembrane protein, putative

Chain BM: 7% 68% 32%



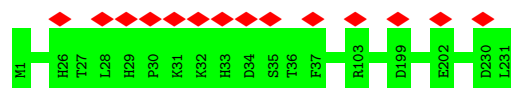
- Molecule 65: NDUC2

Chain C4: 99% .



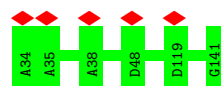
- Molecule 66: Transmembrane protein, putative

Chain AN: 6% 100%



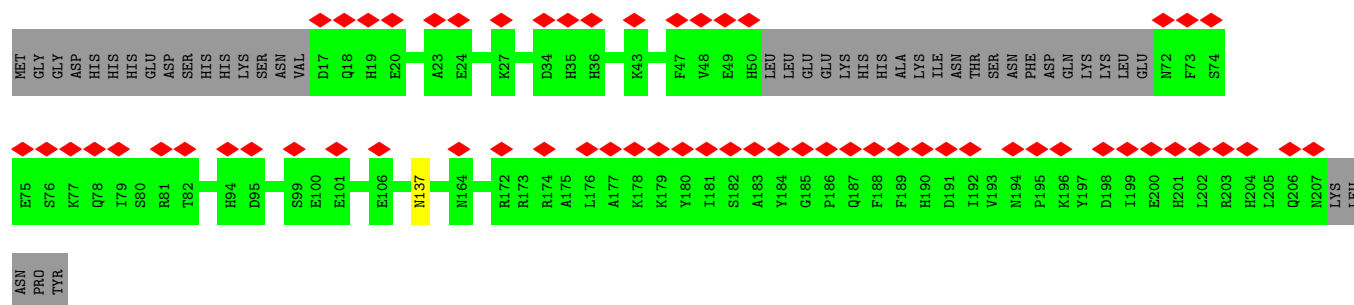
- Molecule 67: NDUB4

Chain B4: 5% 100%

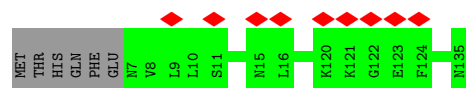


- Molecule 68: NDUTT4

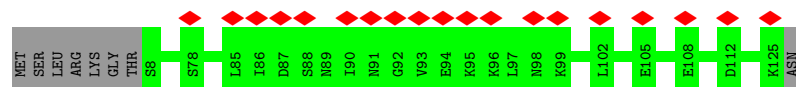
Chain T4: 29% 80% 20%



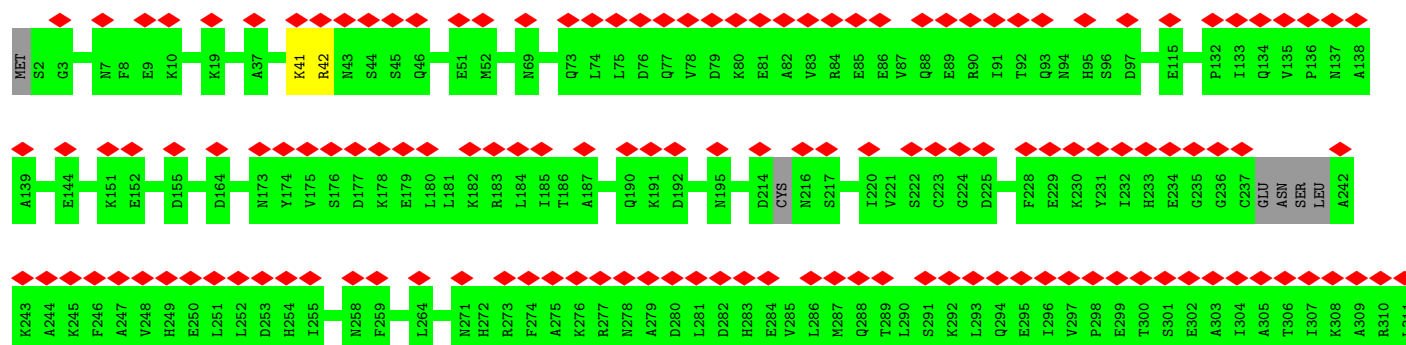
• Molecule 69: NDUTT8



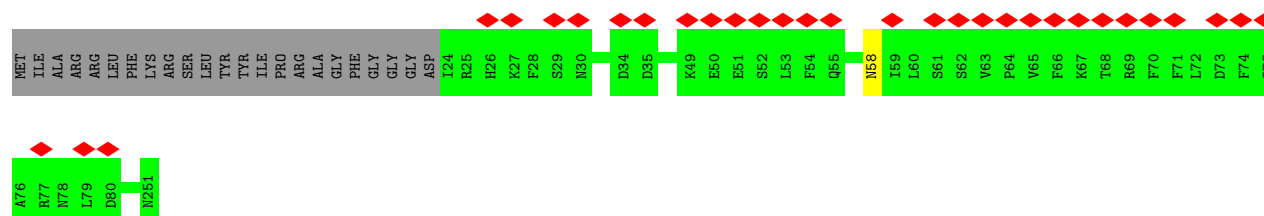
• Molecule 70: NDUB2



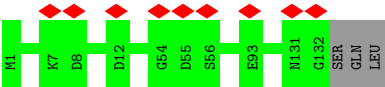
• Molecule 71: NDUTT3



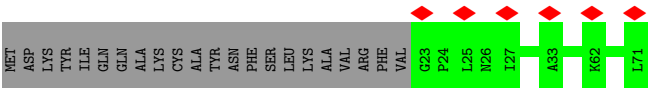
• Molecule 72: Transmembrane protein, putative



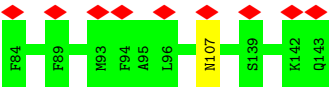
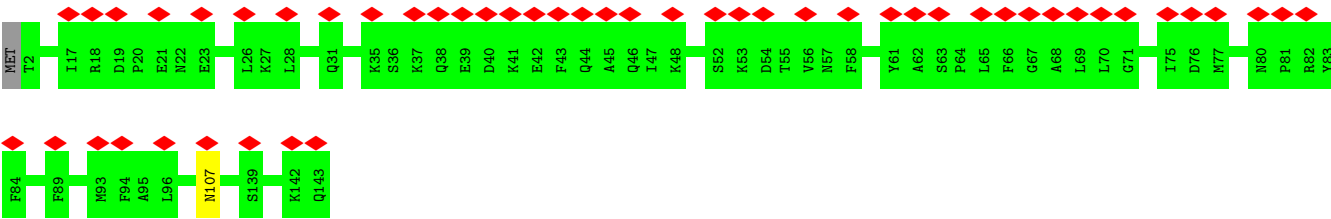
- Chain T9: 



• Molecule 80: Transmembrane protein, putative



• Molecule 81: Transmembrane protein, putative



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203834	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 ($e^-/\text{\AA}^2$)	66.69	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	58616	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	32.050	Depositor
Minimum map value	-15.499	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.092	Depositor
Recommended contour level	6	Depositor
Map size (Å)	501.0, 501.0, 501.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FMN, ZN, CDL, 3PE, FES, ZMP, PC1, ADP, SF4, HEC, U10, HEM

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	1	0.27	0/2384	0.43	0/3244
2	1B	0.27	0/536	0.41	0/727
3	2	0.29	0/3165	0.41	0/4302
4	2B	0.27	0/1520	0.41	0/2058
5	3	0.27	0/1051	0.38	0/1429
6	3A	0.26	0/3563	0.46	0/4827
6	3a	0.25	0/3547	0.46	0/4806
7	3B	0.26	0/3912	0.48	0/5313
7	3b	0.27	0/3901	0.49	0/5299
8	3C	0.27	0/3716	0.43	0/5046
8	3c	0.27	0/3715	0.44	0/5046
9	3D	0.28	0/2579	0.48	0/3491
9	3d	0.27	0/2491	0.48	0/3371
10	3E	0.25	0/1893	0.49	0/2566
10	3e	0.26	0/909	0.48	0/1226
11	3F	0.24	0/717	0.45	0/969
11	3f	0.26	0/608	0.49	0/823
12	3G	0.26	0/2670	0.48	0/3602
12	3g	0.26	0/2759	0.49	0/3724
13	3H	0.26	0/1133	0.50	0/1524
13	3h	0.25	0/1077	0.50	0/1448
14	3I	0.26	0/1005	0.43	0/1365
14	3i	0.26	0/982	0.42	0/1334
15	3J	0.27	0/522	0.47	0/712
15	3j	0.29	0/463	0.49	0/634
16	3M	0.26	0/151	0.55	0/198
17	3l	0.26	0/123	0.32	0/170
18	3m	0.26	0/122	0.56	0/162
19	4	0.28	0/4303	0.42	0/5844
20	4L	0.26	0/982	0.41	0/1335
21	5	0.28	0/4997	0.42	0/6794
22	5B	0.28	0/915	0.41	0/1224

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	6	0.27	0/2137	0.40	0/2906
24	A2	0.26	0/780	0.47	0/1054
25	A5	0.25	0/1336	0.47	0/1797
26	A6	0.26	0/1459	0.47	0/1965
27	A7	0.25	0/2400	0.45	0/3259
28	A9	0.26	0/2789	0.45	0/3777
29	AB	0.24	0/942	0.44	0/1272
30	AC	0.26	0/822	0.47	0/1114
31	AL	0.25	0/1667	0.49	0/2256
32	AM	0.25	0/1379	0.49	0/1841
33	B7	0.27	0/964	0.42	0/1302
34	B8	0.26	0/1445	0.45	0/1952
35	BL	0.25	0/1489	0.48	0/2000
37	C1	0.27	0/1806	0.46	0/2461
38	C2	0.26	0/1653	0.50	0/2257
39	C3	0.25	0/2865	0.46	0/3877
40	TD	0.25	0/626	0.48	0/844
41	J1	0.25	0/2194	0.47	0/2954
42	FX	0.24	0/1186	0.49	0/1607
43	T2	0.25	0/2160	0.46	0/2937
44	T1	0.26	0/3975	0.45	0/5380
45	A1	0.26	0/827	0.50	0/1122
46	X1	0.27	0/1261	0.50	0/1698
47	T6	0.25	0/923	0.44	0/1239
48	T5	0.27	0/1113	0.50	0/1507
49	R	0.27	0/962	0.45	0/1302
50	S1	0.26	0/5502	0.49	0/7454
51	S2	0.27	0/3681	0.49	0/4969
52	S3	0.26	0/1718	0.45	0/2319
53	S4	0.26	0/1505	0.48	0/2035
54	S6	0.25	0/739	0.47	0/1000
55	S7	0.26	0/1319	0.53	1/1789 (0.1%)
56	S8	0.27	0/1867	0.49	0/2538
57	B9	0.26	0/1627	0.43	0/2203
58	TX	0.25	0/1235	0.44	0/1662
59	A8	0.25	0/1099	0.40	0/1477
60	TB	0.27	0/825	0.48	0/1115
61	V1	0.26	0/3485	0.49	0/4713
62	V2	0.25	0/1895	0.47	0/2559
63	B6	0.26	0/623	0.42	0/850
64	BM	0.26	0/1187	0.46	0/1605
65	C4	0.26	0/865	0.43	0/1165
66	AN	0.25	0/1935	0.42	0/2616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
67	B4	0.28	0/935	0.42	0/1277
68	T4	0.25	0/1447	0.43	0/1957
69	T8	0.25	0/1091	0.45	0/1479
70	B2	0.26	0/980	0.46	0/1318
71	T3	0.25	0/2488	0.46	0/3367
72	P1	0.26	0/1951	0.49	0/2642
73	B3	0.26	0/613	0.48	0/829
74	TA	0.26	0/877	0.45	0/1181
75	S5	0.26	0/710	0.44	0/959
76	TC	0.25	0/803	0.45	0/1082
77	P2	0.26	0/1454	0.43	0/1970
78	A3	0.26	0/1103	0.47	0/1491
79	T9	0.26	0/1088	0.48	0/1458
80	TE	0.26	0/425	0.43	0/573
81	T7	0.26	0/1223	0.47	0/1648
All	All	0.26	0/151866	0.46	1/205593 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	S7	31	CYS	CA-CB-SG	5.01	123.02	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	282/284 (99%)	272 (96%)	10 (4%)	0	100	100
2	1B	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
3	2	357/360 (99%)	349 (98%)	8 (2%)	0	100	100
4	2B	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
5	3	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
6	3A	449/482 (93%)	437 (97%)	12 (3%)	0	100	100
6	3a	447/482 (93%)	435 (97%)	12 (3%)	0	100	100
7	3B	477/513 (93%)	468 (98%)	9 (2%)	0	100	100
7	3b	476/513 (93%)	461 (97%)	15 (3%)	0	100	100
8	3C	424/426 (100%)	415 (98%)	9 (2%)	0	100	100
8	3c	424/426 (100%)	404 (95%)	20 (5%)	0	100	100
9	3D	293/319 (92%)	275 (94%)	18 (6%)	0	100	100
9	3d	283/319 (89%)	267 (94%)	16 (6%)	0	100	100
10	3E	226/269 (84%)	215 (95%)	10 (4%)	1 (0%)	30	52
10	3e	100/269 (37%)	91 (91%)	9 (9%)	0	100	100
11	3F	87/90 (97%)	86 (99%)	1 (1%)	0	100	100
11	3f	73/90 (81%)	73 (100%)	0	0	100	100
12	3G	305/328 (93%)	291 (95%)	14 (5%)	0	100	100
12	3g	313/328 (95%)	298 (95%)	15 (5%)	0	100	100
13	3H	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
13	3h	122/130 (94%)	108 (88%)	14 (12%)	0	100	100
14	3I	112/119 (94%)	106 (95%)	6 (5%)	0	100	100
14	3i	109/119 (92%)	101 (93%)	8 (7%)	0	100	100
15	3J	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
15	3j	49/62 (79%)	47 (96%)	2 (4%)	0	100	100
16	3M	17/19 (90%)	14 (82%)	3 (18%)	0	100	100
17	3l	22/24 (92%)	22 (100%)	0	0	100	100
18	3m	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
19	4	503/505 (100%)	481 (96%)	22 (4%)	0	100	100
20	4L	114/116 (98%)	114 (100%)	0	0	100	100
21	5	585/750 (78%)	576 (98%)	9 (2%)	0	100	100
22	5B	98/100 (98%)	86 (88%)	12 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	6	242/255 (95%)	228 (94%)	14 (6%)	0	100	100
24	A2	90/103 (87%)	90 (100%)	0	0	100	100
25	A5	153/206 (74%)	150 (98%)	3 (2%)	0	100	100
26	A6	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
27	A7	279/282 (99%)	274 (98%)	5 (2%)	0	100	100
28	A9	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
29	AB	110/138 (80%)	108 (98%)	2 (2%)	0	100	100
30	AC	96/133 (72%)	95 (99%)	1 (1%)	0	100	100
31	AL	191/194 (98%)	184 (96%)	7 (4%)	0	100	100
32	AM	158/175 (90%)	152 (96%)	6 (4%)	0	100	100
33	B7	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
34	B8	167/207 (81%)	166 (99%)	1 (1%)	0	100	100
35	BL	173/188 (92%)	167 (96%)	6 (4%)	0	100	100
37	C1	227/257 (88%)	213 (94%)	14 (6%)	0	100	100
38	C2	221/233 (95%)	209 (95%)	12 (5%)	0	100	100
39	C3	344/346 (99%)	337 (98%)	7 (2%)	0	100	100
40	TD	69/73 (94%)	68 (99%)	1 (1%)	0	100	100
41	J1	256/317 (81%)	253 (99%)	3 (1%)	0	100	100
42	FX	144/172 (84%)	142 (99%)	2 (1%)	0	100	100
43	T2	269/333 (81%)	259 (96%)	10 (4%)	0	100	100
44	T1	479/516 (93%)	465 (97%)	14 (3%)	0	100	100
45	A1	90/94 (96%)	87 (97%)	3 (3%)	0	100	100
46	X1	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
47	T6	107/144 (74%)	104 (97%)	3 (3%)	0	100	100
48	T5	132/205 (64%)	129 (98%)	3 (2%)	0	100	100
49	R	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
50	S1	685/718 (95%)	667 (97%)	18 (3%)	0	100	100
51	S2	440/442 (100%)	427 (97%)	13 (3%)	0	100	100
52	S3	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
53	S4	173/185 (94%)	166 (96%)	7 (4%)	0	100	100
54	S6	88/132 (67%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	S7	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
56	S8	216/236 (92%)	212 (98%)	4 (2%)	0	100	100
57	B9	184/189 (97%)	177 (96%)	7 (4%)	0	100	100
58	TX	142/166 (86%)	140 (99%)	2 (1%)	0	100	100
59	A8	130/238 (55%)	129 (99%)	1 (1%)	0	100	100
60	TB	94/113 (83%)	89 (95%)	5 (5%)	0	100	100
61	V1	440/474 (93%)	426 (97%)	14 (3%)	0	100	100
62	V2	229/274 (84%)	222 (97%)	7 (3%)	0	100	100
63	B6	68/129 (53%)	64 (94%)	4 (6%)	0	100	100
64	BM	141/214 (66%)	139 (99%)	2 (1%)	0	100	100
65	C4	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
66	AN	229/231 (99%)	226 (99%)	3 (1%)	0	100	100
67	B4	106/108 (98%)	103 (97%)	3 (3%)	0	100	100
68	T4	166/212 (78%)	164 (99%)	2 (1%)	0	100	100
69	T8	127/135 (94%)	124 (98%)	3 (2%)	0	100	100
70	B2	116/126 (92%)	112 (97%)	4 (3%)	0	100	100
71	T3	299/311 (96%)	294 (98%)	4 (1%)	1 (0%)	37	59
72	P1	226/251 (90%)	218 (96%)	8 (4%)	0	100	100
73	B3	66/83 (80%)	63 (96%)	3 (4%)	0	100	100
74	TA	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
75	S5	83/94 (88%)	80 (96%)	3 (4%)	0	100	100
76	TC	89/93 (96%)	87 (98%)	2 (2%)	0	100	100
77	P2	165/189 (87%)	164 (99%)	1 (1%)	0	100	100
78	A3	125/135 (93%)	122 (98%)	3 (2%)	0	100	100
79	T9	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
80	TE	47/71 (66%)	47 (100%)	0	0	100	100
81	T7	140/143 (98%)	135 (96%)	5 (4%)	0	100	100
All	All	17880/19899 (90%)	17305 (97%)	573 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
71	T3	41	LYS

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Mol	Chain	Res	Type
10	3E	229	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	250/250 (100%)	250 (100%)	0	100	100
2	1B	55/55 (100%)	55 (100%)	0	100	100
3	2	345/346 (100%)	344 (100%)	1 (0%)	91	97
4	2B	170/170 (100%)	170 (100%)	0	100	100
5	3	111/112 (99%)	111 (100%)	0	100	100
6	3A	384/409 (94%)	384 (100%)	0	100	100
6	3a	382/409 (93%)	382 (100%)	0	100	100
7	3B	410/440 (93%)	409 (100%)	1 (0%)	92	98
7	3b	409/440 (93%)	407 (100%)	2 (0%)	86	95
8	3C	386/386 (100%)	385 (100%)	1 (0%)	91	97
8	3c	386/386 (100%)	386 (100%)	0	100	100
9	3D	255/274 (93%)	254 (100%)	1 (0%)	89	96
9	3d	247/274 (90%)	247 (100%)	0	100	100
10	3E	200/237 (84%)	199 (100%)	1 (0%)	86	95
10	3e	92/237 (39%)	91 (99%)	1 (1%)	70	86
11	3F	80/81 (99%)	80 (100%)	0	100	100
11	3f	69/81 (85%)	69 (100%)	0	100	100
12	3G	269/289 (93%)	269 (100%)	0	100	100
12	3g	278/289 (96%)	276 (99%)	2 (1%)	81	93
13	3H	117/118 (99%)	116 (99%)	1 (1%)	75	90
13	3h	112/118 (95%)	112 (100%)	0	100	100
14	3I	104/109 (95%)	104 (100%)	0	100	100
14	3i	102/109 (94%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	3J	53/56 (95%)	53 (100%)	0	100	100
15	3j	47/56 (84%)	47 (100%)	0	100	100
16	3M	16/16 (100%)	16 (100%)	0	100	100
17	3l	1/1 (100%)	1 (100%)	0	100	100
18	3m	7/7 (100%)	7 (100%)	0	100	100
19	4	463/463 (100%)	462 (100%)	1 (0%)	92	98
20	4L	108/108 (100%)	108 (100%)	0	100	100
21	5	533/694 (77%)	533 (100%)	0	100	100
22	5B	98/98 (100%)	98 (100%)	0	100	100
23	6	233/244 (96%)	233 (100%)	0	100	100
24	A2	82/93 (88%)	82 (100%)	0	100	100
25	A5	144/186 (77%)	144 (100%)	0	100	100
26	A6	154/154 (100%)	154 (100%)	0	100	100
27	A7	256/257 (100%)	255 (100%)	1 (0%)	89	96
28	A9	288/311 (93%)	288 (100%)	0	100	100
29	AB	104/129 (81%)	103 (99%)	1 (1%)	73	88
30	AC	88/119 (74%)	88 (100%)	0	100	100
31	AL	169/170 (99%)	169 (100%)	0	100	100
32	AM	142/156 (91%)	141 (99%)	1 (1%)	81	93
33	B7	97/99 (98%)	97 (100%)	0	100	100
34	B8	151/180 (84%)	151 (100%)	0	100	100
35	BL	160/172 (93%)	160 (100%)	0	100	100
37	C1	194/218 (89%)	194 (100%)	0	100	100
38	C2	165/197 (84%)	163 (99%)	2 (1%)	67	85
39	C3	309/309 (100%)	309 (100%)	0	100	100
40	TD	63/65 (97%)	63 (100%)	0	100	100
41	J1	220/270 (82%)	220 (100%)	0	100	100
42	FX	130/152 (86%)	130 (100%)	0	100	100
43	T2	230/280 (82%)	230 (100%)	0	100	100
44	T1	421/454 (93%)	421 (100%)	0	100	100
45	A1	87/89 (98%)	86 (99%)	1 (1%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	X1	132/133 (99%)	132 (100%)	0	100	100
47	T6	97/131 (74%)	97 (100%)	0	100	100
48	T5	115/179 (64%)	115 (100%)	0	100	100
49	R	98/98 (100%)	98 (100%)	0	100	100
50	S1	588/617 (95%)	588 (100%)	0	100	100
51	S2	399/399 (100%)	398 (100%)	1 (0%)	91	97
52	S3	191/191 (100%)	190 (100%)	1 (0%)	86	95
53	S4	157/163 (96%)	156 (99%)	1 (1%)	84	94
54	S6	80/116 (69%)	80 (100%)	0	100	100
55	S7	137/137 (100%)	136 (99%)	1 (1%)	81	93
56	S8	197/215 (92%)	196 (100%)	1 (0%)	86	95
57	B9	169/172 (98%)	169 (100%)	0	100	100
58	TX	128/147 (87%)	128 (100%)	0	100	100
59	A8	121/224 (54%)	120 (99%)	1 (1%)	79	91
60	TB	82/97 (84%)	82 (100%)	0	100	100
61	V1	362/392 (92%)	362 (100%)	0	100	100
62	V2	205/236 (87%)	204 (100%)	1 (0%)	86	95
63	B6	64/117 (55%)	64 (100%)	0	100	100
64	BM	125/182 (69%)	125 (100%)	0	100	100
65	C4	88/89 (99%)	88 (100%)	0	100	100
66	AN	199/199 (100%)	199 (100%)	0	100	100
67	B4	94/94 (100%)	94 (100%)	0	100	100
68	T4	151/190 (80%)	150 (99%)	1 (1%)	81	93
69	T8	116/122 (95%)	116 (100%)	0	100	100
70	B2	102/109 (94%)	102 (100%)	0	100	100
71	T3	267/275 (97%)	266 (100%)	1 (0%)	89	96
72	P1	206/223 (92%)	205 (100%)	1 (0%)	86	95
73	B3	63/74 (85%)	63 (100%)	0	100	100
74	TA	94/94 (100%)	94 (100%)	0	100	100
75	S5	76/83 (92%)	76 (100%)	0	100	100
76	TC	82/84 (98%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	P2	158/178 (89%)	158 (100%)	0	100	100
78	A3	107/114 (94%)	107 (100%)	0	100	100
79	T9	118/121 (98%)	118 (100%)	0	100	100
80	TE	44/63 (70%)	44 (100%)	0	100	100
81	T7	124/125 (99%)	123 (99%)	1 (1%)	79	91
All	All	15962/17605 (91%)	15933 (100%)	29 (0%)	91	98

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	241	ASN
7	3B	224	ASN
8	3C	160	LYS
9	3D	101	ARG
10	3E	117	ARG
13	3H	80	ARG
7	3b	224	ASN
7	3b	465	ARG
10	3e	117	ARG
12	3g	11	GLN
12	3g	20	ARG
19	4	462	ASN
27	A7	117	LYS
29	AB	83	ARG
32	AM	87	ARG
38	C2	97	ARG
38	C2	194	ARG
45	A1	44	ARG
51	S2	267	ARG
52	S3	3	ASN
53	S4	76	ARG
55	S7	2	ARG
56	S8	60	ARG
59	A8	187	ASN
62	V2	136	ARG
68	T4	137	ASN
71	T3	42	ARG
72	P1	58	ASN
81	T7	107	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	ASN
5	3	12	ASN
6	3A	88	GLN
7	3B	420	ASN
9	3D	107	GLN
10	3E	32	GLN
10	3E	199	HIS
11	3F	26	GLN
11	3F	27	HIS
11	3f	15	GLN
11	3f	26	GLN
35	BL	114	HIS
39	C3	133	ASN
40	TD	64	GLN
50	S1	599	GLN
54	S6	70	GLN
62	V2	123	GLN
68	T4	137	ASN
77	P2	74	ASN
77	P2	78	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 3 are monoatomic - leaving 101 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	$\# Z > 2$
83	PC1	T1	601	-	25,25,53	0.40	0	31,33,61	0.38	0
83	PC1	X1	201	-	48,48,53	0.30	0	54,56,61	0.35	0
88	3PE	TA	201	-	25,25,50	0.41	0	28,30,55	0.37	0
82	CDL	AL	301	-	52,52,99	0.40	0	58,64,111	0.33	0
83	PC1	C4	403	-	31,31,53	0.37	0	37,39,61	0.41	0
88	3PE	P1	402	-	46,46,50	0.32	0	49,51,55	0.32	0
93	SF4	S1	801	50	0,12,12	-	-	-		
82	CDL	T7	201	-	47,47,99	0.42	0	53,59,111	0.35	0
84	HEM	3c	503	8	42,50,50	1.24	5 (11%)	46,82,82	1.63	9 (19%)
82	CDL	5	803	-	89,89,99	0.31	0	95,101,111	0.26	0
83	PC1	3C	606	-	43,43,53	0.31	0	49,51,61	0.30	0
83	PC1	3I	602	-	45,45,53	0.32	0	51,53,61	0.30	0
86	HEC	3d	401	9	32,50,50	1.94	4 (12%)	30,82,82	2.68	16 (53%)
83	PC1	3c	506	-	37,37,53	0.34	0	43,45,61	0.32	0
83	PC1	AM	201	-	29,29,53	0.38	0	35,37,61	0.34	0
83	PC1	B6	201	-	51,51,53	0.29	0	57,59,61	0.30	0
85	U10	3H	201	-	29,29,63	2.72	13 (44%)	36,38,79	1.60	8 (22%)
83	PC1	5	801	-	53,53,53	0.29	0	59,61,61	0.28	0
83	PC1	AN	303	-	35,35,53	0.35	0	41,43,61	0.39	0
82	CDL	3G	401	-	65,65,99	0.36	0	71,77,111	0.32	0
87	FES	S1	803	50	0,4,4	-	-	-		
83	PC1	3F	102	-	21,21,53	0.39	0	27,29,61	0.43	0
82	CDL	5	805	-	95,95,99	0.31	0	101,107,111	0.36	0
83	PC1	6	301	-	38,38,53	0.33	0	44,46,61	0.33	0
93	SF4	S8	301	56	0,12,12	-	-	-		
83	PC1	3e	301	-	49,49,53	0.31	0	55,57,61	0.30	0
83	PC1	3g	401	-	32,32,53	0.36	0	38,40,61	0.36	0
83	PC1	3b	601	-	29,29,53	0.39	0	35,37,61	0.48	0
82	CDL	3H	203	-	65,65,99	0.36	0	71,77,111	0.31	0
83	PC1	3E	304	-	23,23,53	0.41	0	29,31,61	0.38	0
83	PC1	3I	601	-	31,31,53	0.38	0	37,39,61	0.36	0
83	PC1	3c	501	-	30,30,53	0.38	0	36,38,61	0.45	0
88	3PE	3d	402	-	46,46,50	0.32	0	49,51,55	0.39	0
91	ZMP	AB	201	29	28,33,36	0.72	1 (3%)	32,40,45	3.80	6 (18%)
84	HEM	3C	601	8	42,50,50	1.22	5 (11%)	46,82,82	1.71	7 (15%)
83	PC1	3j	101	-	35,35,53	0.34	0	41,43,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	PC1	3C	607	-	28,28,53	0.38	0	34,36,61	0.37	0
83	PC1	TC	101	-	41,41,53	0.32	0	47,49,61	0.31	0
88	3PE	5	806	-	34,34,50	0.35	0	37,39,55	0.32	0
83	PC1	6	302	-	53,53,53	0.29	0	59,61,61	0.31	0
93	SF4	V1	500	61	0,12,12	-	-	-		
82	CDL	BM	301	-	85,85,99	0.32	0	91,97,111	0.31	0
88	3PE	5B	201	-	23,23,50	0.43	0	26,28,55	0.36	0
83	PC1	3C	604	-	45,45,53	0.31	0	51,53,61	0.31	0
87	FES	FX	201	42	0,4,4	-	-	-		
88	3PE	A3	201	-	44,44,50	0.33	0	47,49,55	0.40	0
83	PC1	3E	302	-	53,53,53	0.29	0	59,61,61	0.32	0
88	3PE	T8	201	-	38,38,50	0.33	0	41,43,55	0.31	0
83	PC1	P1	401	-	39,39,53	0.33	0	45,47,61	0.30	0
88	3PE	S8	303	-	40,40,50	0.34	0	43,45,55	0.32	0
93	SF4	S1	802	50	0,12,12	-	-	-		
93	SF4	S7	201	55	0,12,12	-	-	-		
93	SF4	S8	302	56	0,12,12	-	-	-		
83	PC1	5	802	-	38,38,53	0.33	0	44,46,61	0.33	0
82	CDL	3C	603	-	64,64,99	0.36	0	70,76,111	0.35	0
82	CDL	3b	602	-	67,67,99	0.36	0	73,79,111	0.37	0
94	FMN	V1	501	-	33,33,33	0.21	0	48,50,50	0.34	0
82	CDL	A1	101	-	52,52,99	0.40	0	58,64,111	0.34	0
90	NDP	A9	401	-	47,52,52	0.56	0	61,80,80	0.54	1 (1%)
82	CDL	3	202	-	43,43,99	0.43	0	49,55,111	0.37	0
82	CDL	2B	201	-	52,52,99	0.40	0	58,64,111	0.33	0
85	U10	5B	202	-	63,63,63	2.19	24 (38%)	78,79,79	1.72	22 (28%)
85	U10	3C	605	-	25,25,63	2.84	9 (36%)	24,29,79	1.99	8 (33%)
82	CDL	3i	201	-	70,70,99	0.35	0	76,82,111	0.34	0
82	CDL	B4	201	-	38,38,99	0.42	0	43,49,111	0.40	0
83	PC1	5	807	-	53,53,53	0.29	0	59,61,61	0.30	0
83	PC1	3	201	-	30,30,53	0.37	0	36,38,61	0.36	0
88	3PE	3E	303	-	33,33,50	0.37	0	36,38,55	0.34	0
82	CDL	3c	504	-	63,63,99	0.36	0	69,75,111	0.31	0
82	CDL	AN	304	-	52,52,99	0.39	0	58,64,111	0.35	0
82	CDL	3c	505	-	55,55,99	0.38	0	61,67,111	0.33	0
83	PC1	J1	400	-	39,39,53	0.33	0	45,47,61	0.35	0
87	FES	V2	300	62	0,4,4	-	-	-		
84	HEM	3C	602	8	42,50,50	1.22	5 (11%)	46,82,82	1.63	8 (17%)
84	HEM	3c	502	8	42,50,50	1.23	5 (11%)	46,82,82	1.63	7 (15%)
92	ADP	B8	602	-	24,29,29	0.86	0	29,45,45	1.23	2 (6%)
82	CDL	1	301	-	49,49,99	0.41	0	55,61,111	0.35	0
83	PC1	1	302	-	35,35,53	0.35	0	41,43,61	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	3PE	B8	601	-	35,35,50	0.35	0	38,40,55	0.33	0
87	FES	3E	301	10	0,4,4	-	-	-		
82	CDL	3I	603	-	70,70,99	0.35	0	76,82,111	0.35	0
86	HEC	3D	401	9	32,50,50	1.94	4 (12%)	30,82,82	2.68	16 (53%)
82	CDL	P2	201	-	81,81,99	0.33	0	87,93,111	0.28	0
88	3PE	T4	301	-	24,24,50	0.42	0	27,29,55	0.37	0
82	CDL	C4	401	-	97,97,99	0.30	0	103,109,111	0.33	0
83	PC1	3J	101	-	36,36,53	0.36	0	42,44,61	0.40	0
82	CDL	3H	202	-	61,61,99	0.37	0	67,73,111	0.36	0
82	CDL	B8	603	-	44,44,99	0.43	0	50,56,111	0.36	0
88	3PE	4	602	-	35,35,50	0.35	0	38,40,55	0.33	0
88	3PE	4	601	-	46,46,50	0.32	0	49,51,55	0.37	0
88	3PE	AN	301	-	44,44,50	0.32	0	47,49,55	0.32	0
82	CDL	TD	101	-	65,65,99	0.36	0	71,77,111	0.36	0
82	CDL	3B	701	-	77,77,99	0.33	0	83,89,111	0.31	0
88	3PE	AN	302	-	34,34,50	0.36	0	37,39,55	0.33	0
82	CDL	R	201	-	83,83,99	0.32	0	89,95,111	0.31	0
82	CDL	T1	602	-	54,54,99	0.39	0	60,66,111	0.41	0
83	PC1	B2	201	-	47,47,53	0.31	0	53,55,61	0.35	0
82	CDL	AM	202	-	61,61,99	0.37	0	67,73,111	0.31	0
88	3PE	5	804	-	36,36,50	0.34	0	39,41,55	0.31	0
88	3PE	C4	402	-	50,50,50	0.30	0	53,55,55	0.34	0
82	CDL	3I	604	-	36,36,99	0.43	0	42,48,111	0.39	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
83	PC1	T1	601	-	-	11/29/29/57	-
83	PC1	X1	201	-	-	12/52/52/57	-
88	3PE	TA	201	-	-	5/29/29/54	-
82	CDL	AL	301	-	-	15/63/63/110	-
83	PC1	C4	403	-	-	13/35/35/57	-
88	3PE	P1	402	-	-	11/50/50/54	-
93	SF4	S1	801	50	-	-	0/6/5/5
82	CDL	T7	201	-	-	14/58/58/110	-
84	HEM	3c	503	8	-	7/12/54/54	-
82	CDL	5	803	-	-	22/100/100/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PC1	3C	606	-	-	6/47/47/57	-
83	PC1	3I	602	-	-	7/49/49/57	-
86	HEC	3d	401	9	-	3/10/54/54	-
83	PC1	3c	506	-	-	13/41/41/57	-
83	PC1	AM	201	-	-	12/33/33/57	-
83	PC1	B6	201	-	-	9/55/55/57	-
85	U10	3H	201	-	-	6/23/47/87	0/1/1/1
83	PC1	5	801	-	-	6/57/57/57	-
83	PC1	AN	303	-	-	7/39/39/57	-
82	CDL	3G	401	-	-	19/76/76/110	-
87	FES	S1	803	50	-	-	0/1/1/1
83	PC1	3F	102	-	-	8/23/23/57	-
82	CDL	5	805	-	-	20/106/106/110	-
83	PC1	6	301	-	-	6/42/42/57	-
93	SF4	S8	301	56	-	-	0/6/5/5
83	PC1	3e	301	-	-	6/53/53/57	-
83	PC1	3g	401	-	-	2/36/36/57	-
83	PC1	3b	601	-	-	15/33/33/57	-
82	CDL	3H	203	-	-	11/76/76/110	-
83	PC1	3E	304	-	-	9/26/26/57	-
83	PC1	3I	601	-	-	9/35/35/57	-
83	PC1	3c	501	-	-	7/34/34/57	-
88	3PE	3d	402	-	-	11/50/50/54	-
91	ZMP	AB	201	29	-	8/38/40/43	-
84	HEM	3C	601	8	-	3/12/54/54	-
83	PC1	3j	101	-	-	5/39/39/57	-
83	PC1	3C	607	-	-	9/32/32/57	-
83	PC1	TC	101	-	-	7/45/45/57	-
88	3PE	5	806	-	-	6/38/38/54	-
83	PC1	6	302	-	-	11/57/57/57	-
93	SF4	V1	500	61	-	-	0/6/5/5
88	3PE	5B	201	-	-	7/27/27/54	-
82	CDL	BM	301	-	-	19/96/96/110	-
83	PC1	3C	604	-	-	14/49/49/57	-
88	3PE	A3	201	-	-	6/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	FES	FX	201	42	-	-	0/1/1/1
83	PC1	3E	302	-	-	21/57/57/57	-
88	3PE	T8	201	-	-	9/42/42/54	-
83	PC1	P1	401	-	-	15/43/43/57	-
88	3PE	S8	303	-	-	8/44/44/54	-
93	SF4	S1	802	50	-	-	0/6/5/5
93	SF4	S7	201	55	-	-	0/6/5/5
93	SF4	S8	302	56	-	-	0/6/5/5
83	PC1	5	802	-	-	7/42/42/57	-
82	CDL	3C	603	-	-	20/75/75/110	-
82	CDL	3b	602	-	-	24/78/78/110	-
94	FMN	V1	501	-	-	1/18/18/18	0/3/3/3
82	CDL	A1	101	-	-	15/63/63/110	-
90	NDP	A9	401	-	-	3/30/77/77	0/5/5/5
82	CDL	3	202	-	-	7/54/54/110	-
82	CDL	2B	201	-	-	9/63/63/110	-
85	U10	5B	202	-	-	18/63/87/87	0/1/1/1
85	U10	3C	605	-	-	12/28/28/87	-
82	CDL	3i	201	-	-	15/81/81/110	-
82	CDL	B4	201	-	-	10/44/44/110	-
83	PC1	5	807	-	-	10/57/57/57	-
83	PC1	3	201	-	-	6/34/34/57	-
88	3PE	3E	303	-	-	7/37/37/54	-
82	CDL	3c	504	-	-	15/74/74/110	-
82	CDL	AN	304	-	-	20/62/62/110	-
82	CDL	3c	505	-	-	16/66/66/110	-
83	PC1	J1	400	-	-	9/43/43/57	-
87	FES	V2	300	62	-	-	0/1/1/1
84	HEM	3C	602	8	-	5/12/54/54	-
84	HEM	3c	502	8	-	5/12/54/54	-
92	ADP	B8	602	-	-	1/12/32/32	0/3/3/3
82	CDL	1	301	-	-	11/60/60/110	-
83	PC1	1	302	-	-	12/39/39/57	-
88	3PE	B8	601	-	-	8/39/39/54	-
87	FES	3E	301	10	-	-	0/1/1/1
82	CDL	3I	603	-	-	23/81/81/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	HEC	3D	401	9	-	4/10/54/54	-
82	CDL	P2	201	-	-	20/92/92/110	-
88	3PE	T4	301	-	-	4/28/28/54	-
82	CDL	C4	401	-	-	21/108/108/110	-
83	PC1	3J	101	-	-	16/40/40/57	-
82	CDL	3H	202	-	-	17/72/72/110	-
82	CDL	B8	603	-	-	4/55/55/110	-
88	3PE	4	602	-	-	7/39/39/54	-
88	3PE	4	601	-	-	6/50/50/54	-
88	3PE	AN	301	-	-	6/48/48/54	-
82	CDL	TD	101	-	-	14/76/76/110	-
82	CDL	3B	701	-	-	23/88/88/110	-
88	3PE	AN	302	-	-	8/38/38/54	-
82	CDL	R	201	-	-	17/94/94/110	-
82	CDL	T1	602	-	-	10/65/65/110	-
83	PC1	B2	201	-	-	15/51/51/57	-
82	CDL	AM	202	-	-	14/72/72/110	-
88	3PE	5	804	-	-	5/40/40/54	-
88	3PE	C4	402	-	-	14/54/54/54	-
82	CDL	3I	604	-	-	6/44/44/110	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	3H	201	U10	C6-C1	10.27	1.53	1.35
85	3C	605	U10	C6-C1	10.27	1.56	1.33
85	5B	202	U10	C6-C1	10.25	1.53	1.35
86	3D	401	HEC	C3C-C2C	-5.98	1.34	1.40
86	3d	401	HEC	C3C-C2C	-5.97	1.34	1.40
85	3C	605	U10	C2-C1	-5.86	1.36	1.51
86	3d	401	HEC	C2B-C3B	-5.70	1.34	1.40
86	3D	401	HEC	C2B-C3B	-5.69	1.34	1.40
85	3H	201	U10	C4-C3	4.82	1.53	1.36
85	5B	202	U10	C4-C3	4.79	1.53	1.36
84	3C	601	HEM	C4D-ND	-3.75	1.33	1.40
84	3c	503	HEM	C4D-ND	-3.66	1.33	1.40
84	3c	502	HEM	C4D-ND	-3.66	1.33	1.40
84	3C	602	HEM	C4D-ND	-3.65	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3d	401	HEC	CBC-CAC	-3.43	1.36	1.49
86	3D	401	HEC	CBC-CAC	-3.41	1.36	1.49
84	3C	602	HEM	C1B-NB	-3.08	1.34	1.40
84	3C	601	HEM	C1B-NB	-3.07	1.34	1.40
84	3c	502	HEM	C1B-NB	-3.03	1.35	1.40
84	3c	503	HEM	C1B-NB	-2.99	1.35	1.40
85	5B	202	U10	C41-C39	2.98	1.57	1.51
85	5B	202	U10	C26-C24	2.85	1.57	1.51
85	3C	605	U10	C11-C9	2.78	1.57	1.51
84	3c	503	HEM	C1D-ND	-2.76	1.33	1.38
85	5B	202	U10	C31-C29	2.74	1.56	1.51
84	3C	602	HEM	C1D-ND	-2.72	1.33	1.38
85	5B	202	U10	C21-C19	2.71	1.56	1.51
84	3C	601	HEM	C1D-ND	-2.70	1.33	1.38
84	3c	502	HEM	C1D-ND	-2.69	1.33	1.38
85	3H	201	U10	C7-C8	2.66	1.54	1.50
85	3C	605	U10	C16-C14	2.65	1.56	1.51
85	5B	202	U10	C7-C8	2.59	1.54	1.50
84	3C	601	HEM	CHB-C1B	2.50	1.40	1.34
91	AB	201	ZMP	C9-C10	2.50	1.53	1.50
85	5B	202	U10	C36-C34	2.46	1.56	1.51
85	3C	605	U10	C21-C19	2.45	1.56	1.51
85	5B	202	U10	C46-C44	2.45	1.56	1.51
85	3H	201	U10	C11-C9	2.45	1.56	1.51
85	5B	202	U10	O5-C5	-2.42	1.18	1.23
85	3C	605	U10	C7-C8	2.42	1.57	1.51
84	3C	602	HEM	CHB-C1B	2.41	1.40	1.34
85	3H	201	U10	C6-C5	2.40	1.53	1.46
84	3c	503	HEM	CHB-C1B	2.40	1.40	1.34
85	3H	201	U10	O5-C5	-2.40	1.18	1.23
85	5B	202	U10	C51-C49	2.37	1.56	1.51
84	3c	502	HEM	CHB-C1B	2.35	1.40	1.34
85	5B	202	U10	C27-C28	2.33	1.57	1.50
85	3C	605	U10	C12-C13	2.31	1.57	1.50
86	3D	401	HEC	CBB-CAB	-2.30	1.41	1.49
86	3d	401	HEC	CBB-CAB	-2.30	1.41	1.49
85	5B	202	U10	C6-C5	2.28	1.52	1.46
85	3H	201	U10	O3-C3M	-2.28	1.40	1.45
85	5B	202	U10	O3-C3M	-2.27	1.40	1.45
85	5B	202	U10	O2-C2	-2.27	1.18	1.23
85	5B	202	U10	C16-C14	2.27	1.56	1.51
85	5B	202	U10	C11-C9	2.25	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	5B	202	U10	C22-C23	2.24	1.57	1.50
85	3H	201	U10	O2-C2	-2.24	1.18	1.23
85	3H	201	U10	C16-C14	2.24	1.55	1.51
85	5B	202	U10	C42-C43	2.19	1.57	1.50
85	5B	202	U10	C7-C6	2.17	1.55	1.51
84	3c	502	HEM	C4B-NB	-2.14	1.34	1.38
85	3H	201	U10	C7-C6	2.14	1.55	1.51
85	3H	201	U10	C12-C13	2.14	1.56	1.50
85	5B	202	U10	C17-C18	2.12	1.56	1.50
85	3H	201	U10	C17-C18	2.10	1.56	1.50
85	3C	605	U10	C26-C24	2.10	1.57	1.51
85	5B	202	U10	C32-C33	2.10	1.56	1.50
85	5B	202	U10	C12-C13	2.10	1.56	1.50
85	3H	201	U10	O4-C4M	-2.08	1.40	1.45
85	5B	202	U10	O4-C4M	-2.06	1.40	1.45
85	3C	605	U10	C17-C18	2.05	1.56	1.50
84	3C	602	HEM	C4B-NB	-2.05	1.34	1.38
84	3c	503	HEM	C4B-NB	-2.03	1.34	1.38
84	3C	601	HEM	C4B-NB	-2.02	1.34	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AB	201	ZMP	C19-C18-C17	-12.73	87.07	108.77
91	AB	201	ZMP	C20-C18-C17	-11.76	88.73	108.77
91	AB	201	ZMP	C20-C18-C21	8.27	121.88	108.22
86	3d	401	HEC	CBB-CAB-C3B	-7.47	110.00	127.49
86	3D	401	HEC	CBB-CAB-C3B	-7.31	110.37	127.49
91	AB	201	ZMP	C19-C18-C21	5.91	117.98	108.22
86	3D	401	HEC	CBC-CAC-C3C	-5.74	114.06	127.49
86	3d	401	HEC	CBC-CAC-C3C	-5.69	114.17	127.49
91	AB	201	ZMP	C20-C18-C19	5.33	119.84	109.20
84	3C	601	HEM	CHC-C4B-NB	4.84	129.64	124.44
84	3C	602	HEM	CHC-C4B-NB	4.74	129.54	124.44
84	3c	502	HEM	CHC-C4B-NB	4.68	129.47	124.44
84	3c	503	HEM	CHC-C4B-NB	4.45	129.22	124.44
86	3d	401	HEC	CMD-C2D-C1D	-4.41	121.99	128.46
86	3D	401	HEC	CMD-C2D-C1D	-4.26	122.22	128.46
86	3D	401	HEC	CBD-CAD-C3D	3.95	119.17	112.54
85	3H	201	U10	C7-C8-C9	-3.89	120.13	126.83
84	3c	503	HEM	CHB-C1B-NB	3.69	128.95	124.37
84	3c	502	HEM	CHB-C1B-NB	3.65	128.90	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	3C	601	HEM	CHB-C1B-NB	3.63	128.87	124.37
84	3C	602	HEM	CHB-C1B-NB	3.61	128.85	124.37
92	B8	602	ADP	N3-C2-N1	-3.58	123.81	128.67
86	3d	401	HEC	CMB-C2B-C1B	-3.51	123.31	128.46
86	3D	401	HEC	CMB-C2B-C1B	-3.50	123.33	128.46
85	3C	605	U10	C1M-C1-C2	3.36	120.09	116.13
85	5B	202	U10	C27-C28-C29	-3.34	119.97	127.62
86	3D	401	HEC	CMB-C2B-C3B	3.34	129.75	125.82
85	3C	605	U10	C17-C18-C19	-3.31	120.04	127.62
86	3d	401	HEC	CBD-CAD-C3D	3.30	118.09	112.54
85	3C	605	U10	C25-C24-C26	3.28	119.99	116.13
86	3d	401	HEC	CMB-C2B-C3B	3.28	129.68	125.82
85	3C	605	U10	C12-C13-C14	-3.26	120.16	127.62
84	3C	601	HEM	CHA-C4D-ND	3.25	128.40	124.37
84	3C	601	HEM	C1B-NB-C4B	3.24	109.04	105.21
85	5B	202	U10	C17-C18-C19	-3.22	120.24	127.62
85	3C	605	U10	C22-C23-C24	-3.22	120.25	127.62
85	5B	202	U10	C37-C38-C39	-3.20	120.30	127.62
85	3H	201	U10	C7-C6-C1	-3.19	119.41	124.89
86	3d	401	HEC	CMC-C2C-C3C	3.16	129.54	125.82
84	3C	601	HEM	C4D-ND-C1D	3.15	108.94	105.21
85	5B	202	U10	C7-C8-C9	-3.15	121.41	126.83
85	5B	202	U10	C32-C33-C34	-3.11	120.50	127.62
85	5B	202	U10	C10-C9-C11	3.10	120.60	115.23
85	5B	202	U10	C12-C13-C14	-3.09	120.56	127.62
85	5B	202	U10	C42-C43-C44	-3.08	120.57	127.62
85	3H	201	U10	C20-C19-C21	3.07	119.74	116.13
84	3c	503	HEM	C1B-NB-C4B	3.07	108.84	105.21
85	5B	202	U10	C47-C48-C49	-3.04	120.67	127.62
84	3C	602	HEM	C4D-ND-C1D	3.04	108.80	105.21
86	3D	401	HEC	CMC-C2C-C3C	3.04	129.39	125.82
84	3c	503	HEM	C4D-ND-C1D	3.03	108.80	105.21
85	3H	201	U10	C17-C18-C19	-2.93	120.92	127.62
86	3D	401	HEC	C4C-C3C-C2C	2.93	109.52	106.35
84	3c	502	HEM	C1B-NB-C4B	2.92	108.66	105.21
85	5B	202	U10	C22-C23-C24	-2.90	120.98	127.62
85	5B	202	U10	C35-C34-C36	2.90	120.26	115.23
85	5B	202	U10	C7-C6-C1	-2.88	119.95	124.89
85	3C	605	U10	C15-C14-C16	2.86	120.20	115.23
84	3C	602	HEM	C1B-NB-C4B	2.84	108.57	105.21
84	3c	502	HEM	C4D-ND-C1D	2.84	108.57	105.21
85	3C	605	U10	C20-C19-C21	2.83	120.14	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	3d	401	HEC	O1D-CGD-CBD	-2.82	114.15	123.09
85	5B	202	U10	C25-C24-C26	2.82	120.12	115.23
84	3c	502	HEM	CHA-C4D-ND	2.82	127.86	124.37
85	3H	201	U10	C1M-C1-C6	-2.80	119.85	124.45
86	3D	401	HEC	O1D-CGD-CBD	-2.80	114.21	123.09
84	3C	602	HEM	CHA-C4D-ND	2.80	127.84	124.37
86	3d	401	HEC	C4C-C3C-C2C	2.80	109.37	106.35
85	5B	202	U10	C45-C44-C46	2.77	120.04	115.23
85	5B	202	U10	C1M-C1-C6	-2.77	119.89	124.45
85	5B	202	U10	C30-C29-C31	2.72	119.95	115.23
85	3H	201	U10	C12-C13-C14	-2.70	121.44	127.62
85	5B	202	U10	C20-C19-C21	2.69	119.89	115.23
86	3d	401	HEC	CMC-C2C-C1C	-2.68	124.53	128.46
91	AB	201	ZMP	O1-C10-C9	-2.68	120.89	123.98
85	3H	201	U10	C15-C14-C16	2.66	119.85	115.23
85	5B	202	U10	C15-C14-C16	2.61	119.76	115.23
84	3c	503	HEM	CHA-C4D-ND	2.61	127.60	124.37
85	5B	202	U10	C40-C39-C41	2.61	119.75	115.23
84	3C	602	HEM	CHD-C1D-ND	2.59	127.22	124.44
85	3C	605	U10	C10-C9-C11	2.57	119.69	115.23
84	3C	601	HEM	CHD-C1D-ND	2.54	127.17	124.44
86	3D	401	HEC	CMC-C2C-C1C	-2.54	124.73	128.46
85	5B	202	U10	C50-C49-C51	2.54	119.63	115.23
92	B8	602	ADP	C4-C5-N7	-2.47	106.72	109.34
84	3c	502	HEM	CHD-C1D-ND	2.47	127.09	124.44
85	3H	201	U10	C10-C9-C11	2.46	119.50	115.23
86	3d	401	HEC	CMD-C2D-C3D	2.44	129.55	124.94
90	A9	401	NDP	C5A-C6A-N6A	2.32	123.85	120.31
86	3D	401	HEC	CMD-C2D-C3D	2.29	129.26	124.94
84	3c	503	HEM	CHD-C1D-ND	2.27	126.88	124.44
84	3c	503	HEM	C3B-C4B-NB	-2.24	107.86	109.47
86	3d	401	HEC	CMA-C3A-C2A	2.24	129.16	124.94
86	3D	401	HEC	O1A-CGA-CBA	-2.23	116.03	123.09
85	5B	202	U10	C56-C54-C55	2.22	119.70	114.59
86	3d	401	HEC	O1A-CGA-CBA	-2.22	116.05	123.09
86	3D	401	HEC	C1D-C2D-C3D	2.19	108.52	107.00
85	5B	202	U10	C52-C53-C54	-2.17	120.41	127.64
86	3D	401	HEC	C2B-C3B-C4B	2.16	108.69	106.35
86	3D	401	HEC	CMA-C3A-C2A	2.15	129.00	124.94
84	3C	601	HEM	C3B-C4B-NB	-2.15	107.92	109.47
84	3c	502	HEM	CHB-C1B-C2B	-2.15	120.86	126.94
86	3d	401	HEC	C2B-C3B-C4B	2.14	108.66	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	3c	503	HEM	CHB-C1B-C2B	-2.11	120.97	126.94
84	3C	602	HEM	CHB-C1B-C2B	-2.11	120.98	126.94
86	3d	401	HEC	C1D-C2D-C3D	2.10	108.46	107.00
84	3c	503	HEM	CAD-CBD-CGD	-2.10	108.11	113.67
86	3D	401	HEC	O2A-CGA-O1A	2.08	128.68	123.33
86	3d	401	HEC	O2A-CGA-O1A	2.05	128.62	123.33
84	3C	602	HEM	CMC-C2C-C3C	2.01	128.70	124.68

There are no chirality outliers.

