



Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 12:07 PM EST

PDB ID : 8B6H
EMDB ID : EMD-15867
Title : Cryo-EM structure of cytochrome c oxidase dimer (complex IV) from respiratory supercomplex of *Tetrahymena thermophila*
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2022-09-27
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:

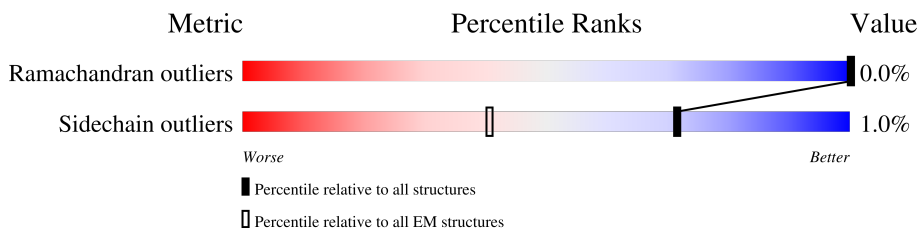
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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



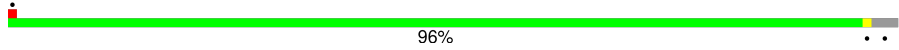
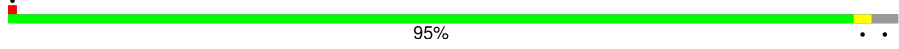
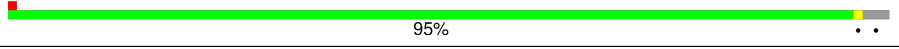
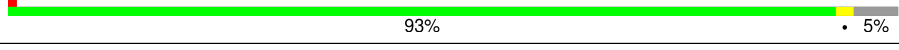
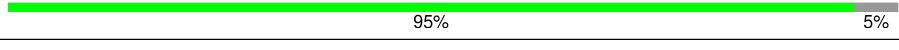
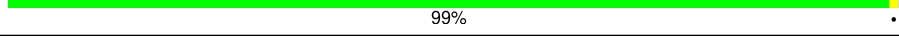
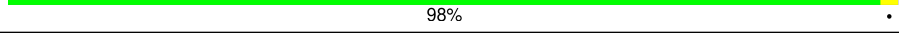
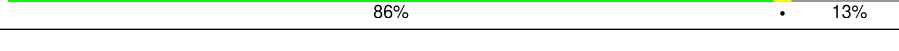
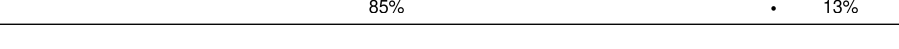
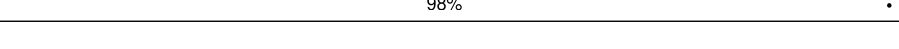
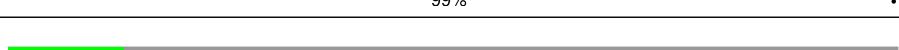

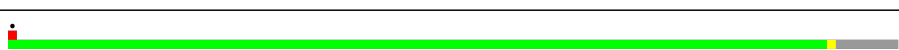
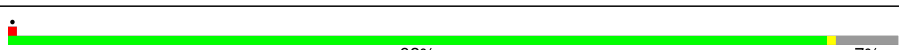
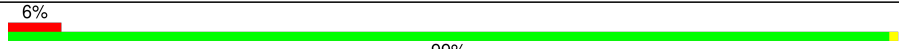
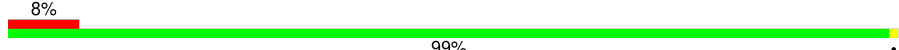

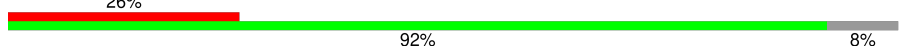


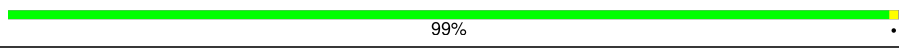
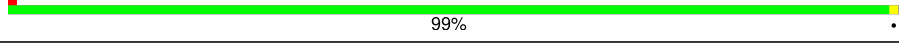



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	DA	688	96%
1	Da	688	96%
2	DB	604	98%
2	Db	604	98%
3	DC	594	6%
3	Dc	594	7%
4	DD	637	86%
4	Dd	637	86%
5	DE	130	97%

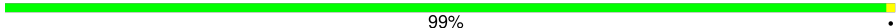
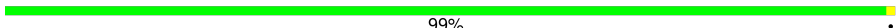


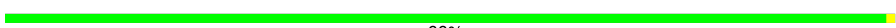








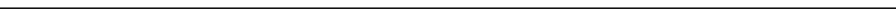





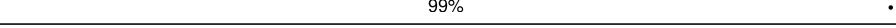
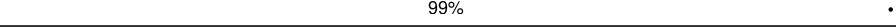
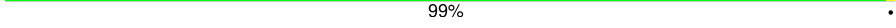
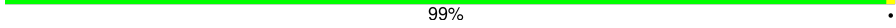
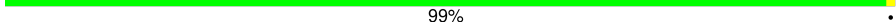
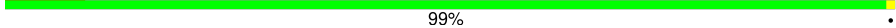
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Mol	Chain	Length	Quality of chain
5	De	130	
6	DF	230	
6	Df	230	
7	DG	103	
7	Dg	103	
8	DH	133	
8	Dh	133	
9	DI	236	
9	Di	236	
10	DJ	220	
10	Dj	220	
11	DK	990	
11	Dk	990	
12	DM	490	
12	Dm	490	
13	DN	453	
13	Dn	453	
14	DO	473	
14	Do	473	
15	DP	402	
15	Dp	402	
16	DQ	385	
16	Dq	385	
17	DR	348	
17	Dr	348	


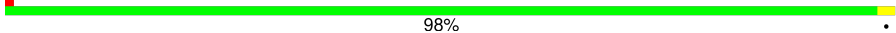
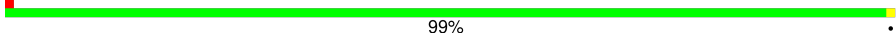
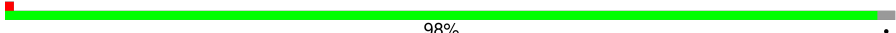

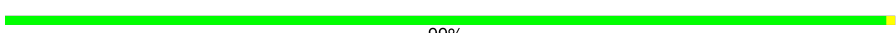









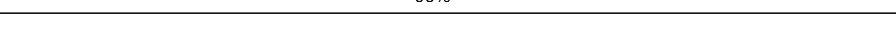
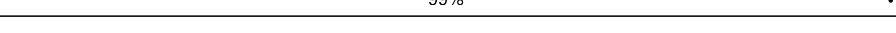
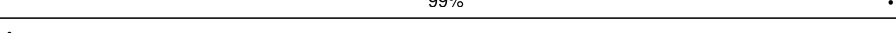
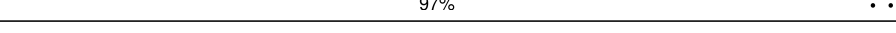
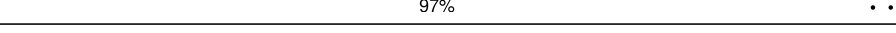
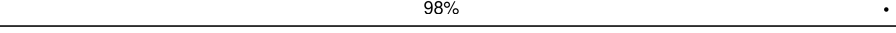
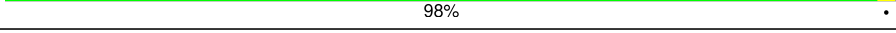


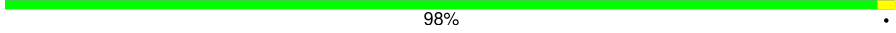
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Mol	Chain	Length	Quality of chain
18	DS	346	 99%
18	Ds	346	 99%
19	DT	318	 92% 8%
19	Dt	318	 92% 8%
20	DU	330	 99%
20	Du	330	 99%
21	DV	318	 99%
21	Dv	318	 99%
22	DW	318	 5% 93% 5%
22	Dw	318	 6% 94% 5%
23	DX	252	 99%
23	Dx	252	 98%
24	DY	234	 79% 20%
24	Dy	234	 79% 20%
25	DZ	231	 90% 10%
25	Dz	231	 90% 10%
26	EA	215	 89% 10%
26	Ea	215	 89% 10%
27	EB	210	 99%
27	Eb	210	 99%
28	EC	212	 21% 99%
28	Ec	212	 38% 99%
29	ED	190	 5% 99%
29	Ed	190	 9% 99%
30	EE	193	 65% 35%

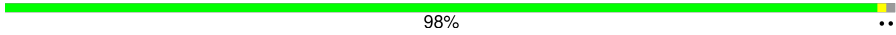
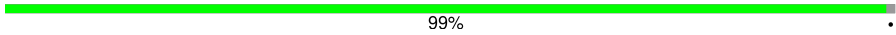




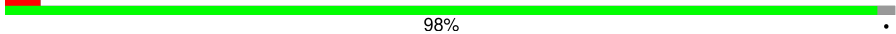
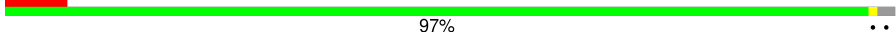
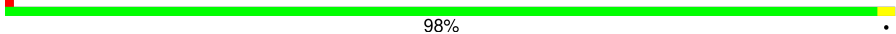
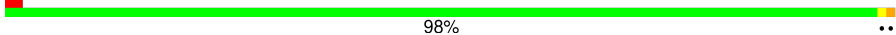



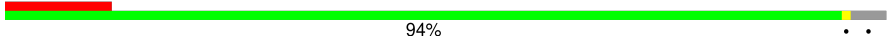
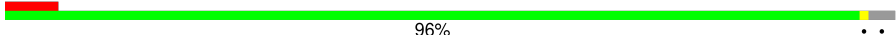
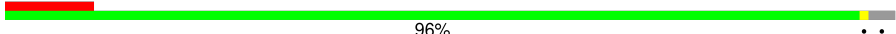


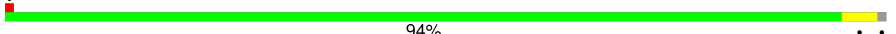
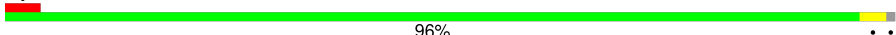


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Mol	Chain	Length	Quality of chain
30	Ee	193	 65% 35%
31	EF	188	 98% .
31	Ef	188	 99% .
32	EG	100	 98% .
32	Eg	100	 97% ..
33	EH	173	 99% .
33	Eh	173	 100%
34	EI	173	 97% ..
34	Ei	173	 97% ..
35	EV	88	 89% 11%
35	Ev	88	 89% 11%
36	EK	170	 98% ..
36	Ek	170	 98% ..
37	EL	158	 96% ..
37	El	158	 96% ..
38	EM	154	 99% ..
38	Em	154	 99% ..
39	EN	149	 97% ..
39	En	149	 97% ..
40	EO	124	 98% ..
40	Eo	124	 98% ..
41	EP	127	 77% . 21%
41	Ep	127	 77% . 21%
42	EQ	122	 98% .
42	Eq	122	 98% .

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Mol	Chain	Length	Quality of chain
43	ER	105	
43	Er	105	
44	ES	89	
44	Es	89	
45	ET	93	
45	Et	93	
46	EU	90	
46	Eu	90	
47	EJ	175	
47	Ej	175	
48	EW	81	
48	Ew	81	
49	EX	72	
49	Ex	72	
50	EY	72	
50	Ey	72	
51	EZ	68	
51	Ez	68	
52	FA	72	
52	Fa	72	
53	DL	536	
53	Dl	536	

2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 436035 atoms, of which 220788 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	DA	671	Total	C	H	N	O	S	0	0
			11168	3720	5609	907	896	36		
1	Da	671	Total	C	H	N	O	S	0	0
			11167	3720	5608	907	896	36		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	288	ALA	GLY	variant	UNP Q950Y4
Da	288	ALA	GLY	variant	UNP Q950Y4

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	DB	604	Total	C	H	N	O	S	0	0
			10232	3340	5101	888	892	11		
2	Db	604	Total	C	H	N	O	S	0	0
			10233	3340	5102	888	892	11		

- Molecule 3 is a protein called Ymf68.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	DC	582	Total	C	H	N	O	S	0	0
			10151	3451	5067	787	838	8		
3	Dc	582	Total	C	H	N	O	S	0	0
			10151	3451	5067	787	838	8		

- Molecule 4 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
4	DD	558	Total	C	H	N	O	P	S	0	0
			9076	2930	4424	782	921	2	17		

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Mol	Chain	Residues	Atoms							AltConf	Trace
4	Dd	558	Total	C	H	N	O	P	S	0	0
			9076	2930	4424	782	921	2	17		

- Molecule 5 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
5	DE	126	Total	C	H	N	O	S		0	0
			2104	698	1021	184	199	2			
5	De	126	Total	C	H	N	O	S		0	0
			2103	698	1020	184	199	2			

- Molecule 6 is a protein called Structural protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
6	DF	222	Total	C	H	N	O	S		0	0
			3681	1238	1768	312	350	13			
6	Df	222	Total	C	H	N	O	S		0	0
			3681	1238	1768	312	350	13			

- Molecule 7 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
7	DG	98	Total	C	H	N	O	S		0	0
			1659	567	788	155	147	2			
7	Dg	98	Total	C	H	N	O	S		0	0
			1659	567	788	155	147	2			

- Molecule 8 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
8	DH	133	Total	C	H	N	O	S		0	0
			2299	771	1129	197	201	1			
8	Dh	133	Total	C	H	N	O	S		0	0
			2299	771	1129	197	201	1			

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms							AltConf	Trace
9	DI	206	Total	C	H	N	O	P	S	0	0
			3381	1134	1604	286	348	1	8		

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Mol	Chain	Residues	Atoms							AltConf	Trace
9	Di	206	Total	C	H	N	O	P	S	0	0
			3381	1134	1604	286	348	1	8		

- Molecule 10 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
10	DJ	220	Total	C	H	N	O	S		0	0
			3653	1223	1772	316	330	12			
10	Dj	220	Total	C	H	N	O	S		0	0
			3653	1223	1772	316	330	12			

- Molecule 11 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
11	DK	130	Total	C	H	N	O	S		0	0
			2133	693	1062	174	196	8			
11	Dk	130	Total	C	H	N	O	S		0	0
			2133	693	1062	174	196	8			

- Molecule 12 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
12	DM	455	Total	C	H	N	O	S		0	0
			7385	2430	3592	645	709	9			
12	Dm	455	Total	C	H	N	O	S		0	0
			7385	2430	3592	645	709	9			

- Molecule 13 is a protein called Ymf67.

Mol	Chain	Residues	Atoms							AltConf	Trace
13	DN	453	Total	C	H	N	O	S		0	0
			7849	2578	3980	618	666	7			
13	Dn	453	Total	C	H	N	O	S		0	0
			7849	2578	3980	618	666	7			

- Molecule 14 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
14	DO	435	Total	C	H	N	O	S		0	0
			6956	2192	3508	603	650	3			
14	Do	435	Total	C	H	N	O	S		0	0
			6956	2192	3508	603	650	3			

- Molecule 15 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	DP	290	Total	C	H	N	O	S	0	0
			4660	1525	2291	400	439	5		
15	Dp	290	Total	C	H	N	O	S	0	0
			4660	1525	2291	400	439	5		

- Molecule 16 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	DQ	383	Total	C	H	N	O	S	0	0
			6271	2041	3102	546	575	7		
16	Dq	383	Total	C	H	N	O	S	0	0
			6271	2041	3102	546	575	7		

- Molecule 17 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	DR	243	Total	C	H	N	O	S	0	0
			3982	1304	1958	335	380	5		
17	Dr	243	Total	C	H	N	O	S	0	0
			3982	1304	1958	335	380	5		

- Molecule 18 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	DS	346	Total	C	H	N	O	S	0	0
			5636	1892	2770	469	492	13		
18	Ds	346	Total	C	H	N	O	S	0	0
			5636	1892	2770	469	492	13		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	DT	293	Total	C	H	N	O	S	0	0
			4733	1555	2290	410	466	12		
19	Dt	293	Total	C	H	N	O	S	0	0
			4733	1555	2290	410	466	12		

- Molecule 20 is a protein called Carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	DU	329	Total	C	H	N	O	S	0	0
			5204	1700	2584	446	470	4		
20	Du	329	Total	C	H	N	O	S	0	0
			5204	1700	2584	446	470	4		

- Molecule 21 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	DV	318	Total	C	H	N	O	S	0	0
			5114	1667	2552	440	451	4		
21	Dv	318	Total	C	H	N	O	S	0	0
			5114	1667	2552	440	451	4		

- Molecule 22 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	DW	301	Total	C	H	N	O	S	0	0
			4738	1515	2344	415	454	10		
22	Dw	301	Total	C	H	N	O	S	0	0
			4738	1515	2344	415	454	10		

- Molecule 23 is a protein called COXTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	DX	251	Total	C	H	N	O	S	0	0
			4126	1358	2018	368	377	5		
23	Dx	251	Total	C	H	N	O	S	0	0
			4126	1358	2018	368	377	5		

- Molecule 24 is a protein called COXTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	DY	187	Total	C	H	N	O	S	0	0
			3135	1023	1562	276	273	1		
24	Dy	187	Total	C	H	N	O	S	0	0
			3135	1023	1562	276	273	1		

- Molecule 25 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	DZ	208	Total	C	H	N	O	S	0	0
			3382	1089	1671	302	317	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
25	Dz	208	Total	C	H	N	O	S	0	0
			3383	1089	1672	302	317	3		

- Molecule 26 is a protein called COXTT12,Transmembrane protein,Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	EA	193	Total	C	H	N	O	S	0	0
			3296	1084	1637	283	290	2		
26	Ea	193	Total	C	H	N	O	S	0	0
			3296	1084	1637	283	290	2		

- Molecule 27 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	EB	209	Total	C	H	N	O	S	0	0
			3417	1131	1678	291	310	7		
27	Eb	209	Total	C	H	N	O	S	0	0
			3417	1131	1678	291	310	7		

- Molecule 28 is a protein called COXTT27.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	EC	212	Total	C	H	N	O	S	0	0
			3307	1045	1660	276	324	2		
28	Ec	212	Total	C	H	N	O	S	0	0
			3307	1045	1660	276	324	2		

- Molecule 29 is a protein called Ymf75.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	ED	190	Total	C	H	N	O	S	0	0
			3384	1141	1725	249	265	4		
29	Ed	190	Total	C	H	N	O	S	0	0
			3384	1141	1725	249	265	4		

- Molecule 30 is a protein called Mobilization protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	EE	125	Total	C	H	N	O	S	0	0
			2073	656	1024	186	201	6		
30	Ee	125	Total	C	H	N	O	S	0	0
			2073	656	1024	186	201	6		

- Molecule 31 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	EF	188	Total	C	H	N	O	S	0	0
			2986	978	1477	260	257	14		
31	Ef	188	Total	C	H	N	O	S	0	0
			2986	978	1477	260	257	14		

- Molecule 32 is a protein called COXTT28.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	EG	98	Total	C	H	N	O	S	0	0
			1523	492	752	136	141	2		
32	Eg	98	Total	C	H	N	O	S	0	0
			1523	492	752	136	141	2		

- Molecule 33 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	EH	173	Total	C	H	N	O	S	0	0
			2820	929	1382	243	257	9		
33	Eh	173	Total	C	H	N	O	S	0	0
			2820	929	1382	243	257	9		

- Molecule 34 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	EI	172	Total	C	H	N	O	S	0	0
			2827	921	1419	231	253	3		
34	Ei	172	Total	C	H	N	O	S	0	0
			2827	921	1419	231	253	3		

- Molecule 35 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	EV	78	Total	C	H	N	O	S	0	0
			1276	411	633	109	117	6		
35	Ev	78	Total	C	H	N	O	S	0	0
			1276	411	633	109	117	6		

- Molecule 36 is a protein called Complex III subunit VII.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	EK	169	Total	C	H	N	O	S	0	0
			2796	878	1407	243	264	4		
36	Ek	169	Total	C	H	N	O	S	0	0
			2796	878	1407	243	264	4		

- Molecule 37 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	EL	153	Total	C	H	N	O	S	0	0
			2544	841	1253	226	220	4		
37	El	153	Total	C	H	N	O	S	0	0
			2544	841	1253	226	220	4		

- Molecule 38 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	EM	153	Total	C	H	N	O	S	0	0
			2603	848	1299	221	230	5		
38	Em	153	Total	C	H	N	O	S	0	0
			2603	848	1299	221	230	5		

- Molecule 39 is a protein called COXTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	EN	145	Total	C	H	N	O	S	0	0
			2417	798	1190	216	211	2		
39	En	145	Total	C	H	N	O	S	0	0
			2417	798	1190	216	211	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
40	EO	123	Total	C	H	N	O	S	0	0
			2128	716	1031	183	194	4		
40	Eo	123	Total	C	H	N	O	S	0	0
			2128	716	1031	183	194	4		

- Molecule 41 is a protein called Phage protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	EP	100	Total	C	H	N	O	S	0	0
			1612	519	795	144	152	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
41	Ep	100	Total	C	H	N	O	S	0	0
			1612	519	795	144	152	2		

- Molecule 42 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	EQ	122	Total	C	H	N	O	S	0	0
			2004	667	989	171	173	4		
42	Eq	122	Total	C	H	N	O	S	0	0
			2004	667	989	171	173	4		

- Molecule 43 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	ER	104	Total	C	H	N	O	S	0	0
			1651	535	800	156	152	8		
43	Er	104	Total	C	H	N	O	S	0	0
			1651	535	800	156	152	8		

- Molecule 44 is a protein called Ymf70.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	ES	89	Total	C	H	N	O	S	0	0
			1574	535	798	115	124	2		
44	Es	89	Total	C	H	N	O	S	0	0
			1574	535	798	115	124	2		

- Molecule 45 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	ET	82	Total	C	H	N	O	S	0	0
			1302	407	655	108	127	5		
45	Et	82	Total	C	H	N	O	S	0	0
			1302	407	655	108	127	5		

- Molecule 46 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	EU	88	Total	C	H	N	O		0	0
			1423	462	699	131	131			
46	Eu	88	Total	C	H	N	O		0	0
			1423	462	699	131	131			

- Molecule 47 is a protein called YftT domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	EJ	175	Total	C	H	N	O	S	0	0
			2802	889	1391	247	274	1		
47	Ej	175	Total	C	H	N	O	S	0	0
			2802	889	1391	247	274	1		

- Molecule 48 is a protein called Cullin domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	EW	63	Total	C	H	N	O	S	0	0
			1025	327	510	90	96	2		
48	Ew	63	Total	C	H	N	O	S	0	0
			1025	327	510	90	96	2		

- Molecule 49 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	EX	69	Total	C	H	N	O	S	0	0
			1117	347	559	98	109	4		
49	Ex	69	Total	C	H	N	O	S	0	0
			1117	347	559	98	109	4		

- Molecule 50 is a protein called Annexin.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	EY	70	Total	C	H	N	O	S	0	0
			1123	362	562	90	105	4		
50	Ey	70	Total	C	H	N	O	S	0	0
			1123	362	562	90	105	4		

- Molecule 51 is a protein called Transposase.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	EZ	58	Total	C	H	N	O	S	0	0
			966	314	474	84	91	3		
51	Ez	58	Total	C	H	N	O	S	0	0
			966	314	474	84	91	3		

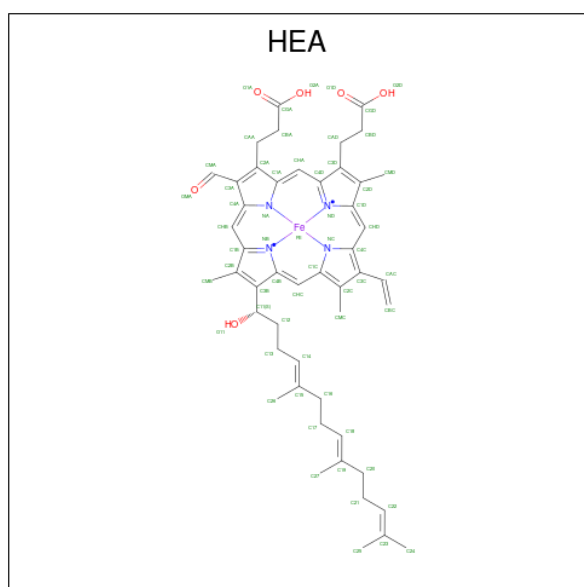
- Molecule 52 is a protein called Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	FA	71	Total	C	H	N	O	S	0	0
			1084	333	536	99	112	4		
52	Fa	71	Total	C	H	N	O	S	0	0
			1084	333	536	99	112	4		

- Molecule 53 is a protein called COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Dl	380	Total	C	H	N	O	S	0	0
			5730	1856	2814	492	566	2		
53	DL	380	Total	C	H	N	O	S	0	0
			5730	1856	2814	492	566	2		

- Molecule 54 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



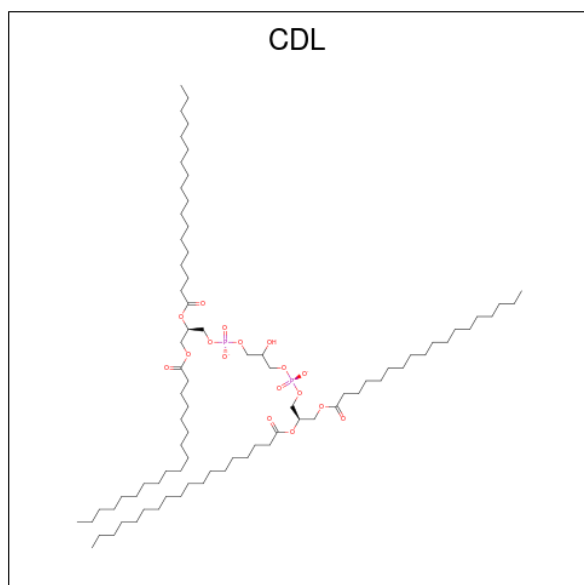
of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
55	DA	1	Total	Cu	0
			1	1	
55	Da	1	Total	Cu	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
56	DA	1	Total	Mg	0
			1	1	
56	Da	1	Total	Mg	0
			1	1	

- Molecule 57 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
57	DA	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	DA	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	DA	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	DC	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
57	DD	1	Total 256	C 81	H 156	O 17	P 2	0
57	DD	1	Total 256	C 81	H 156	O 17	P 2	0
57	DD	1	Total 256	C 81	H 156	O 17	P 2	0
57	DG	1	Total 256	C 81	H 156	O 17	P 2	0
57	DG	1	Total 256	C 81	H 156	O 17	P 2	0
57	DH	1	Total 256	C 81	H 156	O 17	P 2	0
57	DI	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DM	1	Total 256	C 81	H 156	O 17	P 2	0
57	DM	1	Total 256	C 81	H 156	O 17	P 2	0
57	DN	1	Total 256	C 81	H 156	O 17	P 2	0
57	DN	1	Total 256	C 81	H 156	O 17	P 2	0
57	DN	1	Total 256	C 81	H 156	O 17	P 2	0
57	DO	1	Total 256	C 81	H 156	O 17	P 2	0
57	DQ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DQ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DQ	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	DR	1	Total 256	C 81	H 156	O 17	P 2	0
57	DR	1	Total 256	C 81	H 156	O 17	P 2	0
57	DS	1	Total 256	C 81	H 156	O 17	P 2	0
57	DS	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DX	1	Total 256	C 81	H 156	O 17	P 2	0
57	DX	1	Total 256	C 81	H 156	O 17	P 2	0
57	DY	1	Total 256	C 81	H 156	O 17	P 2	0
57	DZ	1	Total 256	C 81	H 156	O 17	P 2	0
57	EA	1	Total 256	C 81	H 156	O 17	P 2	0
57	EB	1	Total 256	C 81	H 156	O 17	P 2	0
57	EB	1	Total 256	C 81	H 156	O 17	P 2	0
57	ED	1	Total 256	C 81	H 156	O 17	P 2	0
57	ED	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	EH	1	Total 256	C 81	H 156	O 17	P 2	0
57	EH	1	Total 255	C 81	H 155	O 17	P 2	0
57	EI	1	Total 256	C 81	H 156	O 17	P 2	0
57	EK	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EN	1	Total 256	C 81	H 156	O 17	P 2	0
57	EN	1	Total 256	C 81	H 156	O 17	P 2	0
57	EO	1	Total 256	C 81	H 156	O 17	P 2	0
57	EU	1	Total 256	C 81	H 156	O 17	P 2	0
57	Da	1	Total 256	C 81	H 156	O 17	P 2	0
57	Da	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dc	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dg	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dg	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	Dh	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dh	1	Total 256	C 81	H 156	O 17	P 2	0
57	Di	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dm	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dm	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Do	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0

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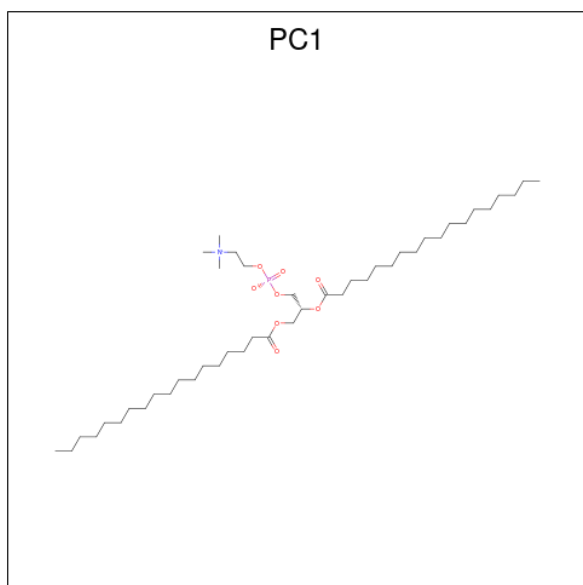
Mol	Chain	Residues	Atoms				AltConf
57	Dr	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dr	1	Total 256	C 81	H 156	O 17 P 2	0
57	Ds	1	Total 256	C 81	H 156	O 17 P 2	0
57	Ds	1	Total 256	C 81	H 156	O 17 P 2	0
57	Du	1	Total 256	C 81	H 156	O 17 P 2	0
57	Du	1	Total 256	C 81	H 156	O 17 P 2	0
57	Du	1	Total 256	C 81	H 156	O 17 P 2	0
57	Du	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dx	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dx	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dy	1	Total 256	C 81	H 156	O 17 P 2	0
57	Dz	1	Total 256	C 81	H 156	O 17 P 2	0
57	Ea	1	Total 256	C 81	H 156	O 17 P 2	0
57	Ed	1	Total 255	C 81	H 155	O 17 P 2	0
57	Ed	1	Total 256	C 81	H 156	O 17 P 2	0
57	Eg	1	Total 256	C 81	H 156	O 17 P 2	0
57	Eh	1	Total 256	C 81	H 156	O 17 P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	Ei	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	Ek	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	El	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	El	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	El	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	En	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	En	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	Ep	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	Eu	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 58 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
58	DA	1	Total	C	H	N	O	P
			141	44	87	1	8	1
58	DA	1	Total	C	H	N	O	P
			142	44	88	1	8	1

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Mol	Chain	Residues	Atoms						AltConf
58	DB	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	DG	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DI	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DJ	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DQ	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DS	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DS	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DX	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DX	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DY	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EB	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EB	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

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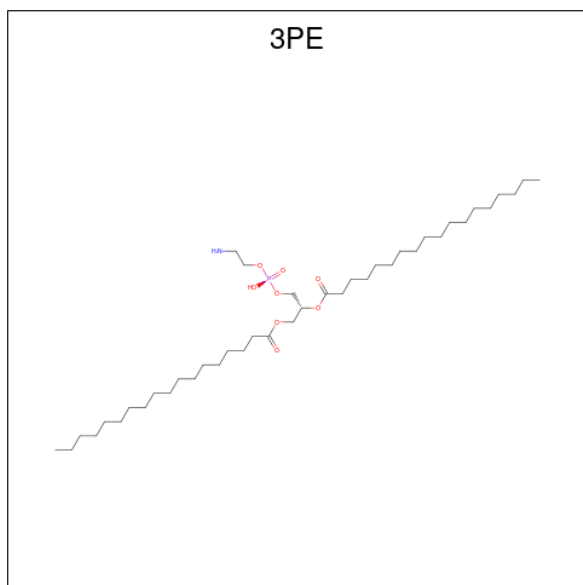
Mol	Chain	Residues	Atoms						AltConf
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Da	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	Da	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Db	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	Dg	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Di	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dj	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dq	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Ds	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dx	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
58	Dx	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dx	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dy	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eb	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eb	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Ef	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	El	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eo	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eo	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eo	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 59 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
59	DA	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

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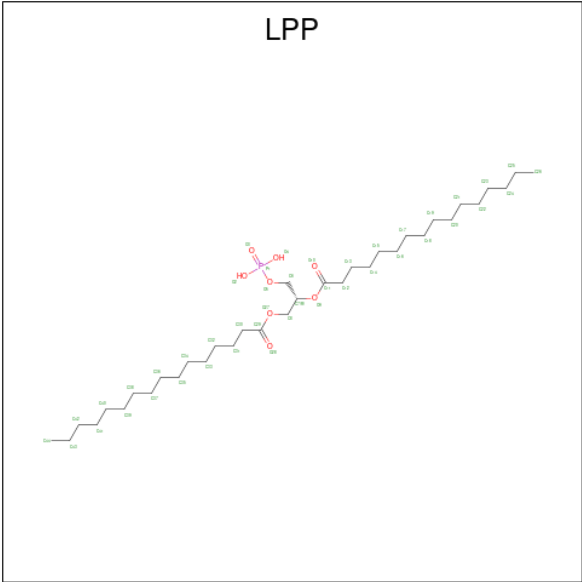
Mol	Chain	Residues	Atoms						AltConf
59	DC	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DC	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DG	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DG	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DJ	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DR	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DS	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DS	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DX	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DX	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DX	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EL	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EM	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EN	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EO	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EO	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Da	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dc	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dd	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dg	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dj	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
59	Dr	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dr	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Ds	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Ds	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Ds	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dx	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dx	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dx	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	El	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Em	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Eo	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Eo	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

- Molecule 60 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).

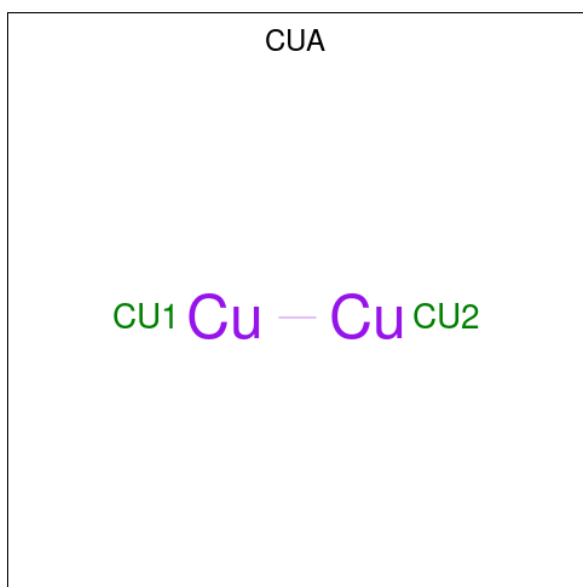


Mol	Chain	Residues	Atoms					AltConf
60	DA	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	EI	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Ed	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dl	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 61 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
61	DA	1	Total	Ca	0
			1	1	
61	Da	1	Total	Ca	0
			1	1	

- Molecule 62 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
62	DB	1	Total	Cu	0
			2	2	
62	Db	1	Total	Cu	0
			2	2	

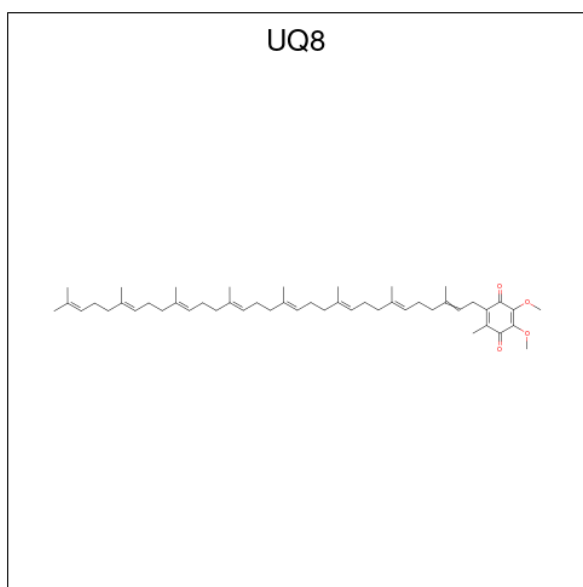
- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
63	DD	1	Total	Zn	0
			1	1	
63	Dd	1	Total	Zn	0
			1	1	

- Molecule 64 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
64	DD	1	Total	K	0
			1	1	

- Molecule 65 is Ubiquinone-8 (three-letter code: UQ8) (formula: C₄₉H₇₄O₄) (labeled as "Ligand of Interest" by depositor).



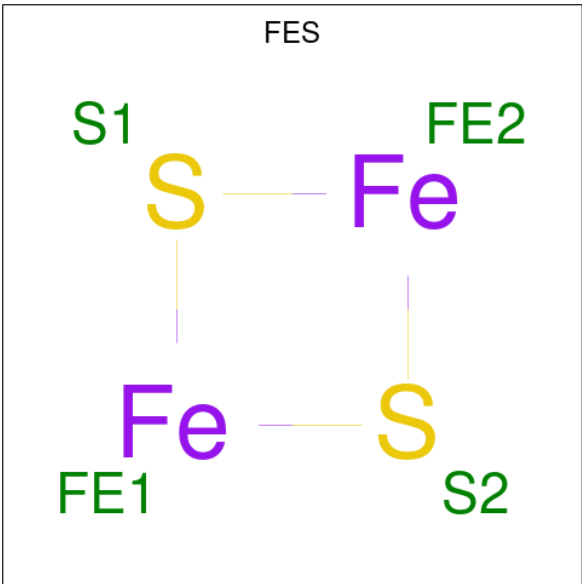
Mol	Chain	Residues	Atoms				AltConf
65	DS	1	Total	C	H	O	0
			127	49	74	4	
65	ED	1	Total	C	H	O	0
			127	49	74	4	
65	EL	1	Total	C	H	O	0
			127	49	74	4	
65	EN	1	Total	C	H	O	0
			127	49	74	4	
65	Ds	1	Total	C	H	O	0
			127	49	74	4	
65	Ed	1	Total	C	H	O	0
			127	49	74	4	
65	El	1	Total	C	H	O	0
			127	49	74	4	
65	En	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 66 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
66	ED	1	Total	C	Fe	H	N	O	0
			65	34	1	22	4	4	
66	Ed	1	Total	C	Fe	H	N	O	0
			67	34	1	24	4	4	

- Molecule 67 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



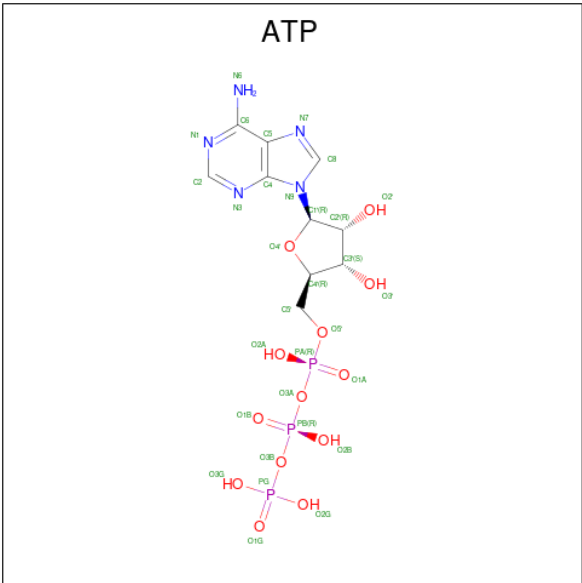
Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	Fe	S	0
			4	2	2	
67	Ef	1	Total	Fe	S	0
			4	2	2	
67	Ef	1	Total	Fe	S	0
			4	2	2	

- Molecule 68 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
68	ER	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
68	Er	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

Chain DA:  96%



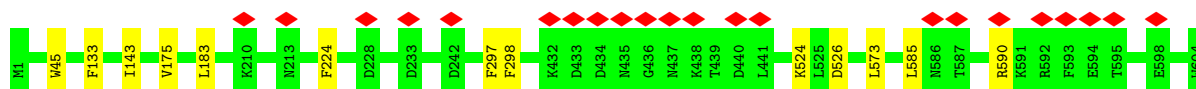
• Molecule 1: Cytochrome c oxidase subunit 1

Chain Da:  96%



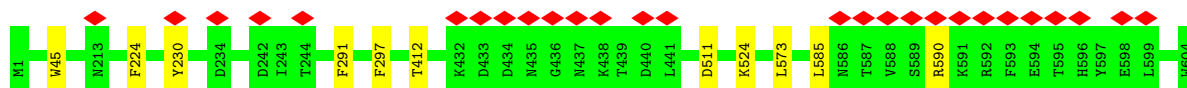
• Molecule 2: Cytochrome c oxidase subunit 2

Chain DB:  98%



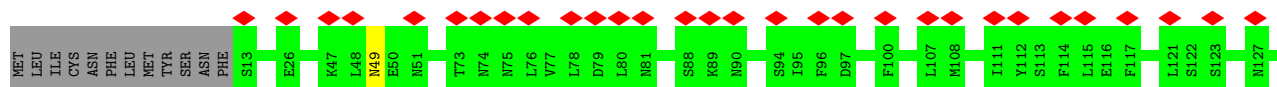
• Molecule 2: Cytochrome c oxidase subunit 2

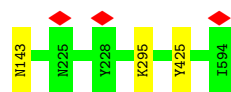
Chain Db:  98%



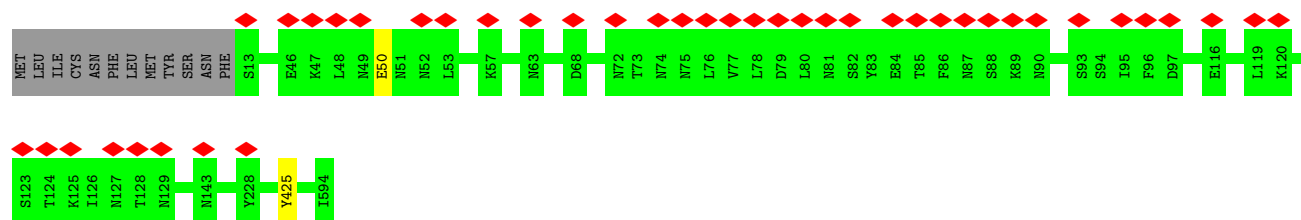
• Molecule 3: Ymf68

Chain DC:  97%

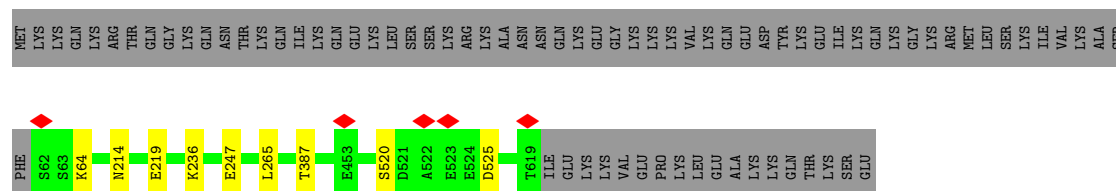
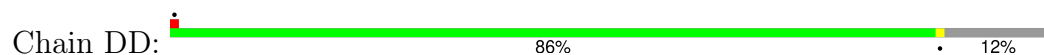




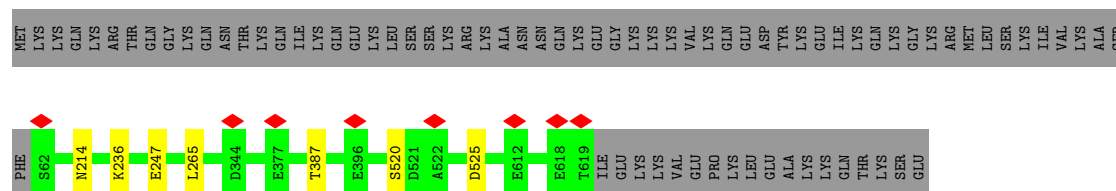
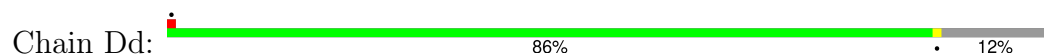
- Molecule 3: Ymf68



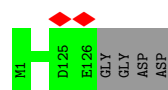
- Molecule 4: Cytochrome C oxidase subunit Vb protein



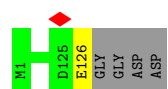
- Molecule 4: Cytochrome C oxidase subunit Vb protein



- Molecule 5: Transmembrane protein, putative

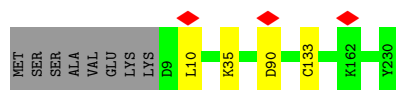


- Molecule 5: Transmembrane protein, putative



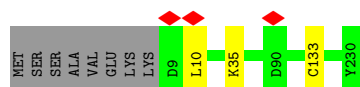
- Molecule 6: Structural protein

Chain DF:  95%



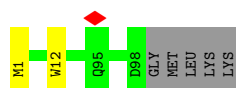
- Molecule 6: Structural protein

Chain Df:  95%



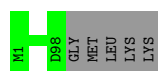
- Molecule 7: Transmembrane protein, putative

Chain DG:  93%



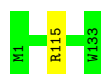
- Molecule 7: Transmembrane protein, putative

Chain Dg:  95%



- Molecule 8: Transmembrane protein, putative

Chain DH:  99%




- Molecule 8: Transmembrane protein, putative

Chain Dh:  98%



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain DI:  86%

GLN
GLU
PHE
SER
SER
MET
ASN
PHE
CYS
GLU
SER
GLY
PRO
LYS
TYR
ASP
ASN
SER
ILE
LEU
SER
PHE
ILE
ASN
LYS
LEU
SER
GLN
GLU
SER
SER
ALA
LEU
ARG
LEU
GLU
ILE
ARG
GLN
ILE
GLY
SER
SER
ALA
SER
GLN
GLY
ARG
ARG
LYS
LYS
GLN
GLN
LYS
GLY
LYS
GLN
ARG
LYS
GLU
LYS
TYR
TYR

LYS
 LYS
 GLN
 GLU
 GLU
 ASN
 LYS
 LEU
 ASN
 ILE
 LYS
 GLN
 TYR
 LYS
 LYS
 GLU
 ARG
 TYR
 ASN
 MET
 A2
 D65
 K66
 L130
 T131

- Molecule 12: Transmembrane protein, putative



MET LEU SER SER LYS VAL THR ARG ARG PHE LEU ASN TYR ASN ASN GLN TYR CYS PHE PHE SER SER GLN HIS GLY ALA GLU HIS HIS
 K28 E34 D206 T386 Q414 S482
 SER GLN PRO LYS LEU LEU LYS

- Molecule 12: Transmembrane protein, putative



MET LEU SER LYS VAL THR ARG ARG PHE LEU ASN TYR ASN GLN ILE TYR CYS PHE ALA SER GLN HIS ALA GLU HIS HIS
 K28 K73 L103 D206 D372 T386 H481 S482
 SER GLN PRO LYS LEU LEU LYS LYS

- Molecule 13: Ymf67

















































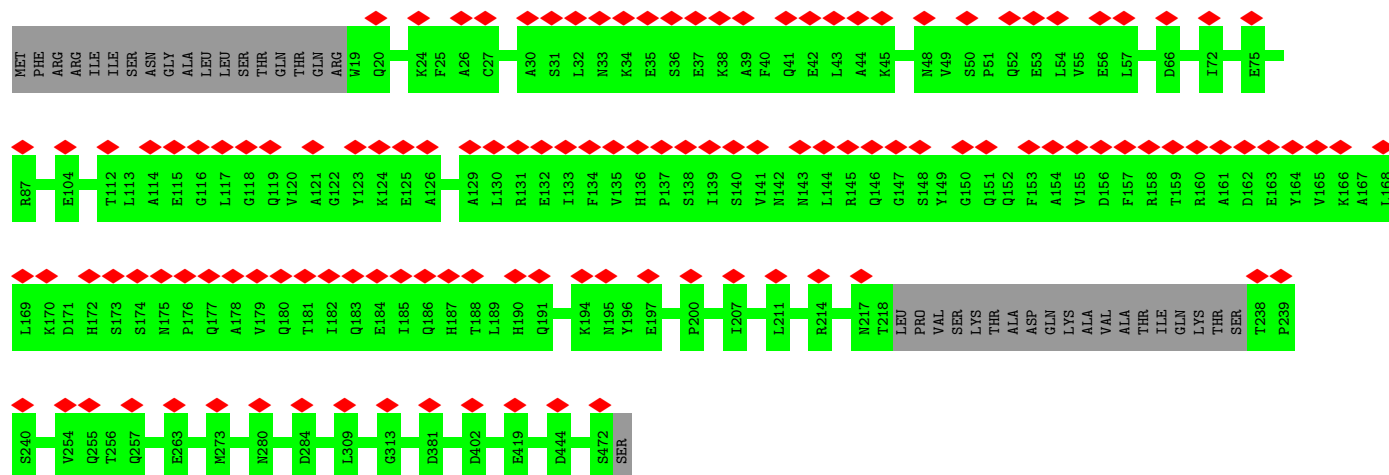
- Molecule 13: Ymf67



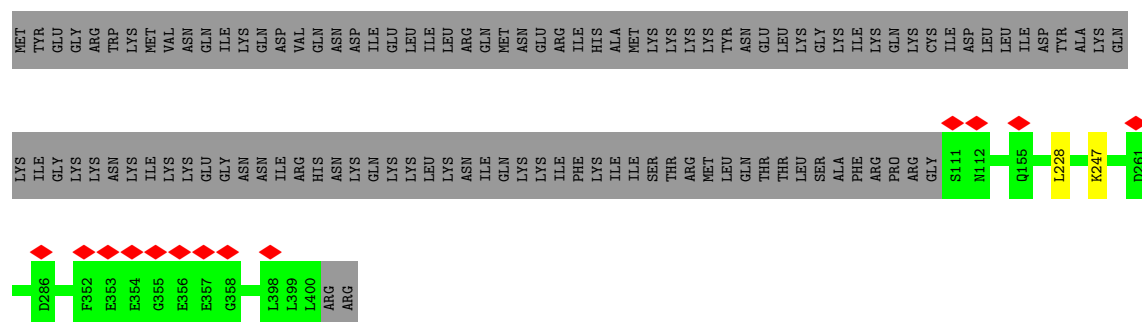
- Molecule 14: Protein phosphatase 2C, putative

[illegible]

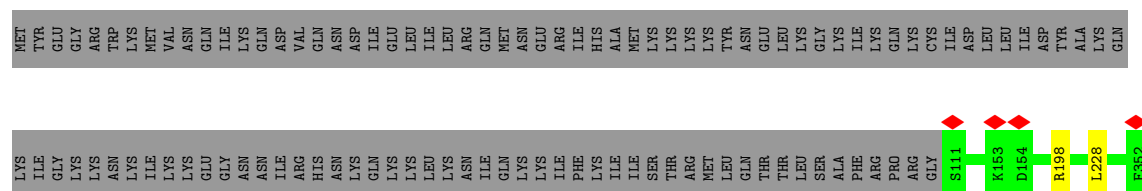
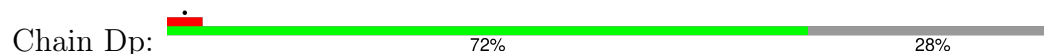
- Molecule 14: Protein phosphatase 2C, putative



- Molecule 15: SURF1-like protein



- Molecule 15: SURF1-like protein

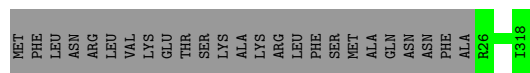






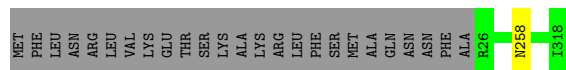
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain DT: 92% 8%



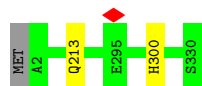
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt: 92% 8%



- Molecule 20: Carrier protein

Chain DU: 99% .



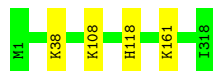
- Molecule 20: Carrier protein

Chain Du: 99% .



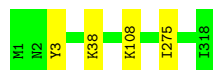
- Molecule 21: 2-oxoglutarate/malate carrier protein

Chain DV: 99% .



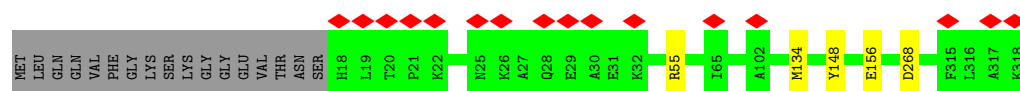
- Molecule 21: 2-oxoglutarate/malate carrier protein

Chain Dv: 99% .



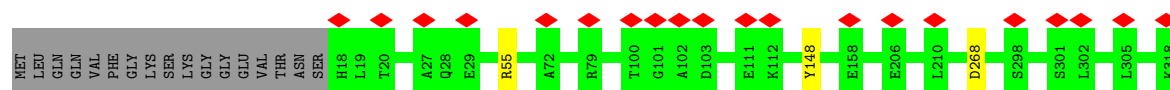
- Molecule 22: SURF1-like protein

Chain DW:  93% 5%



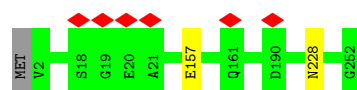
- Molecule 22: SURF1-like protein

Chain Dw:  94% 6% 5%



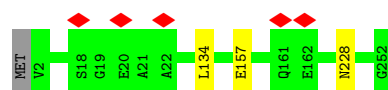
- Molecule 23: COXTT9

Chain DX:  99%




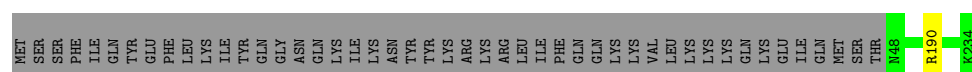
- Molecule 23: COXTT9

Chain Dx:  98%




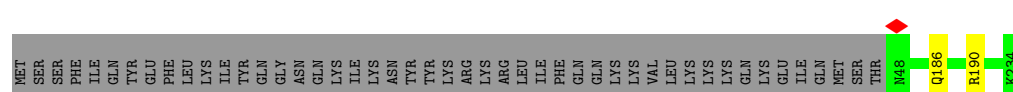
- Molecule 24: COXTT10

Chain DY:  79% 20%




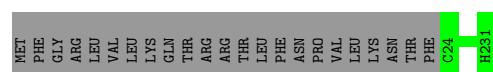
- Molecule 24: COXTT10

Chain Dy:  79% 20%



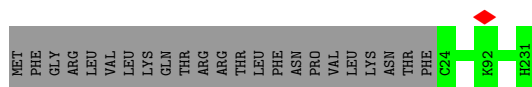
- Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain DZ:  90% 10%



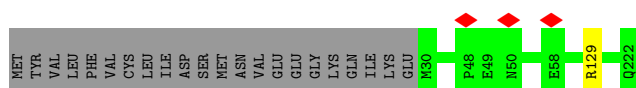
- Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain Dz:  90% 10%



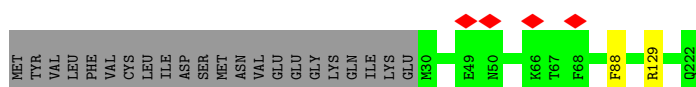
- Molecule 26: COXTT12,Transmembrane protein,Transmembrane protein

Chain EA:  89% 10%



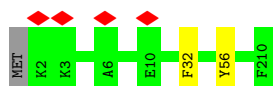
- Molecule 26: COXTT12,Transmembrane protein,Transmembrane protein

Chain Ea:  89% 10%



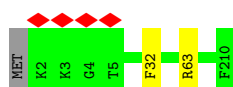
- Molecule 27: Transmembrane protein, putative

Chain EB:  99% .



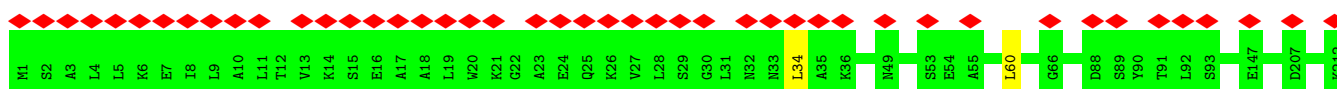
- Molecule 27: Transmembrane protein, putative

Chain Eb:  99% .



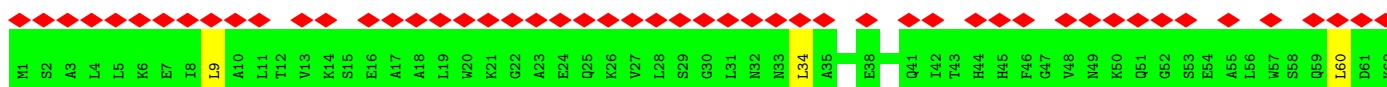
- Molecule 28: COXTT27

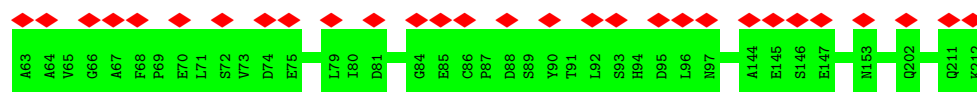
Chain EC:  21% 99% .



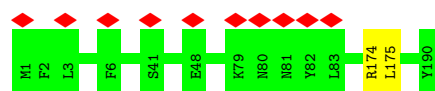
- Molecule 28: COXTT27

Chain Ec:  38% 99% .

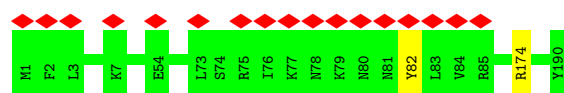




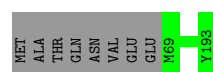
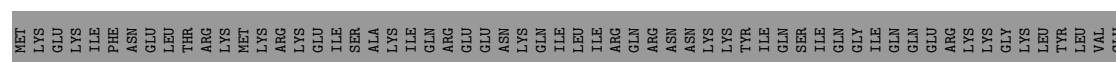
- Molecule 29: Ymf75



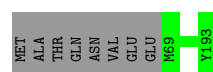
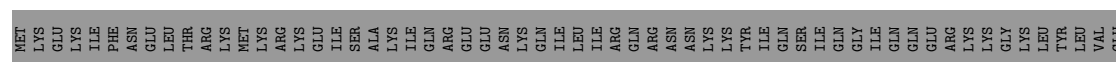
- Molecule 29: Ymf75



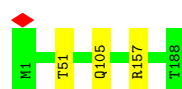
- Molecule 30: Mobilization protein



- Molecule 30: Mobilization protein

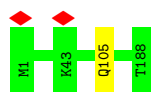


- Molecule 31: Iron-binding zinc finger CDGSH type protein

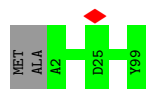


- Molecule 31: Iron-binding zinc finger CDGSH type protein

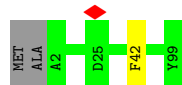




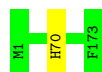
- Molecule 32: COXTT28



- Molecule 32: COXTT28



- Molecule 33: Transmembrane protein, putative



- Molecule 33: Transmembrane protein, putative



There are no outlier residues recorded for this chain.

- Molecule 34: Transmembrane protein



- Molecule 34: Transmembrane protein

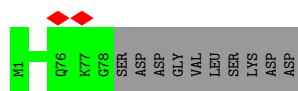
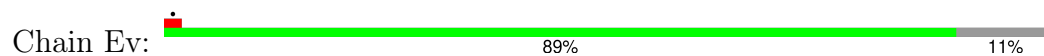


- Molecule 35: Decapping nuclease

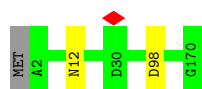




- Molecule 35: Decapping nuclease



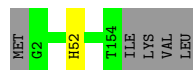
- Molecule 36: Complex III subunit VII



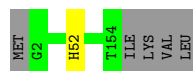
- Molecule 36: Complex III subunit VII



- Molecule 37: Transmembrane protein, putative



- Molecule 37: Transmembrane protein, putative



- Molecule 38: Transmembrane protein, putative



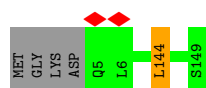
- Molecule 38: Transmembrane protein, putative

Chain Em:  99% ..



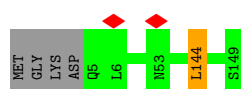
- Molecule 39: COXTT22

Chain EN:  97% ..



- Molecule 39: COXTT22

Chain En:  97% ..



- Molecule 40: Transmembrane protein, putative

Chain EO:  98% ..




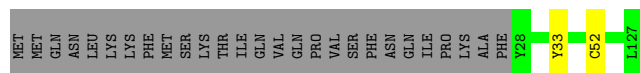
- Molecule 40: Transmembrane protein, putative

Chain Eo:  98% ..



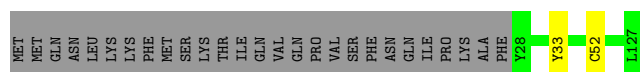
- Molecule 41: Phage protein

Chain EP:  77% 21%



- Molecule 41: Phage protein

Chain Ep:  77% 21%



- Molecule 42: Transmembrane protein, putative

Chain EQ:  98%



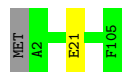
- Molecule 42: Transmembrane protein, putative

Chain Eq:  98%



- Molecule 43: Lysozyme

Chain ER:  98%



- Molecule 43: Lysozyme

Chain Er:  99%



- Molecule 44: Ymf70

Chain ES:  100%


There are no outlier residues recorded for this chain.

- Molecule 44: Ymf70

Chain Es:  100%




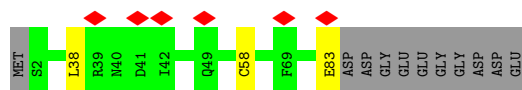
- Molecule 45: Zf-Tim10_DDP domain-containing protein

Chain ET:  8% 85% 12%

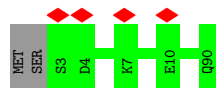


- Molecule 45: Zf-Tim10_DDP domain-containing protein

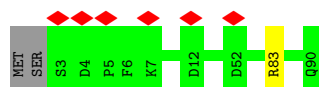
Chain Et:  6% 85% 12%



- Molecule 46: ABC transporter



- Molecule 46: ABC transporter



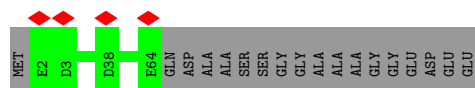
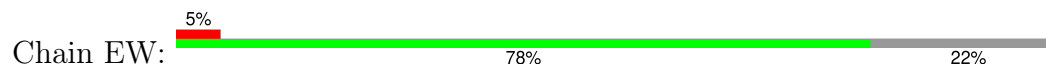
- Molecule 47: YfiT domain-containing protein



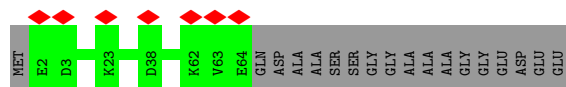
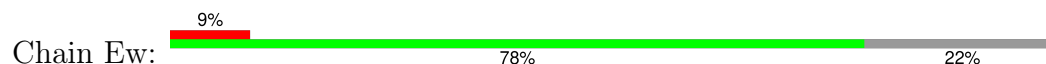
- Molecule 47: YfiT domain-containing protein



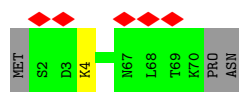
- Molecule 48: Cullin domain-containing protein



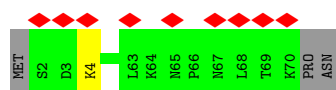
- Molecule 48: Cullin domain-containing protein



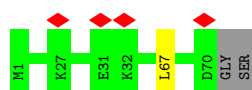
- Molecule 49: Zf-Tim10_DDP domain-containing protein



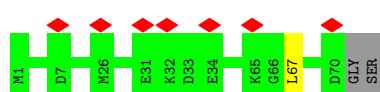
- Molecule 49: Zf-Tim10_DDP domain-containing protein



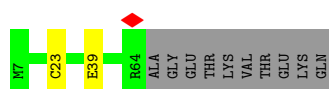
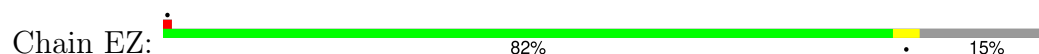
- Molecule 50: Annexin



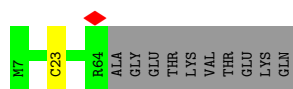
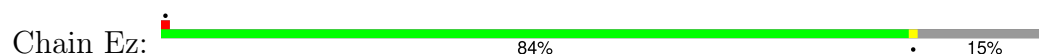
- Molecule 50: Annexin



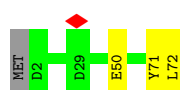
- Molecule 51: Transposase



- Molecule 51: Transposase

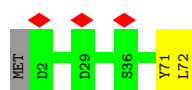


- Molecule 52: Tim10/DDP family zinc finger protein



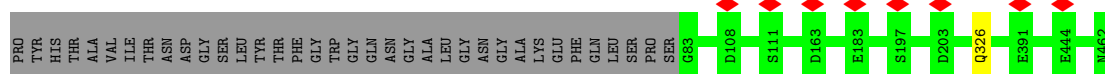
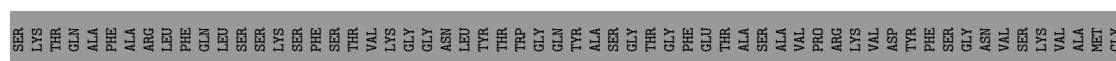
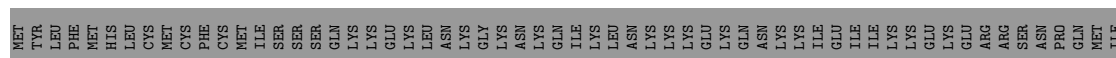
- Molecule 52: Tim10/DDP family zinc finger protein

Chain Fa:  96%



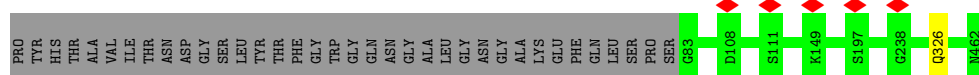
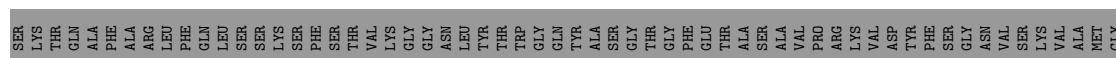
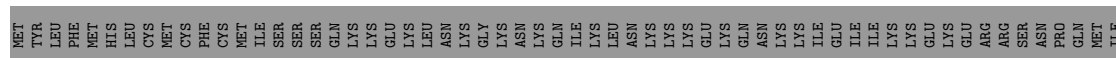
- Molecule 53: COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein

Chain DL:  71% 29%



- Molecule 53: COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein

Chain DL:  71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	138746	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 ($e^-/\text{\AA}^2$)	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	7.005	Depositor
Minimum map value	-3.774	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.539	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	600.912, 600.912, 600.912	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2519, 1.2519, 1.2519	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDL, UQ8, CU, PC1, FES, SEP, HEA, ATP, CUA, CA, HEM, 3PE, K, TPO, ZN, LPP, AME

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	DA	0.25	0/5748	0.44	0/7793
1	Da	0.25	0/5748	0.44	0/7793
2	DB	0.24	0/5282	0.46	2/7159 (0.0%)
2	Db	0.24	0/5282	0.46	2/7159 (0.0%)
3	DC	0.25	0/5256	0.42	0/7142
3	Dc	0.25	0/5256	0.41	0/7142
4	DD	0.24	0/4734	0.46	2/6387 (0.0%)
4	Dd	0.24	0/4734	0.46	2/6387 (0.0%)
5	DE	0.24	0/1116	0.41	0/1512
5	De	0.24	0/1116	0.41	0/1512
6	DF	0.25	0/1977	0.49	2/2673 (0.1%)
6	Df	0.25	0/1977	0.49	2/2673 (0.1%)
7	DG	0.24	0/906	0.46	0/1230
7	Dg	0.25	0/906	0.46	0/1230
8	DH	0.24	0/1199	0.46	0/1621
8	Dh	0.24	0/1199	0.46	0/1621
9	DI	0.24	0/1829	0.42	0/2486
9	Di	0.24	0/1829	0.42	0/2486
10	DJ	0.24	0/1950	0.43	0/2647
10	Dj	0.24	0/1950	0.43	0/2647
11	DK	0.24	0/1100	0.47	2/1495 (0.1%)
11	Dk	0.24	0/1100	0.47	2/1495 (0.1%)
12	DM	0.24	0/3910	0.44	0/5320
12	Dm	0.24	0/3910	0.44	0/5320
13	DN	0.24	0/3963	0.39	0/5359
13	Dn	0.24	0/3963	0.39	0/5359
14	DO	0.24	0/3505	0.42	0/4745
14	Do	0.24	0/3505	0.42	0/4745
15	DP	0.24	0/2433	0.46	0/3307
15	Dp	0.24	0/2433	0.46	0/3307
16	DQ	0.23	0/3247	0.44	0/4410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	Dq	0.24	0/3247	0.44	0/4410
17	DR	0.24	0/2077	0.46	2/2824 (0.1%)
17	Dr	0.24	0/2077	0.46	2/2824 (0.1%)
18	DS	0.25	0/2950	0.44	0/4003
18	Ds	0.25	0/2950	0.44	0/4003
19	DT	0.24	0/2518	0.45	0/3433
19	Dt	0.24	0/2518	0.45	0/3433
20	DU	0.24	0/2689	0.42	0/3657
20	Du	0.24	0/2689	0.42	0/3657
21	DV	0.24	0/2622	0.45	0/3554
21	Dv	0.24	0/2622	0.45	0/3554
22	DW	0.24	0/2449	0.45	0/3312
22	Dw	0.24	0/2449	0.45	0/3312
23	DX	0.24	0/2171	0.44	0/2930
23	Dx	0.24	0/2171	0.44	0/2930
24	DY	0.23	0/1619	0.45	0/2198
24	Dy	0.23	0/1619	0.44	0/2198
25	DZ	0.23	0/1752	0.41	0/2372
25	Dz	0.23	0/1752	0.41	0/2372
26	EA	0.24	0/1709	0.43	0/2321
26	Ea	0.24	0/1709	0.43	0/2321
27	EB	0.24	0/1793	0.42	0/2418
27	Eb	0.24	0/1793	0.42	0/2418
28	EC	0.25	0/1673	0.45	4/2258 (0.2%)
28	Ec	0.24	0/1673	0.46	4/2258 (0.2%)
29	ED	0.26	0/1708	0.38	0/2306
29	Ed	0.26	0/1708	0.38	0/2306
30	EE	0.24	0/1066	0.45	0/1432
30	Ee	0.24	0/1066	0.45	0/1432
31	EF	0.26	0/1562	0.45	0/2123
31	Ef	0.25	0/1562	0.45	0/2123
32	EG	0.25	0/786	0.44	0/1060
32	Eg	0.25	0/786	0.44	0/1060
33	EH	0.24	0/1471	0.44	0/1995
33	Uh	0.24	0/1471	0.44	0/1995
34	EI	0.25	0/1442	0.49	4/1952 (0.2%)
34	Ei	0.25	0/1442	0.49	4/1952 (0.2%)
35	EV	0.23	0/645	0.41	0/866
35	Ev	0.23	0/645	0.42	0/866
36	EK	0.23	0/1410	0.43	0/1900
36	Ek	0.24	0/1410	0.43	0/1900
37	EL	0.24	0/1335	0.44	0/1810
37	El	0.24	0/1335	0.44	0/1810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
38	EM	0.24	0/1335	0.46	0/1794
38	Em	0.24	0/1335	0.46	0/1794
39	EN	0.24	0/1270	0.50	2/1724 (0.1%)
39	En	0.24	0/1270	0.51	2/1724 (0.1%)
40	EO	0.23	0/1137	0.44	0/1545
40	Eo	0.23	0/1137	0.45	0/1545
41	EP	0.23	0/837	0.49	0/1133
41	Ep	0.23	0/837	0.48	0/1133
42	EQ	0.24	0/1035	0.42	0/1403
42	Eq	0.24	0/1035	0.43	0/1403
43	ER	0.24	0/874	0.46	0/1182
43	Er	0.24	0/874	0.46	0/1182
44	ES	0.25	0/802	0.41	0/1087
44	Es	0.25	0/802	0.41	0/1087
45	ET	0.24	0/654	0.43	0/878
45	Et	0.24	0/654	0.43	0/878
46	EU	0.23	0/744	0.44	0/1003
46	Eu	0.23	0/744	0.44	0/1003
47	EJ	0.24	0/1437	0.42	0/1941
47	Ej	0.24	0/1437	0.43	0/1941
48	EW	0.24	0/523	0.41	0/705
48	Ew	0.24	0/523	0.42	0/705
49	EX	0.23	0/564	0.41	0/757
49	Ex	0.24	0/564	0.42	0/757
50	EY	0.25	0/573	0.49	2/770 (0.3%)
50	Ey	0.25	0/573	0.49	2/770 (0.3%)
51	EZ	0.25	0/502	0.43	0/676
51	Ez	0.25	0/502	0.43	0/676
52	FA	0.23	0/554	0.40	0/746
52	Fa	0.23	0/554	0.40	0/746
53	DL	0.25	0/2984	0.45	0/4047
53	Dl	0.25	0/2984	0.45	0/4047
All	All	0.24	0/202854	0.44	44/274802 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
47	Ej	0	1

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Ey	67	LEU	CB-CG-CD2	6.23	121.59	111.00
50	EY	67	LEU	CB-CG-CD2	6.17	121.50	111.00
4	DD	265	LEU	CB-CG-CD2	6.13	121.42	111.00
34	EI	168	LEU	CB-CG-CD2	6.03	121.26	111.00
2	Db	573	LEU	CB-CG-CD2	5.99	121.19	111.00
34	Ei	168	LEU	CB-CG-CD2	5.99	121.18	111.00
4	Dd	265	LEU	CB-CG-CD1	5.97	121.15	111.00
4	Dd	265	LEU	CB-CG-CD2	5.97	121.15	111.00
2	DB	573	LEU	CB-CG-CD2	5.96	121.13	111.00
28	Ec	34	LEU	CB-CG-CD2	5.94	121.10	111.00
4	DD	265	LEU	CB-CG-CD1	5.92	121.07	111.00
28	EC	34	LEU	CB-CG-CD2	5.88	120.99	111.00
17	DR	258	LEU	CB-CG-CD2	5.79	120.85	111.00
6	Df	10	LEU	CB-CG-CD1	5.79	120.84	111.00
17	Dr	258	LEU	CB-CG-CD2	5.79	120.84	111.00
6	DF	10	LEU	CB-CG-CD1	5.78	120.82	111.00
11	DK	130	LEU	CB-CG-CD2	5.77	120.81	111.00
11	Dk	130	LEU	CB-CG-CD2	5.73	120.73	111.00
34	Ei	27	LEU	CB-CG-CD2	5.72	120.73	111.00
28	Ec	60	LEU	CB-CG-CD2	5.71	120.71	111.00
39	EN	144	LEU	CB-CG-CD2	5.70	120.69	111.00
34	EI	27	LEU	CB-CG-CD2	5.70	120.69	111.00
28	EC	60	LEU	CB-CG-CD2	5.64	120.59	111.00
28	EC	60	LEU	CB-CG-CD1	5.63	120.57	111.00
39	En	144	LEU	CB-CG-CD1	5.62	120.56	111.00
28	EC	34	LEU	CB-CG-CD1	5.61	120.53	111.00
39	En	144	LEU	CB-CG-CD2	5.57	120.47	111.00
28	Ec	60	LEU	CB-CG-CD1	5.56	120.45	111.00
39	EN	144	LEU	CB-CG-CD1	5.54	120.42	111.00
6	DF	10	LEU	CB-CG-CD2	5.53	120.40	111.00
34	EI	27	LEU	CB-CG-CD1	5.52	120.38	111.00
11	Dk	130	LEU	CB-CG-CD1	5.50	120.36	111.00
6	Df	10	LEU	CB-CG-CD2	5.47	120.31	111.00
17	Dr	258	LEU	CB-CG-CD1	5.46	120.29	111.00
28	Ec	34	LEU	CB-CG-CD1	5.46	120.28	111.00
17	DR	258	LEU	CB-CG-CD1	5.45	120.27	111.00
11	DK	130	LEU	CB-CG-CD1	5.45	120.26	111.00
2	DB	573	LEU	CB-CG-CD1	5.40	120.18	111.00
34	Ei	27	LEU	CB-CG-CD1	5.37	120.12	111.00
34	Ei	168	LEU	CB-CG-CD1	5.36	120.11	111.00
50	EY	67	LEU	CB-CG-CD1	5.35	120.10	111.00
34	EI	168	LEU	CB-CG-CD1	5.33	120.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Db	573	LEU	CB-CG-CD1	5.33	120.05	111.00
50	Ey	67	LEU	CB-CG-CD1	5.33	120.05	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	Ej	99	PHE	Peptide

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	DA	669/688 (97%)	654 (98%)	15 (2%)	0	100	100
1	Da	669/688 (97%)	657 (98%)	12 (2%)	0	100	100
2	DB	602/604 (100%)	586 (97%)	16 (3%)	0	100	100
2	Db	602/604 (100%)	592 (98%)	10 (2%)	0	100	100
3	DC	580/594 (98%)	569 (98%)	9 (2%)	2 (0%)	37	59
3	Dc	580/594 (98%)	569 (98%)	11 (2%)	0	100	100
4	DD	554/637 (87%)	551 (100%)	3 (0%)	0	100	100
4	Dd	554/637 (87%)	551 (100%)	3 (0%)	0	100	100
5	DE	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
5	De	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
6	DF	220/230 (96%)	216 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Df	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
7	DG	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
7	Dg	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
8	DH	131/133 (98%)	124 (95%)	7 (5%)	0	100	100
8	Dh	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
9	DI	203/236 (86%)	198 (98%)	4 (2%)	1 (0%)	25	47
9	Di	203/236 (86%)	196 (97%)	6 (3%)	1 (0%)	25	47
10	DJ	218/220 (99%)	218 (100%)	0	0	100	100
10	Dj	218/220 (99%)	216 (99%)	2 (1%)	0	100	100
11	DK	128/990 (13%)	120 (94%)	8 (6%)	0	100	100
11	Dk	128/990 (13%)	121 (94%)	7 (6%)	0	100	100
12	DM	453/490 (92%)	446 (98%)	7 (2%)	0	100	100
12	Dm	453/490 (92%)	446 (98%)	7 (2%)	0	100	100
13	DN	451/453 (100%)	444 (98%)	7 (2%)	0	100	100
13	Dn	451/453 (100%)	444 (98%)	7 (2%)	0	100	100
14	DO	431/473 (91%)	429 (100%)	2 (0%)	0	100	100
14	Do	431/473 (91%)	427 (99%)	4 (1%)	0	100	100
15	DP	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
15	Dp	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
16	DQ	381/385 (99%)	368 (97%)	13 (3%)	0	100	100
16	Dq	381/385 (99%)	370 (97%)	11 (3%)	0	100	100
17	DR	241/348 (69%)	237 (98%)	4 (2%)	0	100	100
17	Dr	241/348 (69%)	238 (99%)	3 (1%)	0	100	100
18	DS	344/346 (99%)	343 (100%)	1 (0%)	0	100	100
18	Ds	344/346 (99%)	343 (100%)	1 (0%)	0	100	100
19	DT	291/318 (92%)	290 (100%)	1 (0%)	0	100	100
19	Dt	291/318 (92%)	290 (100%)	1 (0%)	0	100	100
20	DU	327/330 (99%)	321 (98%)	6 (2%)	0	100	100
20	Du	327/330 (99%)	321 (98%)	6 (2%)	0	100	100
21	DV	316/318 (99%)	312 (99%)	4 (1%)	0	100	100
21	Dv	316/318 (99%)	311 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	DW	299/318 (94%)	298 (100%)	1 (0%)	0	100	100
22	Dw	299/318 (94%)	297 (99%)	2 (1%)	0	100	100
23	DX	249/252 (99%)	246 (99%)	3 (1%)	0	100	100
23	Dx	249/252 (99%)	248 (100%)	1 (0%)	0	100	100
24	DY	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
24	Dy	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
25	DZ	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
25	Dz	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
26	EA	191/215 (89%)	187 (98%)	4 (2%)	0	100	100
26	Ea	191/215 (89%)	189 (99%)	2 (1%)	0	100	100
27	EB	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
27	Eb	207/210 (99%)	207 (100%)	0	0	100	100
28	EC	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
28	Ec	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
29	ED	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
29	Ed	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
30	EE	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
30	Ee	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
31	EF	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
31	Ef	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
32	EG	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
32	Eg	96/100 (96%)	96 (100%)	0	0	100	100
33	EH	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
33	Eh	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
34	EI	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
34	Ei	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
35	EV	76/88 (86%)	75 (99%)	1 (1%)	0	100	100
35	Ev	76/88 (86%)	75 (99%)	1 (1%)	0	100	100
36	EK	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
36	Ek	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
37	EL	151/158 (96%)	149 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	El	151/158 (96%)	150 (99%)	1 (1%)	0	100	100
38	EM	151/154 (98%)	150 (99%)	1 (1%)	0	100	100
38	Em	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
39	EN	143/149 (96%)	140 (98%)	3 (2%)	0	100	100
39	En	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
40	EO	121/124 (98%)	118 (98%)	3 (2%)	0	100	100
40	Eo	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
41	EP	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
41	Ep	98/127 (77%)	98 (100%)	0	0	100	100
42	EQ	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
42	Eq	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
43	ER	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
43	Er	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
44	ES	87/89 (98%)	87 (100%)	0	0	100	100
44	Es	87/89 (98%)	87 (100%)	0	0	100	100
45	ET	80/93 (86%)	80 (100%)	0	0	100	100
45	Et	80/93 (86%)	80 (100%)	0	0	100	100
46	EU	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
46	Eu	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
47	EJ	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
47	Ej	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
48	EW	61/81 (75%)	61 (100%)	0	0	100	100
48	Ew	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
49	EX	67/72 (93%)	67 (100%)	0	0	100	100
49	Ex	67/72 (93%)	67 (100%)	0	0	100	100
50	EY	68/72 (94%)	68 (100%)	0	0	100	100
50	Ey	68/72 (94%)	68 (100%)	0	0	100	100
51	EZ	56/68 (82%)	55 (98%)	1 (2%)	0	100	100
51	Ez	56/68 (82%)	56 (100%)	0	0	100	100
52	FA	69/72 (96%)	69 (100%)	0	0	100	100
52	Fa	69/72 (96%)	69 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	DL	378/536 (70%)	364 (96%)	14 (4%)	0	100	100
53	DI	378/536 (70%)	364 (96%)	14 (4%)	0	100	100
All	All	23566/27324 (86%)	23198 (98%)	364 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	DC	143	ASN
9	Di	119	GLU
9	DI	119	GLU
3	DC	49	ASN

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	DA	596/613 (97%)	585 (98%)	11 (2%)	54	77
1	Da	596/613 (97%)	586 (98%)	10 (2%)	56	78
2	DB	569/569 (100%)	557 (98%)	12 (2%)	48	73
2	Db	569/569 (100%)	559 (98%)	10 (2%)	54	77
3	DC	553/565 (98%)	551 (100%)	2 (0%)	89	96
3	Dc	553/565 (98%)	551 (100%)	2 (0%)	89	96
4	DD	506/579 (87%)	500 (99%)	6 (1%)	67	85
4	Dd	506/579 (87%)	502 (99%)	4 (1%)	79	91
5	DE	114/116 (98%)	114 (100%)	0	100	100
5	De	114/116 (98%)	113 (99%)	1 (1%)	75	90
6	DF	200/207 (97%)	197 (98%)	3 (2%)	60	81
6	Df	200/207 (97%)	198 (99%)	2 (1%)	73	88
7	DG	84/88 (96%)	82 (98%)	2 (2%)	44	70
7	Dg	84/88 (96%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	DH	119/119 (100%)	118 (99%)	1 (1%)	79	91
8	Dh	119/119 (100%)	117 (98%)	2 (2%)	56	78
9	DI	193/218 (88%)	191 (99%)	2 (1%)	73	88
9	Di	193/218 (88%)	190 (98%)	3 (2%)	58	79
10	DJ	199/199 (100%)	195 (98%)	4 (2%)	50	74
10	Dj	199/199 (100%)	197 (99%)	2 (1%)	73	88
11	DK	121/943 (13%)	121 (100%)	0	100	100
11	Dk	121/943 (13%)	121 (100%)	0	100	100
12	DM	413/447 (92%)	410 (99%)	3 (1%)	81	93
12	Dm	413/447 (92%)	409 (99%)	4 (1%)	73	88
13	DN	442/442 (100%)	437 (99%)	5 (1%)	70	86
13	Dn	442/442 (100%)	437 (99%)	5 (1%)	70	86
14	DO	380/413 (92%)	380 (100%)	0	100	100
14	Do	380/413 (92%)	380 (100%)	0	100	100
15	DP	253/358 (71%)	251 (99%)	2 (1%)	79	91
15	Dp	253/358 (71%)	251 (99%)	2 (1%)	79	91
16	DQ	340/342 (99%)	337 (99%)	3 (1%)	75	90
16	Dq	340/342 (99%)	338 (99%)	2 (1%)	84	94
17	DR	219/318 (69%)	218 (100%)	1 (0%)	86	95
17	Dr	219/318 (69%)	219 (100%)	0	100	100
18	DS	293/293 (100%)	288 (98%)	5 (2%)	56	78
18	Ds	293/293 (100%)	288 (98%)	5 (2%)	56	78
19	DT	267/289 (92%)	267 (100%)	0	100	100
19	Dt	267/289 (92%)	266 (100%)	1 (0%)	89	96
20	DU	275/276 (100%)	273 (99%)	2 (1%)	81	93
20	Du	275/276 (100%)	272 (99%)	3 (1%)	70	86
21	DV	259/259 (100%)	255 (98%)	4 (2%)	60	81
21	Dv	259/259 (100%)	255 (98%)	4 (2%)	60	81
22	DW	258/272 (95%)	253 (98%)	5 (2%)	52	75
22	Dw	258/272 (95%)	255 (99%)	3 (1%)	67	85
23	DX	218/219 (100%)	216 (99%)	2 (1%)	75	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Dx	218/219 (100%)	215 (99%)	3 (1%)	62	82
24	DY	169/216 (78%)	168 (99%)	1 (1%)	84	94
24	Dy	169/216 (78%)	167 (99%)	2 (1%)	67	85
25	DZ	189/213 (89%)	189 (100%)	0	100	100
25	Dz	189/213 (89%)	189 (100%)	0	100	100
26	EA	180/201 (90%)	179 (99%)	1 (1%)	84	94
26	Ea	180/201 (90%)	178 (99%)	2 (1%)	70	86
27	EB	180/181 (99%)	178 (99%)	2 (1%)	70	86
27	Eb	180/181 (99%)	178 (99%)	2 (1%)	70	86
28	EC	178/178 (100%)	178 (100%)	0	100	100
28	Ec	178/178 (100%)	177 (99%)	1 (1%)	84	94
29	ED	185/185 (100%)	183 (99%)	2 (1%)	70	86
29	Ed	185/185 (100%)	183 (99%)	2 (1%)	70	86
30	EE	116/180 (64%)	116 (100%)	0	100	100
30	Ee	116/180 (64%)	116 (100%)	0	100	100
31	EF	164/164 (100%)	161 (98%)	3 (2%)	54	77
31	Ef	164/164 (100%)	163 (99%)	1 (1%)	84	94
32	EG	77/78 (99%)	77 (100%)	0	100	100
32	Eg	77/78 (99%)	76 (99%)	1 (1%)	65	84
33	EH	156/156 (100%)	155 (99%)	1 (1%)	84	94
33	Eh	156/156 (100%)	156 (100%)	0	100	100
34	EI	156/157 (99%)	153 (98%)	3 (2%)	52	75
34	Ei	156/157 (99%)	153 (98%)	3 (2%)	52	75
35	EV	71/80 (89%)	71 (100%)	0	100	100
35	Ev	71/80 (89%)	71 (100%)	0	100	100
36	EK	153/154 (99%)	151 (99%)	2 (1%)	65	84
36	Ek	153/154 (99%)	150 (98%)	3 (2%)	50	74
37	EL	134/139 (96%)	133 (99%)	1 (1%)	81	93
37	El	134/139 (96%)	133 (99%)	1 (1%)	81	93
38	EM	137/138 (99%)	136 (99%)	1 (1%)	81	93
38	Em	137/138 (99%)	136 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	EN	132/135 (98%)	131 (99%)	1 (1%)	79	91
39	En	132/135 (98%)	131 (99%)	1 (1%)	79	91
40	EO	112/113 (99%)	110 (98%)	2 (2%)	54	77
40	Eo	112/113 (99%)	110 (98%)	2 (2%)	54	77
41	EP	87/113 (77%)	85 (98%)	2 (2%)	45	71
41	Ep	87/113 (77%)	85 (98%)	2 (2%)	45	71
42	EQ	104/104 (100%)	101 (97%)	3 (3%)	37	64
42	Eq	104/104 (100%)	101 (97%)	3 (3%)	37	64
43	ER	87/88 (99%)	86 (99%)	1 (1%)	70	86
43	Er	87/88 (99%)	87 (100%)	0	100	100
44	ES	84/84 (100%)	84 (100%)	0	100	100
44	Es	84/84 (100%)	84 (100%)	0	100	100
45	ET	75/83 (90%)	72 (96%)	3 (4%)	27	52
45	Et	75/83 (90%)	72 (96%)	3 (4%)	27	52
46	EU	78/80 (98%)	78 (100%)	0	100	100
46	Eu	78/80 (98%)	77 (99%)	1 (1%)	65	84
47	EJ	157/157 (100%)	154 (98%)	3 (2%)	52	75
47	Ej	157/157 (100%)	154 (98%)	3 (2%)	52	75
48	EW	57/66 (86%)	57 (100%)	0	100	100
48	Ew	57/66 (86%)	57 (100%)	0	100	100
49	EX	64/67 (96%)	63 (98%)	1 (2%)	58	79
49	Ex	64/67 (96%)	63 (98%)	1 (2%)	58	79
50	EY	62/63 (98%)	62 (100%)	0	100	100
50	Ey	62/63 (98%)	62 (100%)	0	100	100
51	EZ	55/63 (87%)	53 (96%)	2 (4%)	30	56
51	Ez	55/63 (87%)	54 (98%)	1 (2%)	54	77
52	FA	62/63 (98%)	59 (95%)	3 (5%)	21	44
52	Fa	62/63 (98%)	60 (97%)	2 (3%)	34	60
53	DL	308/441 (70%)	307 (100%)	1 (0%)	91	97
53	Dl	308/441 (70%)	307 (100%)	1 (0%)	91	97
All	All	21280/24568 (87%)	21059 (99%)	221 (1%)	71	88

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DA	57	TYR
1	DA	363	ASP
1	DA	389	PHE
1	DA	429	VAL
1	DA	447	LEU
1	DA	503	PHE
1	DA	526	HIS
1	DA	527	PHE
1	DA	530	MET
1	DA	591	HIS
1	DA	630	ARG
2	DB	45	TRP
2	DB	133	PHE
2	DB	143	ILE
2	DB	175	VAL
2	DB	183	LEU
2	DB	224	PHE
2	DB	297	PHE
2	DB	298	PHE
2	DB	524	LYS
2	DB	526	ASP
2	DB	585	LEU
2	DB	590	ARG
3	DC	295	LYS
3	DC	425	TYR
4	DD	64	LYS
4	DD	214	ASN
4	DD	219	GLU
4	DD	236	LYS
4	DD	247	GLU
4	DD	525	ASP
6	DF	35	LYS
6	DF	90	ASP
6	DF	133	CYS
7	DG	1	MET
7	DG	12	TRP
8	DH	115	ARG
9	DI	102	ARG
9	DI	106	TRP
10	DJ	26	LYS
10	DJ	62	HIS
10	DJ	121	TYR

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Mol	Chain	Res	Type
10	DJ	176	MET
12	DM	206	ASP
12	DM	386	THR
12	DM	414	GLN
13	DN	114	TYR
13	DN	191	TYR
13	DN	210	LEU
13	DN	262	LEU
13	DN	420	ASN
15	DP	228	LEU
15	DP	247	LYS
16	DQ	34	THR
16	DQ	202	HIS
16	DQ	280	TRP
17	DR	211	ARG
18	DS	58	GLU
18	DS	96	ARG
18	DS	145	LEU
18	DS	222	LYS
18	DS	232	GLN
20	DU	213	GLN
20	DU	300	HIS
21	DV	38	LYS
21	DV	108	LYS
21	DV	118	HIS
21	DV	161	LYS
22	DW	55	ARG
22	DW	134	MET
22	DW	148	TYR
22	DW	156	GLU
22	DW	268	ASP
23	DX	157	GLU
23	DX	228	ASN
24	DY	190	ARG
26	EA	129	ARG
27	EB	32	PHE
27	EB	56	TYR
29	ED	174	ARG
29	ED	175	LEU
31	EF	51	THR
31	EF	105	GLN
31	EF	157	ARG

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Mol	Chain	Res	Type
33	EH	70	HIS
34	EI	8	TYR
34	EI	111	TYR
34	EI	132	VAL
36	EK	12	ASN
36	EK	98	ASP
37	EL	52	HIS
38	EM	115	PHE
39	EN	144	LEU
40	EO	36	TYR
40	EO	103	TYR
41	EP	33	TYR
41	EP	52	CYS
42	EQ	2	GLU
42	EQ	65	PHE
42	EQ	73	ILE
43	ER	21	GLU
45	ET	38	LEU
45	ET	58	CYS
45	ET	83	GLU
47	EJ	90	PHE
47	EJ	110	ASP
47	EJ	158	LEU
49	EX	4	LYS
51	EZ	23	CYS
51	EZ	39	GLU
52	FA	50	GLU
52	FA	71	TYR
52	FA	72	LEU
1	Da	57	TYR
1	Da	363	ASP
1	Da	429	VAL
1	Da	447	LEU
1	Da	503	PHE
1	Da	519	ASP
1	Da	521	PHE
1	Da	526	HIS
1	Da	527	PHE
1	Da	630	ARG
2	Db	45	TRP
2	Db	224	PHE
2	Db	230	TYR

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Mol	Chain	Res	Type
2	Db	291	PHE
2	Db	297	PHE
2	Db	412	THR
2	Db	511	ASP
2	Db	524	LYS
2	Db	585	LEU
2	Db	590	ARG
3	Dc	50	GLU
3	Dc	425	TYR
4	Dd	214	ASN
4	Dd	236	LYS
4	Dd	247	GLU
4	Dd	525	ASP
5	De	126	GLU
6	Df	35	LYS
6	Df	133	CYS
8	Dh	115	ARG
8	Dh	122	GLU
9	Di	102	ARG
9	Di	106	TRP
9	Di	208	ILE
10	Dj	62	HIS
10	Dj	176	MET
12	Dm	103	LEU
12	Dm	206	ASP
12	Dm	372	ASP
12	Dm	386	THR
13	Dn	30	LEU
13	Dn	114	TYR
13	Dn	210	LEU
13	Dn	262	LEU
13	Dn	420	ASN
15	Dp	198	ARG
15	Dp	228	LEU
16	Dq	202	HIS
16	Dq	280	TRP
18	Ds	58	GLU
18	Ds	65	THR
18	Ds	145	LEU
18	Ds	222	LYS
18	Ds	232	GLN
19	Dt	258	ASN

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Mol	Chain	Res	Type
20	Du	91	VAL
20	Du	131	ARG
20	Du	300	HIS
21	Dv	3	TYR
21	Dv	38	LYS
21	Dv	108	LYS
21	Dv	275	ILE
22	Dw	55	ARG
22	Dw	148	TYR
22	Dw	268	ASP
23	Dx	134	LEU
23	Dx	157	GLU
23	Dx	228	ASN
24	Dy	186	GLN
24	Dy	190	ARG
26	Ea	88	PHE
26	Ea	129	ARG
27	Eb	32	PHE
27	Eb	63	ARG
28	Ec	9	LEU
29	Ed	82	TYR
29	Ed	174	ARG
31	Ef	105	GLN
32	Eg	42	PHE
34	Ei	8	TYR
34	Ei	111	TYR
34	Ei	132	VAL
36	Ek	12	ASN
36	Ek	17	LEU
36	Ek	98	ASP
37	El	52	HIS
38	Em	115	PHE
39	En	144	LEU
40	Eo	24	TYR
40	Eo	36	TYR
41	Ep	33	TYR
41	Ep	52	CYS
42	Eq	2	GLU
42	Eq	65	PHE
42	Eq	73	ILE
45	Et	38	LEU
45	Et	58	CYS

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Mol	Chain	Res	Type
45	Et	83	GLU
46	Eu	83	ARG
47	Ej	90	PHE
47	Ej	99	PHE
47	Ej	110	ASP
49	Ex	4	LYS
51	Ez	23	CYS
52	Fa	71	TYR
52	Fa	72	LEU
53	Dl	326	GLN
53	DL	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	DB	12	GLN
2	DB	198	GLN
2	DB	207	ASN
2	DB	379	ASN
3	DC	224	ASN
13	DN	302	ASN
16	DQ	61	ASN
16	DQ	96	GLN
17	DR	262	GLN
18	DS	120	ASN
21	DV	24	ASN
22	DW	214	ASN
24	DY	226	ASN
26	EA	205	ASN
34	EI	64	ASN
36	EK	55	ASN
39	EN	52	ASN
40	EO	112	GLN
47	EJ	105	GLN
2	Db	198	GLN
2	Db	207	ASN
3	Dc	21	ASN
3	Dc	52	ASN
3	Dc	63	ASN
3	Dc	306	GLN
5	De	56	ASN
5	De	73	GLN

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Mol	Chain	Res	Type
12	Dm	451	GLN
13	Dn	298	ASN
17	Dr	262	GLN
22	Dw	232	HIS
25	Dz	141	GLN
28	Ec	194	GLN
53	Dl	90	GLN
53	Dl	260	ASN
53	DL	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	AME	Dq	1	16	9,10,11	0.27	0	9,11,13	0.44	0
21	AME	DV	1	21	9,10,11	0.26	0	9,11,13	0.54	0
33	AME	EH	1	33	9,10,11	0.25	0	9,11,13	0.41	0
21	AME	Dv	1	21	9,10,11	0.26	0	9,11,13	0.55	0
4	SEP	Dd	520	4	8,9,10	1.61	1 (12%)	7,12,14	1.44	1 (14%)
33	AME	Eh	1	33	9,10,11	0.26	0	9,11,13	0.41	0
9	SEP	Di	120	9	8,9,10	1.60	1 (12%)	7,12,14	1.27	1 (14%)
4	SEP	DD	520	4	8,9,10	1.60	1 (12%)	7,12,14	1.41	1 (14%)
35	AME	EV	1	35	9,10,11	0.27	0	9,11,13	0.43	0
4	TPO	Dd	387	4	8,10,11	1.63	1 (12%)	10,14,16	2.08	1 (10%)
18	AME	Ds	1	18	9,10,11	0.27	0	9,11,13	0.47	0
35	AME	Ev	1	35	9,10,11	0.26	0	9,11,13	0.43	0
16	AME	DQ	1	16	9,10,11	0.26	0	9,11,13	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	AME	DH	1	8	9,10,11	0.28	0	9,11,13	0.44	0
42	AME	Eq	1	42	9,10,11	0.28	0	9,11,13	0.43	0
4	TPO	DD	387	4	8,10,11	1.63	1 (12%)	10,14,16	2.09	1 (10%)
8	AME	Dh	1	8	9,10,11	0.27	0	9,11,13	0.45	0
18	AME	DS	1	18	9,10,11	0.27	0	9,11,13	0.47	0
42	AME	EQ	1	42	9,10,11	0.26	0	9,11,13	0.45	0
9	SEP	DI	120	9	8,9,10	1.60	1 (12%)	7,12,14	1.29	1 (14%)

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
16	AME	Dq	1	16	-	2/9/10/12	-
21	AME	DV	1	21	-	0/9/10/12	-
33	AME	EH	1	33	-	0/9/10/12	-
21	AME	Dv	1	21	-	0/9/10/12	-
4	SEP	Dd	520	4	-	0/6/8/10	-
33	AME	Eh	1	33	-	2/9/10/12	-
9	SEP	Di	120	9	-	0/6/8/10	-
4	SEP	DD	520	4	-	0/6/8/10	-
35	AME	EV	1	35	-	1/9/10/12	-
4	TPO	Dd	387	4	-	2/9/11/13	-
18	AME	Ds	1	18	-	1/9/10/12	-
35	AME	Ev	1	35	-	1/9/10/12	-
16	AME	DQ	1	16	-	2/9/10/12	-
8	AME	DH	1	8	-	0/9/10/12	-
42	AME	Eq	1	42	-	2/9/10/12	-
4	TPO	DD	387	4	-	2/9/11/13	-
8	AME	Dh	1	8	-	0/9/10/12	-
18	AME	DS	1	18	-	0/9/10/12	-
42	AME	EQ	1	42	-	2/9/10/12	-
9	SEP	DI	120	9	-	1/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Dd	520	SEP	P-O1P	3.53	1.61	1.50
9	Di	120	SEP	P-O1P	3.52	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Dd	387	TPO	P-O1P	3.51	1.61	1.50
4	DD	520	SEP	P-O1P	3.50	1.61	1.50
9	DI	120	SEP	P-O1P	3.49	1.61	1.50
4	DD	387	TPO	P-O1P	3.49	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Dd	387	TPO	P-OG1-CB	-6.03	106.95	123.33
4	DD	387	TPO	P-OG1-CB	-6.00	107.02	123.33
4	Dd	520	SEP	OG-CB-CA	3.22	111.28	108.14
4	DD	520	SEP	OG-CB-CA	3.15	111.21	108.14
9	DI	120	SEP	OG-CB-CA	2.76	110.83	108.14
9	Di	120	SEP	OG-CB-CA	2.73	110.80	108.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	EQ	1	AME	O-C-CA-CB
33	Eh	1	AME	O-C-CA-CB
42	Eq	1	AME	O-C-CA-CB
42	Eq	1	AME	CB-CG-SD-CE
42	EQ	1	AME	CB-CG-SD-CE
33	Eh	1	AME	CB-CG-SD-CE
35	EV	1	AME	CB-CG-SD-CE
18	Ds	1	AME	CB-CG-SD-CE
16	Dq	1	AME	C-CA-N-CT1
16	DQ	1	AME	CB-CG-SD-CE
35	Ev	1	AME	CB-CG-SD-CE
16	Dq	1	AME	CB-CA-N-CT1
4	DD	387	TPO	C-CA-CB-CG2
4	Dd	387	TPO	C-CA-CB-CG2
9	DI	120	SEP	CB-OG-P-O3P
16	DQ	1	AME	CB-CA-N-CT1
4	DD	387	TPO	O-C-CA-CB
4	Dd	387	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 245 ligands modelled in this entry, 9 are monoatomic - leaving 236 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$
57	CDL	DV	401	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	Dl	1101	-	43,43,43	0.22	0	46,48,48	0.26	0
58	PC1	Da	707	-	53,53,53	0.29	0	59,61,61	0.28	0
59	3PE	Dj	407	-	50,50,50	0.27	0	53,55,55	0.20	0
58	PC1	Dv	405	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	Dj	402	-	99,99,99	0.29	0	105,111,111	0.25	0
68	ATP	Er	201	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
57	CDL	Dn	503	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dx	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DV	406	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dj	406	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	EO	205	-	53,53,53	0.28	0	59,61,61	0.28	0
59	3PE	Dd	703	-	50,50,50	0.26	0	53,55,55	0.20	0
57	CDL	DC	601	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	Dn	506	-	43,43,43	0.21	0	46,48,48	0.28	0
57	CDL	El	903	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ds	405	-	99,99,99	0.30	0	105,111,111	0.24	0
65	UQ8	Ds	404	-	53,53,53	0.51	0	66,67,67	0.68	2 (3%)
57	CDL	DD	703	-	99,99,99	0.29	0	105,111,111	0.25	0
60	LPP	Ed	203	-	43,43,43	0.21	0	46,48,48	0.26	0
58	PC1	El	904	-	53,53,53	0.27	0	59,61,61	0.29	0
62	CUA	DB	701	2	0,1,1	-	-	-	-	-
57	CDL	En	1202	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DR	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Dy	301	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	EH	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dr	403	-	99,99,99	0.29	0	105,111,111	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	DH	201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DS	407	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	EH	202	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ed	204	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EL	903	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dd	706	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DV	405	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	DS	401	-	50,50,50	0.26	0	53,55,55	0.23	0
60	LPP	EI	402	-	43,43,43	0.21	0	46,48,48	0.26	0
67	FES	EF	201	31	0,4,4	-	-	-	-	-
57	CDL	Dj	408	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ed	205	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	El	902	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DC	608	-	53,53,53	0.27	0	59,61,61	0.27	0
57	CDL	DN	501	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EA	301	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DS	406	-	53,53,53	0.28	0	59,61,61	0.26	0
59	3PE	Dg	204	-	50,50,50	0.26	0	53,55,55	0.23	0
57	CDL	Dn	502	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DZ	501	-	99,99,99	0.29	0	105,111,111	0.24	0
59	3PE	Dc	606	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Dq	402	-	99,99,99	0.29	0	105,111,111	0.25	0
65	UQ8	En	1203	-	53,53,53	0.52	0	66,67,67	0.64	3 (4%)
57	CDL	Dm	502	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DG	204	-	50,50,50	0.26	0	53,55,55	0.20	0
57	CDL	DJ	303	-	99,99,99	0.29	0	105,111,111	0.26	0
57	CDL	DQ	1504	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	501	-	99,99,99	0.29	0	105,111,111	0.26	0
57	CDL	Eu	101	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DR	401	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	DJ	307	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	El	905	-	50,50,50	0.28	0	53,55,55	0.21	0
58	PC1	Dq	405	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Dr	401	-	50,50,50	0.26	0	53,55,55	0.22	0
66	HEM	ED	602	-	42,50,50	1.29	5 (11%)	46,82,82	1.74	8 (17%)
57	CDL	Dq	403	-	99,99,99	0.29	0	105,111,111	0.26	0
59	3PE	Ds	401	-	50,50,50	0.26	0	53,55,55	0.23	0
58	PC1	DA	706	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DA	705	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	Em	901	-	50,50,50	0.27	0	53,55,55	0.19	0
58	PC1	Ds	406	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	Dh	202	-	99,99,99	0.29	0	105,111,111	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Da	709	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dx	1202	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Dx	1205	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	DX	307	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dj	403	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EB	302	-	99,99,99	0.29	0	105,111,111	0.27	0
60	LPP	DN	503	-	43,43,43	0.21	0	46,48,48	0.28	0
57	CDL	El	901	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	DI	702	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	EU	101	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DD	702	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DA	710	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dx	1204	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DJ	305	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Ep	701	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	507	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DC	606	-	50,50,50	0.26	0	53,55,55	0.22	0
57	CDL	Dv	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	EB	304	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dm	501	-	99,99,99	0.29	0	105,111,111	0.25	0
65	UQ8	El	906	-	53,53,53	0.54	0	66,67,67	0.84	4 (6%)
58	PC1	DY	302	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	DN	505	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dr	402	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	EO	206	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	Du	403	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dv	406	-	53,53,53	0.28	0	59,61,61	0.27	0
54	HEA	DA	701	1	58,67,67	2.31	21 (36%)	63,103,103	2.26	26 (41%)
62	CUA	Db	701	2	0,1,1	-	-	-	-	-
57	CDL	DV	404	-	99,99,99	0.29	0	105,111,111	0.26	0
58	PC1	Dc	605	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Ds	407	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Ek	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DA	709	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DY	301	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dc	602	-	53,53,53	0.27	0	59,61,61	0.28	0
57	CDL	Dd	705	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	505	-	99,99,99	0.29	0	105,111,111	0.27	0
57	CDL	DG	202	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DC	603	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	EO	207	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	DM	502	-	99,99,99	0.29	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	3PE	DA	708	-	50,50,50	0.26	0	53,55,55	0.19	0
57	CDL	Ea	301	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DJ	304	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DX	305	-	50,50,50	0.27	0	53,55,55	0.20	0
59	3PE	Dx	1206	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	EN	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dz	501	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	Dn	504	-	43,43,43	0.21	0	46,48,48	0.29	0
57	CDL	En	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Eb	302	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dx	1208	-	53,53,53	0.28	0	59,61,61	0.28	0
54	HEA	DA	702	-	58,67,67	2.30	20 (34%)	63,103,103	2.30	24 (38%)
57	CDL	EL	904	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	Eb	301	-	53,53,53	0.28	0	59,61,61	0.26	0
60	LPP	DA	711	-	43,43,43	0.21	0	46,48,48	0.26	0
57	CDL	Dh	201	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dd	704	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dy	302	-	53,53,53	0.28	0	59,61,61	0.27	0
60	LPP	DN	502	-	43,43,43	0.22	0	46,48,48	0.30	0
57	CDL	Dq	401	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dg	202	-	99,99,99	0.29	0	105,111,111	0.24	0
65	UQ8	EL	906	-	53,53,53	0.53	0	66,67,67	0.80	3 (4%)
57	CDL	Dq	404	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DC	605	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	DC	604	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	DA	707	-	53,53,53	0.29	0	59,61,61	0.28	0
57	CDL	ED	604	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DQ	1502	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dj	401	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DB	702	-	53,53,53	0.29	0	59,61,61	0.27	0
59	3PE	DJ	301	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	Du	402	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DR	402	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EN	1202	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dv	408	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	EO	205	-	53,53,53	0.27	0	59,61,61	0.29	0
57	CDL	DQ	1501	-	99,99,99	0.29	0	105,111,111	0.26	0
59	3PE	EL	905	-	50,50,50	0.27	0	53,55,55	0.22	0
59	3PE	Dr	404	-	50,50,50	0.26	0	53,55,55	0.20	0
65	UQ8	Ed	202	-	53,53,53	0.53	0	66,67,67	0.72	2 (3%)
58	PC1	DX	302	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	DX	306	-	53,53,53	0.28	0	59,61,61	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Dg	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ds	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	EI	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dc	601	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Da	705	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dv	404	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Du	404	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DQ	1503	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	EL	901	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DU	403	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Do	501	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dv	407	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DS	405	-	99,99,99	0.29	0	105,111,111	0.24	0
59	3PE	DG	205	-	50,50,50	0.27	0	53,55,55	0.21	0
57	CDL	DO	501	-	99,99,99	0.29	0	105,111,111	0.24	0
66	HEM	Ed	201	-	42,50,50	1.29	6 (14%)	46,82,82	1.74	8 (17%)
59	3PE	Eo	203	-	50,50,50	0.26	0	53,55,55	0.21	0
59	3PE	Ds	403	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	DN	504	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DV	407	-	53,53,53	0.28	0	59,61,61	0.27	0
54	HEA	Da	701	1	58,67,67	2.31	21 (36%)	63,103,103	2.26	27 (42%)
57	CDL	Dj	405	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Di	701	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Eh	1601	-	99,99,99	0.30	0	105,111,111	0.23	0
58	PC1	DG	203	-	53,53,53	0.28	0	59,61,61	0.28	0
59	3PE	DC	607	-	50,50,50	0.26	0	53,55,55	0.20	0
59	3PE	EO	204	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	DS	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	EO	202	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	EM	901	-	50,50,50	0.26	0	53,55,55	0.20	0
59	3PE	EN	1203	-	50,50,50	0.27	0	53,55,55	0.20	0
58	PC1	Eo	204	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	Dd	702	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DU	404	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dc	603	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	EO	203	-	50,50,50	0.26	0	53,55,55	0.20	0
67	FES	Ef	1002	31	0,4,4	-	-	-	-	-
58	PC1	Dc	607	-	53,53,53	0.27	0	59,61,61	0.28	0
57	CDL	DD	704	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	Db	702	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	Dx	1203	-	99,99,99	0.30	0	105,111,111	0.24	0
67	FES	Ef	1003	31	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	DG	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DX	301	-	99,99,99	0.30	0	105,111,111	0.25	0
67	FES	EF	202	31	0,4,4	-	-	-		
58	PC1	DC	602	-	53,53,53	0.27	0	59,61,61	0.28	0
58	PC1	EB	301	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	DI	701	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dv	401	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DJ	306	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Da	708	-	50,50,50	0.25	0	53,55,55	0.21	0
59	3PE	Dx	1207	-	50,50,50	0.27	0	53,55,55	0.19	0
65	UQ8	DS	404	-	53,53,53	0.51	0	66,67,67	0.68	2 (3%)
57	CDL	DV	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Ei	401	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	EB	303	-	53,53,53	0.29	0	59,61,61	0.28	0
65	UQ8	ED	603	-	53,53,53	0.52	0	66,67,67	0.71	2 (3%)
54	HEA	Da	702	-	58,67,67	2.31	21 (36%)	63,103,103	2.29	23 (36%)
57	CDL	DU	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DJ	302	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EK	201	-	99,99,99	0.29	0	105,111,111	0.25	0
68	ATP	ER	201	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
58	PC1	Eo	201	-	53,53,53	0.29	0	59,61,61	0.28	0
57	CDL	Dj	404	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Du	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DV	403	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	ED	601	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DM	501	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	Ef	1001	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	DX	304	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	EL	902	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dv	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Eg	101	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DX	303	-	50,50,50	0.26	0	53,55,55	0.18	0
59	3PE	Eo	202	-	50,50,50	0.26	0	53,55,55	0.19	0
58	PC1	Dg	203	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Di	702	-	53,53,53	0.29	0	59,61,61	0.27	0
59	3PE	DS	403	-	50,50,50	0.27	0	53,55,55	0.20	0
65	UQ8	EN	1204	-	53,53,53	0.52	0	66,67,67	0.68	2 (3%)
57	CDL	DU	402	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	EO	201	-	53,53,53	0.29	0	59,61,61	0.28	0
58	PC1	Da	706	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dc	604	-	53,53,53	0.27	0	59,61,61	0.28	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
57	CDL	DV	401	-	-	28/110/110/110	-
60	LPP	Dl	1101	-	-	8/45/45/45	-
58	PC1	Da	707	-	-	12/57/57/57	-
59	3PE	Dj	407	-	-	5/54/54/54	-
58	PC1	Dv	405	-	-	10/57/57/57	-
57	CDL	Dj	402	-	-	29/110/110/110	-
68	ATP	Er	201	-	-	2/18/38/38	0/3/3/3
57	CDL	Dn	503	-	-	22/110/110/110	-
57	CDL	Dx	1201	-	-	28/110/110/110	-
58	PC1	DV	406	-	-	11/57/57/57	-
58	PC1	Dj	406	-	-	10/57/57/57	-
58	PC1	Eo	205	-	-	14/57/57/57	-
59	3PE	Dd	703	-	-	17/54/54/54	-
57	CDL	DC	601	-	-	26/110/110/110	-
60	LPP	Dn	506	-	-	7/45/45/45	-
57	CDL	El	903	-	-	31/110/110/110	-
57	CDL	Ds	405	-	-	28/110/110/110	-
65	UQ8	Ds	404	-	-	11/51/75/75	0/1/1/1
57	CDL	DD	703	-	-	25/110/110/110	-
60	LPP	Ed	203	-	-	2/45/45/45	-
58	PC1	El	904	-	-	10/57/57/57	-
57	CDL	En	1202	-	-	23/110/110/110	-
57	CDL	DR	403	-	-	27/110/110/110	-
57	CDL	Dy	301	-	-	25/110/110/110	-
57	CDL	EH	201	-	-	22/110/110/110	-
57	CDL	Dr	403	-	-	23/110/110/110	-
57	CDL	DH	201	-	-	22/110/110/110	-
58	PC1	DS	407	-	-	16/57/57/57	-
57	CDL	EH	202	-	-	24/110/110/110	-
57	CDL	Ed	204	-	-	24/110/110/110	-
57	CDL	EL	903	-	-	37/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	Dd	706	-	-	24/110/110/110	-
58	PC1	DV	405	-	-	13/57/57/57	-
59	3PE	DS	401	-	-	16/54/54/54	-
60	LPP	EI	402	-	-	8/45/45/45	-
67	FES	EF	201	31	-	-	0/1/1/1
57	CDL	Dj	408	-	-	33/110/110/110	-
57	CDL	Ed	205	-	-	25/110/110/110	-
57	CDL	El	902	-	-	38/110/110/110	-
58	PC1	DC	608	-	-	18/57/57/57	-
57	CDL	DN	501	-	-	16/110/110/110	-
57	CDL	EA	301	-	-	27/110/110/110	-
58	PC1	DS	406	-	-	19/57/57/57	-
59	3PE	Dg	204	-	-	11/54/54/54	-
57	CDL	Dn	502	-	-	27/110/110/110	-
57	CDL	DZ	501	-	-	28/110/110/110	-
59	3PE	Dc	606	-	-	18/54/54/54	-
57	CDL	Dq	402	-	-	27/110/110/110	-
65	UQ8	En	1203	-	-	10/51/75/75	0/1/1/1
57	CDL	Dm	502	-	-	18/110/110/110	-
59	3PE	DG	204	-	-	16/54/54/54	-
57	CDL	DJ	303	-	-	33/110/110/110	-
57	CDL	DQ	1504	-	-	33/110/110/110	-
57	CDL	Dn	501	-	-	35/110/110/110	-
57	CDL	Eu	101	-	-	27/110/110/110	-
59	3PE	DR	401	-	-	8/54/54/54	-
57	CDL	DJ	307	-	-	29/110/110/110	-
59	3PE	El	905	-	-	16/54/54/54	-
58	PC1	Dq	405	-	-	10/57/57/57	-
59	3PE	Dr	401	-	-	15/54/54/54	-
66	HEM	ED	602	-	-	2/12/54/54	-
57	CDL	Dq	403	-	-	23/110/110/110	-
59	3PE	Ds	401	-	-	16/54/54/54	-
58	PC1	DA	706	-	-	14/57/57/57	-
57	CDL	DA	705	-	-	26/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Em	901	-	-	13/54/54/54	-
58	PC1	Ds	406	-	-	7/57/57/57	-
57	CDL	Dh	202	-	-	33/110/110/110	-
57	CDL	Da	709	-	-	33/110/110/110	-
58	PC1	Dx	1202	-	-	13/57/57/57	-
59	3PE	Dx	1205	-	-	17/54/54/54	-
57	CDL	DX	307	-	-	26/110/110/110	-
57	CDL	Dj	403	-	-	32/110/110/110	-
57	CDL	EB	302	-	-	24/110/110/110	-
60	LPP	DN	503	-	-	1/45/45/45	-
57	CDL	El	901	-	-	39/110/110/110	-
58	PC1	DI	702	-	-	18/57/57/57	-
57	CDL	EU	101	-	-	30/110/110/110	-
57	CDL	DD	702	-	-	25/110/110/110	-
57	CDL	DA	710	-	-	22/110/110/110	-
58	PC1	Dx	1204	-	-	14/57/57/57	-
57	CDL	DJ	305	-	-	23/110/110/110	-
57	CDL	Ep	701	-	-	28/110/110/110	-
57	CDL	Dn	507	-	-	20/110/110/110	-
59	3PE	DC	606	-	-	9/54/54/54	-
57	CDL	Dv	403	-	-	24/110/110/110	-
57	CDL	EB	304	-	-	34/110/110/110	-
57	CDL	Dm	501	-	-	38/110/110/110	-
65	UQ8	El	906	-	-	12/51/75/75	0/1/1/1
58	PC1	DY	302	-	-	10/57/57/57	-
57	CDL	DN	505	-	-	29/110/110/110	-
57	CDL	Dr	402	-	-	33/110/110/110	-
58	PC1	EO	206	-	-	26/57/57/57	-
57	CDL	Du	403	-	-	29/110/110/110	-
58	PC1	Dv	406	-	-	19/57/57/57	-
54	HEA	DA	701	1	-	3/32/76/76	-
57	CDL	DV	404	-	-	36/110/110/110	-
58	PC1	Dc	605	-	-	16/57/57/57	-
59	3PE	Ds	407	-	-	11/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	Ek	201	-	-	26/110/110/110	-
57	CDL	DA	709	-	-	35/110/110/110	-
57	CDL	DY	301	-	-	27/110/110/110	-
58	PC1	Dc	602	-	-	17/57/57/57	-
57	CDL	Dd	705	-	-	30/110/110/110	-
57	CDL	Dn	505	-	-	25/110/110/110	-
57	CDL	DG	202	-	-	18/110/110/110	-
58	PC1	DC	603	-	-	14/57/57/57	-
58	PC1	EO	207	-	-	17/57/57/57	-
57	CDL	DM	502	-	-	15/110/110/110	-
59	3PE	DA	708	-	-	12/54/54/54	-
57	CDL	Ea	301	-	-	24/110/110/110	-
57	CDL	DJ	304	-	-	33/110/110/110	-
59	3PE	DX	305	-	-	13/54/54/54	-
59	3PE	Dx	1206	-	-	20/54/54/54	-
57	CDL	EN	1201	-	-	28/110/110/110	-
57	CDL	Dz	501	-	-	27/110/110/110	-
60	LPP	Dn	504	-	-	9/45/45/45	-
57	CDL	En	1201	-	-	23/110/110/110	-
58	PC1	Eb	302	-	-	4/57/57/57	-
58	PC1	Dx	1208	-	-	5/57/57/57	-
54	HEA	DA	702	-	-	9/32/76/76	-
57	CDL	EL	904	-	-	29/110/110/110	-
58	PC1	Eb	301	-	-	9/57/57/57	-
60	LPP	DA	711	-	-	7/45/45/45	-
57	CDL	Dh	201	-	-	22/110/110/110	-
57	CDL	Dd	704	-	-	34/110/110/110	-
58	PC1	Dy	302	-	-	10/57/57/57	-
60	LPP	DN	502	-	-	8/45/45/45	-
57	CDL	Dq	401	-	-	23/110/110/110	-
57	CDL	Dg	202	-	-	23/110/110/110	-
65	UQ8	EL	906	-	-	10/51/75/75	0/1/1/1
57	CDL	Dq	404	-	-	20/110/110/110	-
58	PC1	DC	605	-	-	11/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC1	DC	604	-	-	16/57/57/57	-
58	PC1	DA	707	-	-	11/57/57/57	-
57	CDL	ED	604	-	-	25/110/110/110	-
57	CDL	DQ	1502	-	-	22/110/110/110	-
57	CDL	Dj	401	-	-	31/110/110/110	-
58	PC1	DB	702	-	-	23/57/57/57	-
59	3PE	DJ	301	-	-	15/54/54/54	-
57	CDL	Du	402	-	-	18/110/110/110	-
57	CDL	DR	402	-	-	35/110/110/110	-
57	CDL	EN	1202	-	-	29/110/110/110	-
58	PC1	Dv	408	-	-	9/57/57/57	-
58	PC1	EO	205	-	-	10/57/57/57	-
57	CDL	DQ	1501	-	-	30/110/110/110	-
59	3PE	EL	905	-	-	16/54/54/54	-
59	3PE	Dr	404	-	-	10/54/54/54	-
65	UQ8	Ed	202	-	-	9/51/75/75	0/1/1/1
58	PC1	DX	302	-	-	13/57/57/57	-
58	PC1	DX	306	-	-	9/57/57/57	-
57	CDL	Dg	201	-	-	38/110/110/110	-
57	CDL	Ds	402	-	-	30/110/110/110	-
57	CDL	EI	401	-	-	22/110/110/110	-
57	CDL	Dc	601	-	-	28/110/110/110	-
57	CDL	Da	705	-	-	32/110/110/110	-
57	CDL	Dv	404	-	-	40/110/110/110	-
57	CDL	Du	404	-	-	27/110/110/110	-
58	PC1	DQ	1503	-	-	11/57/57/57	-
57	CDL	EL	901	-	-	33/110/110/110	-
57	CDL	DU	403	-	-	20/110/110/110	-
57	CDL	Do	501	-	-	29/110/110/110	-
58	PC1	Dv	407	-	-	12/57/57/57	-
57	CDL	DS	405	-	-	31/110/110/110	-
59	3PE	DG	205	-	-	14/54/54/54	-
57	CDL	DO	501	-	-	26/110/110/110	-
66	HEM	Ed	201	-	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Eo	203	-	-	6/54/54/54	-
59	3PE	Ds	403	-	-	19/54/54/54	-
57	CDL	DN	504	-	-	27/110/110/110	-
58	PC1	DV	407	-	-	10/57/57/57	-
54	HEA	Da	701	1	-	4/32/76/76	-
57	CDL	Dj	405	-	-	22/110/110/110	-
57	CDL	Di	701	-	-	30/110/110/110	-
57	CDL	Eh	1601	-	-	32/110/110/110	-
58	PC1	DG	203	-	-	8/57/57/57	-
59	3PE	DC	607	-	-	15/54/54/54	-
59	3PE	EO	204	-	-	8/54/54/54	-
57	CDL	DS	402	-	-	30/110/110/110	-
57	CDL	EO	202	-	-	30/110/110/110	-
59	3PE	EM	901	-	-	13/54/54/54	-
59	3PE	EN	1203	-	-	14/54/54/54	-
58	PC1	Eo	204	-	-	19/57/57/57	-
57	CDL	Dd	702	-	-	27/110/110/110	-
57	CDL	DU	404	-	-	22/110/110/110	-
58	PC1	Dc	603	-	-	14/57/57/57	-
59	3PE	EO	203	-	-	17/54/54/54	-
67	FES	Ef	1002	31	-	-	0/1/1/1
58	PC1	Dc	607	-	-	16/57/57/57	-
57	CDL	DD	704	-	-	32/110/110/110	-
58	PC1	Db	702	-	-	21/57/57/57	-
57	CDL	Dx	1203	-	-	31/110/110/110	-
67	FES	Ef	1003	31	-	-	0/1/1/1
57	CDL	DG	201	-	-	36/110/110/110	-
57	CDL	DX	301	-	-	30/110/110/110	-
67	FES	EF	202	31	-	-	0/1/1/1
58	PC1	DC	602	-	-	16/57/57/57	-
58	PC1	EB	301	-	-	11/57/57/57	-
57	CDL	DI	701	-	-	25/110/110/110	-
57	CDL	Dv	401	-	-	26/110/110/110	-
58	PC1	DJ	306	-	-	12/57/57/57	-
59	3PE	Da	708	-	-	16/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Dx	1207	-	-	14/54/54/54	-
65	UQ8	DS	404	-	-	8/51/75/75	0/1/1/1
57	CDL	DV	402	-	-	40/110/110/110	-
57	CDL	Ei	401	-	-	21/110/110/110	-
58	PC1	EB	303	-	-	3/57/57/57	-
65	UQ8	ED	603	-	-	8/51/75/75	0/1/1/1
54	HEA	Da	702	-	-	9/32/76/76	-
57	CDL	DU	401	-	-	32/110/110/110	-
57	CDL	DJ	302	-	-	17/110/110/110	-
57	CDL	EK	201	-	-	26/110/110/110	-
68	ATP	ER	201	-	-	7/18/38/38	0/3/3/3
58	PC1	Eo	201	-	-	15/57/57/57	-
57	CDL	Dj	404	-	-	33/110/110/110	-
57	CDL	Du	401	-	-	28/110/110/110	-
57	CDL	DV	403	-	-	25/110/110/110	-
57	CDL	ED	601	-	-	24/110/110/110	-
57	CDL	DM	501	-	-	31/110/110/110	-
58	PC1	Ef	1001	-	-	15/57/57/57	-
59	3PE	DX	304	-	-	18/54/54/54	-
57	CDL	EL	902	-	-	25/110/110/110	-
57	CDL	Dv	402	-	-	37/110/110/110	-
57	CDL	Eg	101	-	-	32/110/110/110	-
59	3PE	DX	303	-	-	13/54/54/54	-
59	3PE	Eo	202	-	-	15/54/54/54	-
58	PC1	Dg	203	-	-	12/57/57/57	-
58	PC1	Di	702	-	-	19/57/57/57	-
59	3PE	DS	403	-	-	19/54/54/54	-
65	UQ8	EN	1204	-	-	15/51/75/75	0/1/1/1
57	CDL	DU	402	-	-	18/110/110/110	-
58	PC1	EO	201	-	-	12/57/57/57	-
58	PC1	Da	706	-	-	17/57/57/57	-
58	PC1	Dc	604	-	-	12/57/57/57	-

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Da	701	HEA	C3A-C2A	6.62	1.49	1.40
54	DA	701	HEA	C3A-C2A	6.53	1.49	1.40
54	Da	702	HEA	C3A-C2A	6.51	1.49	1.40
54	DA	702	HEA	C3A-C2A	6.49	1.49	1.40
54	Da	701	HEA	C3B-C2B	5.46	1.47	1.34
54	DA	701	HEA	C3B-C2B	5.45	1.47	1.34
54	Da	702	HEA	C3C-C2C	5.41	1.47	1.40
54	Da	701	HEA	C3C-C2C	5.39	1.47	1.40
54	DA	702	HEA	C3C-C2C	5.38	1.47	1.40
54	Da	702	HEA	C3B-C2B	5.37	1.46	1.34
54	DA	702	HEA	C3B-C2B	5.37	1.46	1.34
54	DA	701	HEA	C3C-C2C	5.35	1.47	1.40
54	Da	701	HEA	CHC-C4B	5.35	1.47	1.34
54	DA	701	HEA	CHC-C4B	5.34	1.47	1.34
54	Da	702	HEA	C3A-C4A	5.34	1.49	1.41
54	Da	702	HEA	CHC-C4B	5.33	1.47	1.34
54	DA	702	HEA	CHC-C4B	5.30	1.47	1.34
54	DA	702	HEA	C3A-C4A	5.30	1.49	1.41
54	DA	701	HEA	C3A-C4A	5.26	1.49	1.41
54	Da	701	HEA	CHD-C1D	5.26	1.47	1.34
54	DA	701	HEA	CHD-C1D	5.23	1.47	1.34
54	DA	702	HEA	CHD-C1D	5.23	1.47	1.34
54	Da	702	HEA	CHD-C1D	5.23	1.47	1.34
54	Da	701	HEA	C3A-C4A	4.90	1.48	1.41
54	Da	701	HEA	C3D-C2D	4.83	1.47	1.36
54	DA	702	HEA	C3D-C2D	4.81	1.47	1.36
54	Da	702	HEA	C3D-C2D	4.80	1.47	1.36
54	DA	701	HEA	C3D-C2D	4.80	1.47	1.36
54	Da	701	HEA	C2A-C1A	3.43	1.50	1.42
54	DA	701	HEA	C2A-C1A	3.38	1.50	1.42
54	DA	702	HEA	C2A-C1A	3.26	1.49	1.42
54	Da	702	HEA	C2A-C1A	3.26	1.49	1.42
66	Ed	201	HEM	C4D-ND	-3.08	1.34	1.40
66	ED	602	HEM	C4D-ND	-3.04	1.35	1.40
66	ED	602	HEM	C1B-NB	-3.00	1.35	1.40
66	Ed	201	HEM	C1B-NB	-2.95	1.35	1.40
54	Da	702	HEA	C4B-C3B	2.73	1.49	1.44
54	DA	702	HEA	C4B-C3B	2.71	1.49	1.44
54	Da	702	HEA	C1D-ND	-2.71	1.35	1.40
54	Da	701	HEA	C1D-ND	-2.70	1.35	1.40
54	DA	702	HEA	C1D-ND	-2.67	1.35	1.40
54	DA	701	HEA	C1D-ND	-2.64	1.35	1.40
54	Da	701	HEA	C4B-C3B	2.62	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Da	701	HEA	C4B-NB	-2.60	1.35	1.40
54	DA	701	HEA	C4B-NB	-2.58	1.35	1.40
54	DA	701	HEA	C4B-C3B	2.56	1.49	1.44
54	DA	702	HEA	FE-NB	2.52	2.12	1.98
54	Da	701	HEA	C1C-CHC	2.51	1.48	1.41
54	DA	701	HEA	C1C-CHC	2.51	1.48	1.41
54	DA	702	HEA	C4D-C3D	2.51	1.49	1.45
54	Da	702	HEA	FE-NB	2.50	2.12	1.98
54	Da	701	HEA	FE-NB	2.47	2.11	1.98
54	DA	701	HEA	FE-NB	2.47	2.11	1.98
54	DA	702	HEA	FE-ND	2.46	2.11	1.98
66	ED	602	HEM	FE-NB	2.46	2.11	1.98
54	Da	701	HEA	C4C-CHD	2.45	1.47	1.41
66	Ed	201	HEM	CHB-C1B	2.45	1.40	1.34
54	Da	702	HEA	C4D-C3D	2.45	1.49	1.45
54	Da	702	HEA	FE-ND	2.44	2.11	1.98
66	Ed	201	HEM	FE-NB	2.44	2.11	1.98
54	DA	701	HEA	C4C-CHD	2.44	1.47	1.41
54	DA	702	HEA	C4B-NB	-2.43	1.36	1.40
54	Da	702	HEA	C1C-CHC	2.43	1.47	1.41
54	Da	702	HEA	C4B-NB	-2.42	1.36	1.40
54	DA	702	HEA	C1C-CHC	2.42	1.47	1.41
54	Da	702	HEA	C4C-CHD	2.42	1.47	1.41
54	Da	701	HEA	FE-ND	2.40	2.11	1.98
54	DA	702	HEA	C4C-CHD	2.40	1.47	1.41
54	DA	701	HEA	FE-ND	2.39	2.11	1.98
66	ED	602	HEM	CHB-C1B	2.38	1.40	1.34
54	Da	702	HEA	CHA-C4D	2.35	1.47	1.40
54	DA	702	HEA	CHA-C4D	2.33	1.47	1.40
54	Da	701	HEA	CHA-C4D	2.32	1.47	1.40
54	Da	701	HEA	C11-C3B	-2.31	1.48	1.51
54	DA	702	HEA	CHB-C1B	2.31	1.47	1.40
54	Da	702	HEA	CHB-C1B	2.30	1.47	1.40
54	DA	701	HEA	CHB-C1B	2.30	1.47	1.40
54	Da	701	HEA	CHB-C1B	2.27	1.47	1.40
54	Da	701	HEA	C4D-C3D	2.27	1.48	1.45
54	DA	701	HEA	C4D-C3D	2.25	1.48	1.45
54	DA	701	HEA	C11-C3B	-2.23	1.48	1.51
54	DA	701	HEA	CHA-C4D	2.23	1.47	1.40
54	DA	701	HEA	C1D-C2D	2.20	1.49	1.44
54	Da	701	HEA	C1D-C2D	2.19	1.49	1.44
54	DA	702	HEA	C1B-C2B	2.13	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Da	702	HEA	C1D-C2D	2.12	1.48	1.44
54	DA	702	HEA	C1D-C2D	2.11	1.48	1.44
54	Da	702	HEA	C11-C3B	-2.10	1.48	1.51
54	Da	702	HEA	C1B-C2B	2.07	1.48	1.44
54	Da	701	HEA	C1B-C2B	2.06	1.48	1.44
54	DA	701	HEA	C1B-C2B	2.06	1.48	1.44
66	Ed	201	HEM	C1D-ND	-2.02	1.34	1.38
66	ED	602	HEM	C3B-C4B	2.01	1.48	1.44
66	Ed	201	HEM	C3B-C4B	2.01	1.48	1.44

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	701	HEA	C3D-C4D-ND	6.01	116.16	110.35
54	DA	702	HEA	C3D-C4D-ND	5.95	116.10	110.35
54	Da	702	HEA	C3D-C4D-ND	5.93	116.09	110.35
54	Da	701	HEA	C3D-C4D-ND	5.90	116.06	110.35
54	DA	702	HEA	C2D-C1D-ND	5.52	116.19	109.84
54	Da	702	HEA	C2D-C1D-ND	5.47	116.13	109.84
54	Da	701	HEA	C2B-C1B-NB	5.44	116.19	109.90
54	DA	701	HEA	C2D-C1D-ND	5.41	116.06	109.84
54	DA	702	HEA	C3B-C4B-NB	5.40	116.05	109.84
54	DA	701	HEA	C2B-C1B-NB	5.39	116.13	109.90
54	DA	702	HEA	C2B-C1B-NB	5.35	116.09	109.90
54	Da	702	HEA	C2B-C1B-NB	5.34	116.08	109.90
54	Da	701	HEA	C2D-C1D-ND	5.32	115.96	109.84
54	Da	701	HEA	C3B-C4B-NB	5.30	115.93	109.84
54	DA	701	HEA	C3B-C4B-NB	5.29	115.92	109.84
54	Da	702	HEA	C3B-C4B-NB	5.29	115.92	109.84
66	ED	602	HEM	CHC-C4B-NB	5.13	129.95	124.44
66	Ed	201	HEM	CHC-C4B-NB	5.11	129.93	124.44
54	DA	701	HEA	C1D-C2D-C3D	-4.17	102.59	106.98
66	ED	602	HEM	CHD-C1D-ND	4.13	128.88	124.44
54	Da	701	HEA	C1D-C2D-C3D	-4.10	102.66	106.98
54	DA	701	HEA	C3C-C4C-NC	4.07	114.47	109.21
54	Da	702	HEA	C3C-C4C-NC	4.06	114.46	109.21
66	Ed	201	HEM	CHD-C1D-ND	4.06	128.80	124.44
54	Da	701	HEA	C3C-C4C-NC	4.03	114.43	109.21
54	DA	702	HEA	C3C-C4C-NC	3.99	114.37	109.21
54	DA	702	HEA	C1D-C2D-C3D	-3.99	102.78	106.98
54	Da	702	HEA	C1D-C2D-C3D	-3.96	102.81	106.98
65	El	906	UQ8	C8-C7-C6	3.82	121.48	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	El	906	UQ8	C7-C8-C9	3.67	133.16	126.83
66	Ed	201	HEM	CHA-C4D-ND	3.67	128.92	124.37
54	Da	701	HEA	C1B-C2B-C3B	-3.65	102.57	106.80
54	DA	701	HEA	C1B-C2B-C3B	-3.61	102.61	106.80
66	ED	602	HEM	CHA-C4D-ND	3.51	128.72	124.37
65	EL	906	UQ8	C7-C8-C9	3.51	132.87	126.83
54	Da	702	HEA	CMC-C2C-C3C	3.43	131.54	124.68
54	DA	702	HEA	C1B-C2B-C3B	-3.40	102.86	106.80
54	Da	702	HEA	C1B-C2B-C3B	-3.40	102.86	106.80
54	DA	702	HEA	CMC-C2C-C3C	3.36	131.41	124.68
54	DA	702	HEA	C13-C12-C11	-3.27	109.16	114.39
54	Da	701	HEA	CMC-C2C-C3C	3.27	131.22	124.68
54	DA	701	HEA	CMC-C2C-C3C	3.25	131.19	124.68
54	DA	702	HEA	C26-C15-C16	3.22	120.81	115.23
54	Da	702	HEA	C27-C19-C20	3.17	120.73	115.23
54	DA	702	HEA	C4D-C3D-C2D	-3.14	102.33	106.89
54	Da	702	HEA	C4D-C3D-C2D	-3.13	102.33	106.89
66	Ed	201	HEM	C1B-NB-C4B	3.09	108.87	105.21
65	EL	906	UQ8	C8-C7-C6	3.09	119.69	112.08
54	DA	701	HEA	CHA-C4D-C3D	-3.05	120.32	124.77
66	ED	602	HEM	C1B-NB-C4B	3.05	108.82	105.21
54	Da	701	HEA	C4D-C3D-C2D	-3.03	102.48	106.89
54	DA	701	HEA	C4D-C3D-C2D	-3.01	102.51	106.89
54	DA	702	HEA	C4B-C3B-C2B	-2.98	102.43	107.44
54	Da	701	HEA	CHA-C4D-C3D	-2.96	120.45	124.77
65	Ed	202	UQ8	C7-C8-C9	2.94	131.90	126.83
54	Da	702	HEA	C4B-C3B-C2B	-2.94	102.49	107.44
54	DA	701	HEA	CHB-C1B-C2B	-2.94	120.38	125.03
54	Da	702	HEA	CHB-C1B-C2B	-2.89	120.47	125.03
54	Da	701	HEA	CHB-C1B-C2B	-2.89	120.47	125.03
65	ED	603	UQ8	C7-C8-C9	2.87	131.77	126.83
54	DA	701	HEA	C4B-C3B-C2B	-2.86	102.63	107.44
54	Da	701	HEA	C4B-C3B-C2B	-2.85	102.64	107.44
54	DA	702	HEA	CHB-C1B-C2B	-2.85	120.53	125.03
54	Da	702	HEA	CAD-C3D-C4D	2.83	129.63	124.70
54	Da	702	HEA	C13-C12-C11	-2.80	109.92	114.39
54	DA	702	HEA	CAD-C3D-C4D	2.76	129.51	124.70
54	Da	701	HEA	C13-C14-C15	-2.69	121.46	127.62
54	DA	701	HEA	C13-C14-C15	-2.68	121.49	127.62
54	Da	702	HEA	C26-C15-C16	2.66	119.84	115.23
54	DA	702	HEA	C27-C19-C20	2.64	119.81	115.23
65	Ds	404	UQ8	C7-C8-C9	2.63	131.36	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	702	HEA	CMB-C2B-C1B	2.60	129.10	125.03
66	Ed	201	HEM	CHB-C1B-NB	2.58	127.58	124.37
65	EL	906	UQ8	C17-C18-C19	-2.57	121.73	127.62
65	Ed	202	UQ8	C8-C7-C6	2.54	118.34	112.08
65	ED	603	UQ8	C8-C7-C6	2.54	118.33	112.08
54	Da	702	HEA	CHA-C4D-C3D	-2.53	121.08	124.77
54	Da	702	HEA	CHD-C1D-C2D	-2.53	119.78	126.94
54	DA	702	HEA	CHA-C4D-C3D	-2.52	121.10	124.77
54	Da	701	HEA	OMA-CMA-C3A	-2.52	118.83	124.80
54	DA	702	HEA	CHD-C1D-C2D	-2.51	119.83	126.94
54	DA	701	HEA	C12-C11-C3B	-2.51	108.19	112.12
66	ED	602	HEM	CHD-C1D-C2D	-2.51	121.06	125.03
65	EN	1204	UQ8	C17-C18-C19	-2.51	121.88	127.62
65	DS	404	UQ8	C7-C8-C9	2.51	131.15	126.83
66	ED	602	HEM	CHB-C1B-NB	2.50	127.48	124.37
54	Da	702	HEA	CMB-C2B-C1B	2.47	128.90	125.03
66	Ed	201	HEM	CHD-C1D-C2D	-2.46	121.14	125.03
54	Da	701	HEA	CHD-C1D-C2D	-2.45	120.00	126.94
54	Da	701	HEA	C27-C19-C20	2.42	119.43	115.23
54	DA	701	HEA	CHD-C1D-C2D	-2.41	120.11	126.94
54	DA	701	HEA	C27-C19-C20	2.40	119.39	115.23
66	Ed	201	HEM	CHA-C4D-C3D	-2.40	120.80	125.23
54	Da	701	HEA	C12-C11-C3B	-2.40	108.37	112.12
65	El	906	UQ8	C17-C18-C19	-2.39	122.15	127.62
54	Da	702	HEA	C25-C23-C24	2.36	120.03	114.59
54	DA	701	HEA	C25-C23-C24	2.35	120.00	114.59
54	Da	701	HEA	C25-C23-C24	2.35	119.99	114.59
68	ER	201	ATP	C5-C6-N6	2.34	123.87	120.31
66	ED	602	HEM	CHA-C4D-C3D	-2.32	120.95	125.23
54	Da	701	HEA	C17-C18-C19	-2.31	122.33	127.62
68	Er	201	ATP	C5-C6-N6	2.31	123.83	120.31
54	DA	701	HEA	CMD-C2D-C1D	2.28	128.60	125.03
54	DA	702	HEA	C25-C23-C24	2.27	119.81	114.59
54	DA	701	HEA	C17-C18-C19	-2.23	122.52	127.62
54	DA	702	HEA	C4B-NB-C1B	-2.23	102.57	105.21
54	Da	701	HEA	CHC-C4B-C3B	-2.21	120.22	125.80
54	Da	701	HEA	CMD-C2D-C1D	2.21	128.49	125.03
54	DA	702	HEA	C1D-ND-C4D	-2.20	102.60	105.21
65	DS	404	UQ8	C8-C7-C6	2.19	117.49	112.08
54	DA	701	HEA	CHC-C4B-C3B	-2.18	120.31	125.80
54	DA	702	HEA	CMD-C2D-C1D	2.17	128.42	125.03
54	Da	701	HEA	CAD-C3D-C4D	2.17	128.47	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Da	702	HEA	C1D-ND-C4D	-2.17	102.64	105.21
54	Da	702	HEA	C4B-NB-C1B	-2.16	102.65	105.21
54	Da	702	HEA	CMD-C2D-C1D	2.15	128.39	125.03
54	Da	701	HEA	C4B-NB-C1B	-2.14	102.67	105.21
54	DA	701	HEA	CMB-C2B-C1B	2.14	128.38	125.03
54	DA	701	HEA	C1D-ND-C4D	-2.14	102.67	105.21
54	Da	701	HEA	CAA-CBA-CGA	-2.14	108.06	113.83
65	En	1203	UQ8	C7-C8-C9	2.13	130.50	126.83
65	En	1203	UQ8	C17-C18-C19	-2.12	122.78	127.62
54	DA	701	HEA	C4B-NB-C1B	-2.11	102.71	105.21
54	DA	702	HEA	CHC-C4B-C3B	-2.11	120.49	125.80
65	EN	1204	UQ8	C7-C8-C9	2.10	130.45	126.83
54	Da	702	HEA	CHC-C4B-C3B	-2.10	120.51	125.80
54	Da	701	HEA	C26-C15-C16	2.09	118.86	115.23
65	En	1203	UQ8	C8-C7-C6	2.09	117.23	112.08
54	DA	701	HEA	CAD-C3D-C4D	2.09	128.33	124.70
54	Da	701	HEA	CMB-C2B-C1B	2.08	128.28	125.03
54	DA	701	HEA	C26-C15-C16	2.06	118.81	115.23
65	Ds	404	UQ8	C8-C7-C6	2.06	117.15	112.08
66	Ed	201	HEM	CMD-C2D-C1D	2.06	128.25	125.03
54	DA	702	HEA	C13-C14-C15	-2.05	122.94	127.62
54	DA	701	HEA	CAA-CBA-CGA	-2.04	108.33	113.83
65	El	906	UQ8	C7-C6-C5	-2.04	116.15	118.52
66	ED	602	HEM	CMD-C2D-C1D	2.02	128.19	125.03
54	Da	701	HEA	C1D-ND-C4D	-2.00	102.83	105.21

There are no chirality outliers.

All (4627) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	DA	709	CDL	CA2-OA2-PA1-OA3
57	DA	709	CDL	CA2-OA2-PA1-OA4
57	DA	709	CDL	CA2-OA2-PA1-OA5
57	DA	709	CDL	CA3-OA5-PA1-OA4
57	DA	709	CDL	CB2-OB2-PB2-OB3
57	DA	709	CDL	CB3-OB5-PB2-OB2
57	DA	709	CDL	CB3-OB5-PB2-OB4
57	DA	710	CDL	CA3-OA5-PA1-OA2
57	DA	710	CDL	CA3-OA5-PA1-OA3
57	DA	710	CDL	CA3-OA5-PA1-OA4
57	DA	710	CDL	C11-CA5-OA6-CA4
57	DC	601	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
57	DC	601	CDL	CB2-OB2-PB2-OB5
57	DC	601	CDL	CB3-OB5-PB2-OB2
57	DC	601	CDL	CB3-OB5-PB2-OB3
57	DC	601	CDL	CB3-OB5-PB2-OB4
57	DD	702	CDL	O1-C1-CA2-OA2
57	DD	702	CDL	CA3-OA5-PA1-OA2
57	DD	702	CDL	CA3-OA5-PA1-OA3
57	DD	702	CDL	CA3-OA5-PA1-OA4
57	DD	702	CDL	C11-CA5-OA6-CA4
57	DD	702	CDL	OB6-CB4-CB6-OB8
57	DD	703	CDL	CB2-OB2-PB2-OB5
57	DD	704	CDL	CA2-OA2-PA1-OA3
57	DD	704	CDL	CA2-OA2-PA1-OA5
57	DD	704	CDL	C51-CB5-OB6-CB4
57	DG	201	CDL	CB2-C1-CA2-OA2
57	DG	201	CDL	CB2-OB2-PB2-OB3
57	DH	201	CDL	CB2-C1-CA2-OA2
57	DH	201	CDL	CA3-OA5-PA1-OA2
57	DH	201	CDL	CA3-OA5-PA1-OA3
57	DH	201	CDL	OA6-CA4-CA6-OA8
57	DI	701	CDL	C11-CA5-OA6-CA4
57	DI	701	CDL	C51-CB5-OB6-CB4
57	DJ	302	CDL	CB2-C1-CA2-OA2
57	DJ	302	CDL	C1-CA2-OA2-PA1
57	DJ	303	CDL	CA2-OA2-PA1-OA4
57	DJ	303	CDL	CA2-OA2-PA1-OA5
57	DJ	303	CDL	CA3-OA5-PA1-OA2
57	DJ	303	CDL	CA3-OA5-PA1-OA4
57	DJ	303	CDL	C11-CA5-OA6-CA4
57	DJ	303	CDL	CB3-OB5-PB2-OB2
57	DJ	303	CDL	CB3-OB5-PB2-OB4
57	DJ	304	CDL	CA3-OA5-PA1-OA2
57	DJ	305	CDL	O1-C1-CA2-OA2
57	DJ	305	CDL	CB2-C1-CA2-OA2
57	DJ	305	CDL	CA3-OA5-PA1-OA2
57	DJ	305	CDL	CA3-OA5-PA1-OA3
57	DJ	305	CDL	CA3-OA5-PA1-OA4
57	DJ	305	CDL	CB2-OB2-PB2-OB3
57	DJ	307	CDL	O1-C1-CB2-OB2
57	DJ	307	CDL	CB2-OB2-PB2-OB3
57	DJ	307	CDL	OB5-CB3-CB4-OB6
57	DJ	307	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
57	DM	501	CDL	C1-CA2-OA2-PA1
57	DM	501	CDL	CA3-OA5-PA1-OA3
57	DM	501	CDL	CB2-OB2-PB2-OB4
57	DM	501	CDL	CB2-OB2-PB2-OB5
57	DM	501	CDL	C51-CB5-OB6-CB4
57	DM	502	CDL	O1-C1-CB2-OB2
57	DM	502	CDL	C51-CB5-OB6-CB4
57	DN	501	CDL	CA3-OA5-PA1-OA4
57	DN	504	CDL	CB3-OB5-PB2-OB3
57	DN	504	CDL	C51-CB5-OB6-CB4
57	DN	505	CDL	CB2-C1-CA2-OA2
57	DN	505	CDL	C1-CA2-OA2-PA1
57	DN	505	CDL	CA2-OA2-PA1-OA5
57	DN	505	CDL	CA3-OA5-PA1-OA4
57	DN	505	CDL	C11-CA5-OA6-CA4
57	DO	501	CDL	CA3-OA5-PA1-OA2
57	DO	501	CDL	C11-CA5-OA6-CA4
57	DO	501	CDL	CB3-OB5-PB2-OB2
57	DO	501	CDL	C51-CB5-OB6-CB4
57	DQ	1501	CDL	CA3-OA5-PA1-OA2
57	DQ	1501	CDL	CA3-OA5-PA1-OA3
57	DQ	1501	CDL	CA3-OA5-PA1-OA4
57	DQ	1501	CDL	C11-CA5-OA6-CA4
57	DQ	1501	CDL	CB3-OB5-PB2-OB2
57	DQ	1501	CDL	CB3-OB5-PB2-OB3
57	DQ	1502	CDL	CA3-OA5-PA1-OA2
57	DQ	1502	CDL	CA3-OA5-PA1-OA3
57	DQ	1502	CDL	CA3-OA5-PA1-OA4
57	DQ	1502	CDL	CB3-OB5-PB2-OB2
57	DQ	1502	CDL	CB3-OB5-PB2-OB3
57	DQ	1504	CDL	CA2-OA2-PA1-OA3
57	DQ	1504	CDL	CA2-OA2-PA1-OA5
57	DQ	1504	CDL	OA5-CA3-CA4-OA6
57	DQ	1504	CDL	OA7-CA5-OA6-CA4
57	DQ	1504	CDL	C11-CA5-OA6-CA4
57	DQ	1504	CDL	CB3-OB5-PB2-OB2
57	DQ	1504	CDL	CB3-OB5-PB2-OB4
57	DR	402	CDL	CA3-OA5-PA1-OA2
57	DR	402	CDL	CA3-OA5-PA1-OA3
57	DR	402	CDL	CA3-OA5-PA1-OA4
57	DR	402	CDL	CB2-OB2-PB2-OB4
57	DR	402	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
57	DR	402	CDL	CB3-OB5-PB2-OB3
57	DR	402	CDL	CB3-OB5-PB2-OB4
57	DR	403	CDL	O1-C1-CA2-OA2
57	DR	403	CDL	CA2-OA2-PA1-OA3
57	DS	402	CDL	CA2-OA2-PA1-OA3
57	DS	402	CDL	CB3-OB5-PB2-OB2
57	DS	402	CDL	CB3-OB5-PB2-OB4
57	DS	402	CDL	CB4-CB3-OB5-PB2
57	DS	405	CDL	CA2-OA2-PA1-OA3
57	DS	405	CDL	CA2-OA2-PA1-OA5
57	DS	405	CDL	CB3-OB5-PB2-OB2
57	DS	405	CDL	CB3-OB5-PB2-OB3
57	DU	401	CDL	CA2-OA2-PA1-OA3
57	DU	401	CDL	CA2-OA2-PA1-OA5
57	DU	402	CDL	C11-CA5-OA6-CA4
57	DU	402	CDL	CB2-OB2-PB2-OB3
57	DU	403	CDL	CA2-OA2-PA1-OA4
57	DU	403	CDL	CA2-OA2-PA1-OA5
57	DU	403	CDL	CB3-OB5-PB2-OB2
57	DU	403	CDL	CB3-OB5-PB2-OB3
57	DU	404	CDL	CA3-OA5-PA1-OA3
57	DU	404	CDL	CA3-CA4-OA6-CA5
57	DU	404	CDL	CB2-OB2-PB2-OB3
57	DU	404	CDL	CB2-OB2-PB2-OB5
57	DU	404	CDL	OB5-CB3-CB4-OB6
57	DV	401	CDL	CA3-OA5-PA1-OA2
57	DV	401	CDL	CA3-OA5-PA1-OA3
57	DV	401	CDL	CA3-OA5-PA1-OA4
57	DV	401	CDL	OA7-CA5-OA6-CA4
57	DV	402	CDL	CA3-OA5-PA1-OA4
57	DV	402	CDL	C11-CA5-OA6-CA4
57	DV	402	CDL	CB3-OB5-PB2-OB2
57	DV	402	CDL	CB3-OB5-PB2-OB3
57	DV	402	CDL	CB3-OB5-PB2-OB4
57	DV	402	CDL	C51-CB5-OB6-CB4
57	DV	403	CDL	CA3-OA5-PA1-OA2
57	DV	403	CDL	CA3-OA5-PA1-OA3
57	DV	403	CDL	CA3-OA5-PA1-OA4
57	DV	404	CDL	O1-C1-CA2-OA2
57	DV	404	CDL	CA3-OA5-PA1-OA3
57	DV	404	CDL	CB2-OB2-PB2-OB3
57	DV	404	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
57	DV	404	CDL	CB3-OB5-PB2-OB3
57	DV	404	CDL	C51-CB5-OB6-CB4
57	DX	301	CDL	CA3-OA5-PA1-OA2
57	DX	301	CDL	CB2-OB2-PB2-OB5
57	DX	301	CDL	CB3-OB5-PB2-OB4
57	DY	301	CDL	CA3-OA5-PA1-OA2
57	DY	301	CDL	CA3-OA5-PA1-OA3
57	DY	301	CDL	CA3-OA5-PA1-OA4
57	DY	301	CDL	C11-CA5-OA6-CA4
57	DY	301	CDL	OB6-CB4-CB6-OB8
57	DY	301	CDL	C51-CB5-OB6-CB4
57	DZ	501	CDL	CA2-OA2-PA1-OA5
57	EA	301	CDL	CA2-OA2-PA1-OA3
57	EA	301	CDL	CA2-OA2-PA1-OA4
57	EA	301	CDL	CA2-OA2-PA1-OA5
57	EA	301	CDL	CB2-OB2-PB2-OB3
57	EA	301	CDL	CB2-OB2-PB2-OB5
57	EA	301	CDL	CB3-OB5-PB2-OB2
57	EA	301	CDL	CB3-OB5-PB2-OB3
57	EB	302	CDL	C11-CA5-OA6-CA4
57	EB	302	CDL	CB3-OB5-PB2-OB2
57	EB	302	CDL	OB5-CB3-CB4-OB6
57	EB	302	CDL	OB7-CB5-OB6-CB4
57	EB	304	CDL	CA3-OA5-PA1-OA2
57	EB	304	CDL	CA3-OA5-PA1-OA3
57	EB	304	CDL	CA3-OA5-PA1-OA4
57	EB	304	CDL	CB2-OB2-PB2-OB3
57	EB	304	CDL	CB2-OB2-PB2-OB5
57	EB	304	CDL	CB3-OB5-PB2-OB2
57	ED	601	CDL	CA3-OA5-PA1-OA2
57	ED	601	CDL	CA3-OA5-PA1-OA3
57	ED	601	CDL	C11-CA5-OA6-CA4
57	ED	604	CDL	CA3-OA5-PA1-OA2
57	ED	604	CDL	CA3-OA5-PA1-OA3
57	ED	604	CDL	CA3-OA5-PA1-OA4
57	ED	604	CDL	OB5-CB3-CB4-OB6
57	EH	201	CDL	CA3-OA5-PA1-OA3
57	EH	201	CDL	CB3-OB5-PB2-OB2
57	EH	201	CDL	CB3-OB5-PB2-OB3
57	EH	201	CDL	CB3-OB5-PB2-OB4
57	EH	202	CDL	CA3-OA5-PA1-OA2
57	EH	202	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
57	EH	202	CDL	CB2-OB2-PB2-OB5
57	EH	202	CDL	CB3-OB5-PB2-OB2
57	EI	401	CDL	CB3-OB5-PB2-OB2
57	EI	401	CDL	CB3-OB5-PB2-OB3
57	EK	201	CDL	CA2-OA2-PA1-OA5
57	EL	901	CDL	CA3-OA5-PA1-OA3
57	EL	901	CDL	OA6-CA4-CA6-OA8
57	EL	902	CDL	CA2-C1-CB2-OB2
57	EL	902	CDL	CA2-OA2-PA1-OA3
57	EL	902	CDL	C11-CA5-OA6-CA4
57	EL	902	CDL	CB3-OB5-PB2-OB3
57	EL	902	CDL	C51-CB5-OB6-CB4
57	EL	903	CDL	C11-CA5-OA6-CA4
57	EL	903	CDL	CB2-OB2-PB2-OB4
57	EL	903	CDL	CB3-OB5-PB2-OB2
57	EL	903	CDL	CB3-OB5-PB2-OB4
57	EL	904	CDL	CB2-OB2-PB2-OB3
57	EL	904	CDL	CB3-OB5-PB2-OB2
57	EL	904	CDL	CB3-OB5-PB2-OB3
57	EL	904	CDL	CB3-OB5-PB2-OB4
57	EL	904	CDL	C51-CB5-OB6-CB4
57	EN	1201	CDL	O1-C1-CA2-OA2
57	EN	1201	CDL	CA2-OA2-PA1-OA4
57	EN	1201	CDL	CA2-OA2-PA1-OA5
57	EN	1202	CDL	C51-CB5-OB6-CB4
57	EO	202	CDL	C11-CA5-OA6-CA4
57	EO	202	CDL	C51-CB5-OB6-CB4
57	EU	101	CDL	CA3-OA5-PA1-OA2
57	EU	101	CDL	CA3-OA5-PA1-OA3
57	EU	101	CDL	CB2-OB2-PB2-OB3
57	EU	101	CDL	CB3-OB5-PB2-OB2
57	EU	101	CDL	CB3-OB5-PB2-OB4
57	Da	705	CDL	OA6-CA4-CA6-OA8
57	Da	705	CDL	CB3-OB5-PB2-OB2
57	Da	705	CDL	CB3-OB5-PB2-OB4
57	Da	709	CDL	CA3-OA5-PA1-OA2
57	Da	709	CDL	CA3-OA5-PA1-OA4
57	Da	709	CDL	C11-CA5-OA6-CA4
57	Da	709	CDL	CB3-OB5-PB2-OB2
57	Da	709	CDL	CB3-OB5-PB2-OB3
57	Dc	601	CDL	CB2-OB2-PB2-OB5
57	Dc	601	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
57	Dc	601	CDL	CB3-OB5-PB2-OB3
57	Dc	601	CDL	CB3-OB5-PB2-OB4
57	Dd	702	CDL	CB2-C1-CA2-OA2
57	Dd	702	CDL	CA3-OA5-PA1-OA2
57	Dd	702	CDL	CA3-OA5-PA1-OA3
57	Dd	702	CDL	CA3-OA5-PA1-OA4
57	Dd	702	CDL	C11-CA5-OA6-CA4
57	Dd	704	CDL	CB2-C1-CA2-OA2
57	Dd	704	CDL	C1-CB2-OB2-PB2
57	Dd	704	CDL	CB2-OB2-PB2-OB5
57	Dd	705	CDL	CA3-OA5-PA1-OA2
57	Dd	705	CDL	CA3-OA5-PA1-OA3
57	Dd	705	CDL	CA3-OA5-PA1-OA4
57	Dd	706	CDL	CB3-OB5-PB2-OB3
57	Dg	201	CDL	CB2-C1-CA2-OA2
57	Dg	201	CDL	C11-CA5-OA6-CA4
57	Dg	201	CDL	CB3-OB5-PB2-OB2
57	Dg	201	CDL	CB3-OB5-PB2-OB4
57	Dh	201	CDL	CB2-C1-CA2-OA2
57	Dh	201	CDL	CA3-OA5-PA1-OA3
57	Dh	201	CDL	OA6-CA4-CA6-OA8
57	Dh	201	CDL	CB2-OB2-PB2-OB3
57	Dh	202	CDL	CA3-OA5-PA1-OA2
57	Dh	202	CDL	CA3-OA5-PA1-OA3
57	Dh	202	CDL	CA3-OA5-PA1-OA4
57	Dh	202	CDL	CB2-OB2-PB2-OB5
57	Dh	202	CDL	CB3-OB5-PB2-OB2
57	Di	701	CDL	C11-CA5-OA6-CA4
57	Di	701	CDL	OB7-CB5-OB6-CB4
57	Di	701	CDL	C51-CB5-OB6-CB4
57	Dj	401	CDL	CB2-OB2-PB2-OB3
57	Dj	401	CDL	CB3-OB5-PB2-OB2
57	Dj	401	CDL	CB3-OB5-PB2-OB4
57	Dj	401	CDL	C51-CB5-OB6-CB4
57	Dj	402	CDL	O1-C1-CA2-OA2
57	Dj	402	CDL	CA2-OA2-PA1-OA4
57	Dj	402	CDL	CA2-OA2-PA1-OA5
57	Dj	402	CDL	CA3-OA5-PA1-OA2
57	Dj	402	CDL	CA3-OA5-PA1-OA4
57	Dj	402	CDL	C11-CA5-OA6-CA4
57	Dj	403	CDL	CA2-OA2-PA1-OA3
57	Dj	403	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
57	Dj	404	CDL	CA3-OA5-PA1-OA3
57	Dj	404	CDL	CA3-OA5-PA1-OA4
57	Dj	404	CDL	OA7-CA5-OA6-CA4
57	Dj	404	CDL	CB3-OB5-PB2-OB2
57	Dj	404	CDL	CB3-OB5-PB2-OB4
57	Dj	404	CDL	C51-CB5-OB6-CB4
57	Dj	405	CDL	CA3-OA5-PA1-OA2
57	Dj	405	CDL	CA3-OA5-PA1-OA3
57	Dj	405	CDL	CA3-OA5-PA1-OA4
57	Dj	405	CDL	CB2-OB2-PB2-OB3
57	Dj	408	CDL	O1-C1-CB2-OB2
57	Dj	408	CDL	CA2-OA2-PA1-OA4
57	Dj	408	CDL	CA2-OA2-PA1-OA5
57	Dj	408	CDL	OA6-CA4-CA6-OA8
57	Dj	408	CDL	CB2-OB2-PB2-OB5
57	Dj	408	CDL	C51-CB5-OB6-CB4
57	Dm	501	CDL	CA3-OA5-PA1-OA2
57	Dm	501	CDL	CB2-OB2-PB2-OB4
57	Dm	501	CDL	CB2-OB2-PB2-OB5
57	Dm	502	CDL	CA2-OA2-PA1-OA3
57	Dm	502	CDL	CA3-OA5-PA1-OA2
57	Dm	502	CDL	CA3-OA5-PA1-OA3
57	Dm	502	CDL	CA3-OA5-PA1-OA4
57	Dm	502	CDL	C51-CB5-OB6-CB4
57	Dn	501	CDL	CA2-OA2-PA1-OA3
57	Dn	501	CDL	CA2-OA2-PA1-OA4
57	Dn	501	CDL	CA2-OA2-PA1-OA5
57	Dn	501	CDL	CA3-OA5-PA1-OA3
57	Dn	501	CDL	CA3-OA5-PA1-OA4
57	Dn	502	CDL	CA3-OA5-PA1-OA2
57	Dn	502	CDL	CA3-OA5-PA1-OA3
57	Dn	502	CDL	CA3-OA5-PA1-OA4
57	Dn	502	CDL	CA4-CA3-OA5-PA1
57	Dn	502	CDL	CB3-OB5-PB2-OB2
57	Dn	503	CDL	CA3-OA5-PA1-OA2
57	Dn	503	CDL	CA3-OA5-PA1-OA3
57	Dn	503	CDL	OA7-CA5-OA6-CA4
57	Dn	503	CDL	C11-CA5-OA6-CA4
57	Dn	505	CDL	O1-C1-CA2-OA2
57	Dn	505	CDL	OA7-CA5-OA6-CA4
57	Dn	505	CDL	CB3-OB5-PB2-OB2
57	Dn	505	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
57	Dn	505	CDL	CB3-OB5-PB2-OB4
57	Dn	505	CDL	OB7-CB5-OB6-CB4
57	Dn	505	CDL	C51-CB5-OB6-CB4
57	Dn	507	CDL	OB7-CB5-OB6-CB4
57	Dn	507	CDL	C51-CB5-OB6-CB4
57	Do	501	CDL	CA3-OA5-PA1-OA2
57	Do	501	CDL	CA3-OA5-PA1-OA3
57	Do	501	CDL	CA3-OA5-PA1-OA4
57	Do	501	CDL	CB3-OB5-PB2-OB2
57	Do	501	CDL	C51-CB5-OB6-CB4
57	Dq	401	CDL	C1-CB2-OB2-PB2
57	Dq	401	CDL	CB2-OB2-PB2-OB3
57	Dq	401	CDL	CB3-OB5-PB2-OB2
57	Dq	401	CDL	C51-CB5-OB6-CB4
57	Dq	402	CDL	CA2-OA2-PA1-OA5
57	Dq	402	CDL	OA7-CA5-OA6-CA4
57	Dq	402	CDL	C51-CB5-OB6-CB4
57	Dq	403	CDL	CA3-OA5-PA1-OA3
57	Dq	403	CDL	CA3-OA5-PA1-OA4
57	Dq	403	CDL	OA7-CA5-OA6-CA4
57	Dq	403	CDL	C11-CA5-OA6-CA4
57	Dq	403	CDL	CB3-OB5-PB2-OB2
57	Dq	403	CDL	CB3-OB5-PB2-OB3
57	Dq	404	CDL	CA2-OA2-PA1-OA3
57	Dq	404	CDL	CA3-OA5-PA1-OA2
57	Dq	404	CDL	CA3-OA5-PA1-OA4
57	Dq	404	CDL	CB3-OB5-PB2-OB2
57	Dr	402	CDL	CA3-OA5-PA1-OA2
57	Dr	402	CDL	CA3-OA5-PA1-OA3
57	Dr	402	CDL	CA3-OA5-PA1-OA4
57	Dr	402	CDL	CB2-OB2-PB2-OB4
57	Dr	402	CDL	CB2-OB2-PB2-OB5
57	Dr	402	CDL	OB6-CB4-CB6-OB8
57	Dr	403	CDL	O1-C1-CA2-OA2
57	Dr	403	CDL	CA2-OA2-PA1-OA3
57	Dr	403	CDL	CA2-OA2-PA1-OA5
57	Dr	403	CDL	OB6-CB4-CB6-OB8
57	Ds	402	CDL	CA2-OA2-PA1-OA3
57	Ds	402	CDL	CB3-OB5-PB2-OB2
57	Ds	402	CDL	CB3-OB5-PB2-OB4
57	Ds	402	CDL	CB4-CB3-OB5-PB2
57	Ds	405	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
57	Ds	405	CDL	CA2-OA2-PA1-OA5
57	Ds	405	CDL	CB3-OB5-PB2-OB3
57	Du	401	CDL	CA2-OA2-PA1-OA3
57	Du	401	CDL	CA2-OA2-PA1-OA5
57	Du	401	CDL	CA3-OA5-PA1-OA3
57	Du	401	CDL	OB7-CB5-OB6-CB4
57	Du	401	CDL	C51-CB5-OB6-CB4
57	Du	402	CDL	C11-CA5-OA6-CA4
57	Du	402	CDL	CB3-OB5-PB2-OB2
57	Du	402	CDL	CB3-OB5-PB2-OB3
57	Du	402	CDL	CB3-OB5-PB2-OB4
57	Du	403	CDL	CB3-OB5-PB2-OB2
57	Du	403	CDL	CB3-OB5-PB2-OB3
57	Du	403	CDL	CB3-OB5-PB2-OB4
57	Du	404	CDL	CA3-OA5-PA1-OA3
57	Du	404	CDL	CB3-OB5-PB2-OB2
57	Du	404	CDL	CB3-OB5-PB2-OB3
57	Dv	401	CDL	CA3-OA5-PA1-OA2
57	Dv	401	CDL	CA3-OA5-PA1-OA3
57	Dv	401	CDL	CA3-OA5-PA1-OA4
57	Dv	401	CDL	OA7-CA5-OA6-CA4
57	Dv	401	CDL	CB2-OB2-PB2-OB3
57	Dv	402	CDL	CA3-OA5-PA1-OA2
57	Dv	402	CDL	CA3-OA5-PA1-OA3
57	Dv	402	CDL	CA3-OA5-PA1-OA4
57	Dv	402	CDL	OA7-CA5-OA6-CA4
57	Dv	402	CDL	C11-CA5-OA6-CA4
57	Dv	402	CDL	CB3-OB5-PB2-OB2
57	Dv	402	CDL	CB3-OB5-PB2-OB3
57	Dv	402	CDL	CB3-OB5-PB2-OB4
57	Dv	402	CDL	C51-CB5-OB6-CB4
57	Dv	403	CDL	CA3-OA5-PA1-OA2
57	Dv	404	CDL	CA2-OA2-PA1-OA3
57	Dv	404	CDL	CA2-OA2-PA1-OA5
57	Dv	404	CDL	CA3-OA5-PA1-OA2
57	Dv	404	CDL	CA3-OA5-PA1-OA3
57	Dv	404	CDL	CA3-OA5-PA1-OA4
57	Dv	404	CDL	CB2-OB2-PB2-OB3
57	Dv	404	CDL	CB3-OB5-PB2-OB3
57	Dv	404	CDL	C51-CB5-OB6-CB4
57	Dx	1201	CDL	CA2-OA2-PA1-OA4
57	Dx	1201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
57	Dx	1201	CDL	CB2-OB2-PB2-OB4
57	Dx	1201	CDL	CB2-OB2-PB2-OB5
57	Dx	1201	CDL	CB3-OB5-PB2-OB4
57	Dx	1203	CDL	CA2-OA2-PA1-OA3
57	Dx	1203	CDL	CA2-OA2-PA1-OA5
57	Dx	1203	CDL	CA3-OA5-PA1-OA4
57	Dx	1203	CDL	CB3-OB5-PB2-OB2
57	Dx	1203	CDL	OB5-CB3-CB4-OB6
57	Dy	301	CDL	CA3-OA5-PA1-OA2
57	Dy	301	CDL	CA3-OA5-PA1-OA3
57	Dy	301	CDL	CA3-OA5-PA1-OA4
57	Dy	301	CDL	C11-CA5-OA6-CA4
57	Dy	301	CDL	C51-CB5-OB6-CB4
57	Ea	301	CDL	CA2-OA2-PA1-OA4
57	Ea	301	CDL	CA2-OA2-PA1-OA5
57	Ea	301	CDL	C11-CA5-OA6-CA4
57	Ea	301	CDL	CB2-OB2-PB2-OB3
57	Ea	301	CDL	CB2-OB2-PB2-OB5
57	Ed	204	CDL	CA3-OA5-PA1-OA3
57	Ed	204	CDL	CA3-OA5-PA1-OA4
57	Ed	204	CDL	CB2-OB2-PB2-OB3
57	Ed	204	CDL	CB2-OB2-PB2-OB4
57	Ed	204	CDL	CB2-OB2-PB2-OB5
57	Ed	204	CDL	CB3-OB5-PB2-OB2
57	Ed	205	CDL	CA3-OA5-PA1-OA2
57	Ed	205	CDL	CA3-OA5-PA1-OA3
57	Ed	205	CDL	CB3-OB5-PB2-OB2
57	Ed	205	CDL	CB3-OB5-PB2-OB3
57	Eg	101	CDL	CA2-OA2-PA1-OA3
57	Eg	101	CDL	CA2-OA2-PA1-OA5
57	Eg	101	CDL	CA3-OA5-PA1-OA2
57	Eg	101	CDL	C11-CA5-OA6-CA4
57	Eg	101	CDL	CB3-OB5-PB2-OB3
57	Eh	1601	CDL	C11-CA5-OA6-CA4
57	Eh	1601	CDL	CB3-OB5-PB2-OB3
57	Ei	401	CDL	C11-CA5-OA6-CA4
57	Ei	401	CDL	CB3-OB5-PB2-OB2
57	Ei	401	CDL	CB3-OB5-PB2-OB4
57	Ek	201	CDL	CA2-OA2-PA1-OA4
57	Ek	201	CDL	CA2-OA2-PA1-OA5
57	Ek	201	CDL	CA3-OA5-PA1-OA2
57	Ek	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
57	Ek	201	CDL	CA3-OA5-PA1-OA4
57	El	901	CDL	CB2-C1-CA2-OA2
57	El	901	CDL	CA3-OA5-PA1-OA2
57	El	901	CDL	CA3-OA5-PA1-OA3
57	El	901	CDL	CA3-OA5-PA1-OA4
57	El	901	CDL	OB6-CB4-CB6-OB8
57	El	901	CDL	C51-CB5-OB6-CB4
57	El	902	CDL	CA2-C1-CB2-OB2
57	El	902	CDL	C1-CB2-OB2-PB2
57	El	902	CDL	CB2-OB2-PB2-OB4
57	El	902	CDL	CB3-OB5-PB2-OB2
57	El	902	CDL	CB3-OB5-PB2-OB3
57	El	902	CDL	CB3-OB5-PB2-OB4
57	El	902	CDL	OB7-CB5-OB6-CB4
57	El	902	CDL	C51-CB5-OB6-CB4
57	El	903	CDL	CA3-OA5-PA1-OA2
57	El	903	CDL	CA3-OA5-PA1-OA4
57	El	903	CDL	CB2-OB2-PB2-OB3
57	El	903	CDL	CB2-OB2-PB2-OB5
57	El	903	CDL	CB3-OB5-PB2-OB2
57	El	903	CDL	CB3-OB5-PB2-OB3
57	El	903	CDL	CB3-OB5-PB2-OB4
57	El	903	CDL	C51-CB5-OB6-CB4
57	En	1202	CDL	CA3-OA5-PA1-OA2
57	En	1202	CDL	CA3-OA5-PA1-OA3
57	En	1202	CDL	CA3-OA5-PA1-OA4
57	En	1202	CDL	C51-CB5-OB6-CB4
57	Ep	701	CDL	CB2-C1-CA2-OA2
57	Ep	701	CDL	CA3-OA5-PA1-OA2
57	Ep	701	CDL	CA3-OA5-PA1-OA3
57	Ep	701	CDL	CA3-OA5-PA1-OA4
57	Eu	101	CDL	O1-C1-CA2-OA2
57	Eu	101	CDL	CB2-OB2-PB2-OB3
58	DA	706	PC1	C11-O13-P-O14
58	DA	706	PC1	C11-O13-P-O11
58	DA	706	PC1	O21-C2-C3-O31
58	DA	707	PC1	C1-O11-P-O12
58	DA	707	PC1	C1-O11-P-O14
58	DA	707	PC1	C1-O11-P-O13
58	DB	702	PC1	C11-O13-P-O12
58	DB	702	PC1	C11-O13-P-O14
58	DB	702	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
58	DB	702	PC1	O22-C21-O21-C2
58	DC	602	PC1	C1-O11-P-O12
58	DC	602	PC1	C1-O11-P-O14
58	DC	602	PC1	C1-O11-P-O13
58	DC	603	PC1	C11-O13-P-O11
58	DC	603	PC1	O13-C11-C12-N
58	DC	604	PC1	C11-O13-P-O12
58	DC	604	PC1	C11-O13-P-O14
58	DC	604	PC1	C11-O13-P-O11
58	DC	604	PC1	C1-O11-P-O12
58	DC	604	PC1	C1-O11-P-O14
58	DC	605	PC1	C1-O11-P-O13
58	DC	605	PC1	C22-C21-O21-C2
58	DC	608	PC1	C11-O13-P-O12
58	DC	608	PC1	C11-O13-P-O11
58	DC	608	PC1	O22-C21-O21-C2
58	DC	608	PC1	C22-C21-O21-C2
58	DI	702	PC1	C1-O11-P-O12
58	DI	702	PC1	C1-O11-P-O14
58	DI	702	PC1	C1-O11-P-O13
58	DJ	306	PC1	C11-O13-P-O12
58	DJ	306	PC1	C11-O13-P-O11
58	DJ	306	PC1	C1-O11-P-O13
58	DQ	1503	PC1	C11-O13-P-O11
58	DS	406	PC1	C11-O13-P-O14
58	DS	406	PC1	C11-O13-P-O11
58	DS	406	PC1	C1-O11-P-O12
58	DS	406	PC1	C1-O11-P-O14
58	DS	406	PC1	C1-O11-P-O13
58	DS	406	PC1	C12-C11-O13-P
58	DS	407	PC1	C11-O13-P-O14
58	DS	407	PC1	C11-O13-P-O11
58	DV	405	PC1	C11-O13-P-O12
58	DV	405	PC1	C11-O13-P-O11
58	DV	406	PC1	C11-O13-P-O11
58	DV	407	PC1	C11-O13-P-O12
58	DV	407	PC1	C11-O13-P-O14
58	DV	407	PC1	C1-O11-P-O12
58	DV	407	PC1	C1-O11-P-O14
58	DV	407	PC1	C1-O11-P-O13
58	DX	302	PC1	C11-O13-P-O14
58	DX	302	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
58	DX	306	PC1	C11-O13-P-O12
58	DX	306	PC1	C22-C21-O21-C2
58	DY	302	PC1	O13-C11-C12-N
58	DY	302	PC1	O22-C21-O21-C2
58	EB	301	PC1	C11-O13-P-O12
58	EB	301	PC1	C11-O13-P-O11
58	EB	303	PC1	O13-C11-C12-N
58	EO	201	PC1	C11-O13-P-O11
58	EO	201	PC1	C12-C11-O13-P
58	EO	201	PC1	O13-C11-C12-N
58	EO	205	PC1	C11-O13-P-O12
58	EO	205	PC1	C11-O13-P-O11
58	EO	205	PC1	C1-O11-P-O12
58	EO	205	PC1	C1-O11-P-O13
58	EO	206	PC1	C11-O13-P-O12
58	EO	206	PC1	C11-O13-P-O14
58	EO	206	PC1	C11-O13-P-O11
58	EO	206	PC1	C1-O11-P-O12
58	EO	206	PC1	C22-C21-O21-C2
58	EO	207	PC1	C11-O13-P-O12
58	EO	207	PC1	C11-O13-P-O14
58	EO	207	PC1	C11-O13-P-O11
58	EO	207	PC1	C22-C21-O21-C2
58	Da	706	PC1	C11-O13-P-O14
58	Da	706	PC1	O21-C2-C3-O31
58	Da	707	PC1	C1-O11-P-O12
58	Da	707	PC1	C1-O11-P-O14
58	Da	707	PC1	C1-O11-P-O13
58	Da	707	PC1	O13-C11-C12-N
58	Db	702	PC1	C11-O13-P-O11
58	Db	702	PC1	C22-C21-O21-C2
58	Dc	602	PC1	C1-O11-P-O12
58	Dc	602	PC1	C1-O11-P-O14
58	Dc	602	PC1	C1-O11-P-O13
58	Dc	603	PC1	C11-O13-P-O11
58	Dc	604	PC1	C11-O13-P-O11
58	Dc	604	PC1	C1-O11-P-O12
58	Dc	605	PC1	C11-O13-P-O14
58	Dc	605	PC1	C1-O11-P-O14
58	Dc	605	PC1	C1-O11-P-O13
58	Dc	605	PC1	C22-C21-O21-C2
58	Dc	607	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
58	Dc	607	PC1	C11-O13-P-O11
58	Dc	607	PC1	O22-C21-O21-C2
58	Dg	203	PC1	C22-C21-O21-C2
58	Di	702	PC1	C11-O13-P-O12
58	Di	702	PC1	C1-O11-P-O14
58	Di	702	PC1	C1-O11-P-O13
58	Dj	406	PC1	C11-O13-P-O12
58	Dj	406	PC1	C11-O13-P-O11
58	Dj	406	PC1	C1-O11-P-O13
58	Dq	405	PC1	C11-O13-P-O11
58	Ds	406	PC1	O21-C2-C3-O31
58	Dv	406	PC1	C11-O13-P-O14
58	Dv	406	PC1	C11-O13-P-O11
58	Dv	406	PC1	C1-O11-P-O12
58	Dv	406	PC1	C1-O11-P-O14
58	Dv	406	PC1	C1-O11-P-O13
58	Dv	407	PC1	C11-O13-P-O11
58	Dv	407	PC1	C1-O11-P-O14
58	Dv	408	PC1	C11-O13-P-O12
58	Dv	408	PC1	C11-O13-P-O14
58	Dv	408	PC1	C1-O11-P-O12
58	Dv	408	PC1	C1-O11-P-O13
58	Dx	1202	PC1	C11-O13-P-O11
58	Dx	1202	PC1	C1-O11-P-O12
58	Dx	1202	PC1	C1-O11-P-O14
58	Dx	1202	PC1	C1-O11-P-O13
58	Dx	1202	PC1	O13-C11-C12-N
58	Dx	1202	PC1	O11-C1-C2-O21
58	Dx	1204	PC1	C11-O13-P-O14
58	Dy	302	PC1	O13-C11-C12-N
58	Dy	302	PC1	O22-C21-O21-C2
58	Eb	301	PC1	C1-O11-P-O14
58	Eb	302	PC1	O13-C11-C12-N
58	Ef	1001	PC1	C1-O11-P-O13
58	Ef	1001	PC1	O13-C11-C12-N
58	El	904	PC1	C11-O13-P-O12
58	El	904	PC1	C11-O13-P-O11
58	El	904	PC1	C1-O11-P-O12
58	El	904	PC1	C1-O11-P-O13
58	Eo	201	PC1	C11-O13-P-O11
58	Eo	201	PC1	C12-C11-O13-P
58	Eo	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
58	Eo	204	PC1	C11-O13-P-O12
58	Eo	204	PC1	C11-O13-P-O14
58	Eo	204	PC1	C11-O13-P-O11
58	Eo	204	PC1	C22-C21-O21-C2
58	Eo	205	PC1	C11-O13-P-O12
58	Eo	205	PC1	C11-O13-P-O14
58	Eo	205	PC1	C11-O13-P-O11
58	Eo	205	PC1	C22-C21-O21-C2
59	DC	606	3PE	C1-O11-P-O12
59	DC	606	3PE	C1-O11-P-O13
59	DC	606	3PE	C1-O11-P-O14
59	DC	607	3PE	C1-O11-P-O14
59	DC	607	3PE	C11-O13-P-O11
59	DC	607	3PE	C11-O13-P-O14
59	DC	607	3PE	O13-C11-C12-N
59	DG	204	3PE	C11-O13-P-O11
59	DG	204	3PE	C11-O13-P-O12
59	DG	204	3PE	C11-O13-P-O14
59	DG	205	3PE	C1-O11-P-O12
59	DG	205	3PE	C1-O11-P-O13
59	DG	205	3PE	C2-C1-O11-P
59	DJ	301	3PE	C1-O11-P-O12
59	DJ	301	3PE	C1-O11-P-O13
59	DJ	301	3PE	C11-O13-P-O11
59	DJ	301	3PE	C11-O13-P-O12
59	DR	401	3PE	C11-O13-P-O14
59	DR	401	3PE	O21-C2-C3-O31
59	DS	401	3PE	C1-O11-P-O13
59	DS	401	3PE	C1-O11-P-O14
59	DS	401	3PE	C12-C11-O13-P
59	DS	401	3PE	O21-C2-C3-O31
59	DS	403	3PE	C1-O11-P-O13
59	DS	403	3PE	C1-O11-P-O14
59	DS	403	3PE	C11-O13-P-O11
59	DS	403	3PE	C11-O13-P-O12
59	DX	303	3PE	C11-O13-P-O11
59	DX	303	3PE	C11-O13-P-O12
59	DX	303	3PE	C11-O13-P-O14
59	DX	303	3PE	O13-C11-C12-N
59	DX	304	3PE	C1-O11-P-O12
59	DX	304	3PE	C1-O11-P-O13
59	DX	304	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
59	DX	304	3PE	C11-O13-P-O11
59	DX	304	3PE	C11-O13-P-O14
59	DX	305	3PE	C1-O11-P-O12
59	DX	305	3PE	C1-O11-P-O13
59	DX	305	3PE	C1-O11-P-O14
59	DX	305	3PE	C11-O13-P-O11
59	DX	305	3PE	C11-O13-P-O12
59	DX	305	3PE	C11-O13-P-O14
59	EL	905	3PE	C1-O11-P-O12
59	EL	905	3PE	C1-O11-P-O13
59	EL	905	3PE	C1-O11-P-O14
59	EL	905	3PE	C11-O13-P-O11
59	EL	905	3PE	C11-O13-P-O14
59	EM	901	3PE	C1-O11-P-O12
59	EM	901	3PE	C1-O11-P-O13
59	EM	901	3PE	C1-O11-P-O14
59	EN	1203	3PE	C11-O13-P-O12
59	EO	203	3PE	C1-O11-P-O12
59	EO	203	3PE	C1-O11-P-O13
59	EO	203	3PE	C1-O11-P-O14
59	EO	203	3PE	C11-O13-P-O11
59	EO	203	3PE	C11-O13-P-O14
59	EO	203	3PE	O21-C2-C3-O31
59	EO	203	3PE	C22-C21-O21-C2
59	EO	204	3PE	C1-O11-P-O12
59	EO	204	3PE	C1-O11-P-O13
59	Da	708	3PE	C1-O11-P-O12
59	Da	708	3PE	C1-O11-P-O13
59	Da	708	3PE	C1-O11-P-O14
59	Da	708	3PE	C11-O13-P-O14
59	Dc	606	3PE	C1-O11-P-O14
59	Dc	606	3PE	C11-O13-P-O11
59	Dc	606	3PE	C11-O13-P-O12
59	Dc	606	3PE	C11-O13-P-O14
59	Dd	703	3PE	C1-O11-P-O12
59	Dd	703	3PE	C1-O11-P-O13
59	Dr	401	3PE	C1-O11-P-O12
59	Dr	401	3PE	C1-O11-P-O13
59	Dr	401	3PE	C11-O13-P-O14
59	Dr	404	3PE	C1-O11-P-O12
59	Dr	404	3PE	C1-O11-P-O13
59	Ds	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
59	Ds	401	3PE	C1-O11-P-O14
59	Ds	401	3PE	C12-C11-O13-P
59	Ds	401	3PE	O21-C2-C3-O31
59	Ds	403	3PE	C1-O11-P-O13
59	Ds	403	3PE	C1-O11-P-O14
59	Ds	403	3PE	C11-O13-P-O12
59	Ds	407	3PE	C11-O13-P-O14
59	Dx	1205	3PE	C1-O11-P-O12
59	Dx	1205	3PE	C1-O11-P-O13
59	Dx	1205	3PE	C1-O11-P-O14
59	Dx	1205	3PE	C11-O13-P-O11
59	Dx	1205	3PE	C11-O13-P-O12
59	Dx	1205	3PE	C11-O13-P-O14
59	Dx	1205	3PE	O13-C11-C12-N
59	Dx	1206	3PE	C1-O11-P-O13
59	Dx	1206	3PE	C1-O11-P-O14
59	Dx	1206	3PE	C11-O13-P-O11
59	Dx	1206	3PE	C11-O13-P-O12
59	Dx	1206	3PE	C11-O13-P-O14
59	Dx	1207	3PE	C1-O11-P-O12
59	Dx	1207	3PE	C1-O11-P-O13
59	Dx	1207	3PE	C1-O11-P-O14
59	Dx	1207	3PE	C11-O13-P-O12
59	El	905	3PE	C1-O11-P-O12
59	El	905	3PE	C1-O11-P-O13
59	El	905	3PE	C11-O13-P-O11
59	El	905	3PE	C11-O13-P-O14
59	Em	901	3PE	C1-O11-P-O12
59	Em	901	3PE	C1-O11-P-O13
59	Em	901	3PE	C1-O11-P-O14
59	Eo	202	3PE	C22-C21-O21-C2
59	Eo	203	3PE	C1-O11-P-O12
59	Eo	203	3PE	C1-O11-P-O13
59	Eo	203	3PE	C1-O11-P-O14
60	DA	711	LPP	C6-O5-P1-O2
60	DA	711	LPP	C6-O5-P1-O3
60	DA	711	LPP	C6-O5-P1-O4
60	DN	502	LPP	C6-O5-P1-O2
60	DN	502	LPP	C6-O5-P1-O3
60	DN	502	LPP	C6-O5-P1-O4
60	Dn	504	LPP	C6-O5-P1-O2
60	Dn	504	LPP	C6-O5-P1-O3