All (970) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	1	301	CDL	CB2-OB2-PB2-OB3
82	1	301	CDL	OB5-CB3-CB4-OB6
82	2B	201	CDL	CA2-OA2-PA1-OA3
82	2B	201	CDL	CA2-OA2-PA1-OA5
82	2B	201	CDL	CB2-OB2-PB2-OB4
82	2B	201	CDL	CB2-OB2-PB2-OB5
82	2B	201	CDL	CB3-OB5-PB2-OB4
82	3	202	CDL	CA3-OA5-PA1-OA2
82	3	202	CDL	CA3-OA5-PA1-OA3
82	3	202	CDL	CB3-OB5-PB2-OB2
82	3B	701	CDL	CA2-OA2-PA1-OA3
82	3B	701	CDL	CA2-OA2-PA1-OA5
82	3B	701	CDL	CA3-OA5-PA1-OA2
82	3B	701	CDL	CA3-OA5-PA1-OA4
82	3B	701	CDL	CB2-OB2-PB2-OB5
82	3B	701	CDL	CB3-OB5-PB2-OB2
82	3B	701	CDL	CB3-OB5-PB2-OB4
82	3C	603	CDL	CA2-OA2-PA1-OA3
82	3C	603	CDL	CA2-OA2-PA1-OA4
82	3C	603	CDL	CA2-OA2-PA1-OA5
82	3C	603	CDL	CB2-OB2-PB2-OB3
82	3C	603	CDL	CB2-OB2-PB2-OB4
82	3C	603	CDL	CB2-OB2-PB2-OB5
82	3C	603	CDL	CB3-OB5-PB2-OB2
82	3C	603	CDL	CB3-OB5-PB2-OB4
82	3G	401	CDL	CA3-OA5-PA1-OA2
82	3G	401	CDL	CA3-OA5-PA1-OA3
82	3G	401	CDL	CB2-OB2-PB2-OB3
82	3G	401	CDL	CB2-OB2-PB2-OB4
82	3G	401	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
82	3H	202	CDL	CA2-OA2-PA1-OA3
82	3H	202	CDL	CA3-OA5-PA1-OA3
82	3H	202	CDL	CB3-OB5-PB2-OB2
82	3H	202	CDL	CB3-OB5-PB2-OB3
82	3H	202	CDL	CB3-OB5-PB2-OB4
82	3H	203	CDL	CA2-OA2-PA1-OA4
82	3H	203	CDL	CA2-OA2-PA1-OA5
82	3H	203	CDL	CB2-OB2-PB2-OB3
82	3H	203	CDL	CB2-OB2-PB2-OB4
82	3H	203	CDL	CB2-OB2-PB2-OB5
82	3H	203	CDL	CB3-OB5-PB2-OB2
82	3H	203	CDL	CB3-OB5-PB2-OB3
82	3I	603	CDL	CA3-OA5-PA1-OA3
82	3I	603	CDL	CB2-OB2-PB2-OB3
82	3I	603	CDL	CB2-OB2-PB2-OB4
82	3I	603	CDL	CB2-OB2-PB2-OB5
82	3I	603	CDL	CB3-OB5-PB2-OB3
82	3I	604	CDL	CA3-OA5-PA1-OA2
82	3I	604	CDL	CA3-OA5-PA1-OA3
82	3b	602	CDL	CA2-OA2-PA1-OA4
82	3b	602	CDL	CA3-OA5-PA1-OA2
82	3b	602	CDL	CA3-OA5-PA1-OA4
82	3b	602	CDL	CB2-OB2-PB2-OB3
82	3b	602	CDL	CB2-OB2-PB2-OB4
82	3b	602	CDL	CB2-OB2-PB2-OB5
82	3c	504	CDL	CA2-OA2-PA1-OA3
82	3c	504	CDL	CA2-OA2-PA1-OA4
82	3c	504	CDL	CA2-OA2-PA1-OA5
82	3c	504	CDL	CA3-OA5-PA1-OA2
82	3c	504	CDL	CA3-OA5-PA1-OA3
82	3c	504	CDL	CB2-OB2-PB2-OB3
82	3c	504	CDL	CB2-OB2-PB2-OB5
82	3c	504	CDL	CB3-OB5-PB2-OB2
82	3c	504	CDL	CB3-OB5-PB2-OB3
82	3c	504	CDL	CB3-OB5-PB2-OB4
82	3c	505	CDL	CA2-OA2-PA1-OA3
82	3c	505	CDL	CA3-OA5-PA1-OA2
82	3c	505	CDL	CA3-OA5-PA1-OA3
82	3c	505	CDL	CB2-OB2-PB2-OB3
82	3c	505	CDL	CB2-OB2-PB2-OB4
82	3c	505	CDL	CB2-OB2-PB2-OB5
82	3i	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
82	3i	201	CDL	CA2-OA2-PA1-OA4
82	3i	201	CDL	CA3-OA5-PA1-OA2
82	3i	201	CDL	CA3-OA5-PA1-OA3
82	3i	201	CDL	CA3-OA5-PA1-OA4
82	3i	201	CDL	CB2-OB2-PB2-OB3
82	3i	201	CDL	CB3-OB5-PB2-OB3
82	3i	201	CDL	CB3-OB5-PB2-OB4
82	5	803	CDL	CA2-OA2-PA1-OA3
82	5	803	CDL	CA2-OA2-PA1-OA4
82	5	803	CDL	CA2-OA2-PA1-OA5
82	5	803	CDL	CA3-OA5-PA1-OA2
82	5	803	CDL	CA3-OA5-PA1-OA3
82	5	803	CDL	CB2-OB2-PB2-OB4
82	5	803	CDL	CB2-OB2-PB2-OB5
82	5	803	CDL	CB3-OB5-PB2-OB2
82	5	803	CDL	CB3-OB5-PB2-OB3
82	5	803	CDL	CB3-OB5-PB2-OB4
82	5	805	CDL	CA3-OA5-PA1-OA4
82	5	805	CDL	CB3-OB5-PB2-OB2
82	5	805	CDL	CB3-OB5-PB2-OB3
82	AL	301	CDL	CA2-OA2-PA1-OA4
82	AL	301	CDL	CA2-OA2-PA1-OA5
82	AL	301	CDL	CA3-OA5-PA1-OA2
82	AL	301	CDL	CA3-OA5-PA1-OA4
82	AL	301	CDL	CB2-OB2-PB2-OB3
82	AL	301	CDL	CB2-OB2-PB2-OB4
82	AL	301	CDL	CB2-OB2-PB2-OB5
82	AM	202	CDL	CA2-OA2-PA1-OA5
82	AM	202	CDL	CA3-OA5-PA1-OA2
82	AM	202	CDL	CA3-OA5-PA1-OA3
82	AM	202	CDL	CA3-OA5-PA1-OA4
82	B8	603	CDL	CB3-OB5-PB2-OB2
82	B8	603	CDL	CB3-OB5-PB2-OB3
82	B8	603	CDL	CB3-OB5-PB2-OB4
82	TD	101	CDL	CA2-OA2-PA1-OA3
82	TD	101	CDL	CA3-OA5-PA1-OA2
82	TD	101	CDL	CA3-OA5-PA1-OA4
82	TD	101	CDL	CB2-OB2-PB2-OB3
82	TD	101	CDL	CB2-OB2-PB2-OB4
82	TD	101	CDL	CB2-OB2-PB2-OB5
82	T1	602	CDL	CA3-OA5-PA1-OA2
82	T1	602	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
82	T1	602	CDL	CB3-OB5-PB2-OB3
82	A1	101	CDL	CA2-OA2-PA1-OA3
82	A1	101	CDL	CA2-OA2-PA1-OA4
82	A1	101	CDL	CA2-OA2-PA1-OA5
82	R	201	CDL	CA2-OA2-PA1-OA3
82	R	201	CDL	CA2-OA2-PA1-OA4
82	R	201	CDL	CA2-OA2-PA1-OA5
82	BM	301	CDL	CA2-OA2-PA1-OA4
82	BM	301	CDL	CA2-OA2-PA1-OA5
82	BM	301	CDL	CA3-OA5-PA1-OA2
82	BM	301	CDL	CA3-OA5-PA1-OA4
82	BM	301	CDL	CB2-OB2-PB2-OB3
82	BM	301	CDL	CB3-OB5-PB2-OB2
82	BM	301	CDL	CB3-OB5-PB2-OB3
82	BM	301	CDL	CB3-OB5-PB2-OB4
82	BM	301	CDL	OB5-CB3-CB4-OB6
82	C4	401	CDL	CA2-OA2-PA1-OA3
82	C4	401	CDL	CA2-OA2-PA1-OA4
82	C4	401	CDL	CA2-OA2-PA1-OA5
82	C4	401	CDL	CA3-OA5-PA1-OA2
82	C4	401	CDL	CA3-OA5-PA1-OA3
82	C4	401	CDL	CA3-OA5-PA1-OA4
82	C4	401	CDL	CB2-OB2-PB2-OB5
82	AN	304	CDL	CA2-OA2-PA1-OA3
82	AN	304	CDL	CA2-OA2-PA1-OA4
82	AN	304	CDL	CA2-OA2-PA1-OA5
82	AN	304	CDL	CA3-OA5-PA1-OA4
82	AN	304	CDL	CB2-OB2-PB2-OB3
82	AN	304	CDL	CB2-OB2-PB2-OB4
82	AN	304	CDL	CB2-OB2-PB2-OB5
82	AN	304	CDL	CB3-OB5-PB2-OB2
82	AN	304	CDL	CB3-OB5-PB2-OB3
82	B4	201	CDL	CB2-OB2-PB2-OB3
82	B4	201	CDL	CB3-OB5-PB2-OB2
82	B4	201	CDL	CB3-OB5-PB2-OB3
82	B4	201	CDL	CB3-OB5-PB2-OB4
82	P2	201	CDL	CA2-OA2-PA1-OA3
82	P2	201	CDL	CA2-OA2-PA1-OA4
82	P2	201	CDL	CA2-OA2-PA1-OA5
82	P2	201	CDL	CB2-OB2-PB2-OB3
82	P2	201	CDL	CB2-OB2-PB2-OB4
82	P2	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
82	P2	201	CDL	CB3-OB5-PB2-OB3
82	T7	201	CDL	CA2-OA2-PA1-OA3
82	T7	201	CDL	CA2-OA2-PA1-OA5
82	T7	201	CDL	CA3-OA5-PA1-OA2
82	T7	201	CDL	CA3-OA5-PA1-OA3
82	T7	201	CDL	CA3-OA5-PA1-OA4
82	T7	201	CDL	CB2-OB2-PB2-OB5
82	T7	201	CDL	CB3-OB5-PB2-OB2
82	T7	201	CDL	CB3-OB5-PB2-OB3
83	1	302	PC1	C11-O13-P-O14
83	1	302	PC1	C1-O11-P-O14
83	1	302	PC1	C1-O11-P-O13
83	3	201	PC1	C1-O11-P-O14
83	3C	604	PC1	C11-O13-P-O14
83	3C	604	PC1	C1-O11-P-O12
83	3C	604	PC1	C1-O11-P-O14
83	3C	606	PC1	C11-O13-P-O14
83	3C	607	PC1	C1-O11-P-O12
83	3E	302	PC1	C1-O11-P-O14
83	3E	302	PC1	C1-O11-P-O13
83	3E	304	PC1	C11-O13-P-O14
83	3E	304	PC1	C11-O13-P-O11
83	3E	304	PC1	C1-O11-P-O12
83	3E	304	PC1	C1-O11-P-O14
83	3E	304	PC1	C1-O11-P-O13
83	3I	601	PC1	C11-O13-P-O12
83	3I	601	PC1	C1-O11-P-O13
83	3J	101	PC1	C11-O13-P-O12
83	3J	101	PC1	C11-O13-P-O14
83	3J	101	PC1	C11-O13-P-O11
83	3J	101	PC1	C1-O11-P-O12
83	3J	101	PC1	C1-O11-P-O14
83	3J	101	PC1	C1-O11-P-O13
83	3b	601	PC1	C11-O13-P-O12
83	3c	506	PC1	C11-O13-P-O12
83	3c	506	PC1	C11-O13-P-O14
83	3c	506	PC1	C11-O13-P-O11
83	3c	506	PC1	C1-O11-P-O12
83	3c	506	PC1	C1-O11-P-O14
83	3c	506	PC1	C1-O11-P-O13
83	3e	301	PC1	C11-O13-P-O11
83	3g	401	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
83	3j	101	PC1	C11-O13-P-O12
83	3j	101	PC1	C11-O13-P-O11
83	5	801	PC1	C11-O13-P-O12
83	5	801	PC1	C11-O13-P-O14
83	5	801	PC1	C11-O13-P-O11
83	5	801	PC1	C1-O11-P-O12
83	5	802	PC1	C1-O11-P-O12
83	5	802	PC1	C1-O11-P-O13
83	5	807	PC1	C11-O13-P-O12
83	5	807	PC1	C1-O11-P-O14
83	5	807	PC1	C1-O11-P-O13
83	6	301	PC1	C11-O13-P-O14
83	6	301	PC1	C11-O13-P-O11
83	6	301	PC1	C1-O11-P-O12
83	6	301	PC1	C1-O11-P-O14
83	6	301	PC1	C1-O11-P-O13
83	6	302	PC1	C11-O13-P-O12
83	6	302	PC1	C11-O13-P-O11
83	AM	201	PC1	C11-O13-P-O14
83	AM	201	PC1	C11-O13-P-O11
83	AM	201	PC1	C1-O11-P-O12
83	AM	201	PC1	C1-O11-P-O14
83	AM	201	PC1	C1-O11-P-O13
83	J1	400	PC1	C11-O13-P-O12
83	J1	400	PC1	C1-O11-P-O13
83	T1	601	PC1	C11-O13-P-O12
83	T1	601	PC1	C11-O13-P-O14
83	T1	601	PC1	C1-O11-P-O14
83	T1	601	PC1	C1-O11-P-O13
83	X1	201	PC1	C1-O11-P-O12
83	X1	201	PC1	C1-O11-P-O13
83	C4	403	PC1	C11-O13-P-O14
83	C4	403	PC1	C11-O13-P-O11
83	B2	201	PC1	C11-O13-P-O11
83	B2	201	PC1	C1-O11-P-O12
83	B2	201	PC1	C1-O11-P-O14
83	B2	201	PC1	C1-O11-P-O13
83	P1	401	PC1	C11-O13-P-O12
83	P1	401	PC1	C11-O13-P-O14
83	P1	401	PC1	C11-O13-P-O11
83	P1	401	PC1	C1-O11-P-O12
83	P1	401	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
83	P1	401	PC1	C1-O11-P-O13
84	3C	601	HEM	C2B-C3B-CAB-CBB
85	3C	605	U10	C6-C1-C2-C3
85	3C	605	U10	C23-C24-C26-C27
85	3C	605	U10	C25-C24-C26-C27
85	5B	202	U10	C19-C21-C22-C23
88	3E	303	3PE	C11-O13-P-O11
88	3E	303	3PE	C11-O13-P-O12
88	3E	303	3PE	C11-O13-P-O14
88	3d	402	3PE	C11-O13-P-O11
88	3d	402	3PE	C11-O13-P-O14
88	3d	402	3PE	O13-C11-C12-N
88	4	601	3PE	C1-O11-P-O13
88	4	602	3PE	C1-O11-P-O12
88	4	602	3PE	C1-O11-P-O13
88	4	602	3PE	C1-O11-P-O14
88	4	602	3PE	O13-C11-C12-N
88	5	804	3PE	O13-C11-C12-N
88	5	806	3PE	C1-O11-P-O12
88	5	806	3PE	C1-O11-P-O13
88	5	806	3PE	O13-C11-C12-N
88	5B	201	3PE	C1-O11-P-O13
88	5B	201	3PE	C11-O13-P-O11
88	5B	201	3PE	C11-O13-P-O14
88	B8	601	3PE	C1-O11-P-O13
88	B8	601	3PE	C1-O11-P-O14
88	B8	601	3PE	C11-O13-P-O11
88	B8	601	3PE	O13-C11-C12-N
88	S8	303	3PE	O13-C11-C12-N
88	C4	402	3PE	C1-O11-P-O12
88	C4	402	3PE	C1-O11-P-O13
88	C4	402	3PE	C1-O11-P-O14
88	C4	402	3PE	C11-O13-P-O11
88	C4	402	3PE	O13-C11-C12-N
88	AN	301	3PE	C1-O11-P-O13
88	AN	301	3PE	C1-O11-P-O14
88	AN	302	3PE	C11-O13-P-O14
88	AN	302	3PE	O13-C11-C12-N
88	T4	301	3PE	C11-O13-P-O11
88	T4	301	3PE	C11-O13-P-O14
88	T8	201	3PE	C1-O11-P-O13
88	T8	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
88	T8	201	3PE	O13-C11-C12-N
88	P1	402	3PE	C11-O13-P-O14
88	P1	402	3PE	O13-C11-C12-N
88	A3	201	3PE	O13-C11-C12-N
91	AB	201	ZMP	C19-C18-C21-O5
91	AB	201	ZMP	C20-C18-C21-O5
91	AB	201	ZMP	C17-C18-C21-O5
91	AB	201	ZMP	O1-C10-S1-C11
91	AB	201	ZMP	C9-C10-S1-C11
85	3C	605	U10	C12-C11-C9-C10
85	5B	202	U10	C30-C29-C31-C32
85	3C	605	U10	C12-C11-C9-C8
85	5B	202	U10	C28-C29-C31-C32
85	3C	605	U10	C1M-C1-C6-C7
85	3C	605	U10	C2-C1-C6-C7
85	3C	605	U10	C15-C14-C16-C17
85	5B	202	U10	C35-C34-C36-C37
85	3C	605	U10	C13-C14-C16-C17
85	5B	202	U10	C23-C24-C26-C27
85	5B	202	U10	C33-C34-C36-C37
85	5B	202	U10	C9-C11-C12-C13
85	5B	202	U10	C29-C31-C32-C33
85	5B	202	U10	C34-C36-C37-C38
82	3C	603	CDL	CA2-C1-CB2-OB2
82	R	201	CDL	CA2-C1-CB2-OB2
83	3E	304	PC1	C11-C12-N-C15
83	TC	101	PC1	C11-C12-N-C15
85	5B	202	U10	C25-C24-C26-C27
82	3C	603	CDL	O1-C1-CB2-OB2
82	R	201	CDL	O1-C1-CB2-OB2
85	5B	202	U10	C24-C26-C27-C28
85	5B	202	U10	C49-C51-C52-C53
83	3E	304	PC1	C11-C12-N-C14
83	3I	601	PC1	C11-C12-N-C15
83	6	302	PC1	C11-C12-N-C15
83	X1	201	PC1	C11-C12-N-C14
83	B6	201	PC1	C11-C12-N-C13
83	B2	201	PC1	C11-C12-N-C14
83	TC	101	PC1	C11-C12-N-C14
82	5	805	CDL	CA5-C11-C12-C13
82	R	201	CDL	CA5-C11-C12-C13
82	3H	202	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
88	5	806	3PE	C21-C22-C23-C24
82	3c	505	CDL	CA7-C31-C32-C33
82	P2	201	CDL	CB7-C71-C72-C73
83	3I	601	PC1	C11-C12-N-C14
83	3c	501	PC1	C11-C12-N-C15
83	6	302	PC1	C11-C12-N-C13
83	B2	201	PC1	C11-C12-N-C13
83	P1	401	PC1	C11-C12-N-C15
83	B6	201	PC1	C11-C12-N-C15
83	TC	101	PC1	C11-C12-N-C13
82	AN	304	CDL	C34-C35-C36-C37
88	S8	303	3PE	C2A-C2B-C2C-C2D
83	3E	302	PC1	C34-C35-C36-C37
88	A3	201	3PE	C22-C23-C24-C25
82	P2	201	CDL	C12-C13-C14-C15
82	AM	202	CDL	C34-C35-C36-C37
82	3C	603	CDL	C31-C32-C33-C34
83	3C	607	PC1	C11-C12-N-C14
83	3E	304	PC1	C11-C12-N-C13
83	X1	201	PC1	C11-C12-N-C13
83	P1	401	PC1	C11-C12-N-C14
82	P2	201	CDL	CA5-C11-C12-C13
82	3b	602	CDL	C52-C53-C54-C55
82	5	805	CDL	C72-C73-C74-C75
83	B6	201	PC1	C2D-C2E-C2F-C2G
83	B2	201	PC1	C3D-C3E-C3F-C3G
82	3I	603	CDL	C52-C53-C54-C55
82	P2	201	CDL	C52-C53-C54-C55
82	P2	201	CDL	C57-C58-C59-C60
83	1	302	PC1	C34-C35-C36-C37
83	3E	302	PC1	C26-C27-C28-C29
83	3I	601	PC1	C11-C12-N-C13
83	3c	501	PC1	C11-C12-N-C13
83	3c	501	PC1	C11-C12-N-C14
83	3c	506	PC1	C11-C12-N-C14
83	6	302	PC1	C11-C12-N-C14
83	X1	201	PC1	C11-C12-N-C15
83	B6	201	PC1	C11-C12-N-C14
83	B2	201	PC1	C11-C12-N-C15
83	P1	401	PC1	C11-C12-N-C13
82	A1	101	CDL	C51-C52-C53-C54
83	3E	302	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
91	AB	201	ZMP	C2-C3-C4-C5
83	5	807	PC1	C21-C22-C23-C24
82	AM	202	CDL	OB5-CB3-CB4-OB6
82	TD	101	CDL	OB5-CB3-CB4-OB6
88	AN	302	3PE	C23-C24-C25-C26
82	AL	301	CDL	CA5-C11-C12-C13
83	B6	201	PC1	O21-C2-C3-O31
82	BM	301	CDL	C75-C76-C77-C78
83	B6	201	PC1	C25-C26-C27-C28
85	5B	202	U10	C43-C44-C46-C47
83	3I	602	PC1	C35-C36-C37-C38
83	3J	101	PC1	C35-C36-C37-C38
83	B2	201	PC1	C34-C35-C36-C37
83	TC	101	PC1	C25-C26-C27-C28
83	3	201	PC1	C11-C12-N-C14
83	C4	403	PC1	C11-C12-N-C15
83	AN	303	PC1	C11-C12-N-C15
82	3c	504	CDL	OB5-CB3-CB4-CB6
82	R	201	CDL	OB5-CB3-CB4-CB6
82	BM	301	CDL	C76-C77-C78-C79
83	3e	301	PC1	C2D-C2E-C2F-C2G
88	3E	303	3PE	C26-C27-C28-C29
83	3	201	PC1	C31-C32-C33-C34
83	6	302	PC1	C31-C32-C33-C34
82	3I	604	CDL	CB3-CB4-CB6-OB8
82	5	803	CDL	CB3-CB4-CB6-OB8
82	AM	202	CDL	CA3-CA4-CA6-OA8
88	T4	301	3PE	C1-C2-C3-O31
82	3b	602	CDL	C55-C56-C57-C58
88	3E	303	3PE	C24-C25-C26-C27
82	R	201	CDL	CB7-C71-C72-C73
83	3C	607	PC1	C11-C12-N-C13
83	3c	506	PC1	C11-C12-N-C13
83	T1	601	PC1	C11-C12-N-C13
85	5B	202	U10	C45-C44-C46-C47
85	5B	202	U10	C12-C11-C9-C8
82	3B	701	CDL	OA5-CA3-CA4-OA6
82	3B	701	CDL	OB5-CB3-CB4-OB6
82	3c	505	CDL	OB5-CB3-CB4-OB6
88	B8	601	3PE	O11-C1-C2-O21
82	5	805	CDL	C78-C79-C80-C81
82	C4	401	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
83	3E	302	PC1	C24-C25-C26-C27
82	P2	201	CDL	C37-C38-C39-C40
83	3C	606	PC1	O21-C2-C3-O31
83	C4	403	PC1	O21-C2-C3-O31
83	3	201	PC1	C11-C12-N-C13
85	3C	605	U10	C9-C11-C12-C13
82	3I	603	CDL	CA7-C31-C32-C33
85	5B	202	U10	C12-C11-C9-C10
83	6	302	PC1	C35-C36-C37-C38
82	3b	602	CDL	CA4-CA3-OA5-PA1
82	3c	504	CDL	C1-CB2-OB2-PB2
82	AL	301	CDL	CA4-CA3-OA5-PA1
88	TA	201	3PE	C2-C1-O11-P
82	5	805	CDL	C76-C77-C78-C79
82	BM	301	CDL	C35-C36-C37-C38
82	1	301	CDL	OB5-CB3-CB4-CB6
82	3H	202	CDL	OA5-CA3-CA4-CA6
82	3H	203	CDL	OB5-CB3-CB4-CB6
82	3b	602	CDL	OA5-CA3-CA4-CA6
82	5	803	CDL	OB5-CB3-CB4-CB6
82	AM	202	CDL	OB5-CB3-CB4-CB6
82	TD	101	CDL	OB5-CB3-CB4-CB6
82	BM	301	CDL	OB5-CB3-CB4-CB6
83	3C	607	PC1	C11-C12-N-C15
83	T1	601	PC1	C11-C12-N-C15
83	C4	403	PC1	C11-C12-N-C14
83	AN	303	PC1	C11-C12-N-C13
82	5	803	CDL	C17-C18-C19-C20
83	3b	601	PC1	C23-C24-C25-C26
88	C4	402	3PE	C38-C39-C3A-C3B
85	3C	605	U10	C1M-C1-C2-C3
82	A1	101	CDL	CA3-CA4-CA6-OA8
82	R	201	CDL	CA3-CA4-CA6-OA8
83	1	302	PC1	C1-C2-C3-O31
83	B6	201	PC1	C1-C2-C3-O31
83	C4	403	PC1	C1-C2-C3-O31
88	C4	402	3PE	C2F-C2G-C2H-C2I
83	3e	301	PC1	C2F-C2G-C2H-C2I
88	5	804	3PE	C31-C32-C33-C34
82	3b	602	CDL	OA5-CA3-CA4-OA6
82	3c	504	CDL	OB5-CB3-CB4-OB6
82	R	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
82	AN	304	CDL	OB5-CB3-CB4-OB6
82	T7	201	CDL	OB5-CB3-CB4-OB6
88	S8	303	3PE	O11-C1-C2-O21
82	3I	603	CDL	C54-C55-C56-C57
82	C4	401	CDL	C1-CB2-OB2-PB2
84	3C	601	HEM	C3D-CAD-CBD-CGD
84	3c	503	HEM	C3D-CAD-CBD-CGD
82	BM	301	CDL	C38-C39-C40-C41
82	3H	202	CDL	OB6-CB4-CB6-OB8
82	3I	603	CDL	OA6-CA4-CA6-OA8
82	5	803	CDL	OB6-CB4-CB6-OB8
82	R	201	CDL	OA6-CA4-CA6-OA8
83	3C	604	PC1	O21-C2-C3-O31
83	3I	602	PC1	C11-C12-N-C15
83	3j	101	PC1	C11-C12-N-C13
82	BM	301	CDL	O1-C1-CB2-OB2
82	B4	201	CDL	O1-C1-CA2-OA2
82	3I	603	CDL	C31-C32-C33-C34
83	3C	606	PC1	C36-C37-C38-C39
82	3b	602	CDL	C33-C34-C35-C36
88	P1	402	3PE	C37-C38-C39-C3A
82	C4	401	CDL	C35-C36-C37-C38
82	C4	401	CDL	OB5-CB3-CB4-CB6
83	3b	601	PC1	O11-C1-C2-C3
83	X1	201	PC1	O11-C1-C2-C3
88	S8	303	3PE	O11-C1-C2-C3
82	A1	101	CDL	C1-CB2-OB2-PB2
83	B2	201	PC1	C22-C23-C24-C25
91	AB	201	ZMP	C5-C6-C7-C8
83	J1	400	PC1	O31-C31-C32-C33
84	3C	602	HEM	C2B-C3B-CAB-CBB
84	3c	502	HEM	C2B-C3B-CAB-CBB
82	3H	203	CDL	OB5-CB3-CB4-OB6
82	5	803	CDL	OB5-CB3-CB4-OB6
83	3J	101	PC1	O11-C1-C2-O21
82	3B	701	CDL	CA3-CA4-CA6-OA8
85	3C	605	U10	C19-C21-C22-C23
84	3C	601	HEM	C4B-C3B-CAB-CBB
82	AL	301	CDL	C52-C51-CB5-OB6
83	J1	400	PC1	C12-C11-O13-P
82	3B	701	CDL	OA6-CA4-CA6-OA8
82	3I	604	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
82	3b	602	CDL	OB6-CB4-CB6-OB8
82	A1	101	CDL	OA6-CA4-CA6-OA8
83	1	302	PC1	O21-C2-C3-O31
88	3d	402	3PE	O21-C2-C3-O31
88	T4	301	3PE	O21-C2-C3-O31
83	6	302	PC1	C36-C37-C38-C39
88	4	602	3PE	C36-C37-C38-C39
83	3b	601	PC1	C22-C23-C24-C25
88	P1	402	3PE	C2C-C2D-C2E-C2F
83	3I	602	PC1	C11-C12-N-C13
83	3J	101	PC1	C11-C12-N-C14
83	3J	101	PC1	C11-C12-N-C15
83	3j	101	PC1	C11-C12-N-C14
83	AM	201	PC1	C11-C12-N-C14
83	AM	201	PC1	C11-C12-N-C15
82	A1	101	CDL	CA4-CA3-OA5-PA1
83	P1	401	PC1	C2-C1-O11-P
88	S8	303	3PE	C2-C1-O11-P
83	1	302	PC1	O13-C11-C12-N
83	3C	604	PC1	O13-C11-C12-N
83	3E	302	PC1	O13-C11-C12-N
83	3E	304	PC1	O13-C11-C12-N
83	3F	102	PC1	O13-C11-C12-N
83	3b	601	PC1	O13-C11-C12-N
83	3e	301	PC1	O13-C11-C12-N
83	5	802	PC1	O13-C11-C12-N
83	J1	400	PC1	O13-C11-C12-N
83	B2	201	PC1	O13-C11-C12-N
88	P1	402	3PE	C26-C27-C28-C29
82	TD	101	CDL	O1-C1-CA2-OA2
84	3C	602	HEM	C2A-CAA-CBA-CGA
82	AM	202	CDL	C33-C34-C35-C36
83	3c	506	PC1	C11-C12-N-C15
82	3B	701	CDL	OB5-CB3-CB4-CB6
82	3c	505	CDL	OB5-CB3-CB4-CB6
82	B4	201	CDL	OB5-CB3-CB4-CB6
82	T7	201	CDL	OB5-CB3-CB4-CB6
83	3J	101	PC1	O11-C1-C2-C3
85	3H	201	U10	C18-C19-C21-C22
82	5	805	CDL	C13-C14-C15-C16
82	AN	304	CDL	C33-C34-C35-C36
82	3b	602	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
82	5	805	CDL	C36-C37-C38-C39
82	3G	401	CDL	C1-CA2-OA2-PA1
82	B4	201	CDL	C1-CA2-OA2-PA1
83	X1	201	PC1	C2-C1-O11-P
83	TC	101	PC1	C2-C1-O11-P
88	A3	201	3PE	C2-C1-O11-P
82	3C	603	CDL	OB5-CB3-CB4-OB6
82	3H	202	CDL	OA5-CA3-CA4-OA6
82	C4	401	CDL	OB5-CB3-CB4-OB6
82	B4	201	CDL	OB5-CB3-CB4-OB6
83	3b	601	PC1	O11-C1-C2-O21
82	5	803	CDL	C56-C57-C58-C59
83	3	201	PC1	C11-C12-N-C15
83	3b	601	PC1	C11-C12-N-C14
82	AM	202	CDL	OA6-CA4-CA6-OA8
82	1	301	CDL	CB3-CB4-CB6-OB8
82	3I	603	CDL	CA3-CA4-CA6-OA8
83	3C	604	PC1	C1-C2-C3-O31
83	3C	606	PC1	C1-C2-C3-O31
88	3d	402	3PE	C1-C2-C3-O31
82	3I	603	CDL	C56-C57-C58-C59
82	3G	401	CDL	C55-C56-C57-C58
82	5	803	CDL	C22-C23-C24-C25
85	3H	201	U10	C5-C4-O4-C4M
82	P2	201	CDL	C11-C12-C13-C14
82	1	301	CDL	CB2-OB2-PB2-OB4
82	1	301	CDL	CB2-OB2-PB2-OB5
82	2B	201	CDL	CA2-OA2-PA1-OA4
82	2B	201	CDL	CB3-OB5-PB2-OB2
82	3	202	CDL	CB3-OB5-PB2-OB3
82	3B	701	CDL	CA3-OA5-PA1-OA3
82	3B	701	CDL	CB2-OB2-PB2-OB3
82	3B	701	CDL	CB3-OB5-PB2-OB3
82	3C	603	CDL	CA3-OA5-PA1-OA2
82	3C	603	CDL	CA3-OA5-PA1-OA3
82	3C	603	CDL	CA3-OA5-PA1-OA4
82	3G	401	CDL	CA2-OA2-PA1-OA3
82	3G	401	CDL	CA2-OA2-PA1-OA4
82	3G	401	CDL	CA2-OA2-PA1-OA5
82	3G	401	CDL	CA3-OA5-PA1-OA4
82	3H	202	CDL	CA2-OA2-PA1-OA4
82	3H	202	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
82	3H	202	CDL	CA3-OA5-PA1-OA2
82	3H	203	CDL	CA2-OA2-PA1-OA3
82	3I	603	CDL	CA3-OA5-PA1-OA2
82	3I	604	CDL	CA3-OA5-PA1-OA4
82	3b	602	CDL	CA2-OA2-PA1-OA3
82	3b	602	CDL	CA2-OA2-PA1-OA5
82	3b	602	CDL	CA3-OA5-PA1-OA3
82	3c	504	CDL	CA3-OA5-PA1-OA4
82	3c	504	CDL	CB2-OB2-PB2-OB4
82	3c	505	CDL	CA2-OA2-PA1-OA4
82	3c	505	CDL	CA2-OA2-PA1-OA5
82	3c	505	CDL	CA3-OA5-PA1-OA4
82	3i	201	CDL	CA2-OA2-PA1-OA5
82	3i	201	CDL	CB3-OB5-PB2-OB2
82	5	803	CDL	CA3-OA5-PA1-OA4
82	5	805	CDL	CA2-OA2-PA1-OA3
82	5	805	CDL	CA2-OA2-PA1-OA4
82	5	805	CDL	CA2-OA2-PA1-OA5
82	5	805	CDL	CA3-OA5-PA1-OA2
82	5	805	CDL	CA3-OA5-PA1-OA3
82	5	805	CDL	CB3-OB5-PB2-OB4
82	AL	301	CDL	CA3-OA5-PA1-OA3
82	TD	101	CDL	CA2-OA2-PA1-OA5
82	T1	602	CDL	CA3-OA5-PA1-OA4
82	T1	602	CDL	CB3-OB5-PB2-OB2
82	A1	101	CDL	CB3-OB5-PB2-OB2
82	A1	101	CDL	CB3-OB5-PB2-OB3
82	A1	101	CDL	CB3-OB5-PB2-OB4
82	R	201	CDL	CB3-OB5-PB2-OB3
82	BM	301	CDL	CA3-OA5-PA1-OA3
82	C4	401	CDL	CB2-OB2-PB2-OB3
82	AN	304	CDL	CA3-OA5-PA1-OA2
82	AN	304	CDL	CA3-OA5-PA1-OA3
82	AN	304	CDL	CB3-OB5-PB2-OB4
82	B4	201	CDL	CB2-OB2-PB2-OB5
82	P2	201	CDL	CB3-OB5-PB2-OB4
82	T7	201	CDL	CA2-OA2-PA1-OA4
82	T7	201	CDL	CB2-OB2-PB2-OB3
82	T7	201	CDL	CB3-OB5-PB2-OB4
83	1	302	PC1	C11-O13-P-O11
83	1	302	PC1	C1-O11-P-O12
83	3	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
83	3C	604	PC1	C1-O11-P-O13
83	3C	606	PC1	C1-O11-P-O14
83	3C	607	PC1	C11-O13-P-O14
83	3C	607	PC1	C1-O11-P-O14
83	3C	607	PC1	C1-O11-P-O13
83	3E	302	PC1	C1-O11-P-O12
83	3E	302	PC1	C11-C12-N-C13
83	3F	102	PC1	C11-O13-P-O12
83	3F	102	PC1	C11-O13-P-O14
83	3F	102	PC1	C11-O13-P-O11
83	3F	102	PC1	C1-O11-P-O12
83	3I	601	PC1	C11-O13-P-O14
83	3I	601	PC1	C11-O13-P-O11
83	3I	601	PC1	C1-O11-P-O14
83	3b	601	PC1	C11-O13-P-O11
83	3c	501	PC1	C11-O13-P-O12
83	3e	301	PC1	C11-O13-P-O14
83	3g	401	PC1	C11-O13-P-O14
83	5	801	PC1	C1-O11-P-O13
83	5	802	PC1	C11-O13-P-O14
83	5	802	PC1	C1-O11-P-O14
83	5	807	PC1	C11-O13-P-O14
83	5	807	PC1	C11-O13-P-O11
83	5	807	PC1	C1-O11-P-O12
83	AM	201	PC1	C11-O13-P-O12
83	J1	400	PC1	C11-O13-P-O14
83	J1	400	PC1	C11-O13-P-O11
83	J1	400	PC1	C1-O11-P-O14
83	T1	601	PC1	C11-O13-P-O11
83	T1	601	PC1	C1-O11-P-O12
83	T1	601	PC1	C11-C12-N-C14
83	C4	403	PC1	C11-O13-P-O12
83	C4	403	PC1	C11-C12-N-C13
83	AN	303	PC1	C11-C12-N-C14
88	3E	303	3PE	O13-C11-C12-N
88	3d	402	3PE	C11-O13-P-O12
88	4	601	3PE	C1-O11-P-O14
88	4	602	3PE	C11-O13-P-O14
88	5	804	3PE	C11-O13-P-O14
88	5B	201	3PE	C1-O11-P-O14
88	5B	201	3PE	C11-O13-P-O12
88	B8	601	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
88	C4	402	3PE	C11-O13-P-O14
88	AN	302	3PE	C11-O13-P-O11
88	T8	201	3PE	C1-O11-P-O12
83	3E	302	PC1	C3A-C3B-C3C-C3D
82	2B	201	CDL	CA4-CA3-OA5-PA1
82	3B	701	CDL	C1-CB2-OB2-PB2
82	3C	603	CDL	C1-CB2-OB2-PB2
82	3G	401	CDL	C1-CB2-OB2-PB2
82	3c	505	CDL	C1-CA2-OA2-PA1
82	R	201	CDL	C1-CB2-OB2-PB2
83	5	802	PC1	C2-C1-O11-P
83	C4	403	PC1	C2-C1-O11-P
88	3d	402	3PE	C2-C1-O11-P
88	5	804	3PE	C2-C1-O11-P
88	A3	201	3PE	C23-C24-C25-C26
83	3E	302	PC1	C27-C28-C29-C2A
82	3b	602	CDL	C72-C73-C74-C75
83	6	302	PC1	C3C-C3D-C3E-C3F
88	TA	201	3PE	O32-C31-C32-C33
83	3I	602	PC1	C11-C12-N-C14
83	3b	601	PC1	C11-C12-N-C13
82	AN	304	CDL	OB5-CB3-CB4-CB6
83	3C	606	PC1	C23-C24-C25-C26
82	5	803	CDL	C14-C15-C16-C17
83	B2	201	PC1	C25-C26-C27-C28
82	C4	401	CDL	CA5-C11-C12-C13
82	3I	604	CDL	C1-CA2-OA2-PA1
82	5	805	CDL	C52-C51-CB5-OB6
83	3I	602	PC1	C26-C27-C28-C29
83	6	302	PC1	C25-C26-C27-C28
82	R	201	CDL	C72-C73-C74-C75
88	T8	201	3PE	C27-C28-C29-C2A
82	3b	602	CDL	CB3-CB4-CB6-OB8
88	T8	201	3PE	C1-C2-C3-O31
82	R	201	CDL	C33-C34-C35-C36
82	1	301	CDL	C72-C71-CB7-OB8
82	T1	602	CDL	C72-C71-CB7-OB8
84	3c	503	HEM	C2B-C3B-CAB-CBB
83	3j	101	PC1	C11-C12-N-C15
82	5	803	CDL	CA5-C11-C12-C13
88	TA	201	3PE	O31-C31-C32-C33
83	3I	601	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
82	T1	602	CDL	C1-CA2-OA2-PA1
88	4	601	3PE	C2-C1-O11-P
82	AM	202	CDL	C11-C12-C13-C14
82	C4	401	CDL	C20-C21-C22-C23
88	AN	301	3PE	C36-C37-C38-C39
82	3C	603	CDL	OB5-CB3-CB4-CB6
84	3C	602	HEM	C4B-C3B-CAB-CBB
83	AM	201	PC1	O31-C31-C32-C33
83	3E	302	PC1	C11-C12-N-C15
83	3J	101	PC1	C11-C12-N-C13
83	AM	201	PC1	C11-C12-N-C13
88	S8	303	3PE	C27-C28-C29-C2A
83	3I	602	PC1	C21-C22-C23-C24
83	B2	201	PC1	C23-C24-C25-C26
82	T7	201	CDL	CA4-CA3-OA5-PA1
85	3H	201	U10	C20-C19-C21-C22
88	AN	301	3PE	C1-C2-C3-O31
82	AM	202	CDL	C12-C13-C14-C15
83	5	802	PC1	C22-C23-C24-C25
82	3i	201	CDL	CA6-CA4-OA6-CA5
82	5	805	CDL	CB3-CB4-OB6-CB5
88	4	601	3PE	C1-C2-O21-C21
88	A3	201	3PE	C1-C2-O21-C21
88	C4	402	3PE	C23-C24-C25-C26
90	A9	401	NDP	O4D-C1D-N1N-C6N
82	BM	301	CDL	C34-C35-C36-C37
82	3G	401	CDL	CB7-C71-C72-C73
82	3G	401	CDL	OA5-CA3-CA4-OA6
88	C4	402	3PE	C32-C33-C34-C35
82	3H	202	CDL	C32-C33-C34-C35
82	3B	701	CDL	CA4-CA3-OA5-PA1
82	AM	202	CDL	CA4-CA3-OA5-PA1
82	B8	603	CDL	CA4-CA3-OA5-PA1
82	T1	602	CDL	CB4-CB3-OB5-PB2
82	C4	401	CDL	CA4-CA3-OA5-PA1
83	3C	604	PC1	C2-C1-O11-P
83	3J	101	PC1	C2-C1-O11-P
85	3H	201	U10	C15-C14-C16-C17
82	C4	401	CDL	C38-C39-C40-C41
83	3E	302	PC1	C39-C3A-C3B-C3C
82	3b	602	CDL	OB5-CB3-CB4-CB6
88	B8	601	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
83	1	302	PC1	C32-C33-C34-C35
82	1	301	CDL	OB6-CB4-CB6-OB8
83	3E	302	PC1	C2E-C2F-C2G-C2H
83	3C	604	PC1	C11-C12-N-C14
83	3F	102	PC1	C11-C12-N-C15
83	3b	601	PC1	C11-C12-N-C15
82	3B	701	CDL	CA2-C1-CB2-OB2
82	3C	603	CDL	C12-C13-C14-C15
84	3c	502	HEM	CAD-CBD-CGD-O2D
83	B6	201	PC1	C34-C35-C36-C37
86	3d	401	HEC	CAA-CBA-CGA-O2A
84	3C	602	HEM	CAA-CBA-CGA-O1A
84	3C	602	HEM	CAA-CBA-CGA-O2A
82	5	803	CDL	C12-C13-C14-C15
82	3	202	CDL	C1-CB2-OB2-PB2
82	3H	203	CDL	CB4-CB3-OB5-PB2
94	V1	501	FMN	C4'-C5'-O5'-P
91	AB	201	ZMP	C1-C2-C3-C4
84	3c	502	HEM	C3D-CAD-CBD-CGD
83	P1	401	PC1	C33-C34-C35-C36
83	5	807	PC1	C1-C2-C3-O31
85	5B	202	U10	C44-C46-C47-C48
83	X1	201	PC1	C38-C39-C3A-C3B
82	TD	101	CDL	OA5-CA3-CA4-OA6
82	3b	602	CDL	C32-C31-CA7-OA8
83	5	801	PC1	C22-C23-C24-C25
83	3J	101	PC1	C23-C24-C25-C26
88	C4	402	3PE	C36-C37-C38-C39
86	3D	401	HEC	CAA-CBA-CGA-O2A
82	3B	701	CDL	OA5-CA3-CA4-CA6
83	3b	601	PC1	O21-C2-C3-O31
88	AN	301	3PE	O21-C2-C3-O31
82	AM	202	CDL	CB4-CB3-OB5-PB2
82	TD	101	CDL	C1-CA2-OA2-PA1
88	4	601	3PE	O31-C31-C32-C33
90	A9	401	NDP	C2D-C1D-N1N-C6N
84	3c	503	HEM	CAA-CBA-CGA-O2A
86	3d	401	HEC	CAA-CBA-CGA-O1A
82	R	201	CDL	C11-C12-C13-C14
82	3G	401	CDL	C72-C71-CB7-OB8
83	3E	302	PC1	C11-C12-N-C14
84	3c	502	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
83	3c	506	PC1	C22-C23-C24-C25
88	4	602	3PE	O21-C21-C22-C23
82	3C	603	CDL	CA3-CA4-OA6-CA5
82	3C	603	CDL	CA6-CA4-OA6-CA5
82	3I	603	CDL	CA3-CA4-OA6-CA5
82	3I	603	CDL	CA6-CA4-OA6-CA5
82	TD	101	CDL	CA3-CA4-OA6-CA5
82	C4	401	CDL	CA6-CA4-OA6-CA5
83	3J	101	PC1	C3-C2-O21-C21
83	3b	601	PC1	C3-C2-O21-C21
83	X1	201	PC1	C3-C2-O21-C21
83	AN	303	PC1	C3-C2-O21-C21
82	C4	401	CDL	C63-C64-C65-C66
82	3H	202	CDL	C11-C12-C13-C14
82	3I	603	CDL	O1-C1-CB2-OB2
84	3c	503	HEM	CAA-CBA-CGA-O1A
86	3D	401	HEC	CAA-CBA-CGA-O1A
82	AN	304	CDL	C1-CA2-OA2-PA1
83	3c	506	PC1	C2-C1-O11-P
82	3b	602	CDL	OB5-CB3-CB4-OB6
83	3c	501	PC1	O11-C1-C2-O21
88	3d	402	3PE	O11-C1-C2-O21
84	3c	502	HEM	C4B-C3B-CAB-CBB
84	3c	503	HEM	C4B-C3B-CAB-CBB
82	3I	603	CDL	C73-C74-C75-C76
88	TA	201	3PE	C12-C11-O13-P
82	3I	603	CDL	C58-C59-C60-C61
82	AN	304	CDL	C37-C38-C39-C40
83	AN	303	PC1	C34-C35-C36-C37
82	3I	603	CDL	C72-C71-CB7-OB8
82	P2	201	CDL	C52-C51-CB5-OB6
88	5B	201	3PE	O21-C21-C22-C23
82	3I	603	CDL	OB5-CB3-CB4-CB6
82	A1	101	CDL	OB5-CB3-CB4-CB6
82	3B	701	CDL	CA7-C31-C32-C33
83	3C	604	PC1	C31-C32-C33-C34
83	T1	601	PC1	O21-C21-C22-C23
82	3c	505	CDL	C1-CB2-OB2-PB2
82	3	202	CDL	C12-C11-CA5-OA6
82	3G	401	CDL	C52-C51-CB5-OB6
82	AL	301	CDL	C72-C71-CB7-OB8
83	X1	201	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
88	5	806	3PE	O31-C31-C32-C33
83	B6	201	PC1	C27-C28-C29-C2A
83	3c	506	PC1	O31-C31-C32-C33
83	AM	201	PC1	O21-C21-C22-C23
83	P1	401	PC1	O31-C31-C32-C33
88	P1	402	3PE	O31-C31-C32-C33
83	6	302	PC1	C34-C35-C36-C37
83	1	302	PC1	O31-C31-C32-C33
83	3b	601	PC1	O21-C21-C22-C23
82	C4	401	CDL	C60-C61-C62-C63
83	3C	604	PC1	C11-C12-N-C13
88	AN	301	3PE	C22-C23-C24-C25
88	P1	402	3PE	C29-C2A-C2B-C2C
83	B2	201	PC1	O31-C31-C32-C33
83	P1	401	PC1	O21-C21-C22-C23
82	3G	401	CDL	C62-C63-C64-C65
88	3E	303	3PE	C31-C32-C33-C34
82	BM	301	CDL	C52-C51-CB5-OB6
88	C4	402	3PE	C2C-C2D-C2E-C2F
82	3b	602	CDL	C72-C71-CB7-OB8
82	3i	201	CDL	C52-C51-CB5-OB6
82	A1	101	CDL	C52-C51-CB5-OB6
83	C4	403	PC1	O21-C21-C22-C23
88	AN	302	3PE	O21-C21-C22-C23
82	3H	202	CDL	CB3-CB4-CB6-OB8
83	3E	302	PC1	C1-C2-C3-O31
83	3F	102	PC1	C11-C12-N-C13
83	5	807	PC1	C3A-C3B-C3C-C3D
82	3c	505	CDL	C72-C71-CB7-OB8
83	3C	607	PC1	O21-C21-C22-C23
88	T8	201	3PE	O31-C31-C32-C33
82	TD	101	CDL	OA6-CA4-CA6-OA8
83	5	807	PC1	O21-C2-C3-O31
88	S8	303	3PE	O21-C2-C3-O31
83	3E	302	PC1	C3C-C3D-C3E-C3F
82	1	301	CDL	C12-C11-CA5-OA6
82	2B	201	CDL	C72-C71-CB7-OB8
82	P2	201	CDL	C72-C71-CB7-OB8
88	AN	302	3PE	O31-C31-C32-C33
83	TC	101	PC1	C2C-C2D-C2E-C2F
88	P1	402	3PE	C3A-C3B-C3C-C3D
88	TA	201	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
82	T1	602	CDL	C12-C11-CA5-OA6
82	A1	101	CDL	C57-C58-C59-C60
88	4	601	3PE	C26-C27-C28-C29
82	3i	201	CDL	CA3-CA4-OA6-CA5
82	5	805	CDL	CB6-CB4-OB6-CB5
82	C4	401	CDL	CA3-CA4-OA6-CA5
83	3J	101	PC1	C1-C2-O21-C21
83	3c	501	PC1	C1-C2-O21-C21
83	3c	501	PC1	C3-C2-O21-C21
83	X1	201	PC1	C1-C2-O21-C21
83	C4	403	PC1	C1-C2-O21-C21
83	C4	403	PC1	C3-C2-O21-C21
83	AN	303	PC1	C1-C2-O21-C21
88	3d	402	3PE	C1-C2-O21-C21
88	3d	402	3PE	C3-C2-O21-C21
85	3H	201	U10	C3-C4-O4-C4M
88	S8	303	3PE	C25-C26-C27-C28
90	A9	401	NDP	O4B-C4B-C5B-O5B
92	B8	602	ADP	O4'-C4'-C5'-O5'
88	C4	402	3PE	C29-C2A-C2B-C2C
82	R	201	CDL	C34-C35-C36-C37
83	3E	302	PC1	C22-C23-C24-C25
83	AN	303	PC1	O21-C21-C22-C23
88	P1	402	3PE	O32-C31-C32-C33
82	AN	304	CDL	C35-C36-C37-C38
88	P1	402	3PE	C22-C23-C24-C25
82	AL	301	CDL	C1-CA2-OA2-PA1
83	J1	400	PC1	O32-C31-C32-C33
88	5	806	3PE	O32-C31-C32-C33
83	3E	302	PC1	C2D-C2E-C2F-C2G
88	C4	402	3PE	C33-C34-C35-C36
82	5	805	CDL	OB5-CB3-CB4-OB6
82	3H	202	CDL	C72-C73-C74-C75
88	3d	402	3PE	C23-C24-C25-C26
82	3I	603	CDL	C11-C12-C13-C14
82	AL	301	CDL	C52-C51-CB5-OB7
82	A1	101	CDL	C52-C51-CB5-OB7
83	T1	601	PC1	O22-C21-C22-C23
83	P1	401	PC1	O22-C21-C22-C23
83	P1	401	PC1	O32-C31-C32-C33
85	3H	201	U10	C2-C3-O3-C3M
83	3E	302	PC1	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
82	3G	401	CDL	C52-C51-CB5-OB7
82	P2	201	CDL	C16-C17-C18-C19
82	3B	701	CDL	CB7-C71-C72-C73
83	3e	301	PC1	C33-C34-C35-C36
88	B8	601	3PE	C26-C27-C28-C29
83	AM	201	PC1	O22-C21-C22-C23
83	C4	403	PC1	O22-C21-C22-C23
88	P1	402	3PE	C32-C33-C34-C35
82	3G	401	CDL	C32-C31-CA7-OA8
82	3I	603	CDL	C52-C51-CB5-OB6
88	A3	201	3PE	O21-C21-C22-C23
83	3b	601	PC1	C21-C22-C23-C24
82	3	202	CDL	C12-C11-CA5-OA7
82	3I	603	CDL	C72-C71-CB7-OB9
82	3c	505	CDL	C72-C71-CB7-OB9
83	B2	201	PC1	O32-C31-C32-C33
85	5B	202	U10	C31-C32-C33-C34
83	TC	101	PC1	C29-C2A-C2B-C2C
86	3d	401	HEC	CAD-CBD-CGD-O2D
82	3b	602	CDL	C72-C71-CB7-OB9
82	AL	301	CDL	C72-C71-CB7-OB9
83	X1	201	PC1	O32-C31-C32-C33
88	T8	201	3PE	O32-C31-C32-C33
88	T8	201	3PE	O21-C2-C3-O31
82	B4	201	CDL	CB2-C1-CA2-OA2
88	5	804	3PE	C34-C35-C36-C37
82	P2	201	CDL	C52-C51-CB5-OB7
82	P2	201	CDL	C72-C71-CB7-OB9
88	5B	201	3PE	O22-C21-C22-C23
83	3C	604	PC1	O21-C21-C22-C23
83	3I	602	PC1	O31-C31-C32-C33
82	3i	201	CDL	CB3-CB4-CB6-OB8
82	3i	201	CDL	C52-C51-CB5-OB7
82	BM	301	CDL	C52-C51-CB5-OB7
83	3C	607	PC1	O22-C21-C22-C23
83	3b	601	PC1	O22-C21-C22-C23
88	AN	302	3PE	O32-C31-C32-C33
88	AN	302	3PE	O22-C21-C22-C23
83	3C	604	PC1	C11-C12-N-C15
83	3F	102	PC1	C11-C12-N-C14
86	3D	401	HEC	CAD-CBD-CGD-O2D
83	1	302	PC1	O32-C31-C32-C33

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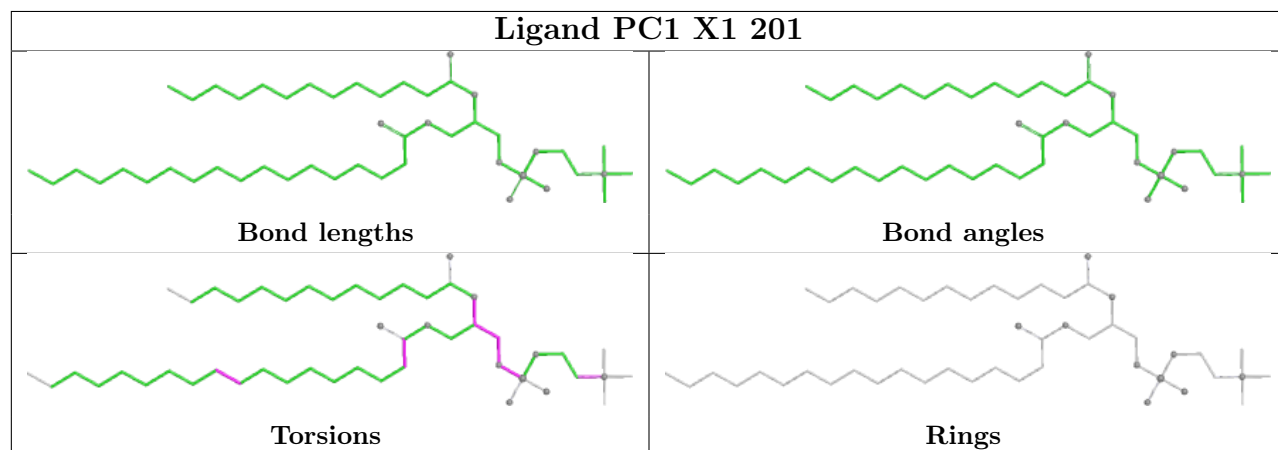
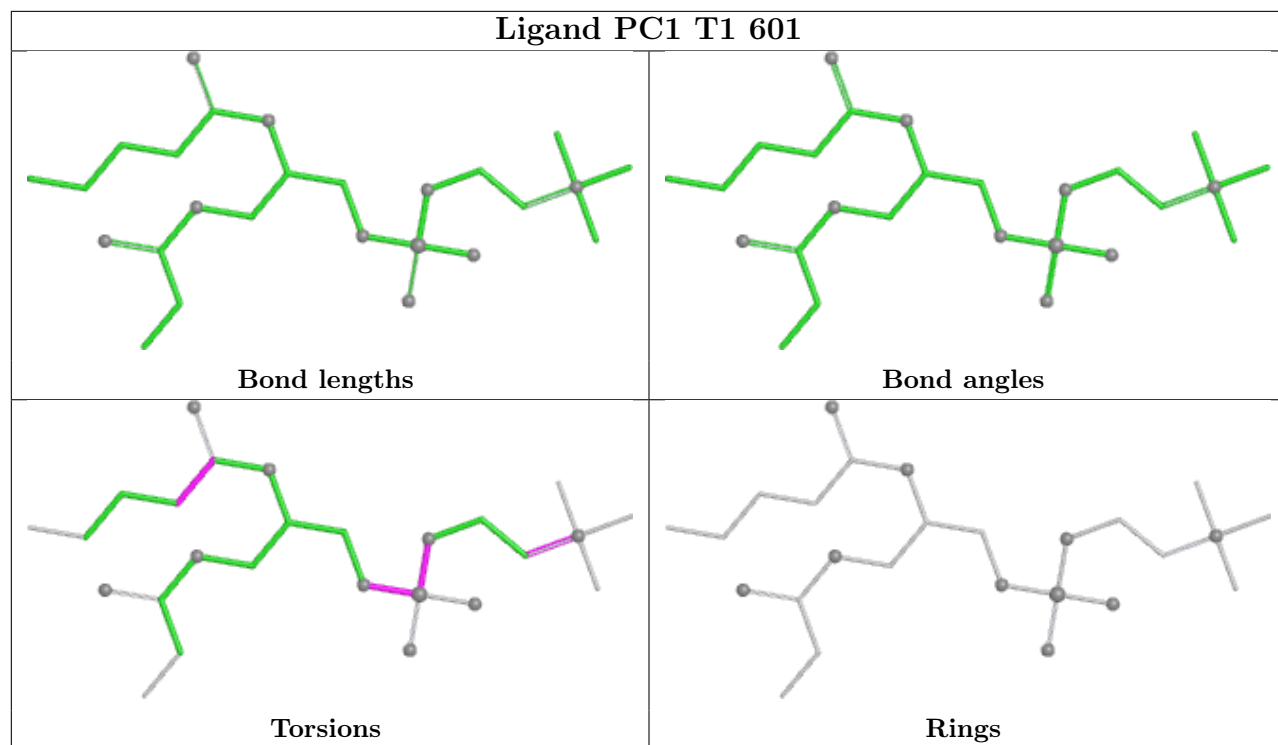
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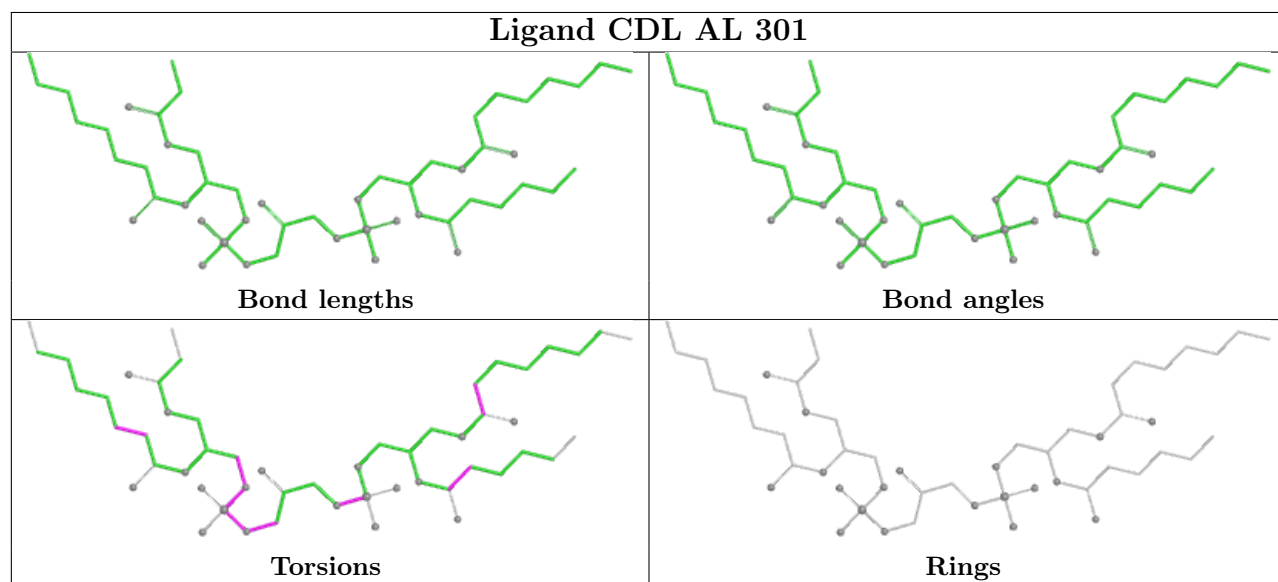
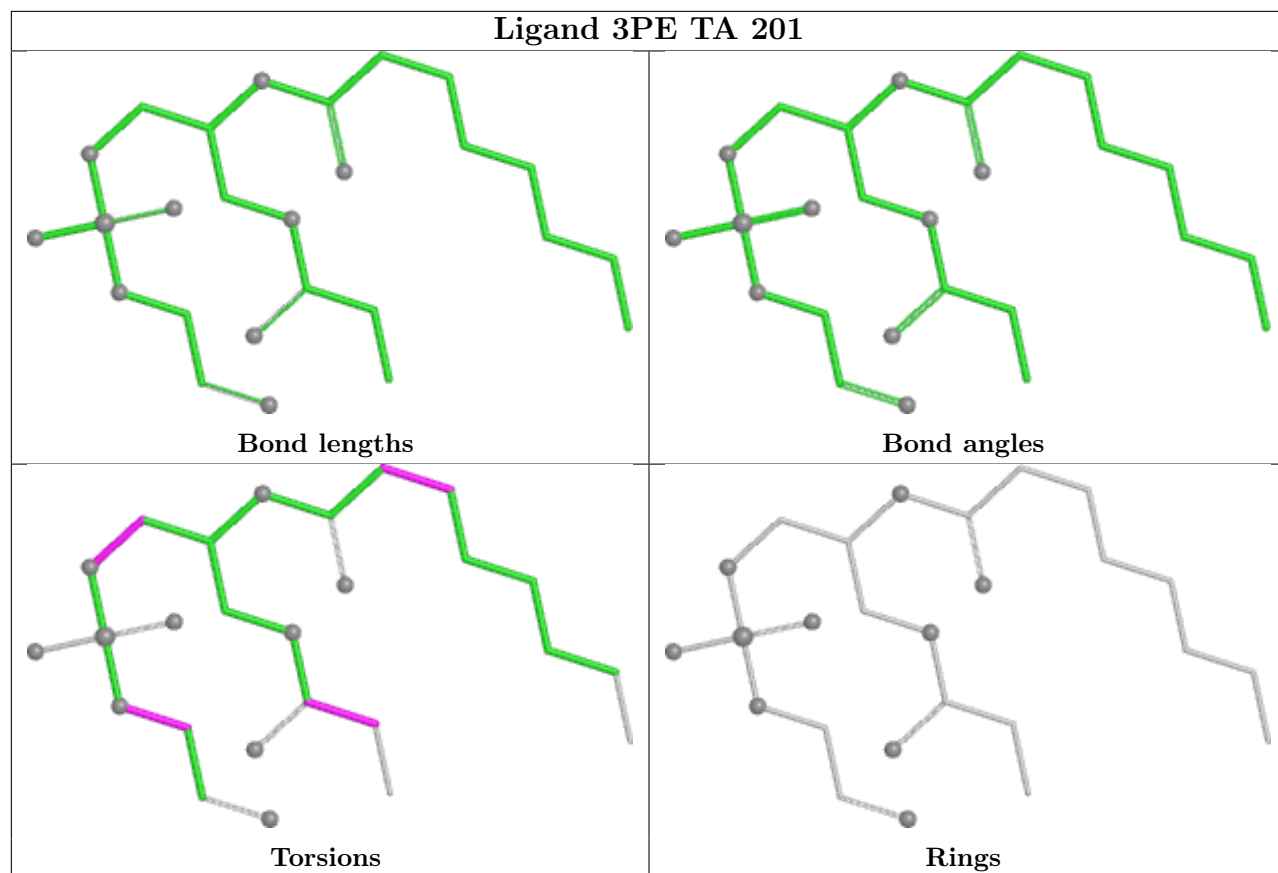
Mol	Chain	Res	Type	Atoms
82	3B	701	CDL	C12-C11-CA5-OA6
82	T1	602	CDL	C12-C11-CA5-OA7
82	AN	304	CDL	CA5-C11-C12-C13
82	5	805	CDL	C37-C38-C39-C40
83	3E	302	PC1	C2B-C2C-C2D-C2E
86	3D	401	HEC	CAD-CBD-CGD-O1D
83	3c	506	PC1	O32-C31-C32-C33
82	3B	701	CDL	C32-C31-CA7-OA8
82	1	301	CDL	C12-C13-C14-C15
82	1	301	CDL	C12-C11-CA5-OA7
82	3H	202	CDL	C72-C71-CB7-OB8
83	6	301	PC1	O31-C31-C32-C33
84	3c	503	HEM	CAD-CBD-CGD-O2D
83	3C	604	PC1	O22-C21-C22-C23
82	5	803	CDL	C59-C60-C61-C62
84	3c	503	HEM	CAD-CBD-CGD-O1D

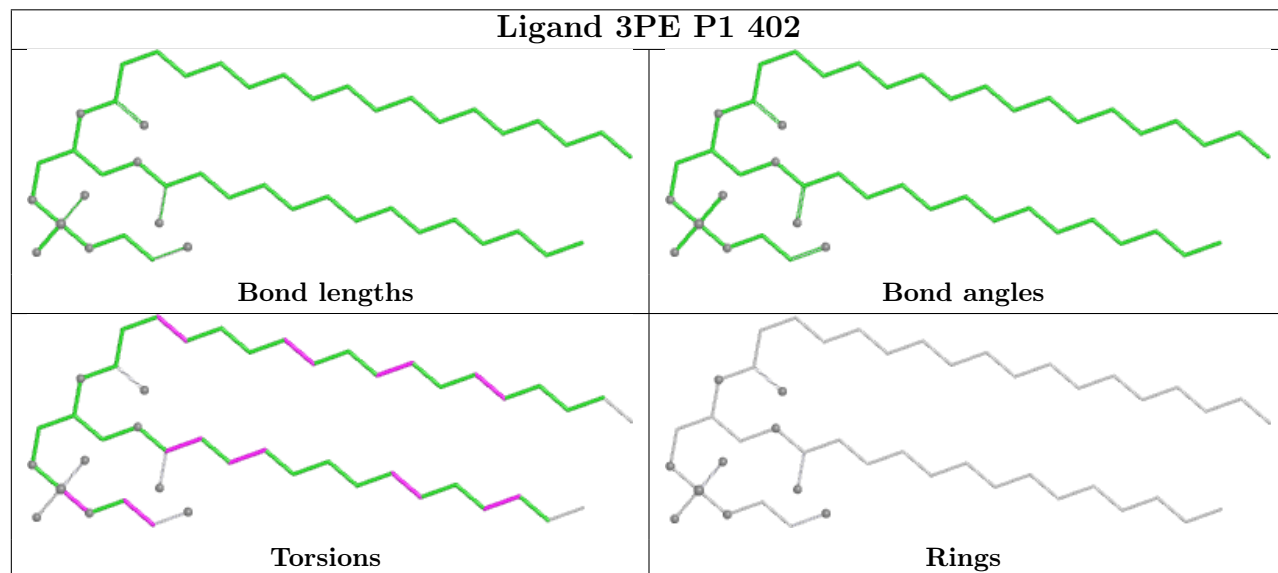
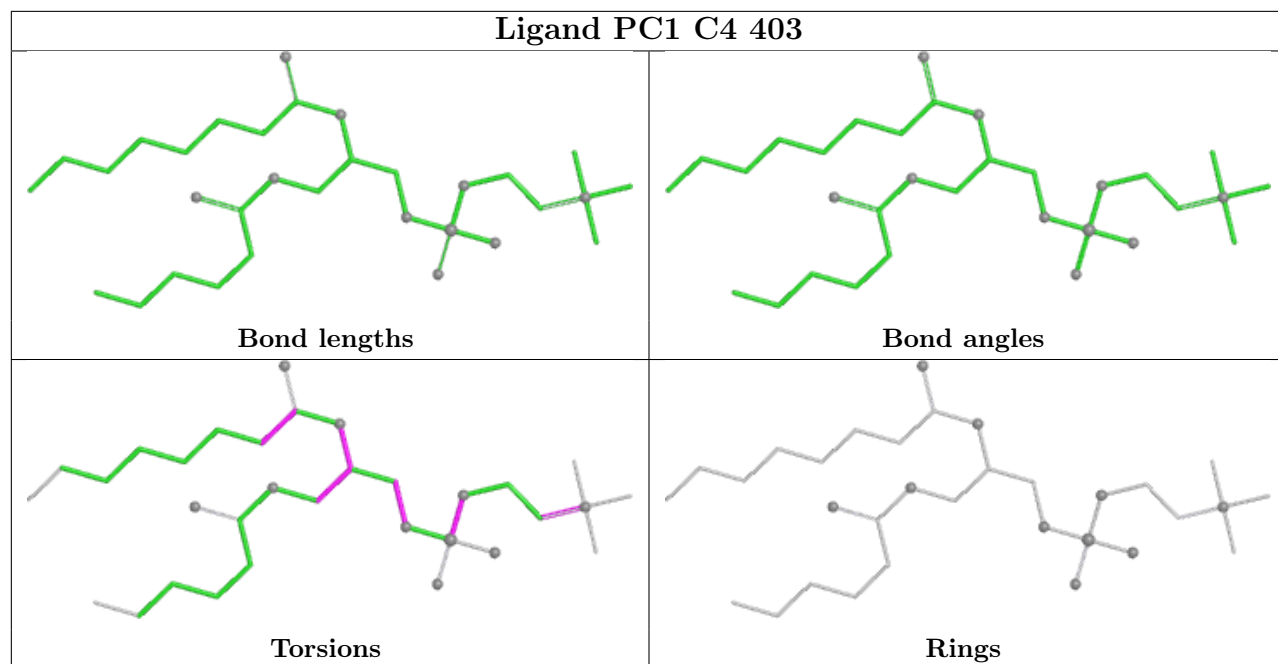
There are no ring outliers.

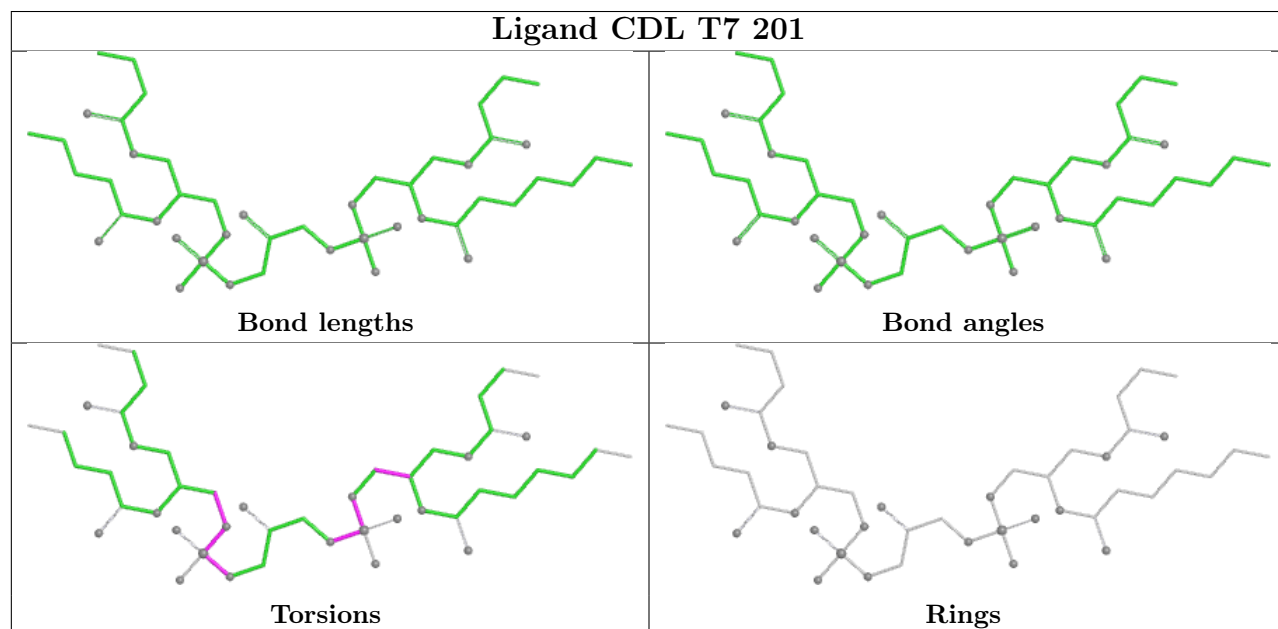
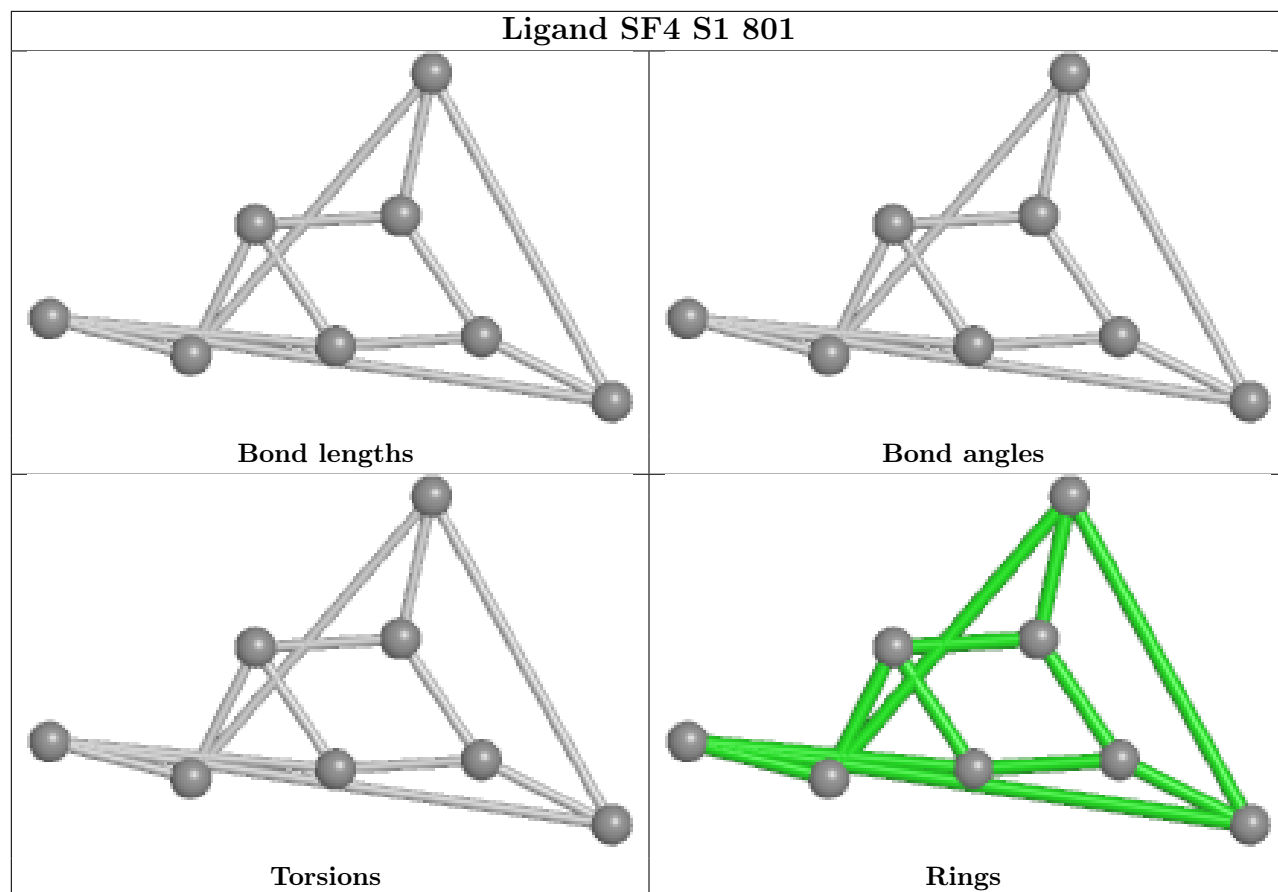
No monomer is involved in short contacts.

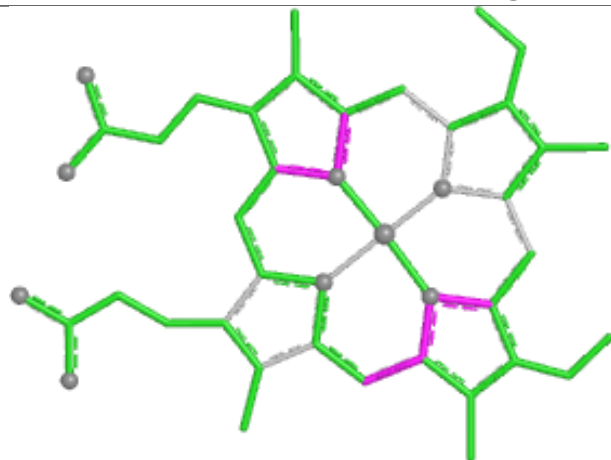
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



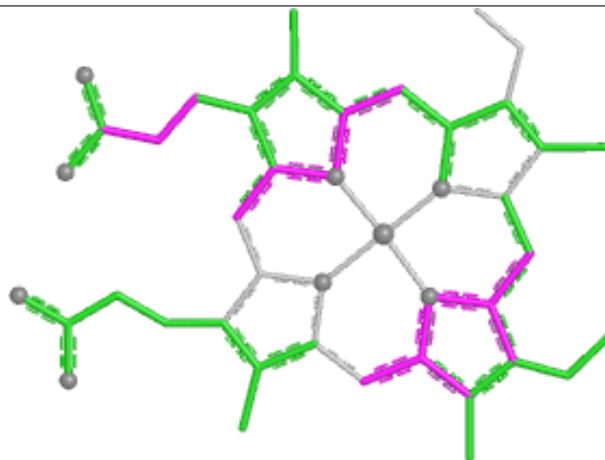




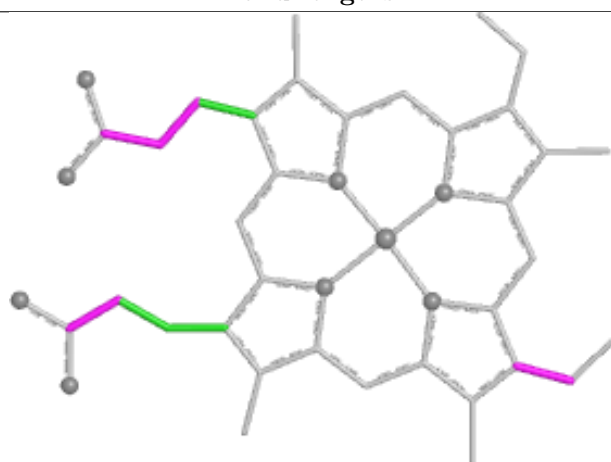


Ligand HEM 3c 503

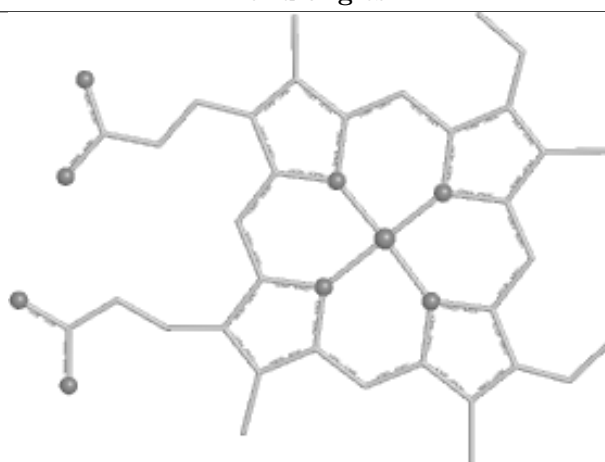
Bond lengths



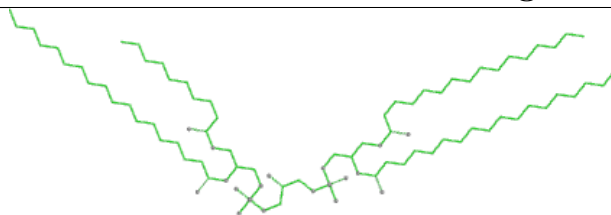
Bond angles



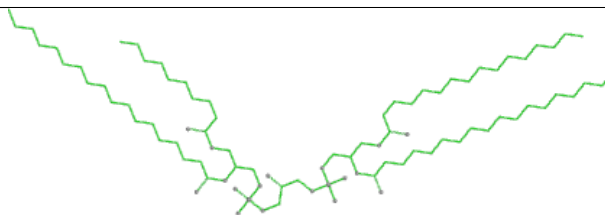
Torsions



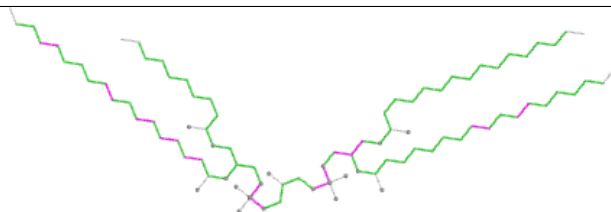
Rings

Ligand CDL 5 803

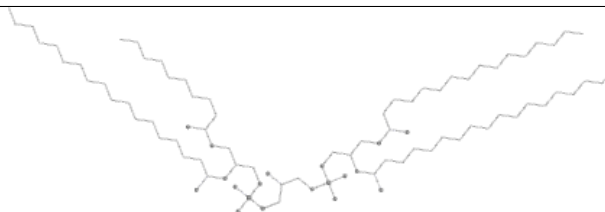
Bond lengths



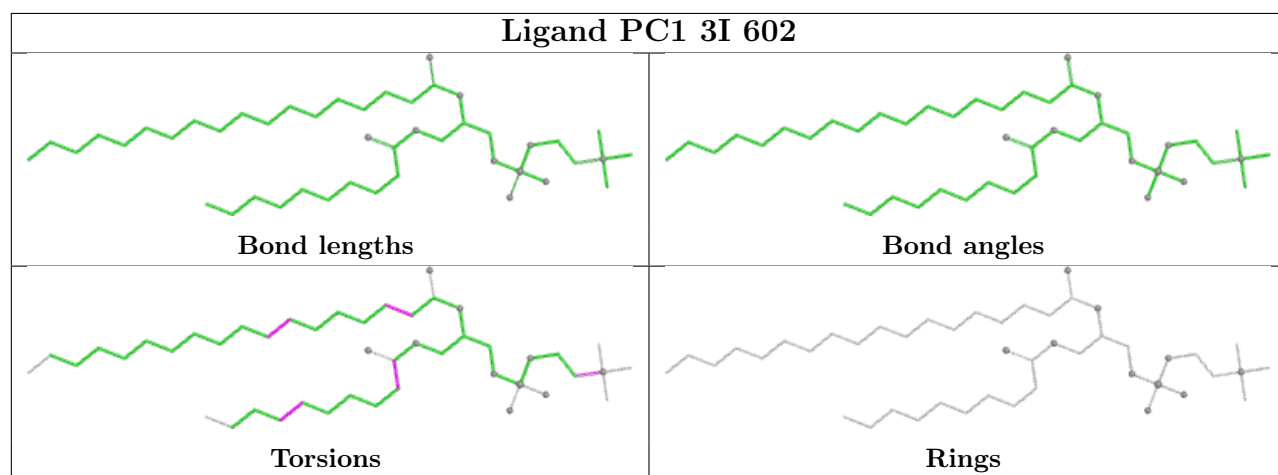
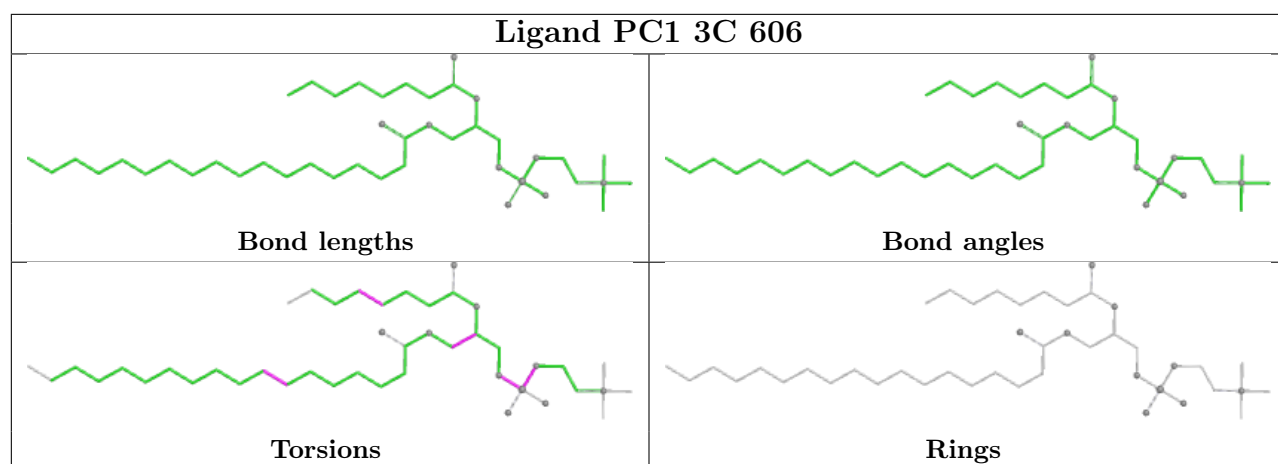
Bond angles