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Mol	Chain	Res	Type	Atoms
60	Dn	504	LPP	C6-O5-P1-O4
60	Dl	1101	LPP	C6-O5-P1-O2
60	Dl	1101	LPP	C6-O5-P1-O4
65	Ds	404	UQ8	C35-C34-C36-C37
65	Ds	404	UQ8	C33-C34-C36-C37
65	El	906	UQ8	C1-C6-C7-C8
65	El	906	UQ8	C5-C6-C7-C8
68	ER	201	ATP	C5'-O5'-PA-O1A
68	ER	201	ATP	C5'-O5'-PA-O2A
68	ER	201	ATP	C5'-O5'-PA-O3A
57	DD	703	CDL	OA9-CA7-OA8-CA6
57	DG	201	CDL	OB9-CB7-OB8-CB6
57	DN	504	CDL	OA9-CA7-OA8-CA6
57	DV	403	CDL	OA9-CA7-OA8-CA6
57	EB	304	CDL	OB9-CB7-OB8-CB6
57	EH	202	CDL	OA9-CA7-OA8-CA6
57	EH	202	CDL	OB9-CB7-OB8-CB6
57	Dh	202	CDL	OB9-CB7-OB8-CB6
57	Dj	402	CDL	OA9-CA7-OA8-CA6
57	Dv	404	CDL	OA9-CA7-OA8-CA6
57	Ed	204	CDL	OA9-CA7-OA8-CA6
57	Ei	401	CDL	OA9-CA7-OA8-CA6
57	Ep	701	CDL	OB9-CB7-OB8-CB6
58	Dj	406	PC1	O32-C31-O31-C3
57	DD	703	CDL	C31-CA7-OA8-CA6
57	DS	405	CDL	C71-CB7-OB8-CB6
57	EI	401	CDL	C31-CA7-OA8-CA6
57	Dd	704	CDL	C31-CA7-OA8-CA6
57	Dj	402	CDL	C31-CA7-OA8-CA6
57	Ei	401	CDL	C31-CA7-OA8-CA6
58	EB	301	PC1	C32-C31-O31-C3
57	DA	709	CDL	OB9-CB7-OB8-CB6
57	DD	703	CDL	OB9-CB7-OB8-CB6
57	DJ	304	CDL	OA9-CA7-OA8-CA6
57	DJ	305	CDL	OB9-CB7-OB8-CB6
57	DQ	1504	CDL	OB9-CB7-OB8-CB6
57	DS	402	CDL	OB9-CB7-OB8-CB6
57	DS	405	CDL	OB9-CB7-OB8-CB6
57	DU	402	CDL	OB9-CB7-OB8-CB6
57	DV	402	CDL	OA9-CA7-OA8-CA6
57	DV	404	CDL	OA9-CA7-OA8-CA6
57	DX	301	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	EA	301	CDL	OA9-CA7-OA8-CA6
57	EI	401	CDL	OA9-CA7-OA8-CA6
57	EK	201	CDL	OB9-CB7-OB8-CB6
57	EL	901	CDL	OB9-CB7-OB8-CB6
57	EL	902	CDL	OB9-CB7-OB8-CB6
57	EO	202	CDL	OB9-CB7-OB8-CB6
57	EU	101	CDL	OA9-CA7-OA8-CA6
57	Dd	704	CDL	OA9-CA7-OA8-CA6
57	Dd	704	CDL	OB9-CB7-OB8-CB6
57	Dg	201	CDL	OA9-CA7-OA8-CA6
57	Dg	201	CDL	OB9-CB7-OB8-CB6
57	Dj	401	CDL	OB9-CB7-OB8-CB6
57	Dj	403	CDL	OA9-CA7-OA8-CA6
57	Dj	404	CDL	OB9-CB7-OB8-CB6
57	Dj	405	CDL	OB9-CB7-OB8-CB6
57	Dn	501	CDL	OB9-CB7-OB8-CB6
57	Dn	507	CDL	OA9-CA7-OA8-CA6
57	Dq	401	CDL	OB9-CB7-OB8-CB6
57	Dq	402	CDL	OA9-CA7-OA8-CA6
57	Ds	405	CDL	OB9-CB7-OB8-CB6
57	Du	403	CDL	OB9-CB7-OB8-CB6
57	Dv	402	CDL	OA9-CA7-OA8-CA6
57	Dv	403	CDL	OA9-CA7-OA8-CA6
57	Ea	301	CDL	OA9-CA7-OA8-CA6
57	El	902	CDL	OB9-CB7-OB8-CB6
57	Eu	101	CDL	OA9-CA7-OA8-CA6
58	DJ	306	PC1	O32-C31-O31-C3
58	DX	302	PC1	O32-C31-O31-C3
58	EB	301	PC1	O32-C31-O31-C3
58	Eb	301	PC1	O32-C31-O31-C3
59	Da	708	3PE	O32-C31-O31-C3
59	Dr	401	3PE	O32-C31-O31-C3
57	DD	704	CDL	OB7-CB5-OB6-CB4
57	DG	201	CDL	OB7-CB5-OB6-CB4
57	DI	701	CDL	OA7-CA5-OA6-CA4
57	DI	701	CDL	OB7-CB5-OB6-CB4
57	DJ	303	CDL	OA7-CA5-OA6-CA4
57	DJ	307	CDL	OB7-CB5-OB6-CB4
57	DM	501	CDL	OB7-CB5-OB6-CB4
57	DM	502	CDL	OB7-CB5-OB6-CB4
57	DN	504	CDL	OB7-CB5-OB6-CB4
57	DN	505	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
57	DO	501	CDL	OA7-CA5-OA6-CA4
57	DO	501	CDL	OB7-CB5-OB6-CB4
57	DQ	1501	CDL	OA7-CA5-OA6-CA4
57	DU	401	CDL	OB7-CB5-OB6-CB4
57	DV	402	CDL	OA7-CA5-OA6-CA4
57	DV	402	CDL	OB7-CB5-OB6-CB4
57	DV	404	CDL	OB7-CB5-OB6-CB4
57	DY	301	CDL	OA7-CA5-OA6-CA4
57	DY	301	CDL	OB7-CB5-OB6-CB4
57	EB	302	CDL	OA7-CA5-OA6-CA4
57	ED	601	CDL	OA7-CA5-OA6-CA4
57	EL	902	CDL	OA7-CA5-OA6-CA4
57	EL	902	CDL	OB7-CB5-OB6-CB4
57	EL	904	CDL	OB7-CB5-OB6-CB4
57	EN	1202	CDL	OB7-CB5-OB6-CB4
57	EO	202	CDL	OB7-CB5-OB6-CB4
57	EU	101	CDL	OA7-CA5-OA6-CA4
57	Da	709	CDL	OA7-CA5-OA6-CA4
57	Dd	702	CDL	OA7-CA5-OA6-CA4
57	Dg	201	CDL	OA7-CA5-OA6-CA4
57	Dj	401	CDL	OB7-CB5-OB6-CB4
57	Dj	402	CDL	OA7-CA5-OA6-CA4
57	Dj	404	CDL	OB7-CB5-OB6-CB4
57	Dj	408	CDL	OB7-CB5-OB6-CB4
57	Dm	501	CDL	OB7-CB5-OB6-CB4
57	Dm	502	CDL	OB7-CB5-OB6-CB4
57	Do	501	CDL	OB7-CB5-OB6-CB4
57	Dq	401	CDL	OB7-CB5-OB6-CB4
57	Dq	402	CDL	OB7-CB5-OB6-CB4
57	Dq	403	CDL	OB7-CB5-OB6-CB4
57	Du	402	CDL	OA7-CA5-OA6-CA4
57	Dv	402	CDL	OB7-CB5-OB6-CB4
57	Dv	404	CDL	OB7-CB5-OB6-CB4
57	Dx	1203	CDL	OB7-CB5-OB6-CB4
57	Ea	301	CDL	OA7-CA5-OA6-CA4
57	Ed	204	CDL	OA7-CA5-OA6-CA4
57	Eg	101	CDL	OA7-CA5-OA6-CA4
57	Eh	1601	CDL	OA7-CA5-OA6-CA4
57	Ei	401	CDL	OA7-CA5-OA6-CA4
57	El	901	CDL	OB7-CB5-OB6-CB4
57	El	902	CDL	OA7-CA5-OA6-CA4
57	El	903	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
57	En	1202	CDL	OB7-CB5-OB6-CB4
58	DC	605	PC1	O22-C21-O21-C2
58	DG	203	PC1	O22-C21-O21-C2
58	DX	306	PC1	O22-C21-O21-C2
58	EO	206	PC1	O22-C21-O21-C2
58	EO	207	PC1	O22-C21-O21-C2
58	Db	702	PC1	O22-C21-O21-C2
58	Dc	605	PC1	O22-C21-O21-C2
58	Dg	203	PC1	O22-C21-O21-C2
58	Eo	204	PC1	O22-C21-O21-C2
58	Eo	205	PC1	O22-C21-O21-C2
59	DG	204	3PE	O22-C21-O21-C2
59	EO	203	3PE	O22-C21-O21-C2
59	Eo	202	3PE	O22-C21-O21-C2
57	DD	703	CDL	C71-CB7-OB8-CB6
57	DG	201	CDL	C71-CB7-OB8-CB6
57	DJ	304	CDL	C31-CA7-OA8-CA6
57	DN	504	CDL	C31-CA7-OA8-CA6
57	DV	403	CDL	C31-CA7-OA8-CA6
57	DX	301	CDL	C31-CA7-OA8-CA6
57	EA	301	CDL	C31-CA7-OA8-CA6
57	EB	304	CDL	C71-CB7-OB8-CB6
57	EH	202	CDL	C31-CA7-OA8-CA6
57	EH	202	CDL	C71-CB7-OB8-CB6
57	EL	904	CDL	C71-CB7-OB8-CB6
57	EN	1201	CDL	C71-CB7-OB8-CB6
57	EN	1202	CDL	C31-CA7-OA8-CA6
57	Dd	704	CDL	C71-CB7-OB8-CB6
57	Dg	201	CDL	C71-CB7-OB8-CB6
57	Dh	202	CDL	C71-CB7-OB8-CB6
57	Dj	403	CDL	C31-CA7-OA8-CA6
57	Ds	405	CDL	C71-CB7-OB8-CB6
57	Du	401	CDL	C31-CA7-OA8-CA6
57	Dv	401	CDL	C31-CA7-OA8-CA6
57	Dv	404	CDL	C31-CA7-OA8-CA6
57	Ea	301	CDL	C31-CA7-OA8-CA6
57	Ed	204	CDL	C31-CA7-OA8-CA6
57	Ep	701	CDL	C71-CB7-OB8-CB6
58	DJ	306	PC1	C32-C31-O31-C3
58	Dc	604	PC1	C32-C31-O31-C3
58	Dj	406	PC1	C32-C31-O31-C3
59	EN	1203	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
59	Da	708	3PE	C32-C31-O31-C3
57	DG	201	CDL	C51-CB5-OB6-CB4
57	DU	401	CDL	C51-CB5-OB6-CB4
57	DV	401	CDL	C11-CA5-OA6-CA4
57	EB	302	CDL	C51-CB5-OB6-CB4
57	EU	101	CDL	C11-CA5-OA6-CA4
57	Dj	404	CDL	C11-CA5-OA6-CA4
57	Dm	501	CDL	C51-CB5-OB6-CB4
57	Dn	505	CDL	C11-CA5-OA6-CA4
57	Dq	402	CDL	C11-CA5-OA6-CA4
57	Dq	403	CDL	C51-CB5-OB6-CB4
57	Dv	401	CDL	C11-CA5-OA6-CA4
57	Dx	1203	CDL	C51-CB5-OB6-CB4
57	Ed	204	CDL	C11-CA5-OA6-CA4
57	El	902	CDL	C11-CA5-OA6-CA4
58	DB	702	PC1	C22-C21-O21-C2
58	DG	203	PC1	C22-C21-O21-C2
58	DY	302	PC1	C22-C21-O21-C2
58	Dc	607	PC1	C22-C21-O21-C2
58	Dy	302	PC1	C22-C21-O21-C2
59	DG	204	3PE	C22-C21-O21-C2
65	DS	404	UQ8	C35-C34-C36-C37
65	EL	906	UQ8	C30-C29-C31-C32
65	El	906	UQ8	C30-C29-C31-C32
65	En	1203	UQ8	C25-C24-C26-C27
65	DS	404	UQ8	C33-C34-C36-C37
65	EL	906	UQ8	C28-C29-C31-C32
65	El	906	UQ8	C28-C29-C31-C32
65	En	1203	UQ8	C23-C24-C26-C27
57	DA	705	CDL	C71-CB7-OB8-CB6
57	DA	709	CDL	C71-CB7-OB8-CB6
57	DJ	305	CDL	C71-CB7-OB8-CB6
57	DQ	1504	CDL	C71-CB7-OB8-CB6
57	DS	402	CDL	C71-CB7-OB8-CB6
57	DU	402	CDL	C71-CB7-OB8-CB6
57	DV	401	CDL	C31-CA7-OA8-CA6
57	DV	402	CDL	C31-CA7-OA8-CA6
57	DV	404	CDL	C31-CA7-OA8-CA6
57	EA	301	CDL	C71-CB7-OB8-CB6
57	EK	201	CDL	C71-CB7-OB8-CB6
57	EL	901	CDL	C71-CB7-OB8-CB6
57	EL	902	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
57	EL	903	CDL	C71-CB7-OB8-CB6
57	EO	202	CDL	C71-CB7-OB8-CB6
57	EU	101	CDL	C31-CA7-OA8-CA6
57	Da	709	CDL	C71-CB7-OB8-CB6
57	Dc	601	CDL	C71-CB7-OB8-CB6
57	Dg	201	CDL	C31-CA7-OA8-CA6
57	Dh	201	CDL	C71-CB7-OB8-CB6
57	Dh	202	CDL	C31-CA7-OA8-CA6
57	Dj	401	CDL	C71-CB7-OB8-CB6
57	Dj	404	CDL	C71-CB7-OB8-CB6
57	Dj	405	CDL	C71-CB7-OB8-CB6
57	Dn	501	CDL	C71-CB7-OB8-CB6
57	Dn	507	CDL	C31-CA7-OA8-CA6
57	Dq	401	CDL	C71-CB7-OB8-CB6
57	Dq	402	CDL	C31-CA7-OA8-CA6
57	Dq	402	CDL	C71-CB7-OB8-CB6
57	Du	402	CDL	C71-CB7-OB8-CB6
57	Du	403	CDL	C71-CB7-OB8-CB6
57	Dv	402	CDL	C31-CA7-OA8-CA6
57	Dv	403	CDL	C31-CA7-OA8-CA6
57	Eh	1601	CDL	C71-CB7-OB8-CB6
57	Ek	201	CDL	C71-CB7-OB8-CB6
57	El	902	CDL	C71-CB7-OB8-CB6
57	En	1202	CDL	C31-CA7-OA8-CA6
57	Eu	101	CDL	C31-CA7-OA8-CA6
58	DC	602	PC1	C32-C31-O31-C3
58	DC	604	PC1	C32-C31-O31-C3
58	DX	302	PC1	C32-C31-O31-C3
58	Eb	301	PC1	C32-C31-O31-C3
58	Ef	1001	PC1	C32-C31-O31-C3
59	Dr	401	3PE	C32-C31-O31-C3
59	Ds	407	3PE	C32-C31-O31-C3
57	DA	705	CDL	OB9-CB7-OB8-CB6
57	DJ	307	CDL	OA9-CA7-OA8-CA6
57	DQ	1504	CDL	OA9-CA7-OA8-CA6
57	DV	401	CDL	OA9-CA7-OA8-CA6
57	EB	304	CDL	OA9-CA7-OA8-CA6
57	EL	903	CDL	OB9-CB7-OB8-CB6
57	EN	1202	CDL	OA9-CA7-OA8-CA6
57	Da	705	CDL	OB9-CB7-OB8-CB6
57	Dc	601	CDL	OB9-CB7-OB8-CB6
57	Dh	202	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	Dj	408	CDL	OA9-CA7-OA8-CA6
57	Du	402	CDL	OB9-CB7-OB8-CB6
57	Dv	401	CDL	OA9-CA7-OA8-CA6
57	Dx	1201	CDL	OB9-CB7-OB8-CB6
57	Eh	1601	CDL	OB9-CB7-OB8-CB6
57	El	901	CDL	OB9-CB7-OB8-CB6
58	DC	602	PC1	O32-C31-O31-C3
58	DC	604	PC1	O32-C31-O31-C3
58	DS	407	PC1	O32-C31-O31-C3
58	Dc	602	PC1	O32-C31-O31-C3
58	Ds	406	PC1	O32-C31-O31-C3
59	EO	204	3PE	O32-C31-O31-C3
57	DA	710	CDL	OA7-CA5-OA6-CA4
57	DD	702	CDL	OA7-CA5-OA6-CA4
57	DU	402	CDL	OA7-CA5-OA6-CA4
57	EL	903	CDL	OA7-CA5-OA6-CA4
57	EO	202	CDL	OA7-CA5-OA6-CA4
57	Di	701	CDL	OA7-CA5-OA6-CA4
57	Dy	301	CDL	OA7-CA5-OA6-CA4
57	Dy	301	CDL	OB7-CB5-OB6-CB4
57	Ek	201	CDL	OA7-CA5-OA6-CA4
57	DA	710	CDL	O1-C1-CB2-OB2
57	DG	201	CDL	O1-C1-CA2-OA2
57	DH	201	CDL	O1-C1-CA2-OA2
57	DJ	302	CDL	O1-C1-CA2-OA2
57	DN	505	CDL	O1-C1-CA2-OA2
57	EB	304	CDL	O1-C1-CA2-OA2
57	EL	902	CDL	O1-C1-CB2-OB2
57	EU	101	CDL	O1-C1-CA2-OA2
57	Dd	704	CDL	O1-C1-CA2-OA2
57	Dd	706	CDL	O1-C1-CA2-OA2
57	Dg	202	CDL	O1-C1-CA2-OA2
57	Dh	201	CDL	O1-C1-CA2-OA2
57	Dj	405	CDL	O1-C1-CA2-OA2
57	Dm	501	CDL	O1-C1-CB2-OB2
57	Du	402	CDL	O1-C1-CB2-OB2
57	Ei	401	CDL	O1-C1-CA2-OA2
57	El	902	CDL	O1-C1-CB2-OB2
57	En	1201	CDL	O1-C1-CA2-OA2
57	DC	601	CDL	C71-CB7-OB8-CB6
57	DH	201	CDL	C71-CB7-OB8-CB6
57	DO	501	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	Dn	503	CDL	C71-CB7-OB8-CB6
57	Dx	1201	CDL	C71-CB7-OB8-CB6
58	DS	407	PC1	C32-C31-O31-C3
58	DV	406	PC1	C32-C31-O31-C3
58	Ds	406	PC1	C32-C31-O31-C3
57	EA	301	CDL	OB9-CB7-OB8-CB6
57	EL	904	CDL	OB9-CB7-OB8-CB6
57	EN	1201	CDL	OB9-CB7-OB8-CB6
57	Da	709	CDL	OB9-CB7-OB8-CB6
57	Dn	503	CDL	OB9-CB7-OB8-CB6
57	Du	401	CDL	OA9-CA7-OA8-CA6
57	Ek	201	CDL	OB9-CB7-OB8-CB6
58	Dc	604	PC1	O32-C31-O31-C3
58	Ef	1001	PC1	O32-C31-O31-C3
59	EN	1203	3PE	O32-C31-O31-C3
57	DJ	304	CDL	C11-CA5-OA6-CA4
57	DJ	305	CDL	C11-CA5-OA6-CA4
57	DJ	305	CDL	C51-CB5-OB6-CB4
57	DM	501	CDL	C11-CA5-OA6-CA4
57	DR	403	CDL	C11-CA5-OA6-CA4
57	DU	404	CDL	C11-CA5-OA6-CA4
57	DV	401	CDL	C51-CB5-OB6-CB4
57	EK	201	CDL	C51-CB5-OB6-CB4
57	EL	903	CDL	C51-CB5-OB6-CB4
57	Dj	403	CDL	C11-CA5-OA6-CA4
57	Dj	405	CDL	C11-CA5-OA6-CA4
57	Dj	408	CDL	C11-CA5-OA6-CA4
57	Dr	403	CDL	C11-CA5-OA6-CA4
57	Ds	402	CDL	C11-CA5-OA6-CA4
57	Ek	201	CDL	C11-CA5-OA6-CA4
57	En	1202	CDL	C11-CA5-OA6-CA4
58	Da	707	PC1	C22-C21-O21-C2
58	Dv	406	PC1	C22-C21-O21-C2
58	Dx	1208	PC1	C22-C21-O21-C2
59	Ds	407	3PE	O32-C31-O31-C3
57	Dd	705	CDL	CA5-C11-C12-C13
59	Dc	606	3PE	C2-C3-O31-C31
57	DJ	307	CDL	C31-CA7-OA8-CA6
57	DQ	1504	CDL	C31-CA7-OA8-CA6
57	EB	304	CDL	C31-CA7-OA8-CA6
57	Da	705	CDL	C71-CB7-OB8-CB6
57	Dj	408	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	El	901	CDL	C71-CB7-OB8-CB6
58	Dc	602	PC1	C32-C31-O31-C3
59	DJ	301	3PE	C32-C31-O31-C3
59	EO	204	3PE	C32-C31-O31-C3
57	DO	501	CDL	OA9-CA7-OA8-CA6
57	Dh	201	CDL	OB9-CB7-OB8-CB6
57	Dq	402	CDL	OB9-CB7-OB8-CB6
57	En	1202	CDL	OA9-CA7-OA8-CA6
58	DV	406	PC1	O32-C31-O31-C3
57	DJ	305	CDL	OB7-CB5-OB6-CB4
58	Dv	406	PC1	O22-C21-O21-C2
58	Dx	1208	PC1	O22-C21-O21-C2
54	DA	702	HEA	C15-C16-C17-C18
54	Da	702	HEA	C19-C20-C21-C22
65	ED	603	UQ8	C39-C41-C42-C43
65	EN	1204	UQ8	C34-C36-C37-C38
65	En	1203	UQ8	C19-C21-C22-C23
57	DJ	304	CDL	CA4-CA3-OA5-PA1
57	EL	903	CDL	C1-CB2-OB2-PB2
57	EU	101	CDL	CA4-CA3-OA5-PA1
57	Dg	201	CDL	CB4-CB3-OB5-PB2
57	El	903	CDL	C1-CB2-OB2-PB2
58	Da	706	PC1	C2-C1-O11-P
57	DC	601	CDL	OB9-CB7-OB8-CB6
57	DH	201	CDL	OB9-CB7-OB8-CB6
59	DJ	301	3PE	O32-C31-O31-C3
57	DA	710	CDL	C31-CA7-OA8-CA6
57	ED	601	CDL	C31-CA7-OA8-CA6
57	Dr	402	CDL	C31-CA7-OA8-CA6
57	Eg	101	CDL	C31-CA7-OA8-CA6
58	Dq	405	PC1	C32-C31-O31-C3
57	DA	705	CDL	C51-CB5-OB6-CB4
57	Dv	401	CDL	C51-CB5-OB6-CB4
59	El	905	3PE	C22-C21-O21-C2
59	Ds	403	3PE	C2-C3-O31-C31
57	DA	710	CDL	OA9-CA7-OA8-CA6
57	ED	601	CDL	OA9-CA7-OA8-CA6
57	Dr	402	CDL	OA9-CA7-OA8-CA6
57	DJ	304	CDL	OA7-CA5-OA6-CA4
57	DR	403	CDL	OA7-CA5-OA6-CA4
57	DU	404	CDL	OA7-CA5-OA6-CA4
57	DV	401	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
57	EK	201	CDL	OB7-CB5-OB6-CB4
57	EL	903	CDL	OB7-CB5-OB6-CB4
57	Dr	403	CDL	OA7-CA5-OA6-CA4
57	Ds	402	CDL	OA7-CA5-OA6-CA4
57	En	1202	CDL	OA7-CA5-OA6-CA4
57	DD	702	CDL	CB2-C1-CA2-OA2
57	DJ	304	CDL	CB2-C1-CA2-OA2
57	DR	403	CDL	CB2-C1-CA2-OA2
57	DY	301	CDL	CB2-C1-CA2-OA2
57	EN	1201	CDL	CB2-C1-CA2-OA2
57	Dj	402	CDL	CB2-C1-CA2-OA2
57	Dj	405	CDL	CB2-C1-CA2-OA2
57	Dj	408	CDL	CA2-C1-CB2-OB2
57	Dm	501	CDL	CA2-C1-CB2-OB2
57	Dn	505	CDL	CB2-C1-CA2-OA2
57	Dq	401	CDL	CB2-C1-CA2-OA2
57	Dr	403	CDL	CB2-C1-CA2-OA2
57	Ds	402	CDL	CA2-C1-CB2-OB2
57	Dy	301	CDL	CB2-C1-CA2-OA2
57	Ei	401	CDL	CB2-C1-CA2-OA2
57	En	1201	CDL	CB2-C1-CA2-OA2
57	DA	709	CDL	C31-CA7-OA8-CA6
57	DD	702	CDL	C71-CB7-OB8-CB6
57	DR	402	CDL	C31-CA7-OA8-CA6
57	ED	601	CDL	C71-CB7-OB8-CB6
57	EH	201	CDL	C71-CB7-OB8-CB6
57	Da	709	CDL	C31-CA7-OA8-CA6
57	Dd	706	CDL	C71-CB7-OB8-CB6
57	Dg	202	CDL	C31-CA7-OA8-CA6
57	Dm	502	CDL	C71-CB7-OB8-CB6
57	Dn	501	CDL	C31-CA7-OA8-CA6
57	Dn	502	CDL	C31-CA7-OA8-CA6
57	Dn	503	CDL	C31-CA7-OA8-CA6
57	Do	501	CDL	C31-CA7-OA8-CA6
57	Dx	1203	CDL	C31-CA7-OA8-CA6
57	Dx	1203	CDL	C71-CB7-OB8-CB6
57	El	903	CDL	C71-CB7-OB8-CB6
58	DA	706	PC1	C32-C31-O31-C3
58	DC	608	PC1	C32-C31-O31-C3
58	DQ	1503	PC1	C32-C31-O31-C3
58	Da	706	PC1	C32-C31-O31-C3
58	Dc	607	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
58	Dv	407	PC1	C32-C31-O31-C3
59	DC	607	3PE	C32-C31-O31-C3
59	DS	403	3PE	C32-C31-O31-C3
59	Dr	404	3PE	C32-C31-O31-C3
59	Ds	403	3PE	C32-C31-O31-C3
65	EN	1204	UQ8	C25-C24-C26-C27
65	EN	1204	UQ8	C23-C24-C26-C27
57	DG	201	CDL	O1-C1-CB2-OB2
57	DJ	304	CDL	O1-C1-CA2-OA2
57	DJ	307	CDL	O1-C1-CA2-OA2
57	EB	302	CDL	O1-C1-CA2-OA2
57	ED	601	CDL	O1-C1-CA2-OA2
57	Dd	702	CDL	O1-C1-CA2-OA2
57	Dd	702	CDL	O1-C1-CB2-OB2
57	Dg	201	CDL	O1-C1-CA2-OA2
57	Dj	408	CDL	O1-C1-CA2-OA2
57	Du	404	CDL	O1-C1-CA2-OA2
57	Dv	404	CDL	O1-C1-CA2-OA2
57	Ep	701	CDL	O1-C1-CA2-OA2
57	DA	709	CDL	OA9-CA7-OA8-CA6
57	EH	201	CDL	OB9-CB7-OB8-CB6
57	Dn	503	CDL	OA9-CA7-OA8-CA6
59	DC	607	3PE	O32-C31-O31-C3
57	DM	502	CDL	CA5-C11-C12-C13
57	El	901	CDL	CA5-C11-C12-C13
58	DA	707	PC1	C3C-C3D-C3E-C3F
57	DD	702	CDL	OB9-CB7-OB8-CB6
57	ED	601	CDL	OB9-CB7-OB8-CB6
57	Dd	706	CDL	OB9-CB7-OB8-CB6
57	Dn	501	CDL	OA9-CA7-OA8-CA6
57	Dn	502	CDL	OA9-CA7-OA8-CA6
57	Do	501	CDL	OA9-CA7-OA8-CA6
57	Dx	1203	CDL	OA9-CA7-OA8-CA6
57	Dx	1203	CDL	OB9-CB7-OB8-CB6
57	El	903	CDL	OB9-CB7-OB8-CB6
58	DA	706	PC1	O32-C31-O31-C3
58	Da	706	PC1	O32-C31-O31-C3
59	DS	403	3PE	O32-C31-O31-C3
59	Ds	403	3PE	O32-C31-O31-C3
57	DJ	305	CDL	OA7-CA5-OA6-CA4
57	DM	501	CDL	OA7-CA5-OA6-CA4
57	Dj	403	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
57	Dj	408	CDL	OA7-CA5-OA6-CA4
57	DJ	304	CDL	OB5-CB3-CB4-OB6
57	DV	404	CDL	OB5-CB3-CB4-OB6
57	Dv	404	CDL	OB5-CB3-CB4-OB6
58	DQ	1503	PC1	O11-C1-C2-O21
57	DD	704	CDL	C11-CA5-OA6-CA4
57	DJ	302	CDL	C11-CA5-OA6-CA4
57	DM	502	CDL	C11-CA5-OA6-CA4
57	Dg	201	CDL	C51-CB5-OB6-CB4
57	Dm	502	CDL	C11-CA5-OA6-CA4
57	Do	501	CDL	C11-CA5-OA6-CA4
57	DA	705	CDL	OA6-CA4-CA6-OA8
57	DJ	303	CDL	OB6-CB4-CB6-OB8
57	DR	402	CDL	OB6-CB4-CB6-OB8
57	DR	403	CDL	OB6-CB4-CB6-OB8
57	Dg	201	CDL	OA6-CA4-CA6-OA8
58	DS	407	PC1	O21-C2-C3-O31
57	DJ	303	CDL	C71-CB7-OB8-CB6
57	DN	505	CDL	C31-CA7-OA8-CA6
57	DN	505	CDL	C71-CB7-OB8-CB6
57	Ed	204	CDL	C71-CB7-OB8-CB6
57	Eh	1601	CDL	C31-CA7-OA8-CA6
57	En	1201	CDL	C71-CB7-OB8-CB6
59	Em	901	3PE	C32-C31-O31-C3
57	DU	404	CDL	CA5-C11-C12-C13
57	EL	901	CDL	CA5-C11-C12-C13
57	DR	402	CDL	OA9-CA7-OA8-CA6
57	Dc	601	CDL	CA5-C11-C12-C13
59	DG	205	3PE	C32-C31-O31-C3
59	Dc	606	3PE	C32-C31-O31-C3
57	Dz	501	CDL	CA7-C31-C32-C33
57	Dj	405	CDL	OA7-CA5-OA6-CA4
57	Dv	401	CDL	OB7-CB5-OB6-CB4
58	Da	707	PC1	O22-C21-O21-C2
65	Ed	202	UQ8	C39-C41-C42-C43
65	En	1203	UQ8	C34-C36-C37-C38
57	DG	202	CDL	CA5-C11-C12-C13
57	DV	402	CDL	CA5-C11-C12-C13
57	Dj	408	CDL	CA5-C11-C12-C13
57	Du	402	CDL	CA5-C11-C12-C13
57	Dv	402	CDL	CA5-C11-C12-C13
57	Dx	1201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
57	Dm	502	CDL	OB9-CB7-OB8-CB6
58	DQ	1503	PC1	O32-C31-O31-C3
58	Dc	607	PC1	O32-C31-O31-C3
57	Eu	101	CDL	C11-CA5-OA6-CA4
59	Eo	203	3PE	C22-C21-O21-C2
57	Ep	701	CDL	C1-CA2-OA2-PA1
57	DJ	304	CDL	CA5-C11-C12-C13
57	DN	501	CDL	CA5-C11-C12-C13
57	EB	304	CDL	CA5-C11-C12-C13
57	ED	601	CDL	CA5-C11-C12-C13
57	Dh	202	CDL	CA5-C11-C12-C13
57	Dm	501	CDL	CA5-C11-C12-C13
57	Dy	301	CDL	CA5-C11-C12-C13
57	Ei	401	CDL	CA5-C11-C12-C13
57	El	902	CDL	CA5-C11-C12-C13
59	EM	901	3PE	C21-C22-C23-C24
57	Dg	202	CDL	OA9-CA7-OA8-CA6
58	Da	707	PC1	C3C-C3D-C3E-C3F
57	DD	704	CDL	O1-C1-CA2-OA2
57	DS	402	CDL	O1-C1-CB2-OB2
57	DX	301	CDL	O1-C1-CB2-OB2
57	DY	301	CDL	O1-C1-CA2-OA2
57	EL	903	CDL	O1-C1-CB2-OB2
57	EN	1202	CDL	O1-C1-CA2-OA2
57	Dd	704	CDL	O1-C1-CB2-OB2
57	Dq	401	CDL	O1-C1-CA2-OA2
57	Ds	402	CDL	O1-C1-CB2-OB2
57	Dy	301	CDL	O1-C1-CA2-OA2
57	El	901	CDL	O1-C1-CA2-OA2
57	En	1202	CDL	O1-C1-CA2-OA2
58	DI	702	PC1	C32-C31-O31-C3
57	Da	709	CDL	OA9-CA7-OA8-CA6
57	Eg	101	CDL	OA9-CA7-OA8-CA6
58	Dq	405	PC1	O32-C31-O31-C3
59	Dr	404	3PE	O32-C31-O31-C3
57	DU	401	CDL	CA5-C11-C12-C13
57	DZ	501	CDL	CA5-C11-C12-C13
58	EO	201	PC1	C31-C32-C33-C34
57	DA	705	CDL	OB7-CB5-OB6-CB4
57	DD	704	CDL	OA7-CA5-OA6-CA4
57	DJ	302	CDL	OA7-CA5-OA6-CA4
57	Dg	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
57	Dm	502	CDL	OA7-CA5-OA6-CA4
59	El	905	3PE	O22-C21-O21-C2
58	DC	608	PC1	O32-C31-O31-C3
58	Dv	407	PC1	O32-C31-O31-C3
59	Em	901	3PE	O32-C31-O31-C3
57	EL	902	CDL	CA5-C11-C12-C13
57	DG	202	CDL	C31-CA7-OA8-CA6
57	Eu	101	CDL	C71-CB7-OB8-CB6
58	Di	702	PC1	C32-C31-O31-C3
57	DQ	1502	CDL	C11-CA5-OA6-CA4
57	DQ	1504	CDL	C51-CB5-OB6-CB4
57	DU	401	CDL	C11-CA5-OA6-CA4
57	EB	304	CDL	C11-CA5-OA6-CA4
57	EI	401	CDL	C11-CA5-OA6-CA4
57	EN	1202	CDL	C11-CA5-OA6-CA4
57	Dh	201	CDL	C11-CA5-OA6-CA4
57	Dh	202	CDL	C11-CA5-OA6-CA4
57	Dr	402	CDL	C51-CB5-OB6-CB4
59	Ds	407	3PE	C22-C21-O21-C2
57	Ed	204	CDL	OB9-CB7-OB8-CB6
57	Eh	1601	CDL	OA9-CA7-OA8-CA6
59	Dc	606	3PE	O32-C31-O31-C3
57	Dq	403	CDL	C19-C20-C21-C22
57	DM	502	CDL	OA7-CA5-OA6-CA4
57	DQ	1502	CDL	OA7-CA5-OA6-CA4
57	DQ	1504	CDL	OB7-CB5-OB6-CB4
57	DU	401	CDL	OA7-CA5-OA6-CA4
57	EB	304	CDL	OA7-CA5-OA6-CA4
57	EI	401	CDL	OA7-CA5-OA6-CA4
57	EN	1202	CDL	OA7-CA5-OA6-CA4
57	Dh	201	CDL	OA7-CA5-OA6-CA4
57	Dh	202	CDL	OA7-CA5-OA6-CA4
57	Do	501	CDL	OA7-CA5-OA6-CA4
57	Dr	402	CDL	OB7-CB5-OB6-CB4
57	Eu	101	CDL	OA7-CA5-OA6-CA4
59	Ds	407	3PE	O22-C21-O21-C2
59	Eo	203	3PE	O22-C21-O21-C2
57	DD	704	CDL	CB2-C1-CA2-OA2
57	DJ	307	CDL	CA2-C1-CB2-OB2
57	DM	502	CDL	CA2-C1-CB2-OB2
57	DV	404	CDL	CB2-C1-CA2-OA2
57	DX	301	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
57	EL	903	CDL	CA2-C1-CB2-OB2
57	EN	1202	CDL	CB2-C1-CA2-OA2
57	Dd	704	CDL	CA2-C1-CB2-OB2
57	En	1202	CDL	CB2-C1-CA2-OA2
57	Eu	101	CDL	CB2-C1-CA2-OA2
57	DR	402	CDL	C71-CB7-OB8-CB6
57	DZ	501	CDL	C71-CB7-OB8-CB6
57	EL	904	CDL	C31-CA7-OA8-CA6
57	Dd	702	CDL	C71-CB7-OB8-CB6
57	Dj	401	CDL	C31-CA7-OA8-CA6
57	Dr	402	CDL	C71-CB7-OB8-CB6
57	Du	401	CDL	C71-CB7-OB8-CB6
57	Du	403	CDL	C31-CA7-OA8-CA6
57	Dv	404	CDL	C71-CB7-OB8-CB6
58	Dx	1204	PC1	C32-C31-O31-C3
57	DU	402	CDL	C14-C15-C16-C17
57	DH	201	CDL	CA5-C11-C12-C13
57	DV	404	CDL	C71-CB7-OB8-CB6
57	Dm	501	CDL	C71-CB7-OB8-CB6
57	Ds	402	CDL	C71-CB7-OB8-CB6
57	DQ	1504	CDL	CB5-C51-C52-C53
57	Dm	502	CDL	CA5-C11-C12-C13
57	DH	201	CDL	C11-CA5-OA6-CA4
57	DS	402	CDL	C11-CA5-OA6-CA4
57	DX	301	CDL	C51-CB5-OB6-CB4
57	DZ	501	CDL	C51-CB5-OB6-CB4
57	EK	201	CDL	C11-CA5-OA6-CA4
57	Dc	601	CDL	C11-CA5-OA6-CA4
57	Dc	601	CDL	C51-CB5-OB6-CB4
57	Dd	705	CDL	C11-CA5-OA6-CA4
57	Dq	404	CDL	C11-CA5-OA6-CA4
58	DA	707	PC1	C22-C21-O21-C2
59	Dg	204	3PE	C22-C21-O21-C2
59	DG	205	3PE	O32-C31-O31-C3
57	DH	201	CDL	OA7-CA5-OA6-CA4
57	DS	402	CDL	OA7-CA5-OA6-CA4
57	EK	201	CDL	OA7-CA5-OA6-CA4
57	Dc	601	CDL	OA7-CA5-OA6-CA4
57	Dc	601	CDL	OB7-CB5-OB6-CB4
59	Dg	204	3PE	O22-C21-O21-C2
57	EN	1201	CDL	CA5-C11-C12-C13
57	Ek	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
65	El	906	UQ8	C14-C16-C17-C18
57	DJ	303	CDL	O1-C1-CB2-OB2
57	EB	302	CDL	O1-C1-CB2-OB2
59	Ds	401	3PE	C32-C31-O31-C3
57	Eh	1601	CDL	CA5-C11-C12-C13
57	Dj	401	CDL	C1-CB2-OB2-PB2
57	Dm	501	CDL	C1-CB2-OB2-PB2
57	Du	401	CDL	C1-CA2-OA2-PA1
57	Eg	101	CDL	C1-CA2-OA2-PA1
57	Ei	401	CDL	CB4-CB3-OB5-PB2
57	DG	202	CDL	OA9-CA7-OA8-CA6
57	DJ	303	CDL	OB9-CB7-OB8-CB6
57	DN	505	CDL	OA9-CA7-OA8-CA6
57	DN	505	CDL	OB9-CB7-OB8-CB6
57	En	1201	CDL	OB9-CB7-OB8-CB6
57	DQ	1501	CDL	C19-C20-C21-C22
57	Du	404	CDL	CA5-C11-C12-C13
57	DV	402	CDL	CB3-CB4-OB6-CB5
57	Dv	402	CDL	CB3-CB4-OB6-CB5
58	EO	206	PC1	C1-C2-O21-C21
57	Dg	201	CDL	C23-C24-C25-C26
58	DI	702	PC1	O32-C31-O31-C3
58	Di	702	PC1	O32-C31-O31-C3
57	DH	201	CDL	C38-C39-C40-C41
57	DZ	501	CDL	OB7-CB5-OB6-CB4
57	Dd	705	CDL	OA7-CA5-OA6-CA4
57	Dq	404	CDL	OA7-CA5-OA6-CA4
58	DA	707	PC1	O22-C21-O21-C2
57	DA	709	CDL	C11-CA5-OA6-CA4
57	DC	601	CDL	C11-CA5-OA6-CA4
57	DD	703	CDL	C11-CA5-OA6-CA4
57	EH	202	CDL	C11-CA5-OA6-CA4
57	EL	904	CDL	C11-CA5-OA6-CA4
57	Dm	501	CDL	C11-CA5-OA6-CA4
57	Dn	501	CDL	C11-CA5-OA6-CA4
57	El	903	CDL	C11-CA5-OA6-CA4
57	DJ	307	CDL	OA6-CA4-CA6-OA8
59	Da	708	3PE	O21-C2-C3-O31
57	DU	401	CDL	C71-CB7-OB8-CB6
57	DR	402	CDL	OB9-CB7-OB8-CB6
57	DZ	501	CDL	OB9-CB7-OB8-CB6
57	EL	904	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	DA	710	CDL	C17-C18-C19-C20
57	Dv	402	CDL	C14-C15-C16-C17
57	DV	402	CDL	C14-C15-C16-C17
57	EA	301	CDL	C11-C12-C13-C14
57	Dd	704	CDL	C75-C76-C77-C78
57	Dj	403	CDL	C55-C56-C57-C58
57	Ds	405	CDL	C14-C15-C16-C17
57	Dz	501	CDL	C39-C40-C41-C42
58	Dc	607	PC1	C3D-C3E-C3F-C3G
57	DU	404	CDL	C80-C81-C82-C83
57	Dr	403	CDL	C13-C14-C15-C16
57	Du	404	CDL	C11-C12-C13-C14
57	El	903	CDL	C74-C75-C76-C77
57	DD	704	CDL	C71-CB7-OB8-CB6
57	DJ	307	CDL	C71-CB7-OB8-CB6
57	DJ	303	CDL	C62-C63-C64-C65
57	EL	904	CDL	C63-C64-C65-C66
57	Dx	1203	CDL	C19-C20-C21-C22
57	El	901	CDL	C55-C56-C57-C58
57	En	1202	CDL	C57-C58-C59-C60
58	EO	207	PC1	C3E-C3F-C3G-C3H
58	Eb	301	PC1	C27-C28-C29-C2A
57	DD	703	CDL	OA7-CA5-OA6-CA4
57	DX	301	CDL	OB7-CB5-OB6-CB4
57	Dm	501	CDL	OA7-CA5-OA6-CA4
57	DQ	1504	CDL	C11-C12-C13-C14
57	Dz	501	CDL	C42-C43-C44-C45
57	El	901	CDL	C80-C81-C82-C83
57	DG	202	CDL	C80-C81-C82-C83
57	Dd	704	CDL	C22-C23-C24-C25
57	Dx	1201	CDL	C14-C15-C16-C17
58	EB	301	PC1	C27-C28-C29-C2A
57	Dm	501	CDL	C55-C56-C57-C58
57	DN	501	CDL	C11-CA5-OA6-CA4
57	DN	504	CDL	C11-CA5-OA6-CA4
57	DU	403	CDL	C11-CA5-OA6-CA4
57	DV	403	CDL	C11-CA5-OA6-CA4
57	DX	307	CDL	C51-CB5-OB6-CB4
57	ED	604	CDL	C11-CA5-OA6-CA4
57	Dn	503	CDL	C51-CB5-OB6-CB4
57	Dn	507	CDL	C11-CA5-OA6-CA4
57	Du	404	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
57	Dv	403	CDL	C11-CA5-OA6-CA4
57	Dx	1201	CDL	C11-CA5-OA6-CA4
57	Dz	501	CDL	C51-CB5-OB6-CB4
57	Ed	205	CDL	C11-CA5-OA6-CA4
59	DA	708	3PE	C22-C21-O21-C2
59	DG	205	3PE	C22-C21-O21-C2
59	Dd	703	3PE	C22-C21-O21-C2
57	DJ	305	CDL	C12-C13-C14-C15
57	DU	404	CDL	C11-C12-C13-C14
57	Dd	705	CDL	C36-C37-C38-C39
57	DM	501	CDL	C81-C82-C83-C84
57	Dc	601	CDL	C13-C14-C15-C16
57	Di	701	CDL	C13-C14-C15-C16
58	DJ	306	PC1	C3D-C3E-C3F-C3G
57	EK	201	CDL	CA5-C11-C12-C13
57	Dg	202	CDL	CA5-C11-C12-C13
57	Dh	201	CDL	CA5-C11-C12-C13
57	Ed	204	CDL	CA5-C11-C12-C13
58	Eo	201	PC1	C31-C32-C33-C34
57	DI	701	CDL	C13-C14-C15-C16
57	DQ	1504	CDL	C34-C35-C36-C37
57	EL	901	CDL	C37-C38-C39-C40
57	Da	705	CDL	C75-C76-C77-C78
57	Dj	403	CDL	C39-C40-C41-C42
57	Eu	101	CDL	C11-C12-C13-C14
58	DB	702	PC1	C3C-C3D-C3E-C3F
58	DC	604	PC1	C3B-C3C-C3D-C3E
58	Eo	204	PC1	C2C-C2D-C2E-C2F
57	DU	402	CDL	C21-C22-C23-C24
59	DS	403	3PE	C2-C3-O31-C31
57	Dq	403	CDL	CA5-C11-C12-C13
58	Dj	406	PC1	C3D-C3E-C3F-C3G
57	Dj	401	CDL	OA9-CA7-OA8-CA6
57	Dr	402	CDL	OB9-CB7-OB8-CB6
57	Du	401	CDL	OB9-CB7-OB8-CB6
57	Du	403	CDL	OA9-CA7-OA8-CA6
57	Dv	404	CDL	OB9-CB7-OB8-CB6
57	Eu	101	CDL	OB9-CB7-OB8-CB6
58	Dx	1204	PC1	O32-C31-O31-C3
57	EL	901	CDL	C39-C40-C41-C42
57	EL	904	CDL	C81-C82-C83-C84
57	El	902	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
57	DA	709	CDL	OA7-CA5-OA6-CA4
57	DC	601	CDL	OA7-CA5-OA6-CA4
57	EH	202	CDL	OA7-CA5-OA6-CA4
57	El	903	CDL	OA7-CA5-OA6-CA4
57	Dq	401	CDL	C35-C36-C37-C38
57	EB	302	CDL	CA2-C1-CB2-OB2
57	EU	101	CDL	CB2-C1-CA2-OA2
57	DM	501	CDL	C71-CB7-OB8-CB6
57	DU	401	CDL	C31-CA7-OA8-CA6
57	DU	403	CDL	C31-CA7-OA8-CA6
57	EU	101	CDL	C71-CB7-OB8-CB6
57	Dd	702	CDL	C31-CA7-OA8-CA6
58	Eo	204	PC1	C32-C31-O31-C3
59	DR	401	3PE	C32-C31-O31-C3
57	Dm	502	CDL	CA3-CA4-CA6-OA8
57	Ed	205	CDL	CA3-CA4-CA6-OA8
58	EO	206	PC1	C1-C2-C3-O31
57	DR	403	CDL	C11-C12-C13-C14
57	EH	201	CDL	C75-C76-C77-C78
57	Dv	403	CDL	C13-C14-C15-C16
57	Dx	1203	CDL	C76-C77-C78-C79
59	DX	303	3PE	C39-C3A-C3B-C3C
57	Dj	403	CDL	CA5-C11-C12-C13
59	EN	1203	3PE	C21-C22-C23-C24
57	DA	705	CDL	C75-C76-C77-C78
57	DX	301	CDL	C11-C12-C13-C14
57	DX	301	CDL	C19-C20-C21-C22
57	Dg	201	CDL	C58-C59-C60-C61
57	Dj	402	CDL	C62-C63-C64-C65
57	Ed	205	CDL	C51-C52-C53-C54
57	Eh	1601	CDL	C61-C62-C63-C64
58	Dc	605	PC1	C29-C2A-C2B-C2C
59	Dd	703	3PE	C25-C26-C27-C28
57	DV	404	CDL	OB9-CB7-OB8-CB6
57	Dd	702	CDL	OB9-CB7-OB8-CB6
57	Dm	501	CDL	OB9-CB7-OB8-CB6
57	Ds	402	CDL	OB9-CB7-OB8-CB6
57	DJ	307	CDL	C54-C55-C56-C57
57	Dn	503	CDL	C17-C18-C19-C20
57	Dq	403	CDL	C12-C13-C14-C15
57	El	902	CDL	C39-C40-C41-C42
58	Dc	603	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
59	Eo	202	3PE	C36-C37-C38-C39
57	DD	702	CDL	C74-C75-C76-C77
57	DR	403	CDL	C13-C14-C15-C16
57	DV	404	CDL	C79-C80-C81-C82
57	Dv	402	CDL	C75-C76-C77-C78
57	Ea	301	CDL	C13-C14-C15-C16
57	DN	504	CDL	C35-C36-C37-C38
57	Dn	507	CDL	C35-C36-C37-C38
57	Dv	401	CDL	C54-C55-C56-C57
57	Dv	404	CDL	C13-C14-C15-C16
57	Dv	404	CDL	C79-C80-C81-C82
57	El	901	CDL	C12-C13-C14-C15
57	En	1201	CDL	C21-C22-C23-C24
57	Ep	701	CDL	C11-C12-C13-C14
57	Dr	402	CDL	CA7-C31-C32-C33
60	EI	402	LPP	C11-C12-C13-C14
59	Ds	401	3PE	O32-C31-O31-C3
57	DU	404	CDL	C33-C34-C35-C36
57	EL	901	CDL	C80-C81-C82-C83
57	Dv	401	CDL	C80-C81-C82-C83
57	El	903	CDL	C81-C82-C83-C84
59	Ds	407	3PE	C27-C28-C29-C2A
57	DS	405	CDL	C51-CB5-OB6-CB4
57	EN	1201	CDL	C11-CA5-OA6-CA4
57	Dd	705	CDL	C51-CB5-OB6-CB4
57	Ds	405	CDL	C11-CA5-OA6-CA4
57	Dx	1201	CDL	C51-CB5-OB6-CB4
58	DS	406	PC1	C22-C21-O21-C2
58	DX	302	PC1	C22-C21-O21-C2
57	Dq	404	CDL	C71-CB7-OB8-CB6
57	Dz	501	CDL	C71-CB7-OB8-CB6
59	DS	401	3PE	C32-C31-O31-C3
57	DG	201	CDL	CA4-CA3-OA5-PA1
57	EH	202	CDL	CA4-CA3-OA5-PA1
57	DV	401	CDL	C54-C55-C56-C57
57	EN	1201	CDL	C77-C78-C79-C80
58	Dy	302	PC1	C2E-C2F-C2G-C2H
59	EL	905	3PE	C26-C27-C28-C29
57	DD	704	CDL	C41-C42-C43-C44
57	DU	402	CDL	C61-C62-C63-C64
57	Dj	408	CDL	C55-C56-C57-C58
60	EI	402	LPP	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
57	DA	710	CDL	CA5-C11-C12-C13
57	DJ	303	CDL	C51-C52-C53-C54
57	DV	403	CDL	C54-C55-C56-C57
57	DV	404	CDL	C72-C73-C74-C75
57	DX	307	CDL	C32-C33-C34-C35
57	DD	704	CDL	OB9-CB7-OB8-CB6
57	DJ	307	CDL	OB9-CB7-OB8-CB6
57	DU	401	CDL	OB9-CB7-OB8-CB6
57	Dn	501	CDL	C73-C74-C75-C76
57	Du	403	CDL	C14-C15-C16-C17
58	DC	603	PC1	C2A-C2B-C2C-C2D
57	DN	501	CDL	OA7-CA5-OA6-CA4
57	DN	504	CDL	OA7-CA5-OA6-CA4
57	ED	604	CDL	OA7-CA5-OA6-CA4
57	EL	904	CDL	OA7-CA5-OA6-CA4
57	Dd	705	CDL	OB7-CB5-OB6-CB4
57	Dn	501	CDL	OA7-CA5-OA6-CA4
57	Dn	503	CDL	OB7-CB5-OB6-CB4
57	Dn	507	CDL	OA7-CA5-OA6-CA4
57	Du	404	CDL	OA7-CA5-OA6-CA4
57	Dv	403	CDL	OA7-CA5-OA6-CA4
57	Dx	1201	CDL	OA7-CA5-OA6-CA4
57	Dz	501	CDL	OB7-CB5-OB6-CB4
57	Ed	205	CDL	OA7-CA5-OA6-CA4
59	DG	205	3PE	O22-C21-O21-C2
59	Dd	703	3PE	O22-C21-O21-C2
65	Ed	202	UQ8	C35-C34-C36-C37
57	DN	505	CDL	C16-C17-C18-C19
57	En	1202	CDL	C11-C12-C13-C14
59	EN	1203	3PE	C38-C39-C3A-C3B
57	DJ	302	CDL	C40-C41-C42-C43
57	DX	301	CDL	C14-C15-C16-C17
57	DX	307	CDL	C11-C12-C13-C14
57	EK	201	CDL	C40-C41-C42-C43
57	EU	101	CDL	C11-C12-C13-C14
57	Dj	403	CDL	C17-C18-C19-C20
57	Dq	402	CDL	C13-C14-C15-C16
57	Ds	402	CDL	C74-C75-C76-C77
57	Eg	101	CDL	C16-C17-C18-C19
57	Ek	201	CDL	C40-C41-C42-C43
58	DX	306	PC1	C3D-C3E-C3F-C3G
58	DY	302	PC1	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
59	Dx	1206	3PE	C3D-C3E-C3F-C3G
57	DU	402	CDL	CA5-C11-C12-C13
57	DD	702	CDL	C31-CA7-OA8-CA6
57	DY	301	CDL	C31-CA7-OA8-CA6
58	Da	707	PC1	C32-C31-O31-C3
59	EO	203	3PE	C32-C31-O31-C3
57	DU	401	CDL	OA9-CA7-OA8-CA6
57	DA	709	CDL	C73-C74-C75-C76
57	DI	701	CDL	C62-C63-C64-C65
57	DJ	304	CDL	C35-C36-C37-C38
57	DS	402	CDL	C16-C17-C18-C19
57	Dh	202	CDL	C21-C22-C23-C24
57	Dv	403	CDL	C54-C55-C56-C57
57	Dx	1203	CDL	C60-C61-C62-C63
58	DB	702	PC1	C27-C28-C29-C2A
58	EO	207	PC1	C3B-C3C-C3D-C3E
58	Eo	205	PC1	C3E-C3F-C3G-C3H
57	DR	402	CDL	C61-C62-C63-C64
57	DV	403	CDL	C13-C14-C15-C16
57	DY	301	CDL	C12-C13-C14-C15
57	DY	301	CDL	C35-C36-C37-C38
57	EN	1202	CDL	C57-C58-C59-C60
57	Dg	201	CDL	C11-C12-C13-C14
57	Dh	202	CDL	C37-C38-C39-C40
57	Ds	402	CDL	C57-C58-C59-C60
57	Du	401	CDL	C36-C37-C38-C39
57	Dv	404	CDL	C72-C73-C74-C75
57	Dx	1203	CDL	C56-C57-C58-C59
57	DA	705	CDL	C41-C42-C43-C44
57	Da	705	CDL	C41-C42-C43-C44
57	Du	401	CDL	C11-C12-C13-C14
58	DC	602	PC1	C3C-C3D-C3E-C3F
57	DJ	304	CDL	C55-C56-C57-C58
57	Dz	501	CDL	C77-C78-C79-C80
58	DI	702	PC1	C27-C28-C29-C2A
58	Dc	602	PC1	C3C-C3D-C3E-C3F
57	Dd	705	CDL	C13-C14-C15-C16
58	Dx	1204	PC1	C24-C25-C26-C27
57	DA	710	CDL	O1-C1-CA2-OA2
57	DM	501	CDL	C58-C59-C60-C61
57	Ds	405	CDL	C11-C12-C13-C14
59	DJ	301	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
57	Dv	401	CDL	C71-CB7-OB8-CB6
57	EN	1201	CDL	C21-C22-C23-C24
59	DX	304	3PE	C3D-C3E-C3F-C3G
57	DC	601	CDL	C51-CB5-OB6-CB4
57	DJ	303	CDL	C51-CB5-OB6-CB4
57	DJ	307	CDL	C11-CA5-OA6-CA4
57	DQ	1501	CDL	C51-CB5-OB6-CB4
57	DQ	1502	CDL	C51-CB5-OB6-CB4
57	DS	405	CDL	C11-CA5-OA6-CA4
57	DU	402	CDL	C51-CB5-OB6-CB4
57	DV	404	CDL	C11-CA5-OA6-CA4
57	DX	307	CDL	C11-CA5-OA6-CA4
57	ED	604	CDL	C51-CB5-OB6-CB4
57	EL	901	CDL	C11-CA5-OA6-CA4
57	Da	705	CDL	C51-CB5-OB6-CB4
57	Dg	202	CDL	C11-CA5-OA6-CA4
57	Dj	405	CDL	C51-CB5-OB6-CB4
57	Ds	405	CDL	C51-CB5-OB6-CB4
57	Du	401	CDL	C11-CA5-OA6-CA4
57	Du	403	CDL	C11-CA5-OA6-CA4
57	Dv	404	CDL	C11-CA5-OA6-CA4
57	Dz	501	CDL	C11-CA5-OA6-CA4
57	Eh	1601	CDL	C51-CB5-OB6-CB4
57	El	901	CDL	C11-CA5-OA6-CA4
57	Ep	701	CDL	C11-CA5-OA6-CA4
58	Dq	405	PC1	C22-C21-O21-C2
58	Dx	1202	PC1	C22-C21-O21-C2
58	Ef	1001	PC1	C22-C21-O21-C2
59	DC	606	3PE	C22-C21-O21-C2
59	DX	304	3PE	C22-C21-O21-C2
59	EO	204	3PE	C22-C21-O21-C2
59	Dx	1205	3PE	C22-C21-O21-C2
59	Dx	1206	3PE	C22-C21-O21-C2
57	DM	501	CDL	OB9-CB7-OB8-CB6
57	Dv	401	CDL	CA5-C11-C12-C13
57	Dh	201	CDL	C38-C39-C40-C41
58	Dx	1208	PC1	C3D-C3E-C3F-C3G
59	Ds	407	3PE	C38-C39-C3A-C3B
57	DG	202	CDL	CA4-CA6-OA8-CA7
57	DJ	303	CDL	OB7-CB5-OB6-CB4
57	DS	405	CDL	OA7-CA5-OA6-CA4
57	DU	403	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
57	DV	403	CDL	OA7-CA5-OA6-CA4
57	DV	404	CDL	OA7-CA5-OA6-CA4
57	EL	901	CDL	OA7-CA5-OA6-CA4
57	Da	705	CDL	OB7-CB5-OB6-CB4
58	Dq	405	PC1	O22-C21-O21-C2
58	Dx	1202	PC1	O22-C21-O21-C2
59	DC	606	3PE	O22-C21-O21-C2
59	EO	204	3PE	O22-C21-O21-C2
57	DD	704	CDL	C36-C37-C38-C39
57	DH	201	CDL	C56-C57-C58-C59
57	DI	701	CDL	C37-C38-C39-C40
57	ED	601	CDL	C17-C18-C19-C20
57	EL	901	CDL	C61-C62-C63-C64
57	Di	701	CDL	C37-C38-C39-C40
57	Dr	402	CDL	C57-C58-C59-C60
57	Eh	1601	CDL	C20-C21-C22-C23
57	El	901	CDL	C33-C34-C35-C36
57	DN	501	CDL	C36-C37-C38-C39
57	DV	404	CDL	C12-C13-C14-C15
57	EB	302	CDL	C34-C35-C36-C37
57	Dq	401	CDL	C11-C12-C13-C14
57	Eg	101	CDL	C81-C82-C83-C84
57	Ei	401	CDL	C61-C62-C63-C64
58	DC	605	PC1	C29-C2A-C2B-C2C
59	DR	401	3PE	O32-C31-O31-C3
57	Dj	408	CDL	C13-C14-C15-C16
57	DZ	501	CDL	CB7-C71-C72-C73
57	Dz	501	CDL	CA5-C11-C12-C13
57	DG	201	CDL	C56-C57-C58-C59
57	DJ	304	CDL	C17-C18-C19-C20
57	EI	401	CDL	C61-C62-C63-C64
57	EL	902	CDL	C20-C21-C22-C23
57	EN	1201	CDL	C34-C35-C36-C37
57	Dj	402	CDL	C52-C53-C54-C55
57	Dx	1201	CDL	C77-C78-C79-C80
57	Eh	1601	CDL	C23-C24-C25-C26
57	DO	501	CDL	C32-C33-C34-C35
57	DA	710	CDL	C16-C17-C18-C19
57	DM	501	CDL	C79-C80-C81-C82
57	Dy	301	CDL	C35-C36-C37-C38
58	DS	406	PC1	C3B-C3C-C3D-C3E
58	Dv	407	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
59	EN	1203	3PE	C27-C28-C29-C2A
65	El	906	UQ8	C15-C14-C16-C17
65	El	906	UQ8	C13-C14-C16-C17
58	DI	702	PC1	C11-C12-N-C14
57	DC	601	CDL	C14-C15-C16-C17
57	DI	701	CDL	C42-C43-C44-C45
57	DS	402	CDL	C57-C58-C59-C60
57	DV	401	CDL	C80-C81-C82-C83
57	Dh	201	CDL	C56-C57-C58-C59
57	Dh	202	CDL	C74-C75-C76-C77
57	Du	404	CDL	C57-C58-C59-C60
59	DA	708	3PE	C28-C29-C2A-C2B
59	DS	403	3PE	C37-C38-C39-C3A
57	EK	201	CDL	C74-C75-C76-C77
57	Da	709	CDL	C14-C15-C16-C17
57	Di	701	CDL	C71-C72-C73-C74
57	Du	402	CDL	C57-C58-C59-C60
57	Dv	403	CDL	C36-C37-C38-C39
58	DV	406	PC1	C3C-C3D-C3E-C3F
60	Ed	203	LPP	C19-C20-C21-C22
57	DG	201	CDL	C14-C15-C16-C17
57	EB	304	CDL	C21-C22-C23-C24
57	DU	403	CDL	OA9-CA7-OA8-CA6
58	EO	204	PC1	O32-C31-O31-C3
57	Dv	404	CDL	C17-C18-C19-C20
57	Eh	1601	CDL	C53-C54-C55-C56
57	El	902	CDL	C78-C79-C80-C81
58	EO	204	PC1	C3A-C3B-C3C-C3D
59	Ds	403	3PE	C37-C38-C39-C3A
57	DJ	303	CDL	CA5-C11-C12-C13
57	DM	502	CDL	CB7-C71-C72-C73
57	DR	402	CDL	CA7-C31-C32-C33
57	DY	301	CDL	CA5-C11-C12-C13
57	Dn	503	CDL	CA5-C11-C12-C13
57	DO	501	CDL	C76-C77-C78-C79
57	EB	304	CDL	C37-C38-C39-C40
57	EN	1201	CDL	C53-C54-C55-C56
57	Ea	301	CDL	C74-C75-C76-C77
59	EO	203	3PE	C36-C37-C38-C39
57	DJ	307	CDL	OA7-CA5-OA6-CA4
57	DX	307	CDL	OB7-CB5-OB6-CB4
57	Dj	405	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
57	Du	403	CDL	OA7-CA5-OA6-CA4
58	DX	302	PC1	O22-C21-O21-C2
58	Ef	1001	PC1	O22-C21-O21-C2
59	DA	708	3PE	O22-C21-O21-C2
57	DX	301	CDL	OB5-CB3-CB4-OB6
57	Dj	403	CDL	OB5-CB3-CB4-OB6
58	DS	407	PC1	O11-C1-C2-O21
58	Dq	405	PC1	O11-C1-C2-O21
57	DI	701	CDL	C71-C72-C73-C74
57	DU	401	CDL	C36-C37-C38-C39
57	EL	903	CDL	C83-C84-C85-C86
57	Dz	501	CDL	C11-C12-C13-C14
57	El	901	CDL	C61-C62-C63-C64
58	DB	702	PC1	C32-C33-C34-C35
58	Di	702	PC1	C27-C28-C29-C2A
58	Ds	406	PC1	C2B-C2C-C2D-C2E
65	ED	603	UQ8	C24-C26-C27-C28
57	Dd	702	CDL	C51-CB5-OB6-CB4
57	Dd	706	CDL	C51-CB5-OB6-CB4
59	Dj	407	3PE	C22-C21-O21-C2
57	DG	201	CDL	C53-C54-C55-C56
57	DJ	302	CDL	C14-C15-C16-C17
57	EN	1201	CDL	C39-C40-C41-C42
57	Dd	704	CDL	C17-C18-C19-C20
57	Dz	501	CDL	C16-C17-C18-C19
57	Ek	201	CDL	C77-C78-C79-C80
59	EL	905	3PE	C37-C38-C39-C3A
57	Dd	702	CDL	OA9-CA7-OA8-CA6
57	Dq	404	CDL	OB9-CB7-OB8-CB6
57	EL	902	CDL	C81-C82-C83-C84
57	EU	101	CDL	C36-C37-C38-C39
57	Dn	505	CDL	C34-C35-C36-C37
57	Eh	1601	CDL	C81-C82-C83-C84
65	EL	906	UQ8	C5-C6-C7-C8
57	DG	201	CDL	CA5-C11-C12-C13
57	Dn	501	CDL	C57-C58-C59-C60
57	El	901	CDL	C23-C24-C25-C26
57	En	1201	CDL	C82-C83-C84-C85
58	DC	602	PC1	C3D-C3E-C3F-C3G
59	DC	606	3PE	C3E-C3F-C3G-C3H
57	DA	710	CDL	OA6-CA4-CA6-OA8
57	DM	501	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
57	DX	307	CDL	OA6-CA4-CA6-OA8
57	EL	901	CDL	OB6-CB4-CB6-OB8
57	Da	709	CDL	OA6-CA4-CA6-OA8
57	Dj	401	CDL	OA6-CA4-CA6-OA8
57	Dy	301	CDL	OB6-CB4-CB6-OB8
57	En	1201	CDL	OA6-CA4-CA6-OA8
58	DV	407	PC1	O21-C2-C3-O31
58	EO	206	PC1	O21-C2-C3-O31
58	Ef	1001	PC1	O21-C2-C3-O31
59	DA	708	3PE	O21-C2-C3-O31
57	DJ	302	CDL	C13-C14-C15-C16
57	Dq	401	CDL	C39-C40-C41-C42
57	Eg	101	CDL	C63-C64-C65-C66
57	Eh	1601	CDL	C55-C56-C57-C58
57	Dj	402	CDL	C71-CB7-OB8-CB6
57	DD	703	CDL	C17-C18-C19-C20
57	DN	501	CDL	C13-C14-C15-C16
57	DR	403	CDL	C41-C42-C43-C44
57	DV	404	CDL	C13-C14-C15-C16
57	Dj	402	CDL	C58-C59-C60-C61
57	Dn	507	CDL	C36-C37-C38-C39
57	Dr	403	CDL	C11-C12-C13-C14
57	Dx	1201	CDL	C20-C21-C22-C23
57	En	1201	CDL	C39-C40-C41-C42
59	Dr	404	3PE	C3E-C3F-C3G-C3H
59	Ds	407	3PE	C35-C36-C37-C38
57	DD	703	CDL	C75-C76-C77-C78
57	DJ	302	CDL	C60-C61-C62-C63
57	Dj	405	CDL	C11-C12-C13-C14
57	DJ	304	CDL	C13-C14-C15-C16
57	Dj	403	CDL	C13-C14-C15-C16
57	Do	501	CDL	C40-C41-C42-C43
57	Du	404	CDL	C80-C81-C82-C83
57	El	901	CDL	C39-C40-C41-C42
57	El	903	CDL	C76-C77-C78-C79
57	DG	201	CDL	CB4-CB3-OB5-PB2
57	DN	501	CDL	CA4-CA3-OA5-PA1
57	DU	401	CDL	C1-CA2-OA2-PA1
57	EI	401	CDL	CB4-CB3-OB5-PB2
57	Da	705	CDL	CB4-CB3-OB5-PB2
57	Dv	404	CDL	CB4-CB3-OB5-PB2
58	DA	706	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
57	DG	201	CDL	C12-C13-C14-C15
57	DO	501	CDL	C40-C41-C42-C43
57	Dj	401	CDL	C53-C54-C55-C56
57	Dj	404	CDL	C16-C17-C18-C19
57	Do	501	CDL	C32-C33-C34-C35
57	Eg	101	CDL	C11-C12-C13-C14
58	Di	702	PC1	C3A-C3B-C3C-C3D
59	EO	203	3PE	C3C-C3D-C3E-C3F
57	EU	101	CDL	OB9-CB7-OB8-CB6
57	DM	501	CDL	C55-C56-C57-C58
58	DS	407	PC1	C2B-C2C-C2D-C2E
59	DS	403	3PE	C39-C3A-C3B-C3C
57	Dg	202	CDL	OA7-CA5-OA6-CA4
57	Du	401	CDL	OA7-CA5-OA6-CA4
57	Dz	501	CDL	OA7-CA5-OA6-CA4
57	El	901	CDL	OA7-CA5-OA6-CA4
57	Ep	701	CDL	OA7-CA5-OA6-CA4
59	DX	304	3PE	O22-C21-O21-C2
57	DR	403	CDL	CA2-C1-CB2-OB2
57	DS	402	CDL	CA2-C1-CB2-OB2
57	EB	304	CDL	CB2-C1-CA2-OA2
57	Dd	706	CDL	CB2-C1-CA2-OA2
57	Du	402	CDL	CA2-C1-CB2-OB2
57	Dv	403	CDL	CA2-C1-CB2-OB2
57	Eg	101	CDL	CB2-C1-CA2-OA2
57	DA	709	CDL	C57-C58-C59-C60
57	DD	703	CDL	C63-C64-C65-C66
57	DN	504	CDL	C36-C37-C38-C39
57	DZ	501	CDL	C16-C17-C18-C19
57	ED	604	CDL	C51-C52-C53-C54
57	Da	709	CDL	C76-C77-C78-C79
57	Dd	702	CDL	C35-C36-C37-C38
57	Dn	503	CDL	C56-C57-C58-C59
57	Dr	403	CDL	C41-C42-C43-C44
57	Ea	301	CDL	C81-C82-C83-C84
57	Ek	201	CDL	C53-C54-C55-C56
57	El	901	CDL	C37-C38-C39-C40
57	El	902	CDL	C75-C76-C77-C78
57	Eu	101	CDL	C36-C37-C38-C39
58	EO	206	PC1	C3A-C3B-C3C-C3D
59	DX	304	3PE	C26-C27-C28-C29
59	EO	203	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
59	Eo	202	3PE	C3C-C3D-C3E-C3F
57	DV	401	CDL	C71-CB7-OB8-CB6
58	EO	207	PC1	C32-C31-O31-C3
57	DR	403	CDL	C12-C13-C14-C15
57	DV	404	CDL	C82-C83-C84-C85
57	Dn	502	CDL	C12-C13-C14-C15
57	Dq	404	CDL	C51-C52-C53-C54
57	Dr	402	CDL	C75-C76-C77-C78
57	Dv	402	CDL	C20-C21-C22-C23
57	Dv	404	CDL	C82-C83-C84-C85
58	Dj	406	PC1	C22-C23-C24-C25
59	DA	708	3PE	C25-C26-C27-C28
59	Dx	1207	3PE	C27-C28-C29-C2A
57	Dg	201	CDL	C44-C45-C46-C47
57	Dg	202	CDL	CB7-C71-C72-C73
59	Em	901	3PE	C21-C22-C23-C24
57	DQ	1502	CDL	C51-C52-C53-C54
57	ED	604	CDL	C61-C62-C63-C64
57	EL	903	CDL	C38-C39-C40-C41
57	Di	701	CDL	C42-C43-C44-C45
57	Ei	401	CDL	C12-C13-C14-C15
57	DD	704	CDL	C62-C63-C64-C65
57	DV	401	CDL	C57-C58-C59-C60
57	DV	402	CDL	C20-C21-C22-C23
57	DX	307	CDL	C14-C15-C16-C17
57	EO	202	CDL	C16-C17-C18-C19
57	Di	701	CDL	C77-C78-C79-C80
57	Dj	405	CDL	C37-C38-C39-C40
57	Ds	402	CDL	C61-C62-C63-C64
57	Dx	1201	CDL	C43-C44-C45-C46
57	Dx	1203	CDL	C17-C18-C19-C20
57	El	902	CDL	C12-C13-C14-C15
59	DG	205	3PE	C3E-C3F-C3G-C3H
59	EO	203	3PE	C2C-C2D-C2E-C2F
59	El	905	3PE	C26-C27-C28-C29
57	DD	702	CDL	OA9-CA7-OA8-CA6
57	Dz	501	CDL	OB9-CB7-OB8-CB6
58	Da	707	PC1	O32-C31-O31-C3
57	DV	404	CDL	C17-C18-C19-C20
57	Ds	405	CDL	C38-C39-C40-C41
57	Ds	405	CDL	C62-C63-C64-C65
57	Eg	101	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
58	EO	207	PC1	C3C-C3D-C3E-C3F
58	Db	702	PC1	C32-C33-C34-C35
59	Dx	1206	3PE	C26-C27-C28-C29
59	Eo	202	3PE	C27-C28-C29-C2A
59	Eo	202	3PE	C2C-C2D-C2E-C2F
57	DG	201	CDL	C63-C64-C65-C66
57	DJ	304	CDL	C60-C61-C62-C63
57	DS	402	CDL	C61-C62-C63-C64
57	DY	301	CDL	C82-C83-C84-C85
57	EK	201	CDL	C33-C34-C35-C36
57	EL	901	CDL	C33-C34-C35-C36
57	Dq	401	CDL	C53-C54-C55-C56
57	Dv	401	CDL	C39-C40-C41-C42
57	Dv	404	CDL	C12-C13-C14-C15
57	En	1201	CDL	C54-C55-C56-C57
60	EI	402	LPP	C15-C16-C17-C18
60	Dn	504	LPP	C31-C32-C33-C34
58	Di	702	PC1	C11-C12-N-C14
57	EB	302	CDL	C71-CB7-OB8-CB6
57	DA	710	CDL	C40-C41-C42-C43
57	DM	502	CDL	C14-C15-C16-C17
57	DV	402	CDL	C37-C38-C39-C40
57	DY	301	CDL	C56-C57-C58-C59
57	EB	304	CDL	C63-C64-C65-C66
57	EO	202	CDL	C11-C12-C13-C14
57	EO	202	CDL	C31-C32-C33-C34
57	Ds	402	CDL	C16-C17-C18-C19
57	Dy	301	CDL	C56-C57-C58-C59
57	Dy	301	CDL	C82-C83-C84-C85
57	Eh	1601	CDL	C57-C58-C59-C60
59	EM	901	3PE	C26-C27-C28-C29
59	EM	901	3PE	C2A-C2B-C2C-C2D
59	Dr	404	3PE	C22-C23-C24-C25
60	DN	502	LPP	C35-C36-C37-C38
60	EI	402	LPP	C20-C21-C22-C23
57	DJ	307	CDL	C51-C52-C53-C54
59	DS	401	3PE	O32-C31-O31-C3
57	DU	403	CDL	C36-C37-C38-C39
57	Ek	201	CDL	C33-C34-C35-C36
58	DC	608	PC1	C2C-C2D-C2E-C2F
58	Dx	1202	PC1	C2B-C2C-C2D-C2E
57	DA	705	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
57	DJ	307	CDL	OB5-CB3-CB4-CB6
57	DQ	1504	CDL	OA5-CA3-CA4-CA6
57	DS	402	CDL	OB5-CB3-CB4-CB6
57	DU	401	CDL	OB5-CB3-CB4-CB6
57	EB	302	CDL	OB5-CB3-CB4-CB6
57	ED	604	CDL	OB5-CB3-CB4-CB6
57	EH	202	CDL	OB5-CB3-CB4-CB6
57	EN	1202	CDL	OA5-CA3-CA4-CA6
57	Dc	601	CDL	OB5-CB3-CB4-CB6
57	Di	701	CDL	OB5-CB3-CB4-CB6
57	Dj	405	CDL	OB5-CB3-CB4-CB6
57	Dm	501	CDL	OA5-CA3-CA4-CA6
57	Do	501	CDL	OA5-CA3-CA4-CA6
57	Dq	402	CDL	OB5-CB3-CB4-CB6
57	Ds	402	CDL	OB5-CB3-CB4-CB6
57	Dx	1203	CDL	OB5-CB3-CB4-CB6
57	Ep	701	CDL	OA5-CA3-CA4-CA6
58	Dc	603	PC1	O11-C1-C2-C3
58	Di	702	PC1	O11-C1-C2-C3
59	Dj	407	3PE	O11-C1-C2-C3
59	Dr	404	3PE	O11-C1-C2-C3
57	DC	601	CDL	OB7-CB5-OB6-CB4
57	DS	405	CDL	OB7-CB5-OB6-CB4
57	ED	604	CDL	OB7-CB5-OB6-CB4
57	EN	1201	CDL	OA7-CA5-OA6-CA4
57	Ds	405	CDL	OA7-CA5-OA6-CA4
57	Ds	405	CDL	OB7-CB5-OB6-CB4
57	Dx	1201	CDL	OB7-CB5-OB6-CB4
58	DS	406	PC1	O22-C21-O21-C2
59	Dx	1206	3PE	O22-C21-O21-C2
57	DJ	304	CDL	C23-C24-C25-C26
57	DS	405	CDL	C62-C63-C64-C65
57	DV	403	CDL	C36-C37-C38-C39
57	DX	307	CDL	C43-C44-C45-C46
57	EA	301	CDL	C81-C82-C83-C84
57	Dd	705	CDL	C62-C63-C64-C65
57	Di	701	CDL	C74-C75-C76-C77
57	Ed	205	CDL	C16-C17-C18-C19
58	DA	706	PC1	C24-C25-C26-C27
58	DI	702	PC1	C2C-C2D-C2E-C2F
58	Da	707	PC1	C3E-C3F-C3G-C3H
57	Dz	501	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
57	DJ	307	CDL	C77-C78-C79-C80
57	DN	505	CDL	C12-C13-C14-C15
57	EN	1201	CDL	C17-C18-C19-C20
57	Dg	201	CDL	C19-C20-C21-C22
57	Dx	1203	CDL	C32-C33-C34-C35
57	Ed	205	CDL	C61-C62-C63-C64
57	Ek	201	CDL	C74-C75-C76-C77
57	El	903	CDL	C20-C21-C22-C23
58	DC	603	PC1	C35-C36-C37-C38
58	EO	206	PC1	C33-C34-C35-C36
57	DY	301	CDL	OA9-CA7-OA8-CA6
59	EO	203	3PE	O32-C31-O31-C3
57	Dr	402	CDL	C60-C61-C62-C63
57	En	1202	CDL	C34-C35-C36-C37
58	Eo	201	PC1	C3B-C3C-C3D-C3E
59	EN	1203	3PE	C35-C36-C37-C38
57	DC	601	CDL	CA5-C11-C12-C13
60	DN	502	LPP	C31-C32-C33-C34
57	DQ	1504	CDL	C53-C54-C55-C56
57	Dj	405	CDL	C41-C42-C43-C44
57	Dn	507	CDL	C14-C15-C16-C17
57	Dv	402	CDL	C37-C38-C39-C40
58	Di	702	PC1	C2C-C2D-C2E-C2F
57	DC	601	CDL	C33-C34-C35-C36
57	DJ	307	CDL	C82-C83-C84-C85
57	DN	501	CDL	C41-C42-C43-C44
57	EH	202	CDL	C80-C81-C82-C83
57	Dj	405	CDL	C20-C21-C22-C23
57	Dj	408	CDL	C82-C83-C84-C85
57	Dv	403	CDL	C62-C63-C64-C65
57	Dx	1201	CDL	C11-C12-C13-C14
57	Ed	204	CDL	C76-C77-C78-C79
57	El	903	CDL	C56-C57-C58-C59
59	Ds	403	3PE	C39-C3A-C3B-C3C
59	DJ	301	3PE	C22-C21-O21-C2
57	DJ	304	CDL	C79-C80-C81-C82
57	DJ	305	CDL	C41-C42-C43-C44
57	DN	505	CDL	C80-C81-C82-C83
57	DU	402	CDL	C11-C12-C13-C14
57	DV	401	CDL	C39-C40-C41-C42
57	ED	601	CDL	C56-C57-C58-C59
57	ED	604	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
57	Dx	1201	CDL	C74-C75-C76-C77
58	DJ	306	PC1	C22-C23-C24-C25
58	EO	206	PC1	C2D-C2E-C2F-C2G
60	DN	502	LPP	C37-C38-C39-C40
57	DJ	303	CDL	C33-C34-C35-C36
57	Dc	601	CDL	C33-C34-C35-C36
57	Dv	402	CDL	C76-C77-C78-C79
57	Eu	101	CDL	C17-C18-C19-C20
59	El	905	3PE	C3E-C3F-C3G-C3H
57	DD	704	CDL	C31-CA7-OA8-CA6
57	DQ	1501	CDL	C71-CB7-OB8-CB6
57	DQ	1502	CDL	C71-CB7-OB8-CB6
57	Dj	404	CDL	C31-C32-C33-C34
57	Du	403	CDL	C37-C38-C39-C40
57	Dv	401	CDL	C21-C22-C23-C24
57	DN	505	CDL	C55-C56-C57-C58
57	DS	405	CDL	C53-C54-C55-C56
57	DX	301	CDL	C74-C75-C76-C77
57	EU	101	CDL	C17-C18-C19-C20
57	Da	709	CDL	C16-C17-C18-C19
57	Dd	704	CDL	C63-C64-C65-C66
57	Dh	202	CDL	C63-C64-C65-C66
57	Dq	404	CDL	C38-C39-C40-C41
57	Dr	402	CDL	C20-C21-C22-C23
57	Eg	101	CDL	C79-C80-C81-C82
58	DX	302	PC1	C33-C34-C35-C36
57	DU	402	CDL	OB7-CB5-OB6-CB4
57	Dv	404	CDL	OA7-CA5-OA6-CA4
57	DA	710	CDL	C12-C13-C14-C15
57	DX	301	CDL	C35-C36-C37-C38
57	Dg	202	CDL	C35-C36-C37-C38
57	Do	501	CDL	C77-C78-C79-C80
57	Dq	401	CDL	C17-C18-C19-C20
59	Dc	606	3PE	C34-C35-C36-C37
57	DA	709	CDL	CA3-CA4-CA6-OA8
57	DA	710	CDL	CA3-CA4-CA6-OA8
57	DC	601	CDL	CA3-CA4-CA6-OA8
57	DD	702	CDL	CB3-CB4-CB6-OB8
57	DH	201	CDL	CA3-CA4-CA6-OA8
57	DJ	303	CDL	CB3-CB4-CB6-OB8
57	DM	501	CDL	CA3-CA4-CA6-OA8
57	DR	402	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
57	DS	402	CDL	CA3-CA4-CA6-OA8
57	DU	401	CDL	CB3-CB4-CB6-OB8
57	EB	304	CDL	CB3-CB4-CB6-OB8
57	EH	201	CDL	CB3-CB4-CB6-OB8
57	EK	201	CDL	CA3-CA4-CA6-OA8
57	Da	705	CDL	CB3-CB4-CB6-OB8
57	Da	709	CDL	CA3-CA4-CA6-OA8
57	Dc	601	CDL	CA3-CA4-CA6-OA8
57	Dd	702	CDL	CA3-CA4-CA6-OA8
57	Dd	704	CDL	CB3-CB4-CB6-OB8
57	Dg	201	CDL	CB3-CB4-CB6-OB8
57	Dh	202	CDL	CB3-CB4-CB6-OB8
57	Dj	401	CDL	CA3-CA4-CA6-OA8
57	Dj	408	CDL	CA3-CA4-CA6-OA8
57	Dr	403	CDL	CB3-CB4-CB6-OB8
57	Du	402	CDL	CA3-CA4-CA6-OA8
57	Du	403	CDL	CB3-CB4-CB6-OB8
57	Dv	404	CDL	CA3-CA4-CA6-OA8
57	Dx	1201	CDL	CA3-CA4-CA6-OA8
57	El	902	CDL	CA3-CA4-CA6-OA8
57	El	903	CDL	CA3-CA4-CA6-OA8
57	Ep	701	CDL	CA3-CA4-CA6-OA8
57	Eu	101	CDL	CB3-CB4-CB6-OB8
58	DC	608	PC1	C1-C2-C3-O31
58	DS	406	PC1	C1-C2-C3-O31
58	DV	407	PC1	C1-C2-C3-O31
58	DX	302	PC1	C1-C2-C3-O31
58	DY	302	PC1	C1-C2-C3-O31
58	EO	207	PC1	C1-C2-C3-O31
58	Dc	605	PC1	C1-C2-C3-O31
58	Ds	406	PC1	C1-C2-C3-O31
58	Dy	302	PC1	C1-C2-C3-O31
59	DR	401	3PE	C1-C2-C3-O31
59	EM	901	3PE	C1-C2-C3-O31
59	EN	1203	3PE	C1-C2-C3-O31
59	EO	203	3PE	C1-C2-C3-O31
59	Da	708	3PE	C1-C2-C3-O31
57	DA	709	CDL	C35-C36-C37-C38
57	DC	601	CDL	C40-C41-C42-C43
57	Dq	402	CDL	C17-C18-C19-C20
57	El	903	CDL	C61-C62-C63-C64
58	Dc	607	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
58	Dx	1204	PC1	C25-C26-C27-C28
59	DX	305	3PE	C27-C28-C29-C2A
57	Dv	401	CDL	OB9-CB7-OB8-CB6
57	DD	703	CDL	C82-C83-C84-C85
57	DJ	304	CDL	C72-C73-C74-C75
57	DV	402	CDL	C57-C58-C59-C60
57	DZ	501	CDL	C38-C39-C40-C41
57	Dd	704	CDL	C82-C83-C84-C85
57	Dg	201	CDL	C63-C64-C65-C66
57	Ds	405	CDL	C53-C54-C55-C56
57	Ed	204	CDL	C80-C81-C82-C83
57	El	902	CDL	C63-C64-C65-C66
57	En	1201	CDL	C17-C18-C19-C20
58	DG	203	PC1	C28-C29-C2A-C2B
58	Eo	201	PC1	C25-C26-C27-C28
59	Dx	1207	3PE	C39-C3A-C3B-C3C
60	Dn	504	LPP	C37-C38-C39-C40
57	DD	703	CDL	C11-C12-C13-C14
57	DG	201	CDL	C31-C32-C33-C34
57	DN	504	CDL	C43-C44-C45-C46
57	DV	401	CDL	C21-C22-C23-C24
57	EK	201	CDL	C77-C78-C79-C80
57	EL	901	CDL	C42-C43-C44-C45
57	Dn	501	CDL	C35-C36-C37-C38
57	Dn	505	CDL	C20-C21-C22-C23
57	Dv	401	CDL	C57-C58-C59-C60
57	Eg	101	CDL	C42-C43-C44-C45
57	En	1202	CDL	C37-C38-C39-C40
58	Dq	405	PC1	C34-C35-C36-C37
59	EL	905	3PE	C3E-C3F-C3G-C3H
59	Em	901	3PE	C2A-C2B-C2C-C2D
60	DA	711	LPP	C40-C41-C42-C43
57	DJ	302	CDL	C71-CB7-OB8-CB6
57	Du	404	CDL	C71-CB7-OB8-CB6
57	Dv	403	CDL	C71-CB7-OB8-CB6
57	Ep	701	CDL	C31-CA7-OA8-CA6
58	DS	406	PC1	C32-C31-O31-C3
58	Dc	603	PC1	C32-C31-O31-C3
58	Dv	406	PC1	C32-C31-O31-C3
57	DU	401	CDL	C11-C12-C13-C14
57	DV	402	CDL	C75-C76-C77-C78
57	EL	904	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
57	Dc	601	CDL	C40-C41-C42-C43
57	Dn	507	CDL	C82-C83-C84-C85
58	DQ	1503	PC1	C34-C35-C36-C37
58	DV	406	PC1	C2D-C2E-C2F-C2G
58	Dx	1208	PC1	C24-C25-C26-C27
58	Eo	204	PC1	C33-C34-C35-C36
57	DV	403	CDL	C23-C24-C25-C26
57	DX	301	CDL	C38-C39-C40-C41
57	EK	201	CDL	C53-C54-C55-C56
57	EL	903	CDL	C63-C64-C65-C66
57	Ds	405	CDL	C55-C56-C57-C58
58	DI	702	PC1	C3A-C3B-C3C-C3D
59	DC	607	3PE	C34-C35-C36-C37
59	Em	901	3PE	C26-C27-C28-C29
57	DX	307	CDL	C20-C21-C22-C23
57	EL	901	CDL	C19-C20-C21-C22
57	Dv	403	CDL	C23-C24-C25-C26
58	EO	201	PC1	C3B-C3C-C3D-C3E
57	DJ	305	CDL	C37-C38-C39-C40
57	El	901	CDL	C51-C52-C53-C54
59	DX	305	3PE	C39-C3A-C3B-C3C
59	El	905	3PE	C37-C38-C39-C3A
57	DD	702	CDL	CA5-C11-C12-C13
57	DR	403	CDL	CA7-C31-C32-C33
57	Dj	402	CDL	OB9-CB7-OB8-CB6
57	Dj	404	CDL	C11-C12-C13-C14
57	Dv	403	CDL	C81-C82-C83-C84
57	Dv	404	CDL	C41-C42-C43-C44
57	Eu	101	CDL	CA4-CA3-OA5-PA1
59	DG	204	3PE	C2-C1-O11-P
59	Dx	1205	3PE	O22-C21-O21-C2
57	Dv	402	CDL	C60-C61-C62-C63
57	DQ	1502	CDL	C38-C39-C40-C41
57	DR	402	CDL	C82-C83-C84-C85
57	DS	405	CDL	C55-C56-C57-C58
57	Da	709	CDL	C21-C22-C23-C24
57	Dj	408	CDL	C59-C60-C61-C62
57	Dq	403	CDL	C53-C54-C55-C56
58	Dv	407	PC1	C2D-C2E-C2F-C2G
57	DV	401	CDL	OB9-CB7-OB8-CB6
57	EB	302	CDL	OB9-CB7-OB8-CB6
58	EO	207	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
60	Dl	1101	LPP	C6-O5-P1-O3
57	DO	501	CDL	C15-C16-C17-C18
57	DV	404	CDL	C43-C44-C45-C46
57	Dm	501	CDL	C58-C59-C60-C61
57	DX	301	CDL	C12-C13-C14-C15
57	Du	402	CDL	C42-C43-C44-C45
58	DX	306	PC1	C24-C25-C26-C27
57	Dd	706	CDL	C75-C76-C77-C78
57	Dr	403	CDL	C34-C35-C36-C37
57	DJ	305	CDL	C77-C78-C79-C80
57	Dd	704	CDL	C11-C12-C13-C14
57	Dv	402	CDL	C79-C80-C81-C82
57	Dm	502	CDL	C31-CA7-OA8-CA6
57	Ed	205	CDL	C31-CA7-OA8-CA6
59	Dd	703	3PE	C32-C31-O31-C3
57	Dq	404	CDL	CB6-CB4-OB6-CB5
57	Dx	1203	CDL	CB6-CB4-OB6-CB5
58	DS	406	PC1	C1-C2-O21-C21
58	Eo	204	PC1	C1-C2-O21-C21
57	DN	505	CDL	C42-C43-C44-C45
57	DQ	1504	CDL	C17-C18-C19-C20
57	EB	302	CDL	C20-C21-C22-C23
57	Dg	201	CDL	C17-C18-C19-C20
57	Dj	401	CDL	C37-C38-C39-C40
57	Dj	403	CDL	C60-C61-C62-C63
57	Dn	502	CDL	C41-C42-C43-C44
57	Dz	501	CDL	C12-C13-C14-C15
57	Ed	205	CDL	C23-C24-C25-C26
58	DB	702	PC1	C2D-C2E-C2F-C2G
57	Dc	601	CDL	C12-C13-C14-C15
57	Dj	404	CDL	C19-C20-C21-C22
57	Dn	502	CDL	C36-C37-C38-C39
58	EO	205	PC1	C3C-C3D-C3E-C3F
58	Da	706	PC1	C24-C25-C26-C27
59	DC	607	3PE	C25-C26-C27-C28
58	Db	702	PC1	C27-C28-C29-C2A
57	DV	403	CDL	C81-C82-C83-C84
59	DS	401	3PE	C35-C36-C37-C38
57	Dj	403	CDL	C58-C59-C60-C61
57	Dn	507	CDL	C43-C44-C45-C46
59	Da	708	3PE	C28-C29-C2A-C2B
57	EB	302	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
57	ED	601	CDL	CB2-C1-CA2-OA2
57	Du	404	CDL	CB2-C1-CA2-OA2
57	Du	404	CDL	CA2-C1-CB2-OB2
57	EL	902	CDL	OA5-CA3-CA4-OA6
57	Di	701	CDL	OB5-CB3-CB4-OB6
57	Du	401	CDL	OA5-CA3-CA4-OA6
57	Dy	301	CDL	OA5-CA3-CA4-OA6
57	Dz	501	CDL	OB5-CB3-CB4-OB6
57	Ed	205	CDL	OB5-CB3-CB4-OB6
58	Ef	1001	PC1	O11-C1-C2-O21
57	DM	501	CDL	C14-C15-C16-C17
57	Dj	403	CDL	C11-C12-C13-C14
57	Dj	404	CDL	C18-C19-C20-C21
57	Do	501	CDL	C15-C16-C17-C18
57	Du	402	CDL	C21-C22-C23-C24
57	DU	404	CDL	C31-CA7-OA8-CA6
57	ED	604	CDL	C31-CA7-OA8-CA6
57	Ed	205	CDL	C71-CB7-OB8-CB6
58	Db	702	PC1	C32-C31-O31-C3
57	EB	304	CDL	C73-C74-C75-C76
57	Dj	401	CDL	C39-C40-C41-C42
57	Dj	401	CDL	C82-C83-C84-C85
58	DB	702	PC1	C2E-C2F-C2G-C2H
58	Db	702	PC1	C2C-C2D-C2E-C2F
58	Dc	604	PC1	C3F-C3G-C3H-C3I
57	ED	604	CDL	C23-C24-C25-C26
57	EL	904	CDL	C20-C21-C22-C23
57	Dz	501	CDL	C34-C35-C36-C37
58	DA	706	PC1	C29-C2A-C2B-C2C
58	DJ	306	PC1	C37-C38-C39-C3A
58	DV	405	PC1	C3B-C3C-C3D-C3E
58	Dc	603	PC1	C35-C36-C37-C38
57	DD	704	CDL	C82-C83-C84-C85
57	DI	701	CDL	C79-C80-C81-C82
57	DQ	1501	CDL	C53-C54-C55-C56
57	DQ	1504	CDL	C40-C41-C42-C43
57	DS	405	CDL	C38-C39-C40-C41
57	DV	402	CDL	C60-C61-C62-C63
57	EL	903	CDL	C36-C37-C38-C39
57	Da	709	CDL	C18-C19-C20-C21
57	Dj	403	CDL	C35-C36-C37-C38
57	Du	403	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
57	Dv	401	CDL	C14-C15-C16-C17
57	Eu	101	CDL	C63-C64-C65-C66
58	Dg	203	PC1	C28-C29-C2A-C2B
57	DG	201	CDL	C13-C14-C15-C16
57	DY	301	CDL	C79-C80-C81-C82
57	Di	701	CDL	C80-C81-C82-C83
57	Dj	403	CDL	C23-C24-C25-C26
57	Dj	408	CDL	C51-C52-C53-C54
57	Dm	501	CDL	C81-C82-C83-C84
57	Dv	404	CDL	C43-C44-C45-C46
57	Dx	1203	CDL	C35-C36-C37-C38
58	DV	405	PC1	C3F-C3G-C3H-C3I
57	DX	307	CDL	CA5-C11-C12-C13
57	EU	101	CDL	CA5-C11-C12-C13
57	DN	501	CDL	C14-C15-C16-C17
57	DV	402	CDL	C17-C18-C19-C20
57	EA	301	CDL	C75-C76-C77-C78
57	EO	202	CDL	C53-C54-C55-C56
57	Dy	301	CDL	C43-C44-C45-C46
57	En	1201	CDL	C53-C54-C55-C56
57	ED	604	CDL	OA6-CA4-CA6-OA8
57	Dd	702	CDL	OB6-CB4-CB6-OB8
57	Dm	502	CDL	OA6-CA4-CA6-OA8
57	Dn	503	CDL	OB6-CB4-CB6-OB8
57	Dv	404	CDL	OA6-CA4-CA6-OA8
57	Dx	1201	CDL	OA6-CA4-CA6-OA8
57	Ed	205	CDL	OA6-CA4-CA6-OA8
58	DA	707	PC1	O21-C2-C3-O31
58	Dy	302	PC1	O21-C2-C3-O31
59	EN	1203	3PE	O21-C2-C3-O31
57	DV	403	CDL	O1-C1-CB2-OB2
57	DX	307	CDL	O1-C1-CA2-OA2
57	Dd	705	CDL	O1-C1-CB2-OB2
57	DN	505	CDL	C60-C61-C62-C63
57	DS	402	CDL	C80-C81-C82-C83
57	DV	404	CDL	C53-C54-C55-C56
57	DZ	501	CDL	C12-C13-C14-C15
57	EO	202	CDL	C62-C63-C64-C65
57	Dj	405	CDL	C77-C78-C79-C80
57	Dq	401	CDL	C82-C83-C84-C85
57	Dq	403	CDL	C36-C37-C38-C39
57	Dv	402	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
58	Db	702	PC1	C2A-C2B-C2C-C2D
59	Ds	401	3PE	C35-C36-C37-C38
57	DU	403	CDL	C71-CB7-OB8-CB6
57	EL	901	CDL	C82-C83-C84-C85
57	Dd	702	CDL	C14-C15-C16-C17
57	Dd	705	CDL	C82-C83-C84-C85
57	Dr	403	CDL	C12-C13-C14-C15
57	Dx	1203	CDL	C54-C55-C56-C57
58	El	904	PC1	C3C-C3D-C3E-C3F
58	Dv	407	PC1	O31-C31-C32-C33
57	EU	101	CDL	C63-C64-C65-C66
57	Dh	201	CDL	C12-C13-C14-C15
57	Eh	1601	CDL	C14-C15-C16-C17
57	DA	710	CDL	C42-C43-C44-C45
57	DU	404	CDL	C23-C24-C25-C26
57	Du	403	CDL	C19-C20-C21-C22
58	Dv	405	PC1	C2A-C2B-C2C-C2D
58	El	904	PC1	C3B-C3C-C3D-C3E
58	EB	301	PC1	C36-C37-C38-C39
54	DA	702	HEA	C3B-C11-C12-C13
65	EN	1204	UQ8	C19-C21-C22-C23
57	DD	703	CDL	C14-C15-C16-C17
57	DY	301	CDL	C14-C15-C16-C17
57	Dq	402	CDL	C35-C36-C37-C38
57	DQ	1502	CDL	OB9-CB7-OB8-CB6
58	Dv	405	PC1	C3F-C3G-C3H-C3I
58	Eo	204	PC1	C3F-C3G-C3H-C3I
57	EA	301	CDL	C13-C14-C15-C16
57	Ds	405	CDL	C58-C59-C60-C61
58	Dv	406	PC1	C3B-C3C-C3D-C3E
57	Dn	505	CDL	C31-CA7-OA8-CA6
57	Eg	101	CDL	C71-CB7-OB8-CB6
58	DC	603	PC1	C32-C31-O31-C3
58	Dy	302	PC1	C32-C31-O31-C3
57	DJ	304	CDL	C51-CB5-OB6-CB4
57	EH	201	CDL	C51-CB5-OB6-CB4
57	DJ	303	CDL	C19-C20-C21-C22
57	DS	405	CDL	C58-C59-C60-C61
57	Dj	404	CDL	C53-C54-C55-C56
60	Dn	504	LPP	C35-C36-C37-C38
58	Eb	301	PC1	C36-C37-C38-C39
59	Dc	606	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
57	EL	903	CDL	CA5-C11-C12-C13
57	Dd	702	CDL	CA5-C11-C12-C13
57	Dd	704	CDL	CA5-C11-C12-C13
57	Du	401	CDL	CA5-C11-C12-C13
57	Dr	402	CDL	C82-C83-C84-C85
58	Dg	203	PC1	C3D-C3E-C3F-C3G
54	DA	701	HEA	C26-C15-C16-C17
54	Da	701	HEA	C26-C15-C16-C17
65	DS	404	UQ8	C30-C29-C31-C32
65	Ds	404	UQ8	C30-C29-C31-C32
57	DV	403	CDL	C62-C63-C64-C65
57	Dh	202	CDL	C42-C43-C44-C45
57	Dn	507	CDL	C40-C41-C42-C43
57	Dr	403	CDL	C35-C36-C37-C38
58	Dj	406	PC1	C37-C38-C39-C3A
59	Ds	401	3PE	C39-C3A-C3B-C3C
57	DC	601	CDL	C80-C81-C82-C83
57	DV	404	CDL	C41-C42-C43-C44
57	DX	301	CDL	C61-C62-C63-C64
57	EL	904	CDL	C61-C62-C63-C64
57	Dc	601	CDL	C14-C15-C16-C17
58	EO	201	PC1	C2B-C2C-C2D-C2E
58	EO	206	PC1	C2E-C2F-C2G-C2H
58	Da	706	PC1	C29-C2A-C2B-C2C
54	DA	702	HEA	C4D-C3D-CAD-CBD
57	DS	405	CDL	C43-C44-C45-C46
57	Dy	301	CDL	C79-C80-C81-C82
58	DV	405	PC1	C2A-C2B-C2C-C2D
57	DQ	1501	CDL	OB7-CB5-OB6-CB4
57	DX	307	CDL	OA7-CA5-OA6-CA4
57	DG	202	CDL	C51-C52-C53-C54
57	Dg	201	CDL	C52-C53-C54-C55
57	Dv	404	CDL	C53-C54-C55-C56
57	El	903	CDL	C79-C80-C81-C82
58	Dc	602	PC1	C3D-C3E-C3F-C3G
57	DD	704	CDL	CA4-CA3-OA5-PA1
57	DJ	305	CDL	C1-CB2-OB2-PB2
57	DS	405	CDL	C1-CA2-OA2-PA1
57	EK	201	CDL	C1-CA2-OA2-PA1
57	Da	705	CDL	CA4-CA3-OA5-PA1
57	Dd	702	CDL	C1-CA2-OA2-PA1
57	Dg	201	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
57	Dj	405	CDL	C1-CB2-OB2-PB2
57	DD	704	CDL	OA9-CA7-OA8-CA6
57	ED	604	CDL	C11-C12-C13-C14
57	EN	1201	CDL	C14-C15-C16-C17
57	Dn	507	CDL	C56-C57-C58-C59
57	Dq	402	CDL	C40-C41-C42-C43
57	En	1202	CDL	C23-C24-C25-C26
58	DB	702	PC1	C2B-C2C-C2D-C2E
58	DC	608	PC1	C3D-C3E-C3F-C3G
58	Eo	205	PC1	C3B-C3C-C3D-C3E
59	Ds	407	3PE	C3E-C3F-C3G-C3H
60	EI	402	LPP	C18-C19-C20-C21
57	Dn	502	CDL	C11-C12-C13-C14
58	DG	203	PC1	C26-C27-C28-C29
58	Db	702	PC1	C2E-C2F-C2G-C2H
57	DR	402	CDL	C33-C34-C35-C36
57	Di	701	CDL	C19-C20-C21-C22
57	Dv	402	CDL	C57-C58-C59-C60
59	EN	1203	3PE	C3E-C3F-C3G-C3H
57	Dv	403	CDL	OB9-CB7-OB8-CB6
57	Dc	601	CDL	C79-C80-C81-C82
57	Dv	403	CDL	C75-C76-C77-C78
57	DJ	305	CDL	C20-C21-C22-C23
57	DN	504	CDL	C14-C15-C16-C17
57	DV	402	CDL	C12-C13-C14-C15
57	DZ	501	CDL	C34-C35-C36-C37
58	DS	406	PC1	C3F-C3G-C3H-C3I
58	Dc	605	PC1	C3F-C3G-C3H-C3I
60	DI	1101	LPP	C41-C42-C43-C44
57	DG	201	CDL	OA5-CA3-CA4-CA6
57	DJ	304	CDL	OB5-CB3-CB4-CB6
57	DO	501	CDL	OA5-CA3-CA4-CA6
57	DU	404	CDL	OB5-CB3-CB4-CB6
57	DV	404	CDL	OB5-CB3-CB4-CB6
57	DX	301	CDL	OB5-CB3-CB4-CB6
57	EB	302	CDL	OA5-CA3-CA4-CA6
57	EI	401	CDL	OB5-CB3-CB4-CB6
57	EL	901	CDL	OB5-CB3-CB4-CB6
57	Da	705	CDL	OB5-CB3-CB4-CB6
57	Dd	705	CDL	OA5-CA3-CA4-CA6
57	Dn	502	CDL	OB5-CB3-CB4-CB6
57	Dq	404	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
57	Ds	405	CDL	OB5-CB3-CB4-CB6
57	Du	401	CDL	OB5-CB3-CB4-CB6
57	Dv	404	CDL	OB5-CB3-CB4-CB6
57	Dz	501	CDL	OB5-CB3-CB4-CB6
57	Eu	101	CDL	OA5-CA3-CA4-CA6
58	DG	203	PC1	O11-C1-C2-C3
58	DI	702	PC1	O11-C1-C2-C3
58	DQ	1503	PC1	O11-C1-C2-C3
58	DS	407	PC1	O11-C1-C2-C3
58	Dg	203	PC1	O11-C1-C2-C3
58	Dq	405	PC1	O11-C1-C2-C3
59	Da	708	3PE	O11-C1-C2-C3
59	Dx	1206	3PE	O11-C1-C2-C3
57	Dg	201	CDL	C56-C57-C58-C59
57	Dn	502	CDL	C19-C20-C21-C22
57	DJ	302	CDL	OB9-CB7-OB8-CB6
57	DQ	1501	CDL	OB9-CB7-OB8-CB6
57	Du	404	CDL	OB9-CB7-OB8-CB6
58	Dv	406	PC1	C3F-C3G-C3H-C3I
57	EL	903	CDL	C74-C75-C76-C77
57	Dm	501	CDL	C76-C77-C78-C79
57	Eh	1601	CDL	C83-C84-C85-C86
59	DS	403	3PE	C2B-C2C-C2D-C2E
58	DI	702	PC1	C11-C12-N-C13
57	Dh	202	CDL	O1-C1-CA2-OA2
57	DV	401	CDL	CA5-C11-C12-C13
58	DC	604	PC1	C3F-C3G-C3H-C3I
57	DU	404	CDL	C13-C14-C15-C16
57	Ds	405	CDL	C43-C44-C45-C46
58	Eo	204	PC1	C2A-C2B-C2C-C2D
59	DS	401	3PE	C39-C3A-C3B-C3C
57	Ea	301	CDL	C71-CB7-OB8-CB6
57	DQ	1502	CDL	OB7-CB5-OB6-CB4
57	DI	701	CDL	C19-C20-C21-C22
57	Da	709	CDL	C74-C75-C76-C77
57	Dn	503	CDL	C83-C84-C85-C86
65	ED	603	UQ8	C40-C39-C41-C42
65	Ds	404	UQ8	C28-C29-C31-C32
65	Ed	202	UQ8	C33-C34-C36-C37
57	DV	401	CDL	C18-C19-C20-C21
57	EB	304	CDL	C42-C43-C44-C45
57	EO	202	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
57	Dc	601	CDL	C80-C81-C82-C83
57	Dh	202	CDL	C53-C54-C55-C56
58	DX	302	PC1	C26-C27-C28-C29
58	DS	406	PC1	O32-C31-O31-C3
58	Dc	603	PC1	O32-C31-O31-C3
58	Dv	406	PC1	O32-C31-O31-C3
58	DC	605	PC1	C32-C31-O31-C3
59	Ds	403	3PE	C2B-C2C-C2D-C2E
57	DN	504	CDL	C56-C57-C58-C59
57	Ep	701	CDL	OA9-CA7-OA8-CA6
57	DG	202	CDL	C35-C36-C37-C38
57	DJ	307	CDL	C59-C60-C61-C62
57	EN	1202	CDL	C23-C24-C25-C26
58	Dx	1204	PC1	C3D-C3E-C3F-C3G
57	DD	704	CDL	C13-C14-C15-C16
57	DJ	303	CDL	C13-C14-C15-C16
57	DN	504	CDL	C40-C41-C42-C43
57	DG	202	CDL	CA7-C31-C32-C33
58	EB	301	PC1	C3C-C3D-C3E-C3F
57	EH	201	CDL	CA2-C1-CB2-OB2
58	DY	302	PC1	C32-C31-O31-C3
57	Dj	401	CDL	C35-C36-C37-C38
57	DA	705	CDL	CA3-CA4-CA6-OA8
57	DA	705	CDL	CB3-CB4-CB6-OB8
57	DG	202	CDL	CB3-CB4-CB6-OB8
57	DJ	307	CDL	CA3-CA4-CA6-OA8
57	DN	505	CDL	CB3-CB4-CB6-OB8
57	DR	403	CDL	CB3-CB4-CB6-OB8
57	DU	401	CDL	CA3-CA4-CA6-OA8
57	DX	307	CDL	CA3-CA4-CA6-OA8
57	DY	301	CDL	CA3-CA4-CA6-OA8
57	DY	301	CDL	CB3-CB4-CB6-OB8
57	ED	601	CDL	CB3-CB4-CB6-OB8
57	ED	604	CDL	CA3-CA4-CA6-OA8
57	EL	901	CDL	CA3-CA4-CA6-OA8
57	EL	901	CDL	CB3-CB4-CB6-OB8
57	EL	903	CDL	CA3-CA4-CA6-OA8
57	EO	202	CDL	CB3-CB4-CB6-OB8
57	EU	101	CDL	CB3-CB4-CB6-OB8
57	Dd	706	CDL	CB3-CB4-CB6-OB8
57	Dg	201	CDL	CA3-CA4-CA6-OA8
57	Dg	202	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
57	Dh	201	CDL	CA3-CA4-CA6-OA8
57	Dn	505	CDL	CB3-CB4-CB6-OB8
57	Dr	402	CDL	CA3-CA4-CA6-OA8
57	Dr	402	CDL	CB3-CB4-CB6-OB8
57	Ds	402	CDL	CA3-CA4-CA6-OA8
57	Dy	301	CDL	CA3-CA4-CA6-OA8
57	Dy	301	CDL	CB3-CB4-CB6-OB8
57	Ei	401	CDL	CA3-CA4-CA6-OA8
58	DA	707	PC1	C1-C2-C3-O31
58	DC	605	PC1	C1-C2-C3-O31
58	DS	407	PC1	C1-C2-C3-O31
58	Da	706	PC1	C1-C2-C3-O31
58	Dc	607	PC1	C1-C2-C3-O31
58	Ef	1001	PC1	C1-C2-C3-O31
58	Eo	201	PC1	C1-C2-C3-O31
59	DA	708	3PE	C1-C2-C3-O31
59	DX	305	3PE	C1-C2-C3-O31
59	EL	905	3PE	C1-C2-C3-O31
59	Ds	401	3PE	C1-C2-C3-O31
59	Em	901	3PE	C1-C2-C3-O31
58	DC	603	PC1	C2C-C2D-C2E-C2F
59	DA	708	3PE	C3A-C3B-C3C-C3D
57	DA	705	CDL	C34-C35-C36-C37
57	Dd	704	CDL	C38-C39-C40-C41
57	Dv	401	CDL	C18-C19-C20-C21
57	Dx	1203	CDL	C36-C37-C38-C39
57	EB	304	CDL	C44-C45-C46-C47
57	EL	901	CDL	C53-C54-C55-C56
57	DN	504	CDL	C82-C83-C84-C85
57	DS	402	CDL	C76-C77-C78-C79
57	EN	1202	CDL	C34-C35-C36-C37
58	DB	702	PC1	C38-C39-C3A-C3B
54	DA	701	HEA	C14-C15-C16-C17
65	ED	603	UQ8	C38-C39-C41-C42
57	Dm	502	CDL	OA9-CA7-OA8-CA6
57	Ed	205	CDL	OA9-CA7-OA8-CA6
58	Db	702	PC1	O32-C31-O31-C3
59	Dd	703	3PE	O32-C31-O31-C3
58	EO	206	PC1	C2B-C2C-C2D-C2E
57	En	1201	CDL	C34-C35-C36-C37
58	Di	702	PC1	C11-C12-N-C13
57	DR	402	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
57	DU	403	CDL	C14-C15-C16-C17
57	EL	902	CDL	C83-C84-C85-C86
57	Eh	1601	CDL	OB7-CB5-OB6-CB4
57	Eu	101	CDL	CA5-C11-C12-C13
57	DQ	1501	CDL	OB5-CB3-CB4-OB6
57	DS	405	CDL	OB5-CB3-CB4-OB6
57	DX	307	CDL	OB5-CB3-CB4-OB6
57	DZ	501	CDL	OB5-CB3-CB4-OB6
57	EA	301	CDL	OA5-CA3-CA4-OA6
57	EI	401	CDL	OB5-CB3-CB4-OB6
57	EN	1202	CDL	OA5-CA3-CA4-OA6
57	Dc	601	CDL	OB5-CB3-CB4-OB6
57	Ds	402	CDL	OB5-CB3-CB4-OB6
57	Ds	405	CDL	OB5-CB3-CB4-OB6
57	Du	401	CDL	OB5-CB3-CB4-OB6
57	Du	404	CDL	OB5-CB3-CB4-OB6
57	Dv	403	CDL	OA5-CA3-CA4-OA6
57	Ep	701	CDL	OA5-CA3-CA4-OA6
58	DI	702	PC1	O11-C1-C2-O21
58	Dc	607	PC1	O11-C1-C2-O21
58	Eo	201	PC1	O11-C1-C2-O21
59	DS	403	3PE	O11-C1-C2-O21
59	DX	303	3PE	O11-C1-C2-O21
59	Dg	204	3PE	O11-C1-C2-O21
59	Dr	404	3PE	O11-C1-C2-O21
59	Ds	403	3PE	O11-C1-C2-O21
59	Dc	606	3PE	C2F-C2G-C2H-C2I
58	EO	205	PC1	C3B-C3C-C3D-C3E
57	Eg	101	CDL	O1-C1-CA2-OA2
57	DQ	1504	CDL	C1-CA2-OA2-PA1
57	EI	401	CDL	C1-CA2-OA2-PA1
57	EO	202	CDL	CB4-CB3-OB5-PB2
57	Dg	201	CDL	CA4-CA3-OA5-PA1
57	Dm	501	CDL	CA4-CA3-OA5-PA1
57	Ds	405	CDL	C1-CA2-OA2-PA1
57	En	1202	CDL	C1-CA2-OA2-PA1
59	DS	401	3PE	C38-C39-C3A-C3B
59	DS	403	3PE	C27-C28-C29-C2A
57	Dh	202	CDL	C44-C45-C46-C47
57	DC	601	CDL	C79-C80-C81-C82
58	Ef	1001	PC1	C2B-C2C-C2D-C2E
57	DI	701	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
57	DJ	303	CDL	C40-C41-C42-C43
57	EI	401	CDL	C11-C12-C13-C14
57	DQ	1501	CDL	C36-C37-C38-C39
57	DV	404	CDL	C40-C41-C42-C43
57	Dx	1203	CDL	C20-C21-C22-C23
58	Dg	203	PC1	C26-C27-C28-C29
58	DC	604	PC1	O21-C21-C22-C23
57	DA	709	CDL	OA6-CA4-CA6-OA8
57	DJ	302	CDL	OA6-CA4-CA6-OA8
57	DS	402	CDL	OA6-CA4-CA6-OA8
57	DY	301	CDL	OA6-CA4-CA6-OA8
57	ED	601	CDL	OB6-CB4-CB6-OB8
57	EH	202	CDL	OA6-CA4-CA6-OA8
57	EI	401	CDL	OA6-CA4-CA6-OA8
57	EL	903	CDL	OB6-CB4-CB6-OB8
57	EO	202	CDL	OB6-CB4-CB6-OB8
57	Dg	201	CDL	OB6-CB4-CB6-OB8
57	Dr	402	CDL	OA6-CA4-CA6-OA8
57	Ds	402	CDL	OA6-CA4-CA6-OA8
57	Eg	101	CDL	OA6-CA4-CA6-OA8
57	Ei	401	CDL	OA6-CA4-CA6-OA8
57	El	902	CDL	OA6-CA4-CA6-OA8
57	El	903	CDL	OA6-CA4-CA6-OA8
57	Ep	701	CDL	OA6-CA4-CA6-OA8
58	DS	406	PC1	O21-C2-C3-O31
58	EO	207	PC1	O21-C2-C3-O31
58	Dc	607	PC1	O21-C2-C3-O31
59	DC	607	3PE	O21-C2-C3-O31
59	DX	305	3PE	O21-C2-C3-O31
59	Dr	401	3PE	O21-C2-C3-O31
59	Dx	1207	3PE	O21-C2-C3-O31
59	Em	901	3PE	O21-C2-C3-O31
57	EU	101	CDL	C72-C73-C74-C75
59	Dx	1205	3PE	C2F-C2G-C2H-C2I
57	DV	403	CDL	C75-C76-C77-C78
57	EI	401	CDL	C76-C77-C78-C79
65	EL	906	UQ8	C2-C3-O3-C3M
57	Dd	702	CDL	OB7-CB5-OB6-CB4
57	DX	301	CDL	CA7-C31-C32-C33
57	Dd	702	CDL	CB7-C71-C72-C73
57	Dy	301	CDL	CB5-C51-C52-C53
57	DZ	501	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
57	Dm	501	CDL	C82-C83-C84-C85
59	Dd	703	3PE	C35-C36-C37-C38
54	Da	701	HEA	C14-C15-C16-C17
57	DU	402	CDL	C56-C57-C58-C59
58	Dc	603	PC1	C3D-C3E-C3F-C3G
60	Dn	506	LPP	C35-C36-C37-C38
57	DG	202	CDL	C14-C15-C16-C17
57	Dq	401	CDL	C37-C38-C39-C40
57	Dh	201	CDL	C31-CA7-OA8-CA6
57	Dq	401	CDL	C31-CA7-OA8-CA6
57	Dj	401	CDL	C13-C14-C15-C16
57	ED	604	CDL	OA9-CA7-OA8-CA6
57	Ek	201	CDL	C51-CB5-OB6-CB4
57	Dv	402	CDL	C42-C43-C44-C45
58	Eo	205	PC1	C29-C2A-C2B-C2C
57	Dr	402	CDL	C84-C85-C86-C87
57	DU	404	CDL	OA9-CA7-OA8-CA6
57	DR	402	CDL	C20-C21-C22-C23
57	Ep	701	CDL	C60-C61-C62-C63
58	DC	603	PC1	C3D-C3E-C3F-C3G
58	Dc	607	PC1	C2B-C2C-C2D-C2E
57	Dd	706	CDL	OB7-CB5-OB6-CB4
58	Eo	204	PC1	C11-C12-N-C13
59	DJ	301	3PE	C35-C36-C37-C38
65	EN	1204	UQ8	C14-C16-C17-C18
57	DM	501	CDL	C77-C78-C79-C80
57	DQ	1504	CDL	C36-C37-C38-C39
57	DU	401	CDL	C60-C61-C62-C63
57	EL	901	CDL	C23-C24-C25-C26
57	Dj	404	CDL	C77-C78-C79-C80
57	Dn	501	CDL	C76-C77-C78-C79
57	Dv	404	CDL	C40-C41-C42-C43
58	Dc	603	PC1	C2C-C2D-C2E-C2F
57	DI	701	CDL	O1-C1-CA2-OA2
57	DR	402	CDL	C84-C85-C86-C87
57	Dd	705	CDL	C84-C85-C86-C87
57	El	902	CDL	C34-C35-C36-C37
60	EI	402	LPP	C38-C39-C40-C41
57	DD	704	CDL	C84-C85-C86-C87
65	DS	404	UQ8	C28-C29-C31-C32
59	EL	905	3PE	C22-C21-O21-C2
57	Dv	402	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
57	DV	402	CDL	C79-C80-C81-C82
57	EL	904	CDL	C77-C78-C79-C80
57	DA	710	CDL	CA2-C1-CB2-OB2
57	DJ	307	CDL	CB2-C1-CA2-OA2
57	DV	403	CDL	CA2-C1-CB2-OB2
57	Dg	202	CDL	CB2-C1-CA2-OA2
57	Dv	404	CDL	CB2-C1-CA2-OA2
57	Ed	204	CDL	CA2-C1-CB2-OB2
57	EB	304	CDL	C53-C54-C55-C56
57	EL	903	CDL	C34-C35-C36-C37
57	Do	501	CDL	C11-C12-C13-C14
58	DA	706	PC1	C37-C38-C39-C3A
60	DI	1101	LPP	C18-C19-C20-C21
58	DV	406	PC1	O31-C31-C32-C33
57	DV	403	CDL	C71-CB7-OB8-CB6
57	Ds	405	CDL	C12-C13-C14-C15
60	DI	1101	LPP	C39-C40-C41-C42
57	EU	101	CDL	C40-C41-C42-C43
57	Dg	201	CDL	C12-C13-C14-C15
57	Dj	401	CDL	C11-C12-C13-C14
57	Dx	1203	CDL	C40-C41-C42-C43
57	DQ	1502	CDL	OB5-CB3-CB4-CB6
57	DS	405	CDL	OB5-CB3-CB4-CB6
57	DX	307	CDL	OB5-CB3-CB4-CB6
57	EH	202	CDL	OA5-CA3-CA4-CA6
57	EO	202	CDL	OA5-CA3-CA4-CA6
57	Da	709	CDL	OB5-CB3-CB4-CB6
57	Dj	403	CDL	OB5-CB3-CB4-CB6
57	Dm	501	CDL	OB5-CB3-CB4-CB6
57	El	901	CDL	OA5-CA3-CA4-CA6
58	Dx	1202	PC1	O11-C1-C2-C3
59	DS	403	3PE	O11-C1-C2-C3
59	Dg	204	3PE	O11-C1-C2-C3
58	DY	302	PC1	O32-C31-O31-C3
57	DR	402	CDL	C41-C42-C43-C44
59	DC	606	3PE	C2A-C2B-C2C-C2D
57	DN	504	CDL	C11-C12-C13-C14
57	DQ	1504	CDL	C57-C58-C59-C60
58	Da	706	PC1	C37-C38-C39-C3A
57	DN	501	CDL	C31-CA7-OA8-CA6
58	EO	206	PC1	C32-C31-O31-C3
57	DQ	1501	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
57	DX	301	CDL	C40-C41-C42-C43
58	Db	702	PC1	C3E-C3F-C3G-C3H
57	DU	403	CDL	OB9-CB7-OB8-CB6
57	Ed	205	CDL	OB9-CB7-OB8-CB6
58	DC	603	PC1	O32-C31-O31-C3
65	EL	906	UQ8	C1-C6-C7-C8
57	Du	403	CDL	C34-C35-C36-C37
59	Dc	606	3PE	C22-C21-O21-C2
59	Dj	407	3PE	O22-C21-O21-C2
57	EL	901	CDL	C11-C12-C13-C14
68	Er	201	ATP	PG-O3B-PB-O3A
58	DC	605	PC1	O32-C31-O31-C3
59	Ds	401	3PE	C38-C39-C3A-C3B
57	Dm	501	CDL	C11-C12-C13-C14
57	Di	701	CDL	C79-C80-C81-C82
57	DG	201	CDL	CB3-CB4-OB6-CB5
57	DI	701	CDL	CA6-CA4-OA6-CA5
57	DJ	305	CDL	CB6-CB4-OB6-CB5
57	DZ	501	CDL	CB6-CB4-OB6-CB5
57	EB	302	CDL	CA6-CA4-OA6-CA5
57	Dg	201	CDL	CA3-CA4-OA6-CA5
57	Dn	502	CDL	CA6-CA4-OA6-CA5
57	Dq	403	CDL	CA6-CA4-OA6-CA5
57	Dy	301	CDL	CB3-CB4-OB6-CB5
57	Dz	501	CDL	CB6-CB4-OB6-CB5
57	Ea	301	CDL	CA6-CA4-OA6-CA5
57	Eh	1601	CDL	CB3-CB4-OB6-CB5
59	Eo	203	3PE	C3-C2-O21-C21
58	Dy	302	PC1	O32-C31-O31-C3
57	DV	402	CDL	C42-C43-C44-C45
57	Dj	402	CDL	C56-C57-C58-C59
57	DU	401	CDL	C13-C14-C15-C16
57	DV	402	CDL	C16-C17-C18-C19
58	DB	702	PC1	C3B-C3C-C3D-C3E
59	Dc	606	3PE	C3B-C3C-C3D-C3E
65	DS	404	UQ8	C5-C4-O4-C4M
65	Ed	202	UQ8	C2-C3-O3-C3M
57	Dn	505	CDL	OA9-CA7-OA8-CA6
57	Ea	301	CDL	OB9-CB7-OB8-CB6
57	Eg	101	CDL	OB9-CB7-OB8-CB6
57	DR	403	CDL	O1-C1-CB2-OB2
57	Dv	403	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
57	El	902	CDL	O1-C1-CA2-OA2
59	Da	708	3PE	C3A-C3B-C3C-C3D
57	Dj	401	CDL	CA5-C11-C12-C13
57	Dx	1203	CDL	C64-C65-C66-C67
57	DJ	304	CDL	OB7-CB5-OB6-CB4
59	DJ	301	3PE	O22-C21-O21-C2
57	DG	201	CDL	OA5-CA3-CA4-OA6
57	DI	701	CDL	OB5-CB3-CB4-OB6
57	DO	501	CDL	OA5-CA3-CA4-OA6
57	DQ	1504	CDL	OB5-CB3-CB4-OB6
57	DS	405	CDL	OA5-CA3-CA4-OA6
57	DV	404	CDL	OA5-CA3-CA4-OA6
57	EB	302	CDL	OA5-CA3-CA4-OA6
57	ED	601	CDL	OB5-CB3-CB4-OB6
57	EL	901	CDL	OB5-CB3-CB4-OB6
57	EL	904	CDL	OA5-CA3-CA4-OA6
57	EO	202	CDL	OA5-CA3-CA4-OA6
57	Da	705	CDL	OB5-CB3-CB4-OB6
57	Dj	402	CDL	OB5-CB3-CB4-OB6
57	Dm	501	CDL	OA5-CA3-CA4-OA6
57	Dm	501	CDL	OB5-CB3-CB4-OB6
57	Do	501	CDL	OA5-CA3-CA4-OA6
57	Dv	404	CDL	OA5-CA3-CA4-OA6
57	Eg	101	CDL	OB5-CB3-CB4-OB6
57	El	901	CDL	OA5-CA3-CA4-OA6
57	Eu	101	CDL	OA5-CA3-CA4-OA6
58	Dc	603	PC1	O11-C1-C2-O21
58	Dg	203	PC1	O11-C1-C2-O21
58	Di	702	PC1	O11-C1-C2-O21
59	Da	708	3PE	O11-C1-C2-O21
59	El	905	3PE	O11-C1-C2-O21
57	DZ	501	CDL	C11-C12-C13-C14
57	DG	201	CDL	CB3-CB4-CB6-OB8
57	DI	701	CDL	CA3-CA4-CA6-OA8
57	DJ	302	CDL	CA3-CA4-CA6-OA8
57	DR	402	CDL	CA3-CA4-CA6-OA8
57	EI	401	CDL	CA3-CA4-CA6-OA8
57	EL	903	CDL	CB3-CB4-CB6-OB8
57	Da	705	CDL	CA3-CA4-CA6-OA8
57	Di	701	CDL	CA3-CA4-CA6-OA8
57	Dn	501	CDL	CA3-CA4-CA6-OA8
57	Eg	101	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
57	El	901	CDL	CB3-CB4-CB6-OB8
57	Ep	701	CDL	CB3-CB4-CB6-OB8
58	DA	706	PC1	C1-C2-C3-O31
58	DC	602	PC1	C1-C2-C3-O31
58	DV	405	PC1	C1-C2-C3-O31
58	Dc	602	PC1	C1-C2-C3-O31
58	Dv	405	PC1	C1-C2-C3-O31
58	Dv	406	PC1	C1-C2-C3-O31
59	DS	401	3PE	C1-C2-C3-O31
57	Dn	502	CDL	C11-CA5-OA6-CA4
57	DA	709	CDL	CB7-C71-C72-C73
57	Dn	501	CDL	CB7-C71-C72-C73
58	DS	406	PC1	C32-C33-C34-C35
57	DJ	304	CDL	C58-C59-C60-C61
57	EL	903	CDL	C78-C79-C80-C81
57	Dg	201	CDL	C83-C84-C85-C86
57	Dj	402	CDL	C54-C55-C56-C57
58	DS	406	PC1	C29-C2A-C2B-C2C
57	Dj	403	CDL	C79-C80-C81-C82
58	EO	206	PC1	C2A-C2B-C2C-C2D
59	DR	401	3PE	C35-C36-C37-C38
65	EN	1204	UQ8	C40-C39-C41-C42
57	El	902	CDL	C52-C53-C54-C55
58	DB	702	PC1	C12-C11-O13-P
58	Db	702	PC1	C12-C11-O13-P
58	Dv	406	PC1	C12-C11-O13-P
58	Dx	1202	PC1	C12-C11-O13-P
59	DX	303	3PE	C12-C11-O13-P
59	Dg	204	3PE	C12-C11-O13-P
59	Dx	1205	3PE	C12-C11-O13-P
57	DH	201	CDL	C21-C22-C23-C24
57	DA	705	CDL	OB6-CB4-CB6-OB8
57	DA	709	CDL	OB6-CB4-CB6-OB8
57	DD	703	CDL	OA6-CA4-CA6-OA8
57	DG	202	CDL	OA6-CA4-CA6-OA8
57	DH	201	CDL	OB6-CB4-CB6-OB8
57	DR	402	CDL	OA6-CA4-CA6-OA8
57	DU	401	CDL	OB6-CB4-CB6-OB8
57	ED	601	CDL	OA6-CA4-CA6-OA8
57	EH	201	CDL	OB6-CB4-CB6-OB8
57	EK	201	CDL	OA6-CA4-CA6-OA8
57	EN	1201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
57	EU	101	CDL	OB6-CB4-CB6-OB8
57	Dd	704	CDL	OB6-CB4-CB6-OB8
57	Dd	706	CDL	OB6-CB4-CB6-OB8
57	Di	701	CDL	OA6-CA4-CA6-OA8
57	Dm	501	CDL	OA6-CA4-CA6-OA8
57	Dn	501	CDL	OA6-CA4-CA6-OA8
57	Dn	505	CDL	OB6-CB4-CB6-OB8
57	Du	402	CDL	OA6-CA4-CA6-OA8
57	Dv	402	CDL	OB6-CB4-CB6-OB8
57	Dy	301	CDL	OA6-CA4-CA6-OA8
57	Eu	101	CDL	OB6-CB4-CB6-OB8
58	DC	602	PC1	O21-C2-C3-O31
58	DV	405	PC1	O21-C2-C3-O31
58	DX	302	PC1	O21-C2-C3-O31
58	DY	302	PC1	O21-C2-C3-O31
58	Dc	602	PC1	O21-C2-C3-O31
58	Dc	605	PC1	O21-C2-C3-O31
58	Eo	204	PC1	O21-C2-C3-O31
59	Dc	606	3PE	O21-C2-C3-O31
59	Eo	202	3PE	O21-C2-C3-O31
57	El	903	CDL	C31-CA7-OA8-CA6
58	DA	707	PC1	C32-C31-O31-C3
58	Dg	203	PC1	C32-C31-O31-C3
57	EL	903	CDL	C79-C80-C81-C82
58	Db	702	PC1	C38-C39-C3A-C3B
57	Dh	201	CDL	OA9-CA7-OA8-CA6
57	Da	709	CDL	C39-C40-C41-C42
59	Ds	403	3PE	C27-C28-C29-C2A
58	EO	206	PC1	C11-C12-N-C13
58	EO	206	PC1	C11-C12-N-C15
58	Eo	204	PC1	C11-C12-N-C15
57	Dv	402	CDL	C77-C78-C79-C80
57	DV	403	CDL	OB9-CB7-OB8-CB6
57	Dq	401	CDL	OA9-CA7-OA8-CA6
57	EO	202	CDL	C77-C78-C79-C80
59	EL	905	3PE	C2B-C2C-C2D-C2E
57	Dj	403	CDL	C51-CB5-OB6-CB4
57	Dm	501	CDL	C52-C51-CB5-OB6
57	EB	302	CDL	C31-CA7-OA8-CA6
57	Dj	403	CDL	C71-CB7-OB8-CB6
58	DX	306	PC1	C32-C31-O31-C3
57	DA	705	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
57	DX	307	CDL	C1-CB2-OB2-PB2
57	EO	202	CDL	CA4-CA3-OA5-PA1
57	Dx	1203	CDL	CA4-CA3-OA5-PA1
57	Ea	301	CDL	CA4-CA3-OA5-PA1
57	DG	201	CDL	C58-C59-C60-C61
57	EO	202	CDL	C63-C64-C65-C66
57	Eu	101	CDL	C40-C41-C42-C43
58	EO	201	PC1	C28-C29-C2A-C2B
57	DU	402	CDL	C42-C43-C44-C45
58	DB	702	PC1	O13-C11-C12-N
58	DC	604	PC1	O13-C11-C12-N
58	DS	406	PC1	O13-C11-C12-N
58	DV	406	PC1	O13-C11-C12-N
58	EO	205	PC1	O13-C11-C12-N
58	Db	702	PC1	O13-C11-C12-N
58	Dc	604	PC1	O13-C11-C12-N
58	Dc	605	PC1	O13-C11-C12-N
58	Dv	406	PC1	O13-C11-C12-N
58	Dv	407	PC1	O13-C11-C12-N
58	El	904	PC1	O13-C11-C12-N
57	Dg	202	CDL	CA4-CA6-OA8-CA7
54	DA	702	HEA	C2D-C3D-CAD-CBD
59	DC	607	3PE	C3B-C3C-C3D-C3E
57	EH	201	CDL	OB7-CB5-OB6-CB4
57	Dd	705	CDL	CA2-C1-CB2-OB2
57	Dj	408	CDL	CB2-C1-CA2-OA2
57	DS	402	CDL	C72-C73-C74-C75
58	DS	407	PC1	C3C-C3D-C3E-C3F
57	Dm	501	CDL	C31-CA7-OA8-CA6
57	El	901	CDL	C64-C65-C66-C67
57	EL	903	CDL	C52-C53-C54-C55
58	EO	206	PC1	O32-C31-O31-C3
57	Dd	705	CDL	C38-C39-C40-C41
58	Dc	602	PC1	C3F-C3G-C3H-C3I
58	DC	608	PC1	C3C-C3D-C3E-C3F
57	DJ	304	CDL	C11-C12-C13-C14
57	DV	404	CDL	C31-C32-C33-C34
57	DN	501	CDL	OA9-CA7-OA8-CA6
57	Do	501	CDL	C76-C77-C78-C79
57	Dv	402	CDL	C12-C13-C14-C15
57	Dx	1201	CDL	C38-C39-C40-C41
57	EO	202	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
57	Eh	1601	CDL	C13-C14-C15-C16
57	Dn	507	CDL	C11-C12-C13-C14
57	Dr	403	CDL	C71-CB7-OB8-CB6
57	DQ	1501	CDL	C81-C82-C83-C84
57	Dr	402	CDL	C61-C62-C63-C64
57	El	901	CDL	C18-C19-C20-C21
58	EB	303	PC1	C2E-C2F-C2G-C2H
58	Dv	406	PC1	C29-C2A-C2B-C2C
60	Dn	506	LPP	C38-C39-C40-C41
58	DC	602	PC1	C3F-C3G-C3H-C3I
65	Ed	202	UQ8	C40-C39-C41-C42
57	Dr	402	CDL	C13-C14-C15-C16
57	DZ	501	CDL	C73-C74-C75-C76
57	EN	1201	CDL	C11-C12-C13-C14
57	Dh	201	CDL	C21-C22-C23-C24
57	DD	702	CDL	C23-C24-C25-C26
57	DI	701	CDL	OB5-CB3-CB4-CB6
57	DQ	1501	CDL	OB5-CB3-CB4-CB6
57	DQ	1504	CDL	OB5-CB3-CB4-CB6
57	DV	404	CDL	OA5-CA3-CA4-CA6
57	DZ	501	CDL	OB5-CB3-CB4-CB6
57	EA	301	CDL	OA5-CA3-CA4-CA6
57	ED	601	CDL	OB5-CB3-CB4-CB6
57	EL	902	CDL	OA5-CA3-CA4-CA6
57	EL	902	CDL	OB5-CB3-CB4-CB6
57	EL	904	CDL	OA5-CA3-CA4-CA6
57	EU	101	CDL	OA5-CA3-CA4-CA6
57	Dd	704	CDL	OA5-CA3-CA4-CA6
57	Dn	503	CDL	OB5-CB3-CB4-CB6
57	Dv	404	CDL	OA5-CA3-CA4-CA6
57	Eg	101	CDL	OB5-CB3-CB4-CB6
57	Eh	1601	CDL	OA5-CA3-CA4-CA6
59	DX	303	3PE	O11-C1-C2-C3
59	Dx	1205	3PE	O11-C1-C2-C3
59	El	905	3PE	O11-C1-C2-C3
58	DC	603	PC1	C3B-C3C-C3D-C3E
57	Dn	502	CDL	OA7-CA5-OA6-CA4
57	Ek	201	CDL	OB7-CB5-OB6-CB4
59	Dc	606	3PE	O22-C21-O21-C2
57	Dq	403	CDL	C17-C18-C19-C20
57	Du	402	CDL	C14-C15-C16-C17
58	Dc	605	PC1	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
58	Eb	301	PC1	C3C-C3D-C3E-C3F
57	DA	705	CDL	C15-C16-C17-C18
57	DG	202	CDL	C63-C64-C65-C66
57	DV	403	CDL	C82-C83-C84-C85
58	EO	201	PC1	C25-C26-C27-C28
59	DS	403	3PE	C34-C35-C36-C37
57	Du	404	CDL	O1-C1-CB2-OB2
58	Dg	203	PC1	O32-C31-O31-C3
57	El	901	CDL	C31-CA7-OA8-CA6
59	Dj	407	3PE	C29-C2A-C2B-C2C
59	Ds	401	3PE	C34-C35-C36-C37
57	Ea	301	CDL	C11-C12-C13-C14
57	DR	403	CDL	C17-C18-C19-C20
57	EB	302	CDL	OA9-CA7-OA8-CA6
57	Dj	403	CDL	OB9-CB7-OB8-CB6
57	Dm	501	CDL	OA9-CA7-OA8-CA6
57	El	903	CDL	OA9-CA7-OA8-CA6
58	DA	707	PC1	O32-C31-O31-C3
58	DX	306	PC1	O32-C31-O31-C3
58	Dx	1204	PC1	C31-C32-C33-C34
57	DD	703	CDL	CB4-CB3-OB5-PB2
57	DG	201	CDL	C1-CA2-OA2-PA1
57	DR	403	CDL	CA4-CA3-OA5-PA1
57	DR	403	CDL	C1-CB2-OB2-PB2
57	DV	402	CDL	C1-CA2-OA2-PA1
57	DX	301	CDL	CA4-CA3-OA5-PA1
57	EA	301	CDL	CA4-CA3-OA5-PA1
57	Dh	202	CDL	C1-CB2-OB2-PB2
57	Dn	502	CDL	C1-CB2-OB2-PB2
57	Dv	402	CDL	C1-CA2-OA2-PA1
57	Dv	404	CDL	C1-CA2-OA2-PA1
57	Dz	501	CDL	C1-CB2-OB2-PB2
57	Ed	204	CDL	C1-CA2-OA2-PA1
57	Ek	201	CDL	C1-CA2-OA2-PA1
58	Db	702	PC1	C2-C1-O11-P
59	Da	708	3PE	C2-C1-O11-P
60	DN	502	LPP	C7-C6-O5-P1
58	DX	302	PC1	C23-C24-C25-C26
57	Dq	404	CDL	OB7-CB5-OB6-CB4
59	EL	905	3PE	O22-C21-O21-C2
57	DC	601	CDL	OB5-CB3-CB4-OB6
57	DD	703	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
57	DJ	304	CDL	OA5-CA3-CA4-OA6
57	DQ	1502	CDL	OB5-CB3-CB4-OB6
57	EH	202	CDL	OA5-CA3-CA4-OA6
57	EH	202	CDL	OB5-CB3-CB4-OB6
57	EL	902	CDL	OB5-CB3-CB4-OB6
57	EU	101	CDL	OA5-CA3-CA4-OA6
57	Da	709	CDL	OB5-CB3-CB4-OB6
57	Dd	704	CDL	OA5-CA3-CA4-OA6
57	Dd	705	CDL	OA5-CA3-CA4-OA6
57	Dj	405	CDL	OB5-CB3-CB4-OB6
57	Dn	502	CDL	OB5-CB3-CB4-OB6
57	Dn	503	CDL	OB5-CB3-CB4-OB6
57	Dq	402	CDL	OA5-CA3-CA4-OA6
57	Dq	402	CDL	OB5-CB3-CB4-OB6
57	Dq	404	CDL	OB5-CB3-CB4-OB6
57	Eh	1601	CDL	OA5-CA3-CA4-OA6
58	DG	203	PC1	O11-C1-C2-O21
58	Db	702	PC1	O11-C1-C2-O21
59	Dx	1206	3PE	O11-C1-C2-O21
57	Da	705	CDL	C62-C63-C64-C65
57	Du	404	CDL	C13-C14-C15-C16
58	EO	201	PC1	C32-C33-C34-C35
57	Dq	404	CDL	C51-CB5-OB6-CB4
57	Ed	205	CDL	C51-CB5-OB6-CB4
58	DI	702	PC1	C11-C12-N-C15
58	DS	407	PC1	C11-C12-N-C13
57	DX	307	CDL	C78-C79-C80-C81
57	Dd	704	CDL	C74-C75-C76-C77
57	Di	701	CDL	C33-C34-C35-C36
57	Dg	202	CDL	C13-C14-C15-C16
57	Dj	408	CDL	C52-C53-C54-C55
58	Dv	405	PC1	C3B-C3C-C3D-C3E
58	Eb	302	PC1	C2E-C2F-C2G-C2H
57	EL	902	CDL	C73-C74-C75-C76
54	Da	702	HEA	C4D-C3D-CAD-CBD
59	El	905	3PE	C33-C34-C35-C36
57	Dr	403	CDL	OB9-CB7-OB8-CB6
57	El	901	CDL	OA9-CA7-OA8-CA6
57	DC	601	CDL	OA6-CA4-CA6-OA8
57	DG	202	CDL	OB6-CB4-CB6-OB8
57	DI	701	CDL	OA6-CA4-CA6-OA8
57	DM	502	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
57	DN	505	CDL	OA6-CA4-CA6-OA8
57	DN	505	CDL	OB6-CB4-CB6-OB8
57	DU	401	CDL	OA6-CA4-CA6-OA8
57	EB	304	CDL	OB6-CB4-CB6-OB8
57	EL	903	CDL	OA6-CA4-CA6-OA8
57	Dc	601	CDL	OA6-CA4-CA6-OA8
57	Dd	702	CDL	OA6-CA4-CA6-OA8
57	Dg	202	CDL	OB6-CB4-CB6-OB8
57	Dh	201	CDL	OB6-CB4-CB6-OB8
57	Du	403	CDL	OB6-CB4-CB6-OB8
57	Ep	701	CDL	OB6-CB4-CB6-OB8
58	DC	605	PC1	O21-C2-C3-O31
58	DC	608	PC1	O21-C2-C3-O31
58	Dv	405	PC1	O21-C2-C3-O31
58	Dv	406	PC1	O21-C2-C3-O31
58	Eo	201	PC1	O21-C2-C3-O31
59	EL	905	3PE	O21-C2-C3-O31
57	Dr	403	CDL	C17-C18-C19-C20
57	DX	307	CDL	CB2-C1-CA2-OA2
59	Dg	204	3PE	C2A-C2B-C2C-C2D
57	DG	202	CDL	CA3-CA4-CA6-OA8
57	DH	201	CDL	CB3-CB4-CB6-OB8
57	DN	505	CDL	CA3-CA4-CA6-OA8
57	DS	402	CDL	CB3-CB4-CB6-OB8
57	ED	601	CDL	CA3-CA4-CA6-OA8
57	EN	1202	CDL	CB3-CB4-CB6-OB8
57	Dd	702	CDL	CB3-CB4-CB6-OB8
57	Dh	201	CDL	CB3-CB4-CB6-OB8
57	Dm	501	CDL	CA3-CA4-CA6-OA8
57	En	1201	CDL	CA3-CA4-CA6-OA8
59	Dc	606	3PE	C1-C2-C3-O31
59	Dr	401	3PE	C1-C2-C3-O31
59	Dx	1207	3PE	C1-C2-C3-O31
57	Dn	507	CDL	C37-C38-C39-C40
58	Dg	203	PC1	C23-C24-C25-C26
57	DJ	307	CDL	C72-C71-CB7-OB8
65	EN	1204	UQ8	C38-C39-C41-C42
57	EN	1202	CDL	C37-C38-C39-C40
57	Da	705	CDL	C34-C35-C36-C37
57	EH	201	CDL	C23-C24-C25-C26
57	EL	901	CDL	C55-C56-C57-C58
57	El	901	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
57	Ep	701	CDL	C84-C85-C86-C87
57	EO	202	CDL	C58-C59-C60-C61
57	Dr	402	CDL	C59-C60-C61-C62
57	DX	307	CDL	C71-CB7-OB8-CB6
57	Dj	404	CDL	C31-CA7-OA8-CA6
57	DR	402	CDL	C13-C14-C15-C16
57	Dv	401	CDL	C78-C79-C80-C81
58	Eo	205	PC1	C3D-C3E-C3F-C3G
57	DA	705	CDL	C62-C63-C64-C65
57	Dh	202	CDL	C71-C72-C73-C74
57	EN	1202	CDL	C58-C59-C60-C61
57	Dx	1203	CDL	C14-C15-C16-C17
57	DX	307	CDL	OB9-CB7-OB8-CB6
57	Dj	403	CDL	OB7-CB5-OB6-CB4
65	EL	906	UQ8	C5-C4-O4-C4M
65	El	906	UQ8	C2-C3-O3-C3M
57	DA	709	CDL	C76-C77-C78-C79
57	Du	401	CDL	C60-C61-C62-C63
58	Dv	406	PC1	C32-C33-C34-C35
57	Dd	704	CDL	C21-C22-C23-C24
57	EI	401	CDL	C52-C51-CB5-OB6
59	Ds	403	3PE	C28-C29-C2A-C2B
57	DA	709	CDL	CA3-OA5-PA1-OA2
57	DA	709	CDL	CA3-OA5-PA1-OA3
57	DA	710	CDL	CB2-OB2-PB2-OB3
57	DC	601	CDL	CA2-OA2-PA1-OA5
57	DC	601	CDL	CB2-OB2-PB2-OB3
57	DD	703	CDL	CB2-OB2-PB2-OB3
57	DD	704	CDL	CA2-OA2-PA1-OA4
57	DD	704	CDL	CA3-OA5-PA1-OA3
57	DD	704	CDL	CB3-OB5-PB2-OB2
57	DG	201	CDL	CB3-OB5-PB2-OB2
57	DG	202	CDL	CA3-OA5-PA1-OA3
57	DH	201	CDL	CB2-OB2-PB2-OB3
57	DJ	302	CDL	CA2-OA2-PA1-OA3
57	DJ	303	CDL	CA3-OA5-PA1-OA3
57	DJ	303	CDL	CB3-OB5-PB2-OB3
57	DJ	304	CDL	CA3-OA5-PA1-OA3
57	DJ	305	CDL	CB3-OB5-PB2-OB3
57	DM	502	CDL	CB2-OB2-PB2-OB3
57	DN	501	CDL	CA3-OA5-PA1-OA2
57	DN	501	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
57	DN	504	CDL	CB3-OB5-PB2-OB2
57	DN	505	CDL	CA2-OA2-PA1-OA3
57	DN	505	CDL	CA3-OA5-PA1-OA2
57	DN	505	CDL	CA3-OA5-PA1-OA3
57	DN	505	CDL	CB3-OB5-PB2-OB3
57	DO	501	CDL	CA3-OA5-PA1-OA3
57	DO	501	CDL	CB3-OB5-PB2-OB3
57	DQ	1501	CDL	CB3-OB5-PB2-OB4
57	DQ	1502	CDL	CA2-OA2-PA1-OA3
57	DR	402	CDL	CB3-OB5-PB2-OB2
57	DS	405	CDL	CA2-OA2-PA1-OA4
57	DS	405	CDL	CB3-OB5-PB2-OB4
57	DU	401	CDL	CA2-OA2-PA1-OA4
57	DU	403	CDL	CB3-OB5-PB2-OB4
57	DU	404	CDL	CB2-OB2-PB2-OB4
57	DV	401	CDL	CB2-OB2-PB2-OB3
57	DV	402	CDL	CA3-OA5-PA1-OA2
57	DV	402	CDL	CA3-OA5-PA1-OA3
57	DV	403	CDL	CB2-OB2-PB2-OB3
57	DX	301	CDL	CB2-OB2-PB2-OB3
57	DX	301	CDL	CB3-OB5-PB2-OB2
57	DX	301	CDL	CB3-OB5-PB2-OB3
57	DY	301	CDL	CA2-OA2-PA1-OA3
57	DY	301	CDL	CB3-OB5-PB2-OB3
57	DZ	501	CDL	CA2-OA2-PA1-OA3
57	EA	301	CDL	CB2-OB2-PB2-OB4
57	EB	302	CDL	CB3-OB5-PB2-OB3
57	EB	304	CDL	CB3-OB5-PB2-OB3
57	ED	601	CDL	CA2-OA2-PA1-OA3
57	EH	202	CDL	CA3-OA5-PA1-OA3
57	EH	202	CDL	CB3-OB5-PB2-OB3
57	EI	401	CDL	CB3-OB5-PB2-OB4
57	EK	201	CDL	CA2-OA2-PA1-OA3
57	EK	201	CDL	CA3-OA5-PA1-OA2
57	EK	201	CDL	CA3-OA5-PA1-OA3
57	EK	201	CDL	CA3-OA5-PA1-OA4
57	EL	902	CDL	CB3-OB5-PB2-OB2
57	EL	903	CDL	CB2-OB2-PB2-OB3
57	EL	903	CDL	CB2-OB2-PB2-OB5
57	EL	904	CDL	CB2-OB2-PB2-OB5
57	EN	1201	CDL	CB2-OB2-PB2-OB3
57	EN	1202	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
57	EU	101	CDL	CA2-OA2-PA1-OA3
57	EU	101	CDL	CA3-OA5-PA1-OA4
57	Da	705	CDL	CB3-OB5-PB2-OB3
57	Da	709	CDL	CA3-OA5-PA1-OA3
57	Da	709	CDL	CB3-OB5-PB2-OB4
57	Dc	601	CDL	CB2-OB2-PB2-OB3
57	Dd	704	CDL	CB2-OB2-PB2-OB3
57	Dg	202	CDL	CA3-OA5-PA1-OA3
57	Dh	202	CDL	CB2-OB2-PB2-OB3
57	Dh	202	CDL	CB3-OB5-PB2-OB3
57	Di	701	CDL	CB3-OB5-PB2-OB2
57	Dj	401	CDL	CB3-OB5-PB2-OB3
57	Dj	403	CDL	CA3-OA5-PA1-OA2
57	Dj	403	CDL	CA3-OA5-PA1-OA3
57	Dj	403	CDL	CB2-OB2-PB2-OB5
57	Dj	403	CDL	CB3-OB5-PB2-OB3
57	Dj	404	CDL	CA2-OA2-PA1-OA3
57	Dj	404	CDL	CA3-OA5-PA1-OA2
57	Dj	408	CDL	CB2-OB2-PB2-OB3
57	Dm	501	CDL	CA3-OA5-PA1-OA3
57	Dn	501	CDL	CA3-OA5-PA1-OA2
57	Dn	501	CDL	CB2-OB2-PB2-OB3
57	Dn	501	CDL	CB3-OB5-PB2-OB3
57	Dn	502	CDL	CB3-OB5-PB2-OB3
57	Dn	503	CDL	CA2-OA2-PA1-OA3
57	Do	501	CDL	CB3-OB5-PB2-OB3
57	Dq	401	CDL	CB3-OB5-PB2-OB3
57	Dq	402	CDL	CA2-OA2-PA1-OA3
57	Dq	403	CDL	CA3-OA5-PA1-OA2
57	Dq	403	CDL	CB3-OB5-PB2-OB4
57	Dq	404	CDL	CA3-OA5-PA1-OA3
57	Dq	404	CDL	CB3-OB5-PB2-OB3
57	Ds	405	CDL	CA2-OA2-PA1-OA4
57	Ds	405	CDL	CB3-OB5-PB2-OB2
57	Ds	405	CDL	CB3-OB5-PB2-OB4
57	Du	401	CDL	CA2-OA2-PA1-OA4
57	Du	401	CDL	CA3-OA5-PA1-OA2
57	Du	403	CDL	CA2-OA2-PA1-OA5
57	Du	403	CDL	CA3-OA5-PA1-OA2
57	Du	403	CDL	CA3-OA5-PA1-OA3
57	Du	403	CDL	CA3-OA5-PA1-OA4
57	Du	404	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
57	Dv	403	CDL	CA3-OA5-PA1-OA3
57	Dv	404	CDL	CB2-OB2-PB2-OB5
57	Dx	1201	CDL	CB3-OB5-PB2-OB2
57	Dx	1201	CDL	CB3-OB5-PB2-OB3
57	Dx	1203	CDL	CA3-OA5-PA1-OA2
57	Dx	1203	CDL	CA3-OA5-PA1-OA3
57	Dx	1203	CDL	CB3-OB5-PB2-OB3
57	Dy	301	CDL	CA2-OA2-PA1-OA3
57	Dz	501	CDL	CA2-OA2-PA1-OA3
57	Ea	301	CDL	CA2-OA2-PA1-OA3
57	Ea	301	CDL	CB2-OB2-PB2-OB4
57	Ed	204	CDL	CA2-OA2-PA1-OA3
57	Ed	204	CDL	CA3-OA5-PA1-OA2
57	Ed	204	CDL	CB3-OB5-PB2-OB3
57	Ed	205	CDL	CA3-OA5-PA1-OA4
57	Eh	1601	CDL	CA2-OA2-PA1-OA3
57	Ei	401	CDL	CA2-OA2-PA1-OA5
57	Ei	401	CDL	CB3-OB5-PB2-OB3
57	El	902	CDL	CB2-OB2-PB2-OB3
57	El	902	CDL	CB2-OB2-PB2-OB5
57	El	903	CDL	CA3-OA5-PA1-OA3
57	El	903	CDL	CB2-OB2-PB2-OB4
57	En	1201	CDL	CA2-OA2-PA1-OA5
57	En	1201	CDL	CB2-OB2-PB2-OB3
57	En	1202	CDL	CB2-OB2-PB2-OB3
57	Eu	101	CDL	CA3-OA5-PA1-OA3
58	DC	602	PC1	C11-O13-P-O12
58	DC	602	PC1	C11-O13-P-O14
58	DC	602	PC1	C11-O13-P-O11
58	DC	603	PC1	C11-O13-P-O14
58	DC	604	PC1	C1-O11-P-O13
58	DC	605	PC1	C1-O11-P-O12
58	DI	702	PC1	C11-O13-P-O12
58	DI	702	PC1	C11-O13-P-O14
58	DI	702	PC1	C11-O13-P-O11
58	DJ	306	PC1	C11-O13-P-O14
58	DJ	306	PC1	C1-O11-P-O14
58	DQ	1503	PC1	C11-O13-P-O14
58	DS	407	PC1	C11-O13-P-O12
58	DS	407	PC1	C1-O11-P-O14
58	DS	407	PC1	C11-C12-N-C15
58	DV	405	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
58	DV	405	PC1	C1-O11-P-O14
58	DV	406	PC1	C11-O13-P-O14
58	DV	406	PC1	C1-O11-P-O14
58	DV	407	PC1	C11-O13-P-O11
58	DX	302	PC1	C1-O11-P-O14
58	DX	302	PC1	C1-O11-P-O13
58	DX	306	PC1	C11-O13-P-O14
58	DX	306	PC1	C11-O13-P-O11
58	EB	301	PC1	C1-O11-P-O12
58	EB	301	PC1	C1-O11-P-O14
58	EB	301	PC1	C1-O11-P-O13
58	EO	201	PC1	C11-O13-P-O14
58	EO	206	PC1	C1-O11-P-O14
58	EO	206	PC1	C1-O11-P-O13
58	Da	706	PC1	C11-O13-P-O12
58	Da	706	PC1	C11-O13-P-O11
58	Db	702	PC1	C11-O13-P-O14
58	Dc	602	PC1	C11-O13-P-O12
58	Dc	602	PC1	C11-O13-P-O14
58	Dc	602	PC1	C11-O13-P-O11
58	Dc	603	PC1	C11-O13-P-O14
58	Dc	604	PC1	C11-O13-P-O14
58	Dc	604	PC1	C1-O11-P-O14
58	Dc	604	PC1	C1-O11-P-O13
58	Dc	605	PC1	C1-O11-P-O12
58	Di	702	PC1	C11-O13-P-O14
58	Di	702	PC1	C11-O13-P-O11
58	Di	702	PC1	C1-O11-P-O12
58	Di	702	PC1	C11-C12-N-C15
58	Dj	406	PC1	C11-O13-P-O14
58	Dj	406	PC1	C1-O11-P-O14
58	Dq	405	PC1	C11-O13-P-O14
58	Dv	405	PC1	C11-O13-P-O12
58	Dv	405	PC1	C1-O11-P-O14
58	Dv	407	PC1	C11-O13-P-O14
58	Dv	408	PC1	C11-O13-P-O11
58	Dv	408	PC1	C1-O11-P-O14
58	Dx	1208	PC1	C11-O13-P-O14
58	Dy	302	PC1	C1-O11-P-O14
58	Eb	301	PC1	C1-O11-P-O12
58	Eb	301	PC1	C1-O11-P-O13
58	Ef	1001	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
58	Eo	201	PC1	C11-O13-P-O14
59	DA	708	3PE	O13-C11-C12-N
59	DC	607	3PE	C1-O11-P-O12
59	DC	607	3PE	C1-O11-P-O13
59	DC	607	3PE	C11-O13-P-O12
59	DG	204	3PE	C1-O11-P-O12
59	DG	204	3PE	C1-O11-P-O13
59	DG	204	3PE	C1-O11-P-O14
59	DG	204	3PE	O13-C11-C12-N
59	DS	403	3PE	C1-O11-P-O12
59	DX	304	3PE	C11-O13-P-O12
59	EL	905	3PE	C11-O13-P-O12
59	EN	1203	3PE	C11-O13-P-O11
59	Da	708	3PE	O13-C11-C12-N
59	Dd	703	3PE	C11-O13-P-O14
59	Dg	204	3PE	O13-C11-C12-N
59	Dr	401	3PE	C11-O13-P-O11
59	Dr	401	3PE	C11-O13-P-O12
59	Ds	403	3PE	C1-O11-P-O12
59	Ds	403	3PE	C11-O13-P-O11
59	Ds	407	3PE	C11-O13-P-O11
59	Dx	1206	3PE	C1-O11-P-O12
59	Dx	1207	3PE	C11-O13-P-O11
59	Dx	1207	3PE	C11-O13-P-O14
59	El	905	3PE	C11-O13-P-O12
59	Eo	202	3PE	C11-O13-P-O14
57	DQ	1504	CDL	C51-C52-C53-C54
57	DV	402	CDL	C76-C77-C78-C79
57	EL	903	CDL	C13-C14-C15-C16
57	DS	405	CDL	C33-C34-C35-C36
57	Dj	404	CDL	C63-C64-C65-C66
58	DG	203	PC1	C23-C24-C25-C26
58	DG	203	PC1	C3B-C3C-C3D-C3E
57	Ei	401	CDL	C52-C51-CB5-OB6
57	Dj	402	CDL	C16-C17-C18-C19
57	DA	705	CDL	CB4-CB3-OB5-PB2
57	DD	702	CDL	C1-CA2-OA2-PA1
57	DG	201	CDL	C1-CB2-OB2-PB2
57	DJ	305	CDL	CB4-CB3-OB5-PB2
57	DN	504	CDL	C1-CB2-OB2-PB2
57	DN	505	CDL	CA4-CA3-OA5-PA1
57	DU	404	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
57	DV	404	CDL	CB4-CB3-OB5-PB2
57	EB	304	CDL	C1-CB2-OB2-PB2
57	ED	604	CDL	C1-CB2-OB2-PB2
57	EN	1202	CDL	C1-CA2-OA2-PA1
57	Dd	706	CDL	CA4-CA3-OA5-PA1
57	Dj	404	CDL	CB4-CB3-OB5-PB2
57	Dn	502	CDL	C1-CA2-OA2-PA1
57	Dn	507	CDL	C1-CB2-OB2-PB2
57	Dq	402	CDL	C1-CA2-OA2-PA1
57	Dr	403	CDL	CA4-CA3-OA5-PA1
57	Dr	403	CDL	C1-CB2-OB2-PB2
57	Du	403	CDL	C1-CA2-OA2-PA1
57	Du	404	CDL	C1-CA2-OA2-PA1
57	Eh	1601	CDL	C1-CA2-OA2-PA1
57	Ei	401	CDL	C1-CB2-OB2-PB2
59	Dc	606	3PE	C2-C1-O11-P
57	Da	705	CDL	C82-C83-C84-C85
54	Da	702	HEA	C2D-C3D-CAD-CBD
57	Dn	505	CDL	C54-C55-C56-C57
57	El	901	CDL	C13-C14-C15-C16
57	Dn	502	CDL	CA5-C11-C12-C13
57	Dr	402	CDL	C53-C54-C55-C56
57	DM	502	CDL	C19-C20-C21-C22
57	DQ	1501	CDL	O1-C1-CA2-OA2
57	DQ	1504	CDL	C61-C62-C63-C64
58	Eo	201	PC1	C2B-C2C-C2D-C2E
57	DA	709	CDL	CB6-CB4-OB6-CB5
57	DC	601	CDL	CB6-CB4-OB6-CB5
57	DD	703	CDL	CA6-CA4-OA6-CA5
57	DD	703	CDL	CB3-CB4-OB6-CB5
57	DJ	303	CDL	CB3-CB4-OB6-CB5
57	DN	501	CDL	CA6-CA4-OA6-CA5
57	DN	504	CDL	CA3-CA4-OA6-CA5
57	DO	501	CDL	CB6-CB4-OB6-CB5
57	DQ	1502	CDL	CB6-CB4-OB6-CB5
57	DQ	1504	CDL	CA6-CA4-OA6-CA5
57	DR	403	CDL	CA6-CA4-OA6-CA5
57	DS	402	CDL	CB3-CB4-OB6-CB5
57	EK	201	CDL	CB3-CB4-OB6-CB5
57	EL	901	CDL	CA3-CA4-OA6-CA5
57	EO	202	CDL	CB3-CB4-OB6-CB5
57	Da	709	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
57	Dc	601	CDL	CB6-CB4-OB6-CB5
57	Di	701	CDL	CA6-CA4-OA6-CA5
57	Dj	405	CDL	CB6-CB4-OB6-CB5
57	Dn	505	CDL	CA6-CA4-OA6-CA5
57	Dn	507	CDL	CA3-CA4-OA6-CA5
57	Dq	402	CDL	CA6-CA4-OA6-CA5
57	Dr	403	CDL	CA6-CA4-OA6-CA5
57	Ds	402	CDL	CB3-CB4-OB6-CB5
57	Du	404	CDL	CA3-CA4-OA6-CA5
57	Dv	404	CDL	CA3-CA4-OA6-CA5
57	Ek	201	CDL	CB3-CB4-OB6-CB5
57	El	903	CDL	CA3-CA4-OA6-CA5
57	En	1202	CDL	CB6-CB4-OB6-CB5
58	Db	702	PC1	C1-C2-O21-C21
58	Dc	605	PC1	C3-C2-O21-C21
58	Dv	406	PC1	C1-C2-O21-C21
58	Eo	205	PC1	C3-C2-O21-C21
59	DC	606	3PE	C1-C2-O21-C21
59	EO	203	3PE	C1-C2-O21-C21
59	EO	204	3PE	C1-C2-O21-C21
59	Dr	401	3PE	C1-C2-O21-C21
57	DR	403	CDL	C34-C35-C36-C37
57	DX	301	CDL	C33-C34-C35-C36
58	Db	702	PC1	C3B-C3C-C3D-C3E
57	Dd	704	CDL	C20-C21-C22-C23
59	El	905	3PE	C2F-C2G-C2H-C2I
58	Eo	204	PC1	C11-C12-N-C14
57	DD	703	CDL	OB5-CB3-CB4-CB6
57	DJ	304	CDL	OA5-CA3-CA4-CA6
57	DS	405	CDL	OA5-CA3-CA4-CA6
57	Du	404	CDL	OB5-CB3-CB4-CB6
57	Dv	403	CDL	OA5-CA3-CA4-CA6
59	Ds	403	3PE	O11-C1-C2-C3
57	DD	704	CDL	C40-C41-C42-C43
57	Dx	1201	CDL	C32-C33-C34-C35
57	Dc	601	CDL	C31-CA7-OA8-CA6
57	Dj	404	CDL	OA9-CA7-OA8-CA6
57	EB	304	CDL	CB5-C51-C52-C53
57	EL	901	CDL	C83-C84-C85-C86
57	EK	201	CDL	CB2-C1-CA2-OA2
57	DA	705	CDL	OB5-CB3-CB4-OB6
57	DS	402	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
57	DU	401	CDL	OB5-CB3-CB4-OB6
59	Dj	407	3PE	O11-C1-C2-O21
59	Dx	1205	3PE	O11-C1-C2-O21
58	EO	201	PC1	C29-C2A-C2B-C2C
57	DI	701	CDL	C33-C34-C35-C36
57	Dn	503	CDL	C14-C15-C16-C17
57	Dc	601	CDL	OA9-CA7-OA8-CA6
65	ED	603	UQ8	C35-C34-C36-C37
57	Da	705	CDL	C17-C18-C19-C20
58	DI	702	PC1	C35-C36-C37-C38
65	EN	1204	UQ8	C2-C3-O3-C3M
65	Ds	404	UQ8	C2-C3-O3-C3M
65	Ds	404	UQ8	C5-C4-O4-C4M
57	Dj	402	CDL	CA4-CA6-OA8-CA7
57	Eh	1601	CDL	C21-C22-C23-C24
65	DS	404	UQ8	C31-C32-C33-C34
57	DG	202	CDL	C72-C73-C74-C75
57	Dr	402	CDL	CA4-CA3-OA5-PA1
57	En	1201	CDL	C14-C15-C16-C17
58	Ds	406	PC1	C3C-C3D-C3E-C3F
57	EN	1202	CDL	OB6-CB4-CB6-OB8
57	Da	705	CDL	OB6-CB4-CB6-OB8
57	Dh	202	CDL	OB6-CB4-CB6-OB8
57	Dn	501	CDL	OB6-CB4-CB6-OB8
57	Eh	1601	CDL	OB6-CB4-CB6-OB8
59	EM	901	3PE	O21-C2-C3-O31
57	Dv	401	CDL	C72-C71-CB7-OB8
57	En	1201	CDL	C12-C11-CA5-OA6
57	DV	402	CDL	O1-C1-CB2-OB2
57	DH	201	CDL	C12-C13-C14-C15
57	ED	601	CDL	C35-C36-C37-C38
57	EL	904	CDL	C84-C85-C86-C87
57	Eu	101	CDL	C51-CB5-OB6-CB4
58	DC	604	PC1	C27-C28-C29-C2A
57	DV	401	CDL	C72-C71-CB7-OB8
57	El	903	CDL	CA5-C11-C12-C13
57	Dd	702	CDL	C23-C24-C25-C26
57	DZ	501	CDL	C31-CA7-OA8-CA6
57	Ds	402	CDL	OA9-CA7-OA8-CA6
65	DS	404	UQ8	C40-C39-C41-C42
57	EH	201	CDL	C44-C45-C46-C47
57	Dj	408	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
58	DC	608	PC1	O31-C31-C32-C33
58	Dc	607	PC1	O31-C31-C32-C33
60	Dl	1101	LPP	O27-C29-C30-C31
57	Eu	101	CDL	C72-C73-C74-C75
57	Dn	503	CDL	CB3-CB4-CB6-OB8
57	Ek	201	CDL	CA3-CA4-CA6-OA8
65	El	906	UQ8	C39-C41-C42-C43
57	Dj	401	CDL	C17-C18-C19-C20
57	El	901	CDL	CB5-C51-C52-C53
57	Dh	202	CDL	C79-C80-C81-C82
58	Dx	1204	PC1	C2B-C2C-C2D-C2E
59	EL	905	3PE	C2F-C2G-C2H-C2I
57	Dj	404	CDL	C62-C63-C64-C65
57	Dj	404	CDL	C61-C62-C63-C64
57	DV	404	CDL	C14-C15-C16-C17
57	Ds	405	CDL	C33-C34-C35-C36
57	DG	202	CDL	C34-C35-C36-C37
59	DS	401	3PE	C34-C35-C36-C37
57	DA	709	CDL	C12-C13-C14-C15
57	Dd	704	CDL	C12-C13-C14-C15
57	EH	201	CDL	O1-C1-CB2-OB2
57	EO	202	CDL	O1-C1-CA2-OA2
57	DS	405	CDL	C14-C15-C16-C17
57	Dn	505	CDL	C39-C40-C41-C42
65	En	1203	UQ8	C35-C34-C36-C37
65	DS	404	UQ8	C38-C39-C41-C42
58	EO	206	PC1	C11-C12-N-C14
57	DO	501	CDL	C11-C12-C13-C14
57	DI	701	CDL	C74-C75-C76-C77
57	Ed	205	CDL	OB7-CB5-OB6-CB4
57	Eu	101	CDL	OB7-CB5-OB6-CB4
57	El	901	CDL	C36-C37-C38-C39
57	DA	705	CDL	C31-CA7-OA8-CA6
57	ED	604	CDL	C71-CB7-OB8-CB6
57	Do	501	CDL	C71-CB7-OB8-CB6
57	Ds	402	CDL	C31-CA7-OA8-CA6
57	Da	705	CDL	C1-CB2-OB2-PB2
57	Dj	403	CDL	C1-CA2-OA2-PA1
57	Dj	403	CDL	CA4-CA3-OA5-PA1
60	Dn	504	LPP	C7-C6-O5-P1
57	DS	402	CDL	OA9-CA7-OA8-CA6
57	DO	501	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
57	Di	701	CDL	C62-C63-C64-C65
57	Dj	401	CDL	C18-C19-C20-C21
57	DV	401	CDL	C78-C79-C80-C81
57	DS	402	CDL	C31-CA7-OA8-CA6
57	DV	402	CDL	C71-CB7-OB8-CB6
57	Dd	705	CDL	C71-CB7-OB8-CB6
59	EM	901	3PE	C32-C31-O31-C3
57	DR	402	CDL	C36-C37-C38-C39
57	DA	705	CDL	OA9-CA7-OA8-CA6
57	DZ	501	CDL	OA9-CA7-OA8-CA6
57	Dd	705	CDL	OB9-CB7-OB8-CB6
57	Do	501	CDL	OB9-CB7-OB8-CB6
65	Ds	404	UQ8	C40-C39-C41-C42
57	DG	201	CDL	OA7-CA5-OA6-CA4
58	Dg	203	PC1	O31-C31-C32-C33
58	Dv	407	PC1	O21-C21-C22-C23
57	Dj	408	CDL	C77-C78-C79-C80
65	Ed	202	UQ8	C38-C39-C41-C42
57	DJ	307	CDL	OA5-CA3-CA4-OA6
57	DO	501	CDL	OB5-CB3-CB4-OB6
57	Dn	505	CDL	OB5-CB3-CB4-OB6
57	El	902	CDL	OB5-CB3-CB4-OB6
58	DB	702	PC1	O11-C1-C2-O21
58	Dv	407	PC1	O32-C31-C32-C33
57	DR	402	CDL	C42-C43-C44-C45
57	Dv	403	CDL	C82-C83-C84-C85
58	DA	706	PC1	C35-C36-C37-C38
59	Ds	403	3PE	C34-C35-C36-C37
57	ED	604	CDL	OB9-CB7-OB8-CB6
57	Ep	701	CDL	C76-C77-C78-C79
57	DJ	304	CDL	C71-CB7-OB8-CB6
59	EN	1203	3PE	C36-C37-C38-C39
57	DV	402	CDL	C78-C79-C80-C81
58	Dc	603	PC1	C34-C35-C36-C37
58	Eb	302	PC1	C34-C35-C36-C37
57	Do	501	CDL	C12-C13-C14-C15
57	Dq	403	CDL	C21-C22-C23-C24
57	DO	501	CDL	C77-C78-C79-C80
57	EL	901	CDL	C44-C45-C46-C47
57	DG	201	CDL	C31-CA7-OA8-CA6
57	DQ	1504	CDL	C55-C56-C57-C58
57	Dj	402	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
59	DG	205	3PE	C29-C2A-C2B-C2C
57	DV	402	CDL	OB9-CB7-OB8-CB6
57	DX	307	CDL	C39-C40-C41-C42
57	EL	902	CDL	C78-C79-C80-C81
57	Dj	401	CDL	C36-C37-C38-C39
57	Dj	401	CDL	C59-C60-C61-C62
57	DD	704	CDL	OA6-CA4-CA6-OA8
57	DQ	1501	CDL	OB6-CB4-CB6-OB8
57	DV	402	CDL	OB6-CB4-CB6-OB8
57	EN	1202	CDL	OA6-CA4-CA6-OA8
57	Dd	705	CDL	OA6-CA4-CA6-OA8
57	Dn	502	CDL	OB6-CB4-CB6-OB8
57	Dq	401	CDL	OB6-CB4-CB6-OB8
58	Dv	408	PC1	O21-C2-C3-O31
57	DA	705	CDL	C55-C56-C57-C58
65	EN	1204	UQ8	C12-C11-C9-C10
65	Ds	404	UQ8	C31-C32-C33-C34
65	En	1203	UQ8	C33-C34-C36-C37
57	DM	501	CDL	C62-C63-C64-C65
57	EH	202	CDL	C74-C75-C76-C77
57	EB	304	CDL	C74-C75-C76-C77
57	Do	501	CDL	C36-C37-C38-C39
58	DJ	306	PC1	C23-C24-C25-C26
57	Dm	502	CDL	CB7-C71-C72-C73
59	EM	901	3PE	O32-C31-O31-C3
59	Dd	703	3PE	C39-C3A-C3B-C3C
60	DA	711	LPP	C17-C18-C19-C20
57	Dd	706	CDL	OA7-CA5-OA6-CA4
57	Da	705	CDL	C55-C56-C57-C58
54	DA	702	HEA	CAD-CBD-CGD-O1D
57	Di	701	CDL	C55-C56-C57-C58
58	Eo	205	PC1	C3C-C3D-C3E-C3F
57	DA	705	CDL	C82-C83-C84-C85
57	DU	401	CDL	C20-C21-C22-C23
57	DA	709	CDL	CB4-CB3-OB5-PB2
57	ED	601	CDL	C1-CB2-OB2-PB2
57	EL	903	CDL	CB4-CB3-OB5-PB2
57	Dj	404	CDL	C1-CB2-OB2-PB2
57	Dx	1201	CDL	C1-CB2-OB2-PB2
58	Eb	302	PC1	C2-C1-O11-P
59	Dd	703	3PE	C2-C1-O11-P
54	DA	702	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
57	DU	402	CDL	C60-C61-C62-C63
57	DQ	1504	CDL	C72-C73-C74-C75
57	Dd	706	CDL	C77-C78-C79-C80
57	El	901	CDL	C11-C12-C13-C14
57	DJ	302	CDL	C84-C85-C86-C87
57	DU	402	CDL	C58-C59-C60-C61
57	DU	403	CDL	C17-C18-C19-C20
57	EO	202	CDL	C18-C19-C20-C21
57	Dv	402	CDL	C72-C73-C74-C75
57	Dx	1201	CDL	C81-C82-C83-C84
66	Ed	201	HEM	CAA-CBA-CGA-O1A
54	Da	702	HEA	C27-C19-C20-C21
65	EN	1204	UQ8	C35-C34-C36-C37
57	DA	705	CDL	C17-C18-C19-C20
59	DR	401	3PE	C3D-C3E-C3F-C3G
57	DV	402	CDL	CA2-C1-CB2-OB2
57	Dd	702	CDL	CA2-C1-CB2-OB2
57	DA	709	CDL	CB3-CB4-CB6-OB8
57	DM	502	CDL	CB3-CB4-CB6-OB8
57	Dj	402	CDL	CB3-CB4-CB6-OB8
57	Dj	404	CDL	CA3-CA4-CA6-OA8
57	Dq	402	CDL	CB3-CB4-CB6-OB8
57	Ds	405	CDL	C31-C32-C33-C34
58	DV	406	PC1	C3B-C3C-C3D-C3E
60	DA	711	LPP	C18-C19-C20-C21
59	Dx	1206	3PE	C3F-C3G-C3H-C3I
57	Ei	401	CDL	C76-C77-C78-C79
54	Da	702	HEA	CAD-CBD-CGD-O1D
57	DJ	304	CDL	OB9-CB7-OB8-CB6
57	EL	903	CDL	OA9-CA7-OA8-CA6
58	Dg	203	PC1	C3F-C3G-C3H-C3I
57	Dg	202	CDL	C80-C81-C82-C83
57	Dn	501	CDL	C78-C79-C80-C81
58	Dy	302	PC1	C3B-C3C-C3D-C3E
60	DA	711	LPP	O27-C29-C30-C31
57	DJ	307	CDL	CB6-CB4-OB6-CB5
57	DQ	1501	CDL	CA6-CA4-OA6-CA5
57	DV	401	CDL	CB3-CB4-OB6-CB5
57	DV	404	CDL	CA3-CA4-OA6-CA5
57	EA	301	CDL	CA6-CA4-OA6-CA5
57	EN	1202	CDL	CB6-CB4-OB6-CB5
57	Dd	704	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
57	Dg	201	CDL	CB3-CB4-OB6-CB5
57	Dj	404	CDL	CB3-CB4-OB6-CB5
57	Dn	501	CDL	CB6-CB4-OB6-CB5
57	Dv	401	CDL	CB3-CB4-OB6-CB5
58	DC	608	PC1	C1-C2-O21-C21
58	DC	608	PC1	C3-C2-O21-C21
58	EO	207	PC1	C1-C2-O21-C21
58	Eo	205	PC1	C1-C2-O21-C21
59	Dg	204	3PE	C1-C2-O21-C21
57	DQ	1502	CDL	C12-C13-C14-C15
57	Ds	402	CDL	C80-C81-C82-C83
58	DQ	1503	PC1	O22-C21-O21-C2
59	Dr	401	3PE	O22-C21-O21-C2
59	Dr	401	3PE	C22-C21-O21-C2
57	EH	201	CDL	C76-C77-C78-C79
57	EI	401	CDL	C14-C15-C16-C17
57	Do	501	CDL	C33-C34-C35-C36
57	DS	402	CDL	C11-C12-C13-C14
58	Dv	406	PC1	O31-C31-C32-C33
54	Da	702	HEA	C18-C19-C20-C21
57	Di	701	CDL	C32-C33-C34-C35
54	Da	702	HEA	CAD-CBD-CGD-O2D
57	EB	304	CDL	C51-C52-C53-C54
59	Dx	1205	3PE	C3A-C3B-C3C-C3D
57	Ds	402	CDL	C78-C79-C80-C81
58	Eo	201	PC1	C33-C34-C35-C36
57	DM	501	CDL	C52-C51-CB5-OB6
58	DS	407	PC1	C11-C12-N-C14
57	DU	404	CDL	C71-CB7-OB8-CB6
57	EL	903	CDL	C31-CA7-OA8-CA6
57	En	1201	CDL	C31-CA7-OA8-CA6
57	EB	302	CDL	C11-C12-C13-C14
59	DJ	301	3PE	C3C-C3D-C3E-C3F
59	DX	305	3PE	C2E-C2F-C2G-C2H
57	DN	504	CDL	C37-C38-C39-C40
57	Ep	701	CDL	C80-C81-C82-C83
57	DU	401	CDL	OA5-CA3-CA4-OA6
57	EL	903	CDL	OB5-CB3-CB4-OB6
58	DC	608	PC1	O11-C1-C2-O21
58	Ds	406	PC1	O11-C1-C2-O21
57	El	902	CDL	C83-C84-C85-C86
57	EN	1201	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
57	DD	704	CDL	O1-C1-CB2-OB2
57	Dd	706	CDL	C11-CA5-OA6-CA4
58	DQ	1503	PC1	C22-C21-O21-C2
57	DJ	304	CDL	CA7-C31-C32-C33
66	ED	602	HEM	CAA-CBA-CGA-O1A
59	Ds	401	3PE	C32-C33-C34-C35
58	EO	201	PC1	C23-C24-C25-C26
59	Ds	401	3PE	C3A-C3B-C3C-C3D
57	DD	703	CDL	C1-CB2-OB2-PB2
57	DR	402	CDL	C1-CB2-OB2-PB2
57	DV	401	CDL	C1-CA2-OA2-PA1
57	DV	403	CDL	C1-CA2-OA2-PA1
57	DZ	501	CDL	C1-CB2-OB2-PB2
57	Dn	501	CDL	CB4-CB3-OB5-PB2
57	Dv	401	CDL	C1-CA2-OA2-PA1
58	EO	205	PC1	C2-C1-O11-P
58	El	904	PC1	C2-C1-O11-P
59	DX	304	3PE	C2-C1-O11-P
59	DX	304	3PE	C3F-C3G-C3H-C3I
54	DA	702	HEA	O11-C11-C12-C13
57	Da	709	CDL	C22-C23-C24-C25
57	Du	403	CDL	C79-C80-C81-C82
65	Ed	202	UQ8	C12-C11-C9-C10
65	En	1203	UQ8	C30-C29-C31-C32
65	En	1203	UQ8	C12-C11-C9-C10
58	Dc	603	PC1	C3B-C3C-C3D-C3E
57	DD	704	CDL	OB5-CB3-CB4-CB6
57	DR	402	CDL	OB5-CB3-CB4-CB6
57	Dd	706	CDL	OA5-CA3-CA4-CA6
57	Dj	402	CDL	OA5-CA3-CA4-CA6
57	Ed	205	CDL	OB5-CB3-CB4-CB6
58	Db	702	PC1	O11-C1-C2-C3
65	Ds	404	UQ8	C38-C39-C41-C42
57	Dj	402	CDL	C51-C52-C53-C54
58	Di	702	PC1	O22-C21-O21-C2
57	Dg	201	CDL	C21-C22-C23-C24
57	ED	604	CDL	CA5-C11-C12-C13
54	Da	701	HEA	CAD-CBD-CGD-O1D
57	EB	302	CDL	C12-C13-C14-C15
57	EL	904	CDL	C43-C44-C45-C46
57	DG	201	CDL	OB6-CB4-CB6-OB8
57	Dq	402	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
57	Ek	201	CDL	OA6-CA4-CA6-OA8
58	Da	707	PC1	O21-C2-C3-O31
57	Eh	1601	CDL	C18-C19-C20-C21
57	El	902	CDL	C13-C14-C15-C16
57	EB	304	CDL	C79-C80-C81-C82
58	DV	407	PC1	C32-C33-C34-C35
59	Ds	403	3PE	C3E-C3F-C3G-C3H
59	Dx	1207	3PE	C2B-C2C-C2D-C2E
58	Dc	604	PC1	O21-C21-C22-C23
57	DG	201	CDL	C43-C44-C45-C46
57	EL	904	CDL	C41-C42-C43-C44
57	EN	1201	CDL	C79-C80-C81-C82
57	Dr	402	CDL	C51-C52-C53-C54
57	DM	501	CDL	C54-C55-C56-C57
57	En	1202	CDL	C32-C33-C34-C35
65	EN	1204	UQ8	C15-C14-C16-C17
65	El	906	UQ8	C12-C11-C9-C10
57	EL	901	CDL	C78-C79-C80-C81
65	EN	1204	UQ8	C12-C11-C9-C8
57	Dj	403	CDL	C34-C35-C36-C37
57	DU	404	CDL	OB9-CB7-OB8-CB6
57	En	1201	CDL	OA9-CA7-OA8-CA6
57	DN	505	CDL	C81-C82-C83-C84
57	Dq	403	CDL	O1-C1-CA2-OA2
58	DS	406	PC1	O31-C31-C32-C33
57	DN	504	CDL	C13-C14-C15-C16
57	DG	201	CDL	OA9-CA7-OA8-CA6
58	Di	702	PC1	C22-C21-O21-C2
57	DS	402	CDL	C13-C14-C15-C16
57	Da	705	CDL	C77-C78-C79-C80
68	ER	201	ATP	PA-O3A-PB-O1B
57	DJ	307	CDL	C52-C53-C54-C55
60	Dn	506	LPP	C37-C38-C39-C40
65	EN	1204	UQ8	C11-C12-C13-C14
57	DM	501	CDL	C82-C83-C84-C85
57	Dd	706	CDL	C80-C81-C82-C83
58	DC	608	PC1	C2B-C2C-C2D-C2E
54	Da	701	HEA	CAD-CBD-CGD-O2D
57	DU	403	CDL	C12-C13-C14-C15
57	En	1202	CDL	C36-C37-C38-C39
59	DX	303	3PE	C2C-C2D-C2E-C2F
59	EM	901	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
66	ED	602	HEM	CAA-CBA-CGA-O2A
57	DH	201	CDL	CA4-CA3-OA5-PA1
57	DJ	303	CDL	C1-CB2-OB2-PB2
57	DR	402	CDL	CA4-CA3-OA5-PA1
57	EB	304	CDL	CB4-CB3-OB5-PB2
57	EK	201	CDL	CB4-CB3-OB5-PB2
57	EL	902	CDL	CB4-CB3-OB5-PB2
57	EL	904	CDL	C1-CB2-OB2-PB2
57	Dm	501	CDL	C1-CA2-OA2-PA1
57	Dv	403	CDL	C1-CB2-OB2-PB2
57	Dz	501	CDL	CA4-CA3-OA5-PA1
57	DS	402	CDL	C74-C75-C76-C77
65	EN	1204	UQ8	C33-C34-C36-C37
65	En	1203	UQ8	C12-C11-C9-C8
57	EH	201	CDL	C39-C40-C41-C42
59	Dr	401	3PE	C3D-C3E-C3F-C3G
59	Eo	202	3PE	C32-C31-O31-C3
57	DH	201	CDL	C18-C19-C20-C21
57	DG	201	CDL	C11-CA5-OA6-CA4
57	EN	1202	CDL	C36-C37-C38-C39
57	Eu	101	CDL	C71-C72-C73-C74
59	Dr	404	3PE	C29-C2A-C2B-C2C
57	DJ	307	CDL	C32-C31-CA7-OA8
57	EO	202	CDL	C59-C60-C61-C62
57	Da	705	CDL	C15-C16-C17-C18
57	DD	702	CDL	CA3-CA4-CA6-OA8
57	DD	704	CDL	CA3-CA4-CA6-OA8
57	DJ	302	CDL	CB3-CB4-CB6-OB8
57	DX	301	CDL	CB3-CB4-CB6-OB8
57	Dd	705	CDL	CA3-CA4-CA6-OA8
57	Dm	502	CDL	CB3-CB4-CB6-OB8
57	Dn	501	CDL	CB3-CB4-CB6-OB8
57	Dq	402	CDL	CA3-CA4-CA6-OA8
57	Dv	402	CDL	CB3-CB4-CB6-OB8
57	Eh	1601	CDL	CB3-CB4-CB6-OB8
57	En	1202	CDL	CB3-CB4-CB6-OB8
58	Dv	408	PC1	C1-C2-C3-O31
58	Dx	1204	PC1	C1-C2-C3-O31
58	Eo	204	PC1	C1-C2-C3-O31
59	DC	606	3PE	C1-C2-C3-O31
59	El	905	3PE	C1-C2-C3-O31
66	Ed	201	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
57	En	1201	CDL	C52-C53-C54-C55
59	DS	401	3PE	C3A-C3B-C3C-C3D
59	EO	203	3PE	C26-C27-C28-C29
59	Ds	407	3PE	C36-C37-C38-C39
57	Dh	201	CDL	C18-C19-C20-C21
57	Eg	101	CDL	C54-C55-C56-C57
57	DZ	501	CDL	O1-C1-CA2-OA2
57	DR	402	CDL	OB5-CB3-CB4-OB6
57	EU	101	CDL	OB5-CB3-CB4-OB6
57	Dj	402	CDL	OA5-CA3-CA4-OA6
57	Dn	505	CDL	OA5-CA3-CA4-OA6
57	Do	501	CDL	OB5-CB3-CB4-OB6
57	Dz	501	CDL	OA5-CA3-CA4-OA6
59	DG	205	3PE	O11-C1-C2-O21
57	Dz	501	CDL	C72-C71-CB7-OB8
57	Eh	1601	CDL	C73-C74-C75-C76
59	Ds	401	3PE	C36-C37-C38-C39
57	DJ	304	CDL	C16-C17-C18-C19
57	Dg	202	CDL	C14-C15-C16-C17
57	Dg	202	CDL	C42-C43-C44-C45
59	Eo	202	3PE	O32-C31-O31-C3
57	Dq	403	CDL	C76-C77-C78-C79
65	ED	603	UQ8	C2-C3-O3-C3M
57	Ed	205	CDL	C11-C12-C13-C14
58	DA	707	PC1	C3E-C3F-C3G-C3H
58	DC	604	PC1	C26-C27-C28-C29
60	DI	1101	LPP	C17-C18-C19-C20
57	DJ	302	CDL	C52-C51-CB5-OB6
57	Dd	705	CDL	C40-C41-C42-C43
57	Du	402	CDL	C24-C25-C26-C27
57	DI	701	CDL	C53-C54-C55-C56
57	DV	401	CDL	C43-C44-C45-C46
57	Dq	402	CDL	C72-C73-C74-C75
57	Ds	402	CDL	C12-C13-C14-C15
58	EO	207	PC1	C3D-C3E-C3F-C3G
57	EO	202	CDL	C12-C13-C14-C15
57	Da	709	CDL	C38-C39-C40-C41
57	Dj	404	CDL	C55-C56-C57-C58
57	EL	904	CDL	C71-C72-C73-C74
57	EN	1202	CDL	C14-C15-C16-C17
58	Dx	1204	PC1	O22-C21-O21-C2
57	DG	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
57	El	902	CDL	C44-C45-C46-C47
59	EO	204	3PE	C2F-C2G-C2H-C2I
59	El	905	3PE	C22-C23-C24-C25
57	El	902	CDL	OA9-CA7-OA8-CA6
57	Dd	706	CDL	C44-C45-C46-C47
57	DR	402	CDL	CA5-C11-C12-C13
57	En	1202	CDL	C59-C60-C61-C62
57	DI	701	CDL	C57-C58-C59-C60
59	DX	305	3PE	C35-C36-C37-C38
57	DU	402	CDL	OA9-CA7-OA8-CA6
57	DC	601	CDL	OB5-CB3-CB4-CB6
57	DJ	305	CDL	OB5-CB3-CB4-CB6
57	EH	201	CDL	OA5-CA3-CA4-CA6
57	EL	901	CDL	OA5-CA3-CA4-CA6
57	Dj	401	CDL	OA5-CA3-CA4-CA6
57	Du	401	CDL	OA5-CA3-CA4-CA6
57	Dy	301	CDL	OA5-CA3-CA4-CA6
57	Dz	501	CDL	OA5-CA3-CA4-CA6
57	Ed	204	CDL	OB5-CB3-CB4-CB6
57	El	902	CDL	OB5-CB3-CB4-CB6
58	DC	603	PC1	O11-C1-C2-C3
58	Dc	607	PC1	O11-C1-C2-C3
58	Ef	1001	PC1	O11-C1-C2-C3
59	DG	204	3PE	O11-C1-C2-C3
65	ED	603	UQ8	C12-C11-C9-C10
57	DY	301	CDL	C57-C58-C59-C60
57	DV	404	CDL	OA6-CA4-CA6-OA8
57	Dj	404	CDL	OA6-CA4-CA6-OA8
65	EN	1204	UQ8	C13-C14-C16-C17
65	El	906	UQ8	C11-C12-C13-C14
57	Ds	402	CDL	C56-C57-C58-C59
58	Dv	405	PC1	C29-C2A-C2B-C2C
59	DG	204	3PE	C2A-C2B-C2C-C2D
59	DS	401	3PE	C36-C37-C38-C39
57	EO	202	CDL	C1-CB2-OB2-PB2
57	Dd	705	CDL	C1-CB2-OB2-PB2
57	Ek	201	CDL	CB4-CB3-OB5-PB2
57	DA	709	CDL	C36-C37-C38-C39
57	EN	1201	CDL	C13-C14-C15-C16
58	Dv	407	PC1	C3B-C3C-C3D-C3E
59	DX	305	3PE	C26-C27-C28-C29
59	Dd	703	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
57	DV	401	CDL	C14-C15-C16-C17
57	EB	304	CDL	C35-C36-C37-C38
59	Em	901	3PE	C25-C26-C27-C28
57	DM	501	CDL	C41-C42-C43-C44
57	DQ	1501	CDL	C21-C22-C23-C24
57	EL	902	CDL	C14-C15-C16-C17
57	EN	1201	CDL	C40-C41-C42-C43
57	Di	701	CDL	C57-C58-C59-C60
57	Ds	402	CDL	C11-C12-C13-C14
57	Ed	204	CDL	O1-C1-CA2-OA2
57	Ed	204	CDL	O1-C1-CB2-OB2
57	DN	501	CDL	C12-C13-C14-C15
57	DJ	303	CDL	C75-C76-C77-C78
57	ED	601	CDL	C80-C81-C82-C83
58	DC	604	PC1	O22-C21-C22-C23
57	DU	404	CDL	C22-C23-C24-C25
57	Da	705	CDL	OA9-CA7-OA8-CA6
57	Dn	505	CDL	C12-C13-C14-C15
57	Du	401	CDL	C71-C72-C73-C74
57	Da	709	CDL	C40-C41-C42-C43
58	Eb	301	PC1	O31-C31-C32-C33
58	Eo	201	PC1	C3F-C3G-C3H-C3I
57	DM	502	CDL	C12-C13-C14-C15
57	Di	701	CDL	CA7-C31-C32-C33
58	DY	302	PC1	C3E-C3F-C3G-C3H
57	EN	1202	CDL	C11-C12-C13-C14
57	Di	701	CDL	C61-C62-C63-C64
57	El	903	CDL	C43-C44-C45-C46
58	DB	702	PC1	O32-C31-O31-C3
57	EL	903	CDL	C16-C17-C18-C19
57	Dg	202	CDL	C40-C41-C42-C43
57	DU	402	CDL	C31-CA7-OA8-CA6
57	DZ	501	CDL	C72-C71-CB7-OB8
57	EH	202	CDL	CA5-C11-C12-C13
57	DQ	1501	CDL	CA3-CA4-OA6-CA5
57	DR	403	CDL	CA3-CA4-OA6-CA5
57	Dd	705	CDL	CB6-CB4-OB6-CB5
57	Do	501	CDL	CB3-CB4-OB6-CB5
57	Do	501	CDL	CB6-CB4-OB6-CB5
57	Dr	403	CDL	CA3-CA4-OA6-CA5
58	Db	702	PC1	C3-C2-O21-C21
59	Dg	204	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
57	EL	902	CDL	C35-C36-C37-C38
57	Dd	706	CDL	C39-C40-C41-C42
57	DM	502	CDL	C52-C53-C54-C55
57	DS	405	CDL	C31-C32-C33-C34
58	DC	602	PC1	C2E-C2F-C2G-C2H
59	DX	303	3PE	C2B-C2C-C2D-C2E
65	ED	603	UQ8	C33-C34-C36-C37
57	Dh	201	CDL	C59-C60-C61-C62
59	DX	304	3PE	C32-C33-C34-C35
57	DJ	304	CDL	C1-CB2-OB2-PB2
57	DV	402	CDL	C72-C73-C74-C75
57	EA	301	CDL	CB2-C1-CA2-OA2
57	Da	705	CDL	CB2-C1-CA2-OA2
57	EH	201	CDL	OA5-CA3-CA4-OA6
57	Dd	706	CDL	OA5-CA3-CA4-OA6
57	Dd	706	CDL	OB5-CB3-CB4-OB6
57	Dj	408	CDL	OB5-CB3-CB4-OB6
59	DG	204	3PE	O11-C1-C2-O21
57	En	1201	CDL	C83-C84-C85-C86
57	Da	705	CDL	C31-CA7-OA8-CA6
57	El	902	CDL	C31-CA7-OA8-CA6
57	Dn	505	CDL	C14-C15-C16-C17
57	EA	301	CDL	CA3-CA4-CA6-OA8
57	EN	1202	CDL	CA3-CA4-CA6-OA8
58	Da	707	PC1	C1-C2-C3-O31
59	DC	607	3PE	C1-C2-C3-O31
59	Eo	202	3PE	C1-C2-C3-O31
65	EL	906	UQ8	C14-C16-C17-C18
57	Ds	405	CDL	C41-C42-C43-C44
58	Ef	1001	PC1	C2A-C2B-C2C-C2D
57	Du	403	CDL	C57-C58-C59-C60
57	DR	402	CDL	C76-C77-C78-C79
57	Dd	706	CDL	C56-C57-C58-C59
59	DS	403	3PE	C28-C29-C2A-C2B
59	Dx	1207	3PE	C35-C36-C37-C38
58	DS	407	PC1	C12-C11-O13-P
59	DG	204	3PE	C12-C11-O13-P
58	DV	407	PC1	C3D-C3E-C3F-C3G
57	EH	201	CDL	C34-C35-C36-C37
58	DB	702	PC1	C3E-C3F-C3G-C3H
57	DQ	1504	CDL	C13-C14-C15-C16
57	Dm	501	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
57	Dh	202	CDL	CB5-C51-C52-C53
57	Dq	401	CDL	CA4-CA6-OA8-CA7
57	Dd	705	CDL	C12-C11-CA5-OA6
57	Dj	408	CDL	C52-C51-CB5-OB6
58	Da	706	PC1	O31-C31-C32-C33
59	DG	204	3PE	O21-C21-C22-C23
59	DX	303	3PE	O21-C21-C22-C23
59	Dx	1206	3PE	O21-C21-C22-C23
60	Dn	504	LPP	O27-C29-C30-C31
59	DC	607	3PE	C2F-C2G-C2H-C2I
57	DV	404	CDL	C83-C84-C85-C86
57	Dj	401	CDL	C60-C61-C62-C63
59	DR	401	3PE	C3F-C3G-C3H-C3I
57	DV	402	CDL	C77-C78-C79-C80
57	Dj	408	CDL	OB9-CB7-OB8-CB6
57	DU	403	CDL	C15-C16-C17-C18
58	DQ	1503	PC1	C3D-C3E-C3F-C3G
57	EB	304	CDL	C20-C21-C22-C23
57	En	1201	CDL	C43-C44-C45-C46
57	DQ	1501	CDL	C72-C71-CB7-OB8
58	EO	207	PC1	O21-C21-C22-C23
57	DN	504	CDL	C81-C82-C83-C84
57	Da	705	CDL	OA5-CA3-CA4-CA6
57	Dd	704	CDL	OB5-CB3-CB4-CB6
57	Dn	505	CDL	OA5-CA3-CA4-CA6
57	Ed	204	CDL	OA5-CA3-CA4-CA6
58	Eo	201	PC1	O11-C1-C2-C3
59	Em	901	3PE	C3B-C3C-C3D-C3E
68	ER	201	ATP	PG-O3B-PB-O3A
65	Ed	202	UQ8	C4-C3-O3-C3M
57	DV	403	CDL	C77-C78-C79-C80
60	DN	503	LPP	C35-C36-C37-C38
57	DJ	303	CDL	C12-C11-CA5-OA6
57	Da	709	CDL	C52-C51-CB5-OB6
57	Ed	205	CDL	C12-C11-CA5-OA6
58	DC	603	PC1	O21-C21-C22-C23
58	Dx	1202	PC1	O31-C31-C32-C33
59	DG	205	3PE	O31-C31-C32-C33
59	DS	401	3PE	O21-C21-C22-C23
59	DS	403	3PE	O21-C21-C22-C23
59	Dd	703	3PE	O21-C21-C22-C23
57	DN	501	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
58	DV	405	PC1	C29-C2A-C2B-C2C
57	DS	402	CDL	C56-C57-C58-C59
57	DD	702	CDL	C35-C36-C37-C38
57	Dn	507	CDL	C81-C82-C83-C84
58	Da	706	PC1	C2C-C2D-C2E-C2F
57	DJ	304	CDL	C19-C20-C21-C22
57	DV	402	CDL	C81-C82-C83-C84
57	Dg	202	CDL	C78-C79-C80-C81
57	Ep	701	CDL	C78-C79-C80-C81
57	DD	702	CDL	C51-CB5-OB6-CB4
58	Dx	1204	PC1	C22-C21-O21-C2
57	DU	401	CDL	C72-C71-CB7-OB8
57	DD	702	CDL	OB7-CB5-OB6-CB4
57	DX	301	CDL	C24-C25-C26-C27
57	EL	904	CDL	C83-C84-C85-C86
58	Di	702	PC1	C34-C35-C36-C37
57	DM	501	CDL	C1-CB2-OB2-PB2
57	EL	901	CDL	CB4-CB3-OB5-PB2
57	Dn	503	CDL	CB4-CB3-OB5-PB2
57	Eg	101	CDL	CB4-CB3-OB5-PB2
57	Ds	402	CDL	C82-C83-C84-C85
65	EL	906	UQ8	C39-C41-C42-C43
65	Ds	404	UQ8	C39-C41-C42-C43
57	Dd	702	CDL	C78-C79-C80-C81
59	EL	905	3PE	C34-C35-C36-C37
57	DD	703	CDL	C52-C51-CB5-OB6
57	ED	604	CDL	C12-C11-CA5-OA6
57	Dh	202	CDL	C72-C71-CB7-OB8
57	Dm	501	CDL	C72-C71-CB7-OB8
57	Dn	502	CDL	C32-C31-CA7-OA8
58	Dv	405	PC1	O31-C31-C32-C33
59	DJ	301	3PE	O21-C21-C22-C23
59	Dc	606	3PE	O21-C21-C22-C23
57	DG	202	CDL	C31-C32-C33-C34
57	EL	901	CDL	C77-C78-C79-C80
57	Dd	704	CDL	C35-C36-C37-C38
57	EK	201	CDL	C13-C14-C15-C16
57	Dg	202	CDL	C63-C64-C65-C66
58	DB	702	PC1	C26-C27-C28-C29
68	ER	201	ATP	PA-O3A-PB-O2B
68	Er	201	ATP	PG-O3B-PB-O1B
57	Dj	401	CDL	CA4-CA6-OA8-CA7

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Mol	Chain	Res	Type	Atoms
57	Dg	202	CDL	C31-C32-C33-C34
57	DN	505	CDL	CA5-C11-C12-C13
57	Dx	1201	CDL	C52-C51-CB5-OB6
57	Ea	301	CDL	C72-C71-CB7-OB8
58	DA	706	PC1	O31-C31-C32-C33
58	EO	205	PC1	O21-C21-C22-C23
59	Ds	403	3PE	O21-C21-C22-C23
57	DQ	1504	CDL	C76-C77-C78-C79
57	Du	401	CDL	C37-C38-C39-C40
59	Eo	202	3PE	C38-C39-C3A-C3B
57	DX	301	CDL	C78-C79-C80-C81
57	Dn	501	CDL	C12-C13-C14-C15
57	Du	403	CDL	C58-C59-C60-C61
57	EA	301	CDL	C52-C51-CB5-OB6
57	Da	709	CDL	C12-C11-CA5-OA6
57	Du	401	CDL	C72-C71-CB7-OB8
57	Dv	401	CDL	C52-C51-CB5-OB6
58	DV	405	PC1	O31-C31-C32-C33
58	El	904	PC1	O21-C21-C22-C23
57	DA	705	CDL	C77-C78-C79-C80
57	DN	504	CDL	C59-C60-C61-C62
57	DX	301	CDL	C32-C33-C34-C35
57	DS	405	CDL	C18-C19-C20-C21
57	Dr	402	CDL	C41-C42-C43-C44
59	Dr	401	3PE	C3F-C3G-C3H-C3I
57	Dq	404	CDL	C14-C15-C16-C17
57	Dv	404	CDL	C83-C84-C85-C86
57	DM	501	CDL	C12-C11-CA5-OA6
57	DR	403	CDL	C52-C51-CB5-OB6
57	DV	401	CDL	C52-C51-CB5-OB6
57	EH	202	CDL	C72-C71-CB7-OB8
57	Dj	408	CDL	C32-C31-CA7-OA8
57	Dq	402	CDL	C32-C31-CA7-OA8
57	Dr	403	CDL	C52-C51-CB5-OB6
57	Ek	201	CDL	C32-C31-CA7-OA8
57	El	901	CDL	C32-C31-CA7-OA8
58	Dc	603	PC1	O21-C21-C22-C23
59	DJ	301	3PE	O31-C31-C32-C33
59	Dx	1206	3PE	O31-C31-C32-C33
57	DM	501	CDL	C17-C18-C19-C20
57	El	901	CDL	C62-C63-C64-C65
58	Dc	602	PC1	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
57	DD	704	CDL	OB5-CB3-CB4-OB6
57	DY	301	CDL	OA5-CA3-CA4-OA6
57	Dn	502	CDL	OA5-CA3-CA4-OA6
58	DY	302	PC1	O11-C1-C2-O21
60	EI	402	LPP	C40-C41-C42-C43
57	DR	403	CDL	C52-C53-C54-C55
57	DZ	501	CDL	C39-C40-C41-C42
57	DN	504	CDL	C72-C71-CB7-OB8
57	DO	501	CDL	C72-C71-CB7-OB8
57	DQ	1501	CDL	C32-C31-CA7-OA8
57	Do	501	CDL	C72-C71-CB7-OB8
57	Dv	404	CDL	C52-C51-CB5-OB6
57	Dz	501	CDL	C32-C31-CA7-OA8
57	Ea	301	CDL	C52-C51-CB5-OB6
57	Eu	101	CDL	C72-C71-CB7-OB8
58	Dx	1204	PC1	O31-C31-C32-C33
59	DX	304	3PE	O21-C21-C22-C23
59	Eo	202	3PE	O31-C31-C32-C33
59	DA	708	3PE	C2C-C2D-C2E-C2F
58	DB	702	PC1	C32-C31-O31-C3
57	Dv	402	CDL	C81-C82-C83-C84
57	EN	1201	CDL	C54-C55-C56-C57
57	Da	705	CDL	C16-C17-C18-C19
57	DA	709	CDL	C77-C78-C79-C80
57	DX	307	CDL	C63-C64-C65-C66
57	EA	301	CDL	C78-C79-C80-C81
57	Du	403	CDL	C33-C34-C35-C36
57	Eg	101	CDL	C73-C74-C75-C76
54	Da	702	HEA	CAA-CBA-CGA-O1A
57	DV	402	CDL	C12-C11-CA5-OA6
57	DV	404	CDL	C52-C51-CB5-OB6
57	Da	705	CDL	C72-C71-CB7-OB8
57	Dd	705	CDL	C72-C71-CB7-OB8
57	Dm	501	CDL	C12-C11-CA5-OA6
57	Dv	402	CDL	C12-C11-CA5-OA6
57	Dv	403	CDL	C72-C71-CB7-OB8
58	DC	602	PC1	O21-C21-C22-C23
60	Dn	506	LPP	O27-C29-C30-C31
57	El	903	CDL	C83-C84-C85-C86
58	DV	405	PC1	C2D-C2E-C2F-C2G
60	EI	402	LPP	C21-C22-C23-C24
59	DA	708	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
58	Dc	604	PC1	O22-C21-O21-C2
57	DV	403	CDL	C11-C12-C13-C14
59	DS	403	3PE	C3E-C3F-C3G-C3H
57	DS	405	CDL	C78-C79-C80-C81
54	Da	702	HEA	CAA-CBA-CGA-O2A
58	Da	706	PC1	C35-C36-C37-C38
58	DB	702	PC1	C2-C1-O11-P
57	DA	709	CDL	C72-C71-CB7-OB8
57	DU	403	CDL	C32-C31-CA7-OA8
57	DV	403	CDL	C72-C71-CB7-OB8
57	EI	401	CDL	C72-C71-CB7-OB8
57	EL	904	CDL	C12-C11-CA5-OA6
57	Dq	401	CDL	C72-C71-CB7-OB8
58	DC	608	PC1	O21-C21-C22-C23
59	DG	205	3PE	O21-C21-C22-C23
59	EN	1203	3PE	O21-C21-C22-C23
57	Di	701	CDL	C53-C54-C55-C56
59	Dr	404	3PE	C28-C29-C2A-C2B
57	Du	403	CDL	O1-C1-CB2-OB2
57	DD	703	CDL	CA3-CA4-CA6-OA8
57	EB	302	CDL	CB3-CB4-CB6-OB8
57	EH	202	CDL	CA3-CA4-CA6-OA8
57	EN	1201	CDL	CA3-CA4-CA6-OA8
57	DJ	303	CDL	C24-C25-C26-C27
57	Dn	502	CDL	C61-C62-C63-C64
57	Ds	402	CDL	C54-C55-C56-C57
57	DO	501	CDL	C33-C34-C35-C36
58	Dc	604	PC1	C22-C21-O21-C2
57	DZ	501	CDL	C32-C31-CA7-OA8
57	Dg	201	CDL	C12-C11-CA5-OA6
57	Dn	501	CDL	C72-C71-CB7-OB8
57	Dq	404	CDL	C72-C71-CB7-OB8
57	Du	403	CDL	C32-C31-CA7-OA8
57	Du	404	CDL	C72-C71-CB7-OB8
57	Ea	301	CDL	C12-C11-CA5-OA6
57	Eh	1601	CDL	C52-C51-CB5-OB6
57	Ei	401	CDL	C72-C71-CB7-OB8
57	Ep	701	CDL	C12-C11-CA5-OA6
58	Eo	205	PC1	O21-C21-C22-C23
59	DX	304	3PE	O31-C31-C32-C33
59	Ds	401	3PE	O21-C21-C22-C23
59	Dx	1205	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
60	DN	502	LPP	O27-C29-C30-C31
57	DA	709	CDL	C11-C12-C13-C14
57	Du	401	CDL	C13-C14-C15-C16
58	Dc	607	PC1	C3C-C3D-C3E-C3F
59	DS	401	3PE	C32-C33-C34-C35
57	DQ	1504	CDL	OB6-CB4-CB6-OB8
57	Ed	205	CDL	OB6-CB4-CB6-OB8
57	El	901	CDL	OA6-CA4-CA6-OA8
54	DA	702	HEA	CAA-CBA-CGA-O1A
57	DU	401	CDL	C37-C38-C39-C40
57	Dj	403	CDL	C19-C20-C21-C22
57	DU	401	CDL	CA7-C31-C32-C33
57	Dh	202	CDL	C55-C56-C57-C58
59	Dx	1207	3PE	C2E-C2F-C2G-C2H
58	DV	406	PC1	O32-C31-C32-C33
54	DA	702	HEA	CAA-CBA-CGA-O2A
57	DQ	1502	CDL	C32-C31-CA7-OA8
57	DQ	1502	CDL	C72-C71-CB7-OB8
57	DU	401	CDL	C32-C31-CA7-OA8
57	EI	401	CDL	C12-C11-CA5-OA6
57	Di	701	CDL	C72-C71-CB7-OB8
57	El	902	CDL	C52-C51-CB5-OB6
58	EO	206	PC1	O21-C21-C22-C23
58	Dc	602	PC1	O21-C21-C22-C23
59	EM	901	3PE	O21-C21-C22-C23
57	DU	401	CDL	C71-C72-C73-C74
57	Dg	202	CDL	C36-C37-C38-C39
58	Da	706	PC1	C3A-C3B-C3C-C3D
59	Eo	202	3PE	C26-C27-C28-C29
57	DQ	1501	CDL	C14-C15-C16-C17
58	Dv	408	PC1	C3C-C3D-C3E-C3F
60	Dn	506	LPP	C30-C31-C32-C33
57	EN	1202	CDL	C32-C33-C34-C35
57	Dj	402	CDL	OB5-CB3-CB4-CB6
57	EK	201	CDL	C32-C31-CA7-OA8
58	EO	206	PC1	O31-C31-C32-C33
59	Dg	204	3PE	O21-C21-C22-C23
57	EL	901	CDL	C73-C74-C75-C76
57	Dd	704	CDL	C37-C38-C39-C40
57	DM	501	CDL	C40-C41-C42-C43
57	DS	405	CDL	C41-C42-C43-C44
57	Ds	402	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
58	DA	706	PC1	C2C-C2D-C2E-C2F
57	DD	704	CDL	C72-C71-CB7-OB8
57	Dq	403	CDL	C72-C71-CB7-OB8
57	Dj	401	CDL	C79-C80-C81-C82
57	Dj	408	CDL	C71-CB7-OB8-CB6
65	En	1203	UQ8	C28-C29-C31-C32
57	DJ	304	CDL	C83-C84-C85-C86
59	Dx	1206	3PE	C32-C33-C34-C35
57	Dh	202	CDL	C20-C21-C22-C23
57	DA	710	CDL	CA3-CA4-OA6-CA5
57	DJ	307	CDL	CB3-CB4-OB6-CB5
57	DO	501	CDL	CB3-CB4-OB6-CB5
57	DV	401	CDL	CA3-CA4-OA6-CA5
57	EA	301	CDL	CA3-CA4-OA6-CA5
57	EN	1202	CDL	CB3-CB4-OB6-CB5
57	EO	202	CDL	CB6-CB4-OB6-CB5
57	Dd	705	CDL	CB3-CB4-OB6-CB5
57	Dd	706	CDL	CB6-CB4-OB6-CB5
57	Dj	402	CDL	CB3-CB4-OB6-CB5
57	Dj	404	CDL	CA3-CA4-OA6-CA5
58	EO	207	PC1	C3-C2-O21-C21
58	Dc	607	PC1	C1-C2-O21-C21
57	DS	402	CDL	C54-C55-C56-C57
57	ED	604	CDL	C75-C76-C77-C78
57	Dh	202	CDL	C51-C52-C53-C54
65	EL	906	UQ8	C3-C4-O4-C4M
65	Ds	404	UQ8	C4-C3-O3-C3M
59	DA	708	3PE	C36-C37-C38-C39
57	EN	1202	CDL	OB9-CB7-OB8-CB6
57	Dv	402	CDL	OB9-CB7-OB8-CB6
57	Dj	401	CDL	C72-C71-CB7-OB8
57	DI	701	CDL	C36-C37-C38-C39
57	Dg	201	CDL	C75-C76-C77-C78
57	Dj	404	CDL	C58-C59-C60-C61
57	DG	201	CDL	C41-C42-C43-C44
57	El	902	CDL	C79-C80-C81-C82
57	DD	702	CDL	C73-C74-C75-C76
60	Ed	203	LPP	C18-C19-C20-C21
57	DA	709	CDL	C83-C84-C85-C86
57	DN	504	CDL	C20-C21-C22-C23
65	El	906	UQ8	C36-C37-C38-C39
57	DM	501	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
57	EU	101	CDL	C71-C72-C73-C74
57	DJ	303	CDL	C72-C71-CB7-OB8
57	Dr	402	CDL	C52-C51-CB5-OB6
57	DJ	303	CDL	C12-C11-CA5-OA7
57	Dj	408	CDL	C52-C51-CB5-OB7
57	DH	201	CDL	C60-C61-C62-C63
57	DR	403	CDL	C20-C21-C22-C23
65	Ed	202	UQ8	C24-C26-C27-C28
59	DA	708	3PE	C3C-C3D-C3E-C3F
59	Da	708	3PE	C3C-C3D-C3E-C3F
59	Da	708	3PE	C2D-C2E-C2F-C2G
57	DA	705	CDL	C1-CB2-OB2-PB2
57	Dg	201	CDL	C1-CB2-OB2-PB2
57	Eg	101	CDL	CA4-CA3-OA5-PA1
58	EB	301	PC1	C2-C1-O11-P
58	EB	303	PC1	C2-C1-O11-P
57	DD	702	CDL	C14-C15-C16-C17
57	Dn	501	CDL	C83-C84-C85-C86
65	EL	906	UQ8	C15-C14-C16-C17
57	DO	501	CDL	C72-C71-CB7-OB9
57	DV	403	CDL	C72-C71-CB7-OB9
58	DC	603	PC1	O22-C21-C22-C23
58	Dc	603	PC1	O22-C21-C22-C23
58	Dv	405	PC1	O32-C31-C32-C33
57	DA	710	CDL	C12-C11-CA5-OA6
57	Dn	503	CDL	C32-C31-CA7-OA8
58	Ef	1001	PC1	O31-C31-C32-C33
57	EN	1201	CDL	C42-C43-C44-C45
57	Dd	704	CDL	C40-C41-C42-C43
57	DA	709	CDL	C55-C56-C57-C58
57	DG	201	CDL	C17-C18-C19-C20
57	Da	709	CDL	C36-C37-C38-C39
57	Dd	704	CDL	C83-C84-C85-C86
57	Dj	403	CDL	C63-C64-C65-C66
57	Du	402	CDL	C20-C21-C22-C23
57	Ea	301	CDL	C72-C71-CB7-OB9
58	Dx	1204	PC1	O32-C31-C32-C33
59	DS	403	3PE	O22-C21-C22-C23
59	Ds	403	3PE	O22-C21-C22-C23
59	Dx	1206	3PE	O22-C21-C22-C23
60	Dn	506	LPP	O28-C29-C30-C31
57	DU	404	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
57	EL	901	CDL	C32-C33-C34-C35
57	Dd	704	CDL	OB5-CB3-CB4-OB6
59	Dr	401	3PE	O11-C1-C2-O21
57	Du	404	CDL	C76-C77-C78-C79
59	DX	303	3PE	C26-C27-C28-C29
57	DD	704	CDL	C52-C51-CB5-OB6
57	DS	405	CDL	C12-C11-CA5-OA6
57	DQ	1501	CDL	C72-C71-CB7-OB9
57	EA	301	CDL	C52-C51-CB5-OB7
57	Dm	501	CDL	C52-C51-CB5-OB7
57	Dn	502	CDL	C32-C31-CA7-OA9
57	Dv	401	CDL	C52-C51-CB5-OB7
58	EO	205	PC1	O22-C21-C22-C23
59	DX	303	3PE	O22-C21-C22-C23
57	DZ	501	CDL	C33-C34-C35-C36
57	EL	903	CDL	C33-C34-C35-C36
57	Ep	701	CDL	C55-C56-C57-C58
57	EO	202	CDL	C72-C73-C74-C75
57	Dv	403	CDL	C77-C78-C79-C80
57	EN	1202	CDL	C71-CB7-OB8-CB6
57	Dv	402	CDL	C82-C83-C84-C85
57	EH	202	CDL	C72-C71-CB7-OB9
57	Da	705	CDL	C72-C71-CB7-OB9
57	Dq	404	CDL	C72-C71-CB7-OB9
57	Ea	301	CDL	C12-C11-CA5-OA7
57	Ep	701	CDL	C12-C11-CA5-OA7
58	El	904	PC1	O22-C21-C22-C23
59	DJ	301	3PE	O32-C31-C32-C33
59	DX	304	3PE	O32-C31-C32-C33
57	Ds	402	CDL	C76-C77-C78-C79
57	Dm	501	CDL	C41-C42-C43-C44
57	Dn	501	CDL	C43-C44-C45-C46
57	DJ	303	CDL	C59-C60-C61-C62
57	DR	403	CDL	C37-C38-C39-C40
57	DU	401	CDL	C72-C71-CB7-OB9
57	Dd	705	CDL	C12-C11-CA5-OA7
57	Dj	408	CDL	C32-C31-CA7-OA9
57	Ek	201	CDL	C32-C31-CA7-OA9
58	DV	405	PC1	O32-C31-C32-C33
58	Da	706	PC1	O32-C31-C32-C33
59	Dd	703	3PE	O22-C21-C22-C23
60	Dn	504	LPP	O28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
57	DX	307	CDL	C42-C43-C44-C45
57	DN	505	CDL	C53-C54-C55-C56
57	DR	402	CDL	C31-C32-C33-C34
57	Dv	402	CDL	C71-CB7-OB8-CB6
59	Dd	703	3PE	O31-C31-C32-C33
57	DQ	1501	CDL	C32-C31-CA7-OA9
57	DR	403	CDL	C52-C51-CB5-OB7
57	EI	401	CDL	C12-C11-CA5-OA7
57	Da	709	CDL	C52-C51-CB5-OB7
57	Dm	501	CDL	C72-C71-CB7-OB9
57	Dn	501	CDL	C72-C71-CB7-OB9
57	Du	404	CDL	C72-C71-CB7-OB9
57	Dv	403	CDL	C72-C71-CB7-OB9
57	Ed	205	CDL	C12-C11-CA5-OA7
57	El	901	CDL	C32-C31-CA7-OA9
58	EO	207	PC1	O22-C21-C22-C23
59	DG	204	3PE	O22-C21-C22-C23
59	DS	401	3PE	O22-C21-C22-C23
59	Dg	204	3PE	O22-C21-C22-C23
57	DS	405	CDL	CA7-C31-C32-C33
57	DD	704	CDL	C37-C38-C39-C40
57	Dh	201	CDL	C60-C61-C62-C63
57	Dn	501	CDL	C77-C78-C79-C80
57	DN	504	CDL	C74-C75-C76-C77
57	DU	403	CDL	C33-C34-C35-C36
57	DV	402	CDL	C71-C72-C73-C74
54	DA	701	HEA	CAD-CBD-CGD-O2D
59	Dx	1206	3PE	C38-C39-C3A-C3B
57	DD	703	CDL	C52-C51-CB5-OB7
57	DU	403	CDL	C32-C31-CA7-OA9
57	ED	604	CDL	C12-C11-CA5-OA7
57	EI	401	CDL	C72-C71-CB7-OB9
57	Dg	201	CDL	C12-C11-CA5-OA7
57	Dm	501	CDL	C12-C11-CA5-OA7
57	Du	401	CDL	C72-C71-CB7-OB9
57	Ea	301	CDL	C52-C51-CB5-OB7
57	El	902	CDL	C52-C51-CB5-OB7
58	Dc	602	PC1	O22-C21-C22-C23
59	DG	205	3PE	O22-C21-C22-C23
59	DJ	301	3PE	O22-C21-C22-C23
59	Dc	606	3PE	O22-C21-C22-C23
57	DA	705	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
57	DR	402	CDL	C75-C76-C77-C78
57	EL	904	CDL	C14-C15-C16-C17
57	DD	702	CDL	OA6-CA4-CA6-OA8
57	EA	301	CDL	OA6-CA4-CA6-OA8
57	Dj	402	CDL	OB6-CB4-CB6-OB8
57	Dq	402	CDL	OA6-CA4-CA6-OA8
57	DJ	303	CDL	C16-C17-C18-C19
57	DJ	307	CDL	C61-C62-C63-C64
57	DQ	1501	CDL	C12-C13-C14-C15
59	Dx	1206	3PE	C35-C36-C37-C38
57	DQ	1502	CDL	C32-C31-CA7-OA9
57	DV	402	CDL	C12-C11-CA5-OA7
57	DZ	501	CDL	C32-C31-CA7-OA9
57	EK	201	CDL	C32-C31-CA7-OA9
57	Eu	101	CDL	C72-C71-CB7-OB9
58	Dx	1202	PC1	O32-C31-C32-C33
59	DG	205	3PE	O32-C31-C32-C33
59	EN	1203	3PE	O22-C21-C22-C23
57	Dj	402	CDL	C12-C11-CA5-OA6
57	Dg	202	CDL	C43-C44-C45-C46
57	Dr	402	CDL	C42-C43-C44-C45
57	DS	402	CDL	C22-C23-C24-C25
57	DN	504	CDL	CA3-CA4-CA6-OA8
57	DX	307	CDL	CB3-CB4-CB6-OB8
57	Eg	101	CDL	CB3-CB4-CB6-OB8
58	DC	603	PC1	C1-C2-C3-O31
57	DZ	501	CDL	C35-C36-C37-C38
57	Dn	507	CDL	C18-C19-C20-C21
57	Ek	201	CDL	C11-C12-C13-C14
57	En	1201	CDL	C40-C41-C42-C43
57	DQ	1502	CDL	C72-C71-CB7-OB9
57	DV	404	CDL	C52-C51-CB5-OB7
57	Do	501	CDL	C72-C71-CB7-OB9
59	DX	304	3PE	O22-C21-C22-C23
59	Ds	401	3PE	O22-C21-C22-C23
59	Dx	1205	3PE	O22-C21-C22-C23
57	Di	701	CDL	C23-C24-C25-C26
57	Dj	408	CDL	C1-CA2-OA2-PA1
57	EN	1201	CDL	C12-C11-CA5-OA6
57	Dd	702	CDL	C32-C31-CA7-OA8
58	Eo	201	PC1	O31-C31-C32-C33
57	DU	403	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
57	EN	1201	CDL	C52-C53-C54-C55
57	Dn	501	CDL	C36-C37-C38-C39
57	DD	704	CDL	C72-C71-CB7-OB9
57	DM	501	CDL	C12-C11-CA5-OA7
57	DV	401	CDL	C52-C51-CB5-OB7
57	Da	709	CDL	C12-C11-CA5-OA7
57	Dq	402	CDL	C32-C31-CA7-OA9
57	Dq	403	CDL	C72-C71-CB7-OB9
57	Dv	402	CDL	C12-C11-CA5-OA7
57	Dv	404	CDL	C52-C51-CB5-OB7
57	Dz	501	CDL	C32-C31-CA7-OA9
58	DA	706	PC1	O32-C31-C32-C33
57	DD	703	CDL	C74-C75-C76-C77
57	DH	201	CDL	C59-C60-C61-C62
57	Eg	101	CDL	C12-C13-C14-C15
58	DJ	306	PC1	C33-C34-C35-C36
57	Ds	405	CDL	CA7-C31-C32-C33
57	DX	307	CDL	C34-C35-C36-C37
57	EL	903	CDL	C84-C85-C86-C87
57	DG	201	CDL	C21-C22-C23-C24
57	EB	304	CDL	C72-C71-CB7-OB8
57	EH	201	CDL	C32-C31-CA7-OA8
57	EU	101	CDL	C72-C71-CB7-OB8
57	Dg	201	CDL	C32-C31-CA7-OA8
57	Dm	502	CDL	C12-C11-CA5-OA6
57	Dn	505	CDL	C12-C11-CA5-OA6
57	Dy	301	CDL	C72-C71-CB7-OB8
57	El	901	CDL	C72-C71-CB7-OB8
59	Em	901	3PE	O21-C21-C22-C23
59	Dx	1205	3PE	C2-C3-O31-C31
57	Dj	401	CDL	C72-C71-CB7-OB9
58	DC	602	PC1	O22-C21-C22-C23
58	Eo	205	PC1	O22-C21-C22-C23
57	Du	401	CDL	C40-C41-C42-C43
57	Du	404	CDL	C61-C62-C63-C64
59	Dx	1207	3PE	C26-C27-C28-C29
57	DO	501	CDL	OB5-CB3-CB4-CB6
57	Eg	101	CDL	OA5-CA3-CA4-CA6
58	DB	702	PC1	O11-C1-C2-C3
59	Dd	703	3PE	O11-C1-C2-C3
57	DY	301	CDL	C20-C21-C22-C23
57	Ek	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
57	Eh	1601	CDL	C52-C51-CB5-OB7
58	EO	206	PC1	O32-C31-C32-C33
59	Eo	202	3PE	O32-C31-C32-C33
57	DC	601	CDL	C72-C71-CB7-OB8
57	Dn	505	CDL	C72-C71-CB7-OB8
57	Du	403	CDL	C12-C11-CA5-OA6
58	DC	605	PC1	O21-C21-C22-C23
58	DI	702	PC1	O21-C21-C22-C23
58	Dc	605	PC1	O21-C21-C22-C23
57	DI	701	CDL	C23-C24-C25-C26
57	EH	201	CDL	C80-C81-C82-C83
57	Dd	706	CDL	C34-C35-C36-C37
57	Dr	402	CDL	C74-C75-C76-C77
57	Dx	1203	CDL	C57-C58-C59-C60
57	DA	709	CDL	C82-C83-C84-C85
57	DR	403	CDL	C74-C75-C76-C77
57	Dr	402	CDL	C40-C41-C42-C43
59	DX	304	3PE	C38-C39-C3A-C3B
57	DA	709	CDL	C72-C71-CB7-OB9
57	DN	504	CDL	C72-C71-CB7-OB9
57	Dd	705	CDL	C72-C71-CB7-OB9
57	Dr	403	CDL	C52-C51-CB5-OB7
57	Dx	1201	CDL	C52-C51-CB5-OB7
59	Dx	1206	3PE	O32-C31-C32-C33
57	Dj	405	CDL	C61-C62-C63-C64
57	El	902	CDL	C16-C17-C18-C19
58	DC	604	PC1	C3C-C3D-C3E-C3F
57	DA	705	CDL	C72-C71-CB7-OB8
57	DD	702	CDL	C32-C31-CA7-OA8
57	DI	701	CDL	C72-C71-CB7-OB8
57	DJ	305	CDL	C72-C71-CB7-OB8
57	DM	501	CDL	C72-C71-CB7-OB8
57	DR	403	CDL	C72-C71-CB7-OB8
57	DV	402	CDL	C52-C51-CB5-OB6
57	ED	601	CDL	C52-C51-CB5-OB6
57	Da	709	CDL	C32-C31-CA7-OA8
57	Dc	601	CDL	C72-C71-CB7-OB8
57	Dd	706	CDL	C32-C31-CA7-OA8
57	Dq	403	CDL	C52-C51-CB5-OB6
57	Eg	101	CDL	C12-C11-CA5-OA6
58	DQ	1503	PC1	O31-C31-C32-C33
57	Dj	404	CDL	C76-C77-C78-C79