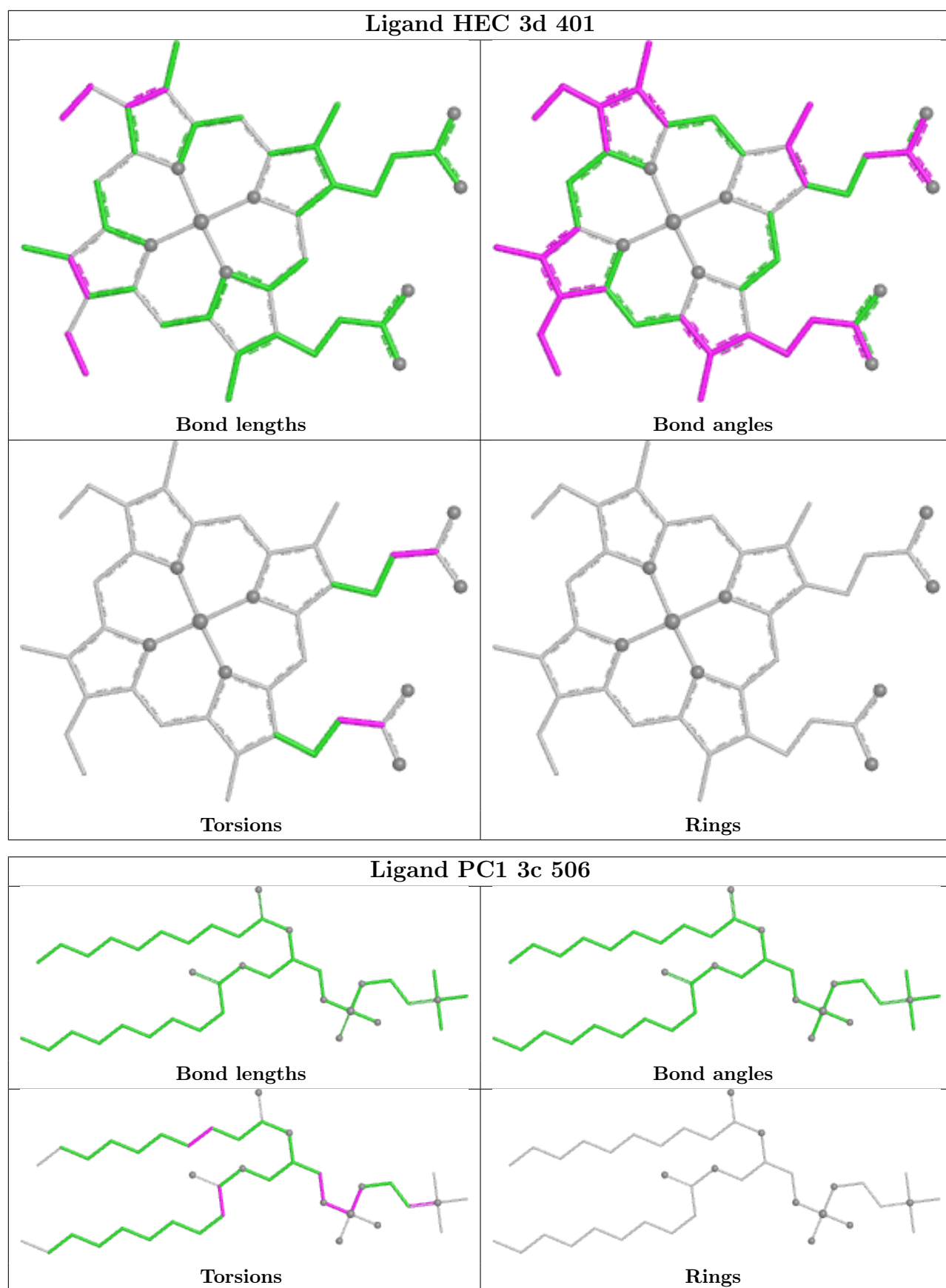


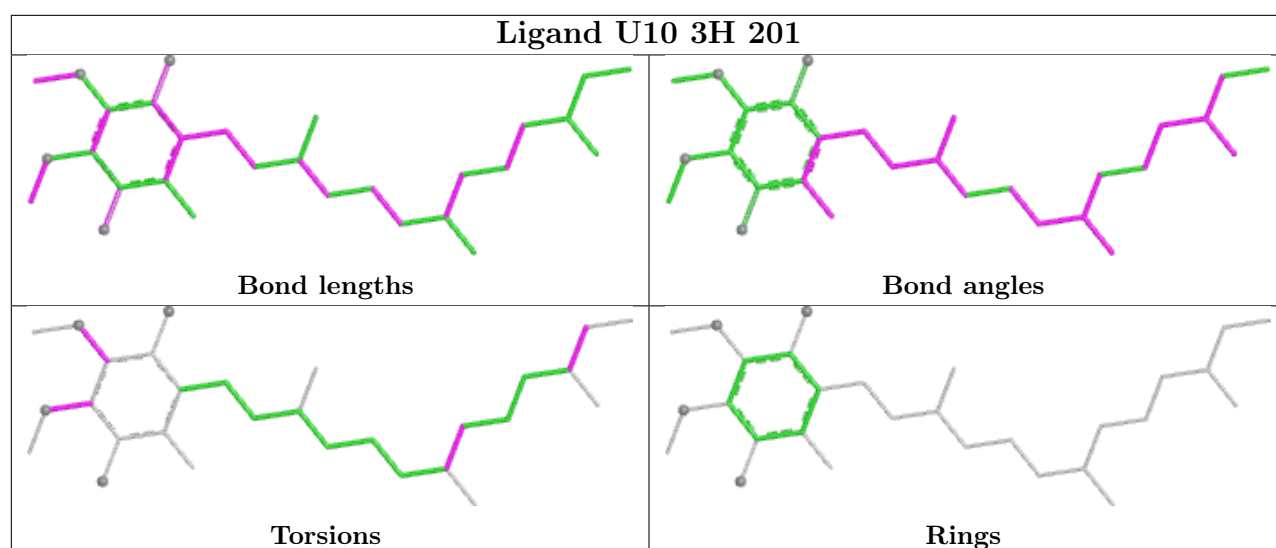
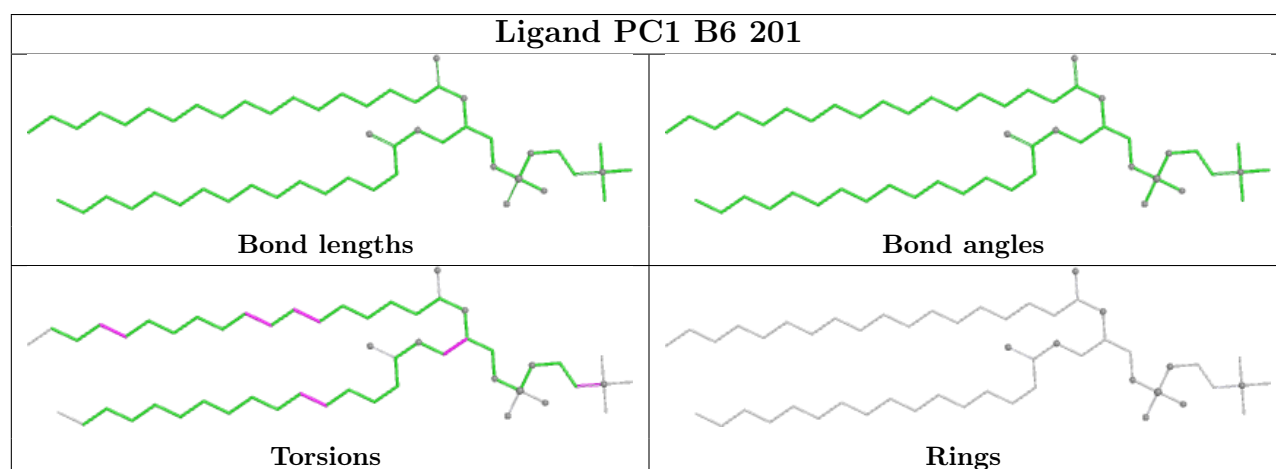
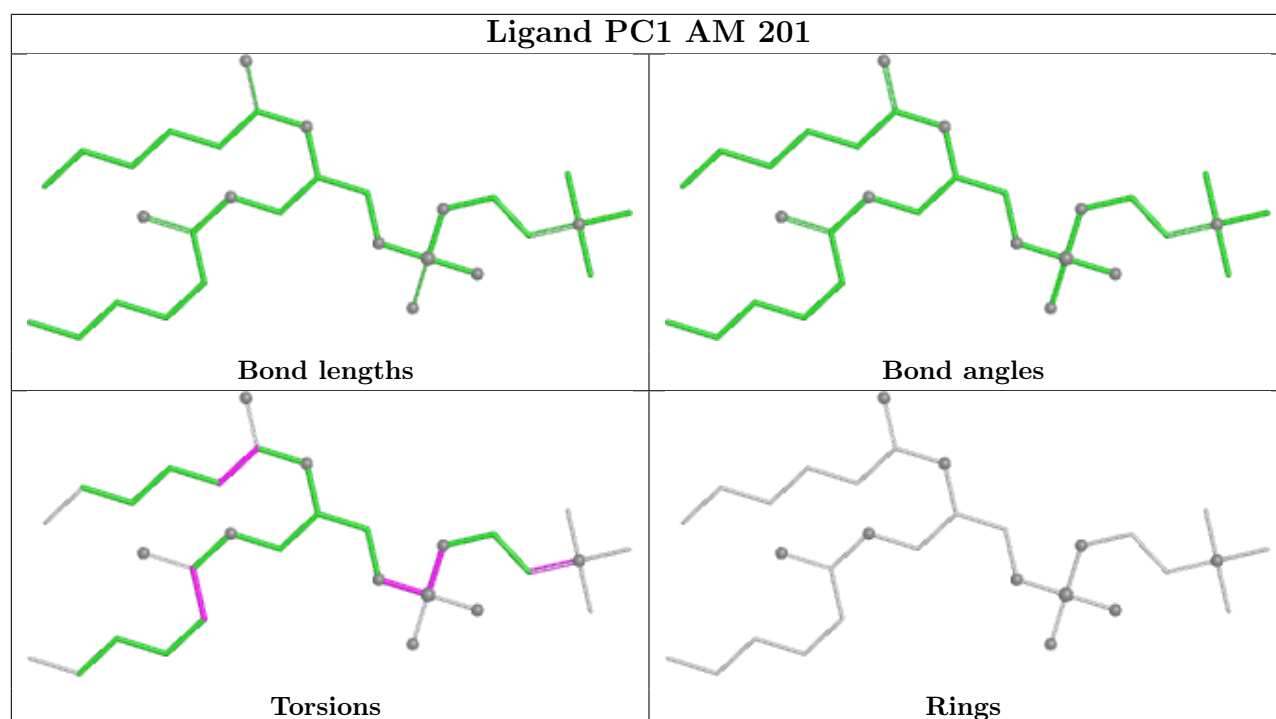
Torsions

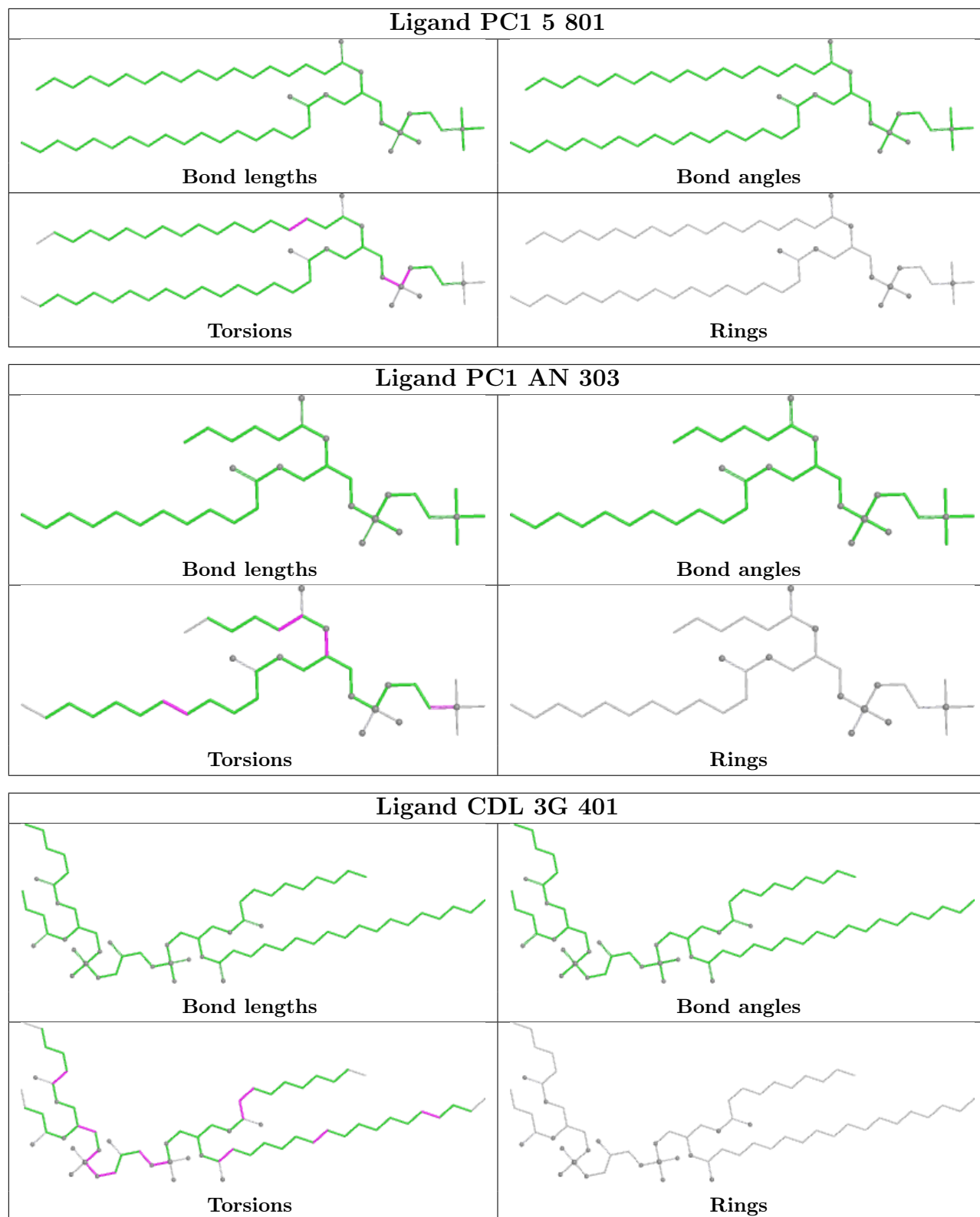


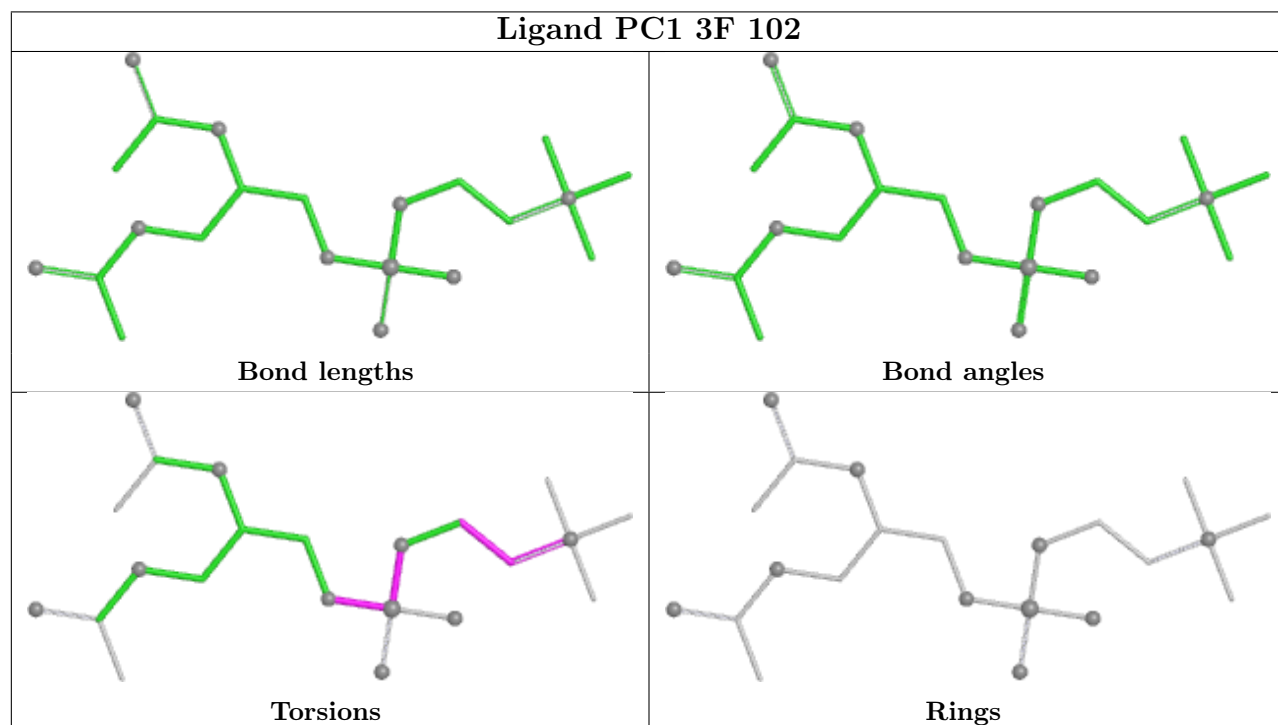
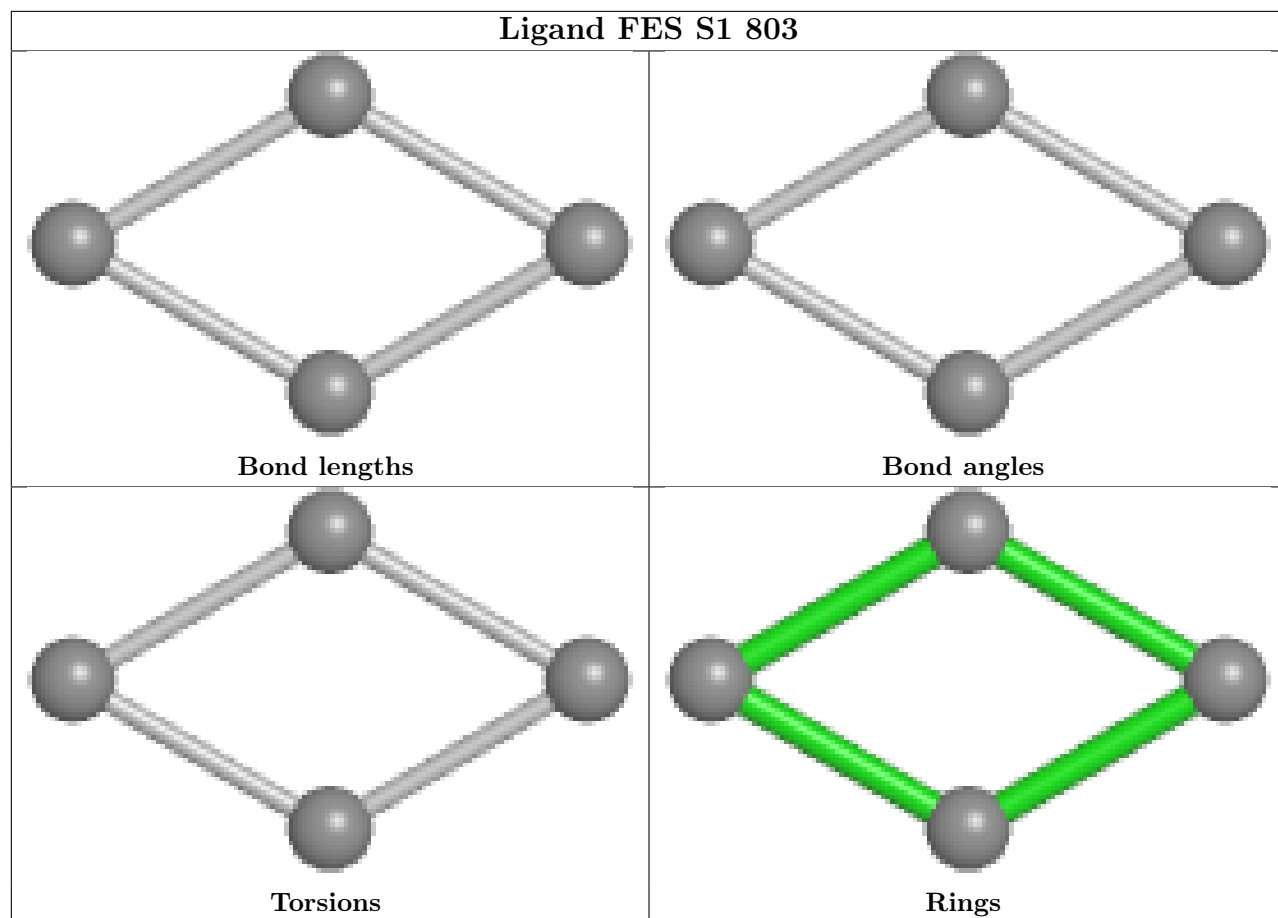
Rings

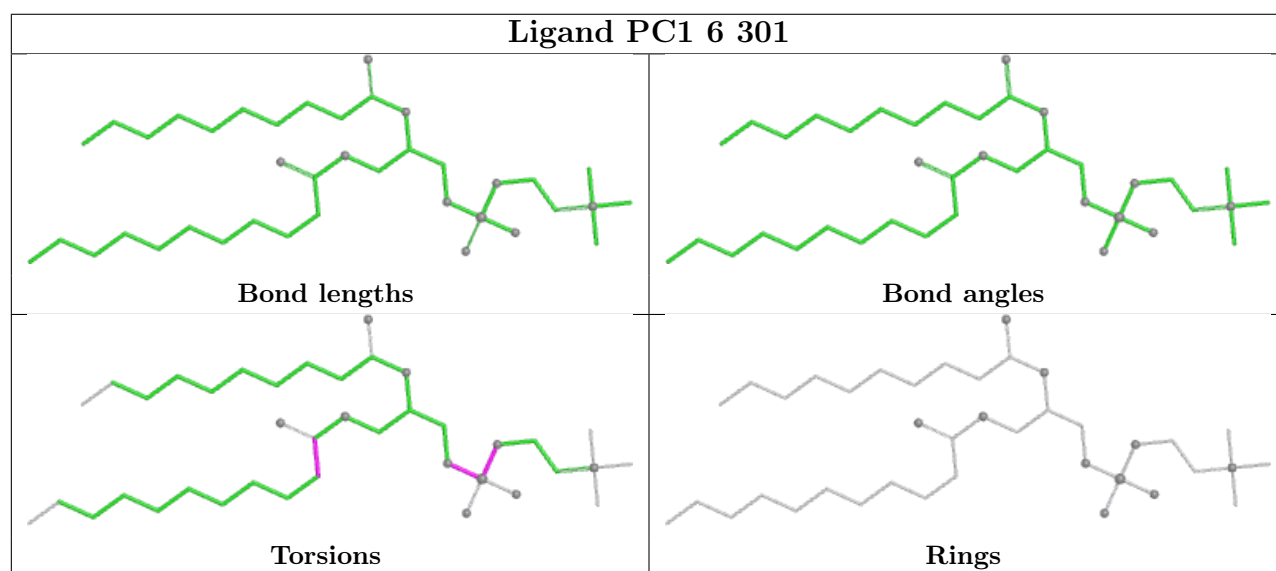
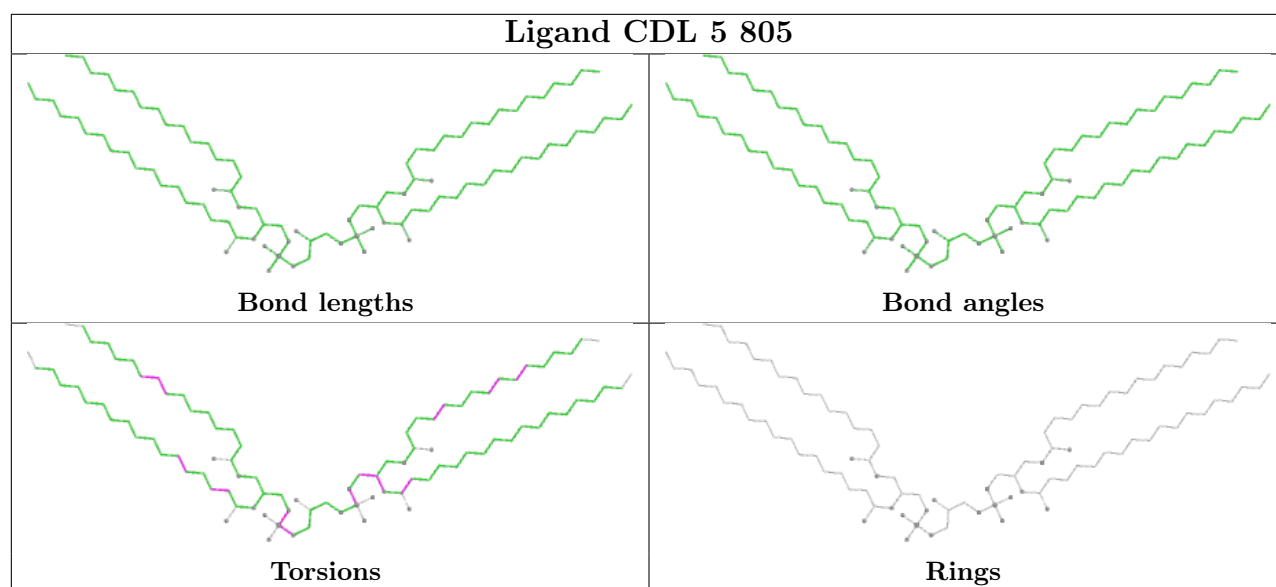


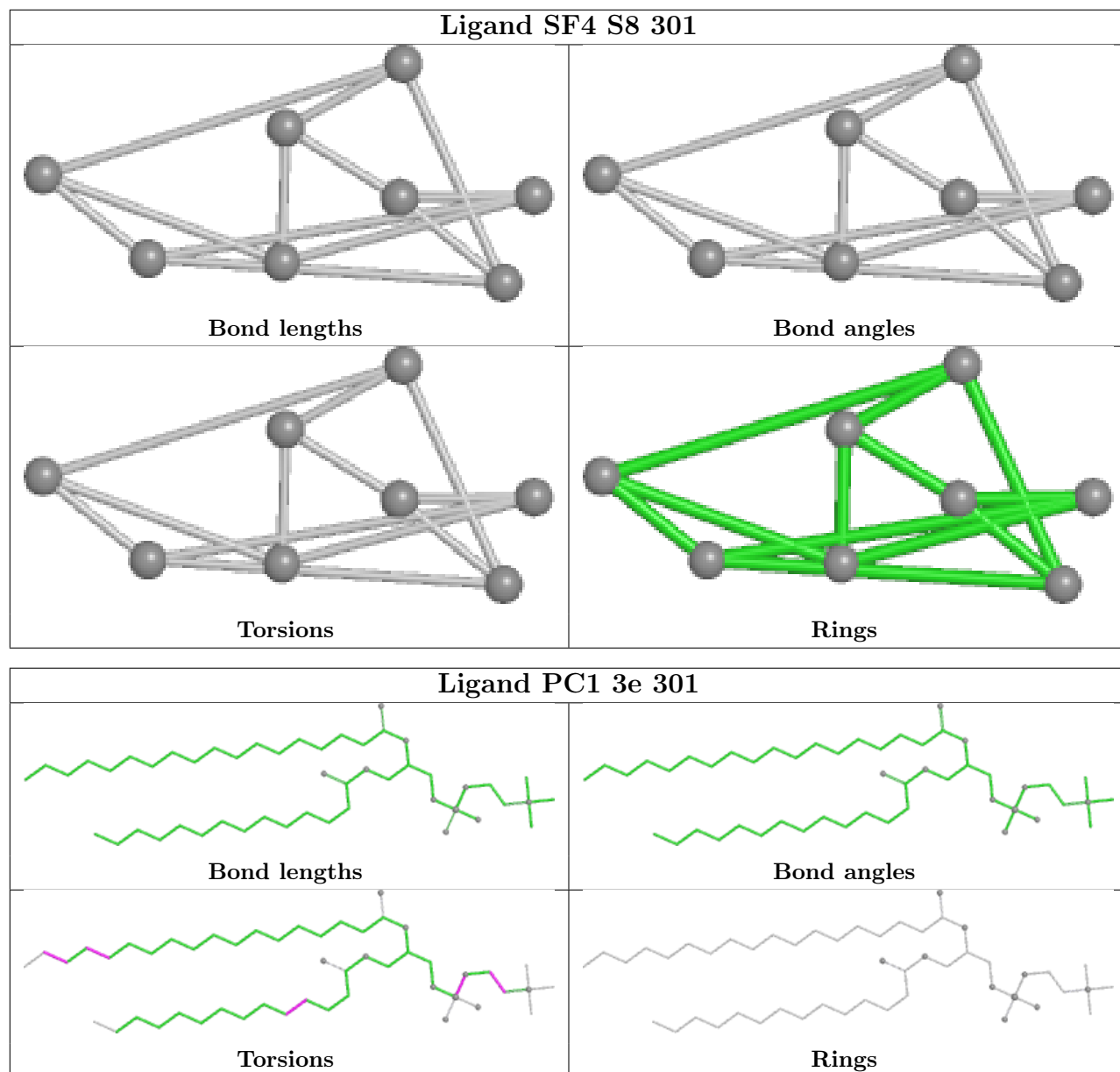


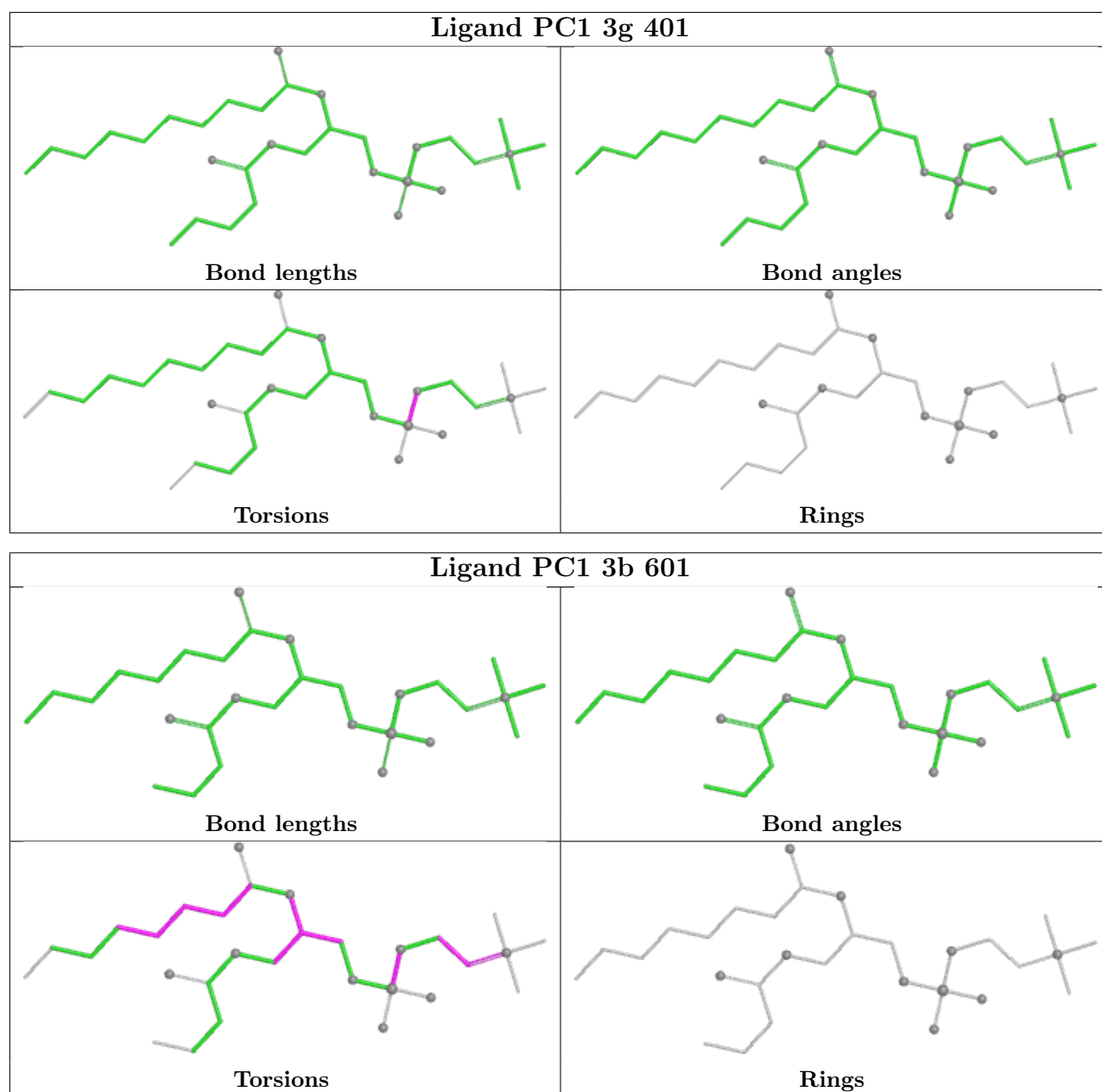


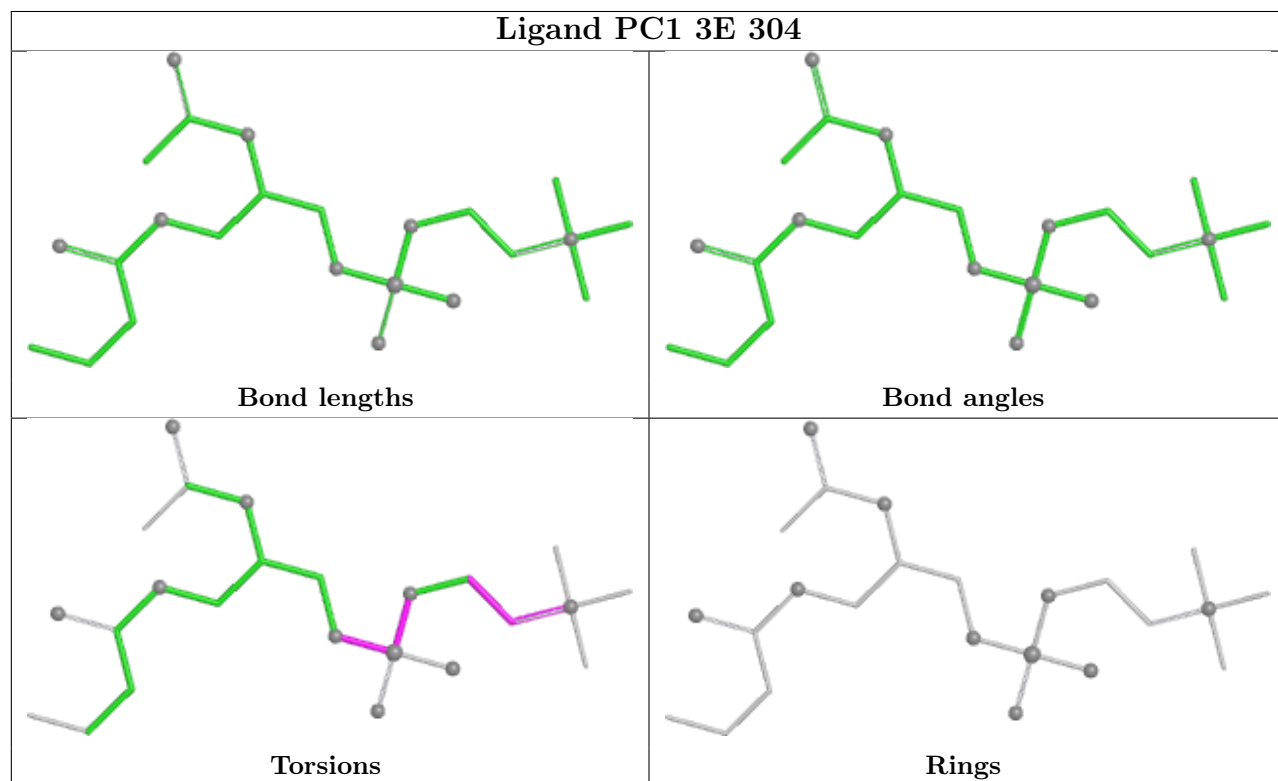
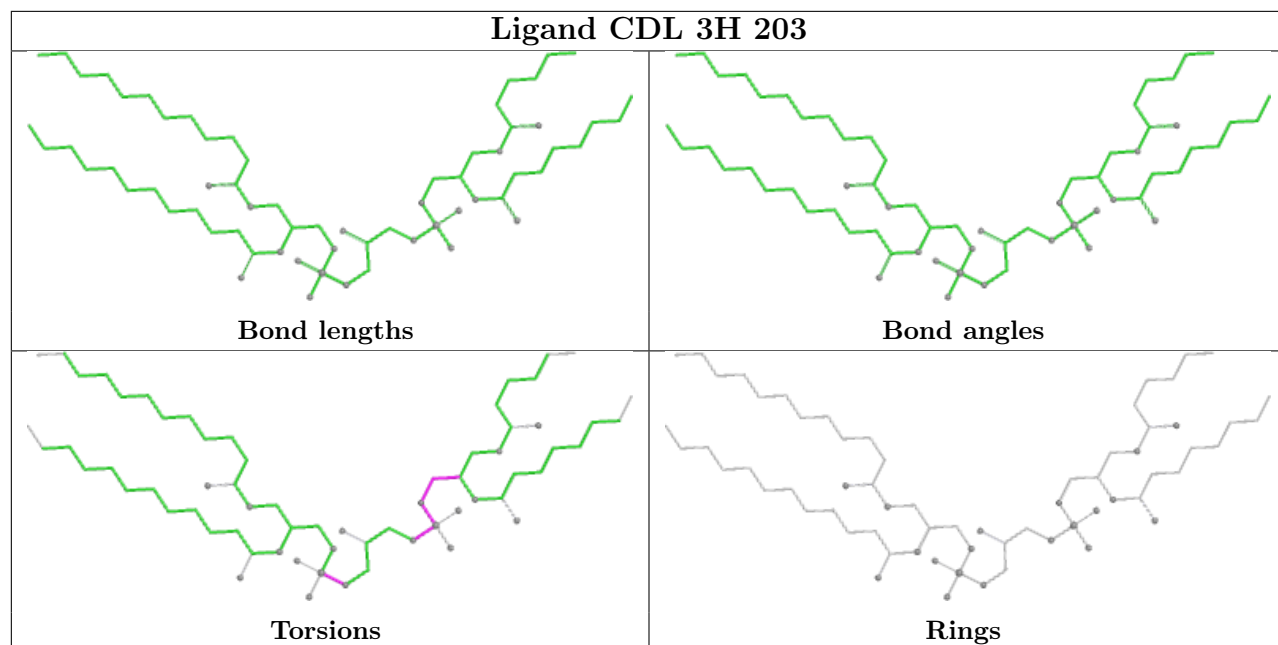


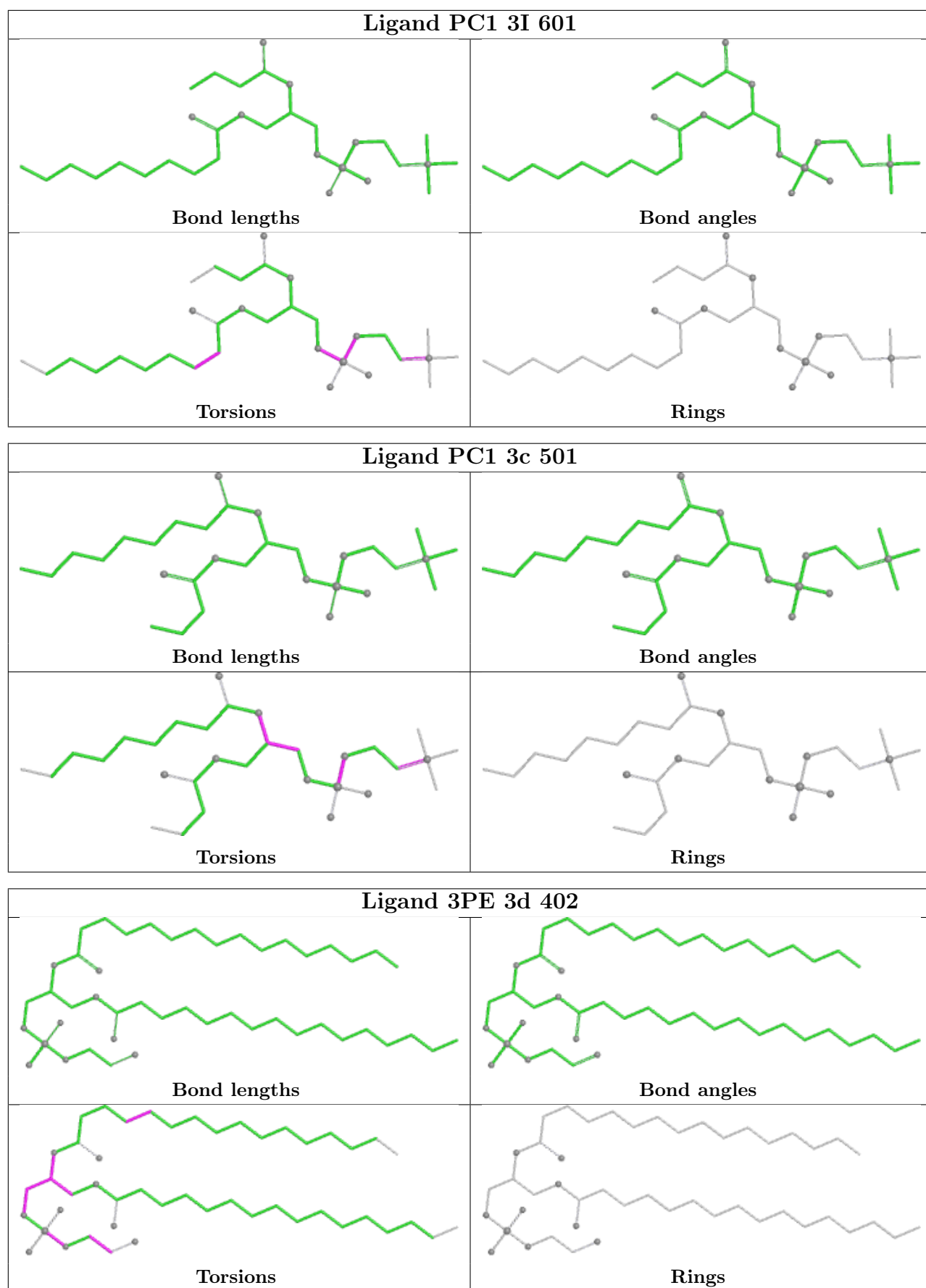


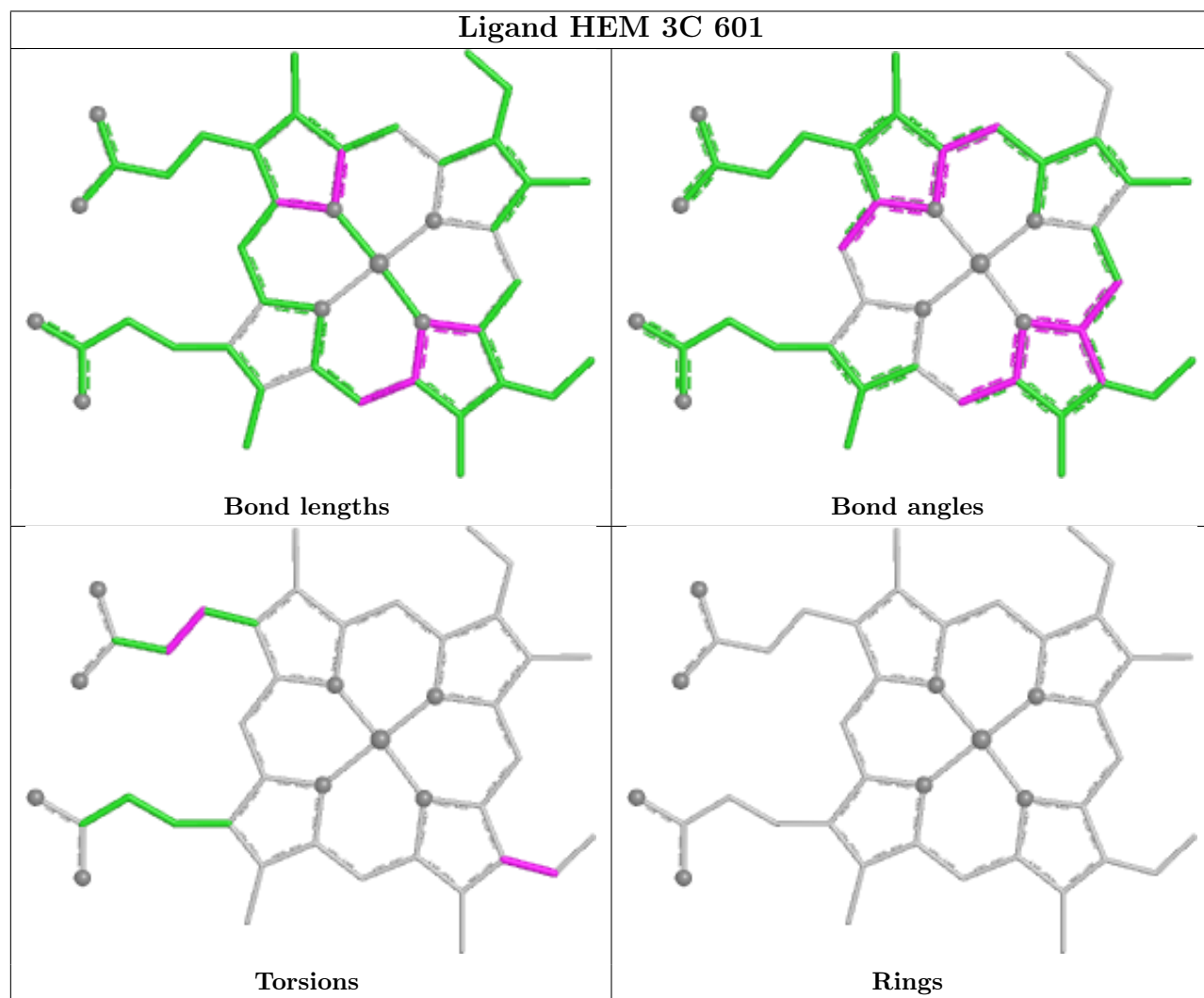
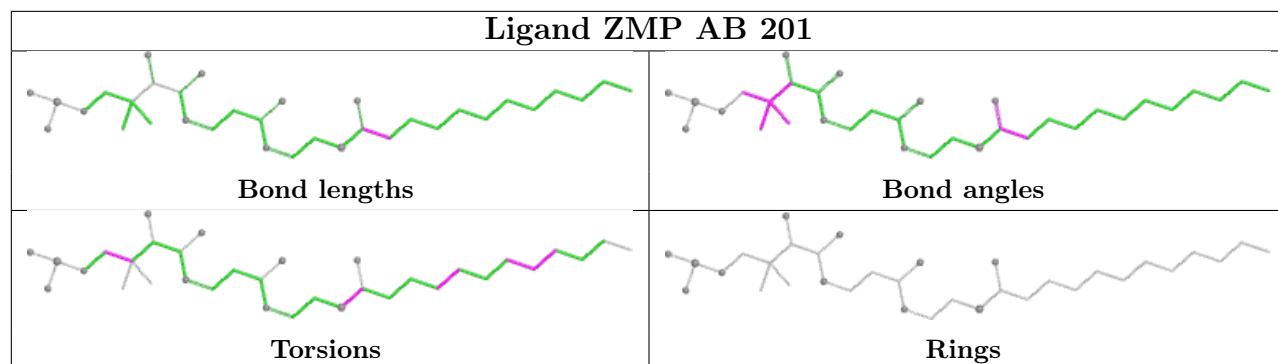


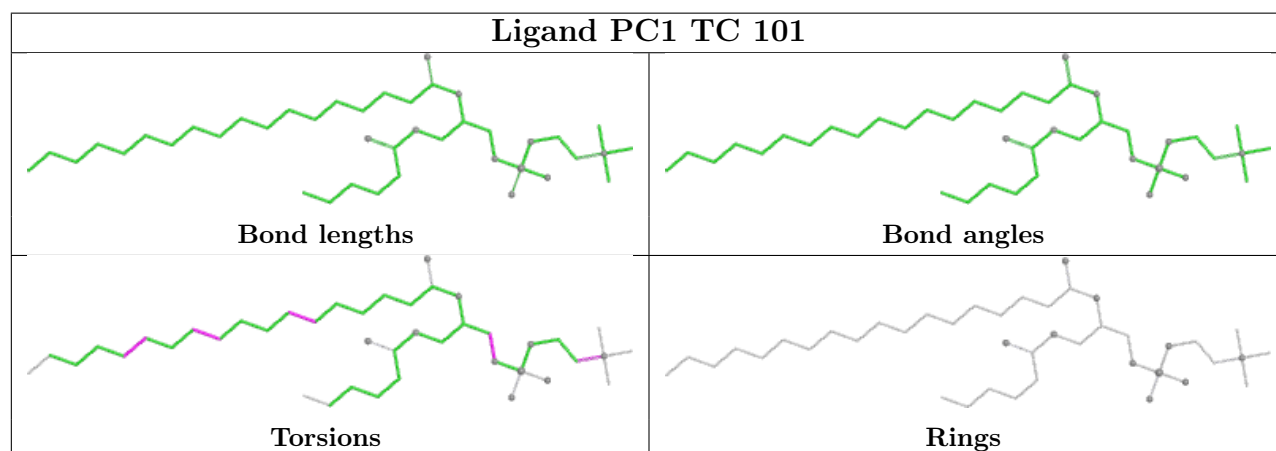
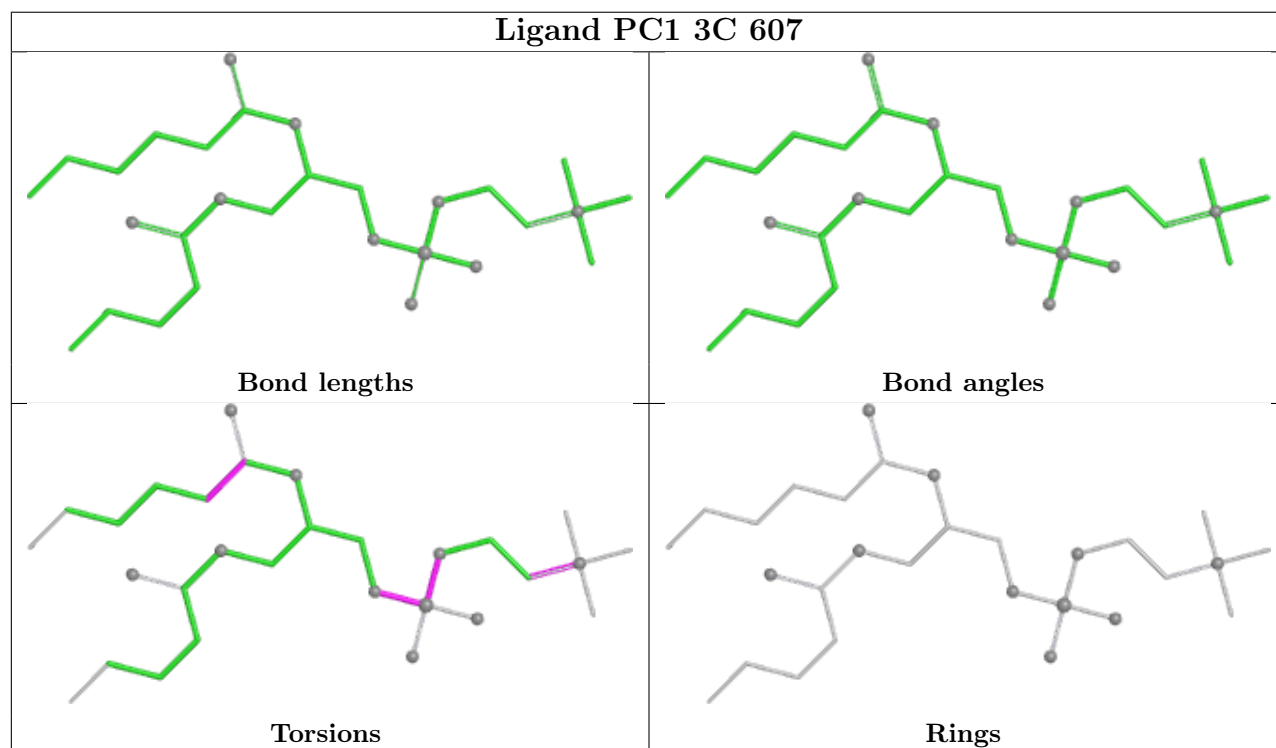
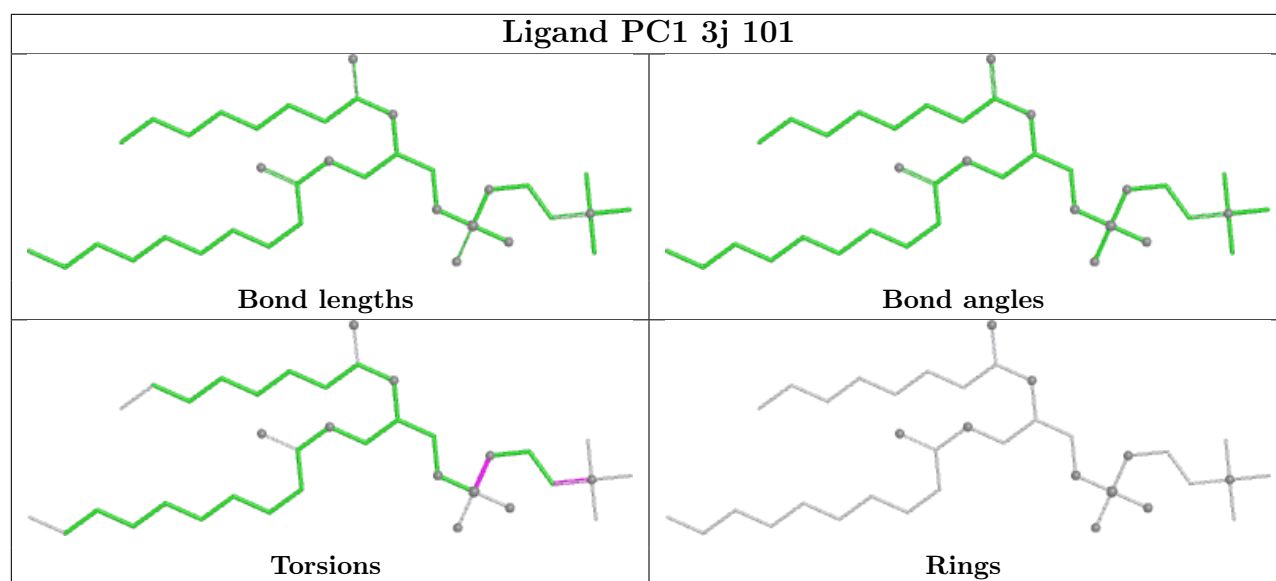