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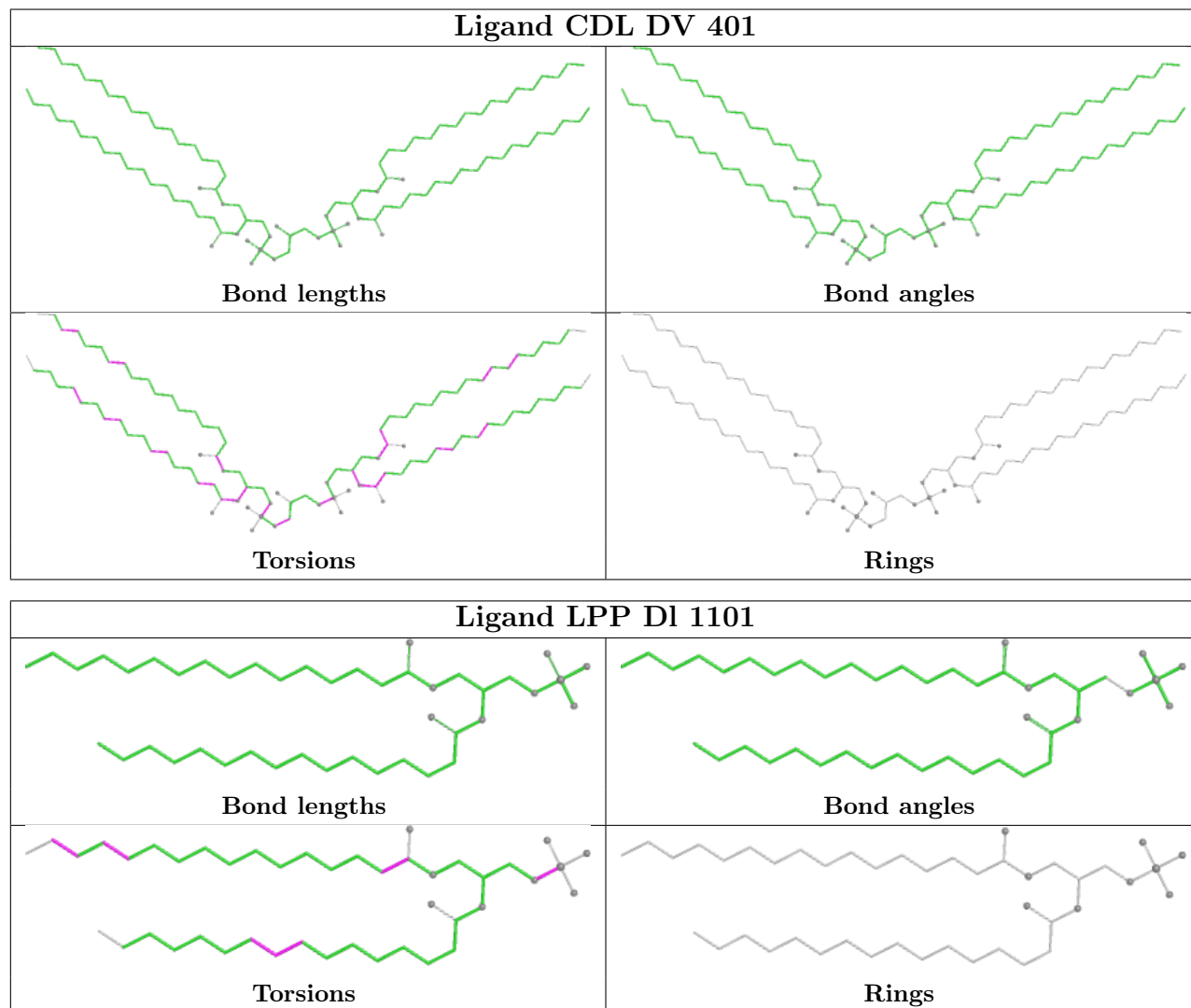
Mol	Chain	Res	Type	Atoms
58	Da	706	PC1	C2D-C2E-C2F-C2G
68	ER	201	ATP	PG-O3B-PB-O1B
57	DA	710	CDL	C12-C11-CA5-OA7
57	DC	601	CDL	C72-C71-CB7-OB9
57	Dc	601	CDL	C72-C71-CB7-OB9
57	Dq	401	CDL	C72-C71-CB7-OB9
58	Ef	1001	PC1	O32-C31-C32-C33
57	Dn	501	CDL	C82-C83-C84-C85
57	Dn	507	CDL	C74-C75-C76-C77
58	Eo	204	PC1	C32-C33-C34-C35
57	Du	404	CDL	C22-C23-C24-C25
57	DM	501	CDL	C32-C31-CA7-OA8
57	DX	307	CDL	C52-C51-CB5-OB6
57	EL	903	CDL	C32-C31-CA7-OA8
57	Dn	502	CDL	C52-C51-CB5-OB6
57	Ep	701	CDL	C32-C31-CA7-OA8
58	Dc	602	PC1	O31-C31-C32-C33
58	Dq	405	PC1	O21-C21-C22-C23
58	Dx	1204	PC1	O21-C21-C22-C23
58	DB	702	PC1	C39-C3A-C3B-C3C
58	Dc	605	PC1	O32-C31-O31-C3
57	Dn	501	CDL	C64-C65-C66-C67
60	Dn	506	LPP	C41-C42-C43-C44
57	DU	401	CDL	C32-C31-CA7-OA9
57	Di	701	CDL	C72-C71-CB7-OB9
57	Du	403	CDL	C32-C31-CA7-OA9
57	Ei	401	CDL	C72-C71-CB7-OB9
58	DC	608	PC1	O22-C21-C22-C23
58	Dc	605	PC1	O22-C21-C22-C23
59	EM	901	3PE	O22-C21-C22-C23
59	Dd	703	3PE	O32-C31-C32-C33
57	Dq	402	CDL	C21-C22-C23-C24
57	Du	404	CDL	C35-C36-C37-C38
58	EO	206	PC1	C3E-C3F-C3G-C3H
57	EL	902	CDL	C64-C65-C66-C67
57	Dh	202	CDL	C35-C36-C37-C38
58	DC	605	PC1	C3B-C3C-C3D-C3E

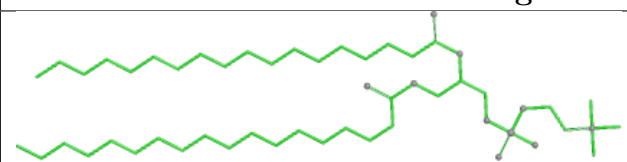
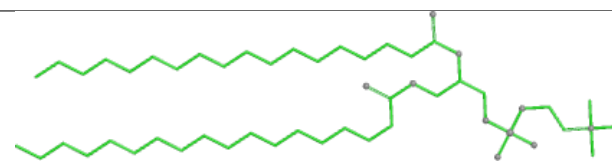
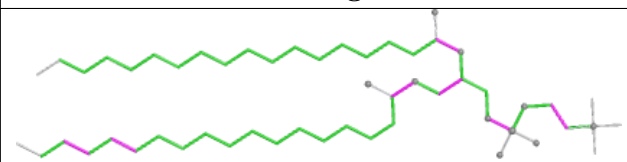
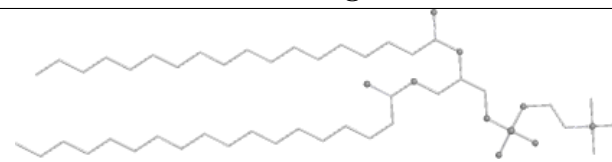
There are no ring outliers.

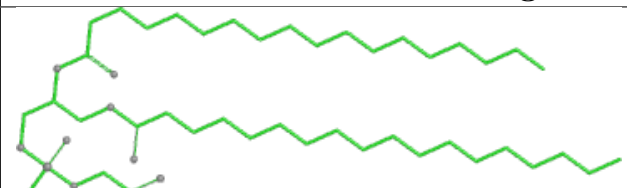
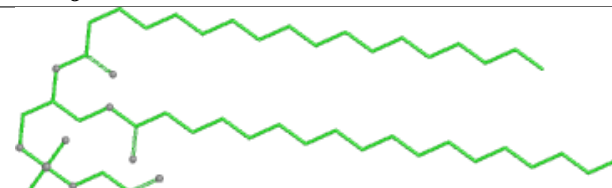
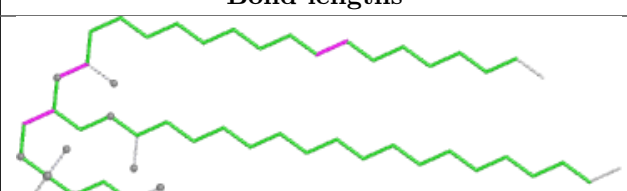
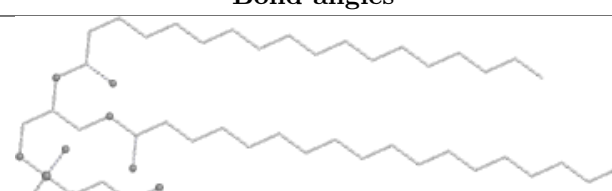
No monomer is involved in short contacts.

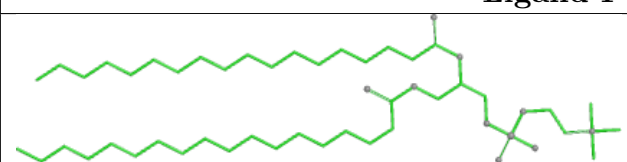
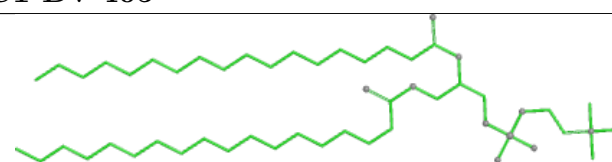
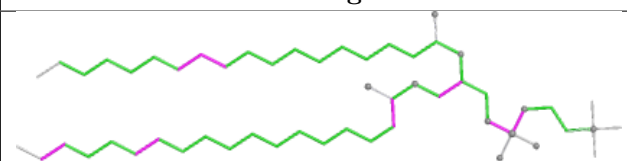
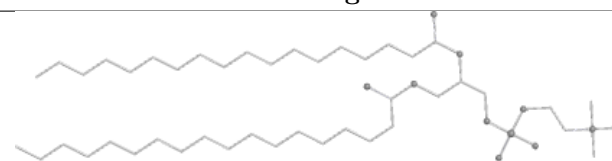
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

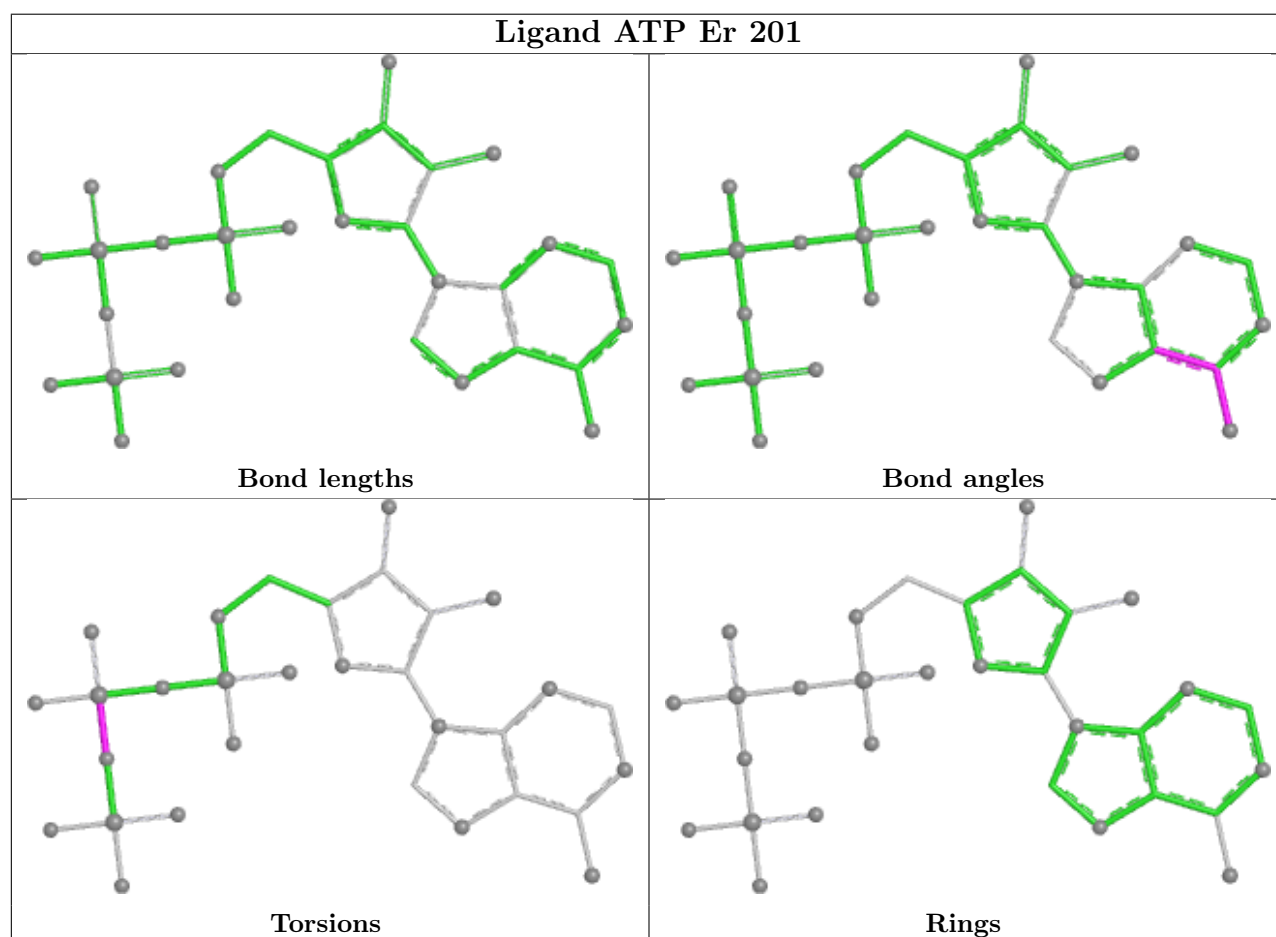
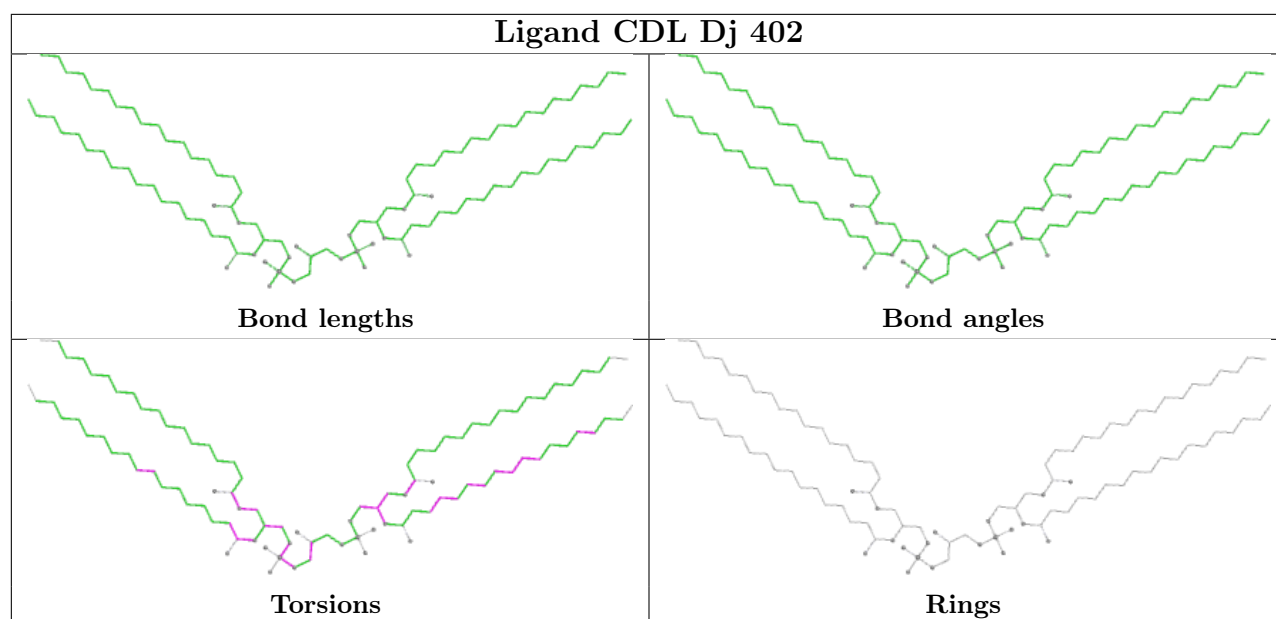
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

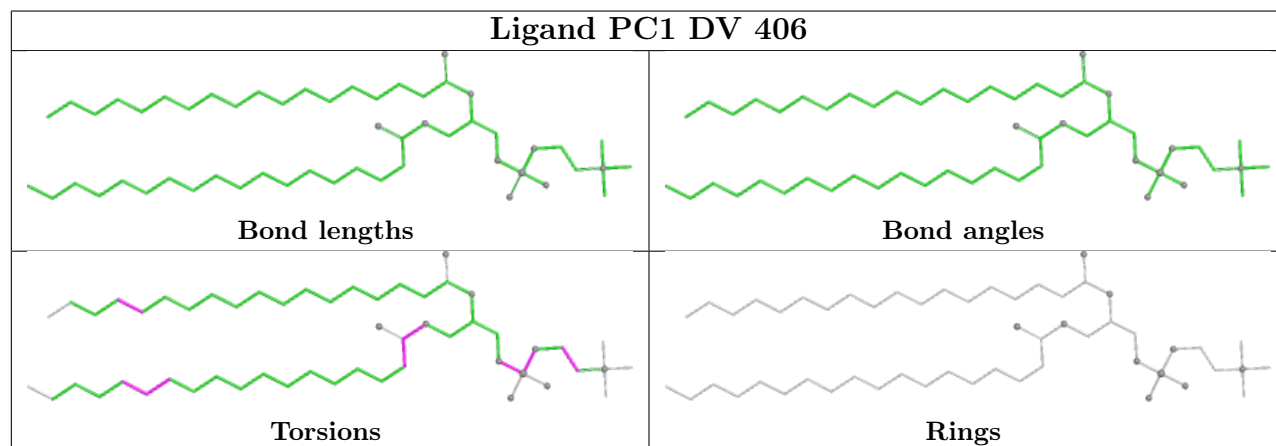
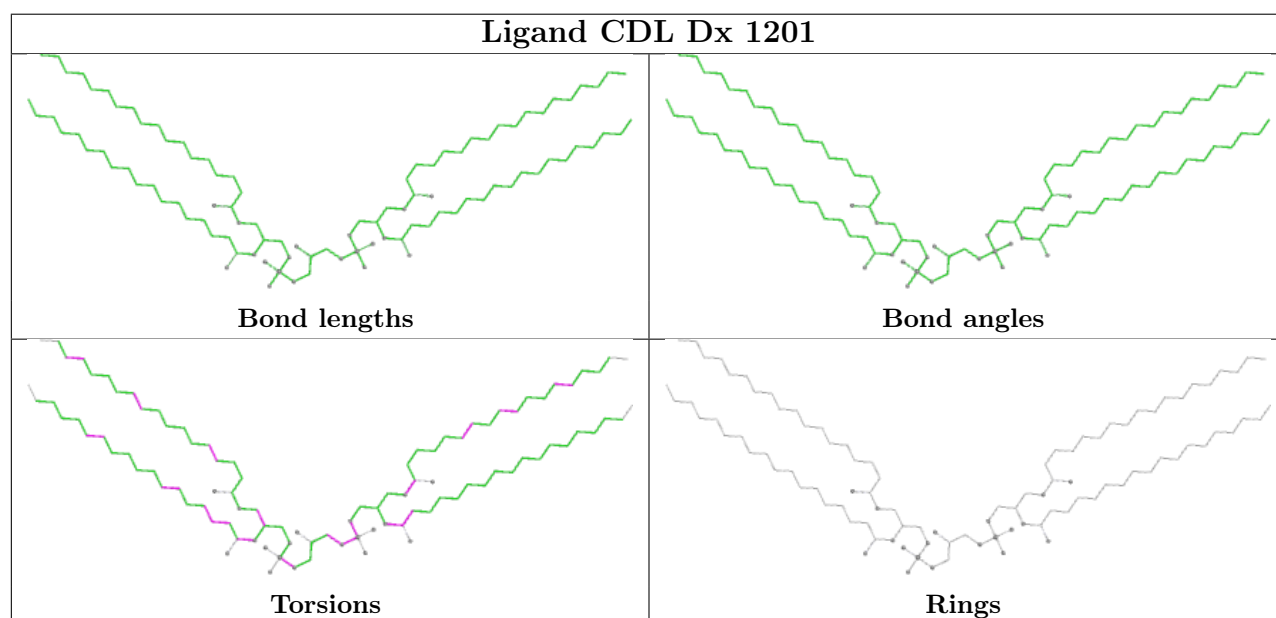
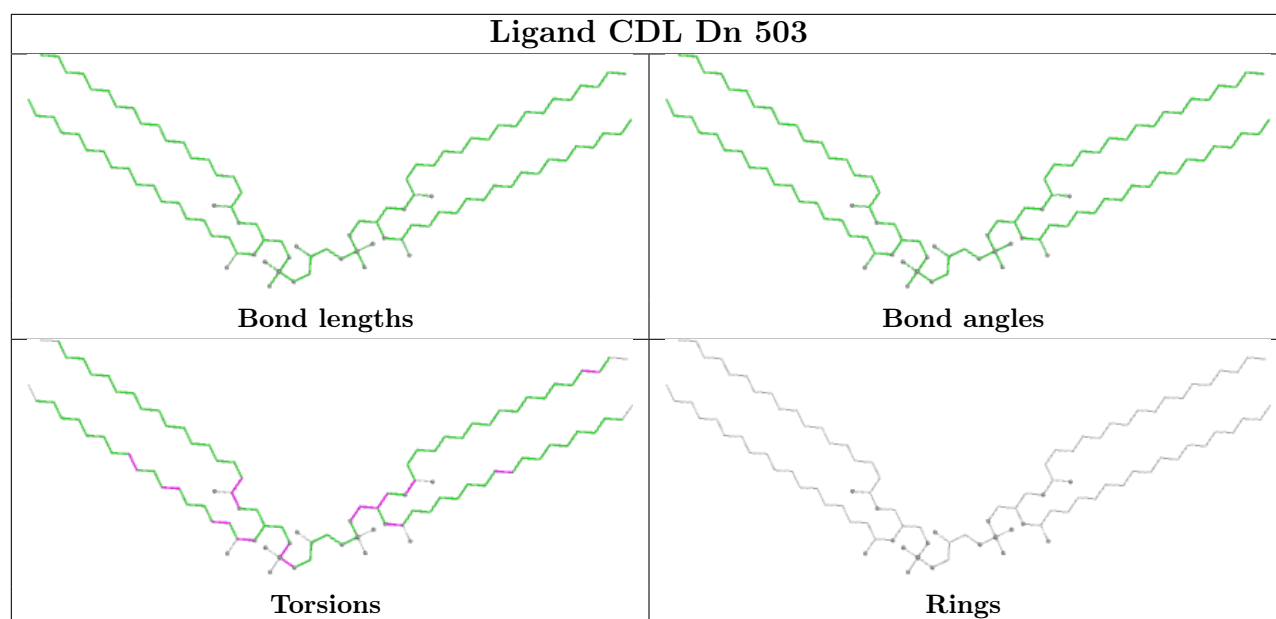


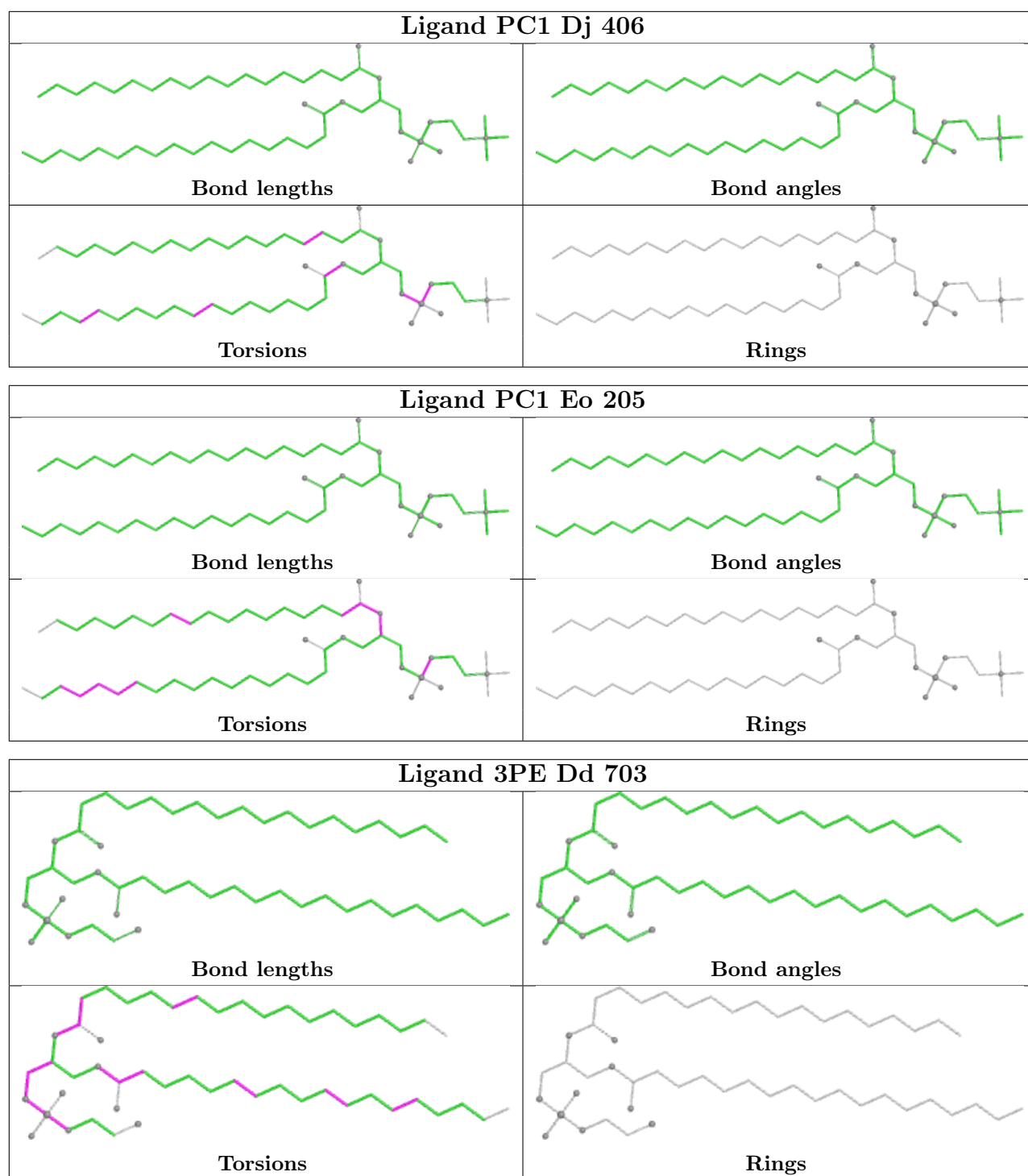
Ligand PC1 Da 707	
	
Bond lengths	Bond angles
	
Torsions	Rings

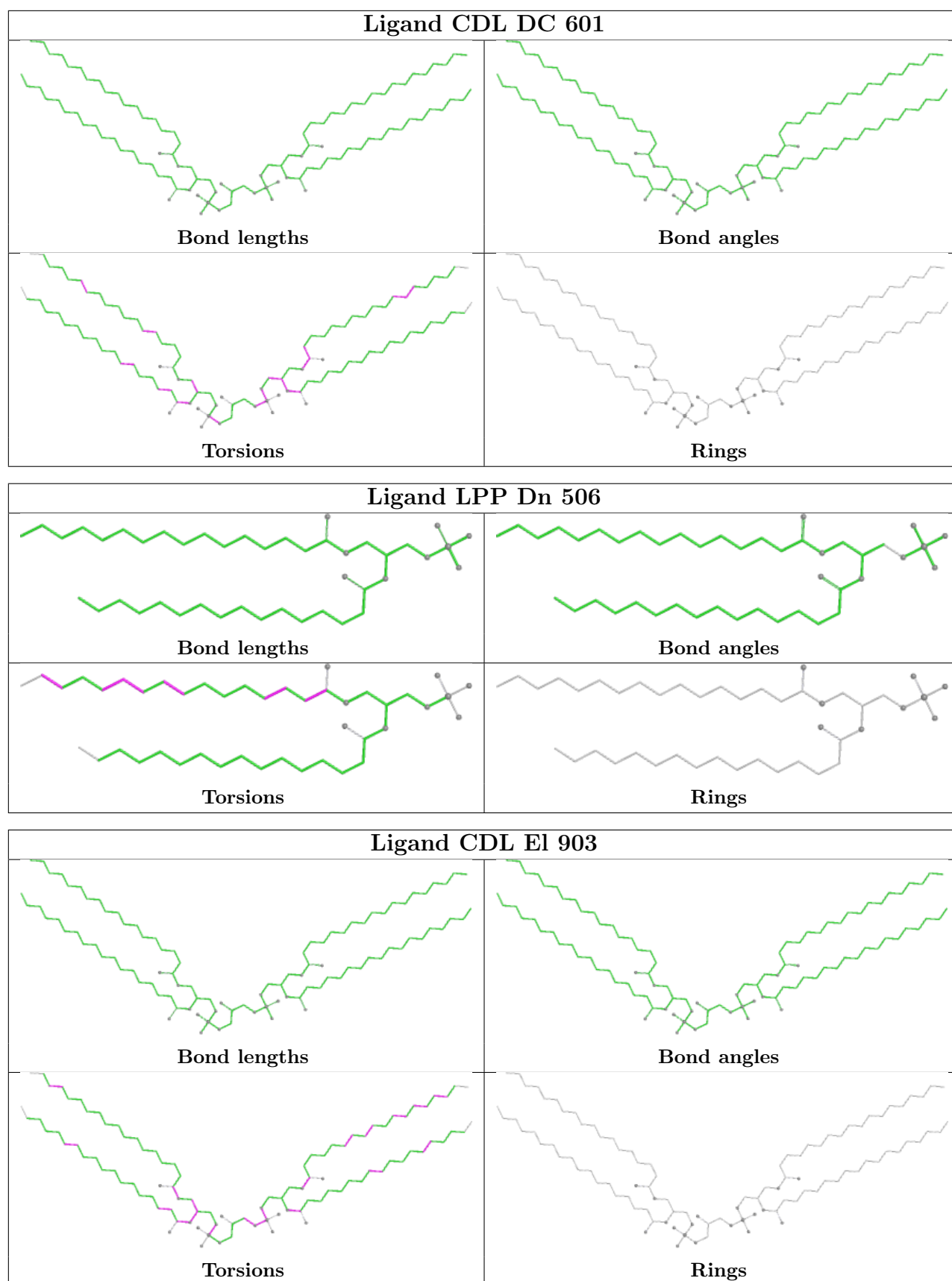
Ligand 3PE Dj 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

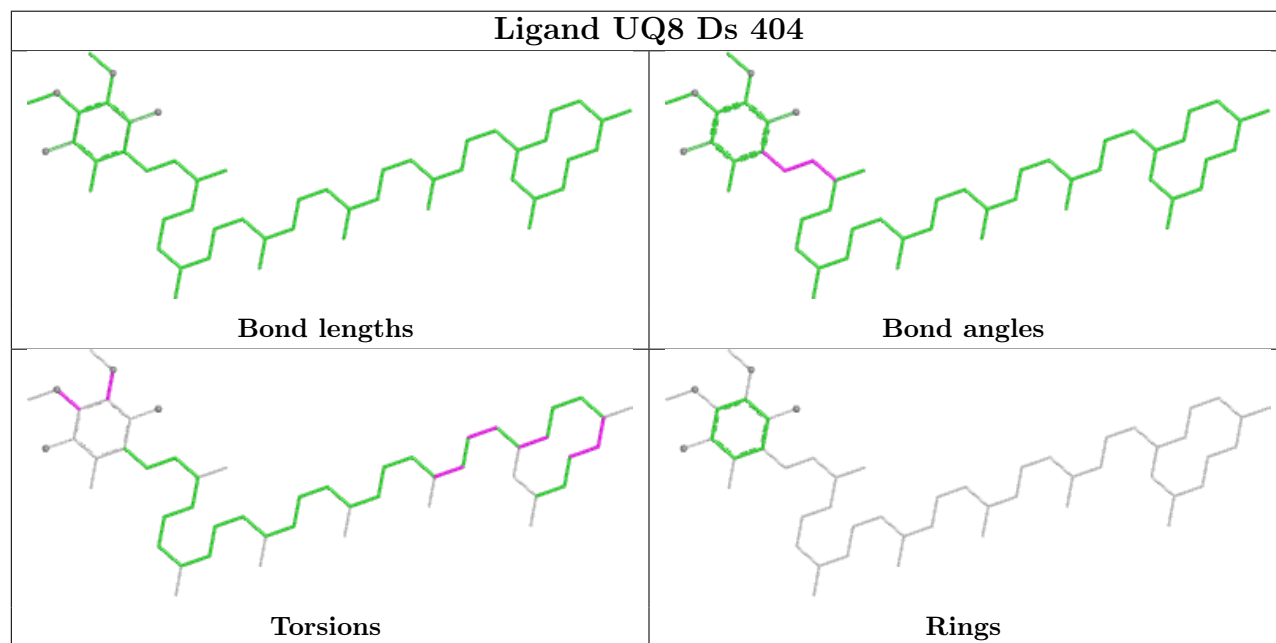
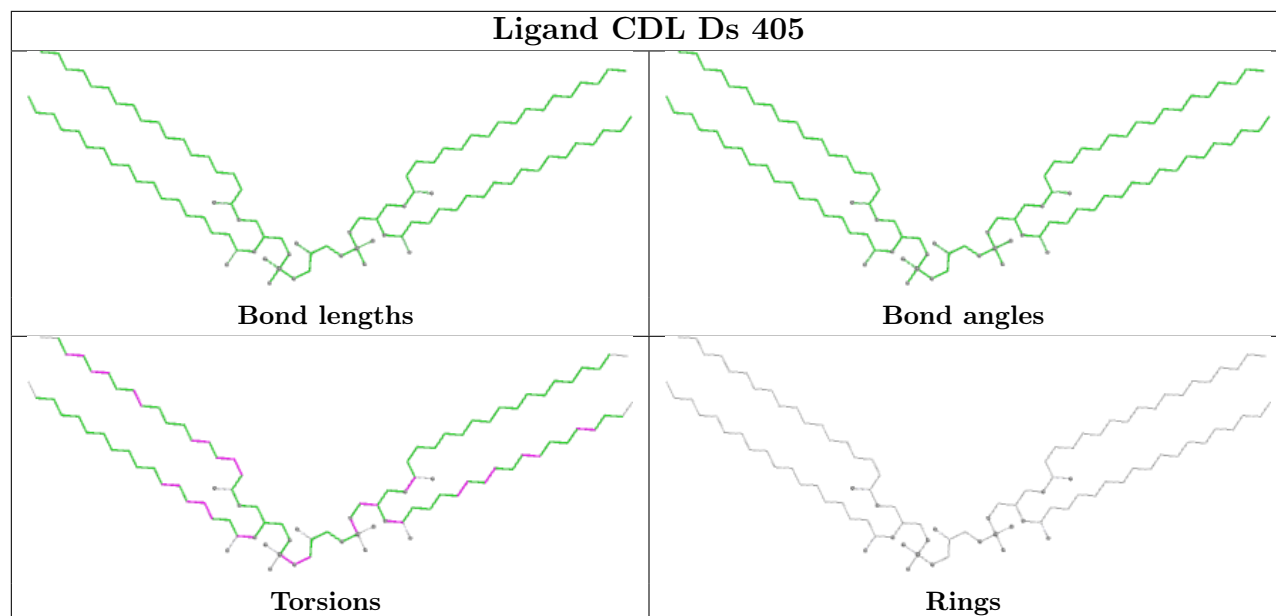
Ligand PC1 Dv 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

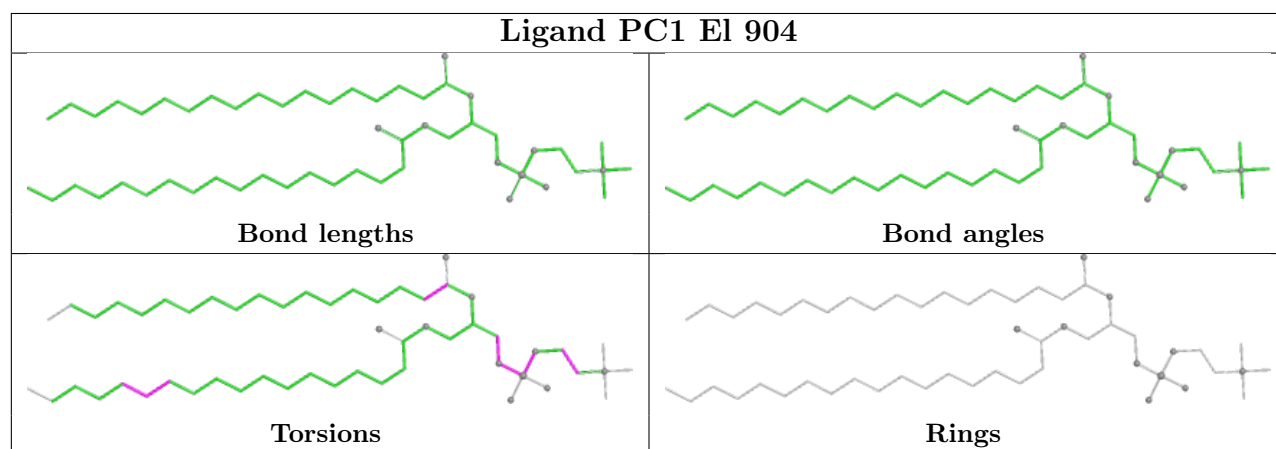
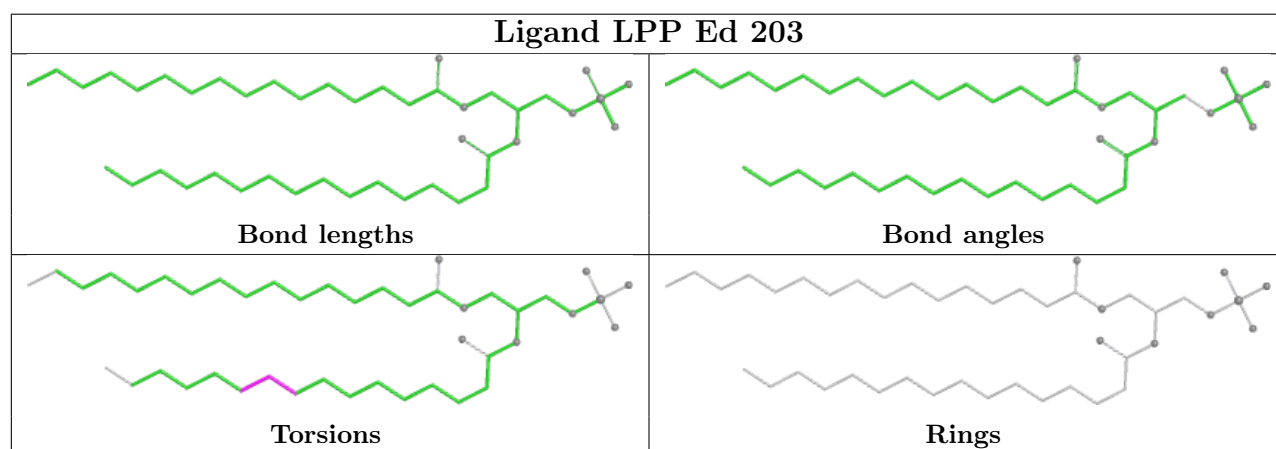
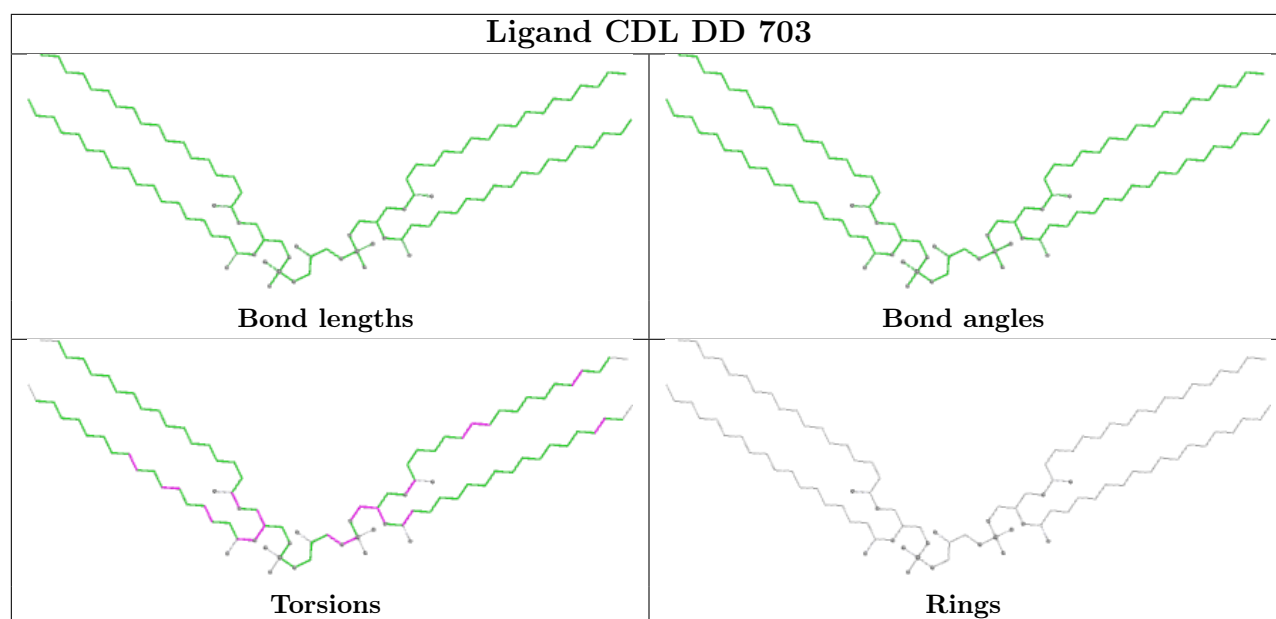


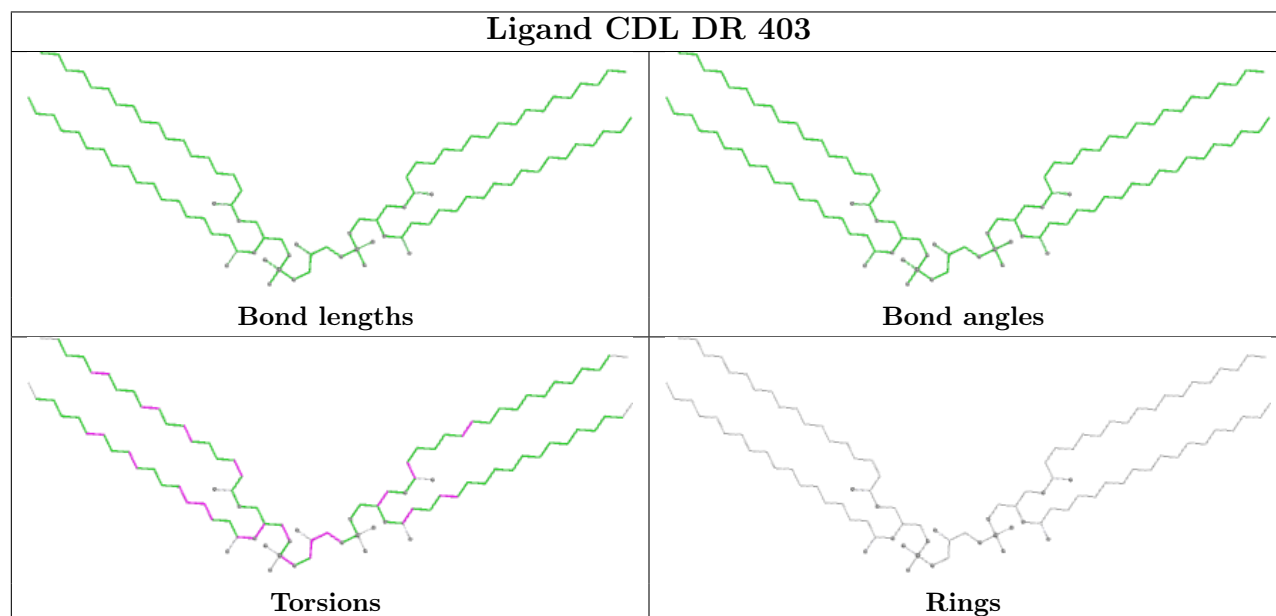
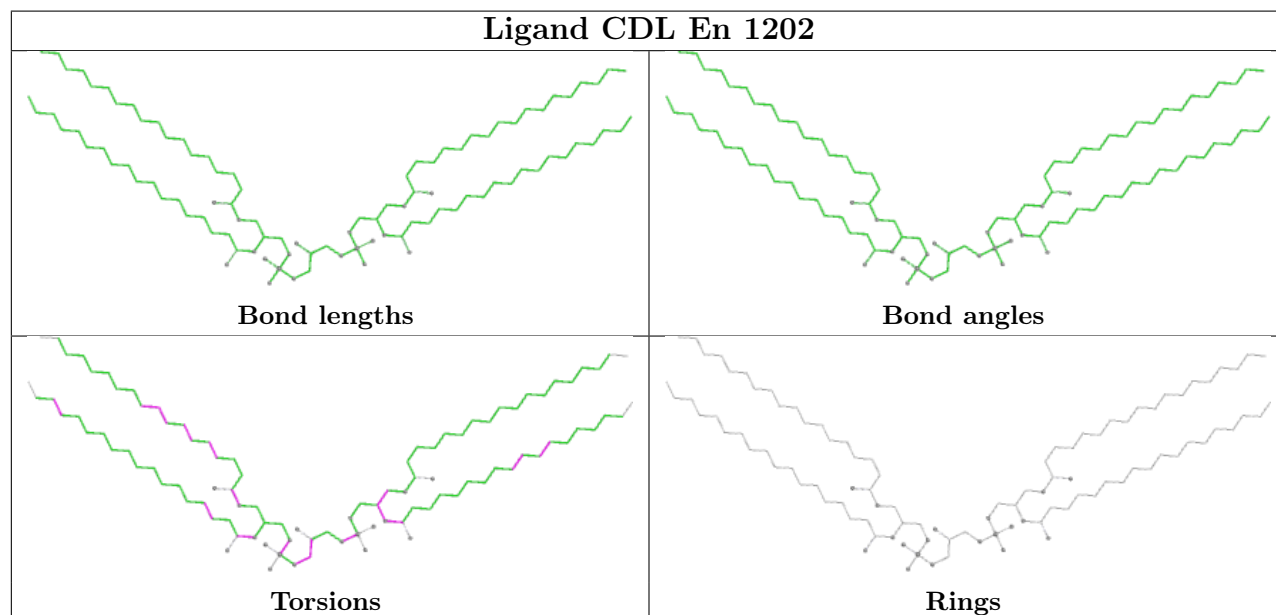
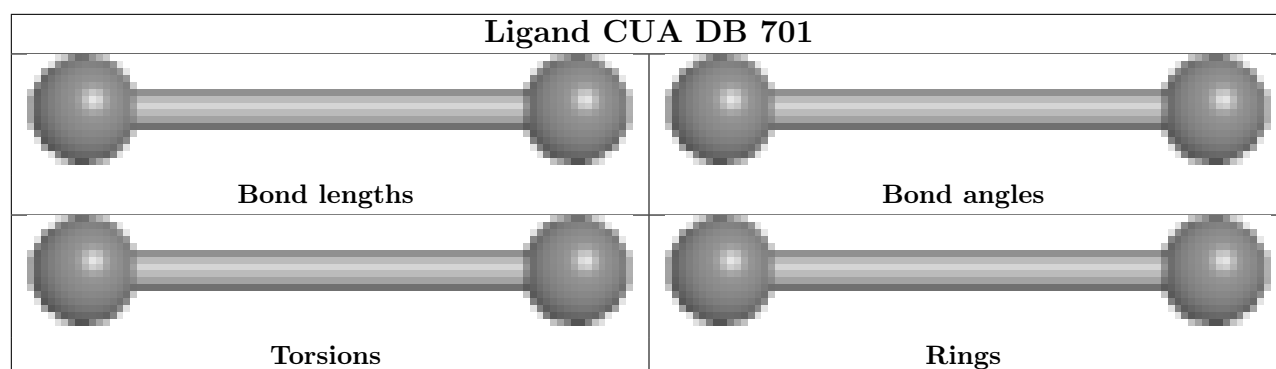


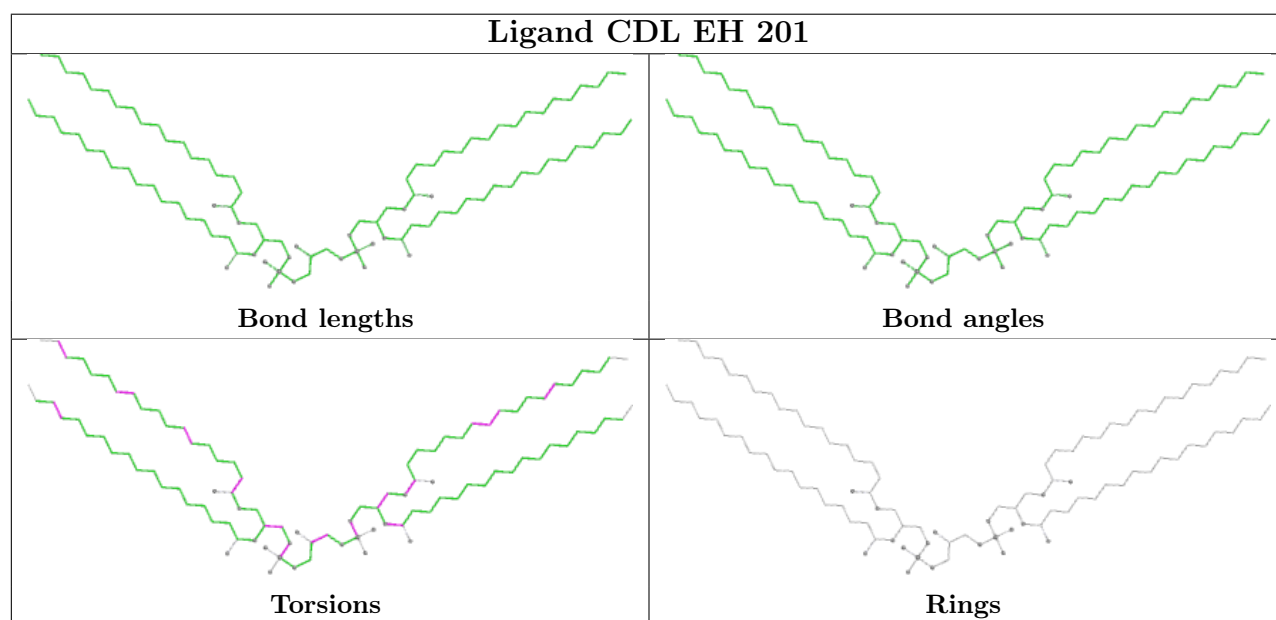
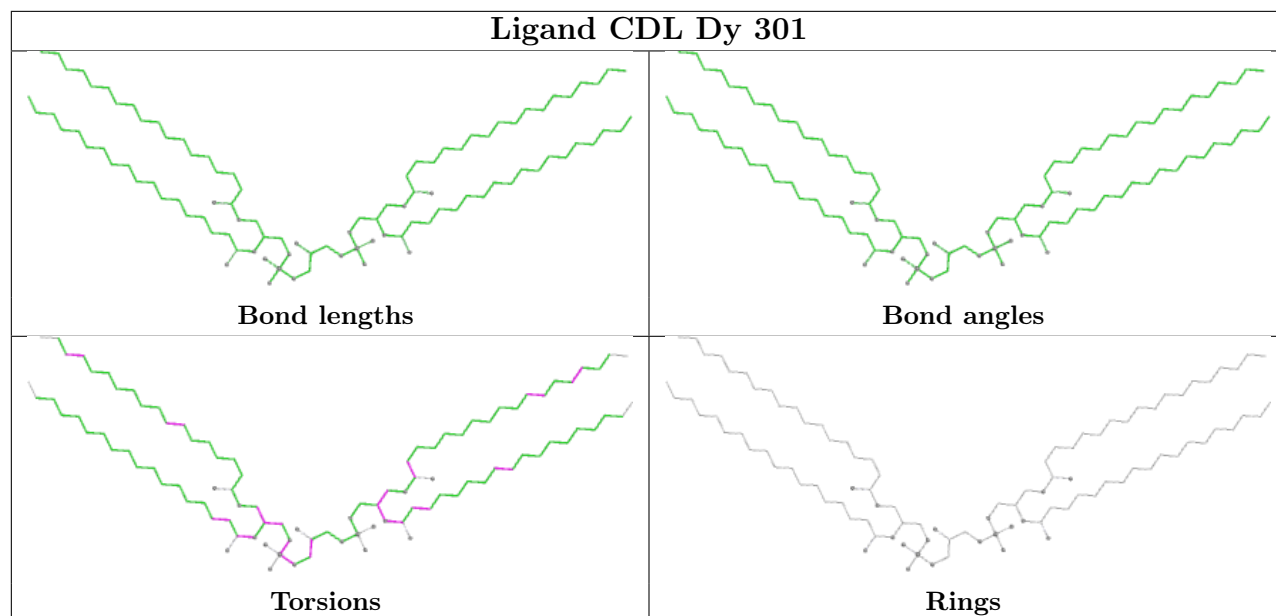


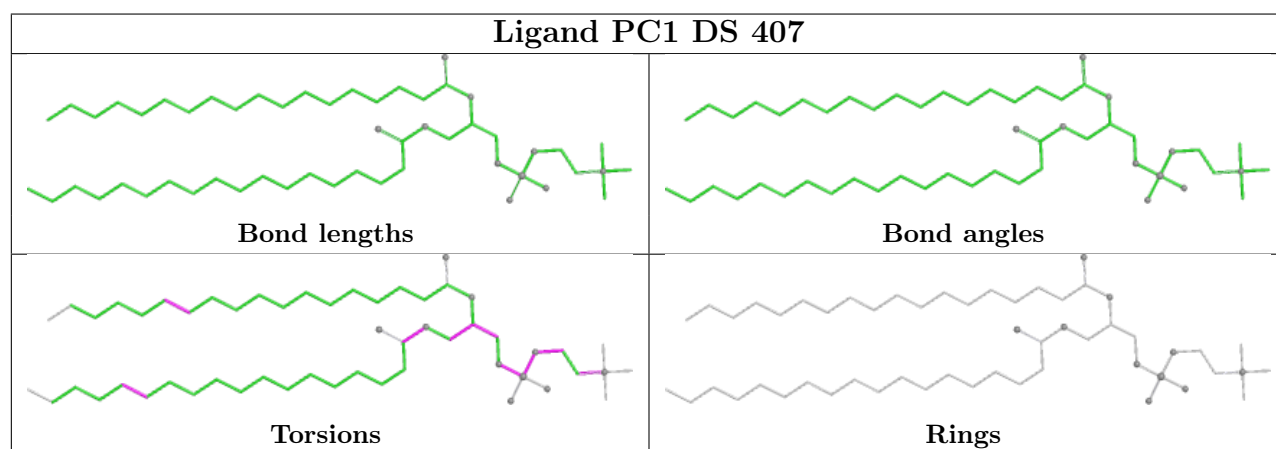
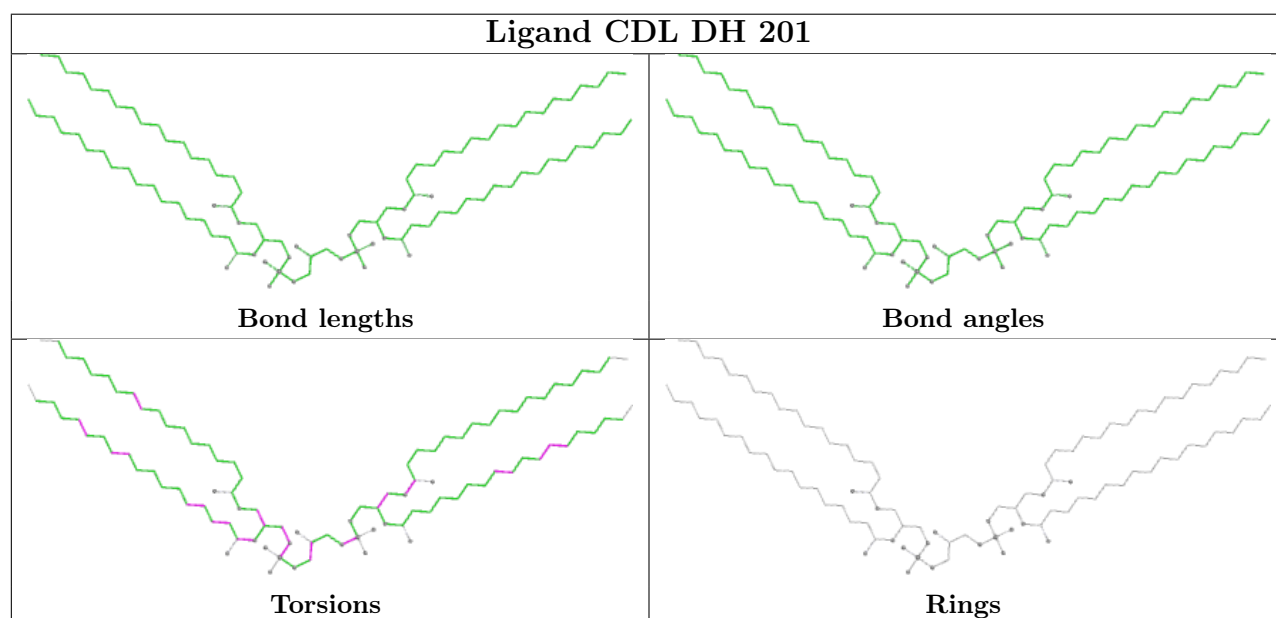
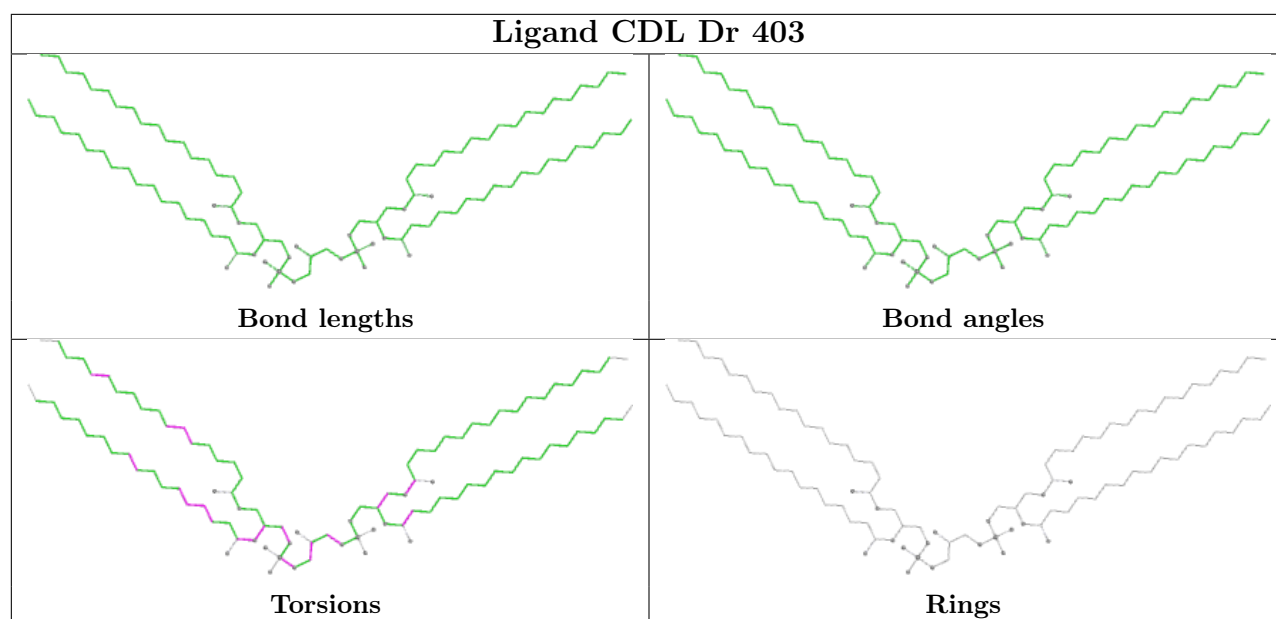


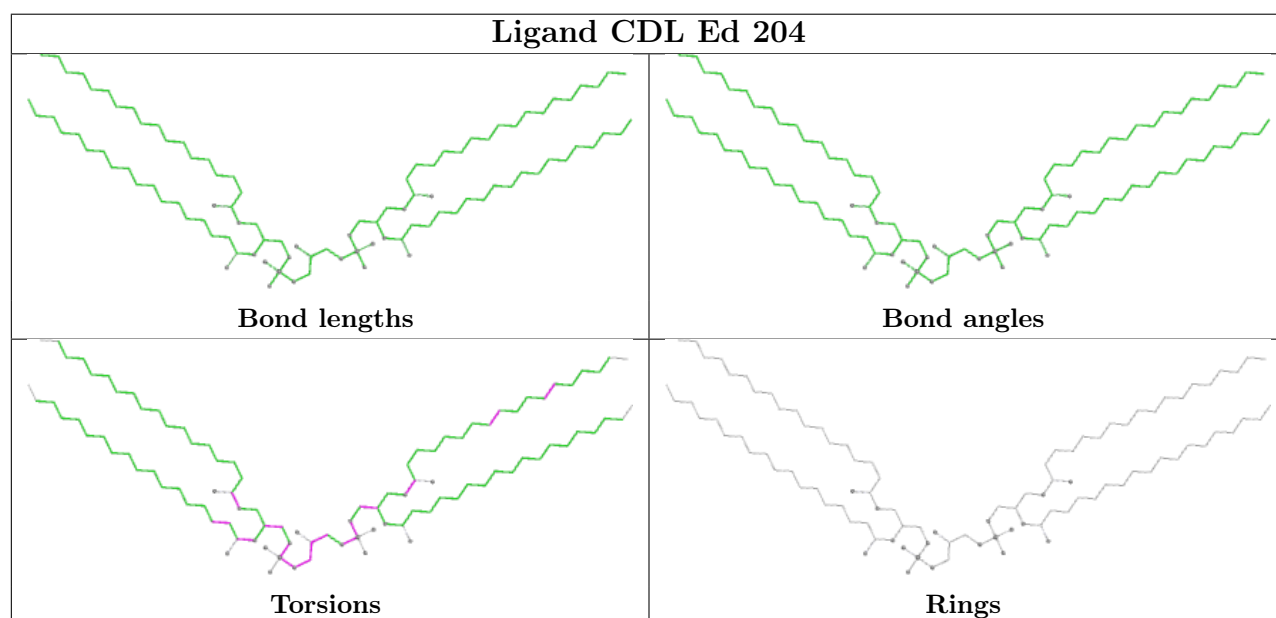
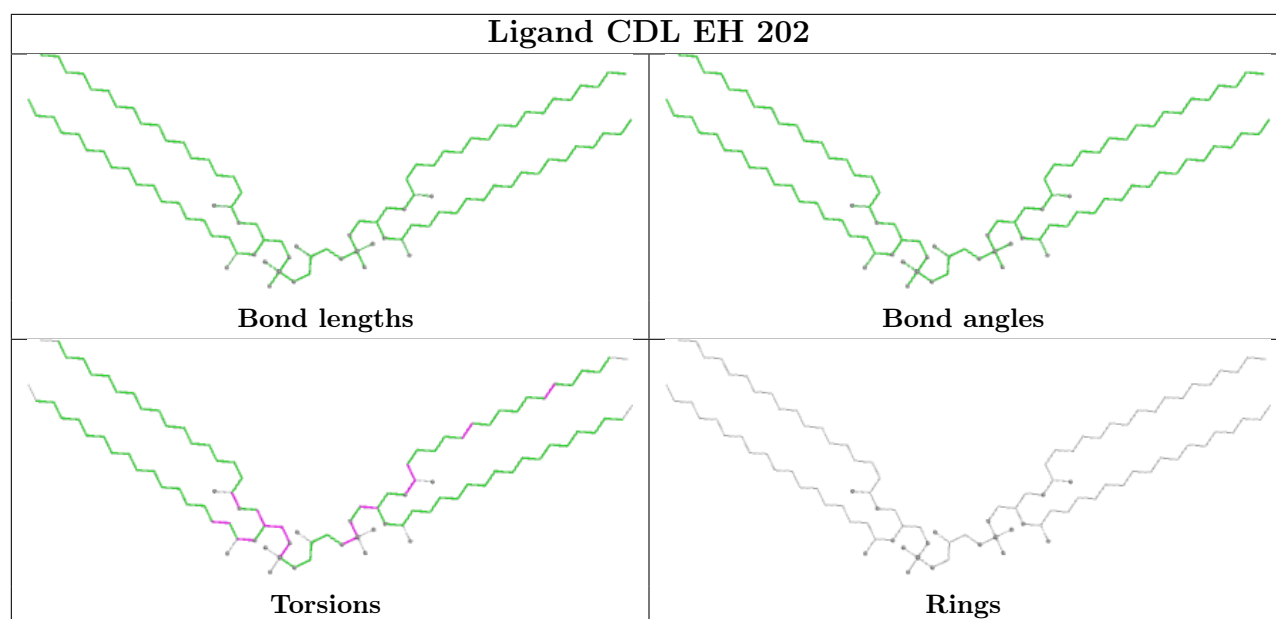


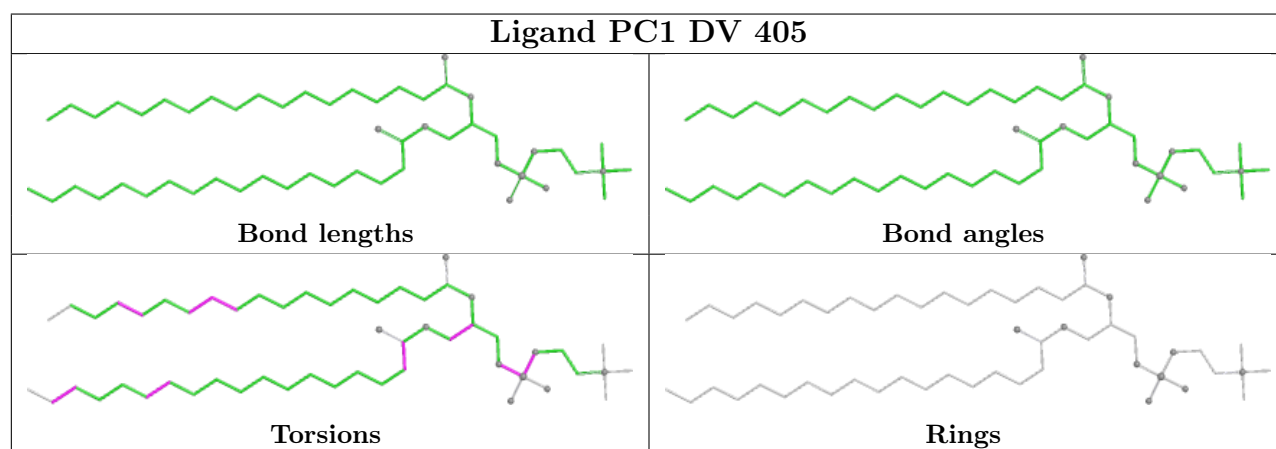
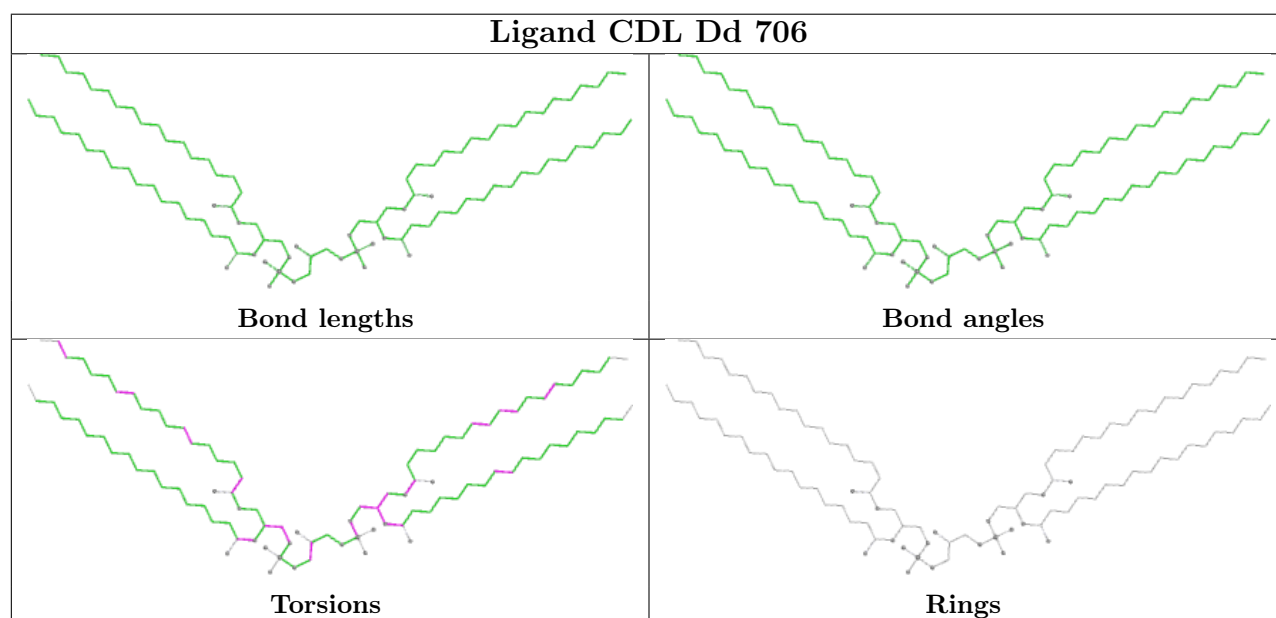
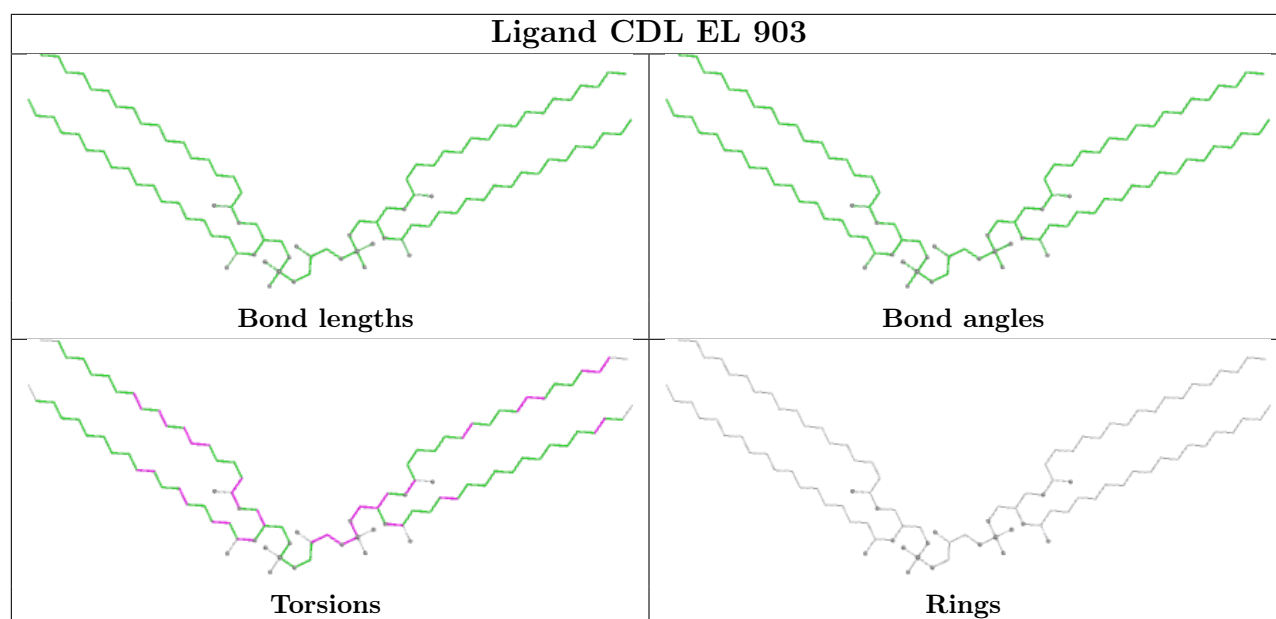


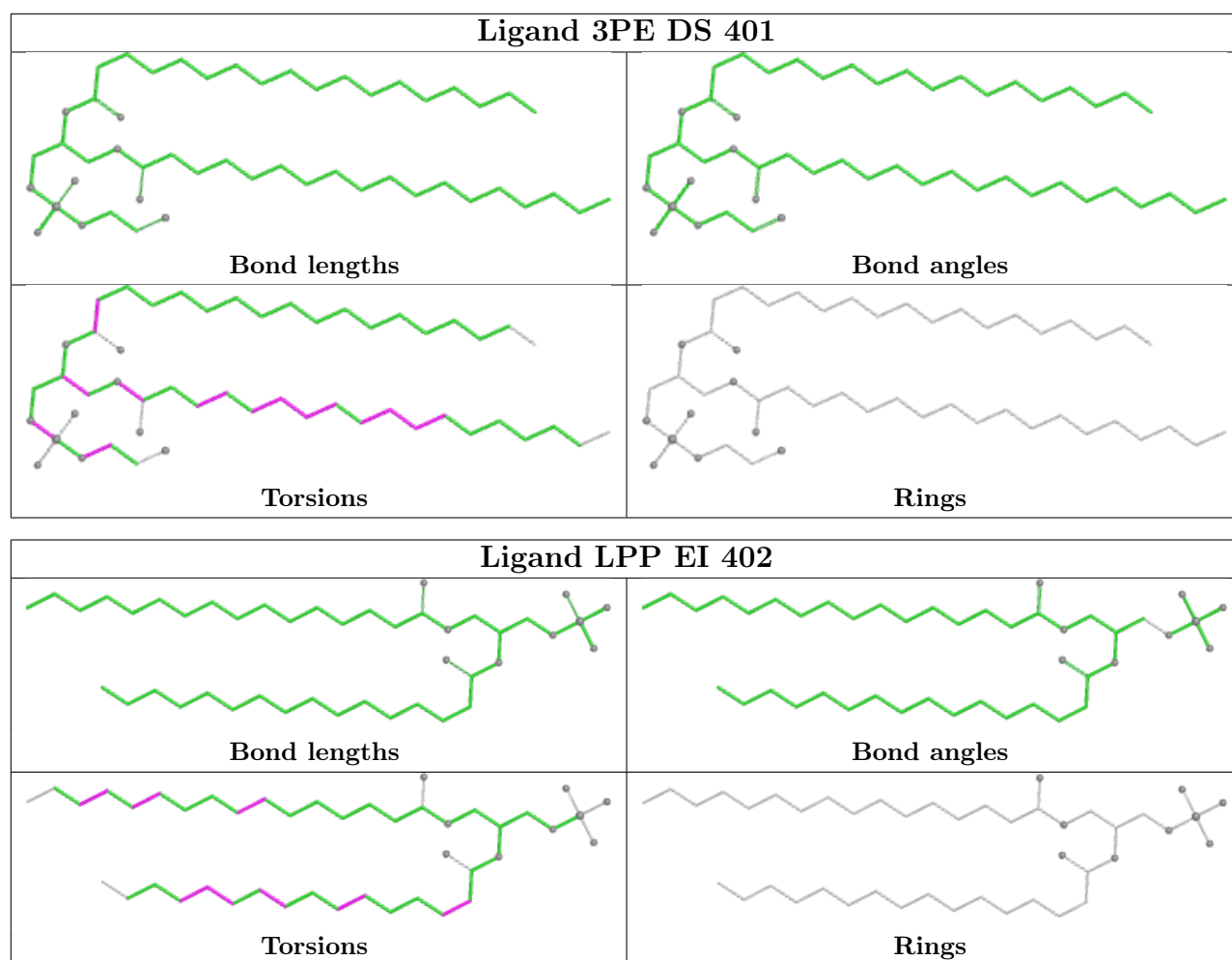


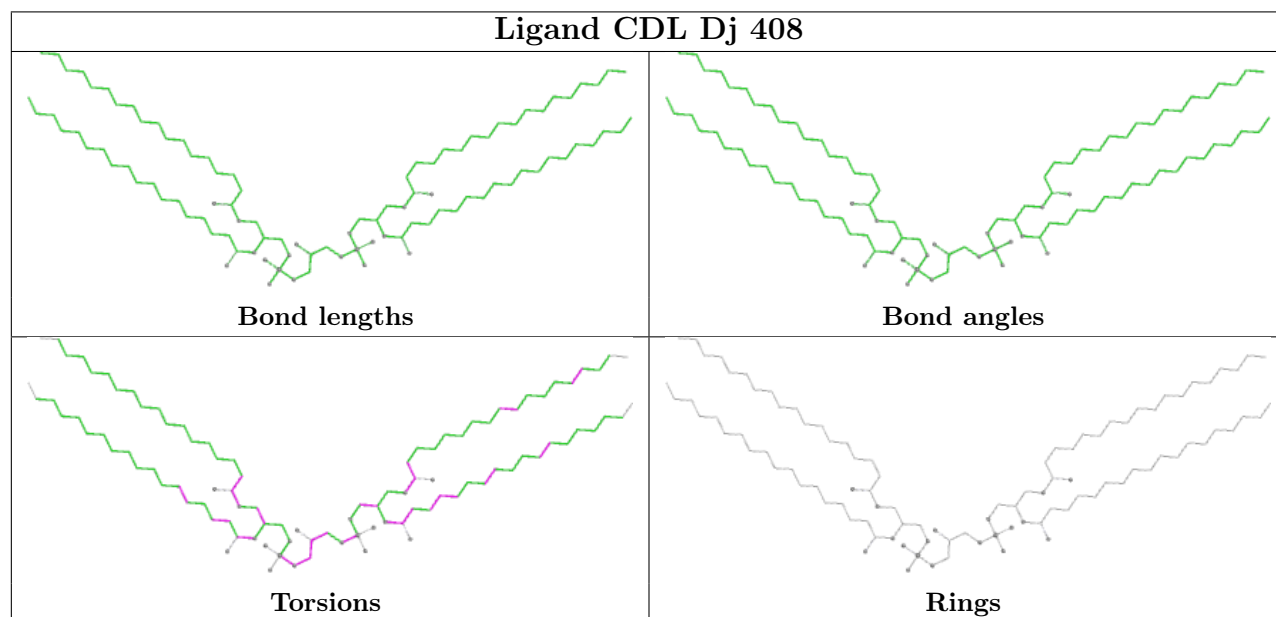
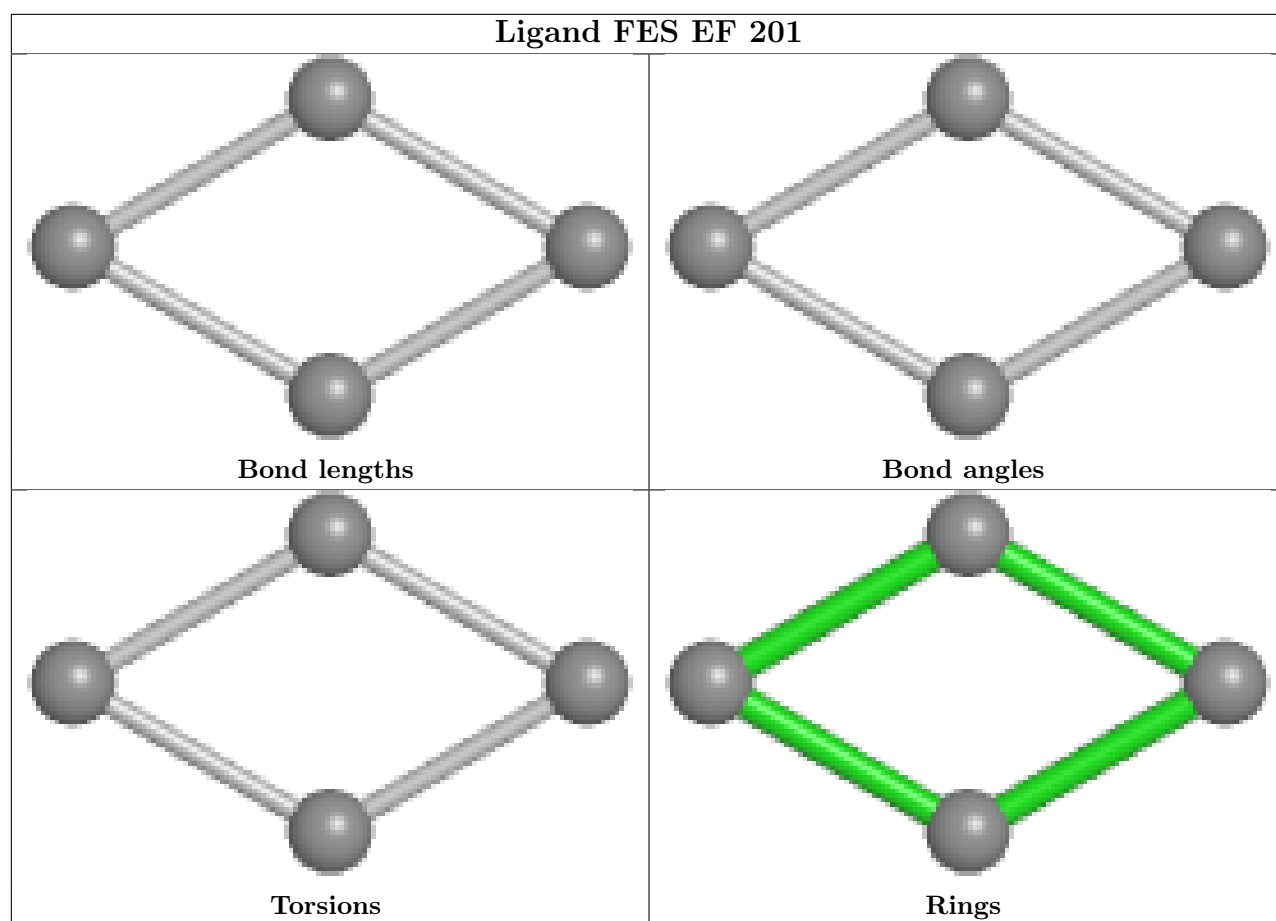


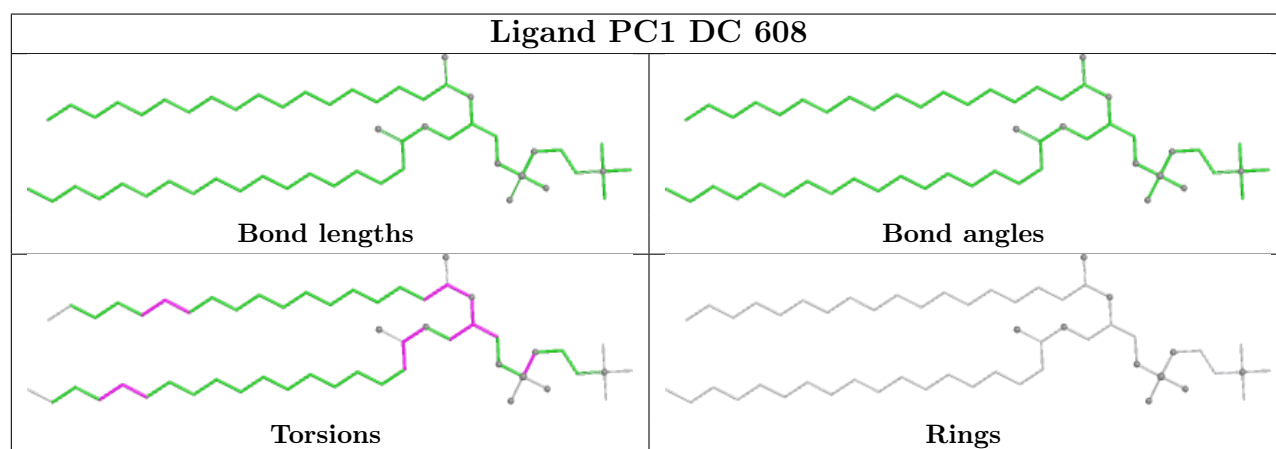
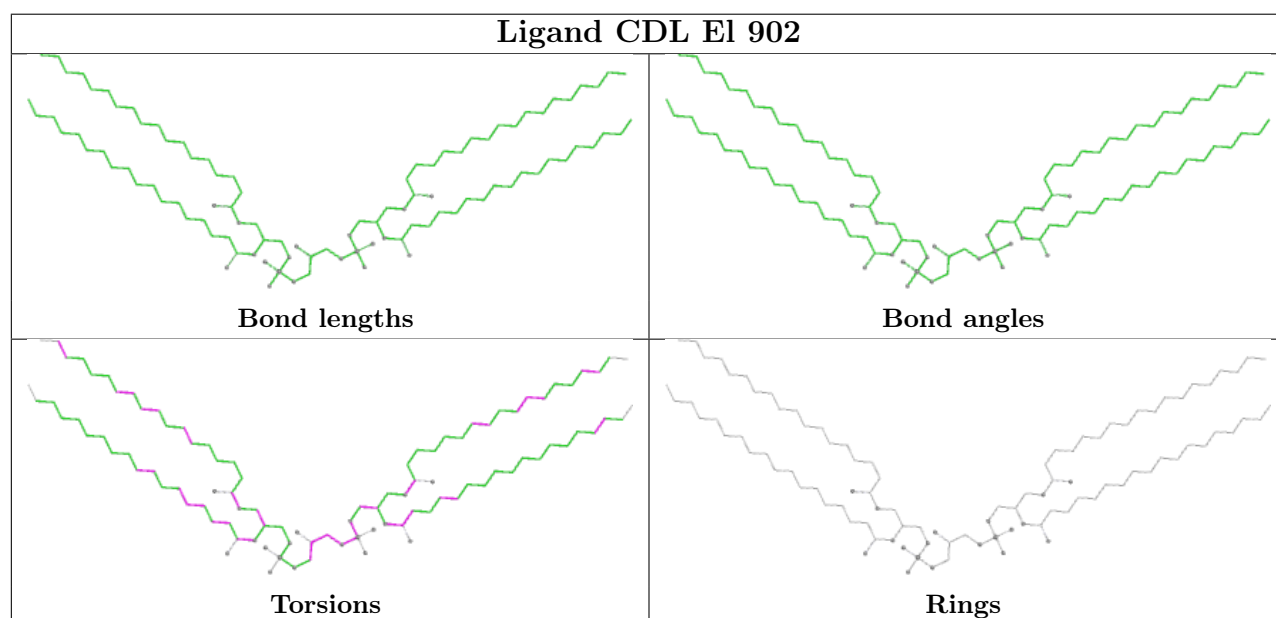
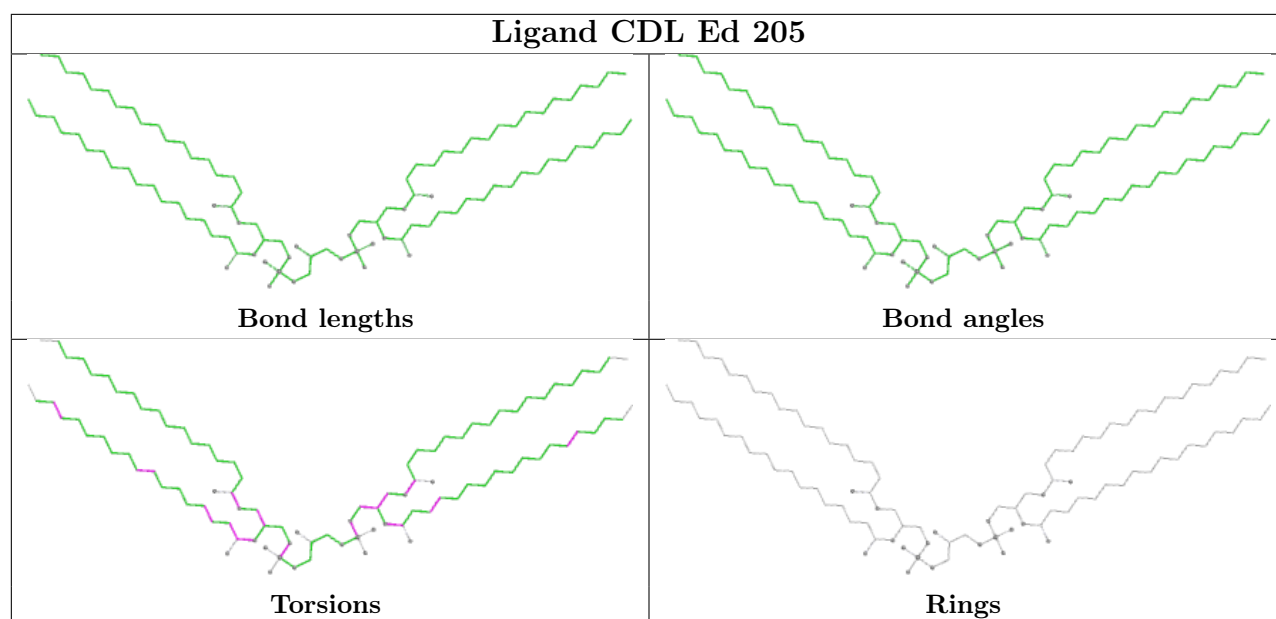


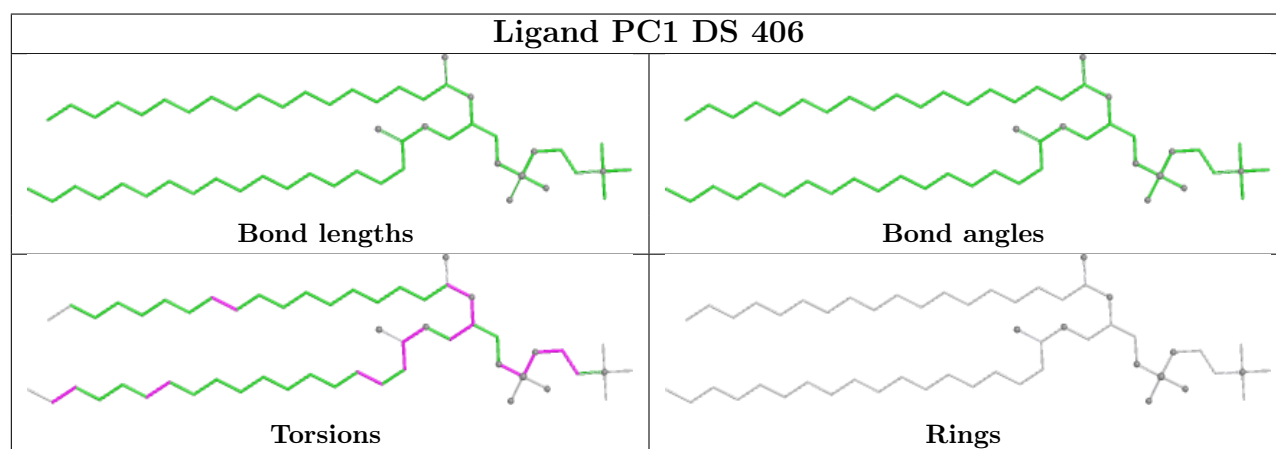
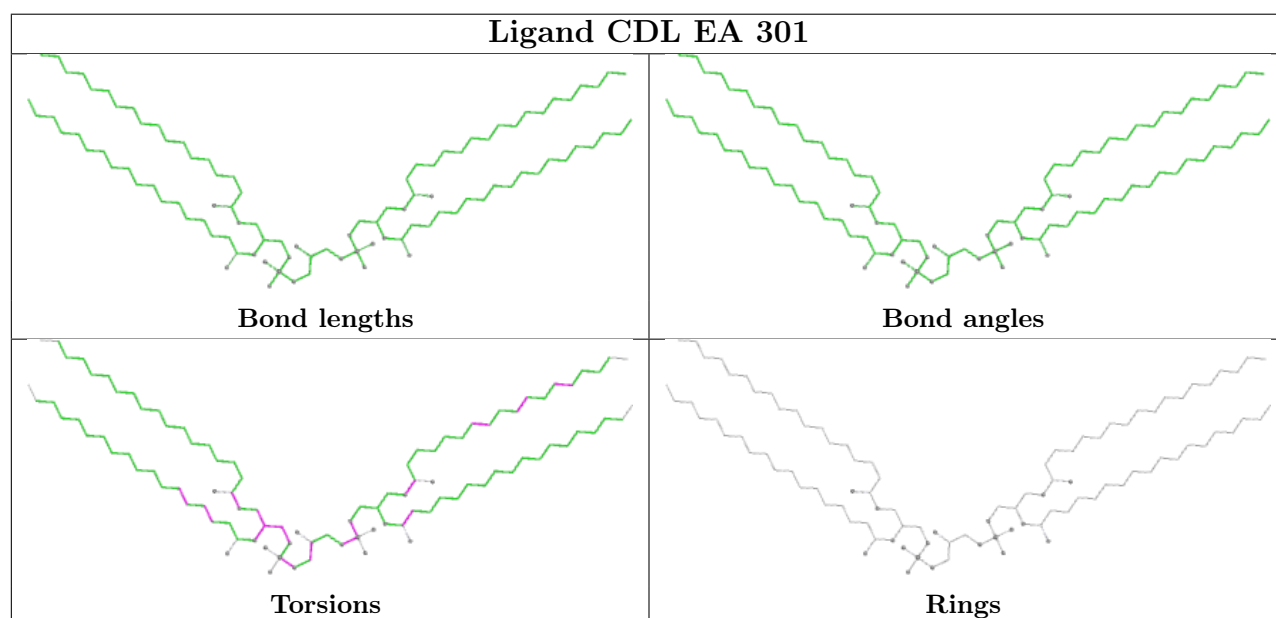
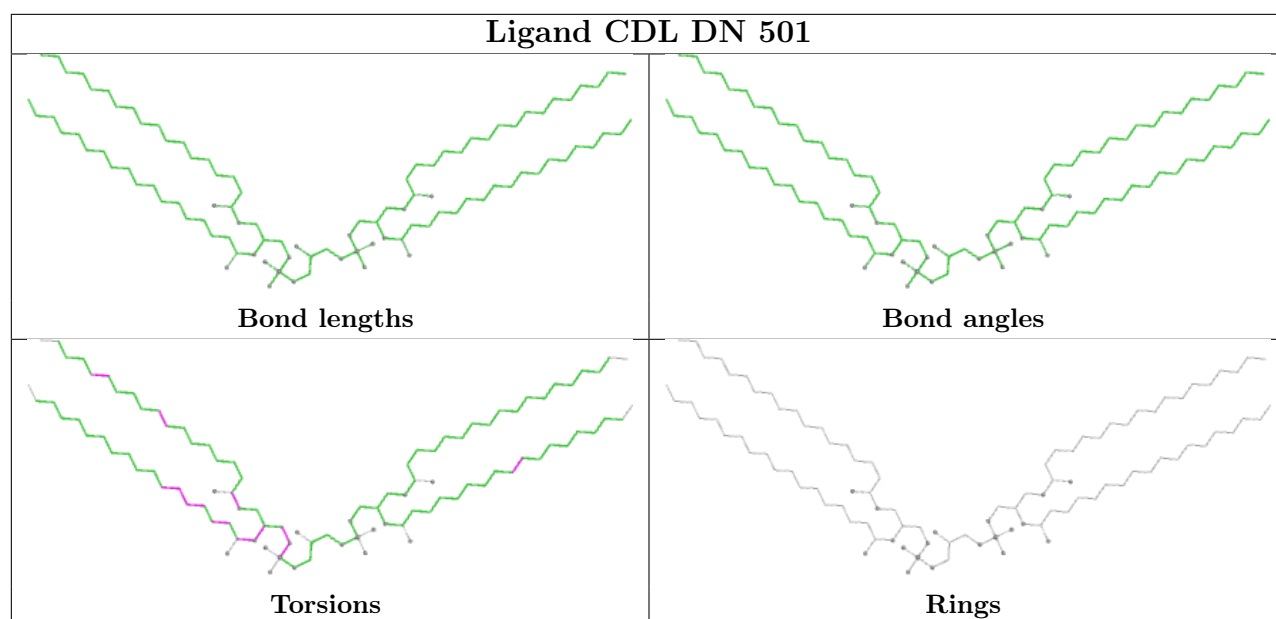