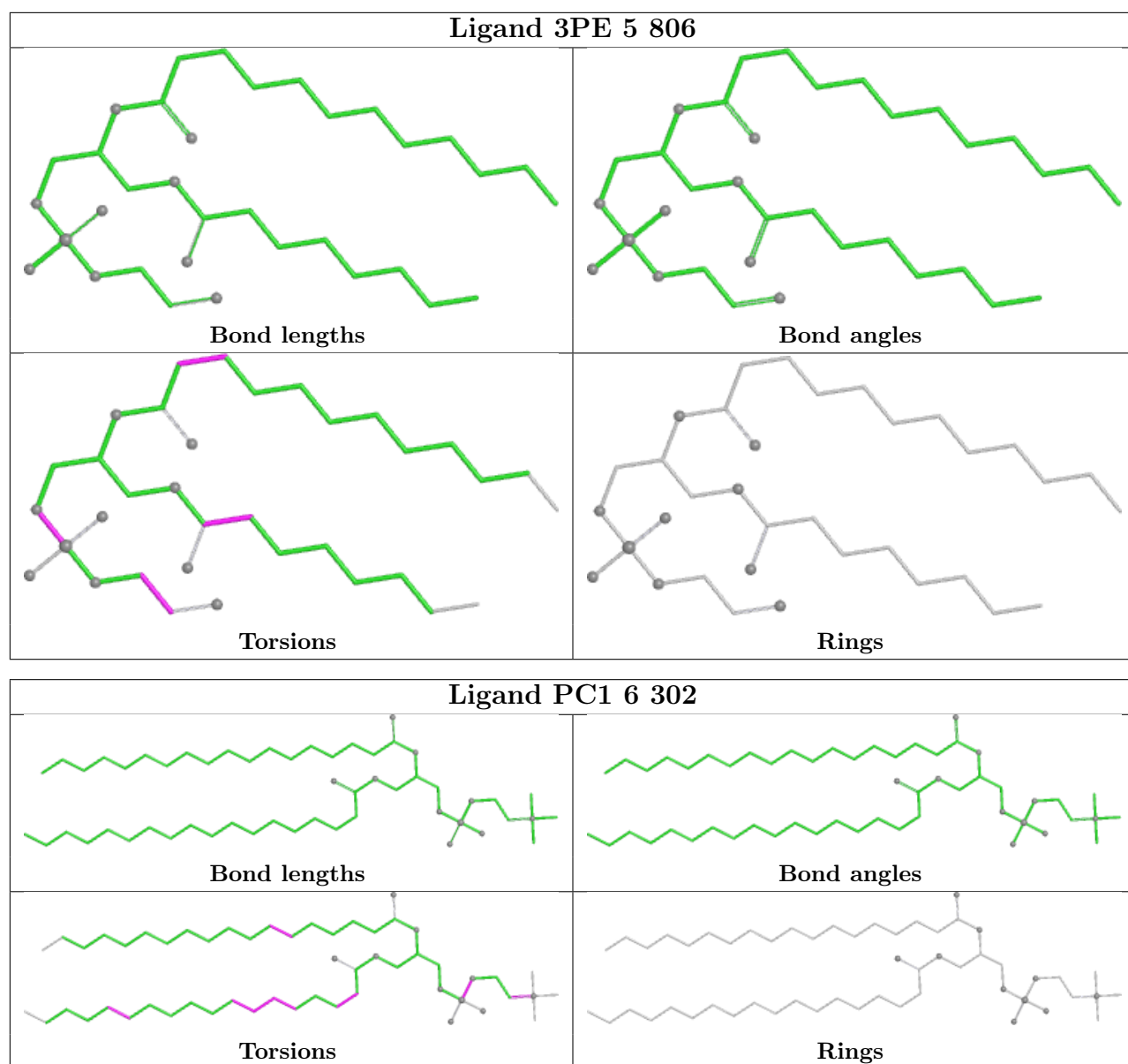


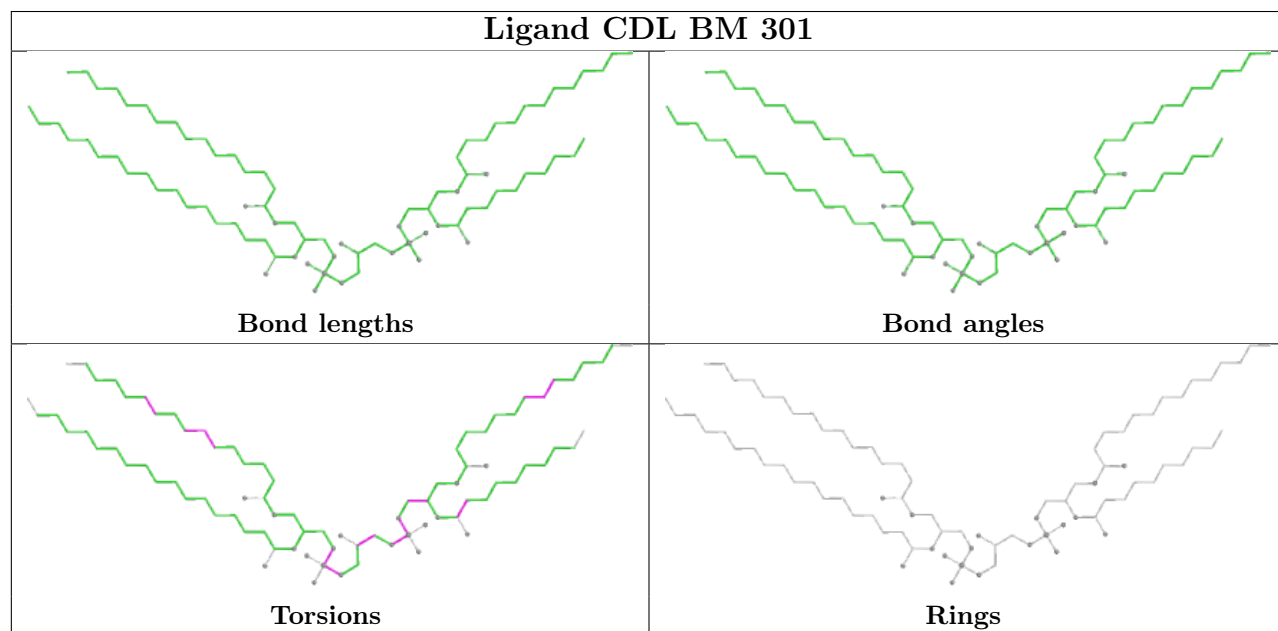
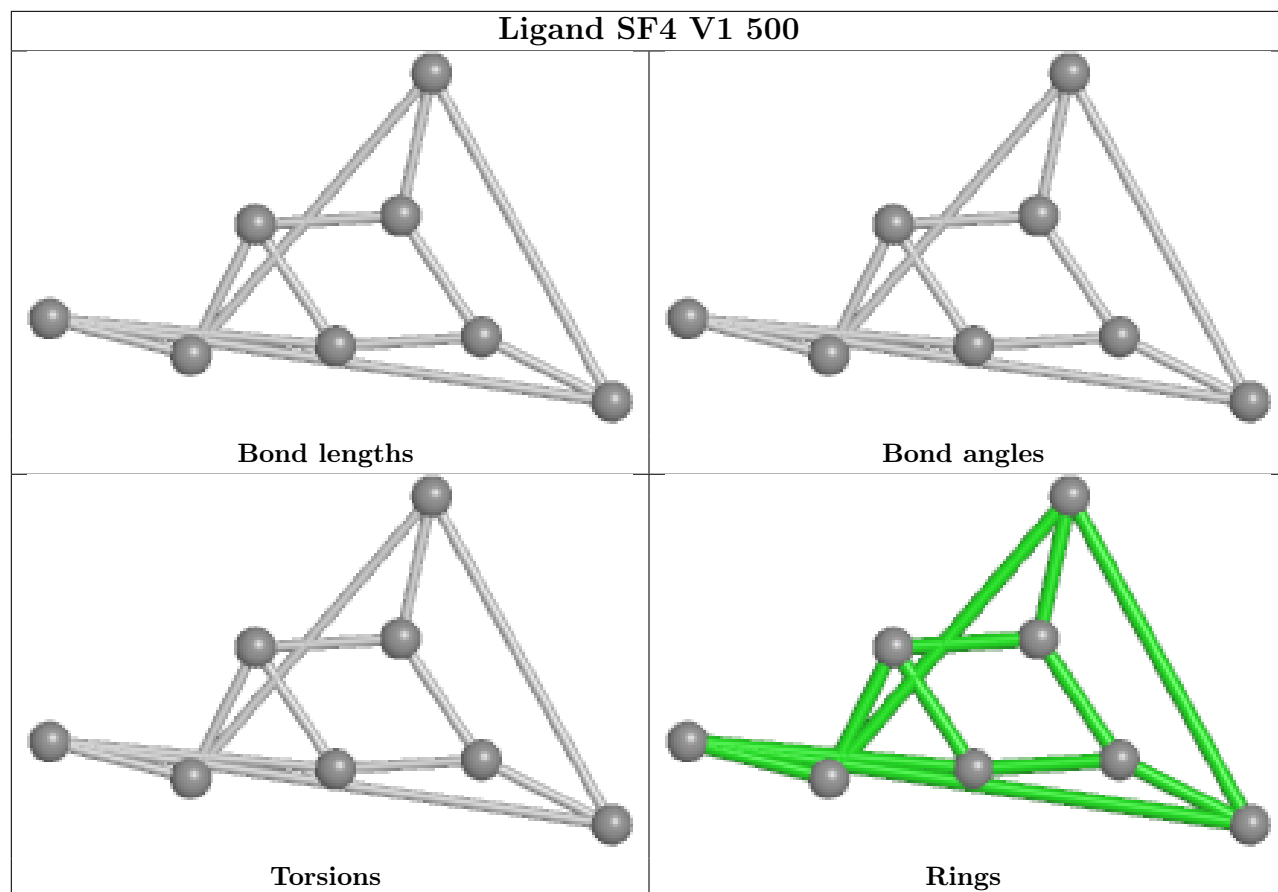


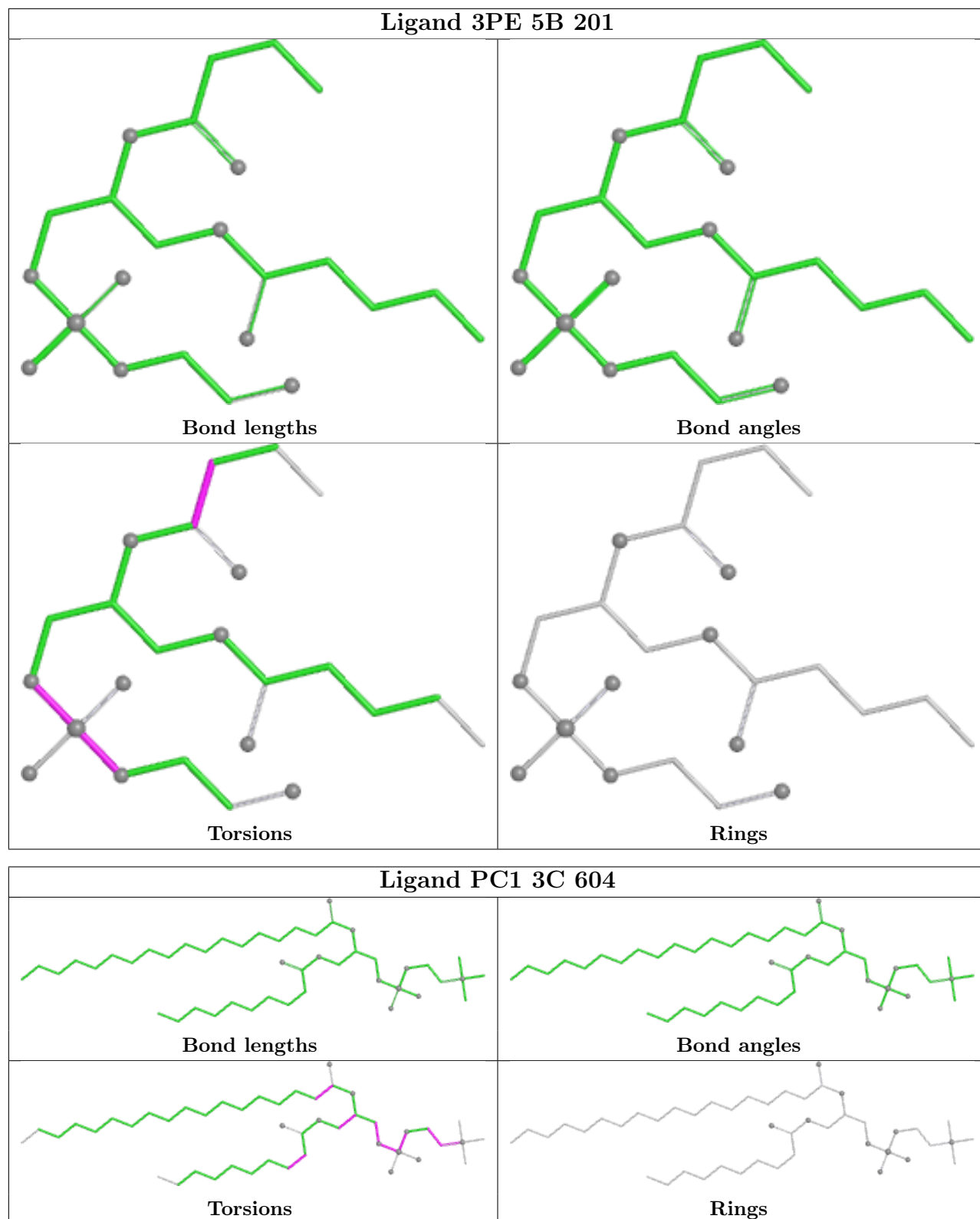


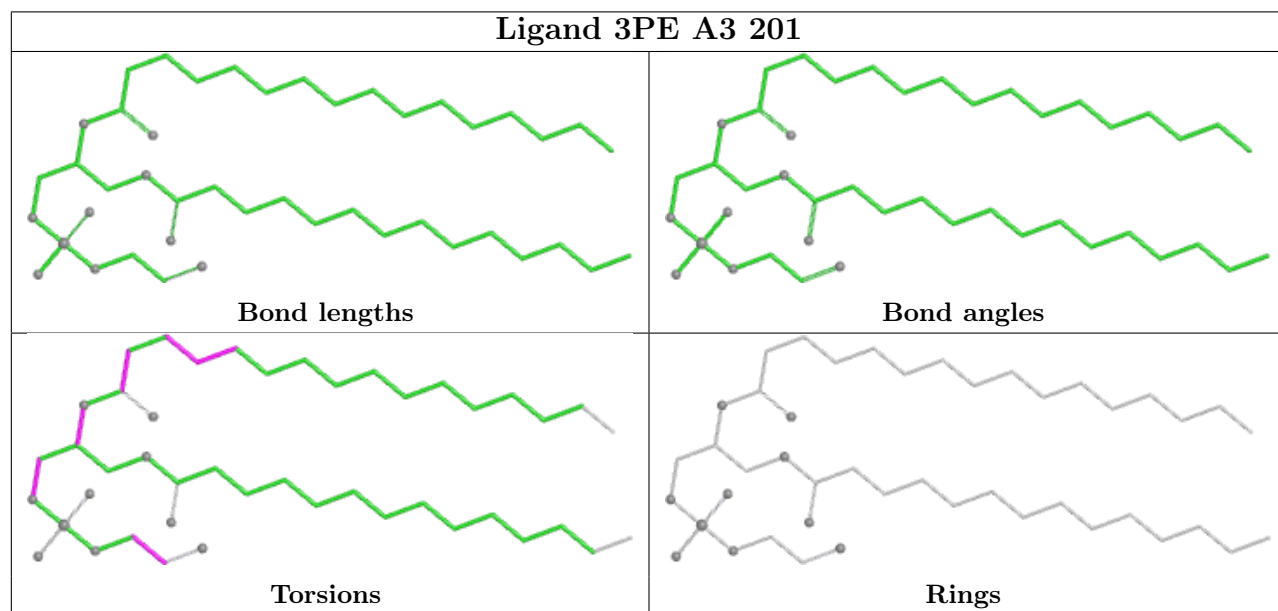
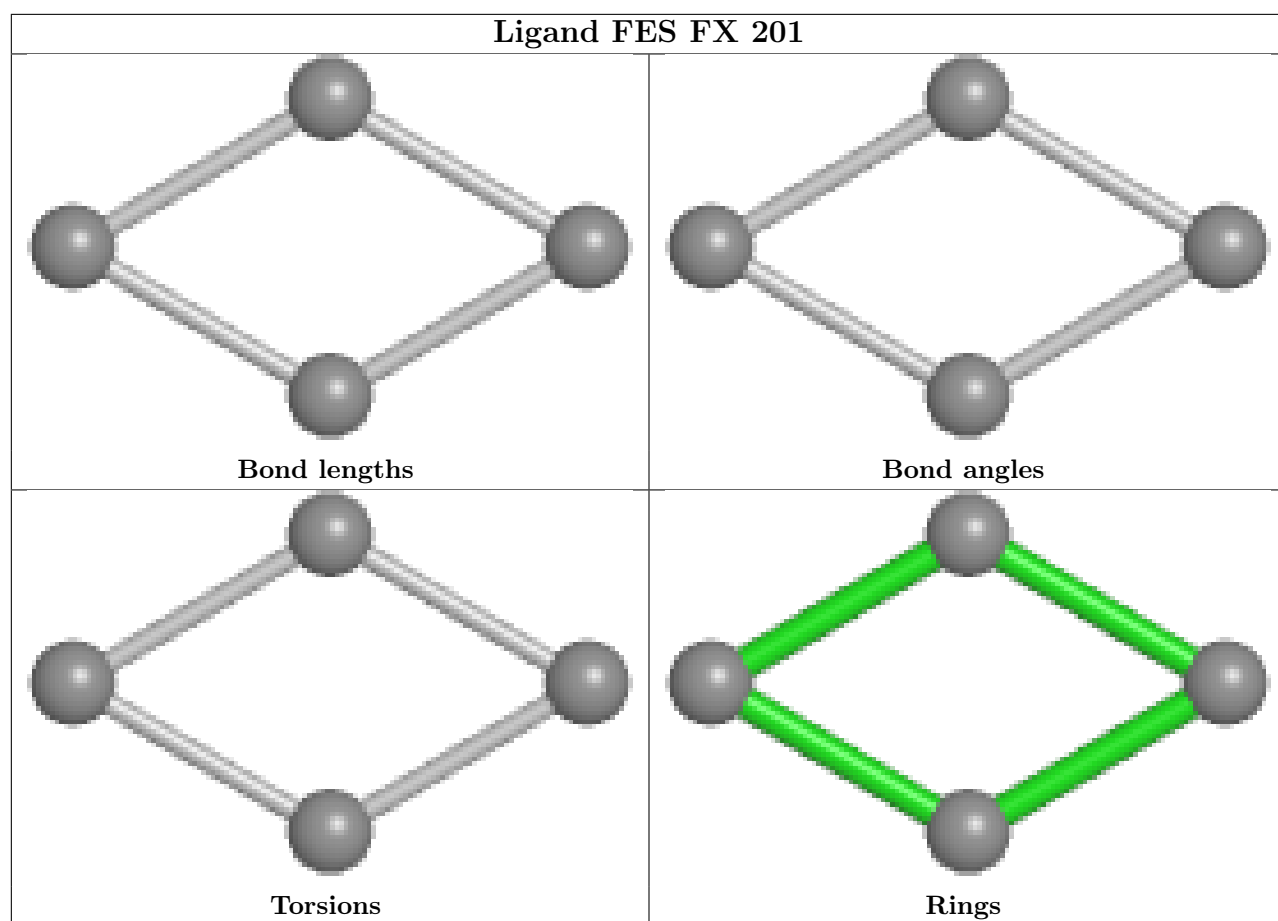


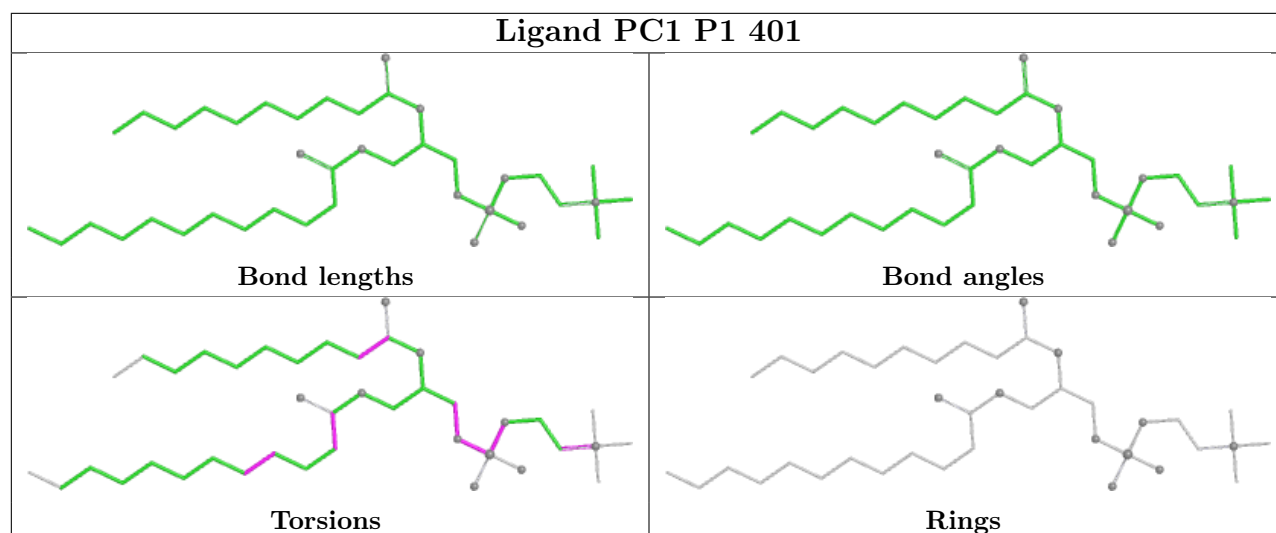
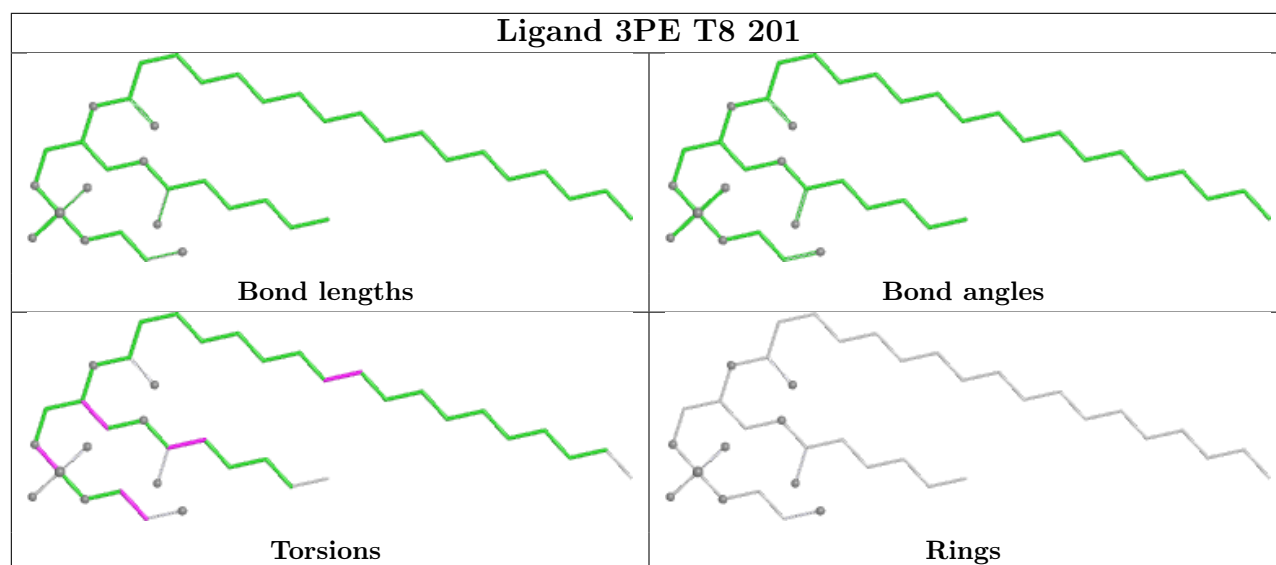
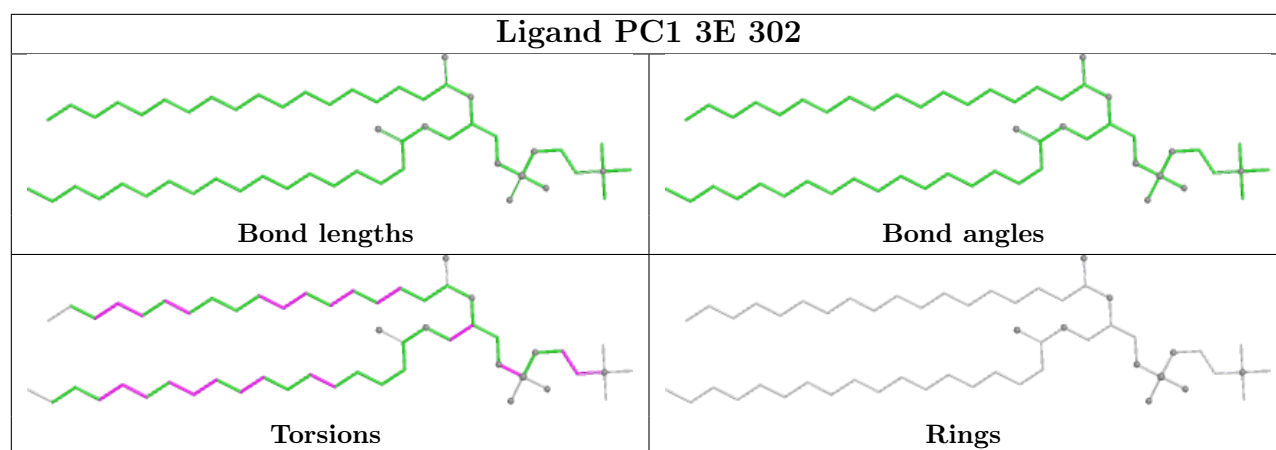


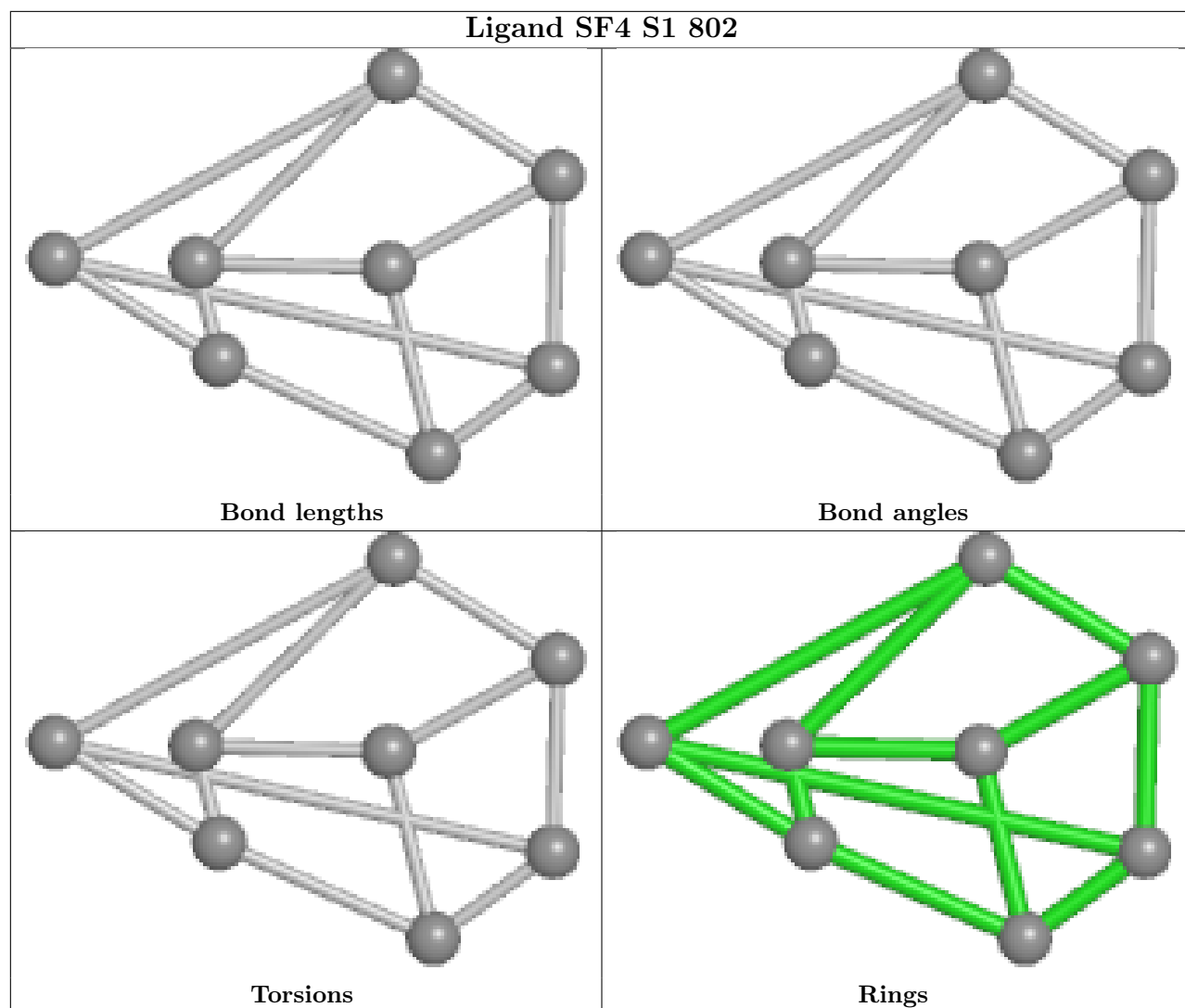
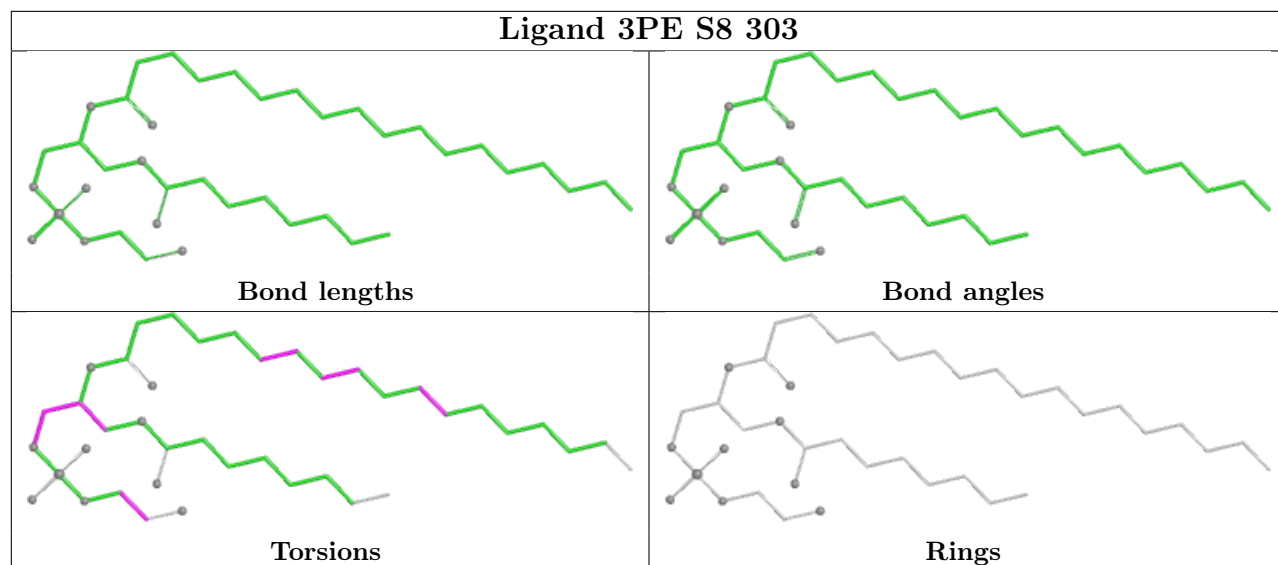




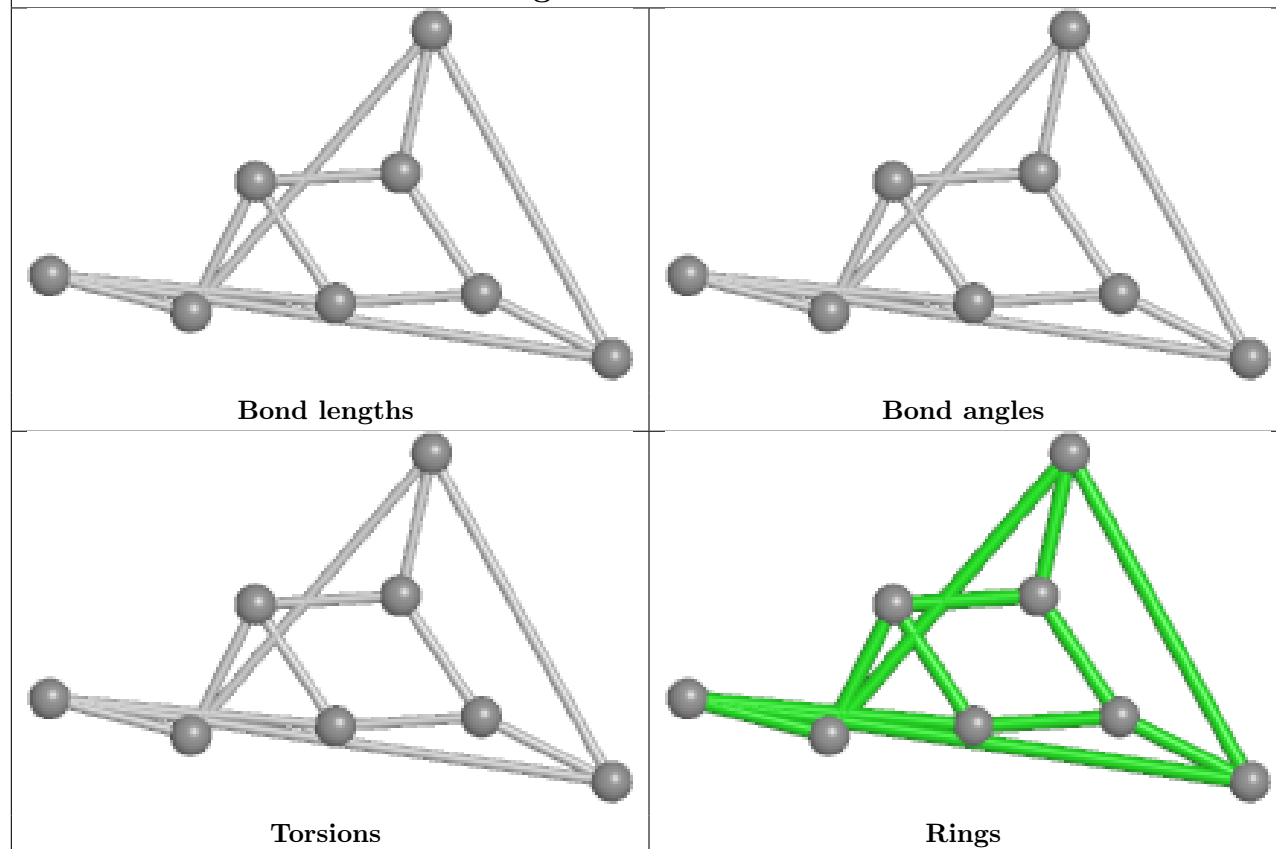




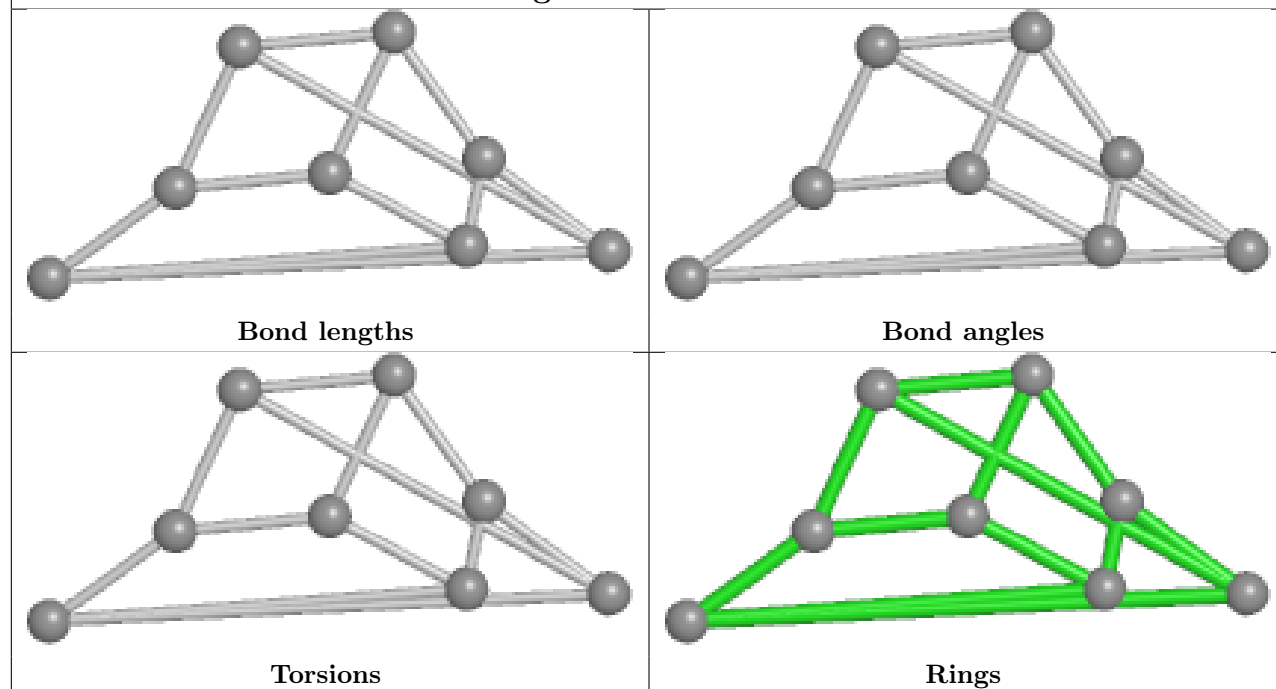


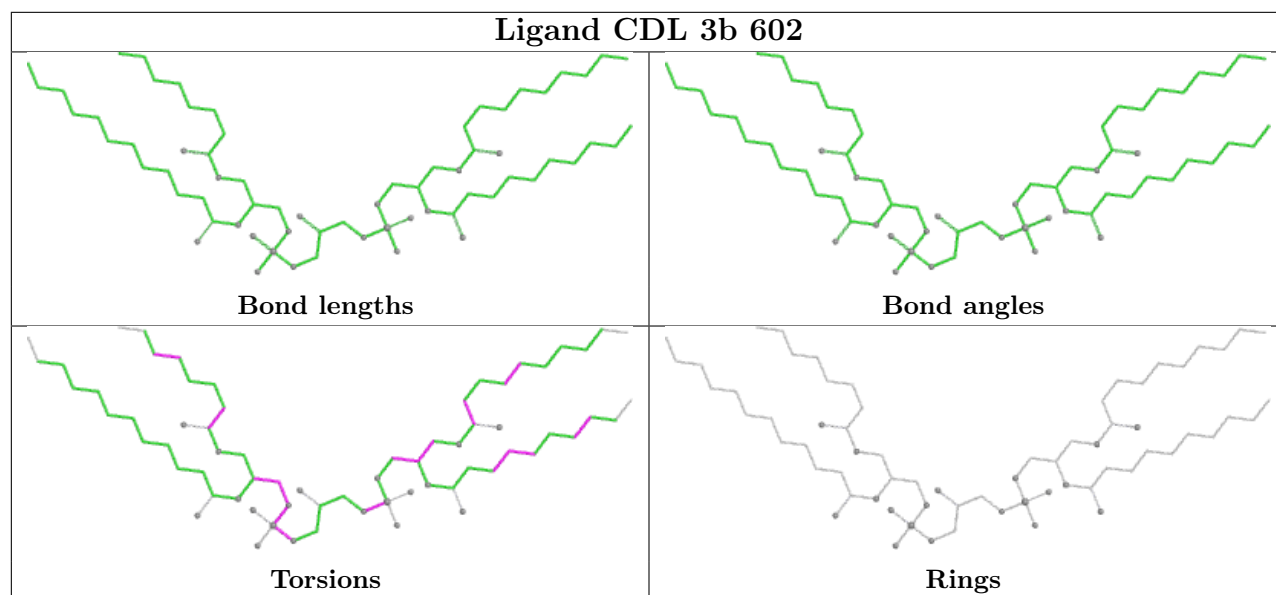
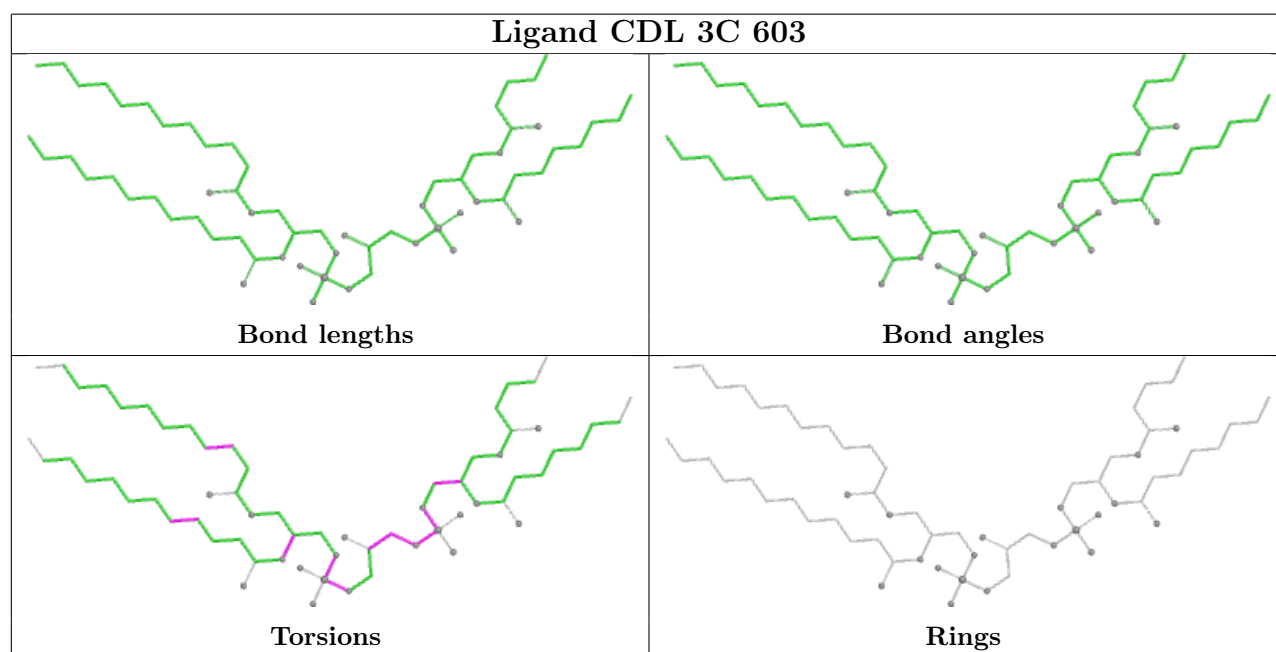
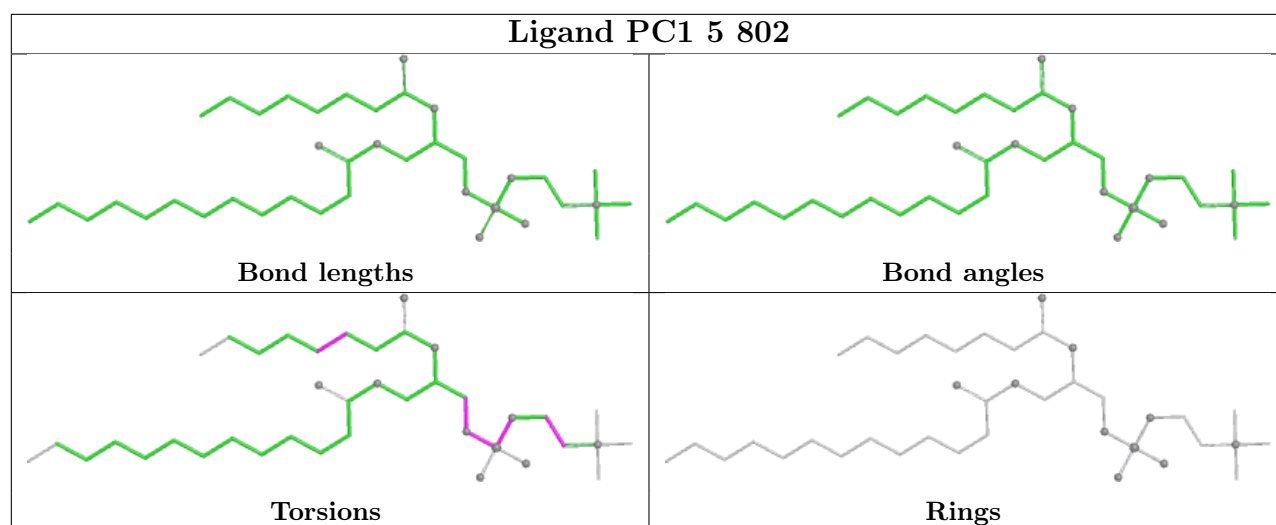