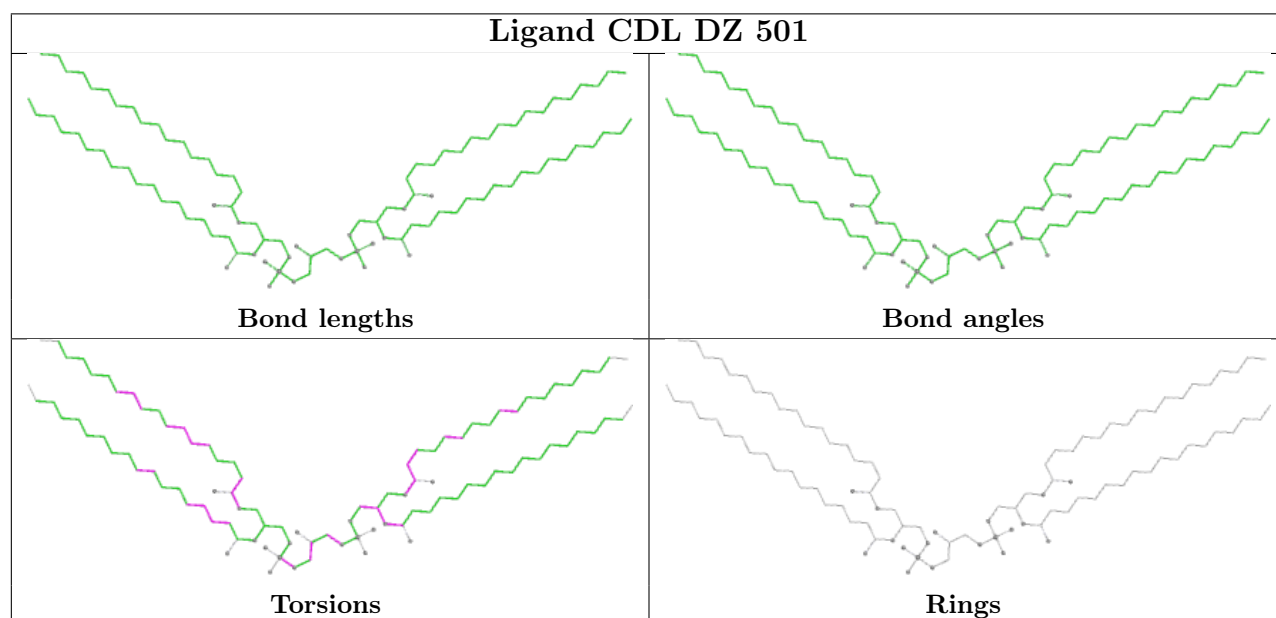
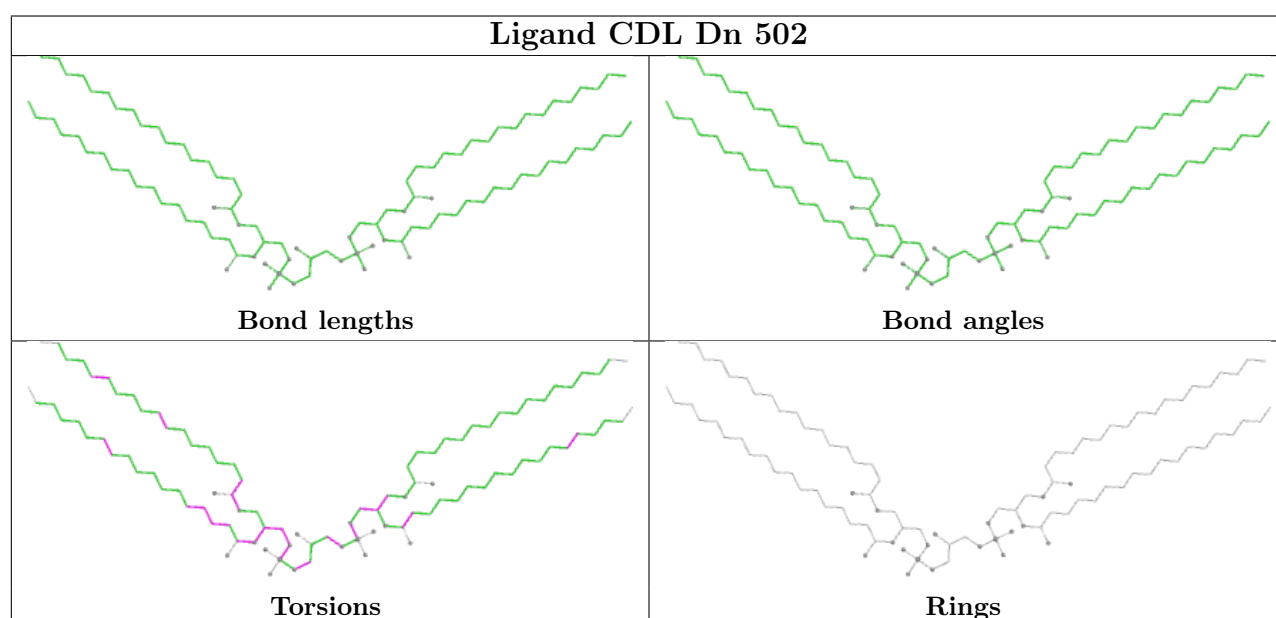
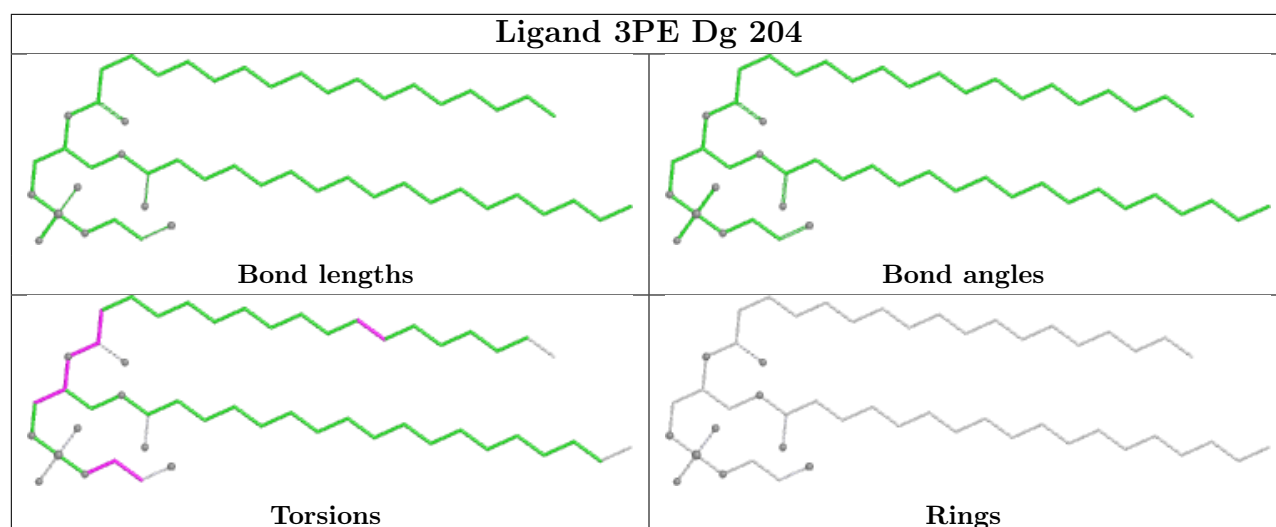


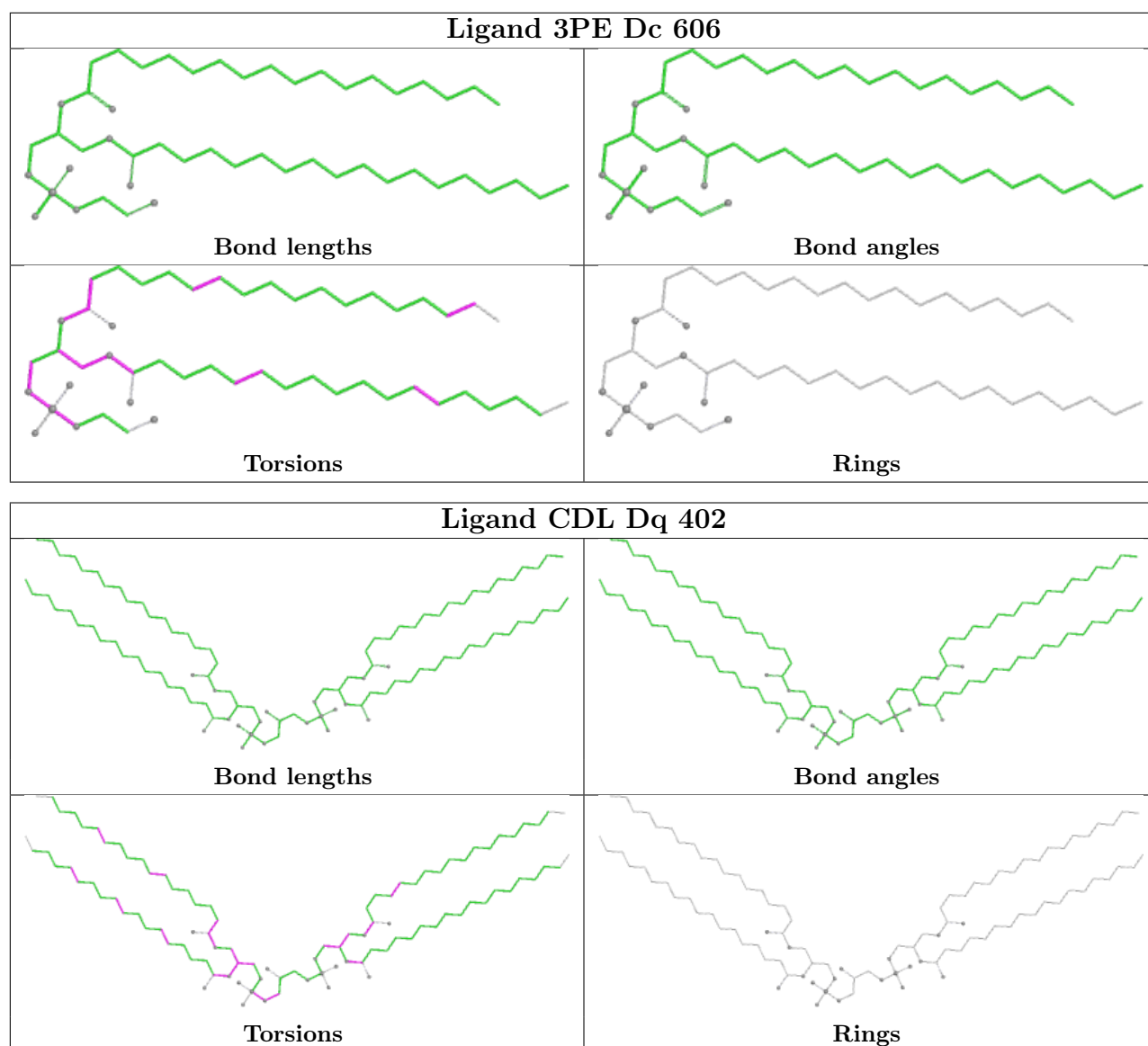


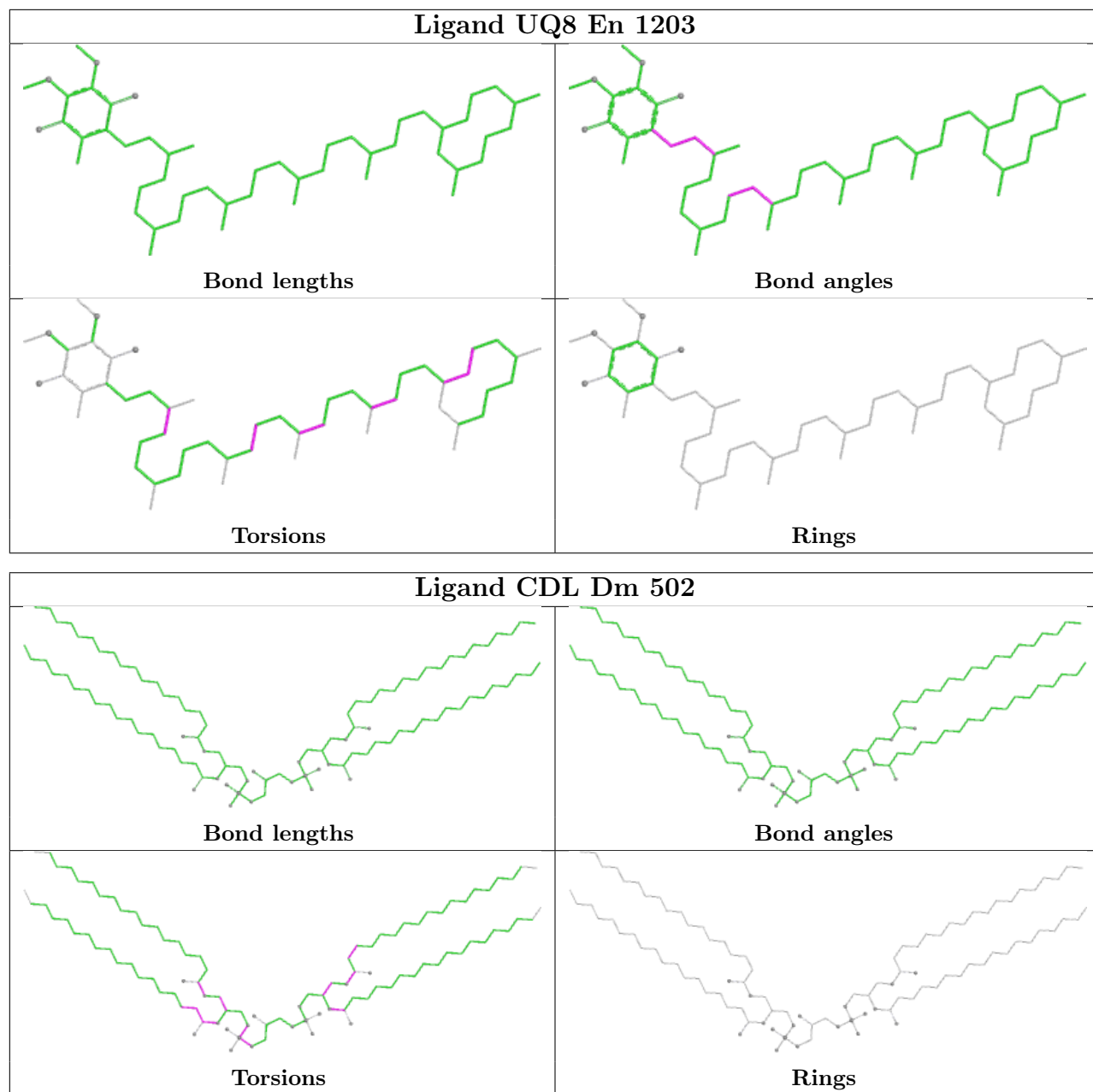


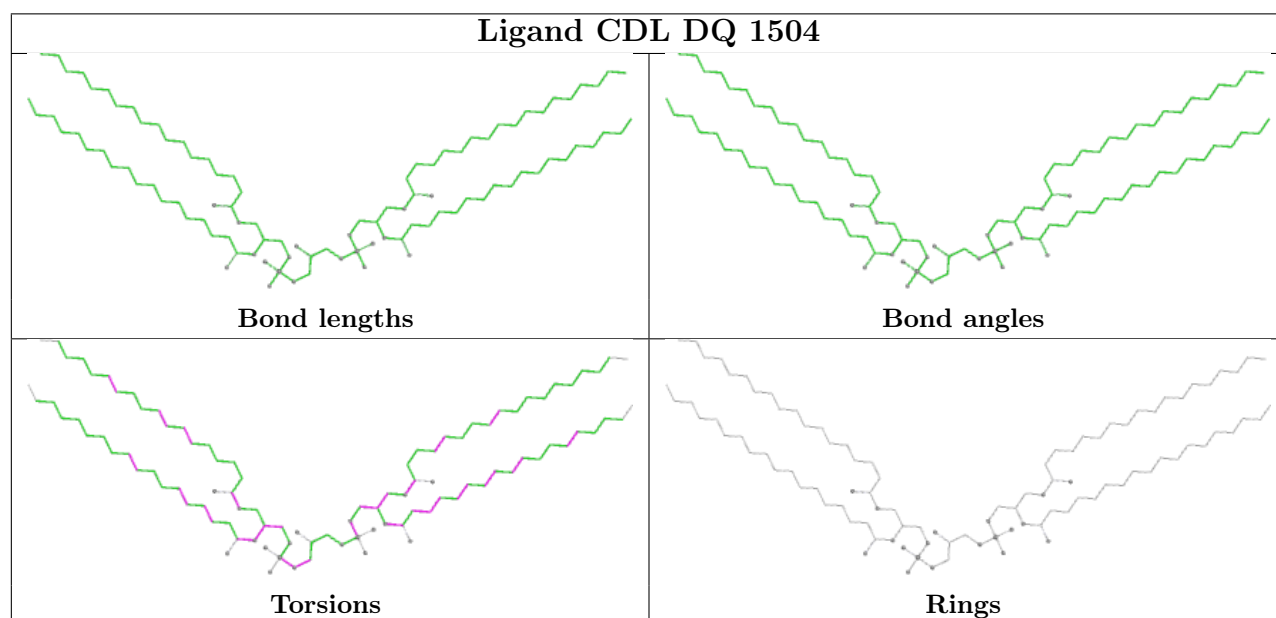
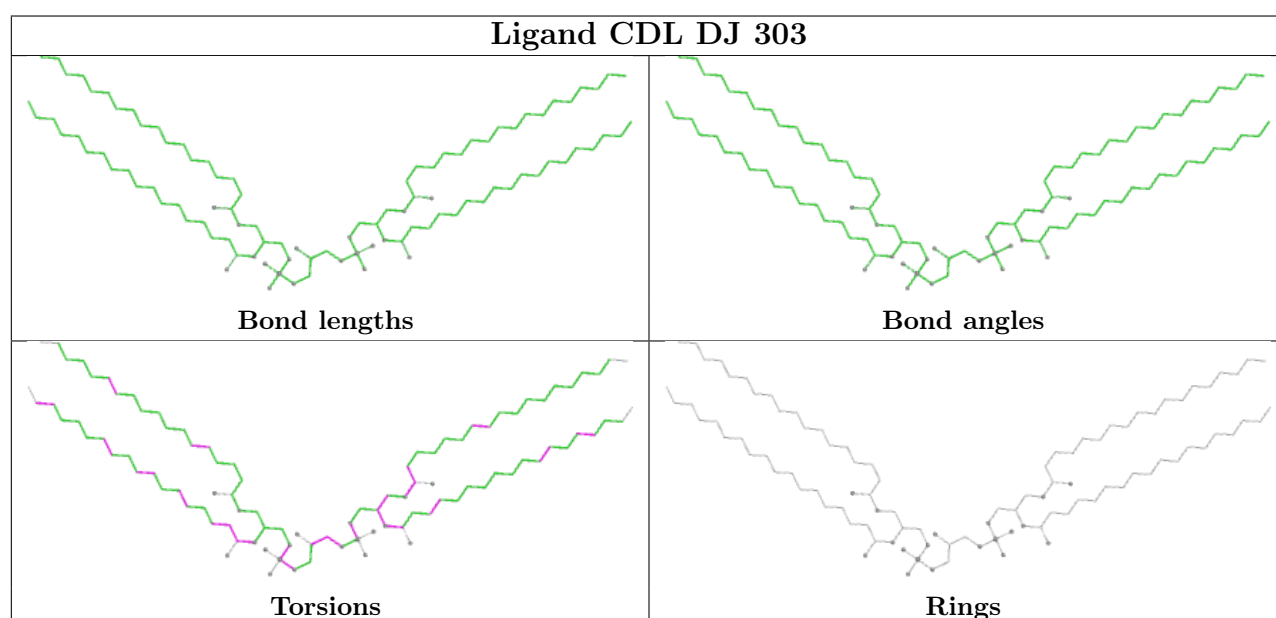
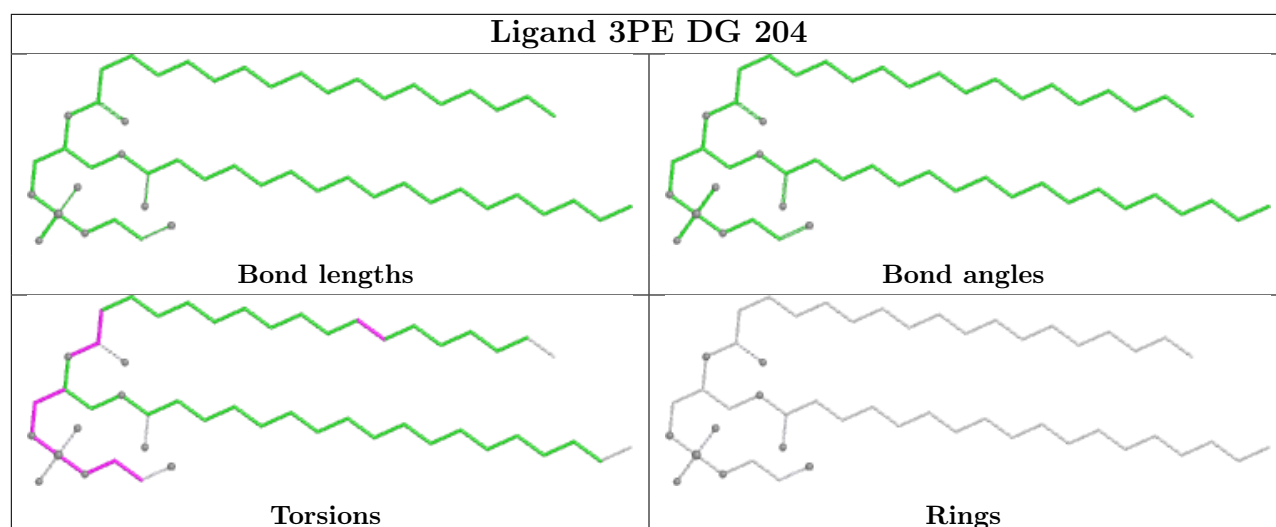


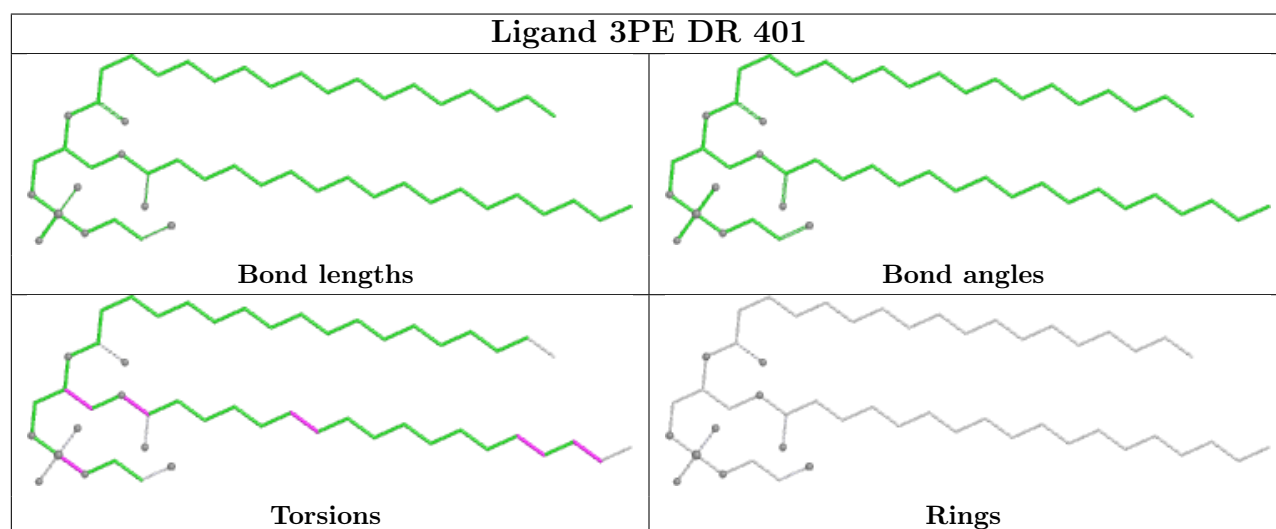
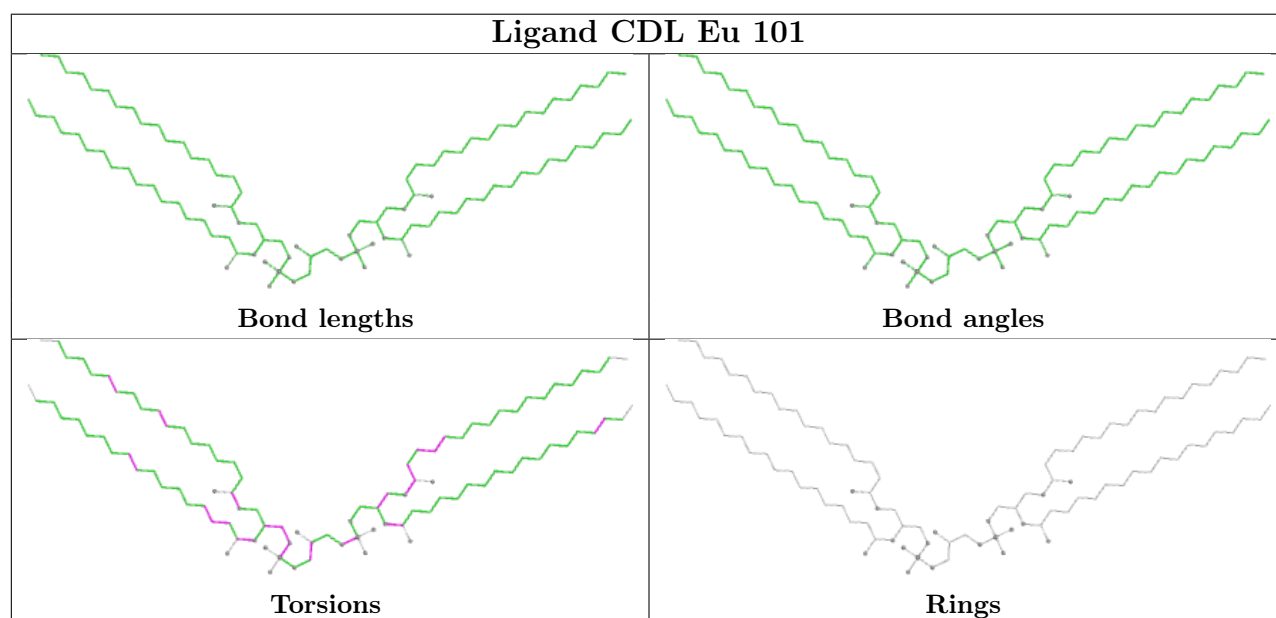
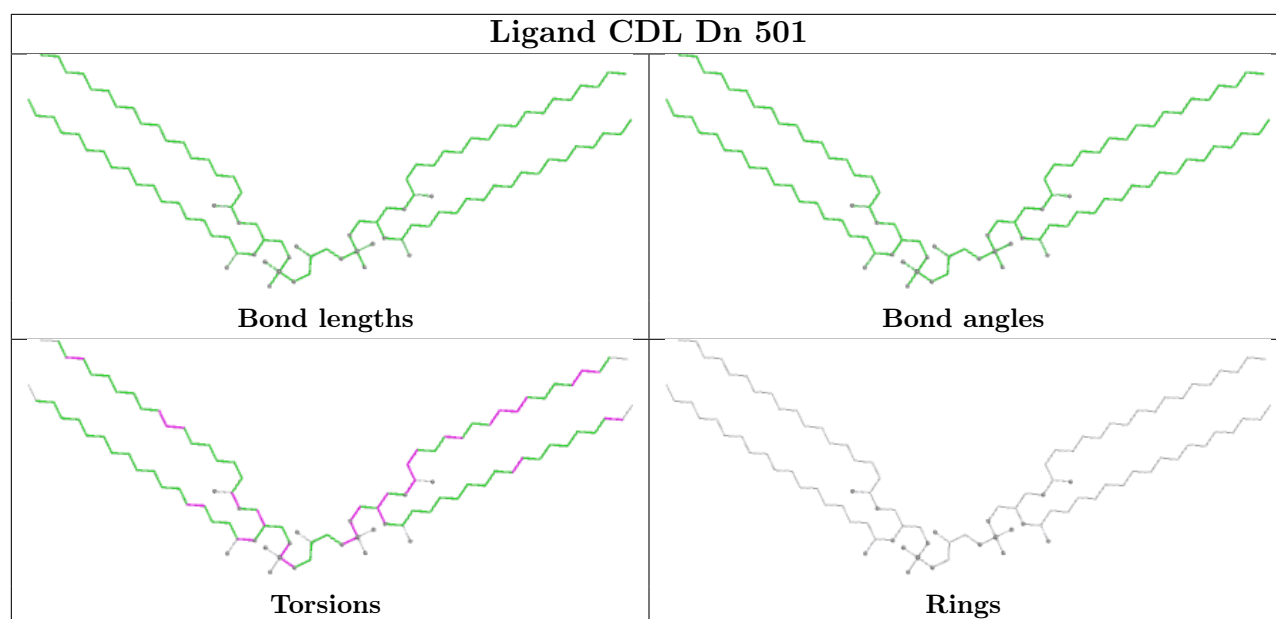


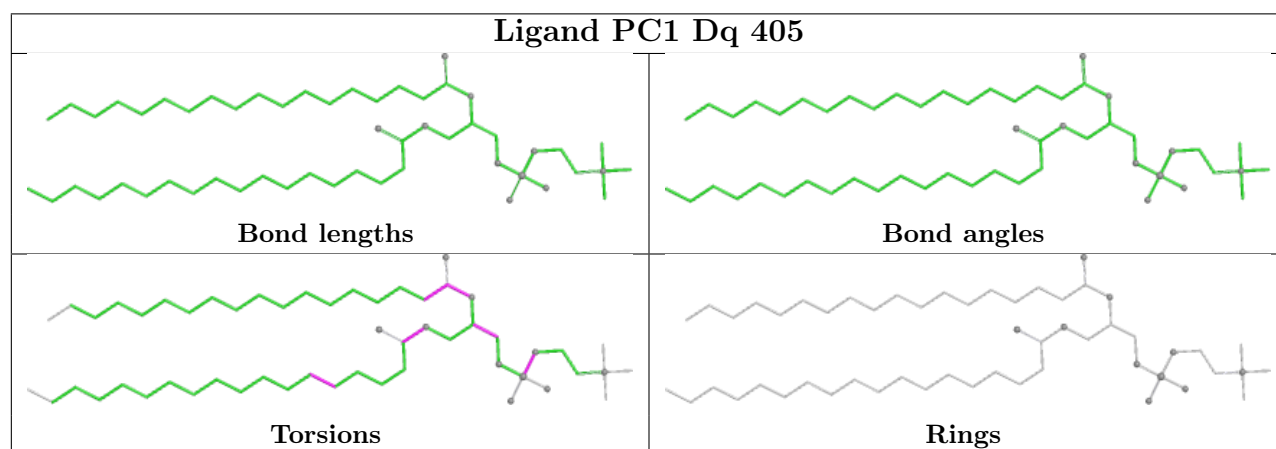
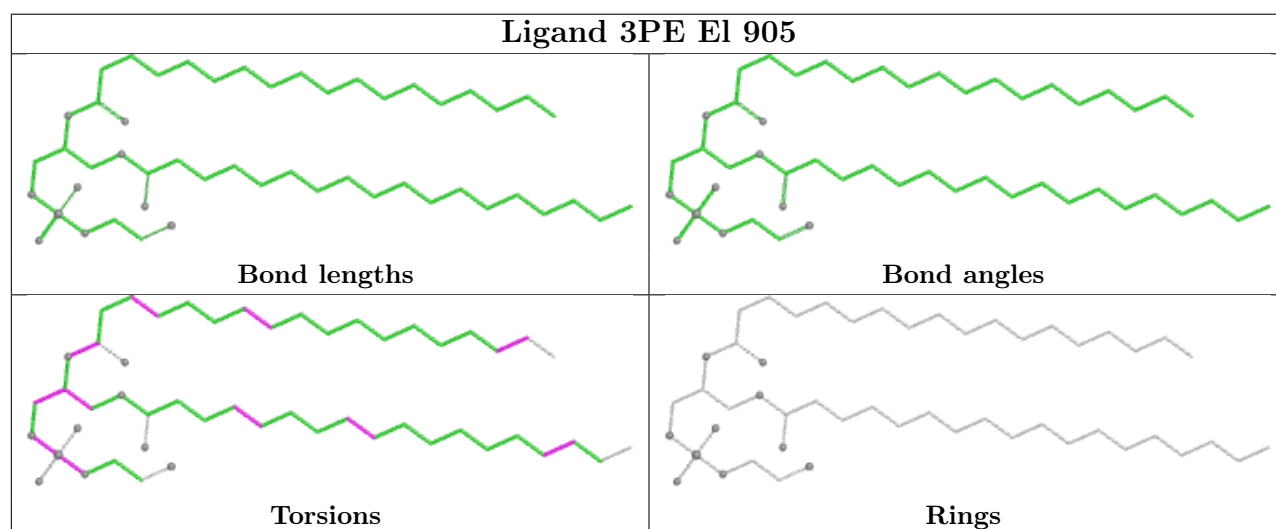
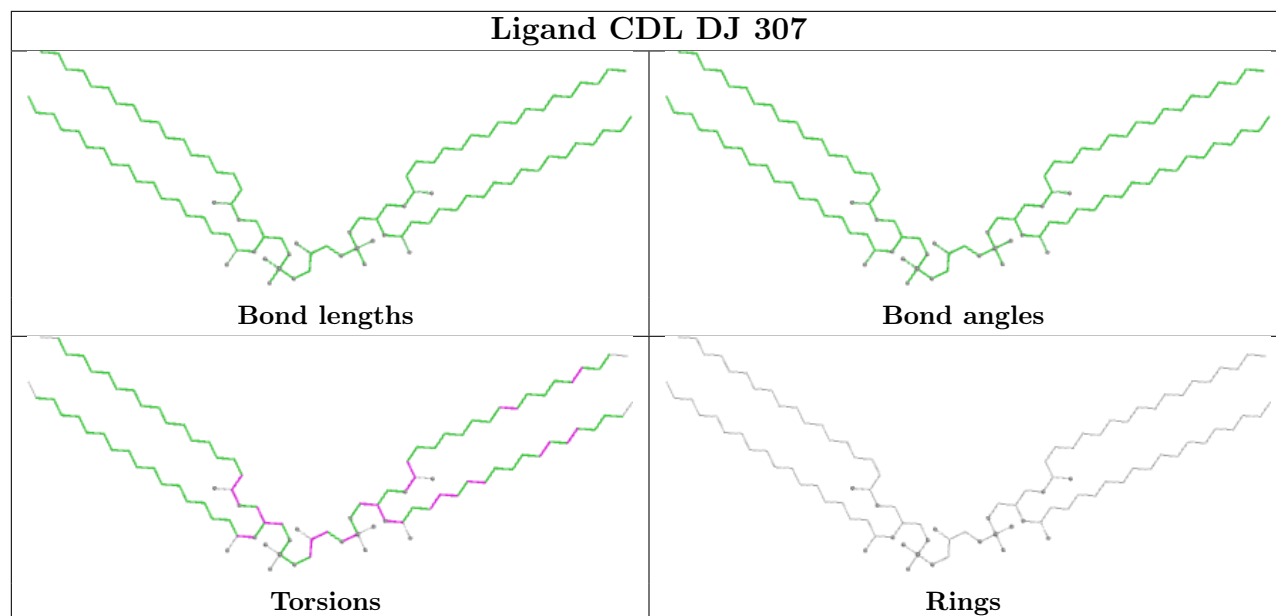


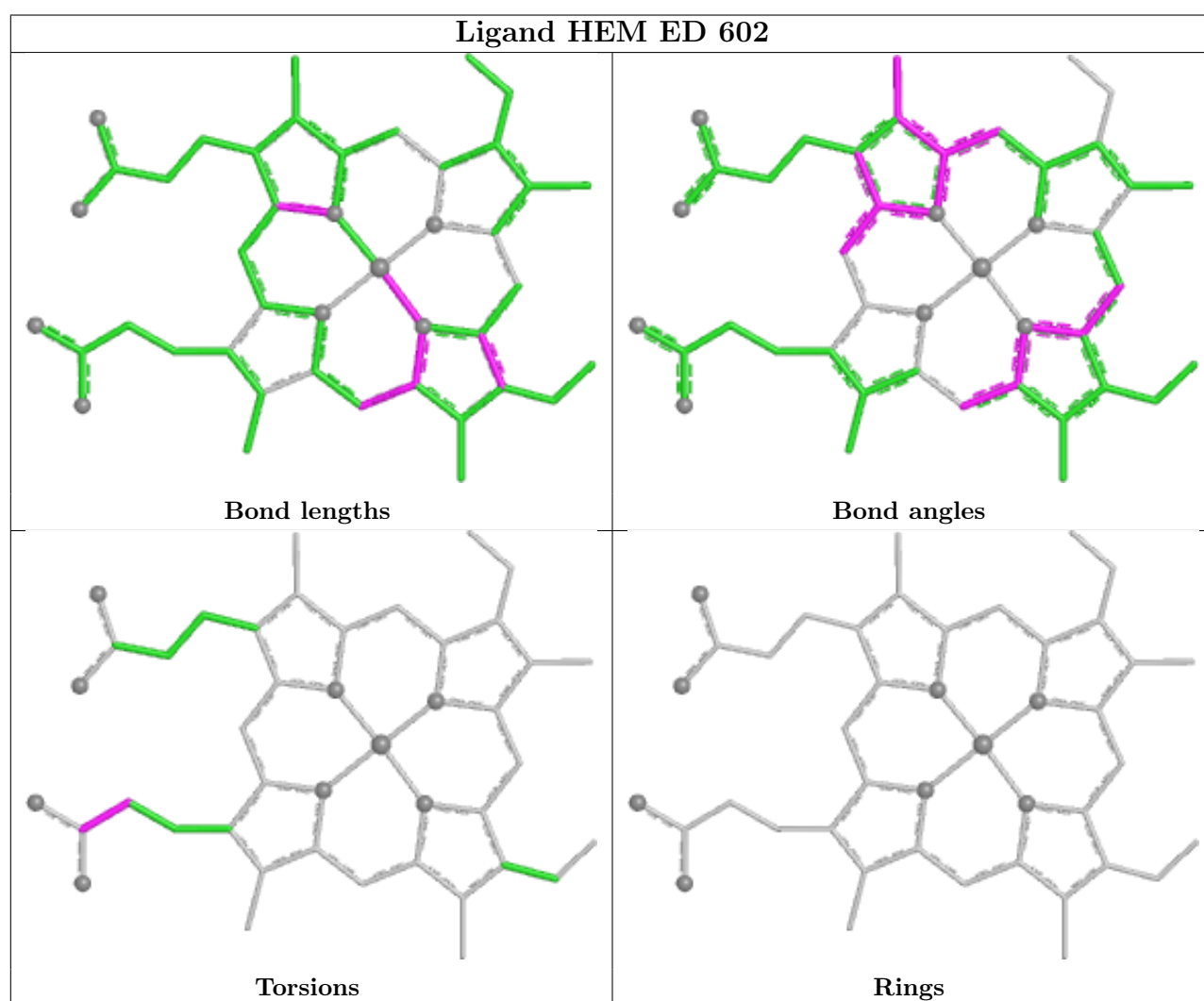
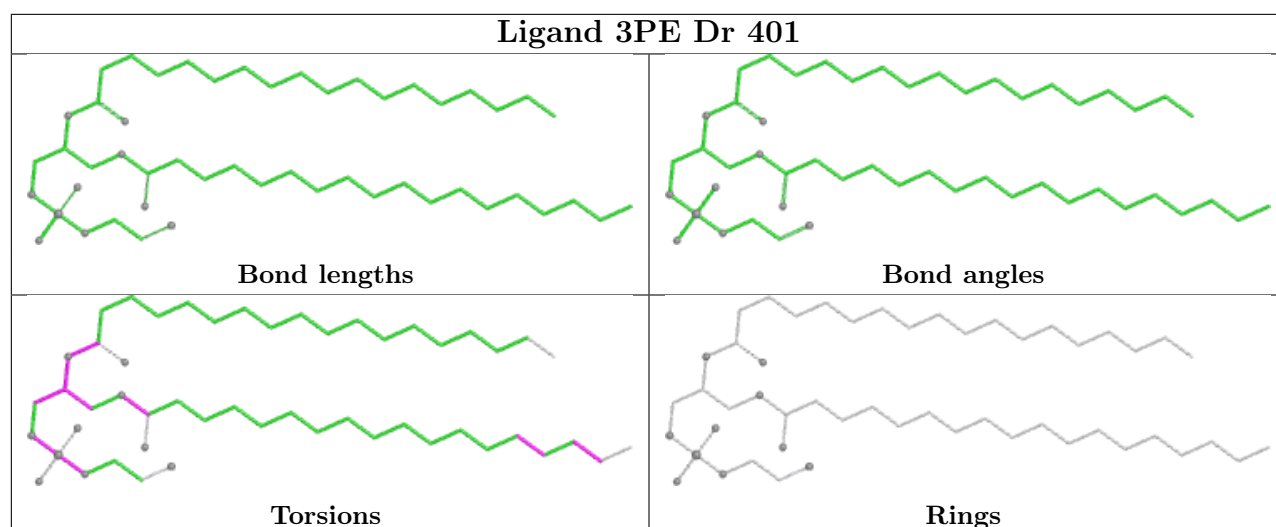


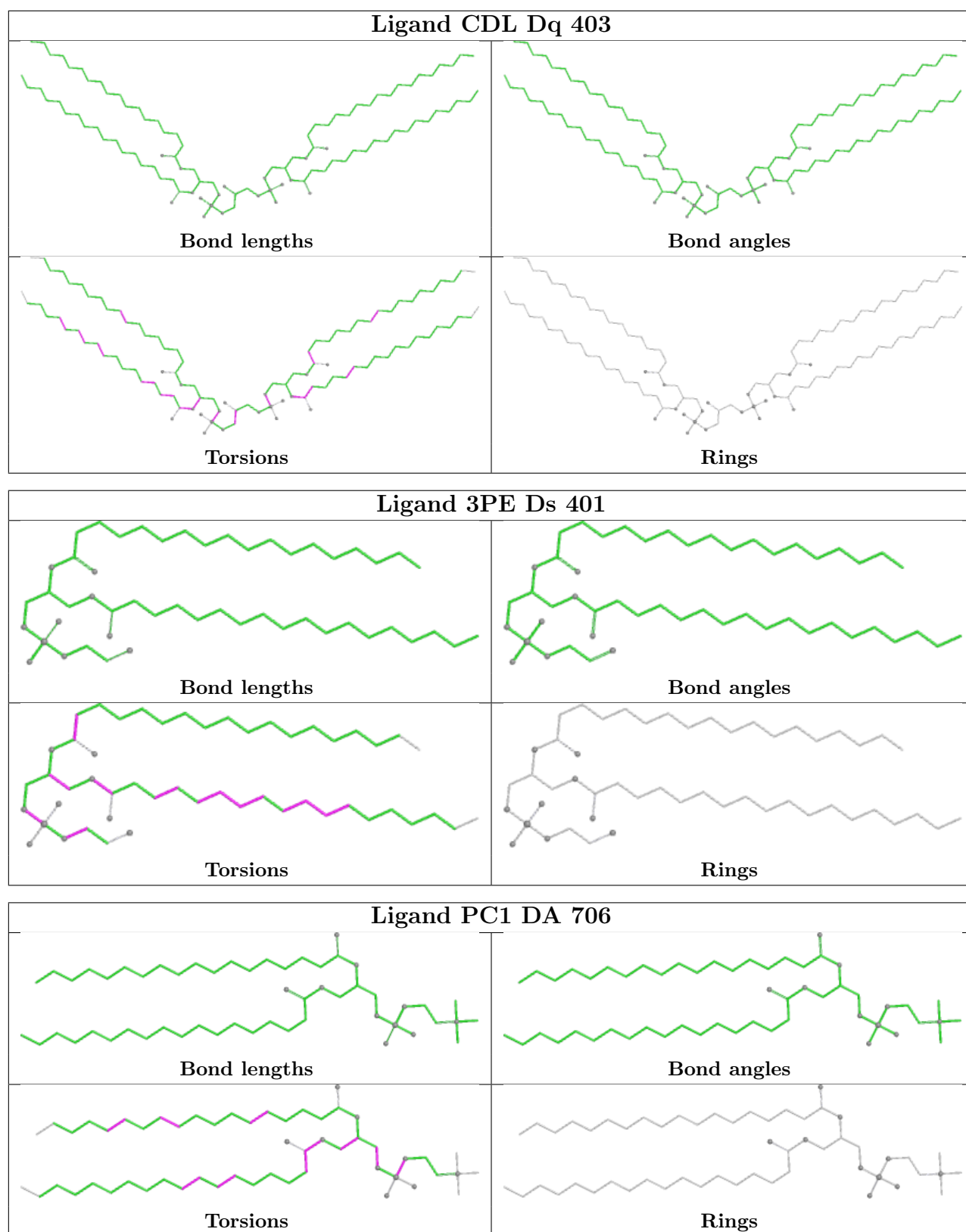


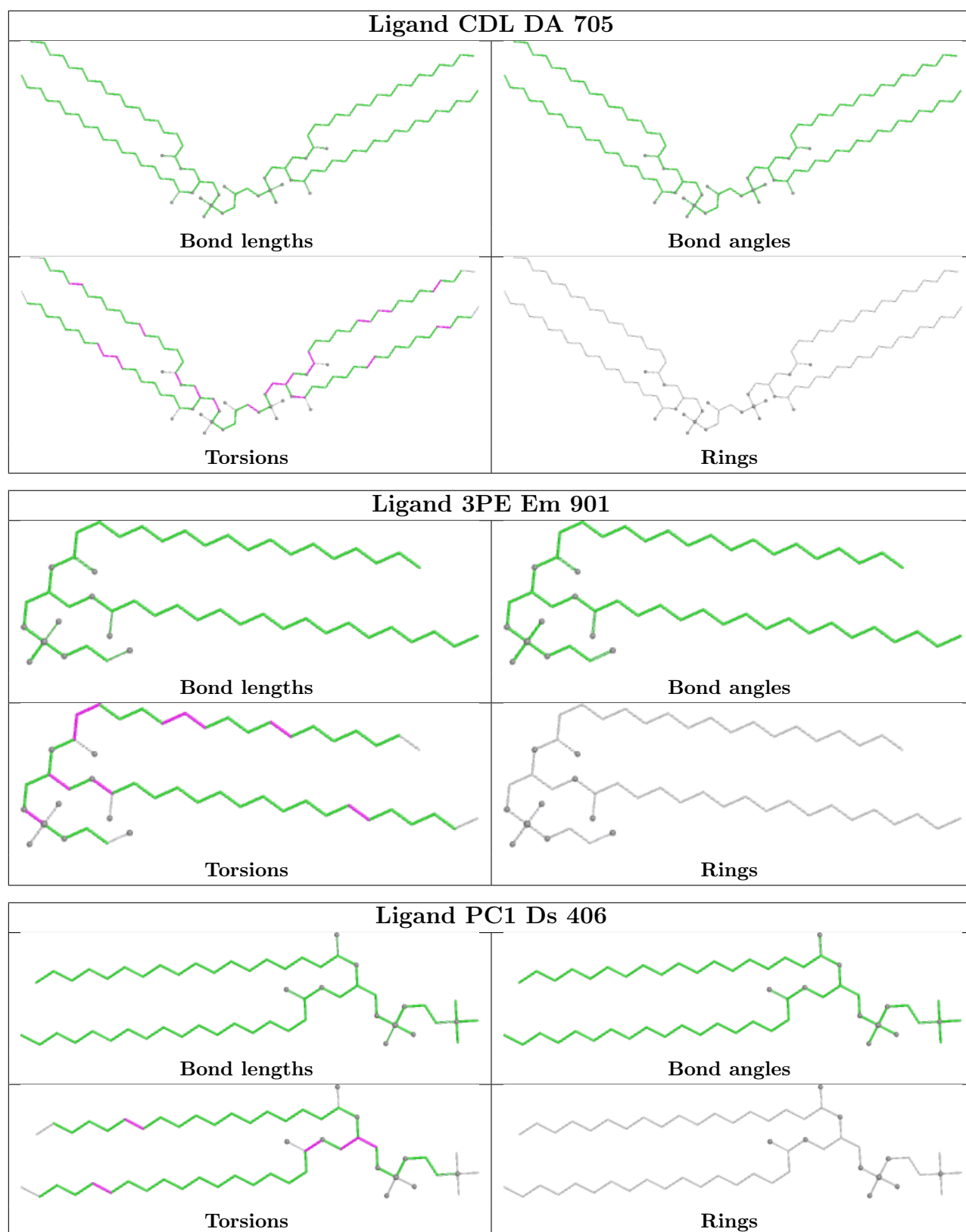


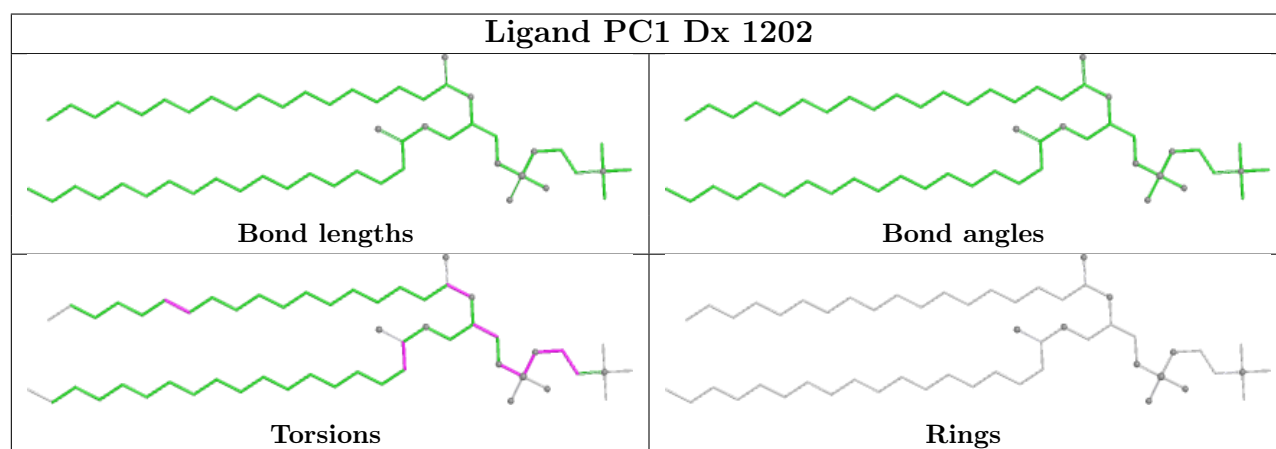
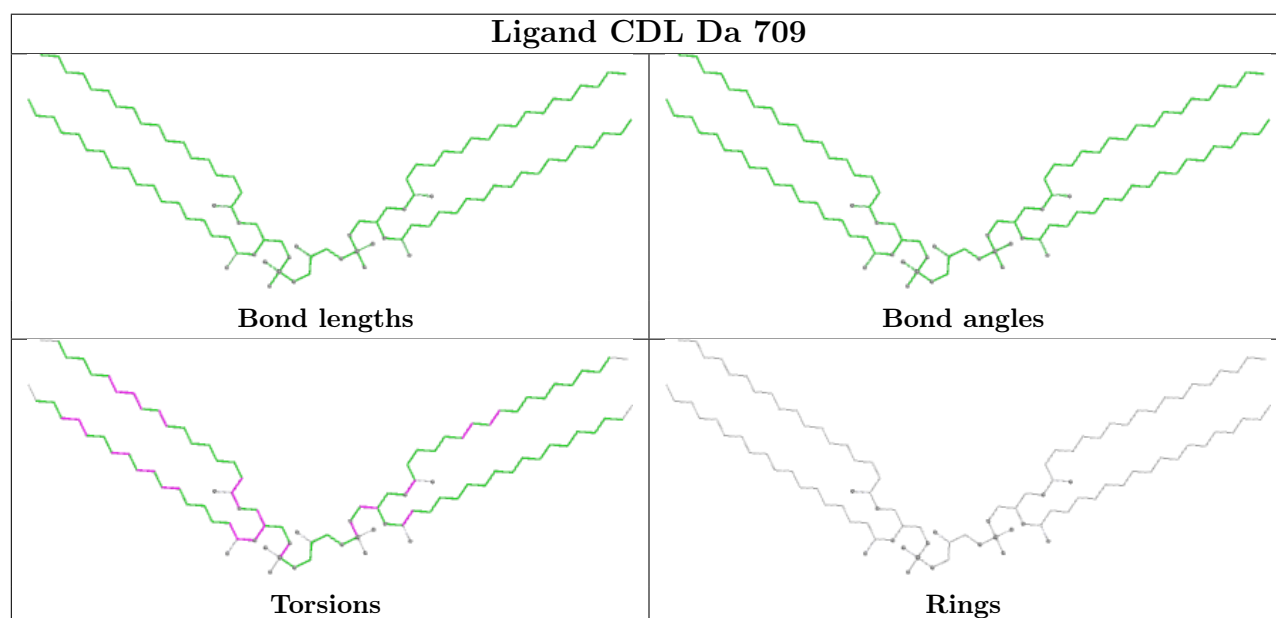
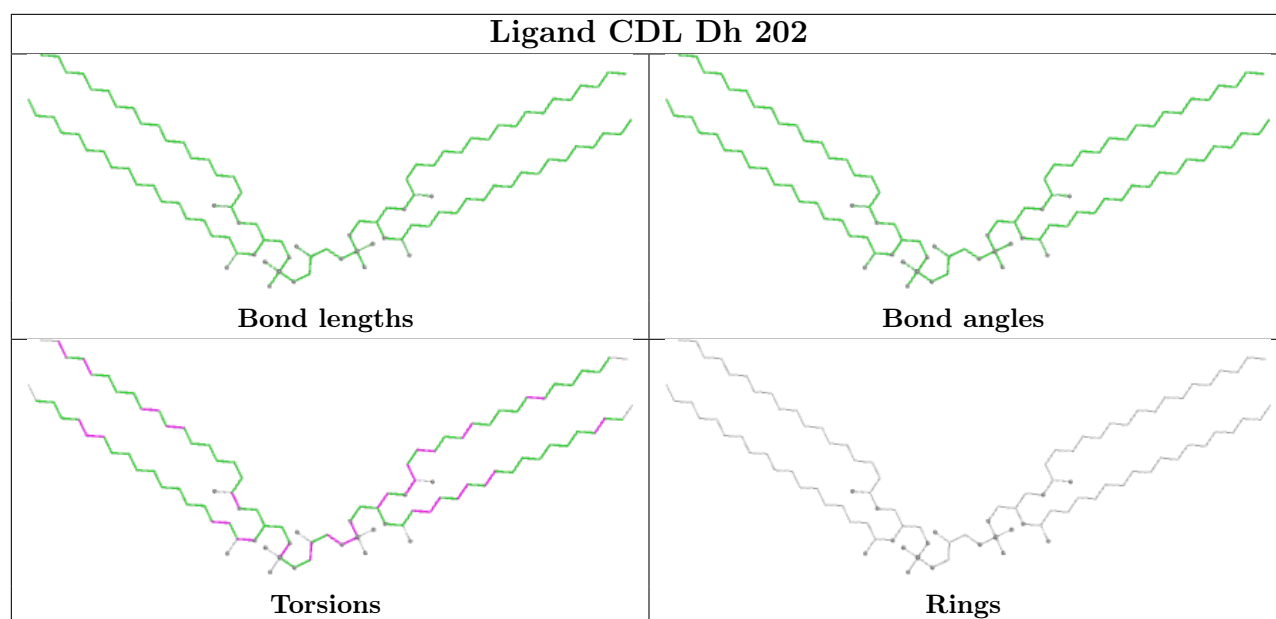


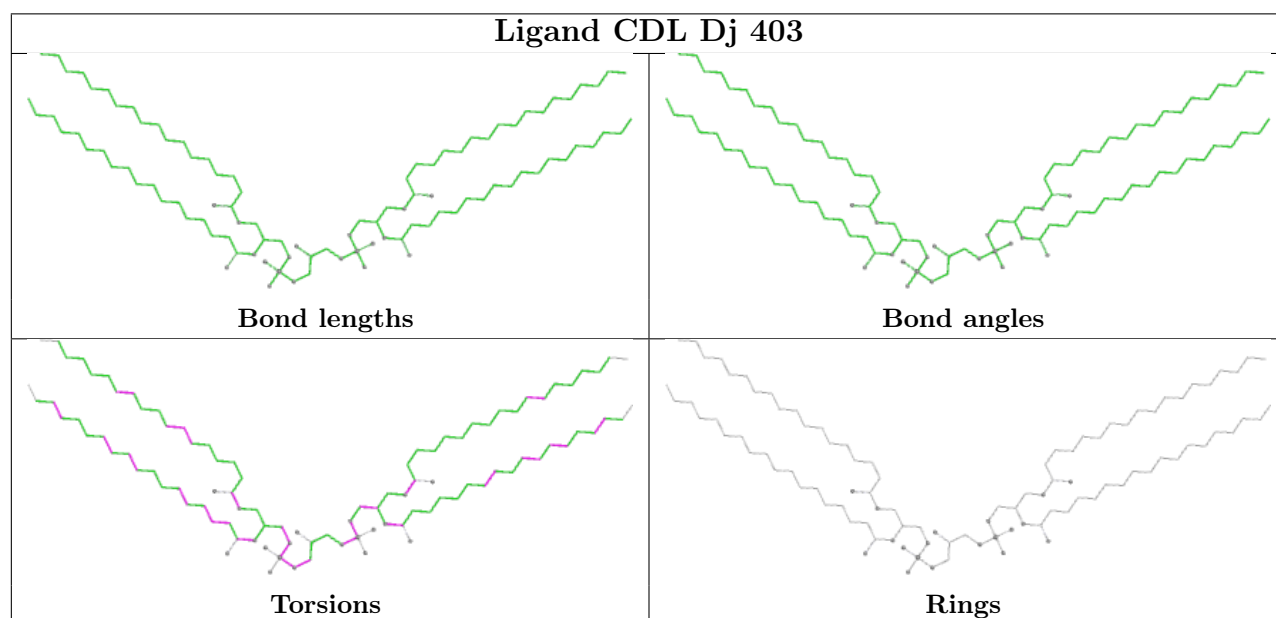
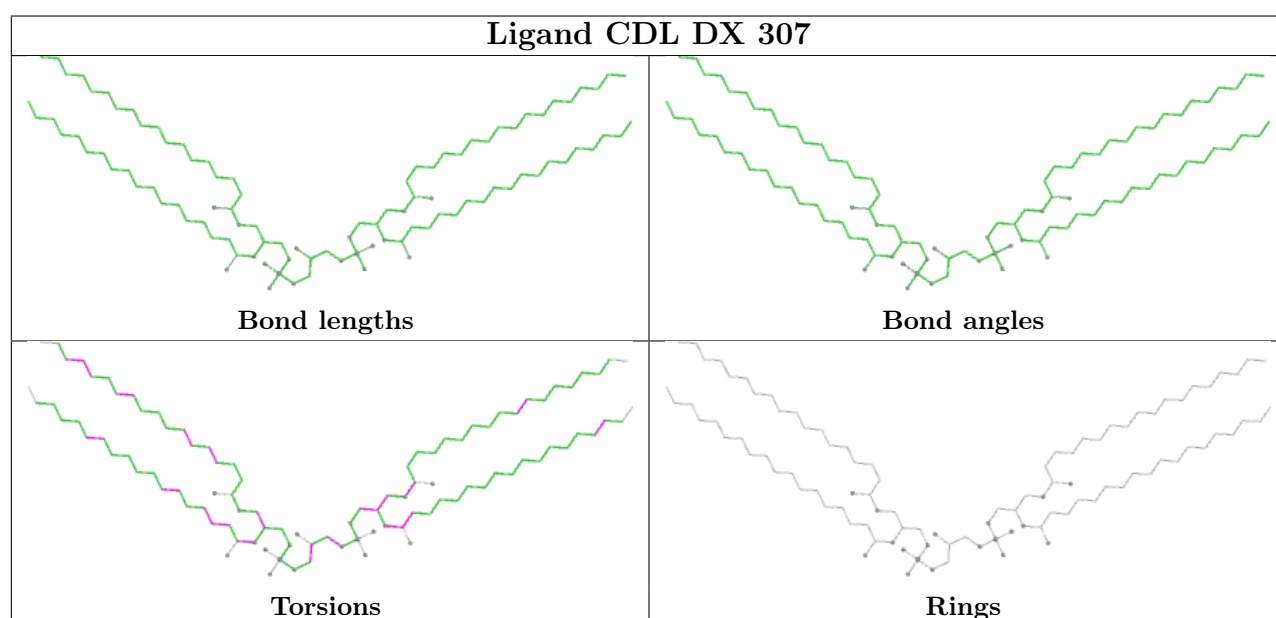
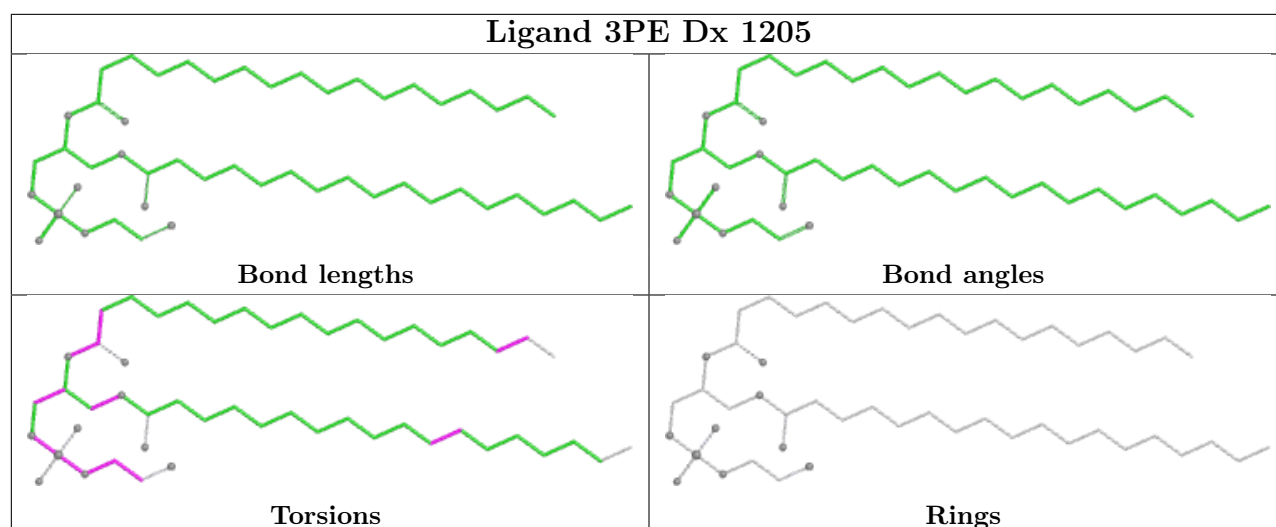


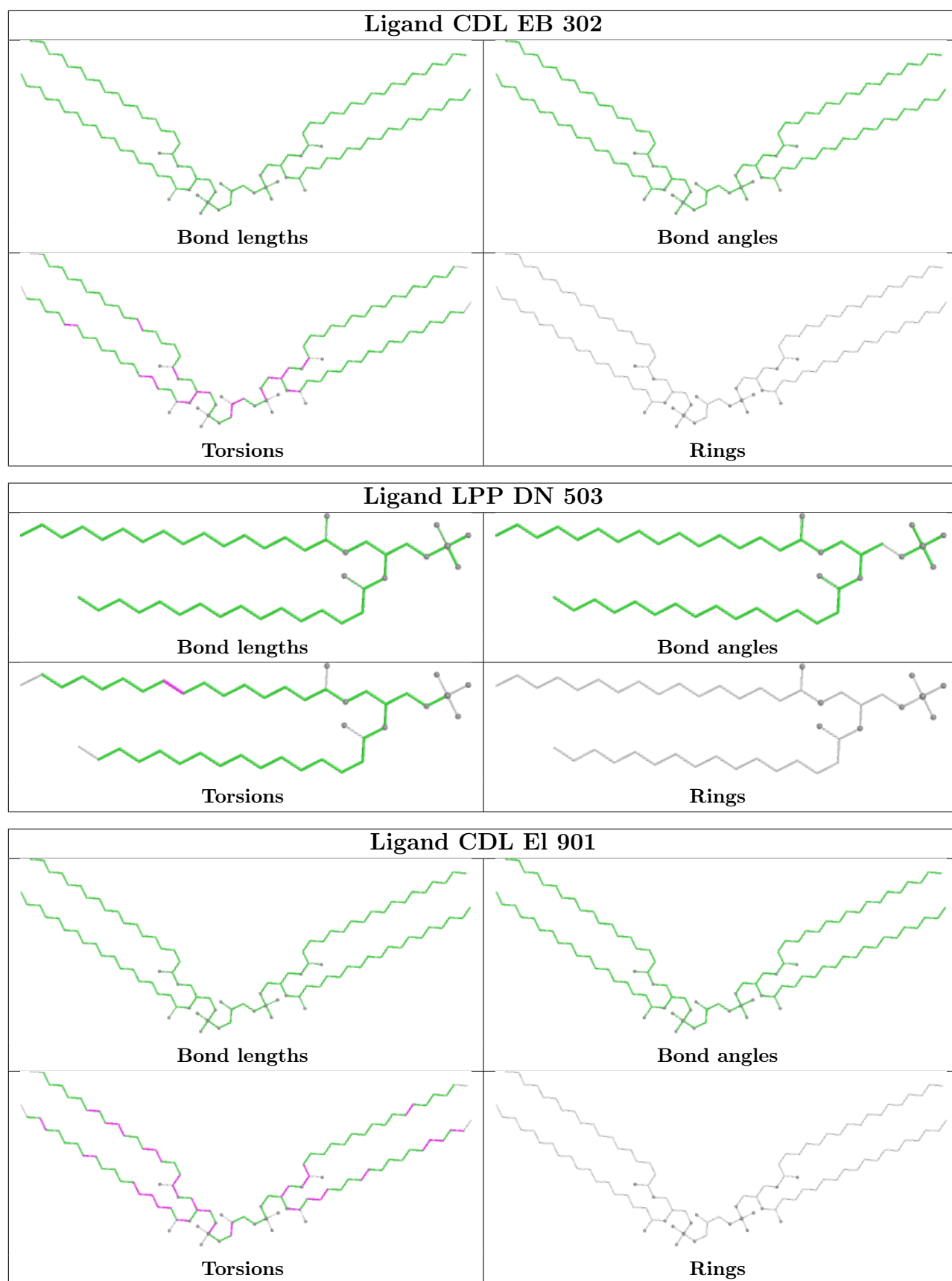


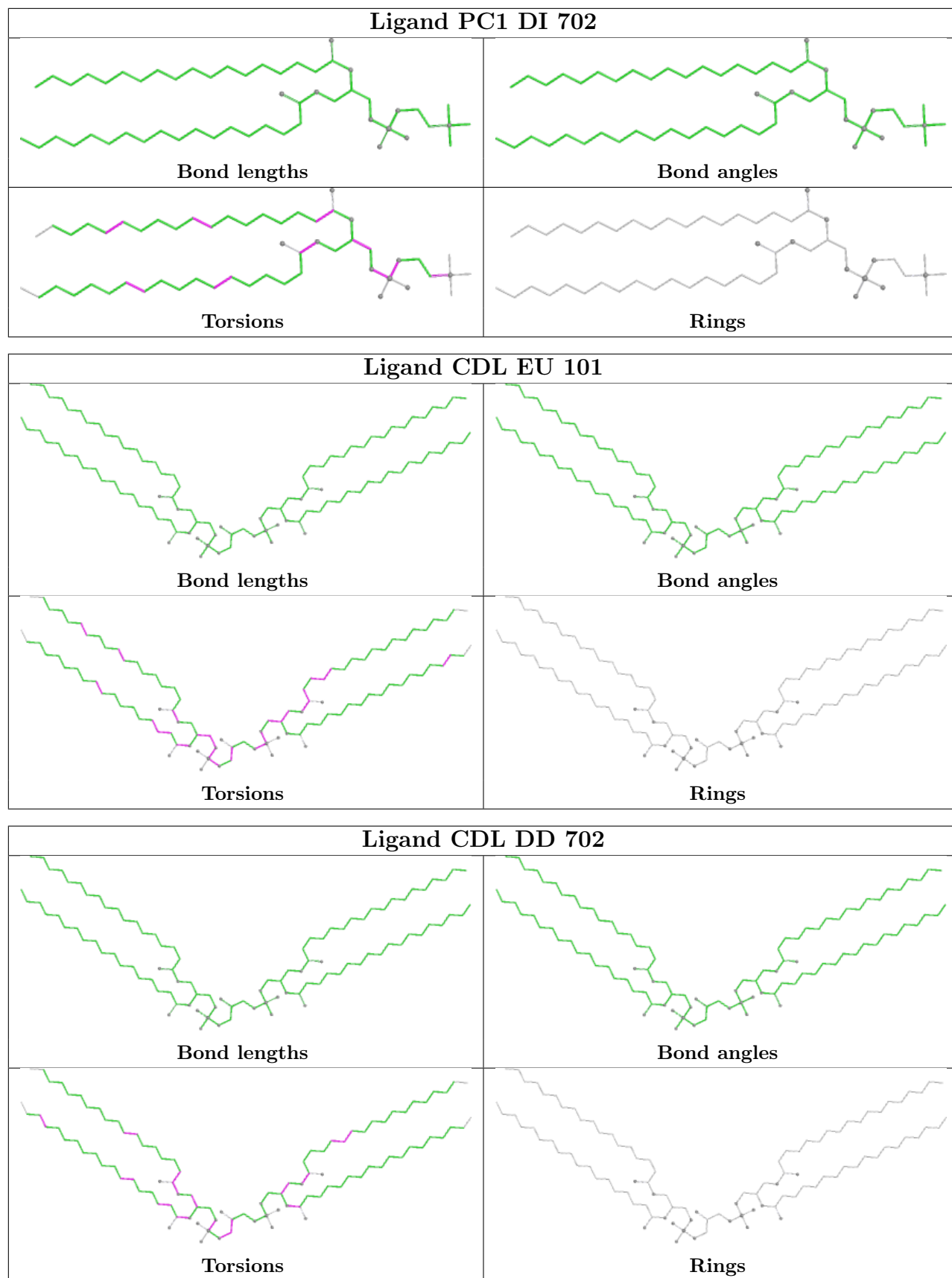


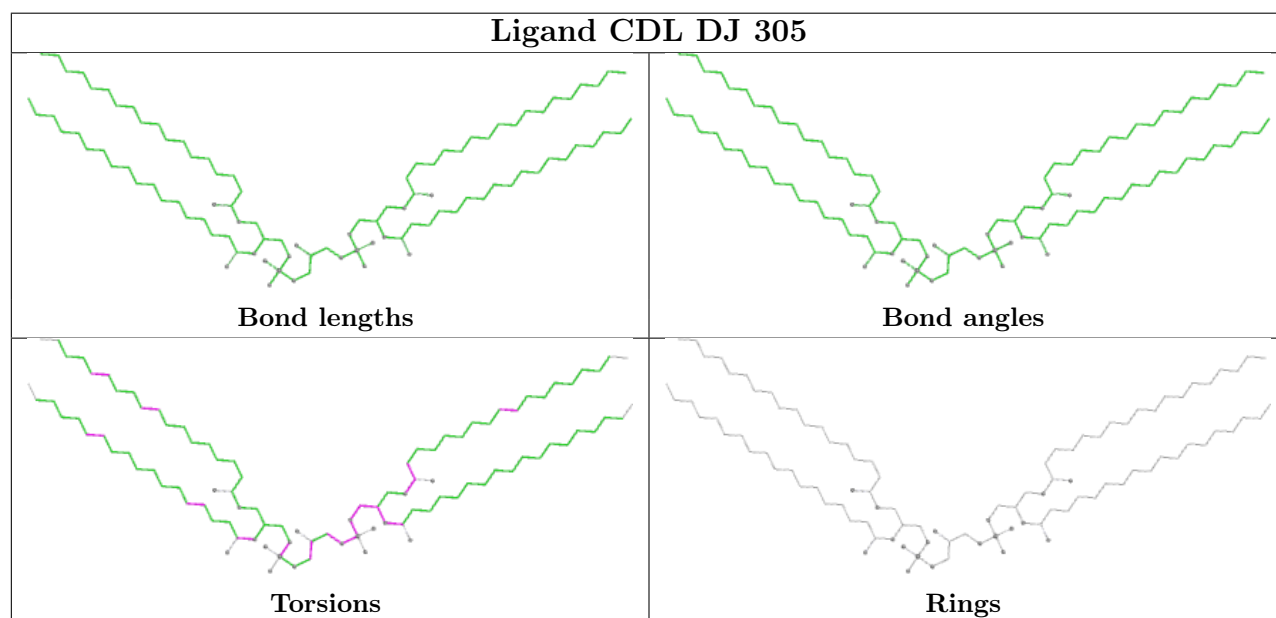
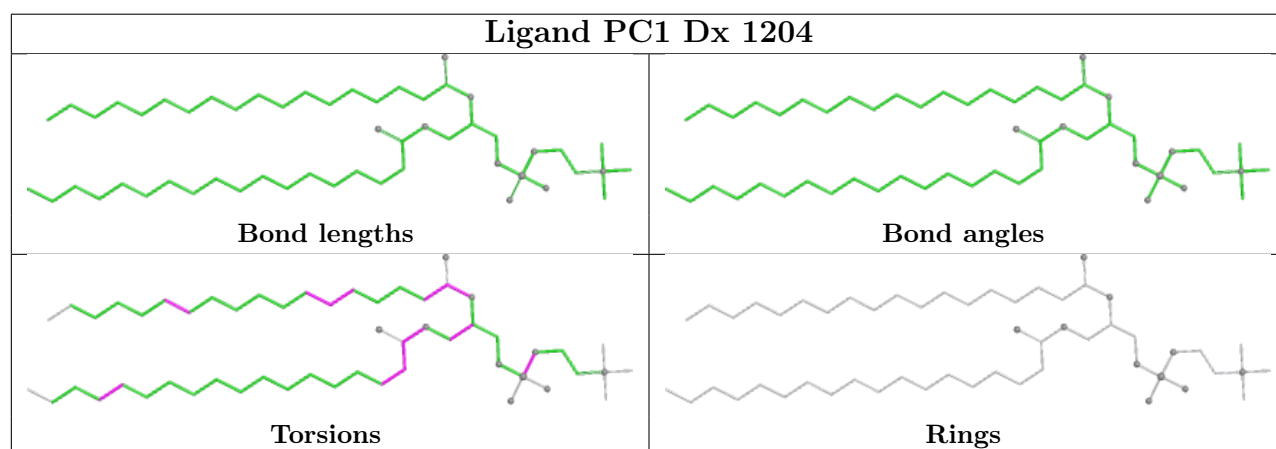
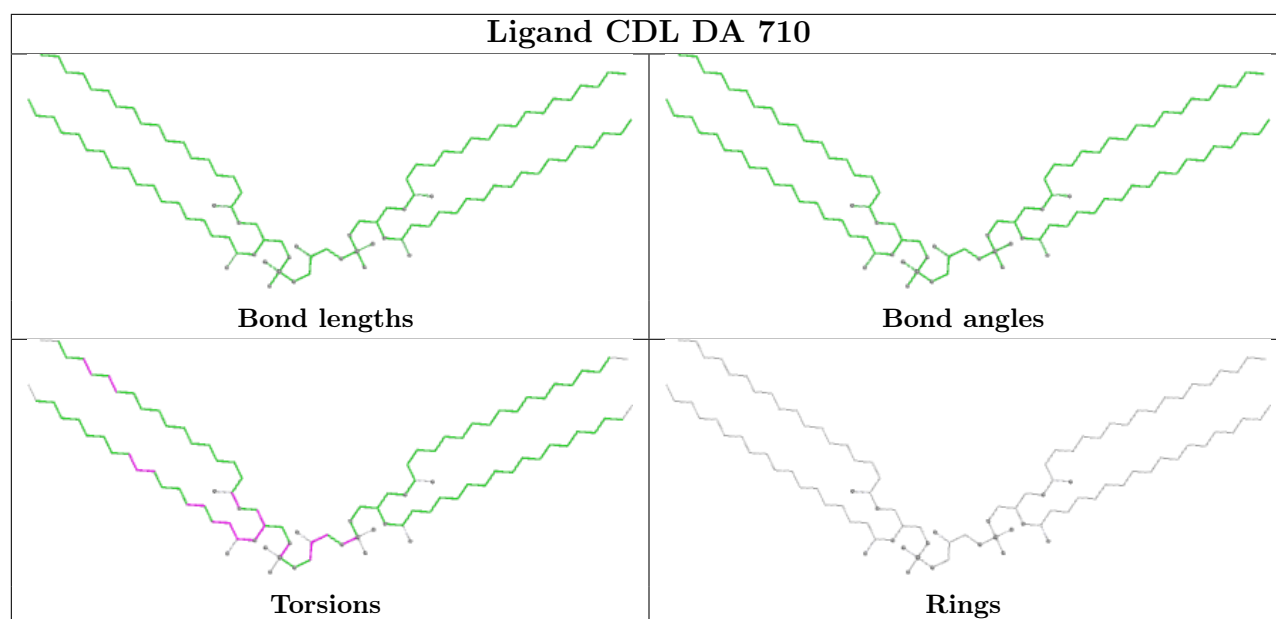


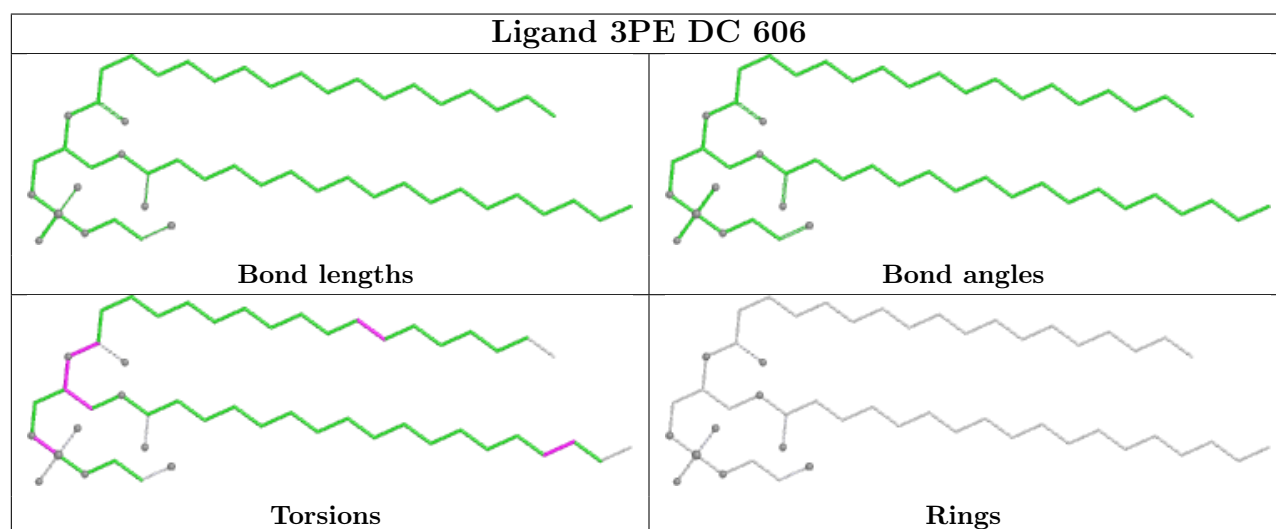
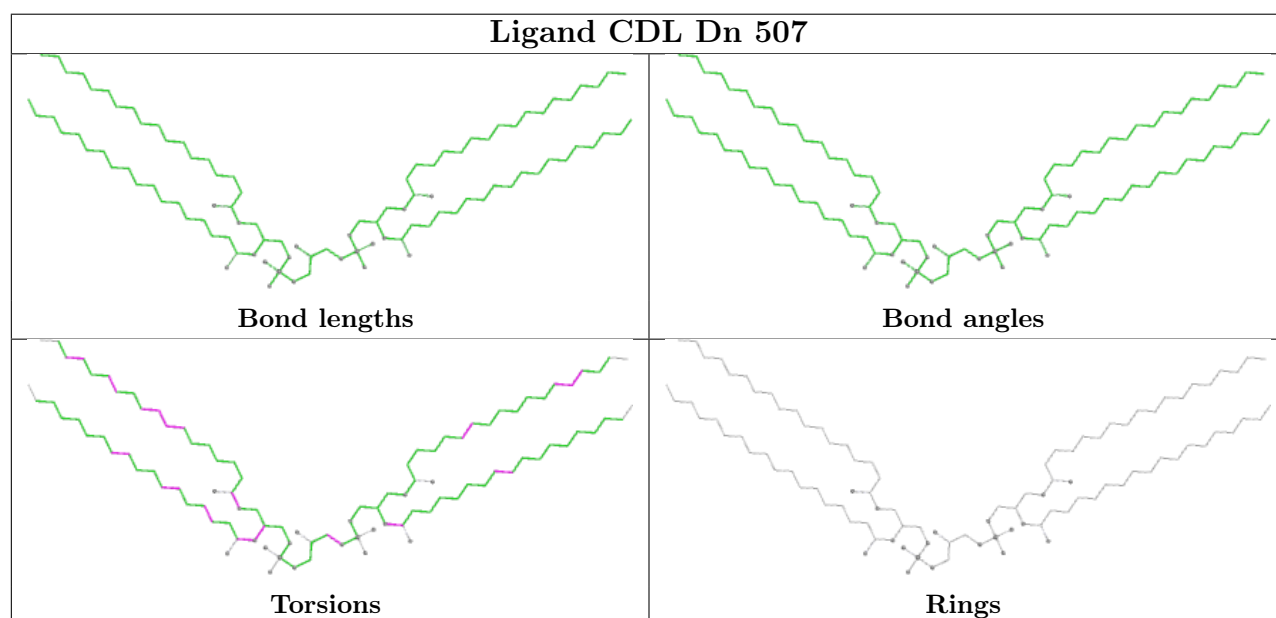
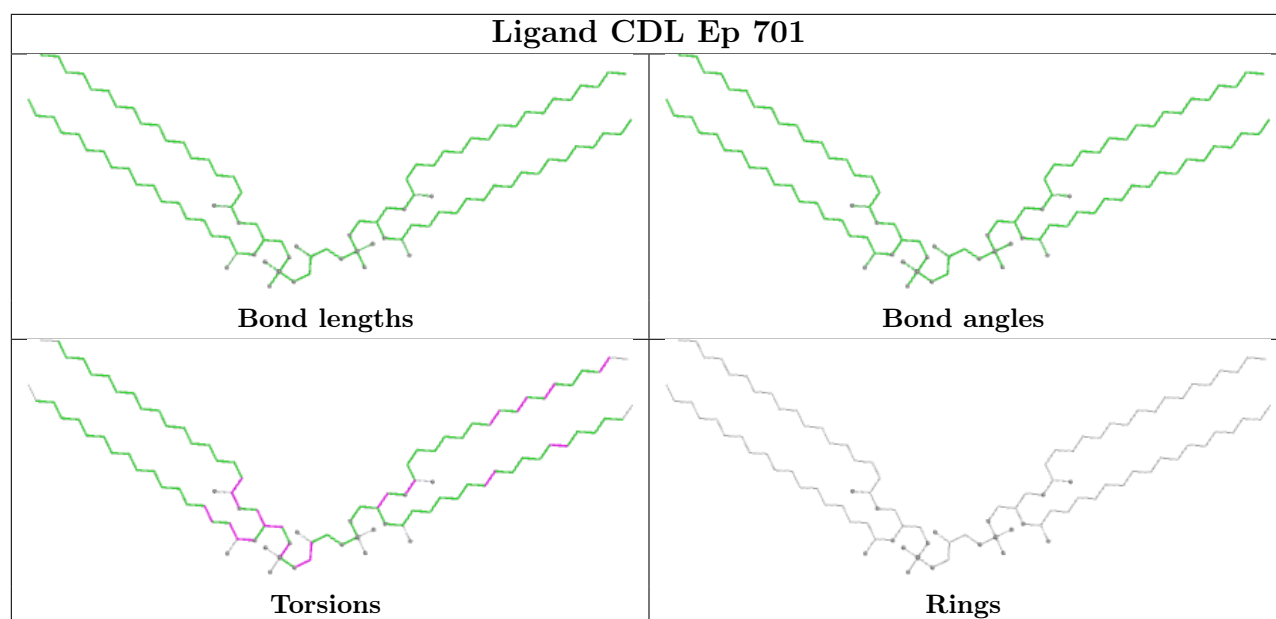


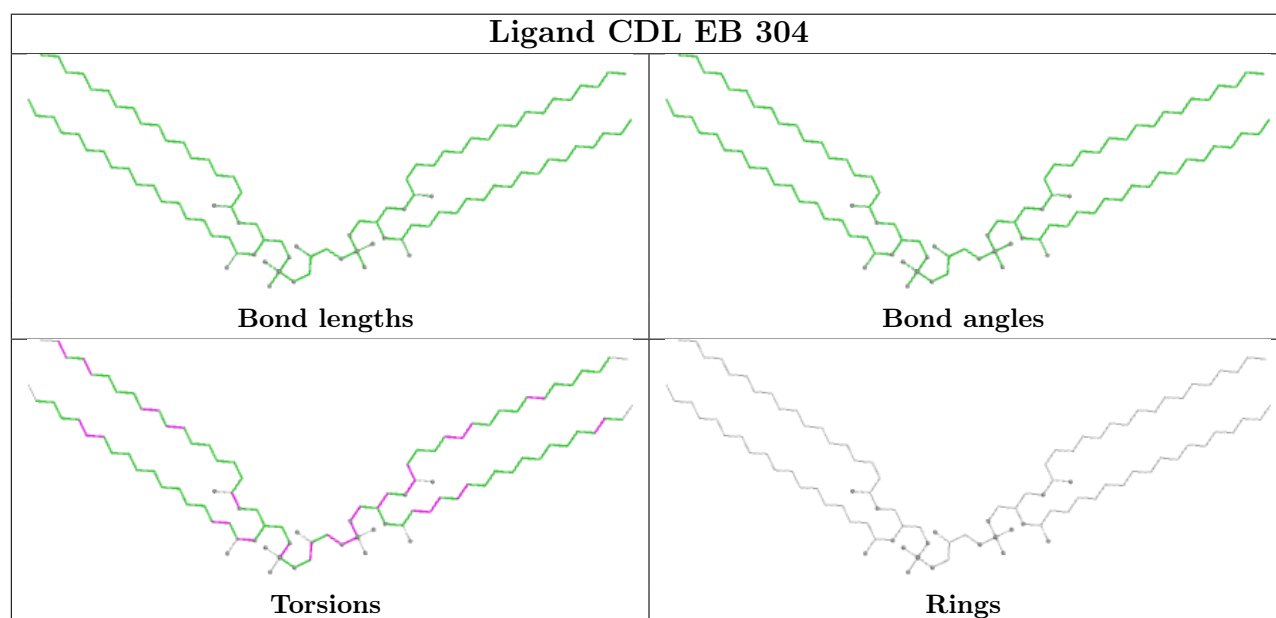
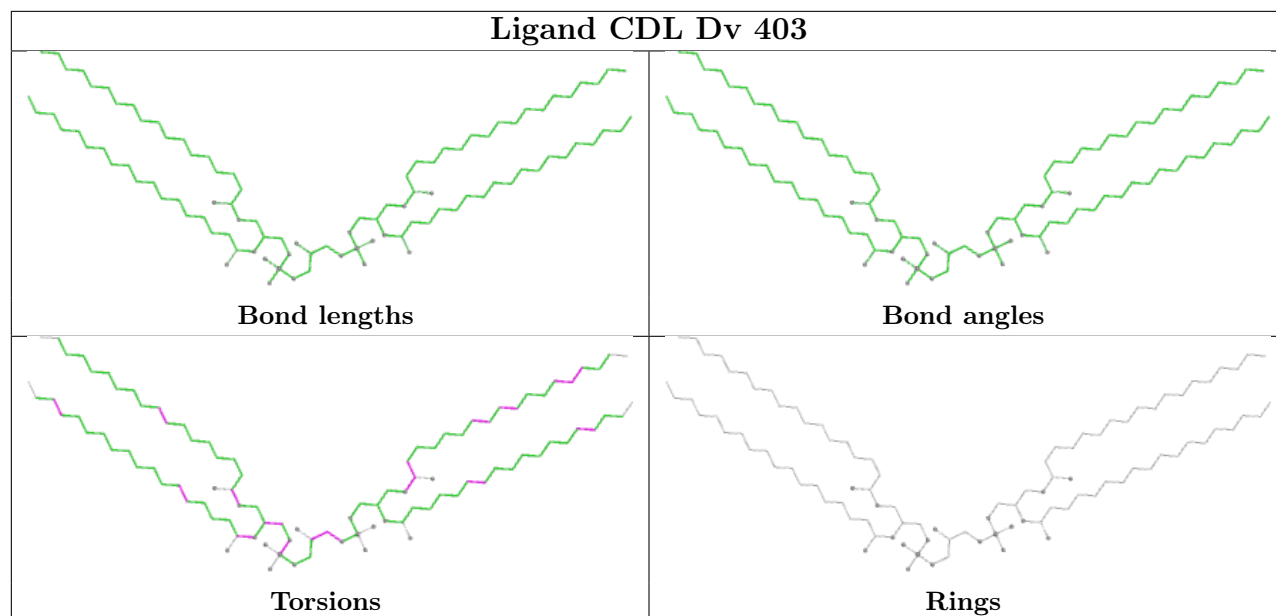