Ligand SF4 S7 201

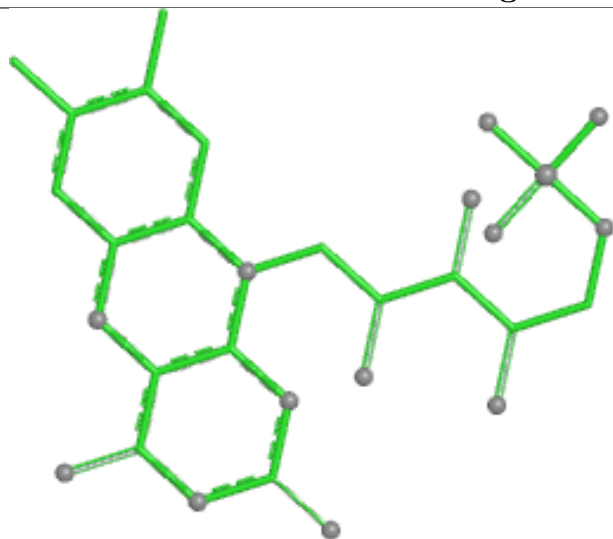


Ligand SF4 S8 302

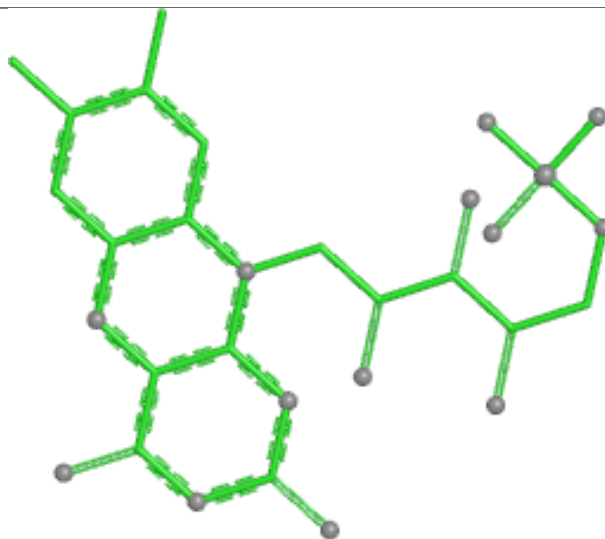




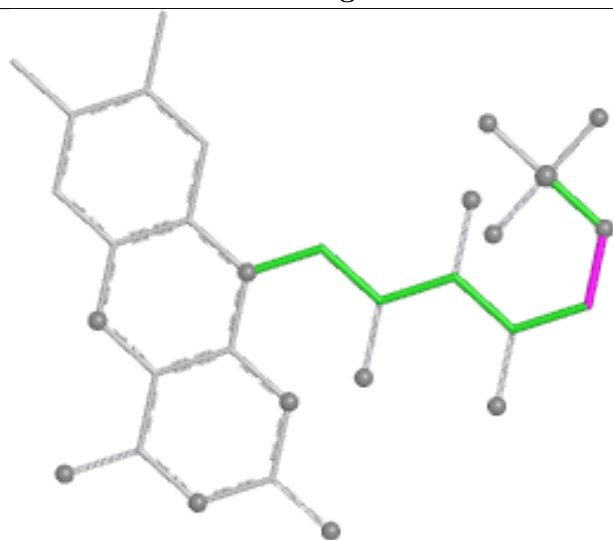
Ligand FMN V1 501



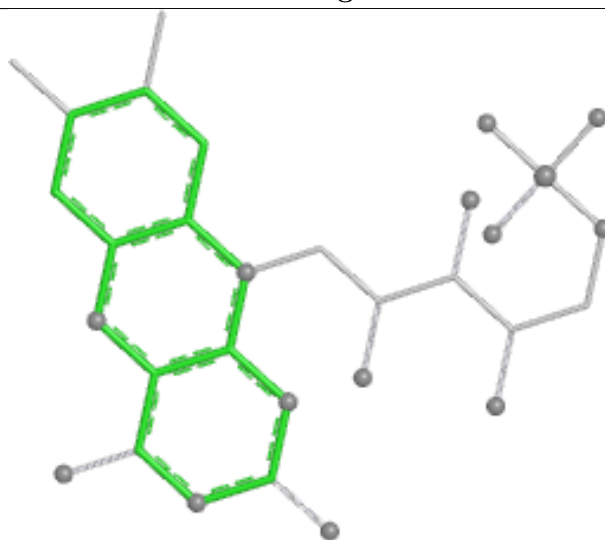
Bond lengths



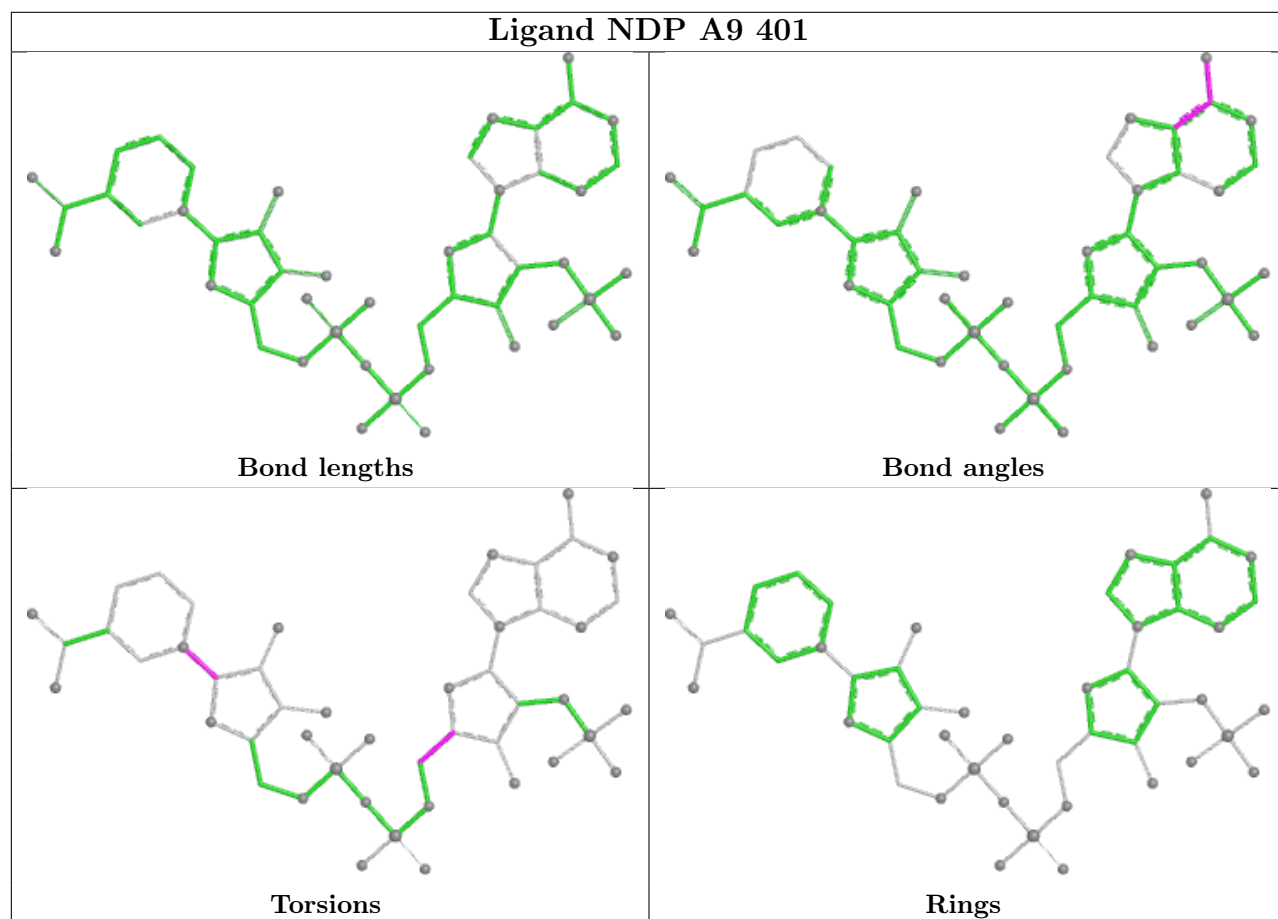
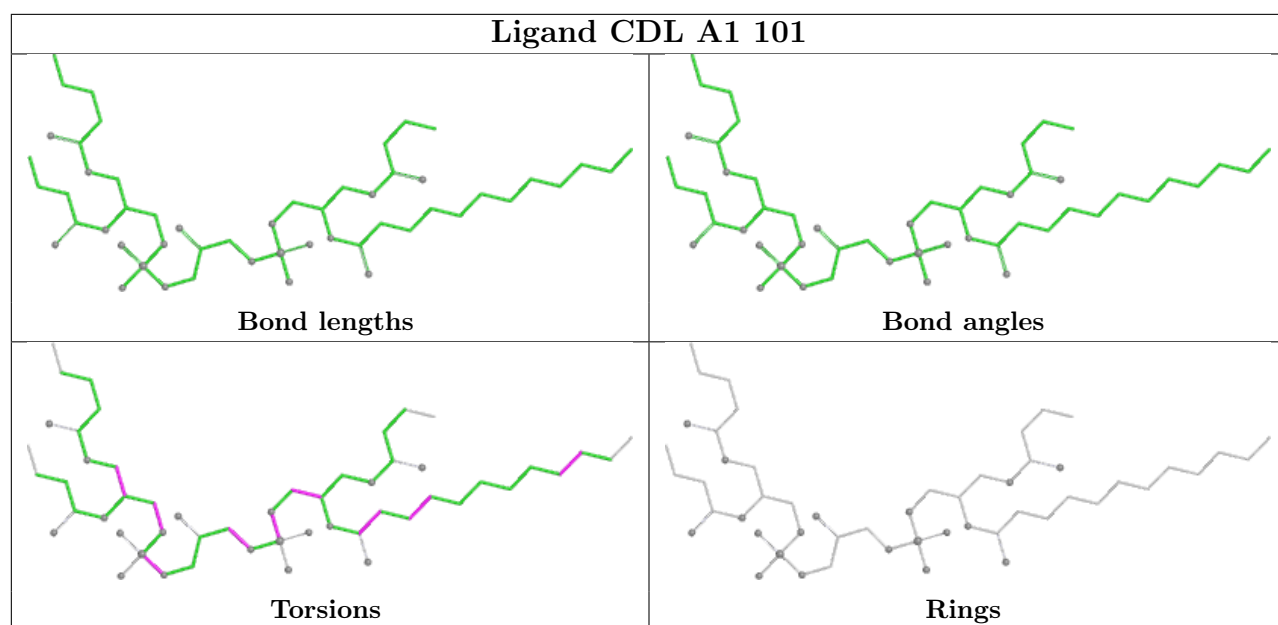
Bond angles

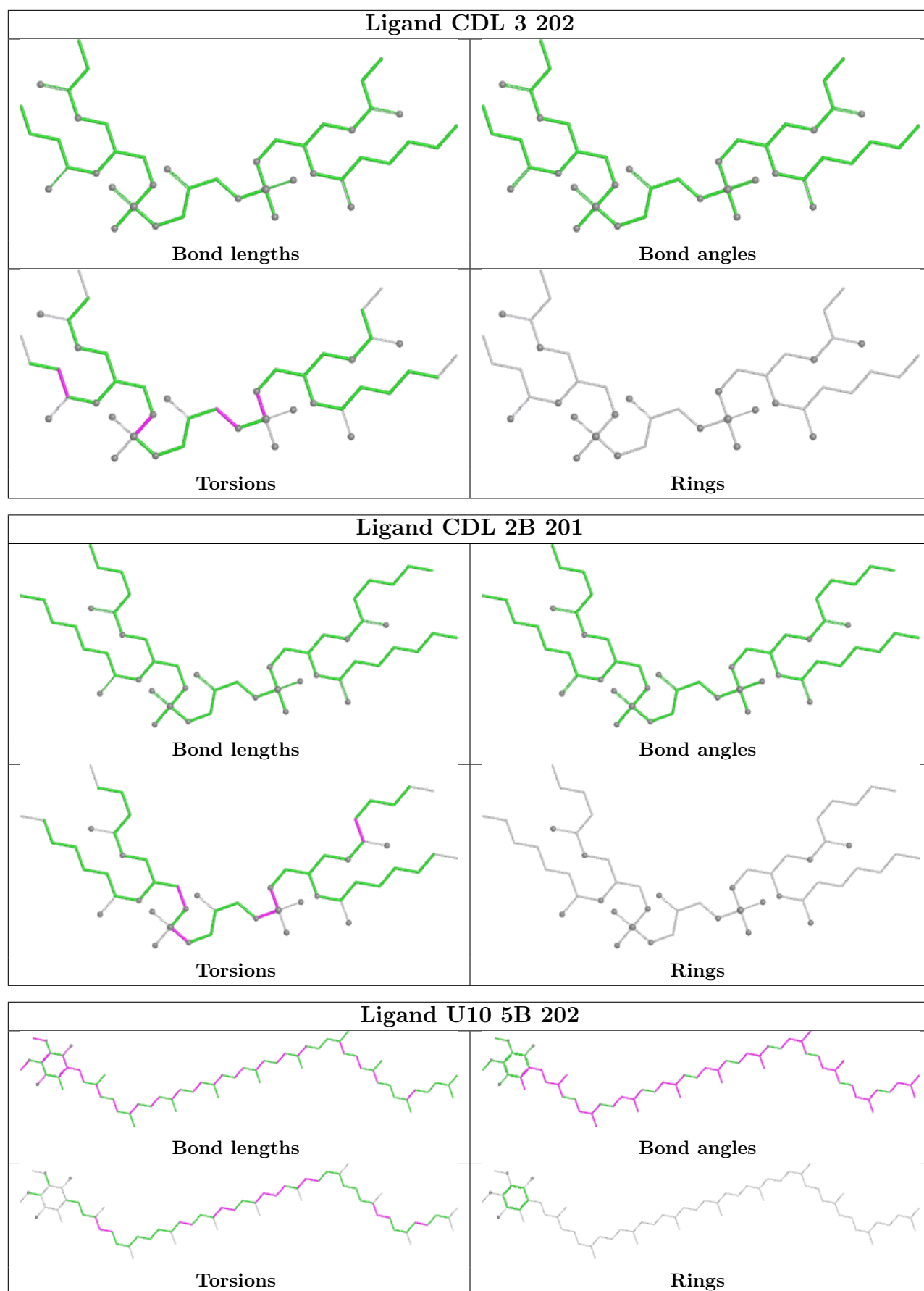


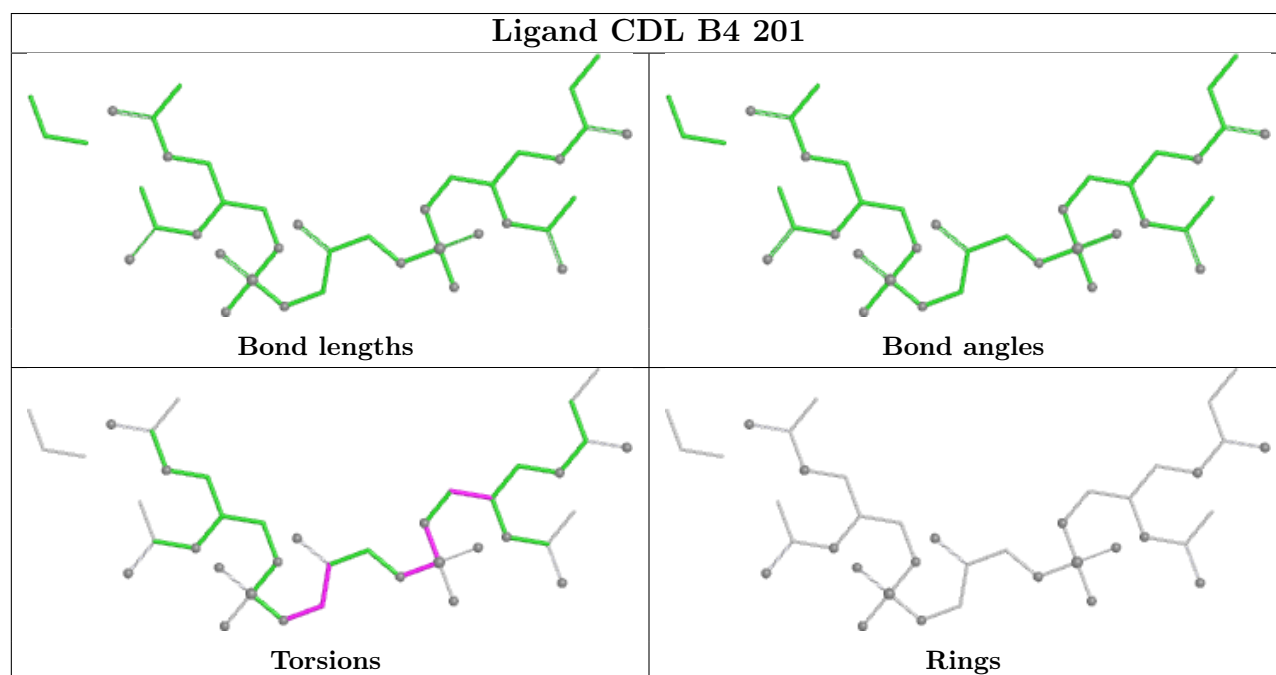
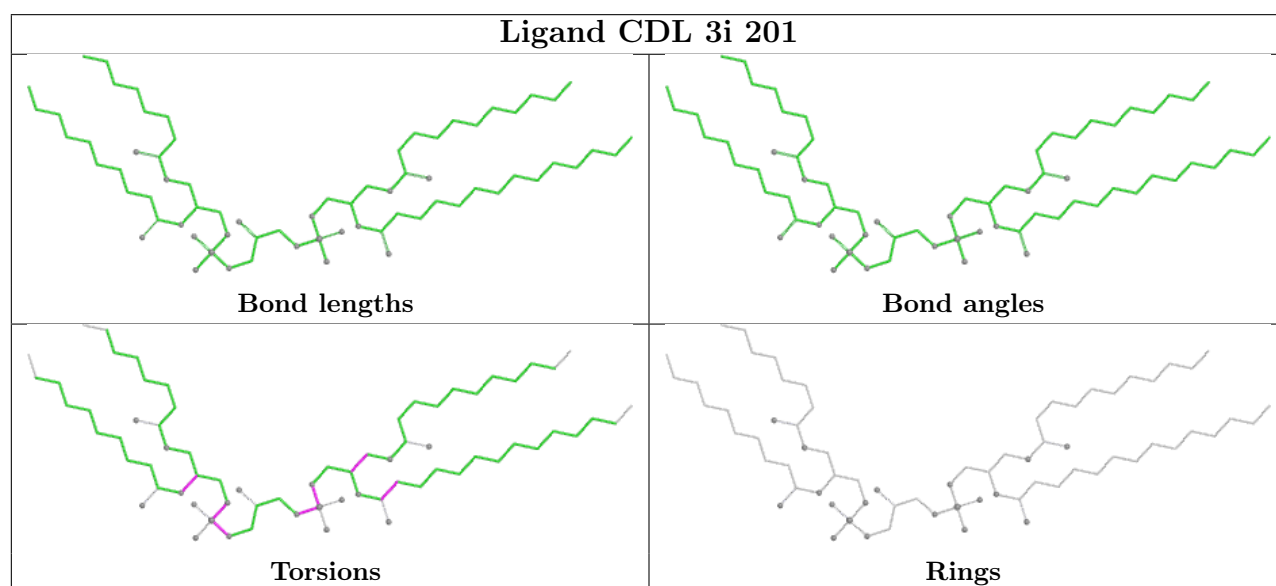
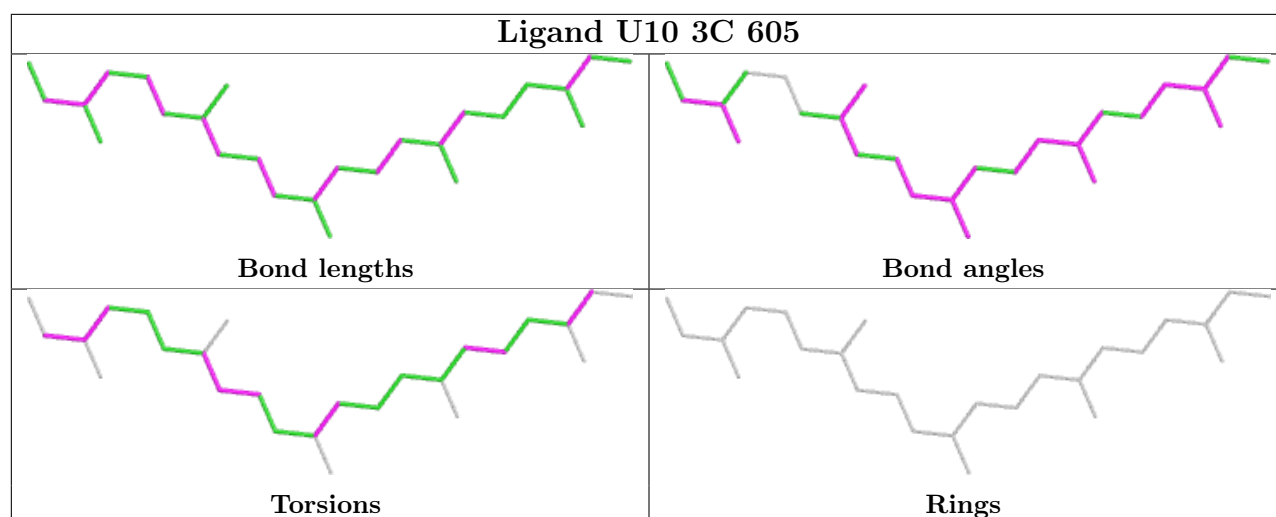
Torsions

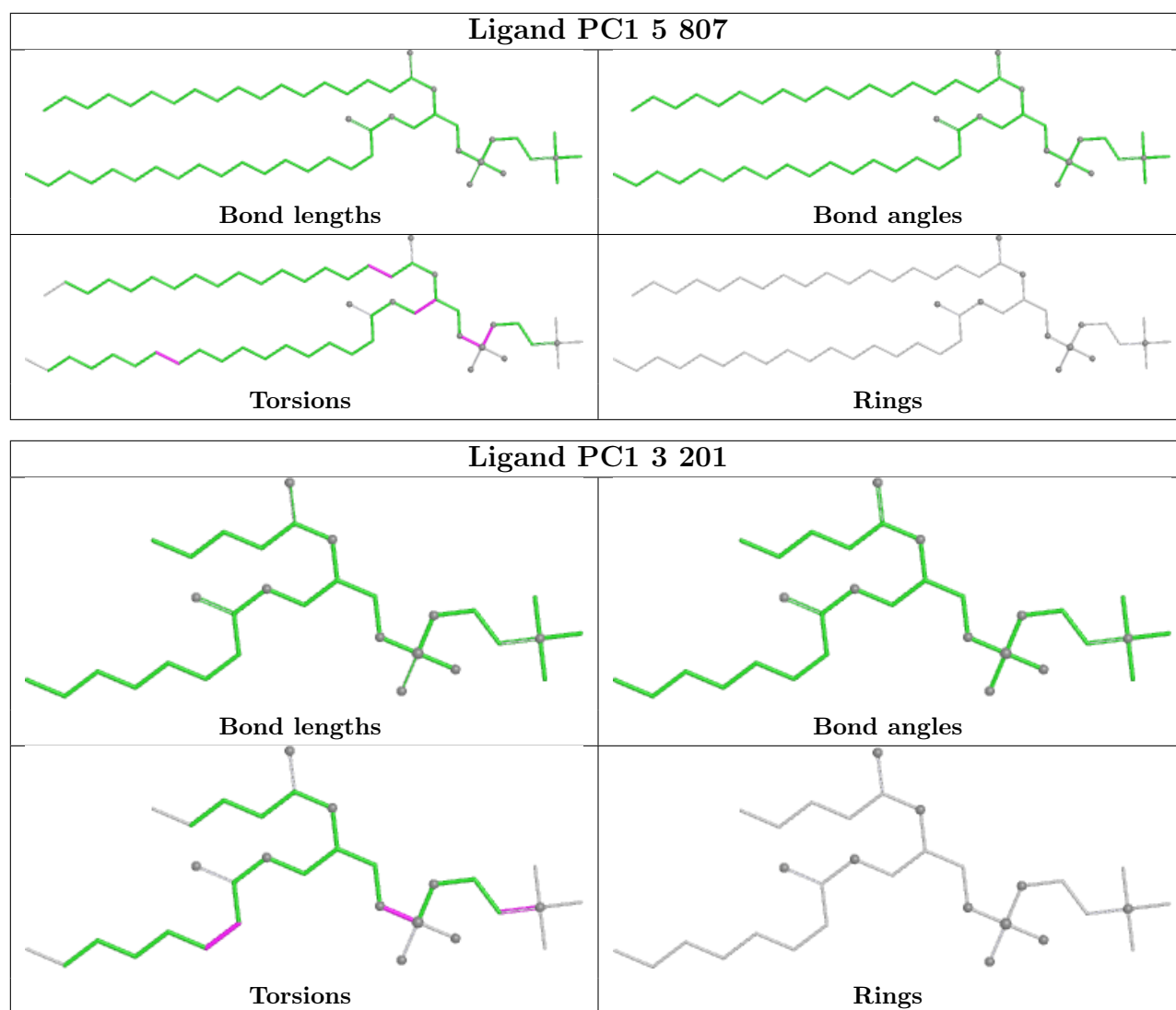


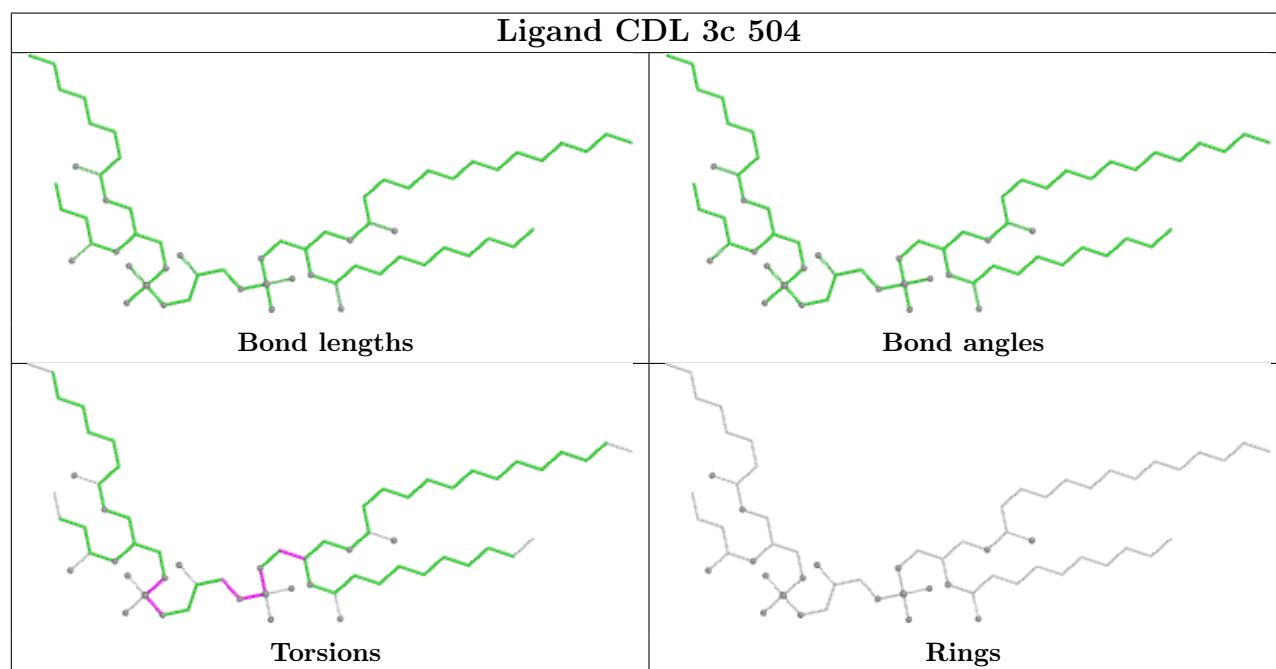
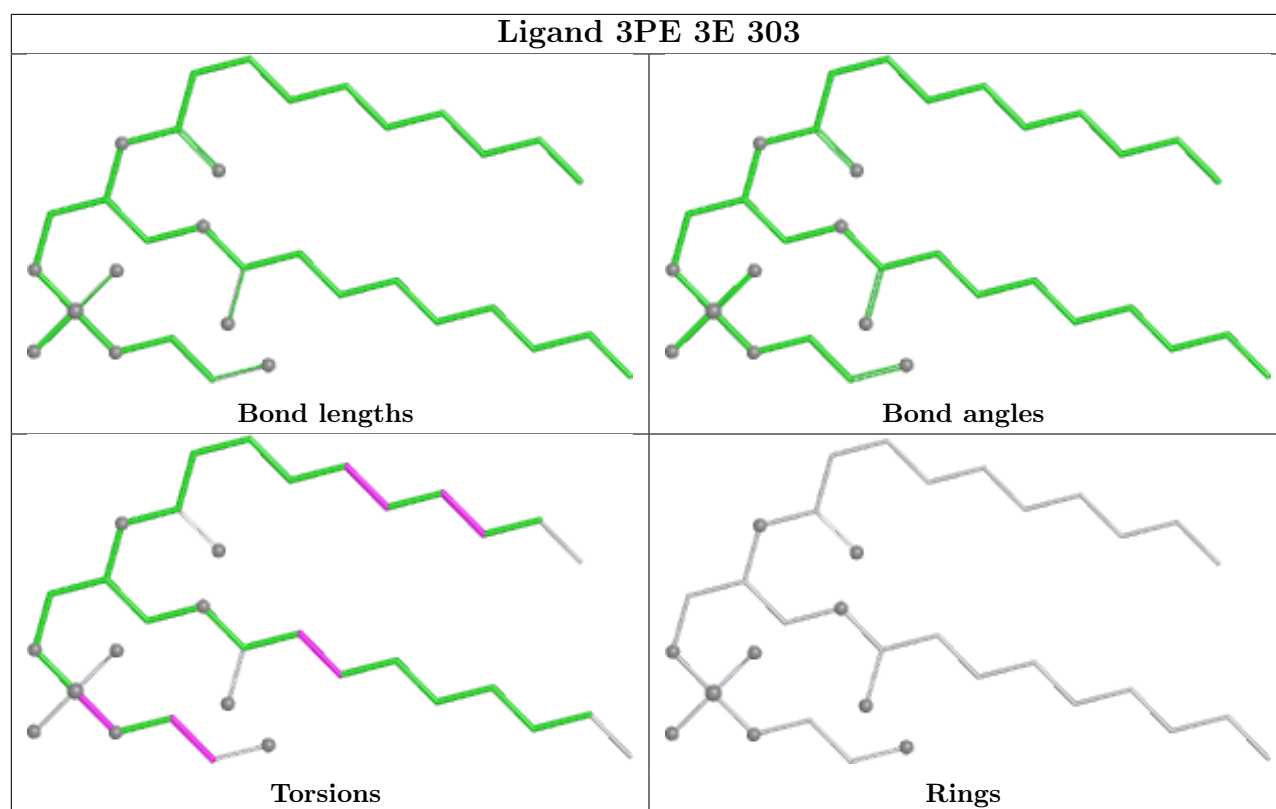
Rings

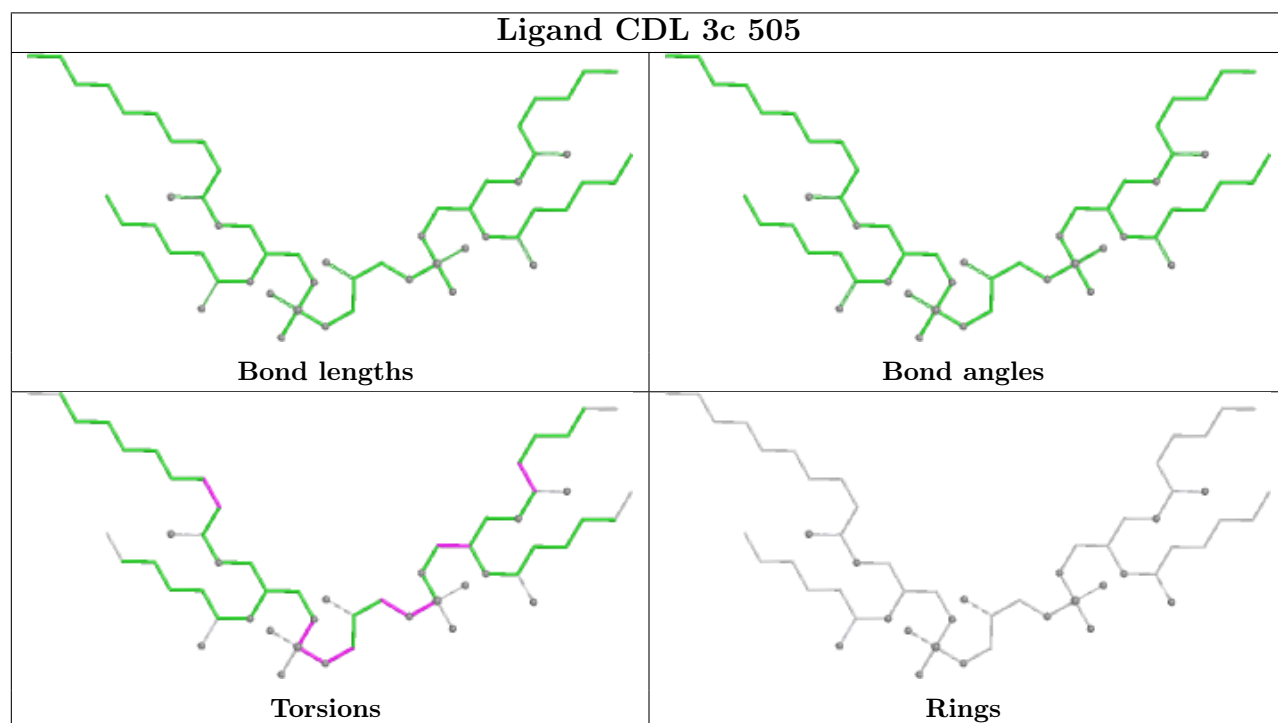
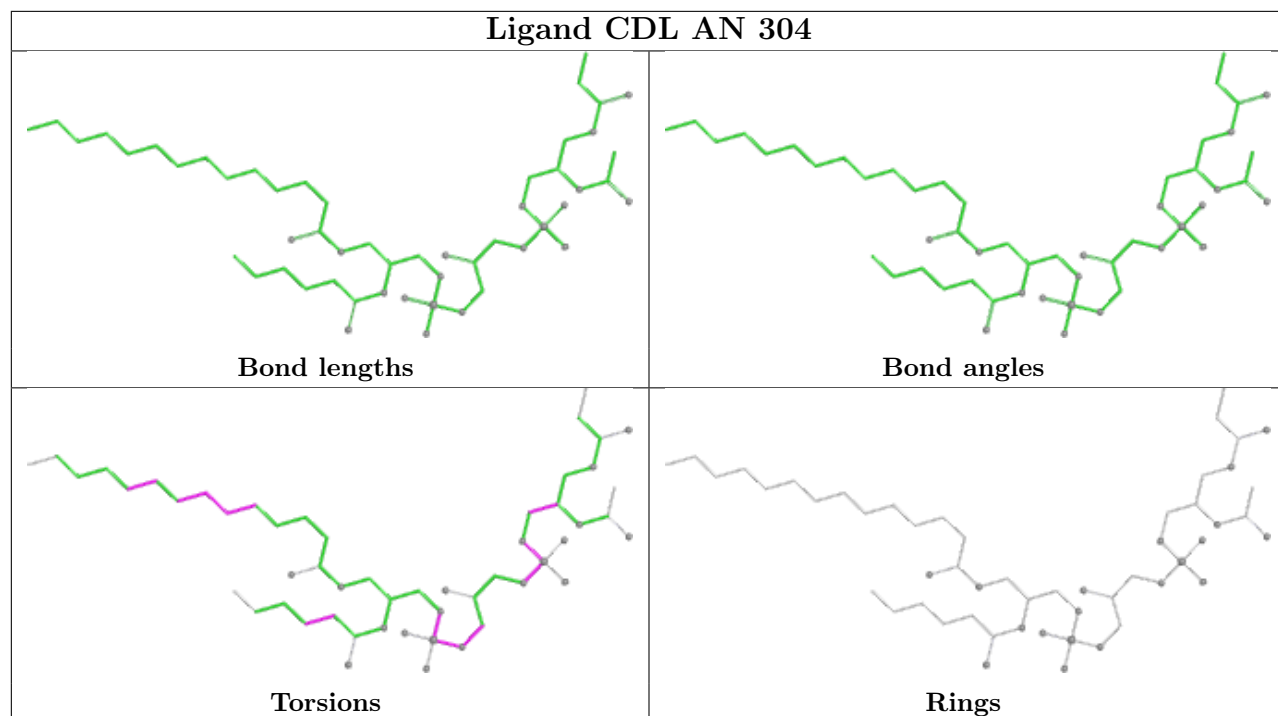


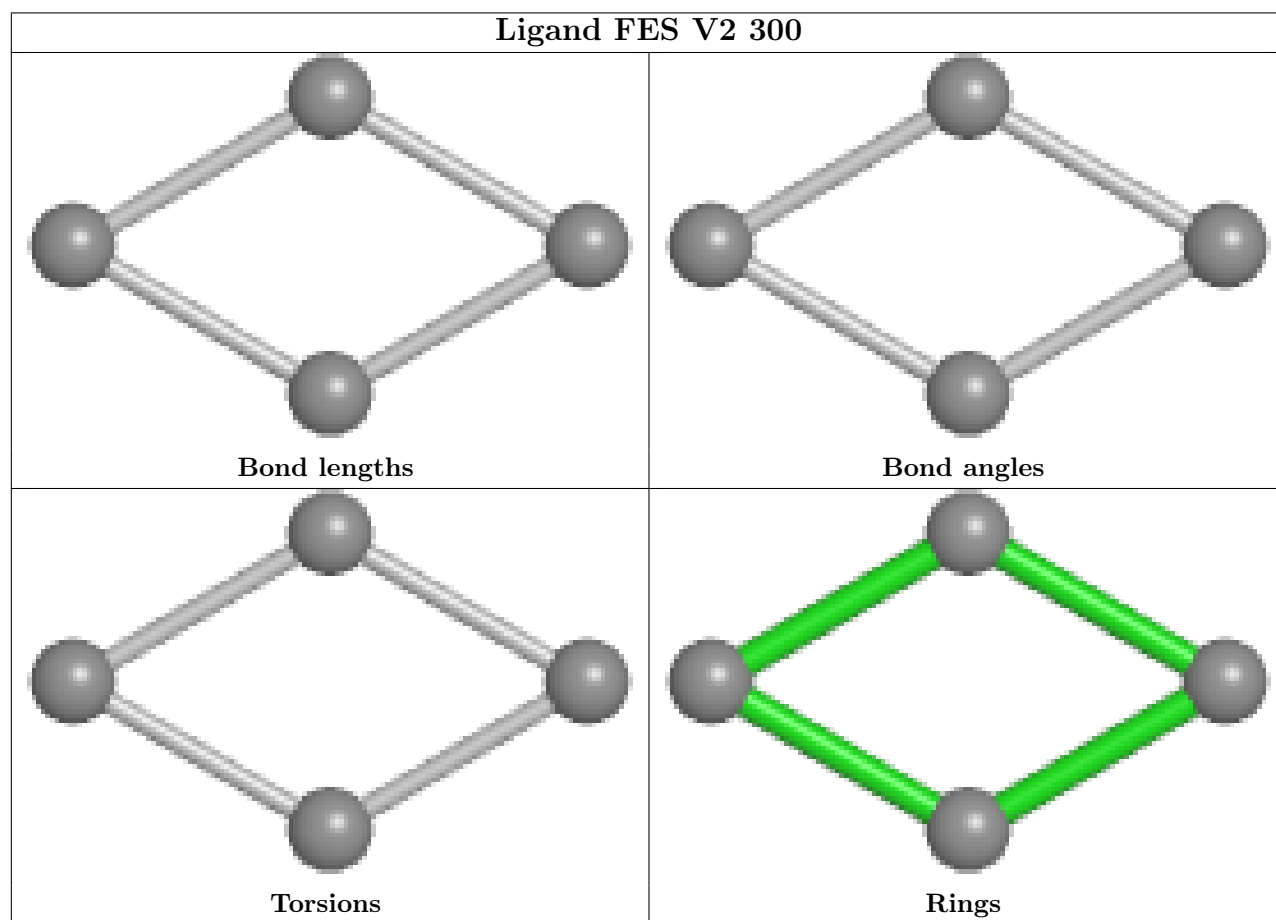
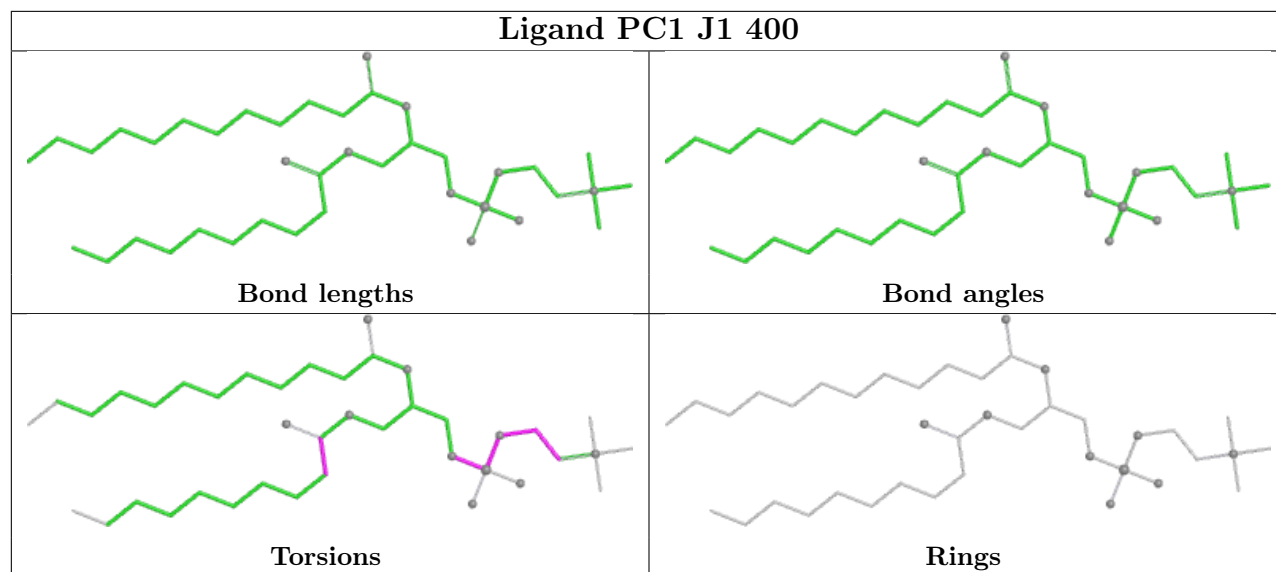


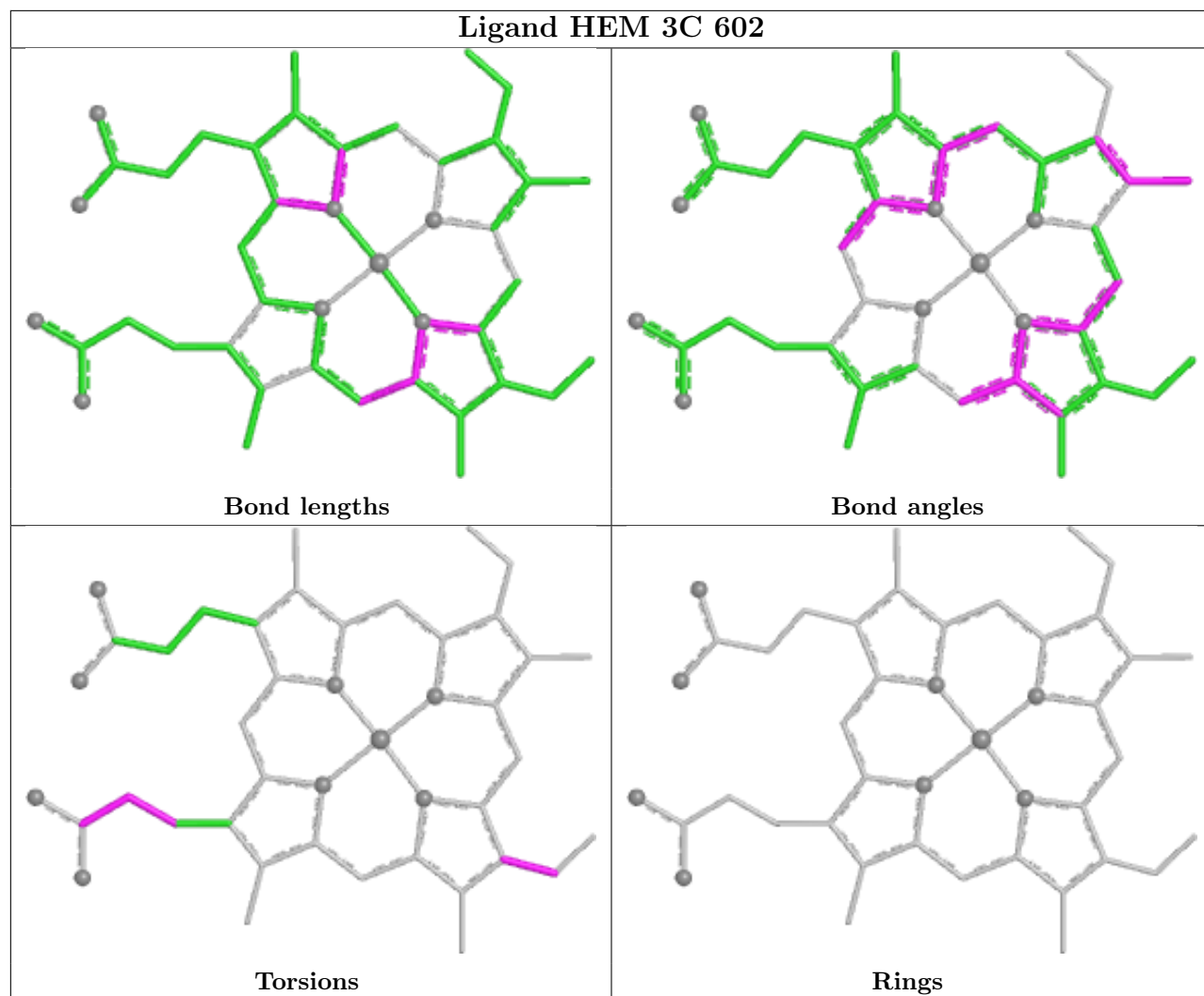




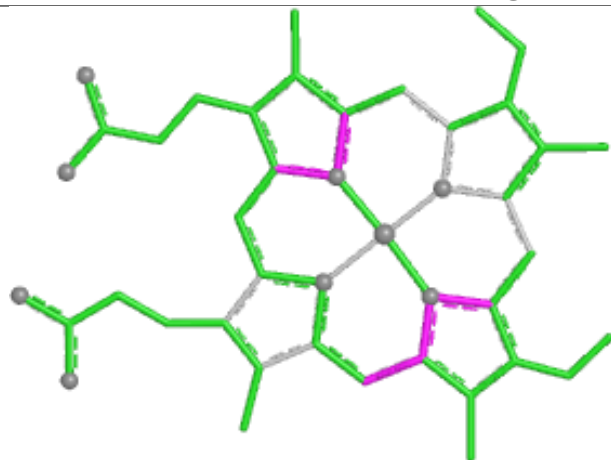




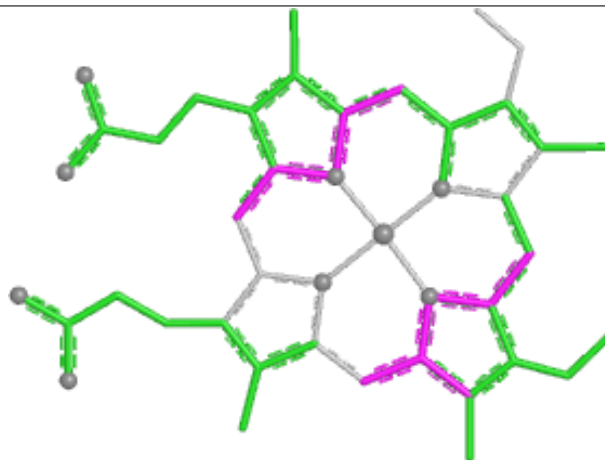




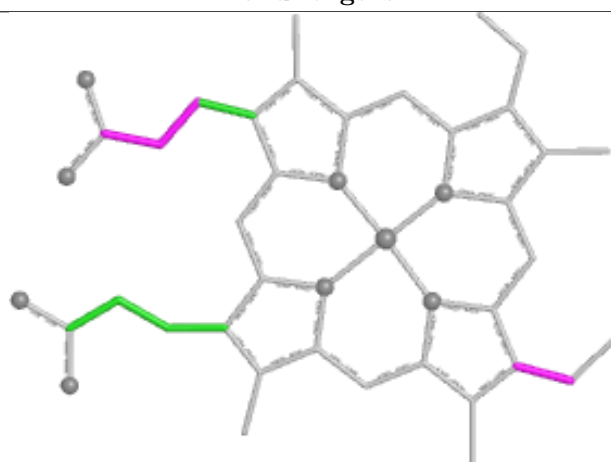
Ligand HEM 3c 502



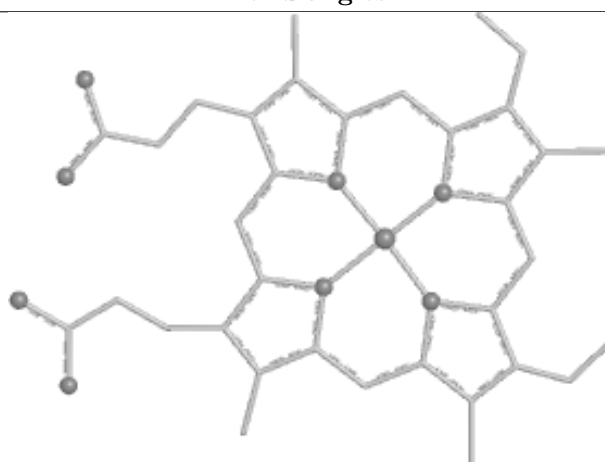
Bond lengths



Bond angles

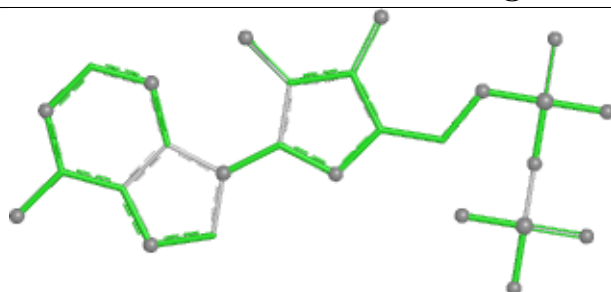


Torsions

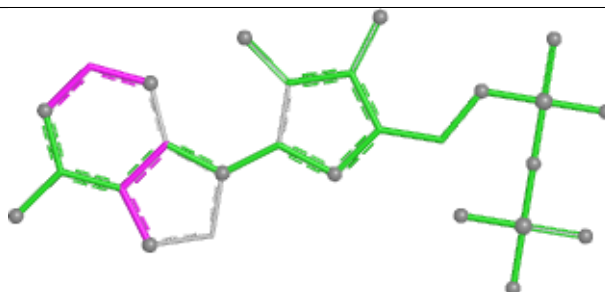


Rings

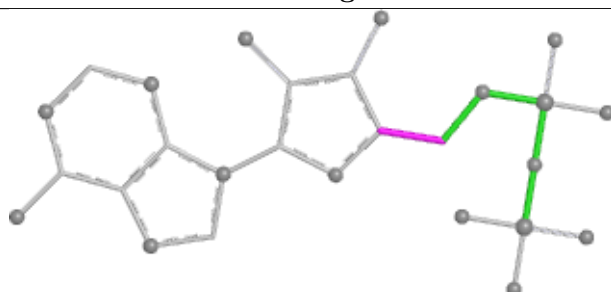
Ligand ADP B8 602



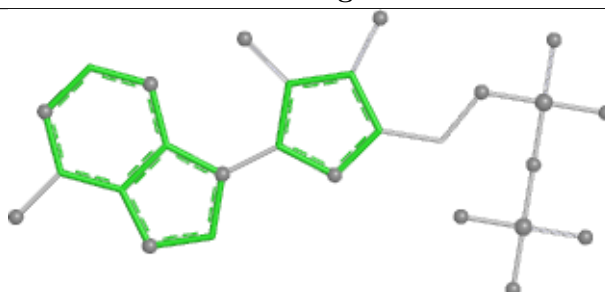
Bond lengths



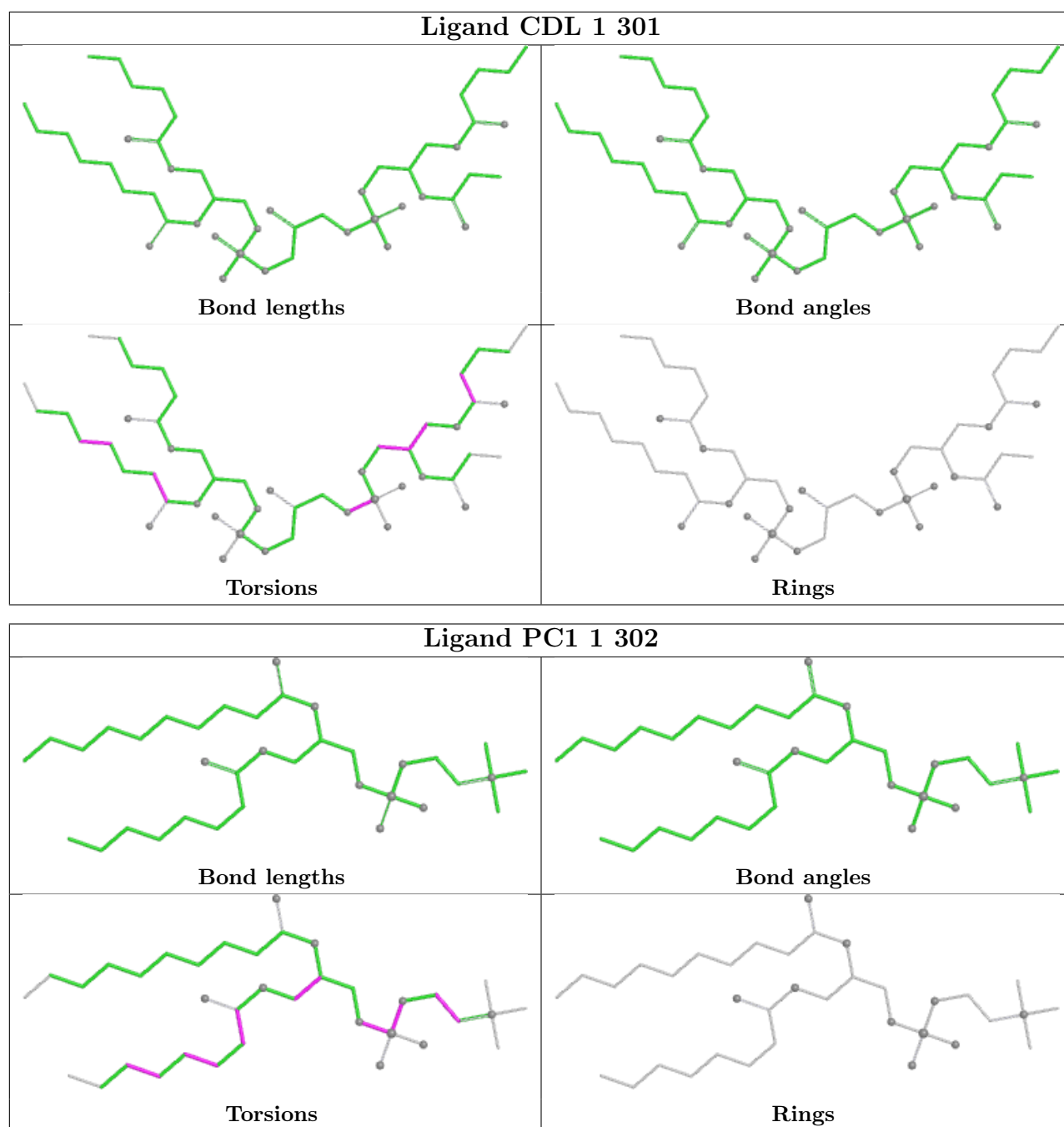
Bond angles

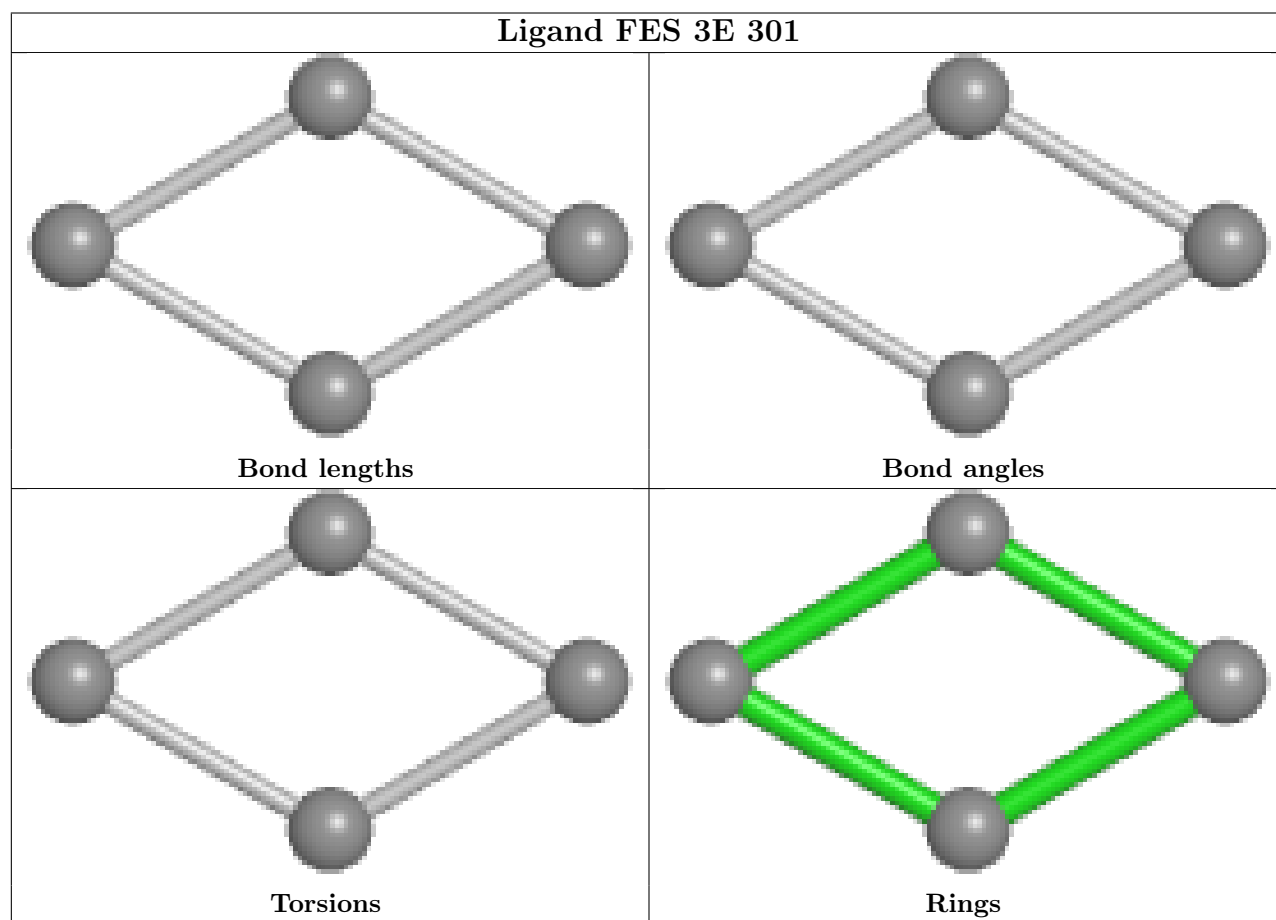
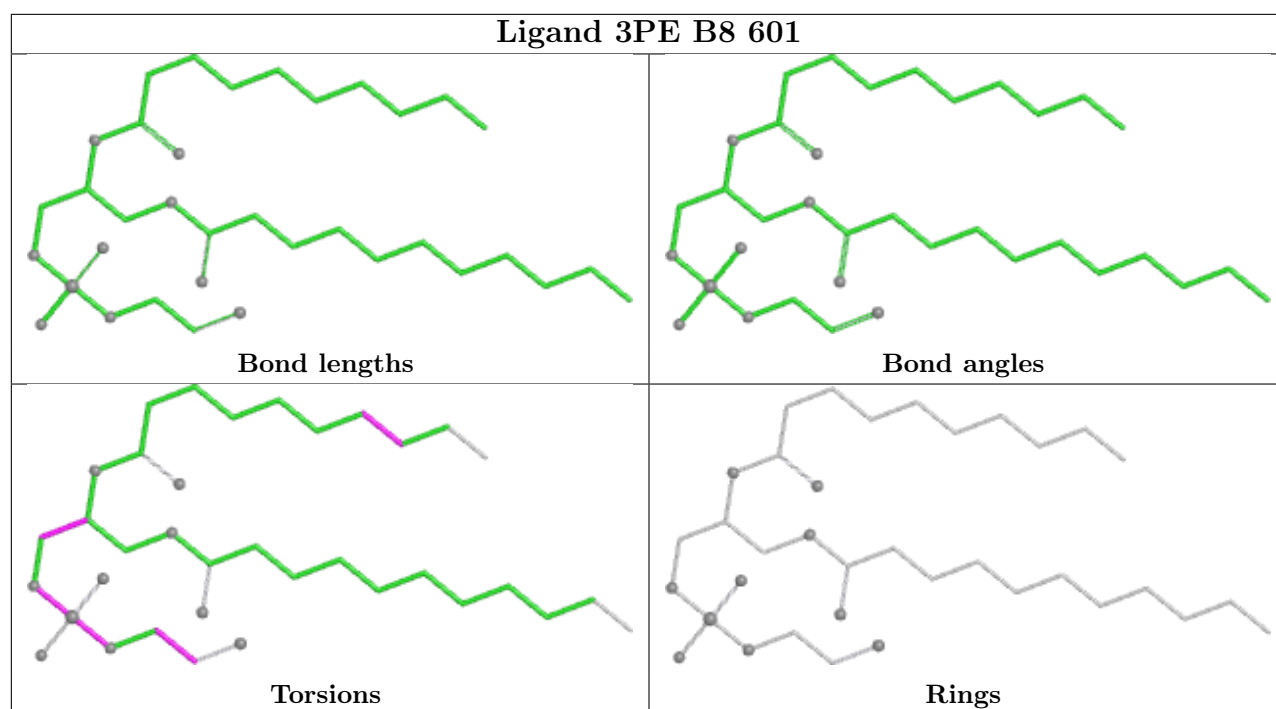


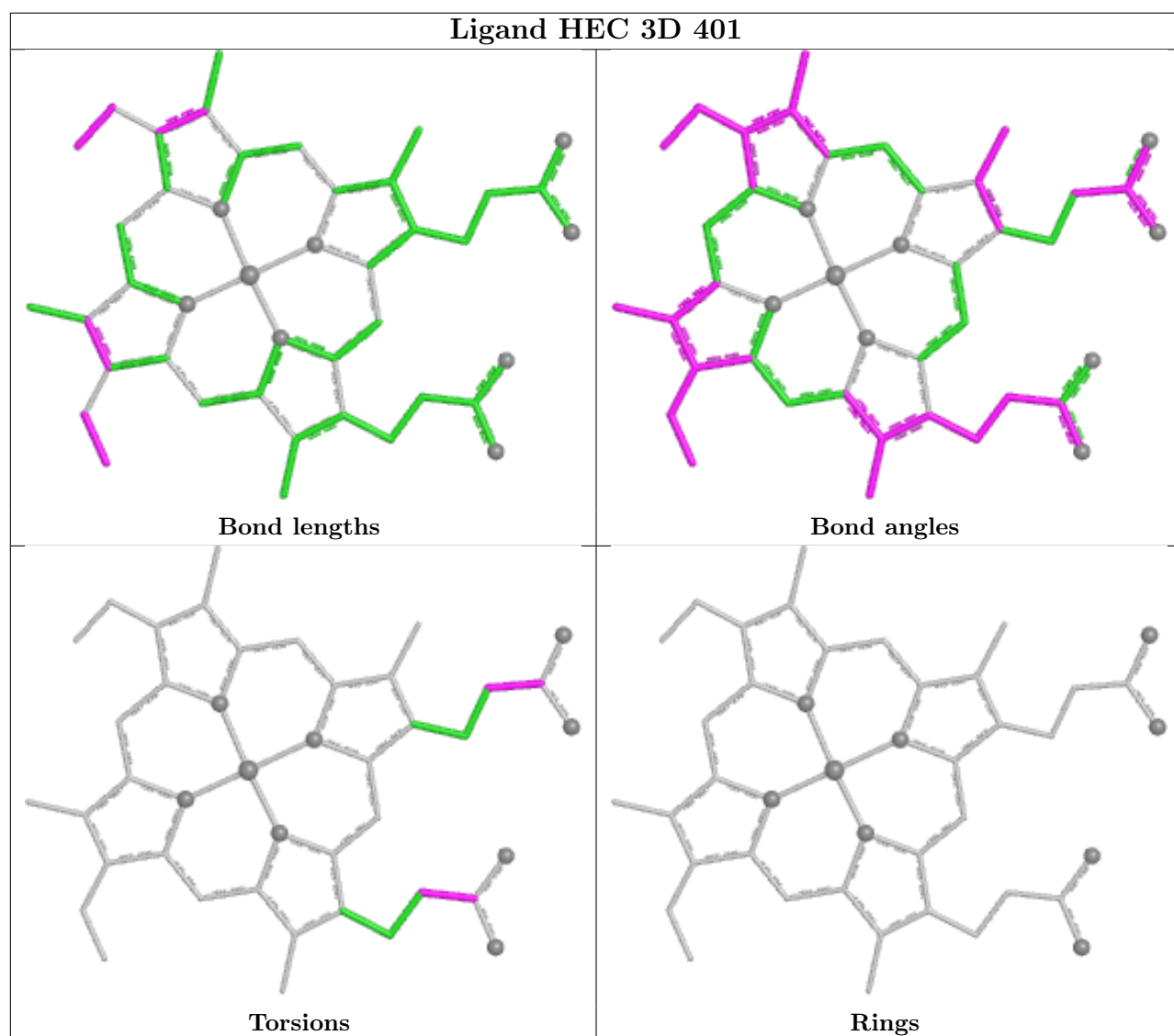
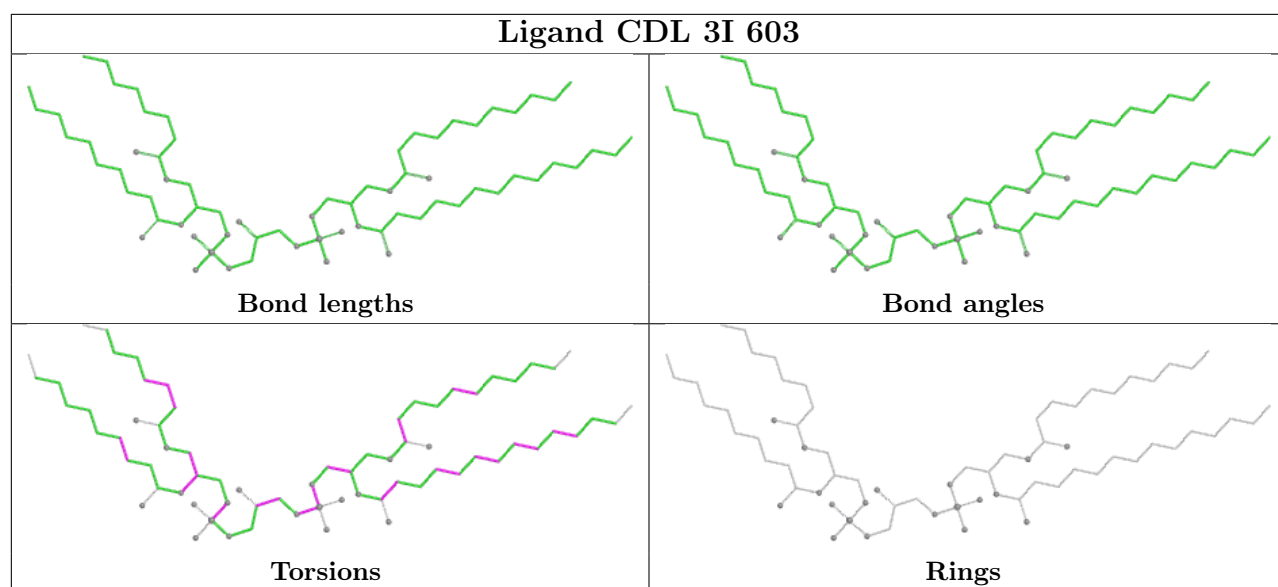
Torsions

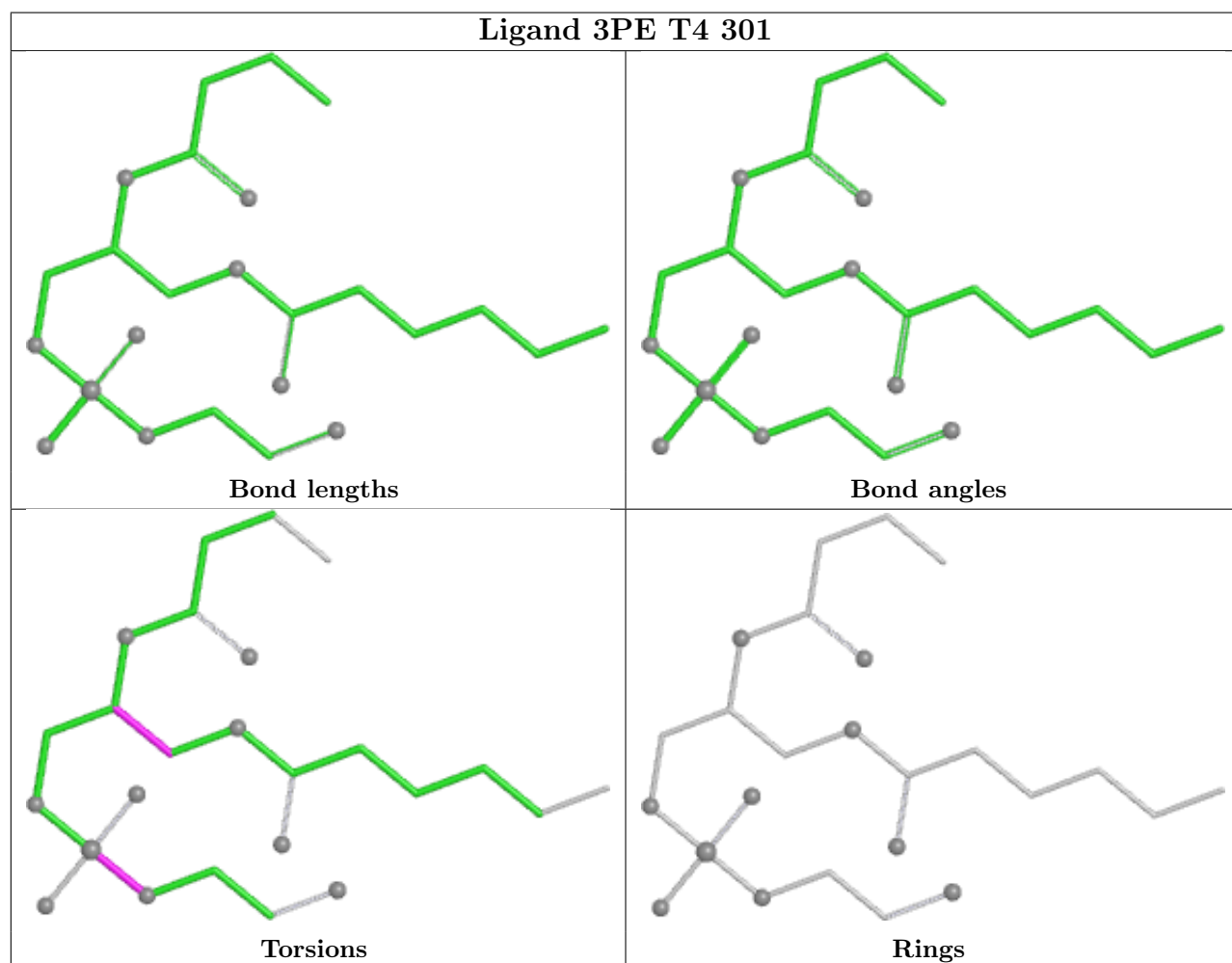
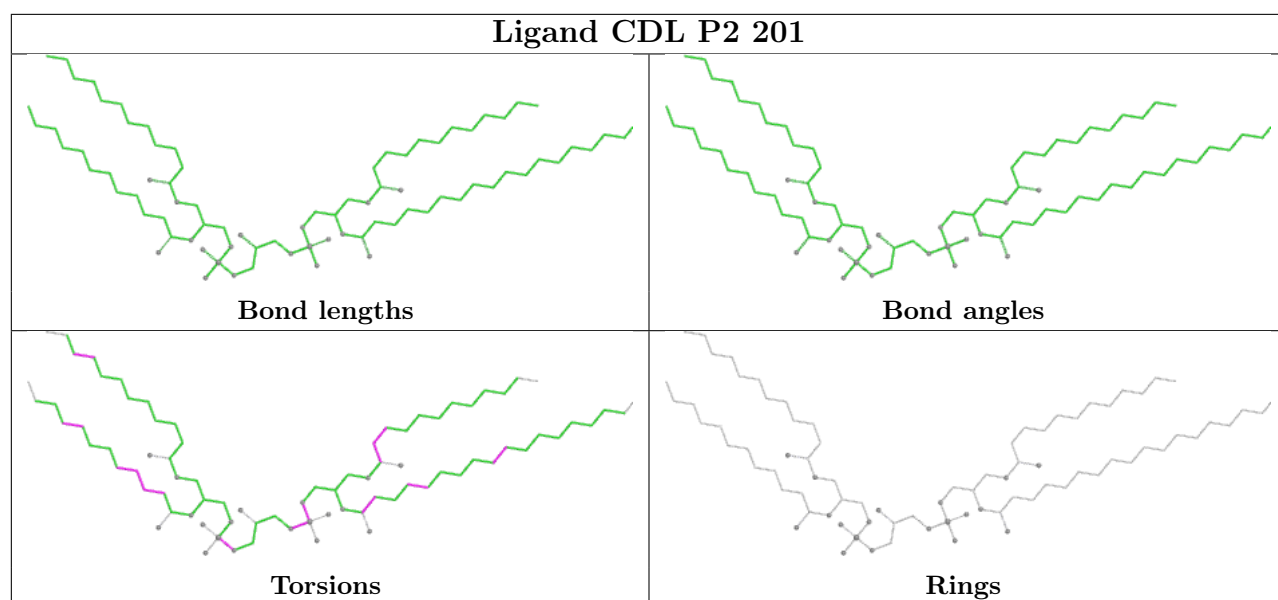


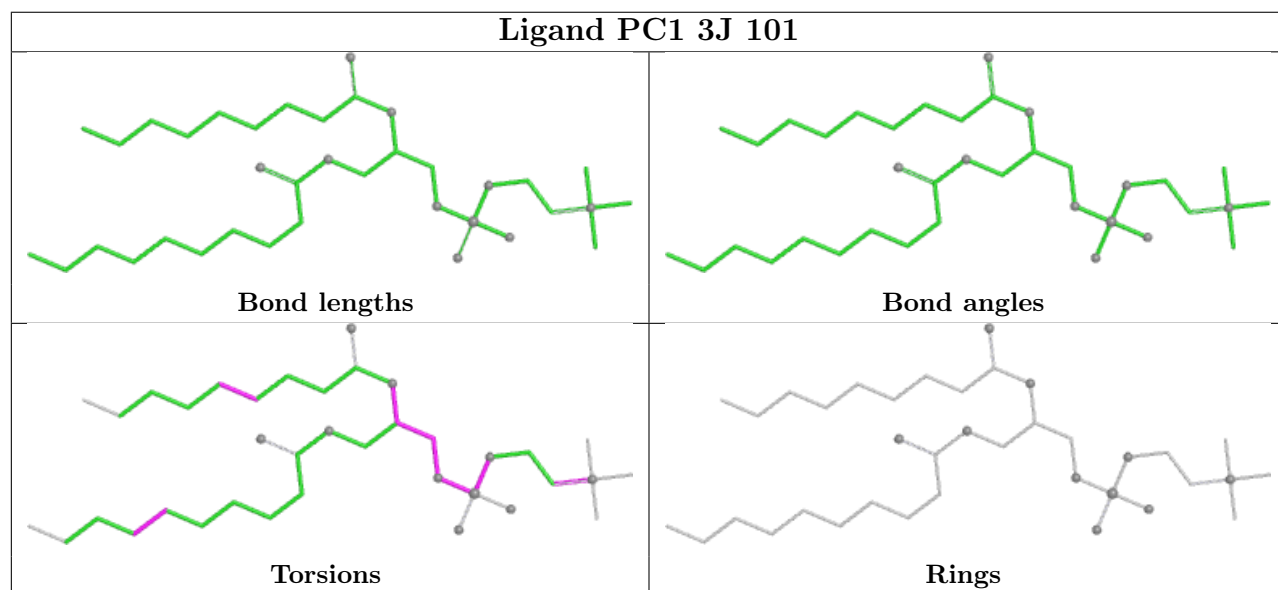
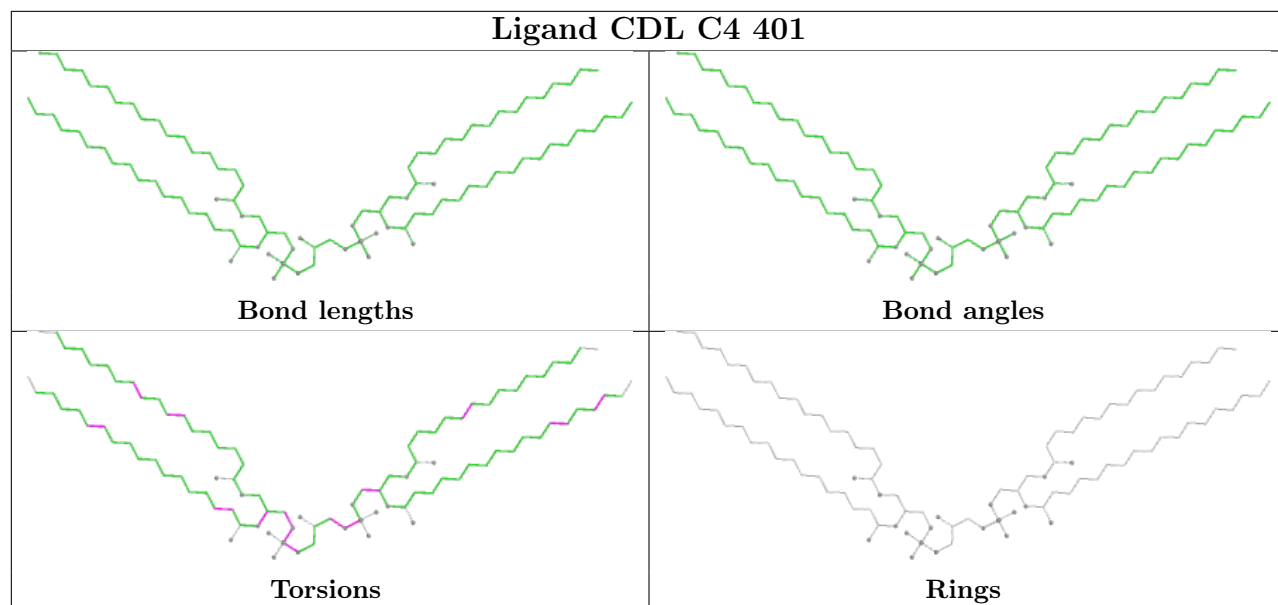
Rings

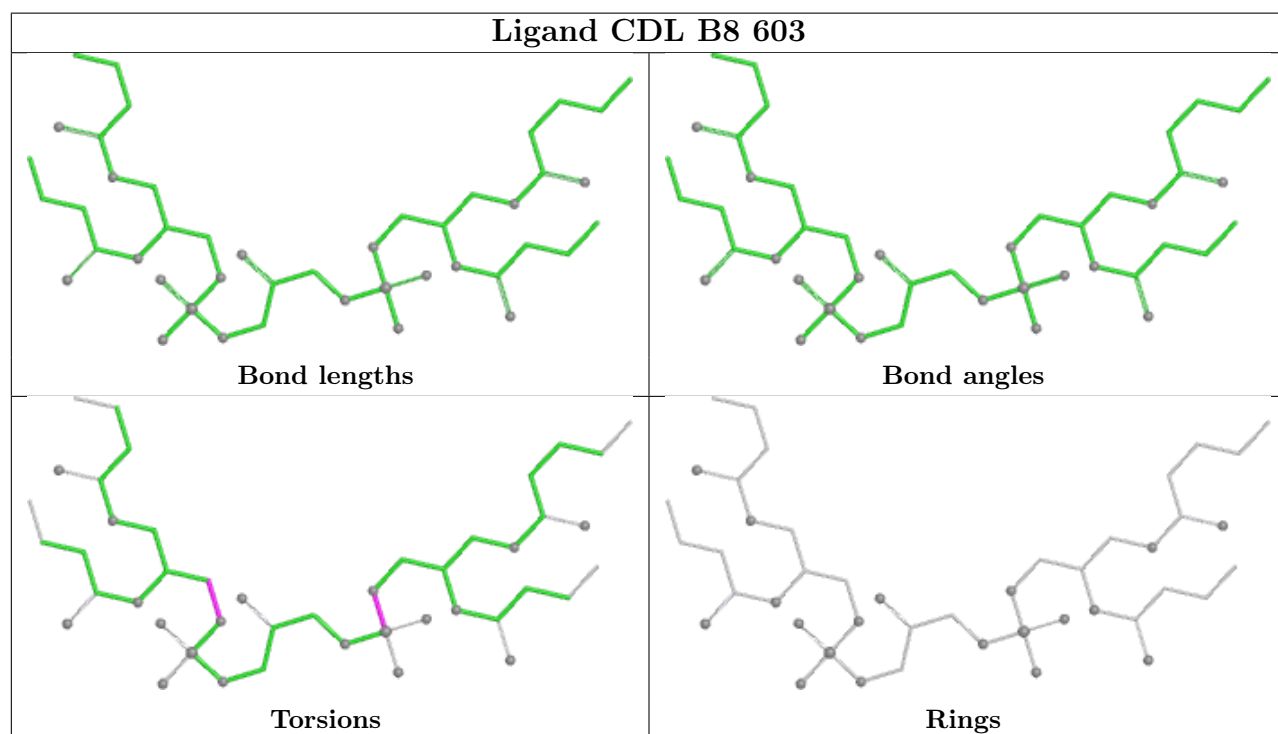
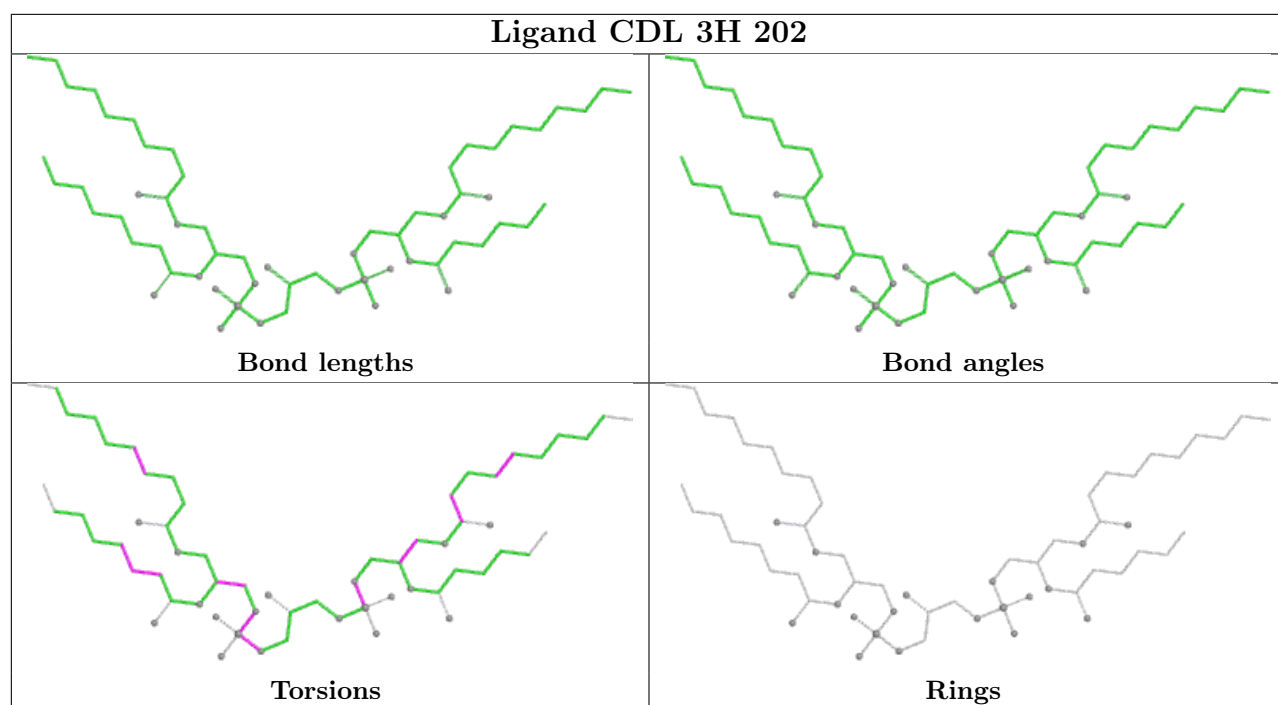


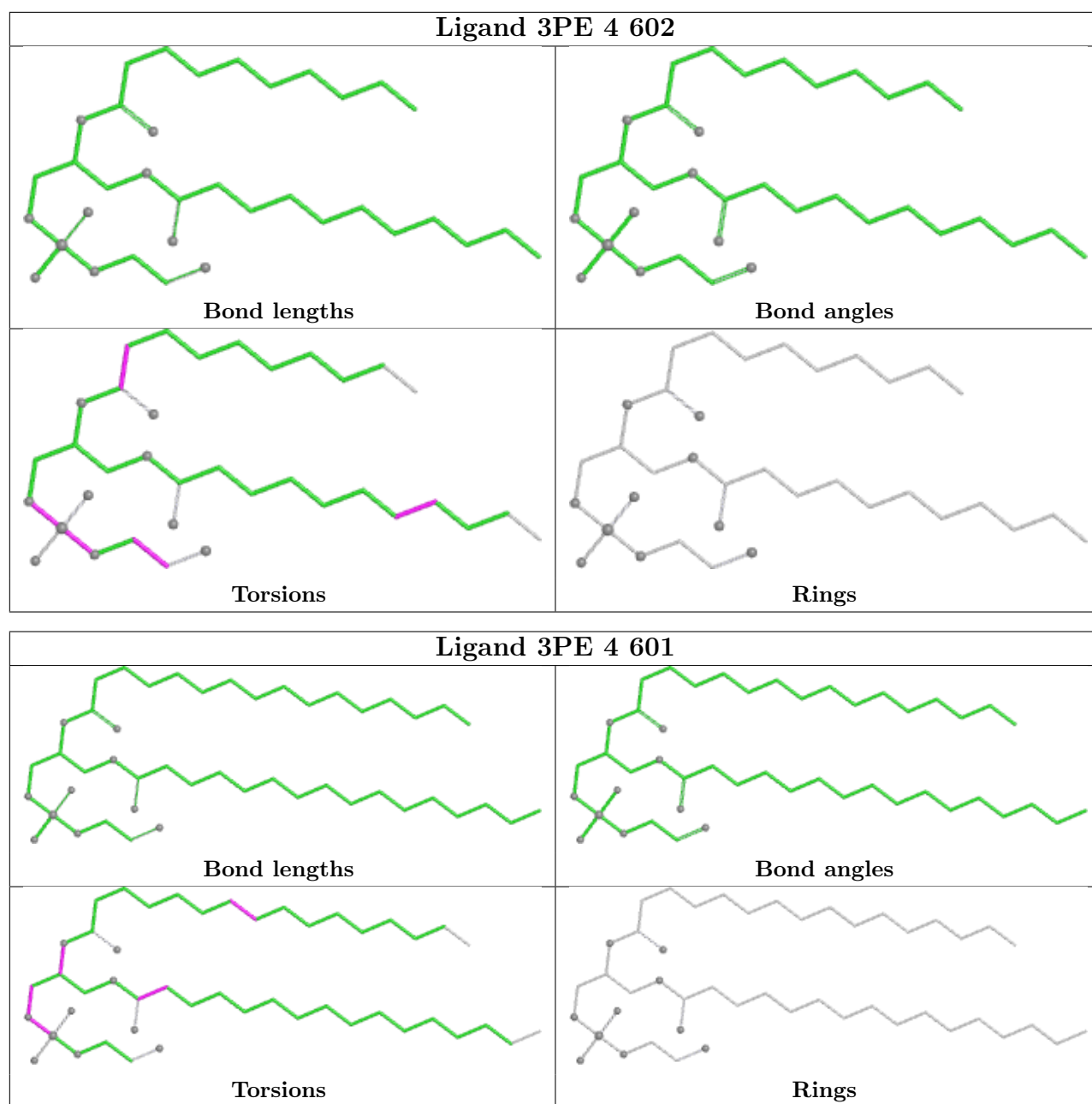


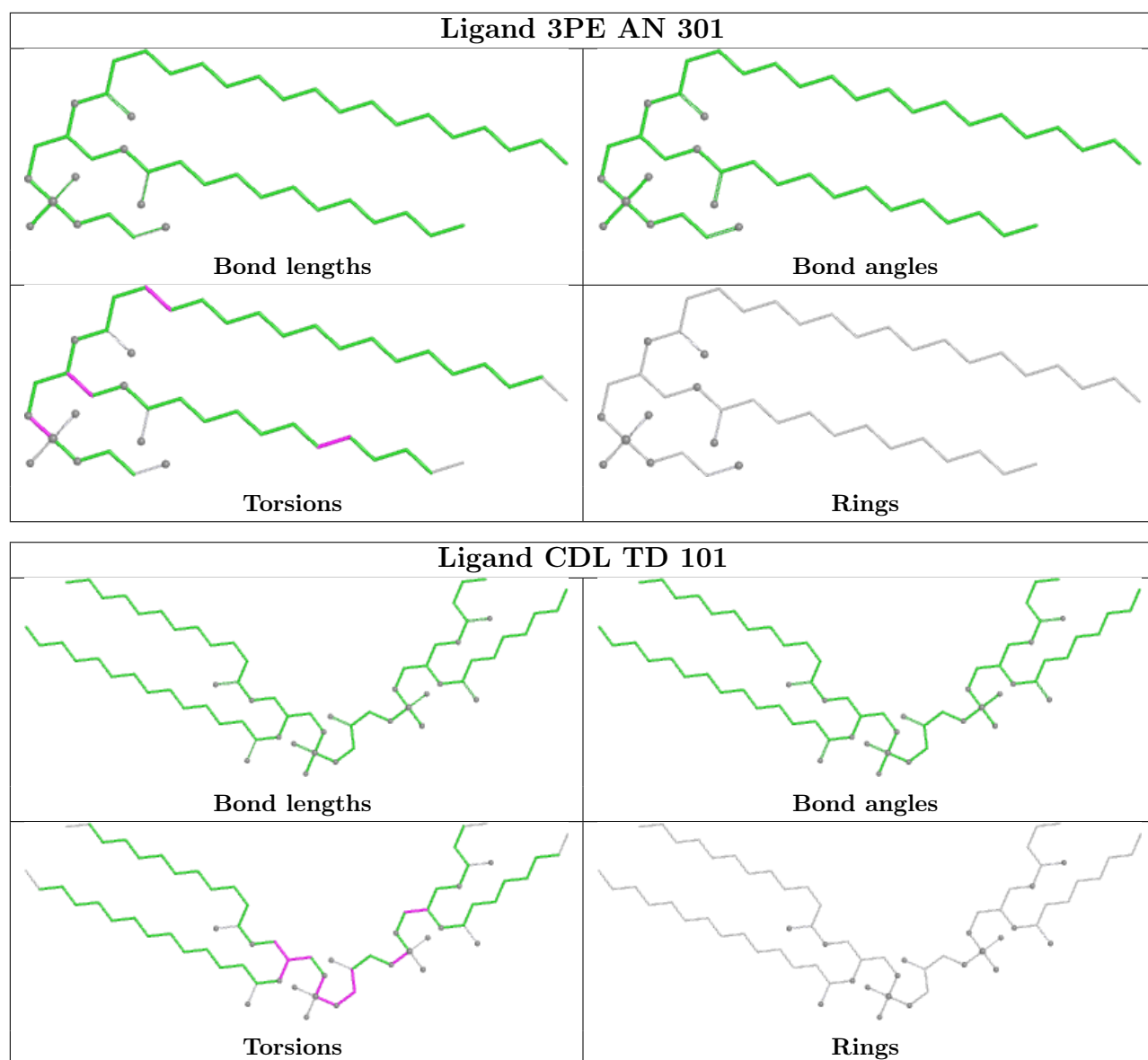


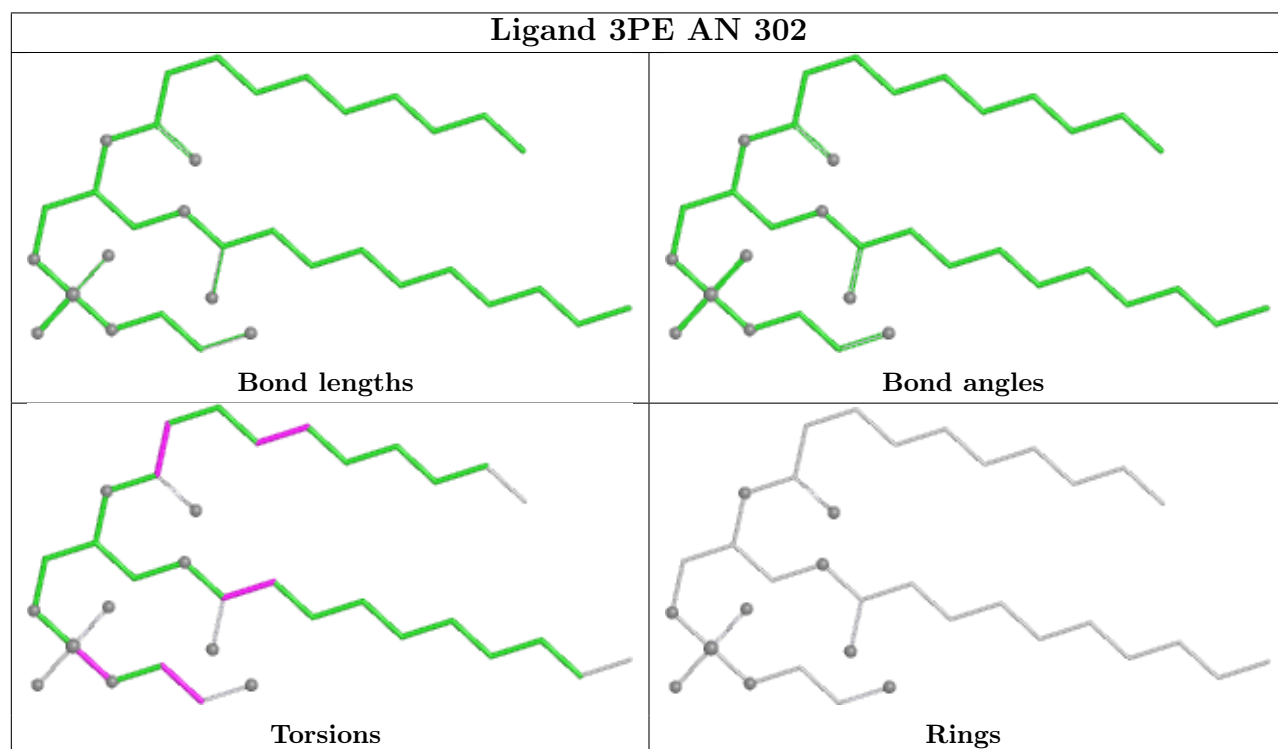
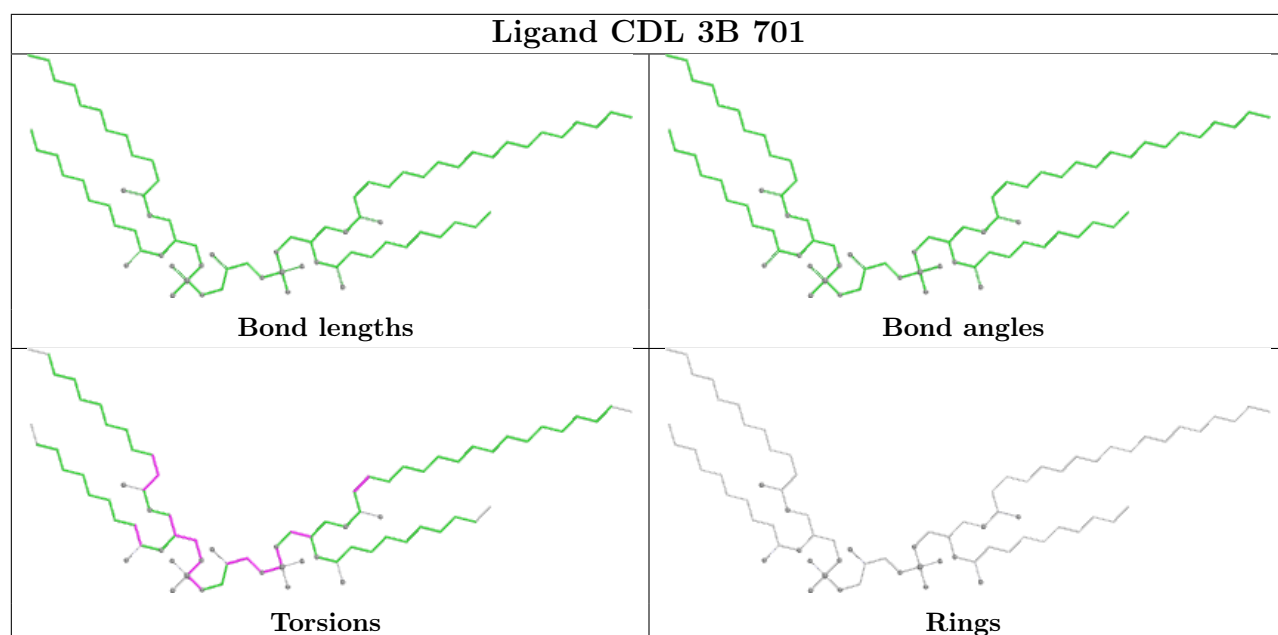


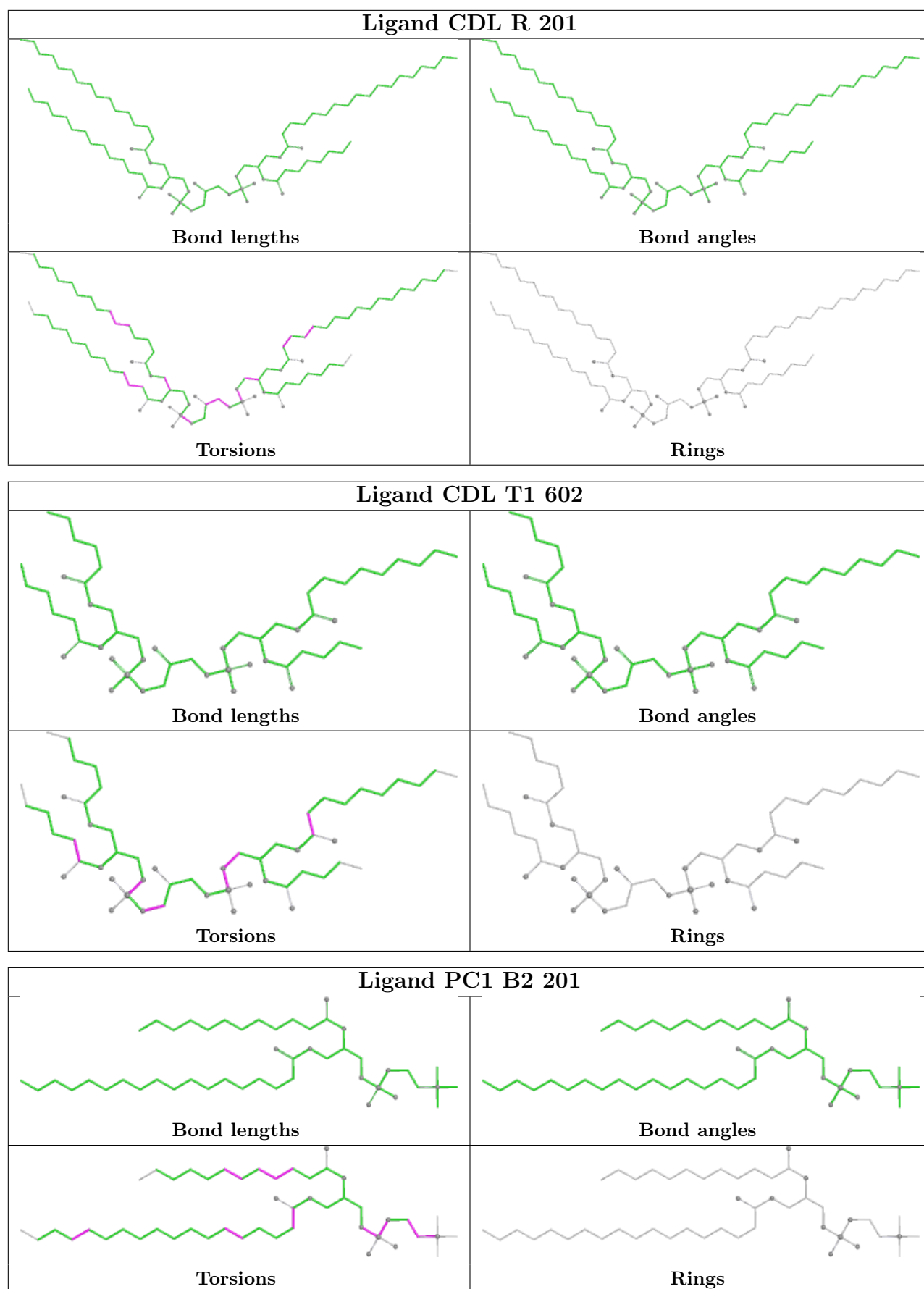


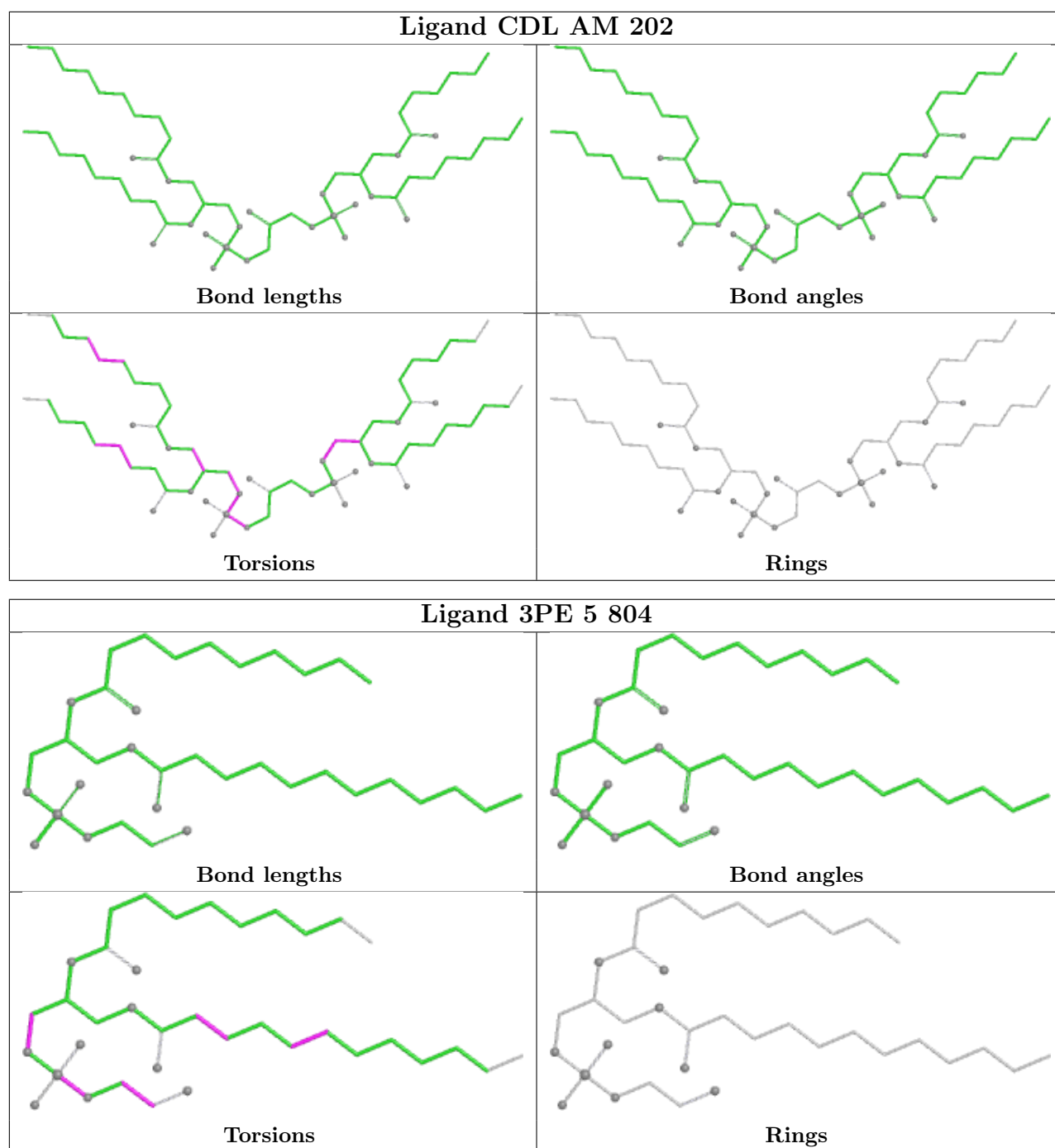


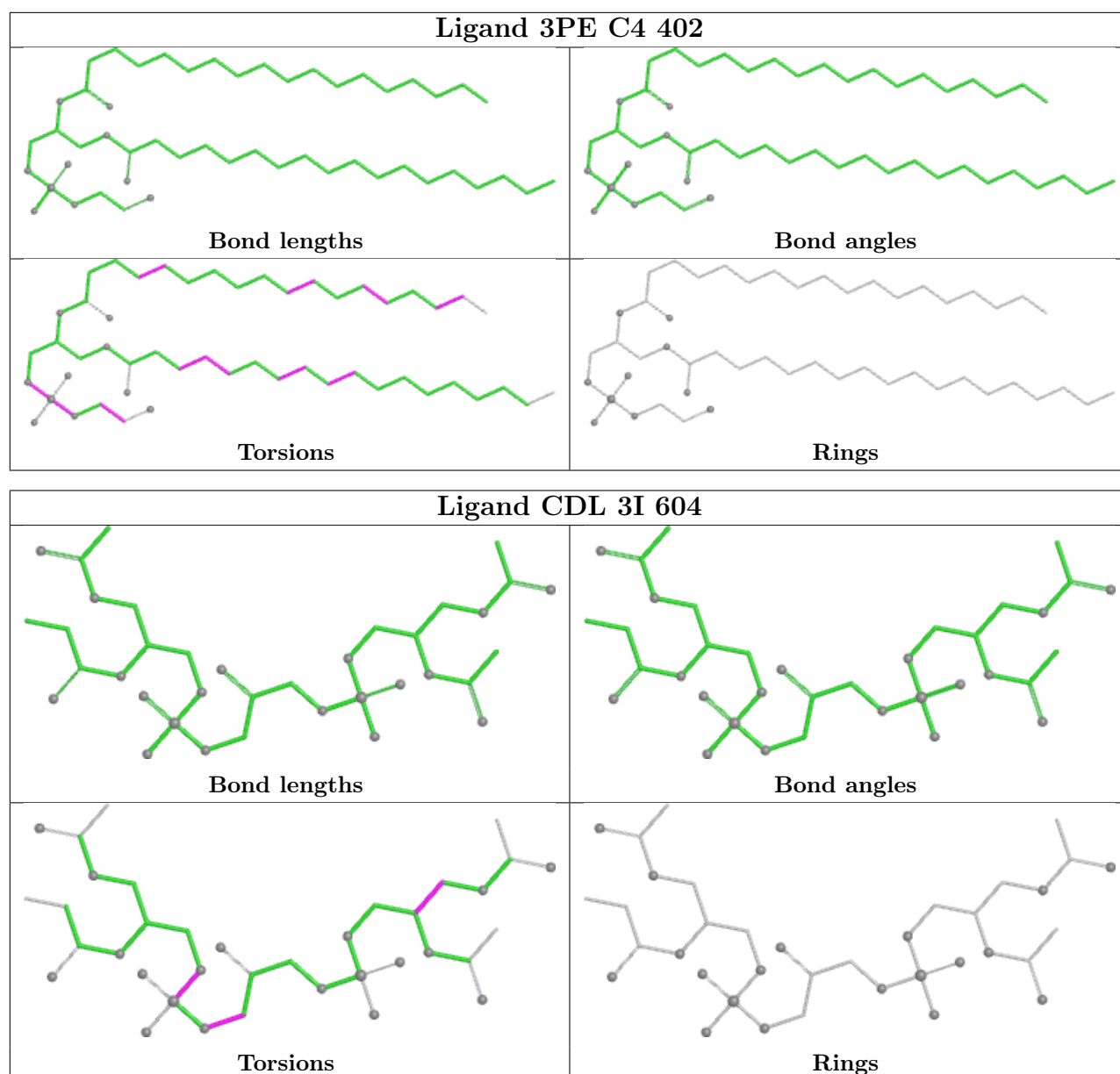












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

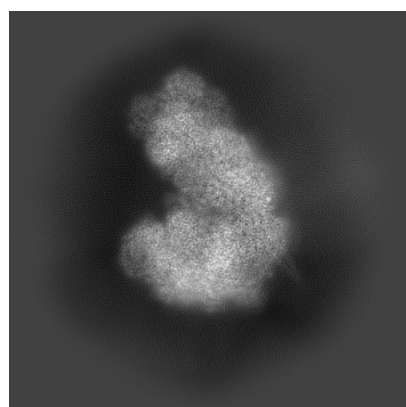
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25882. These allow visual inspection of the internal detail of the map and identification of artifacts.

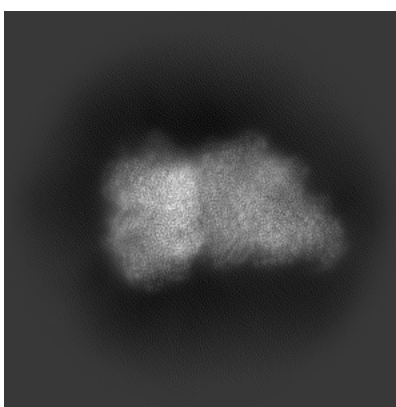
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

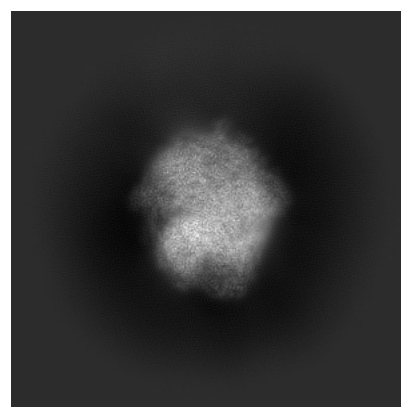
6.1.1 Primary map



X



Y

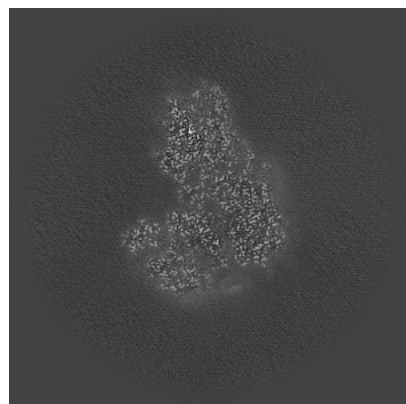


Z

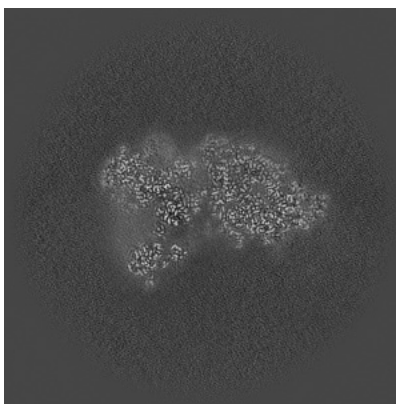
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

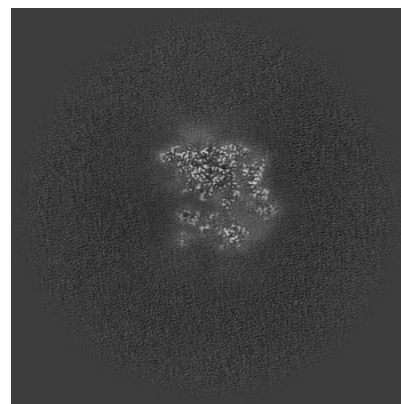
6.2.1 Primary map



X Index: 300



Y Index: 300

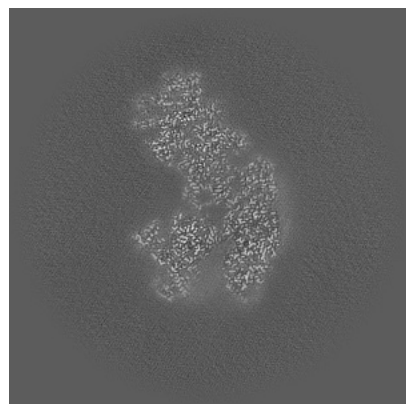


Z Index: 300

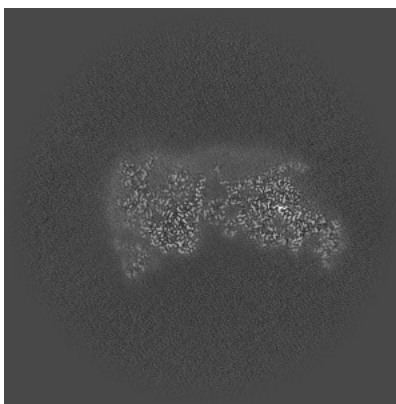
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

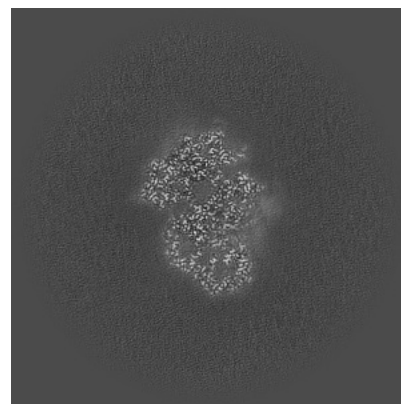
6.3.1 Primary map



X Index: 276



Y Index: 271

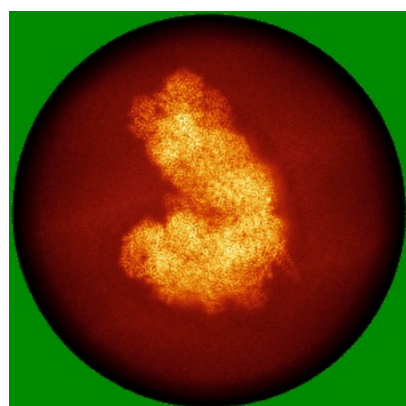


Z Index: 248

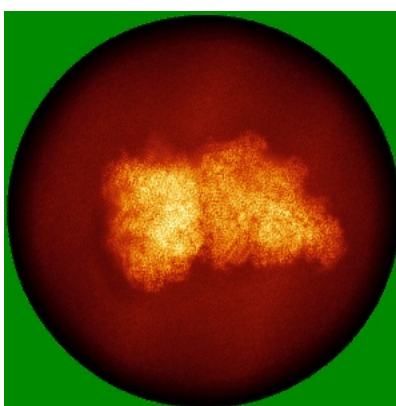
The images above show the largest variance slices of the map in three orthogonal directions.

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

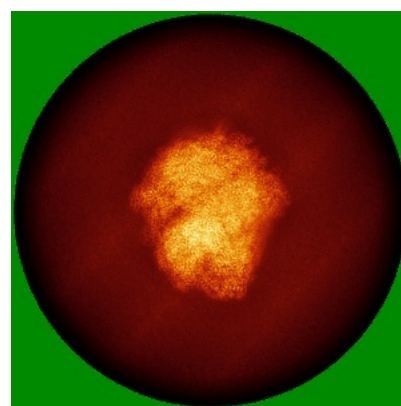
6.4.1 Primary map



X



Y

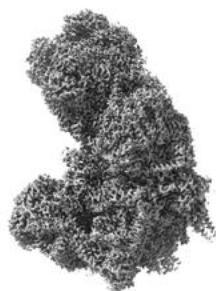


Z

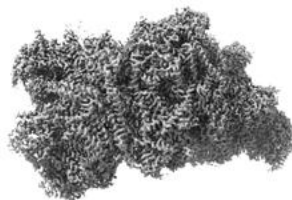
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

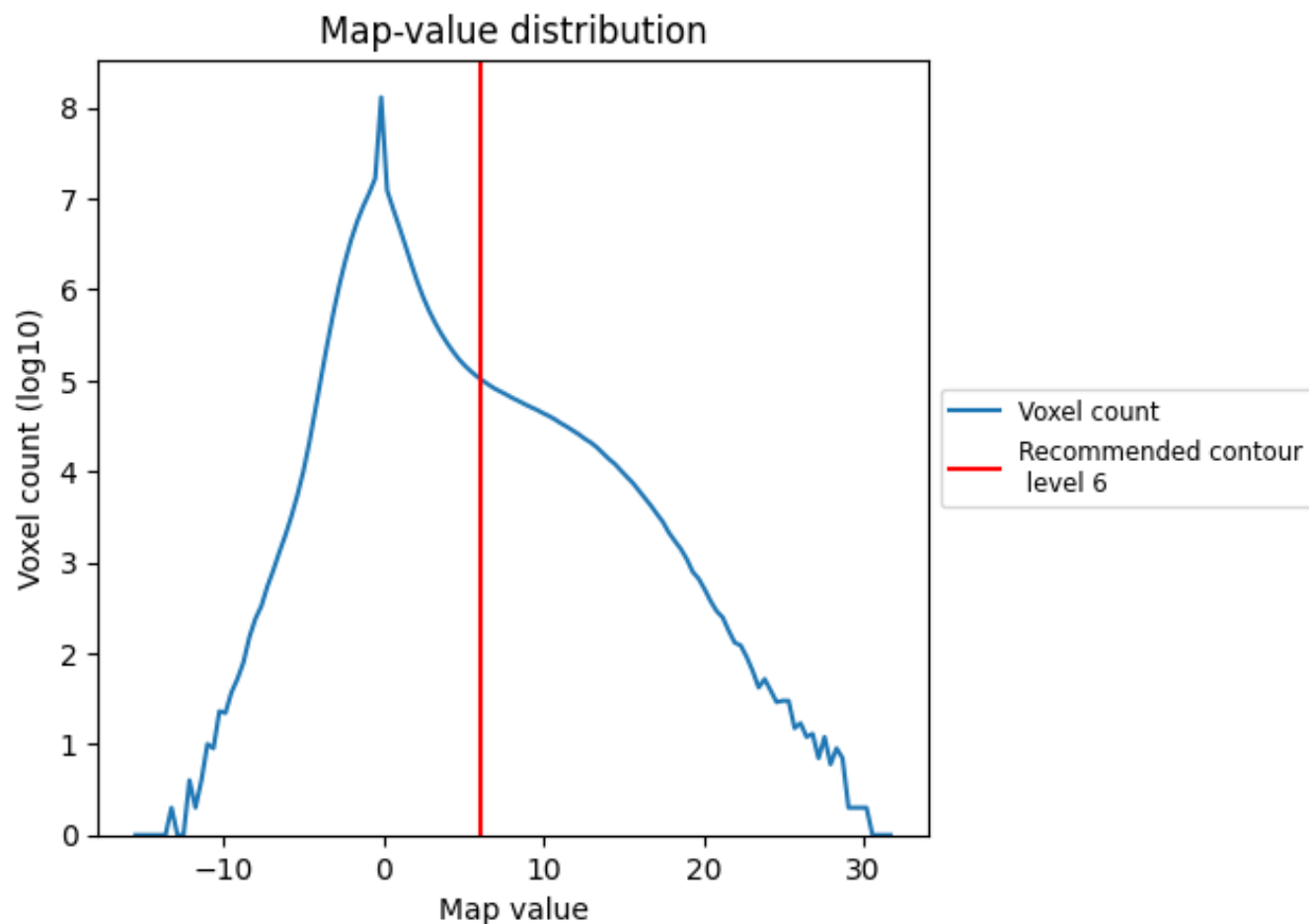
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

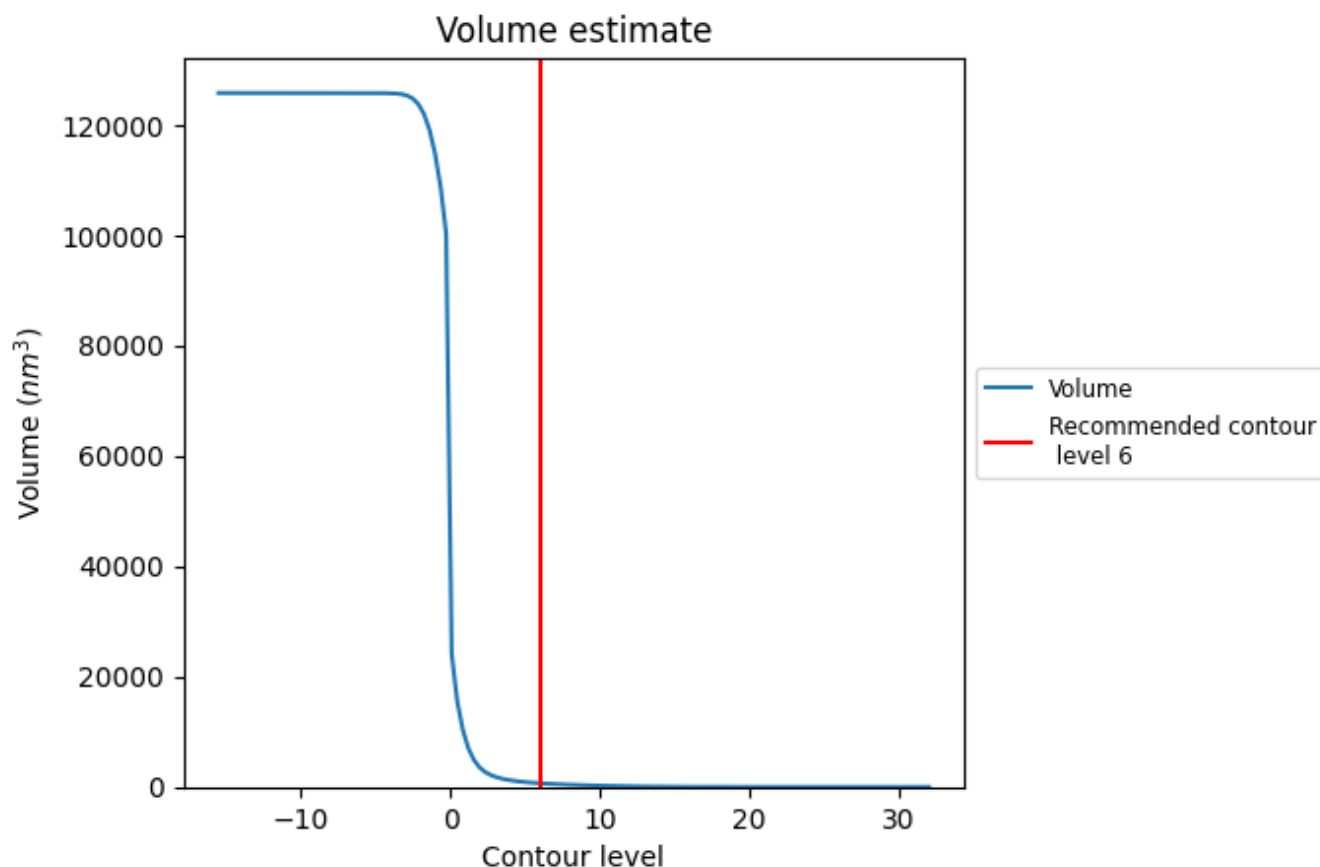
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

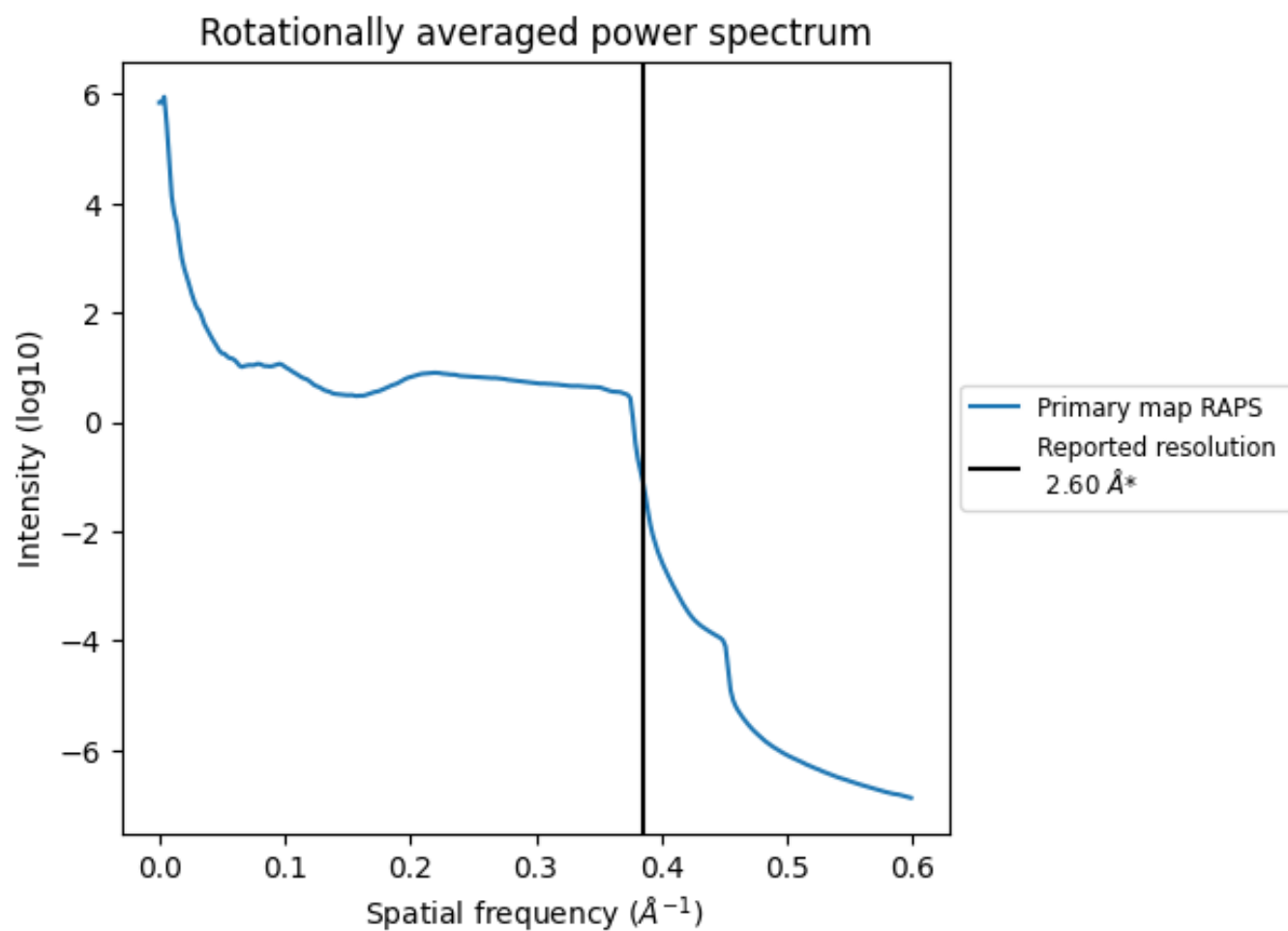
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 673 nm³; this corresponds to an approximate mass of 608 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 ⓘ

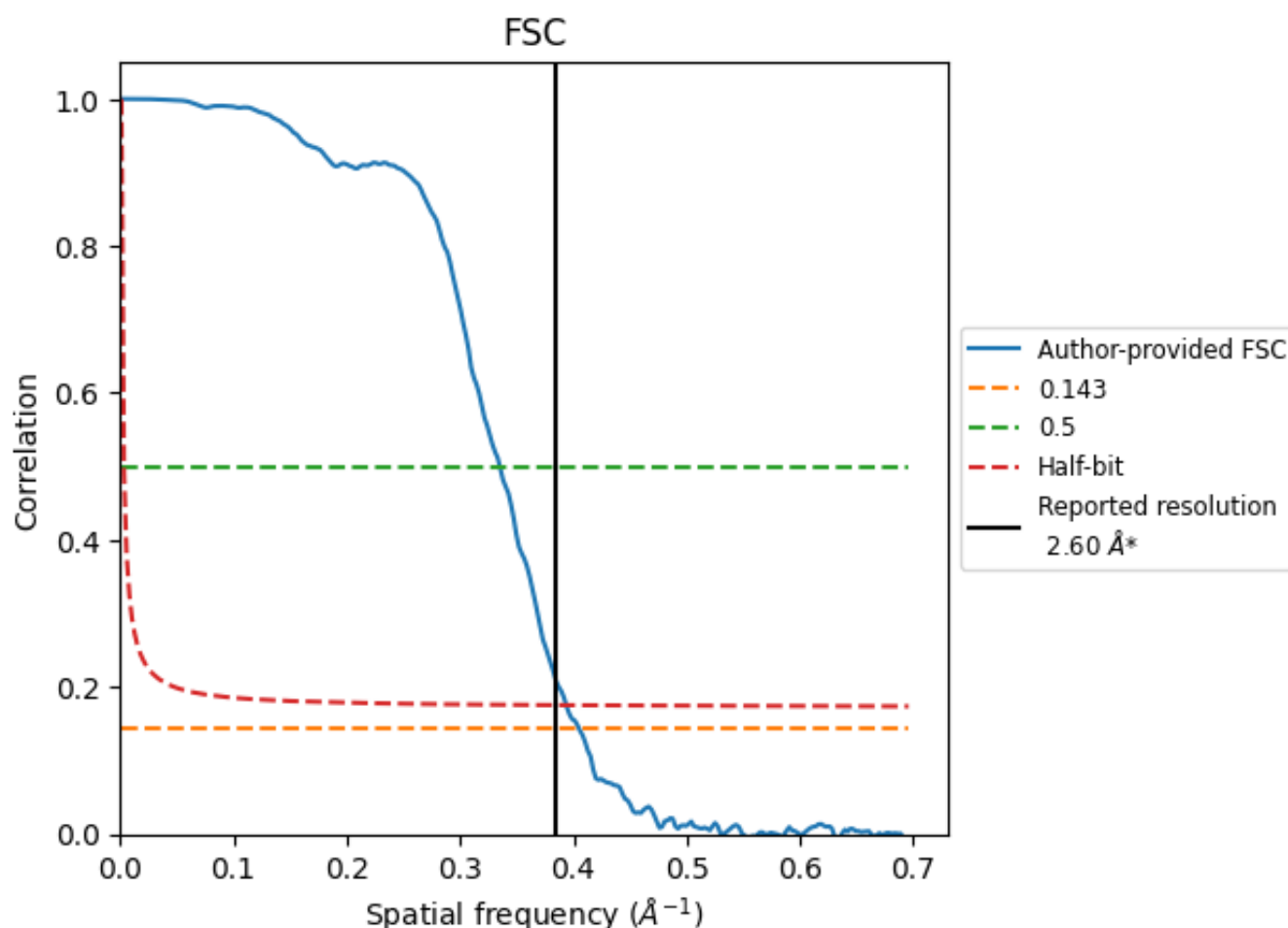


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

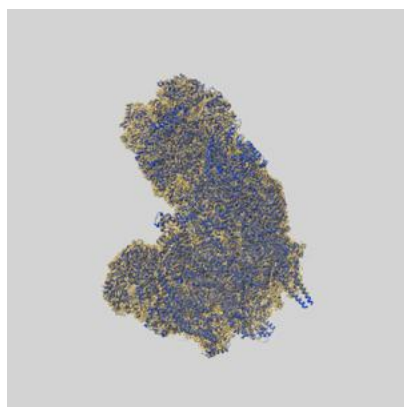
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.47	2.99	2.54
Unmasked-calculated*	-	-	-

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

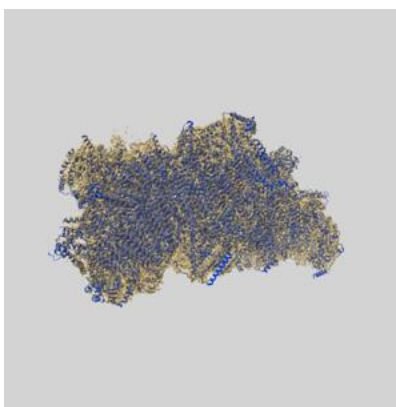
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25882 and PDB model 7TGH. Per-residue inclusion information can be found in section [3](#) on page [31](#).

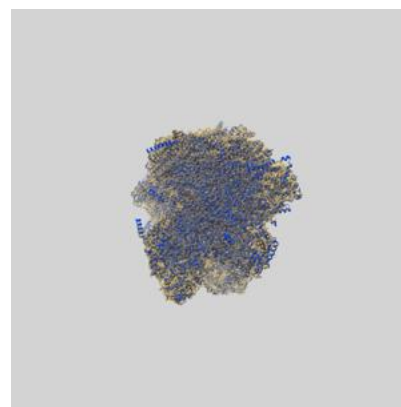
9.1 Map-model overlay [i](#)



X



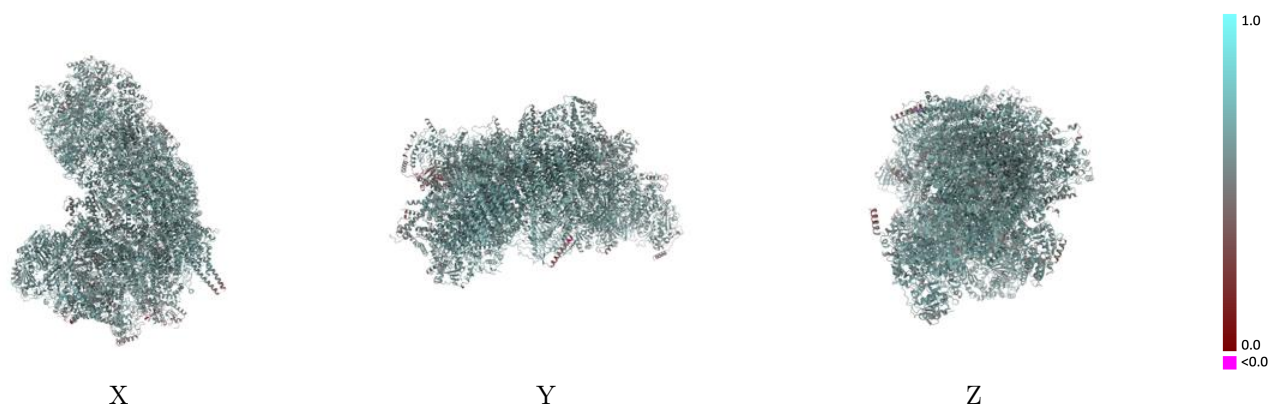
Y



Z

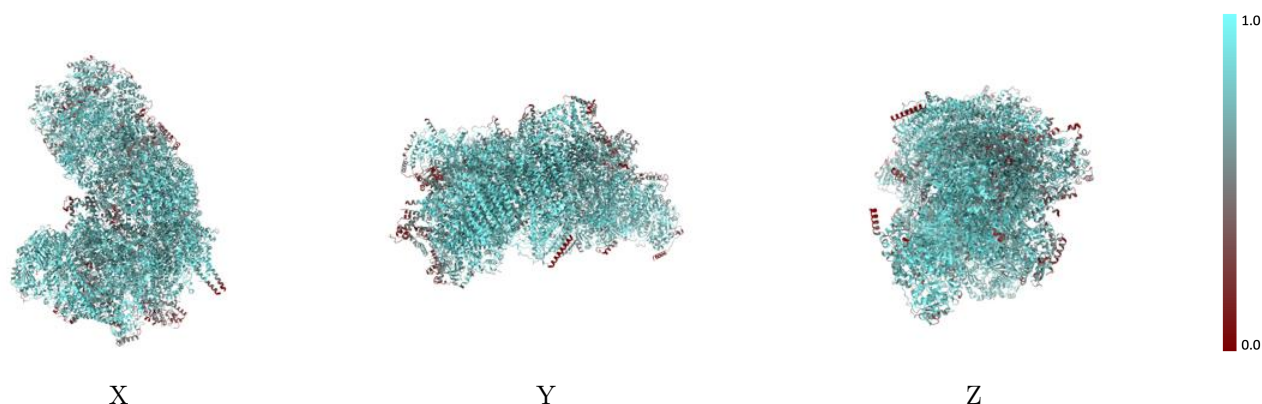
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



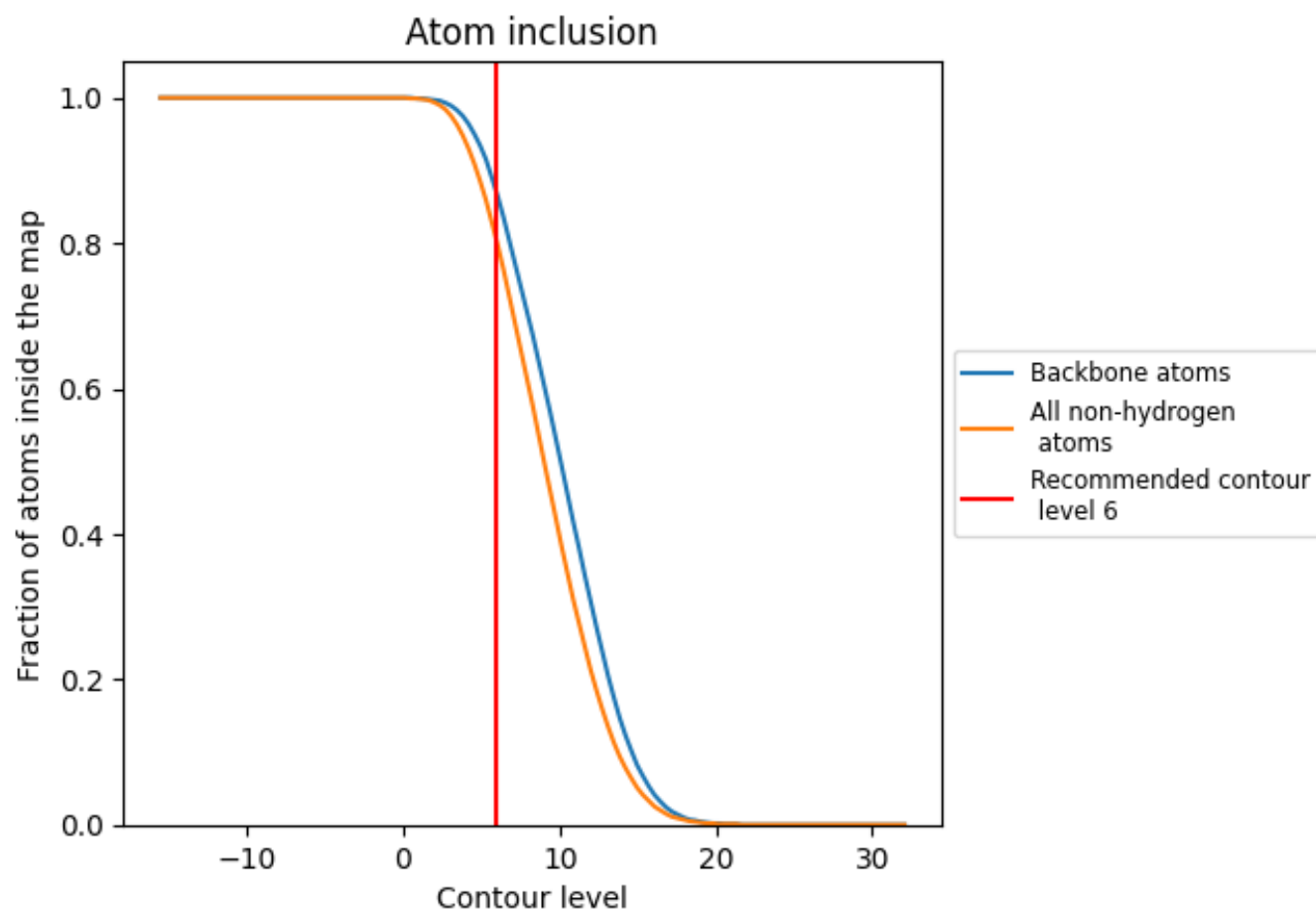
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.6050
1	 0.7560	 0.6000
1B	 0.8320	 0.6230
2	 0.9050	 0.6450
2B	 0.9020	 0.6420
3	 0.8080	 0.6230
3A	 0.8860	 0.6160
3B	 0.9010	 0.6320
3C	 0.7980	 0.5920
3D	 0.9260	 0.6340
3E	 0.6380	 0.5290
3F	 0.7560	 0.5760
3G	 0.7280	 0.5750
3H	 0.8030	 0.6080
3I	 0.8340	 0.6220
3J	 0.8060	 0.6210
3M	 0.7720	 0.5900
3a	 0.8340	 0.6060
3b	 0.8590	 0.6030
3c	 0.7600	 0.5770
3d	 0.8820	 0.6020
3e	 0.8320	 0.5980
3f	 0.5320	 0.4700
3g	 0.7150	 0.5560
3h	 0.7450	 0.5700
3i	 0.7890	 0.5870
3j	 0.7850	 0.5630
3l	 0.4350	 0.4300
3m	 0.8710	 0.6070
4	 0.9010	 0.6390
4L	 0.8760	 0.6250
5	 0.9060	 0.6420
5B	 0.8430	 0.6410
6	 0.8340	 0.6270
A1	 0.7800	 0.6080

































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Chain	Atom inclusion	Q-score
A2	 0.7560	 0.5850
A3	 0.8090	 0.6140
A5	 0.7690	 0.5900
A6	 0.9140	 0.6430
A7	 0.6990	 0.5830
A8	 0.8040	 0.5990
A9	 0.9040	 0.6420
AB	 0.7690	 0.6210
AC	 0.8360	 0.6250
AL	 0.8330	 0.6240
AM	 0.7340	 0.5920
AN	 0.7350	 0.6020
B2	 0.7240	 0.5860
B3	 0.8300	 0.6310
B4	 0.8500	 0.6380
B6	 0.9310	 0.6580
B7	 0.8550	 0.6170
B8	 0.8420	 0.6290
B9	 0.8390	 0.6230
BL	 0.8960	 0.6330
BM	 0.7830	 0.6100
C	 0.7170	 0.5510
C1	 0.8850	 0.6350
C2	 0.8060	 0.5960
C3	 0.7680	 0.6020
C4	 0.8080	 0.6180
FX	 0.8640	 0.6390
J1	 0.6580	 0.5900
P1	 0.7600	 0.6040
P2	 0.6870	 0.5940
R	 0.8150	 0.5970
S1	 0.8850	 0.6300
S2	 0.8860	 0.6270
S3	 0.8910	 0.6330
S4	 0.8630	 0.6280
S5	 0.8470	 0.6230
S6	 0.8810	 0.6330
S7	 0.9160	 0.6390
S8	 0.7870	 0.6150
T1	 0.6840	 0.5720
T2	 0.7770	 0.5890
T3	 0.4530	 0.5160

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Chain	Atom inclusion	Q-score
T4	 0.4930	 0.5340
T5	 0.8230	 0.5990
T6	 0.8250	 0.6030
T7	 0.5040	 0.5310
T8	 0.7910	 0.6090
T9	 0.8080	 0.6010
TA	 0.6410	 0.5690
TB	 0.8380	 0.6220
TC	 0.7950	 0.6130
TD	 0.4560	 0.5450
TE	 0.6210	 0.5920
TX	 0.7130	 0.6110
V1	 0.7910	 0.5870
V2	 0.7040	 0.5690
X1	 0.8380	 0.6200