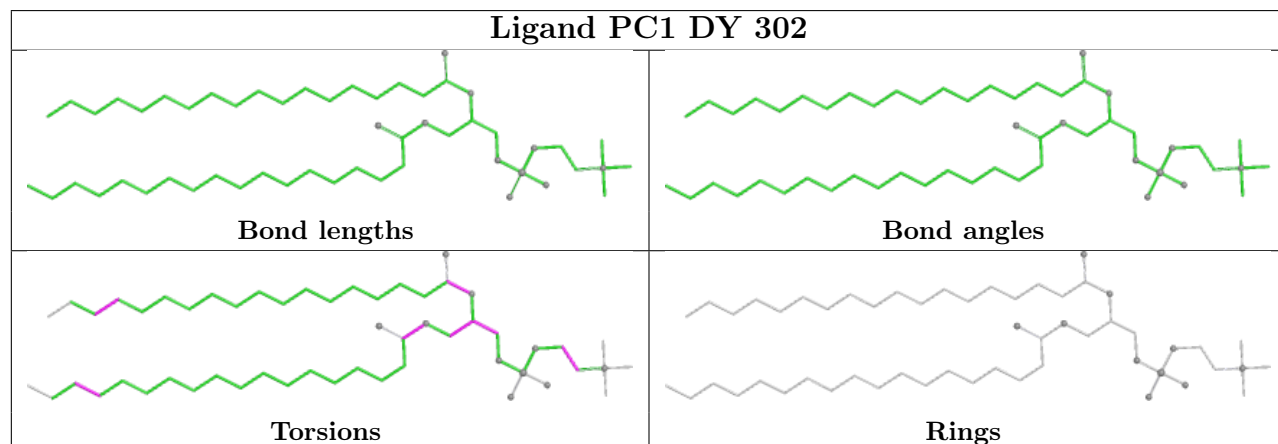
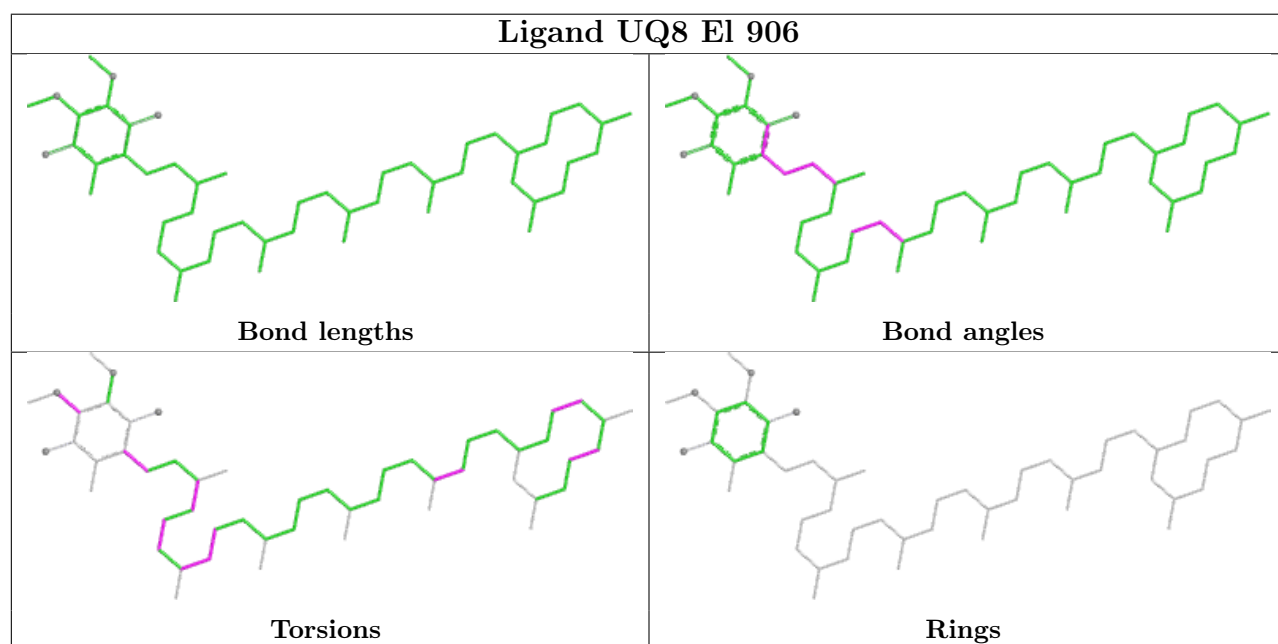
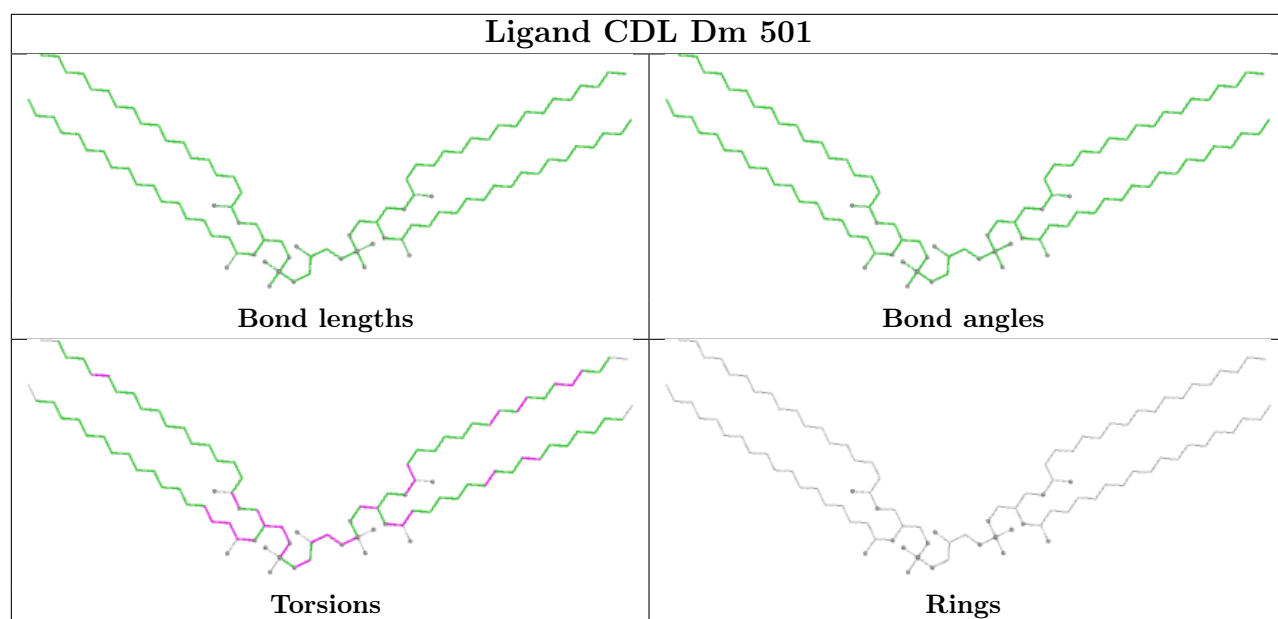


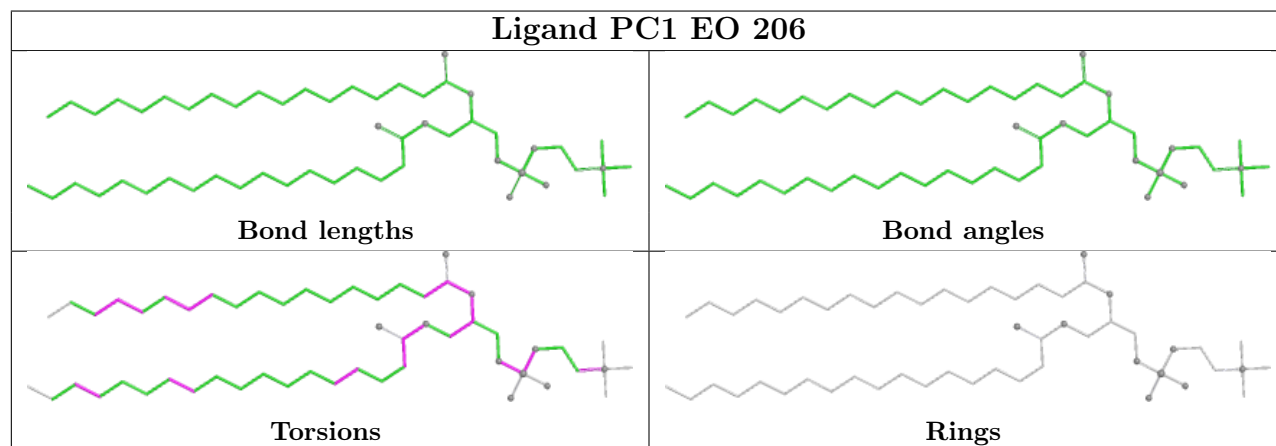
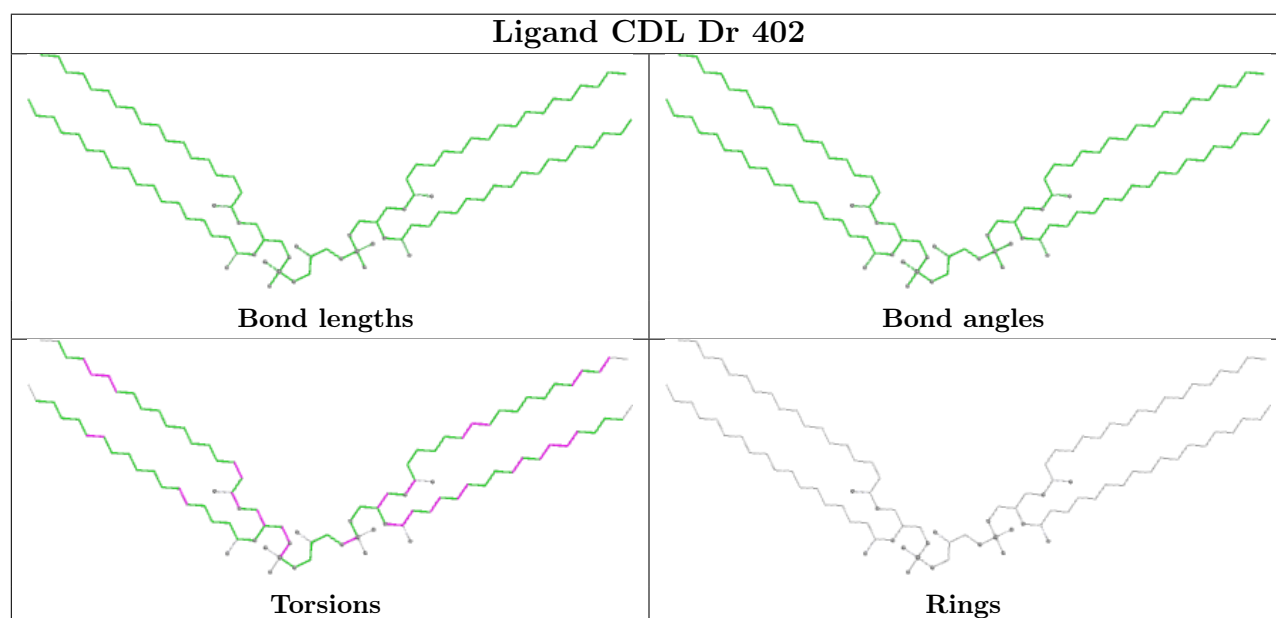
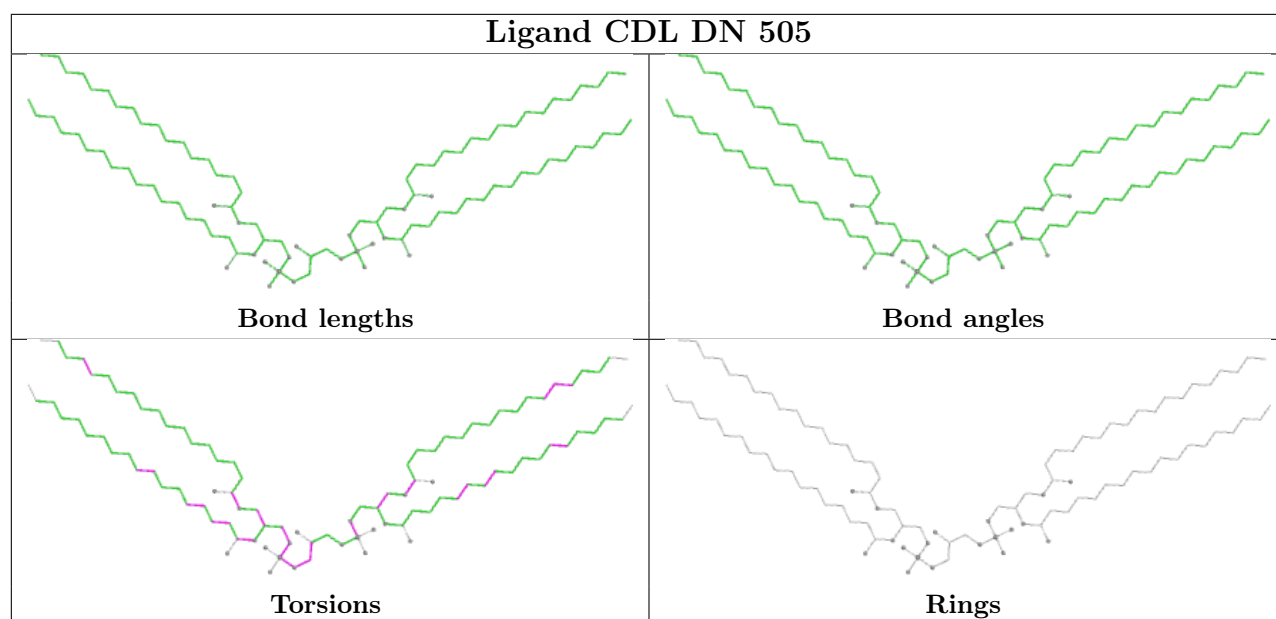


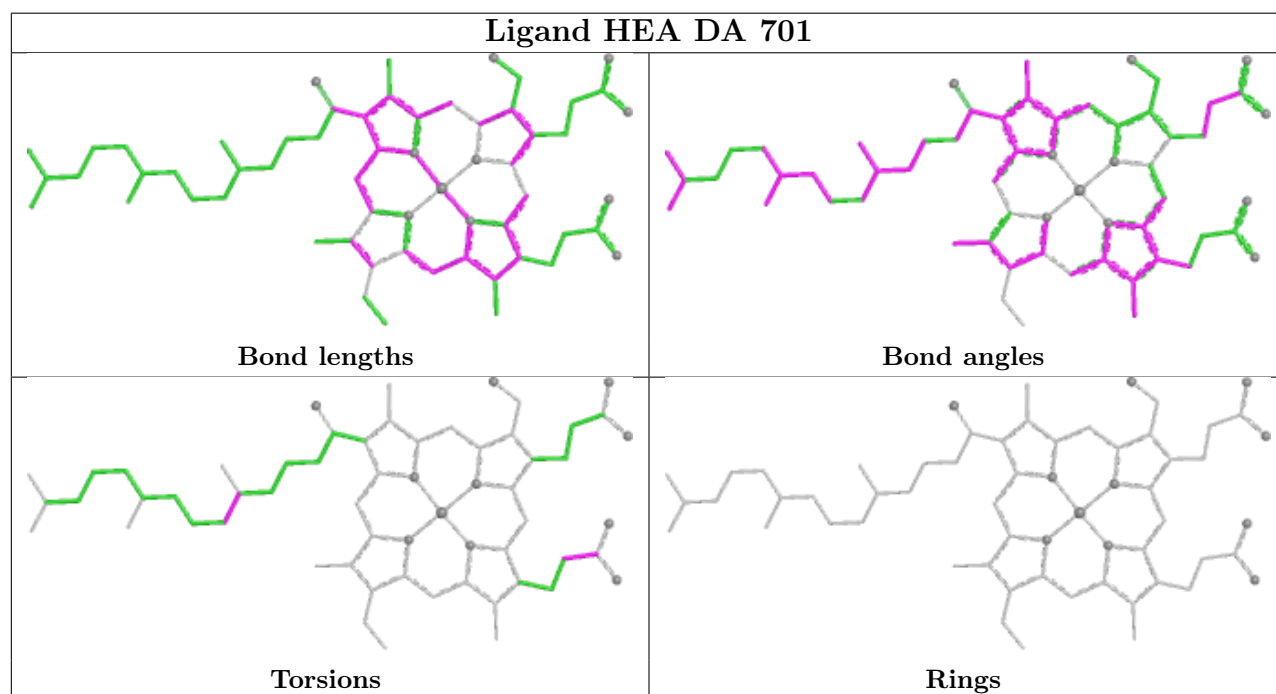
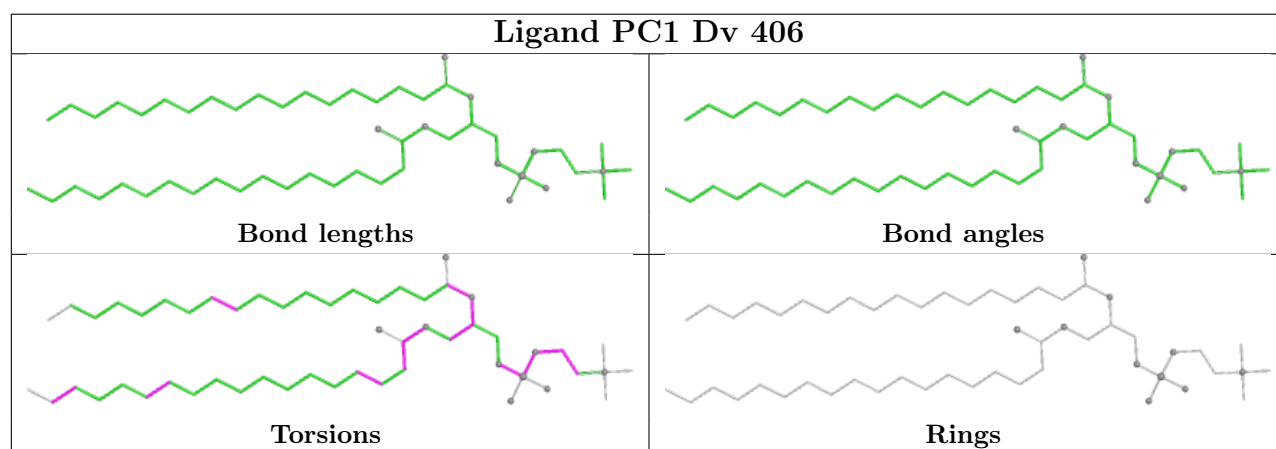
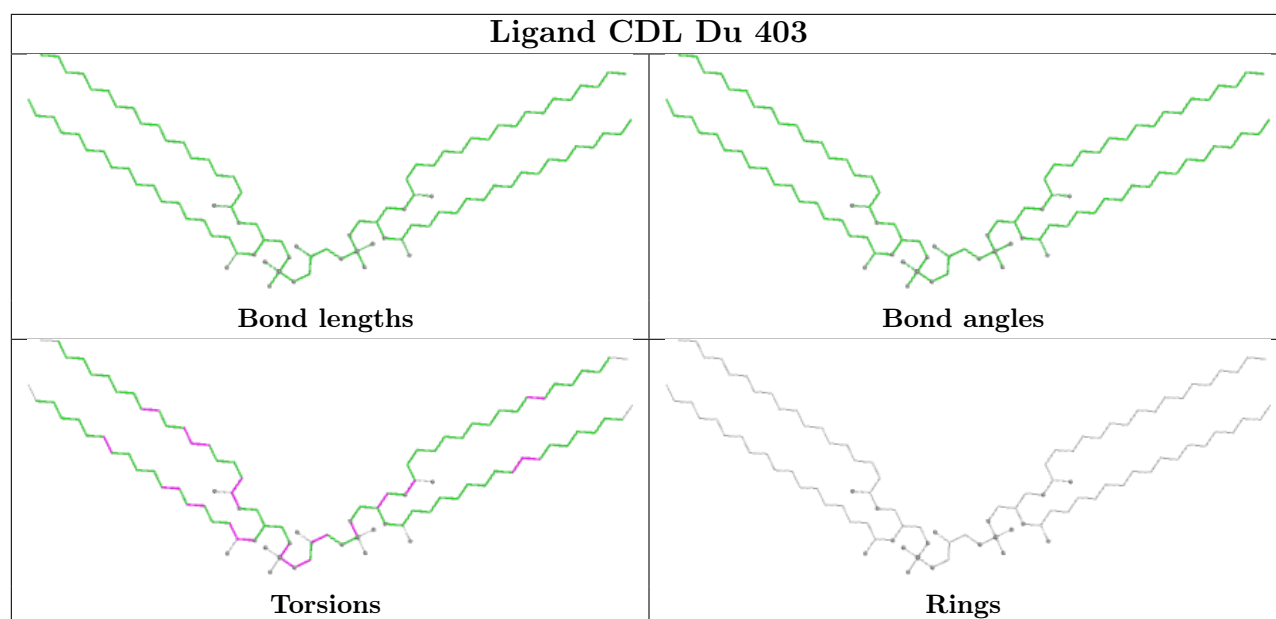


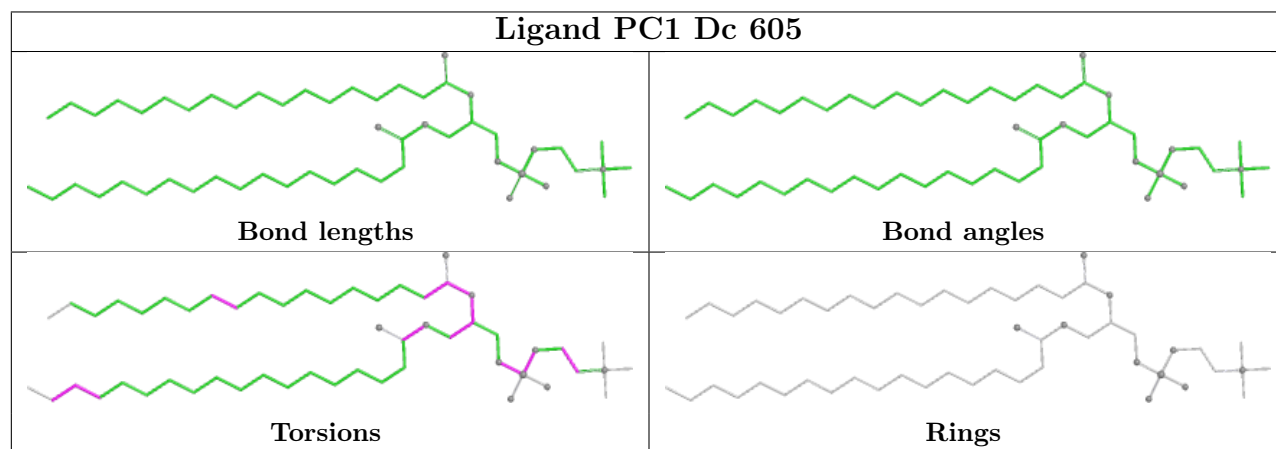
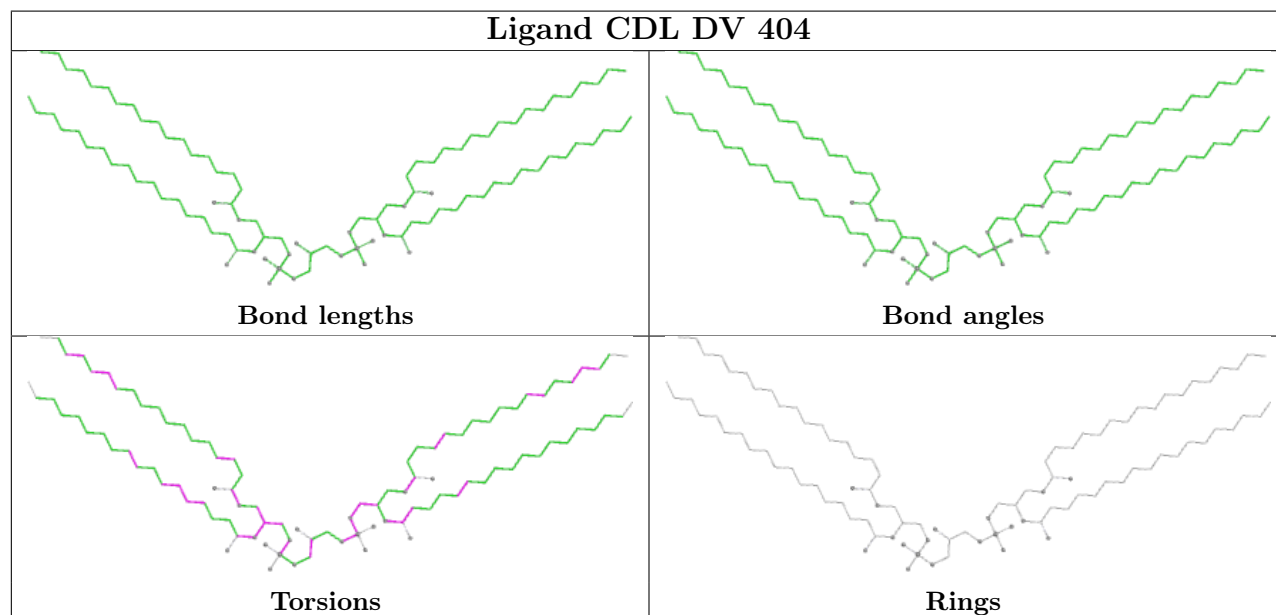
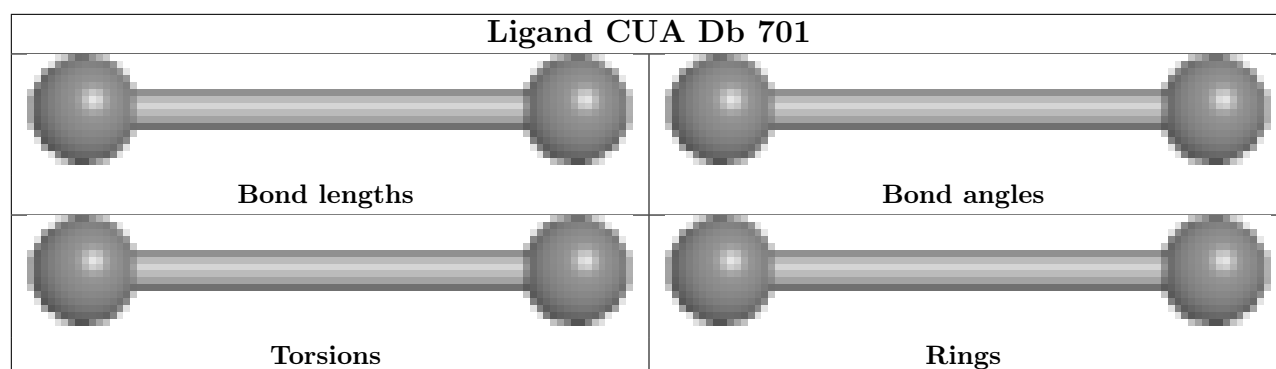


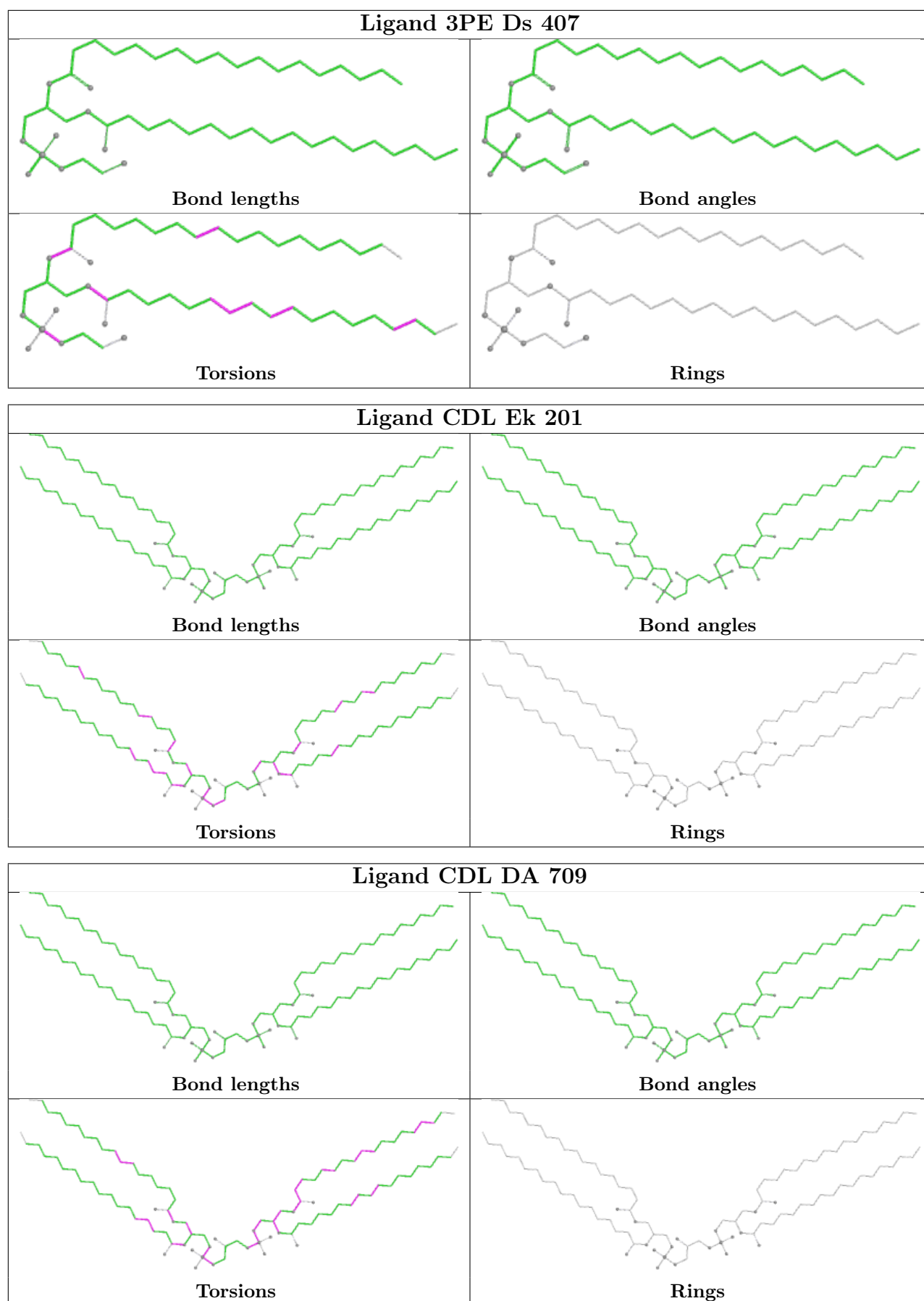


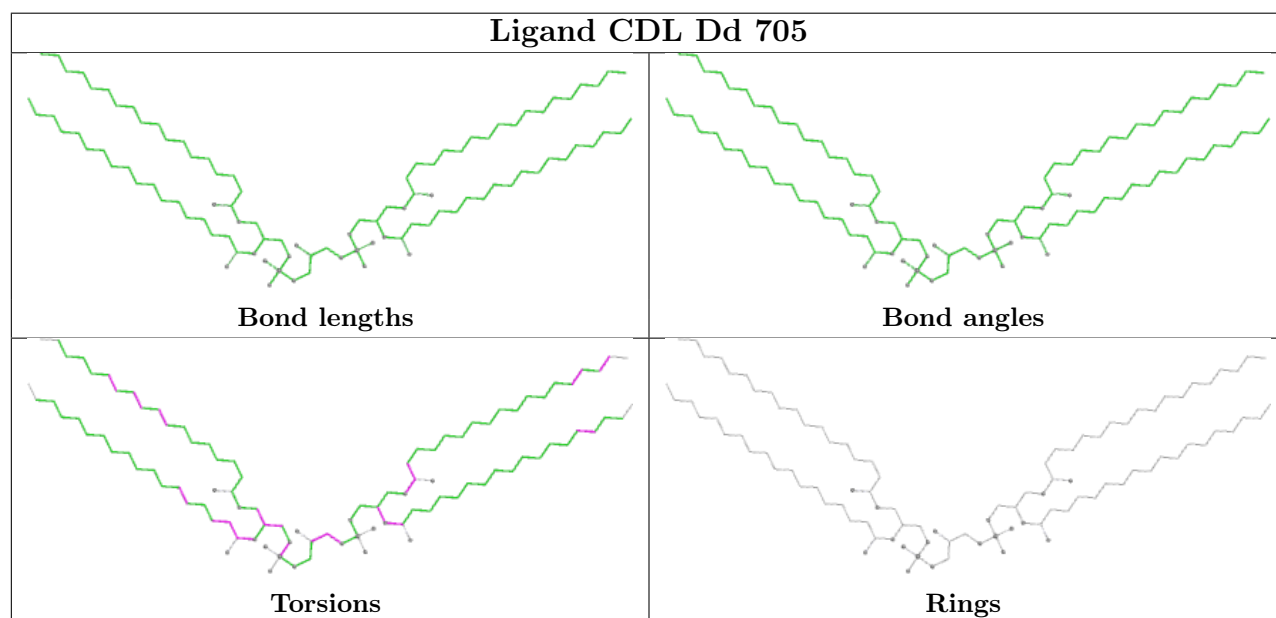
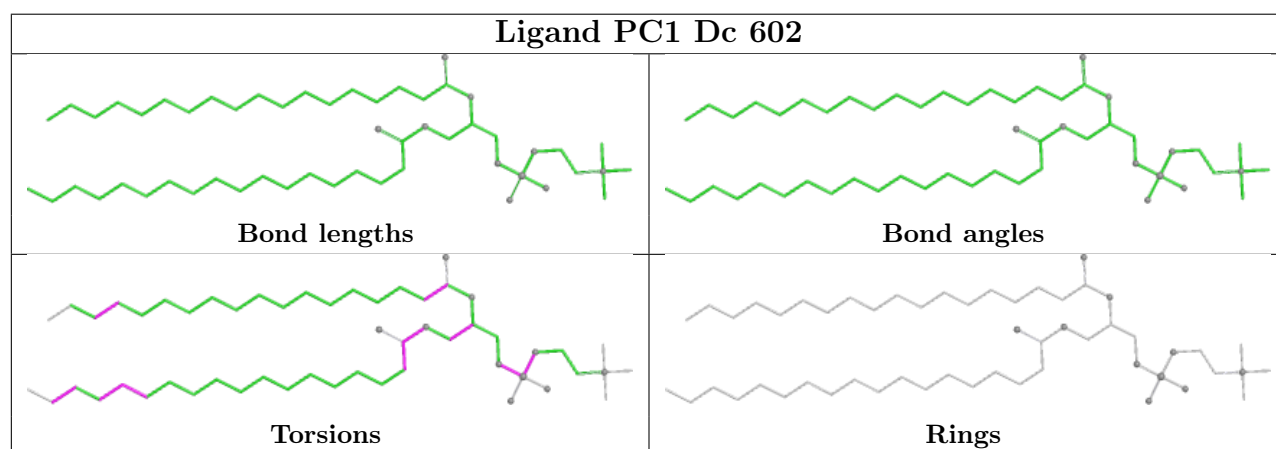
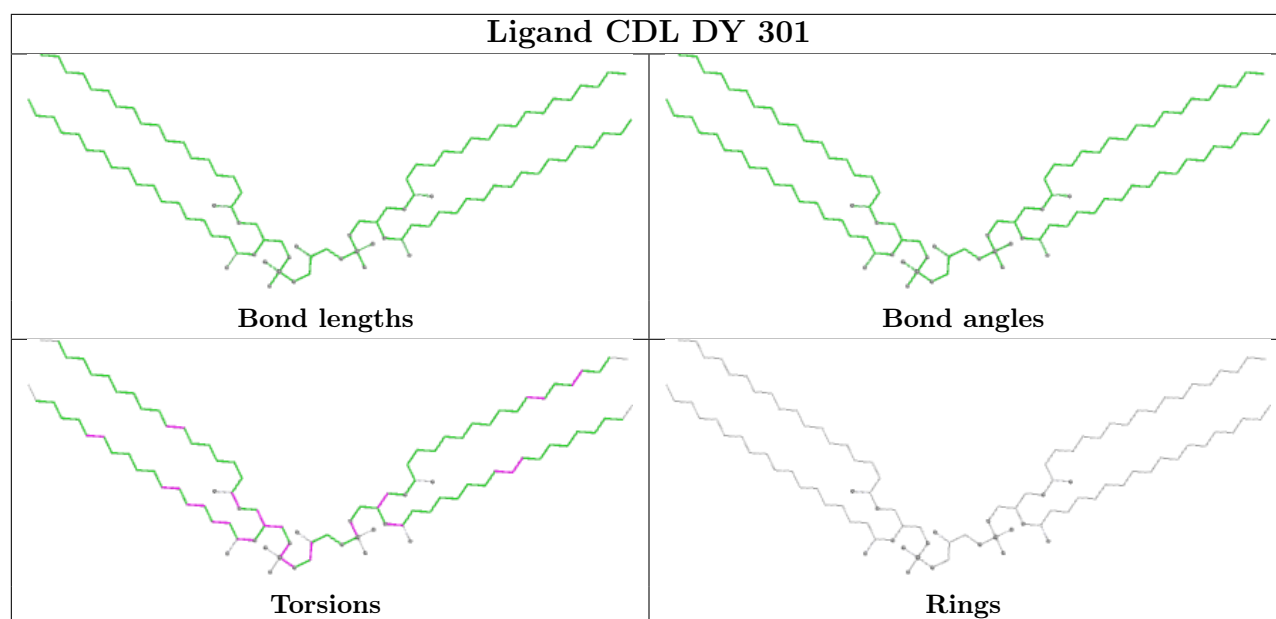


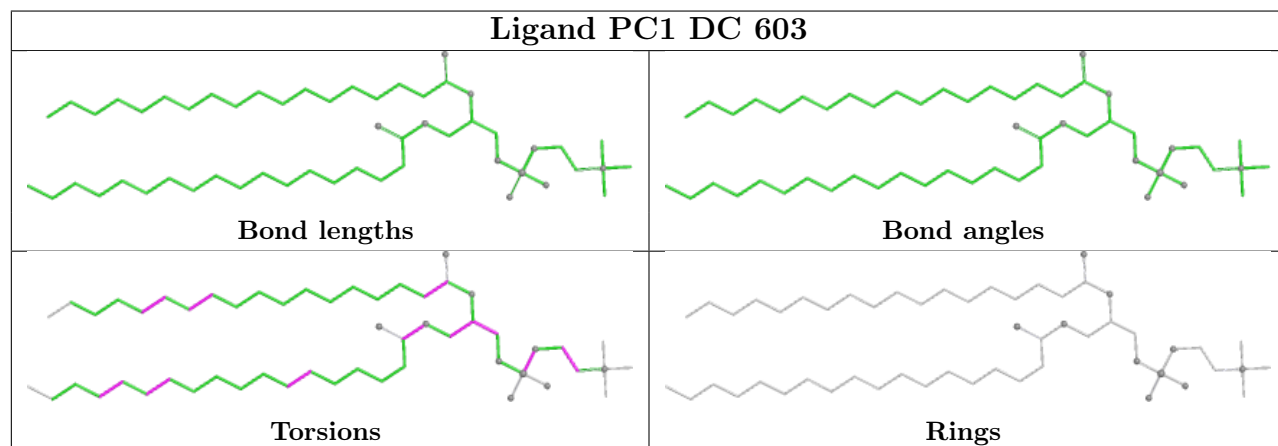
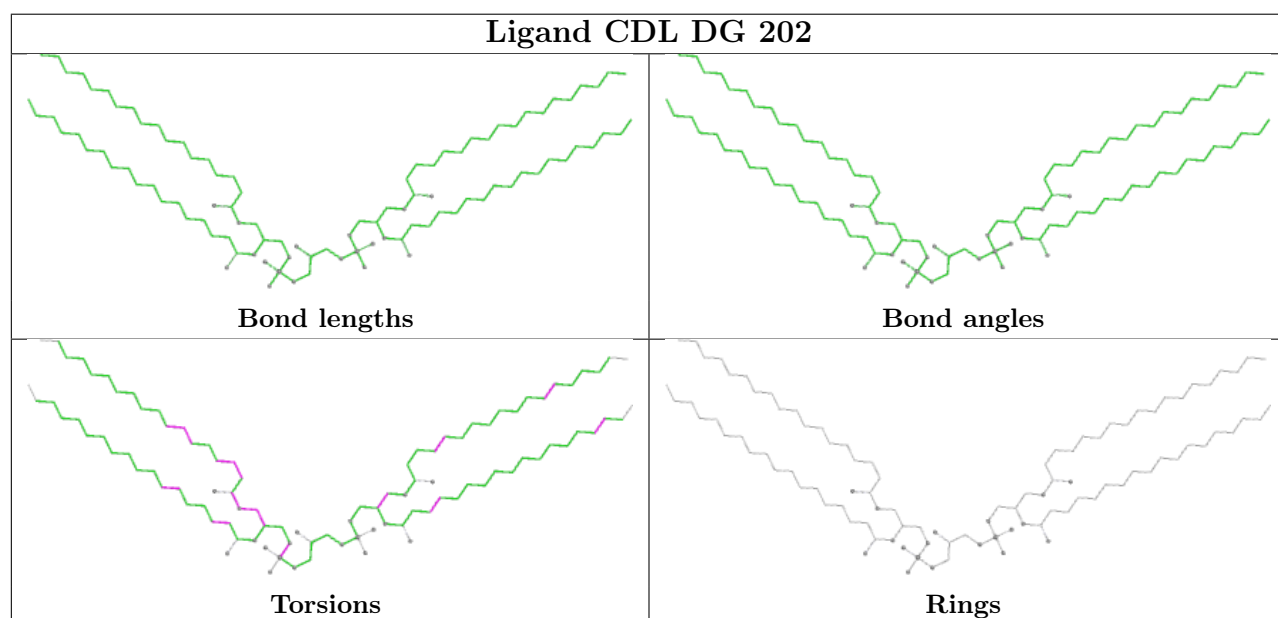
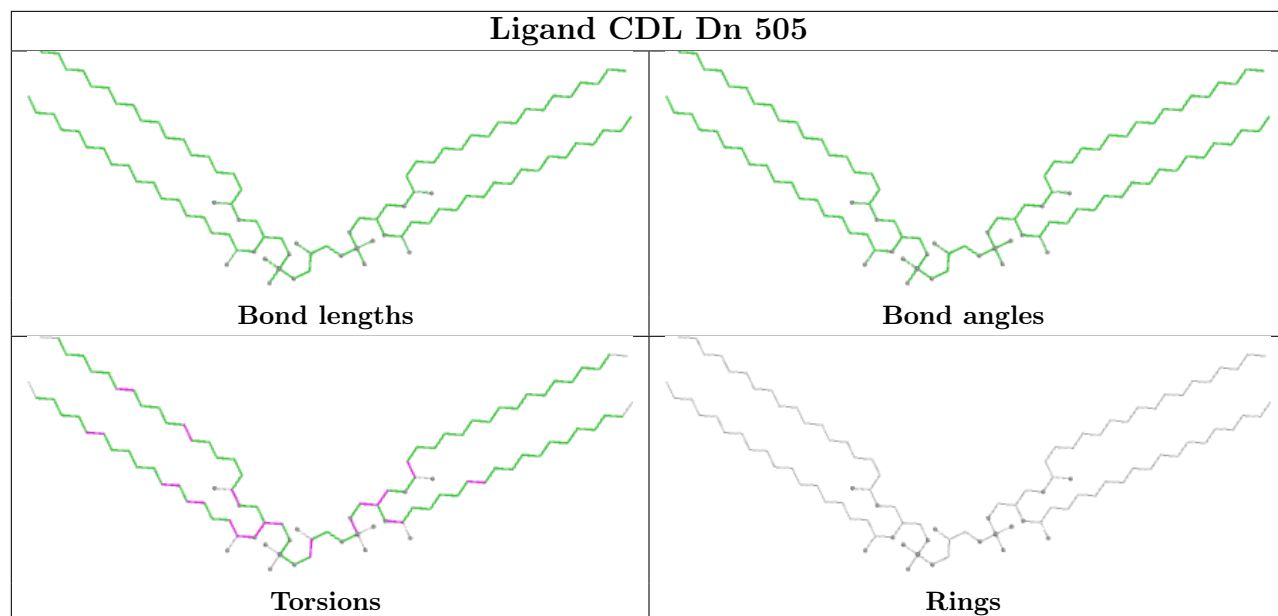


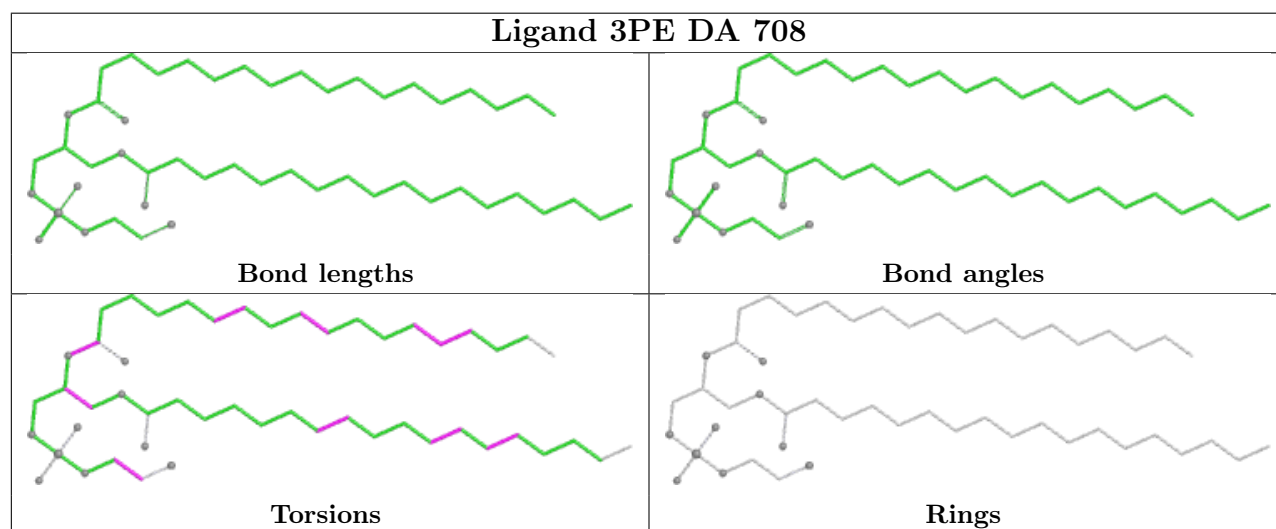
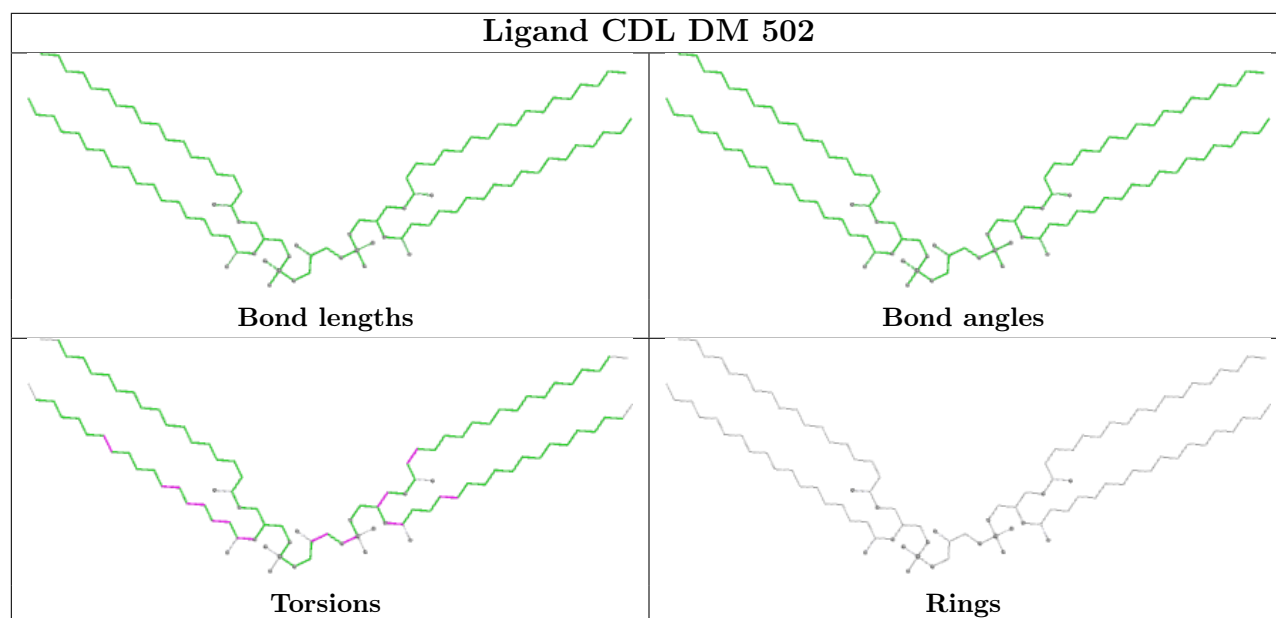
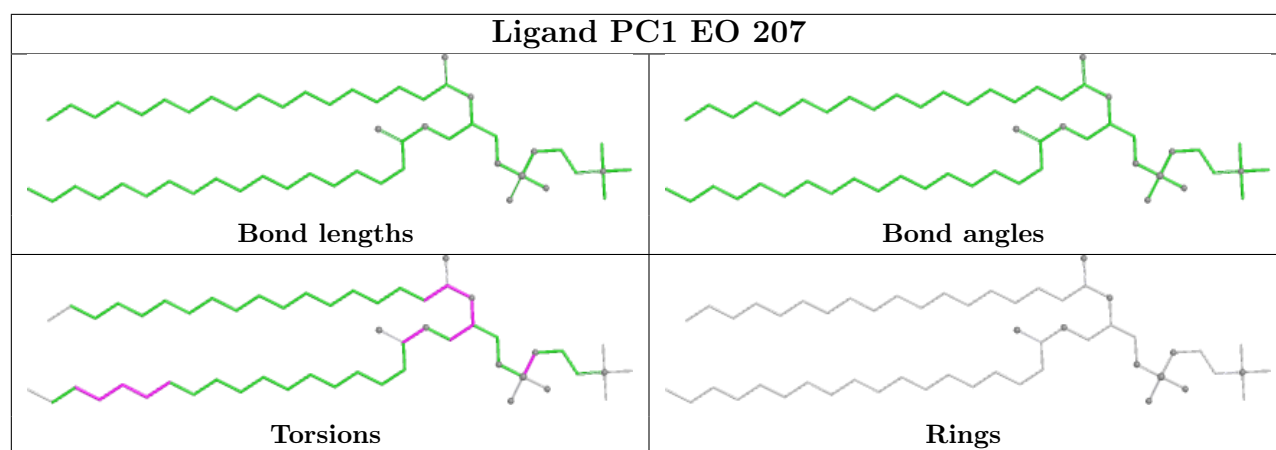


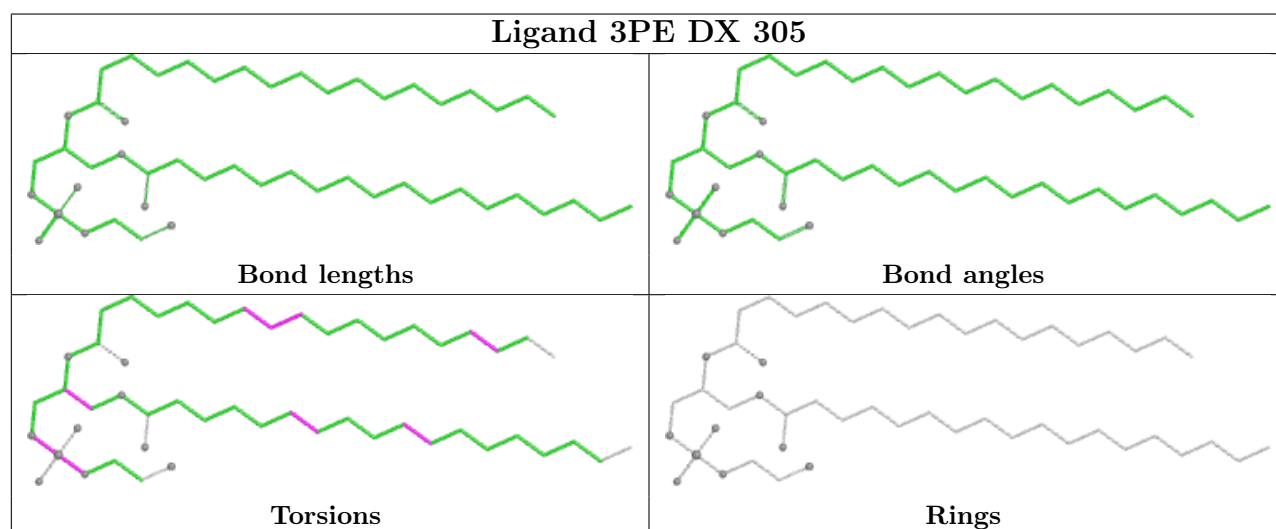
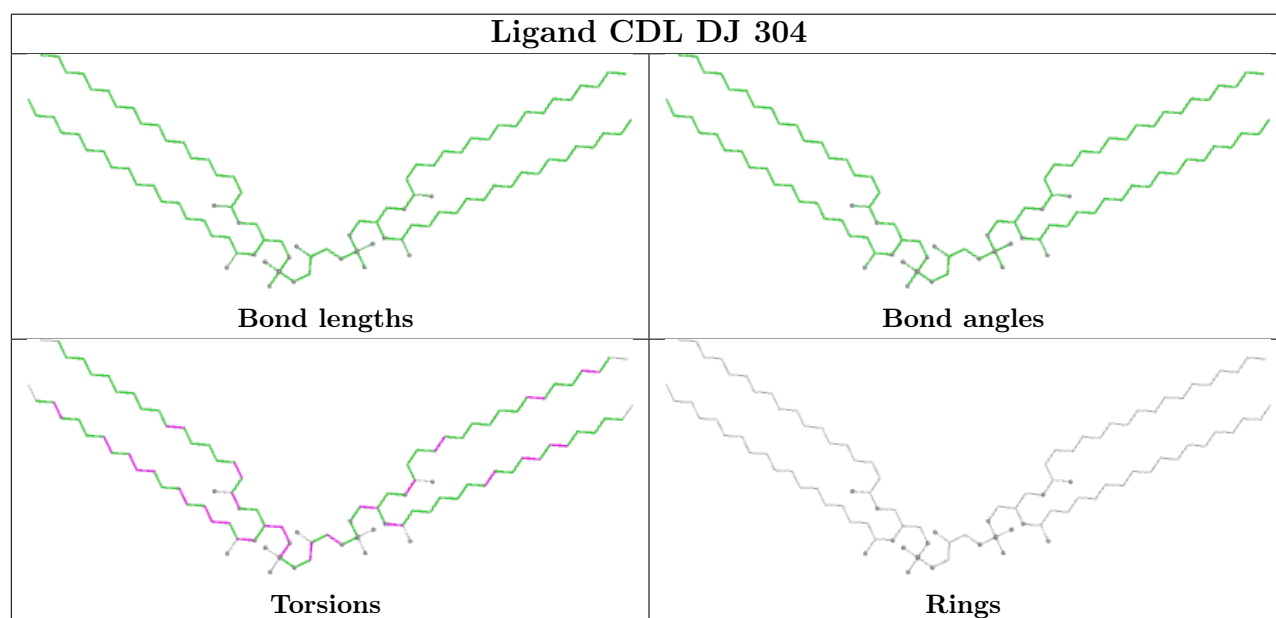
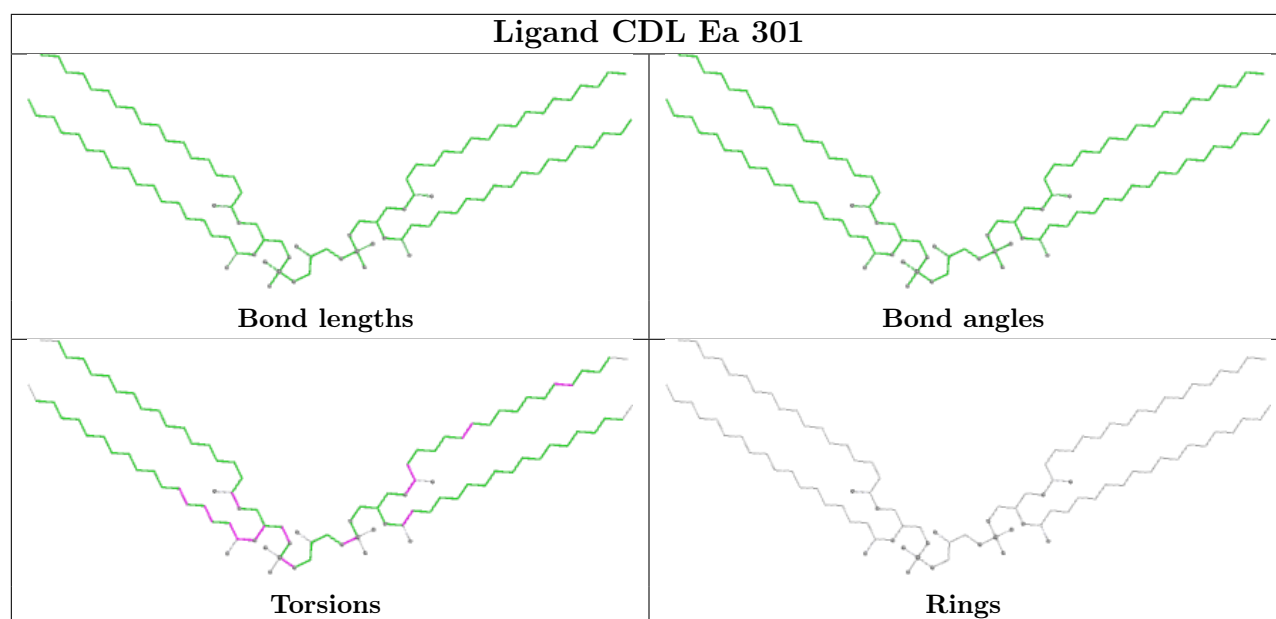


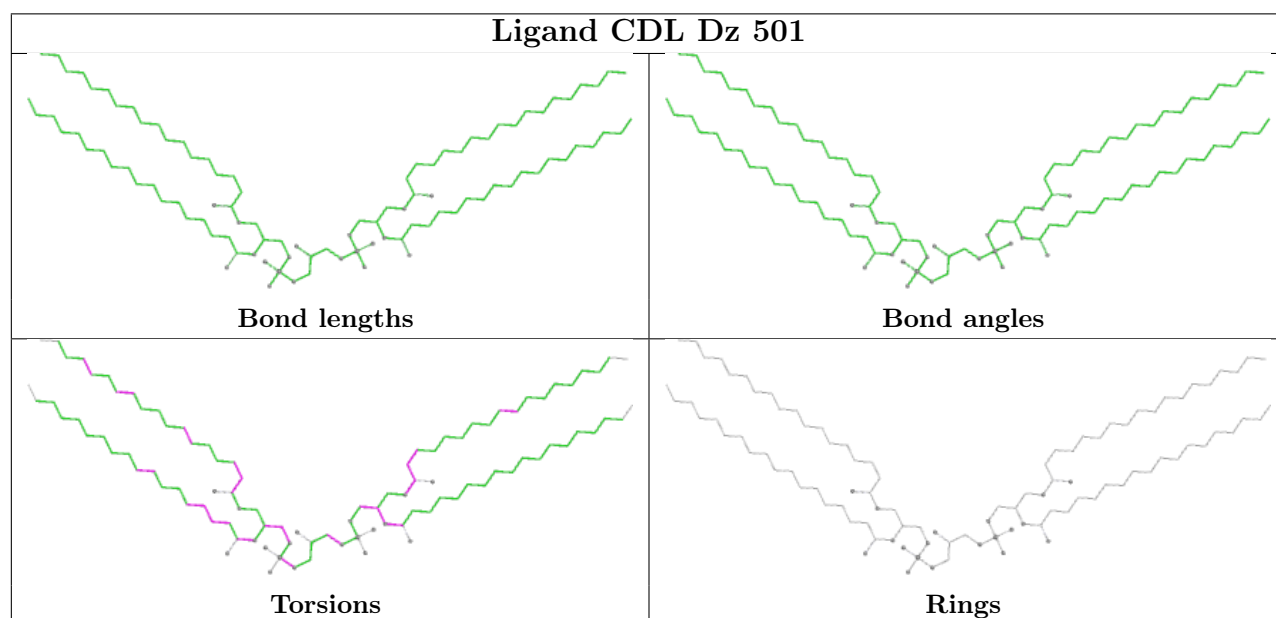
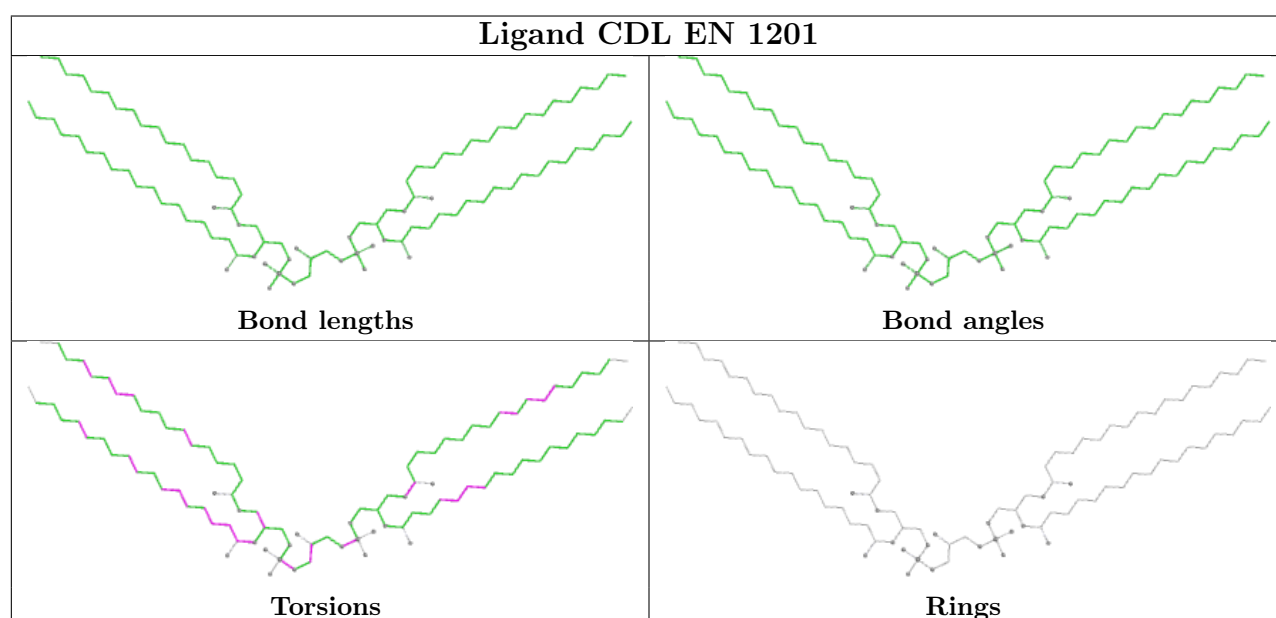
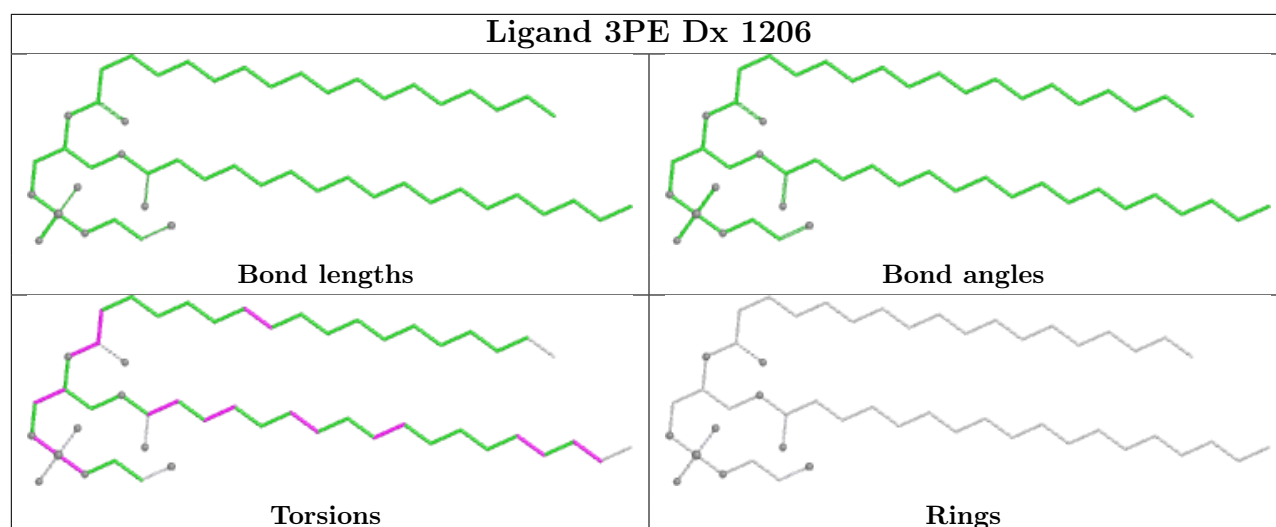


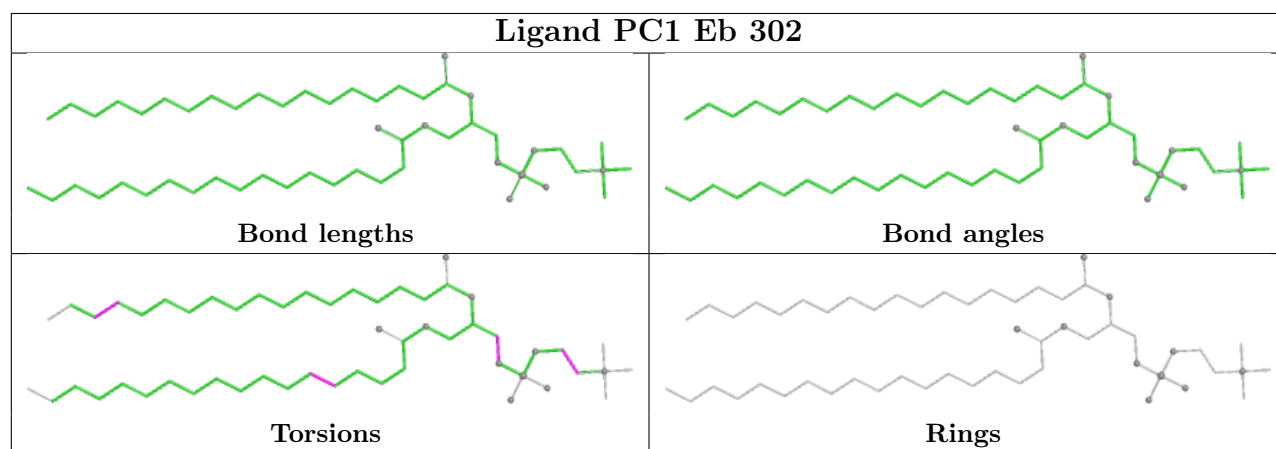
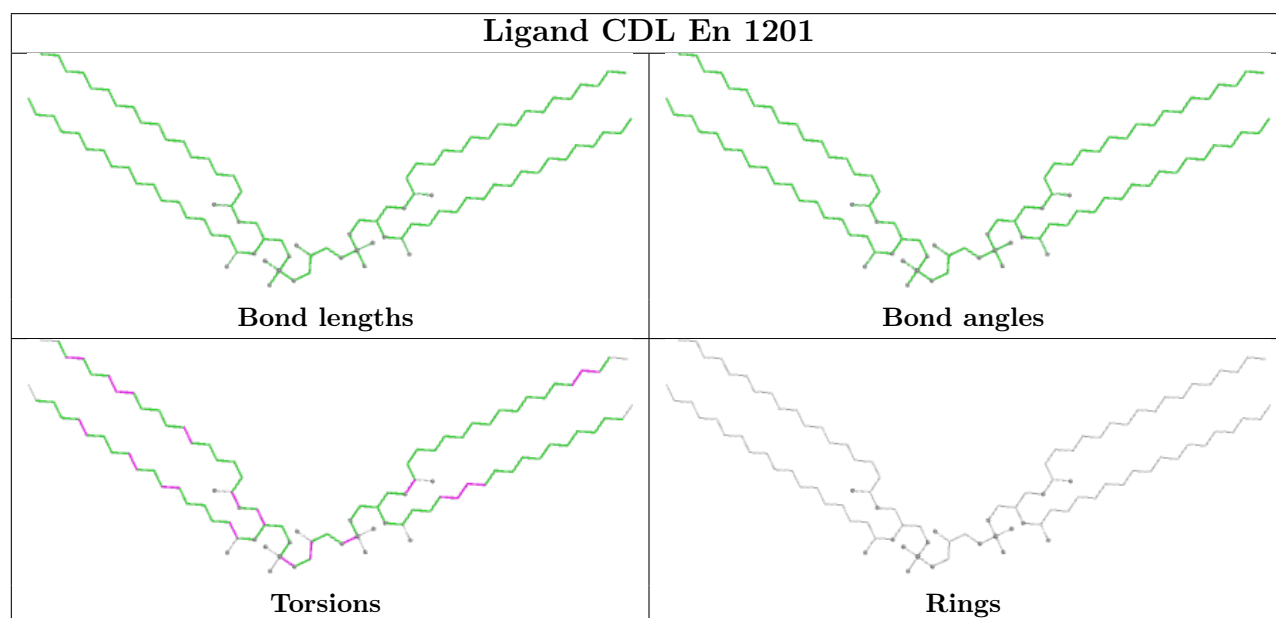
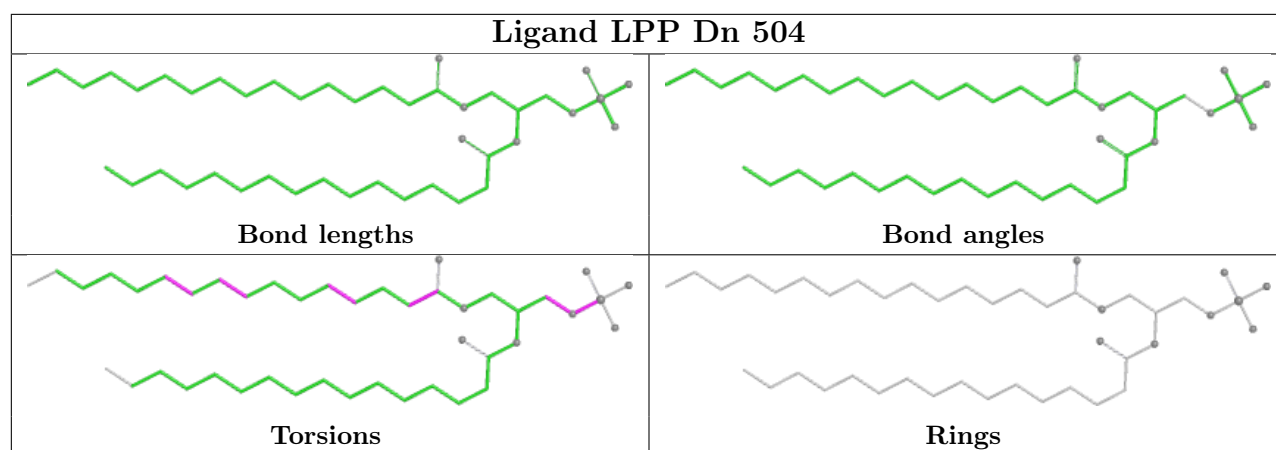


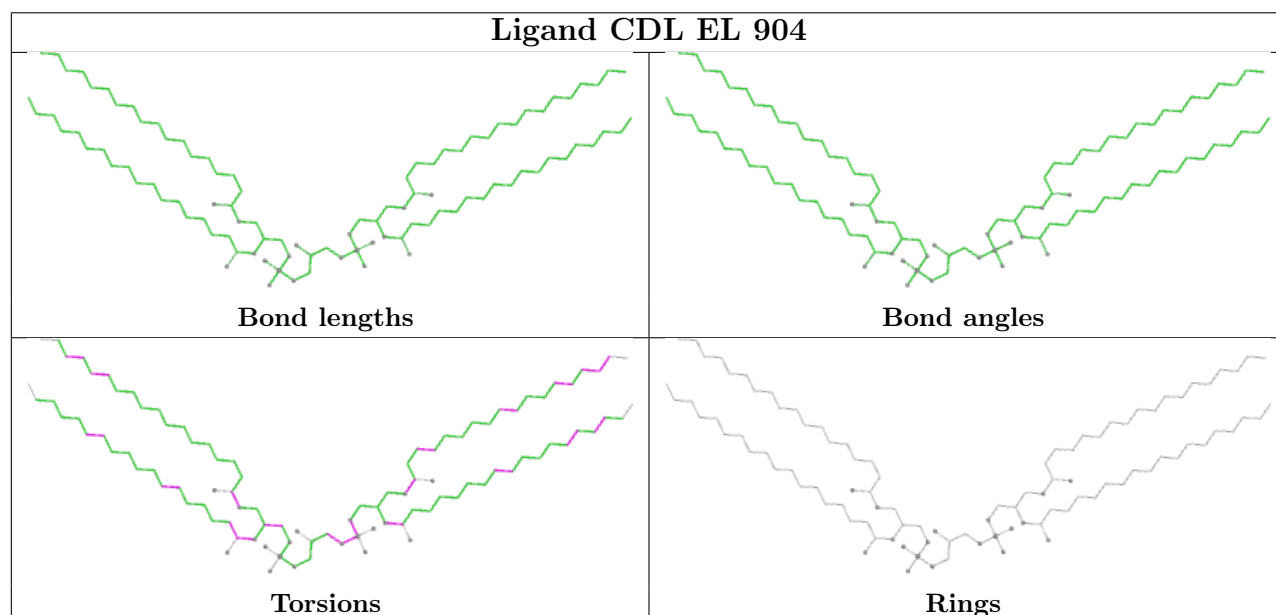
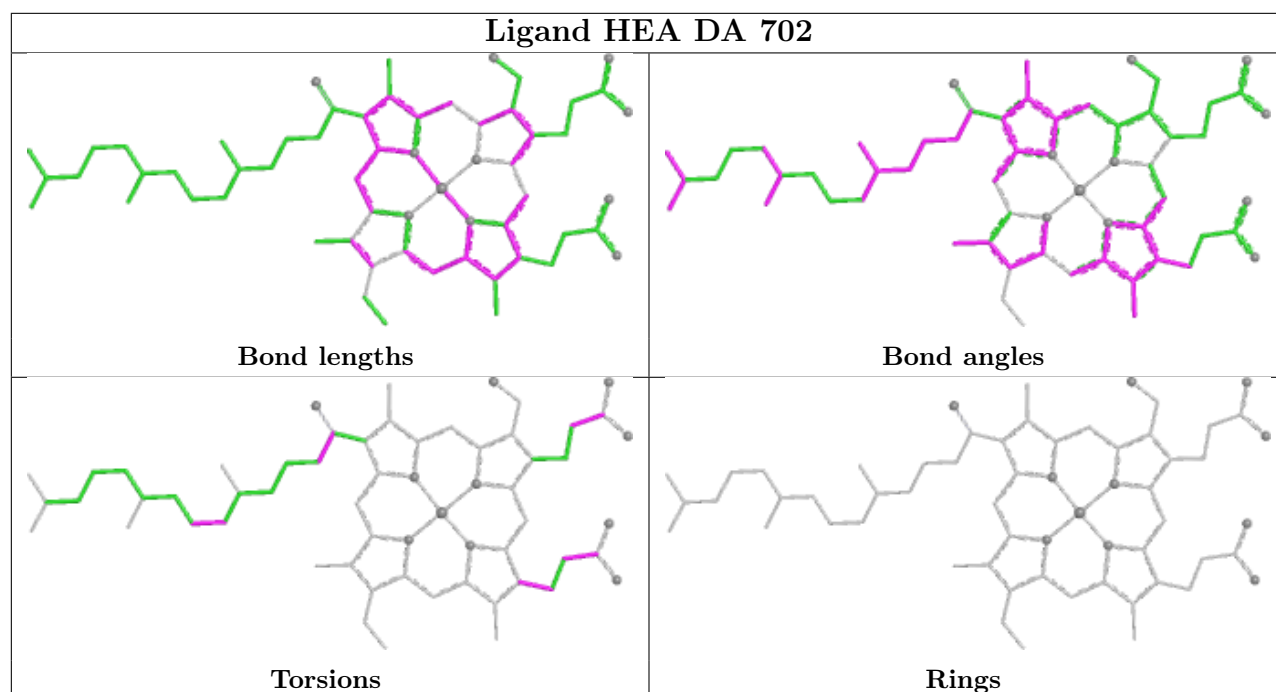
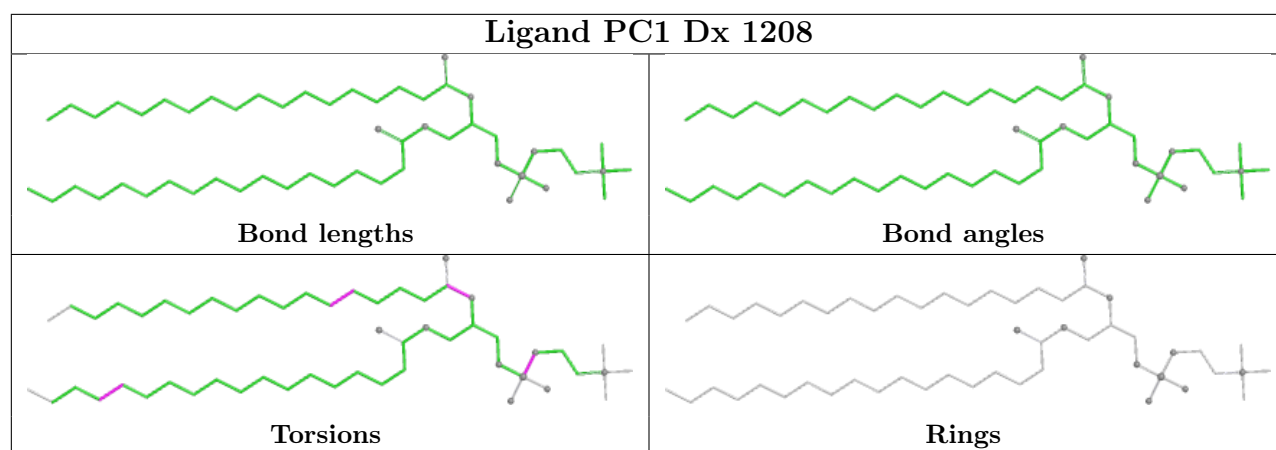


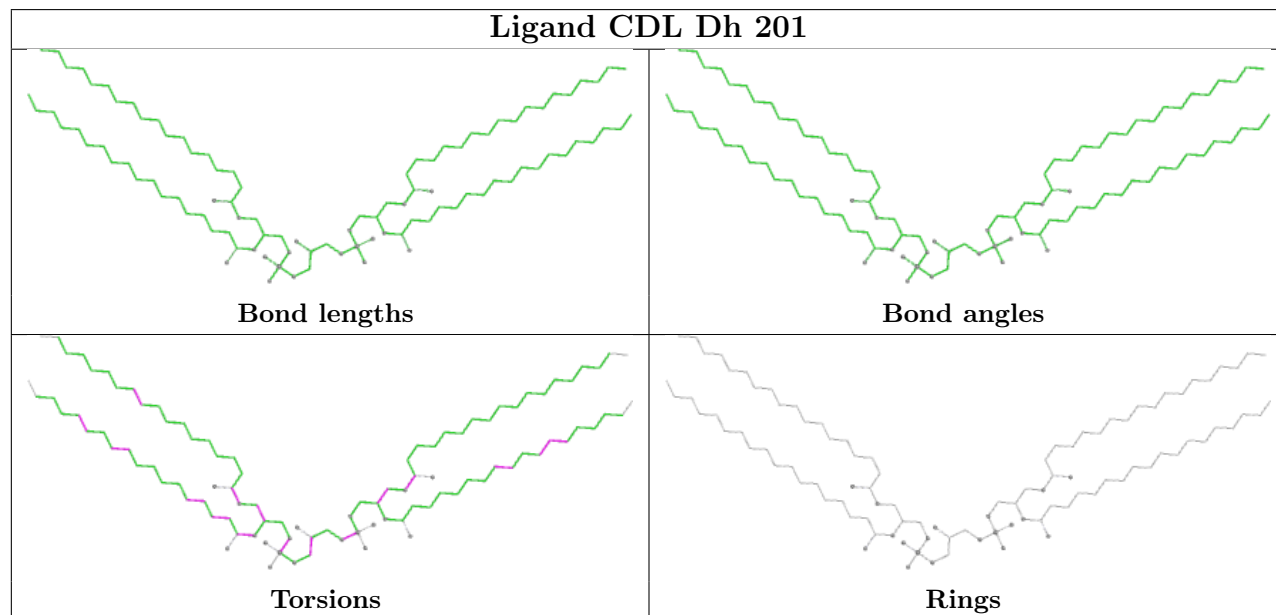
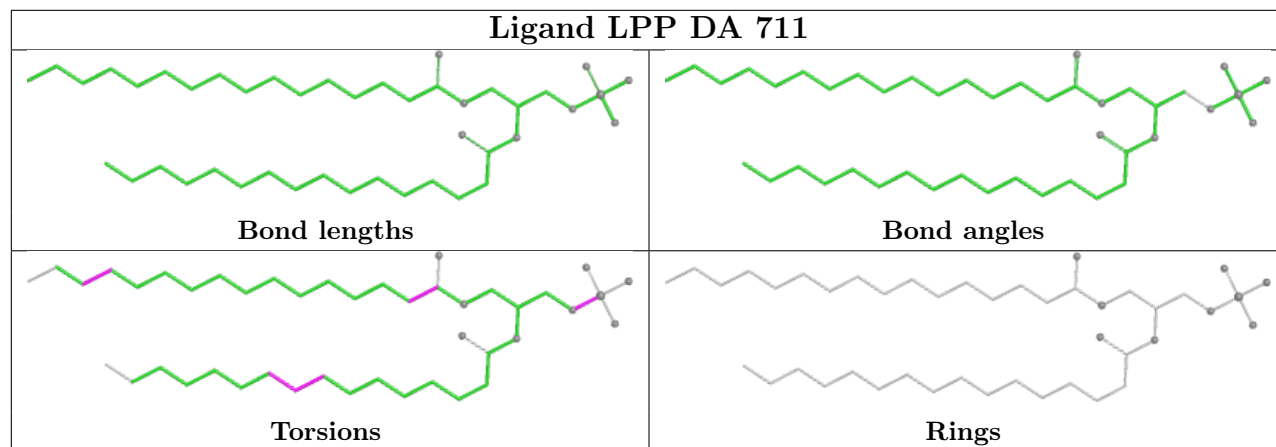
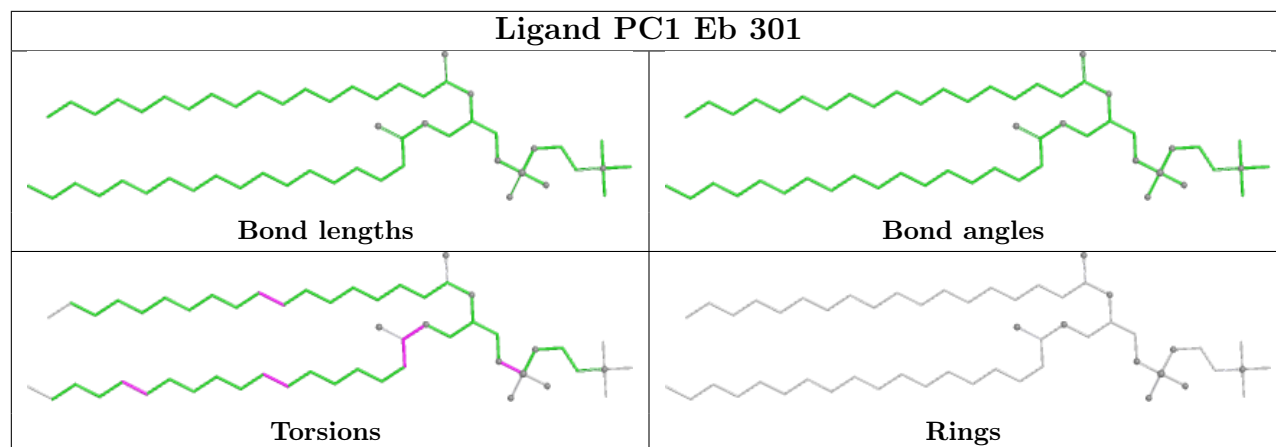


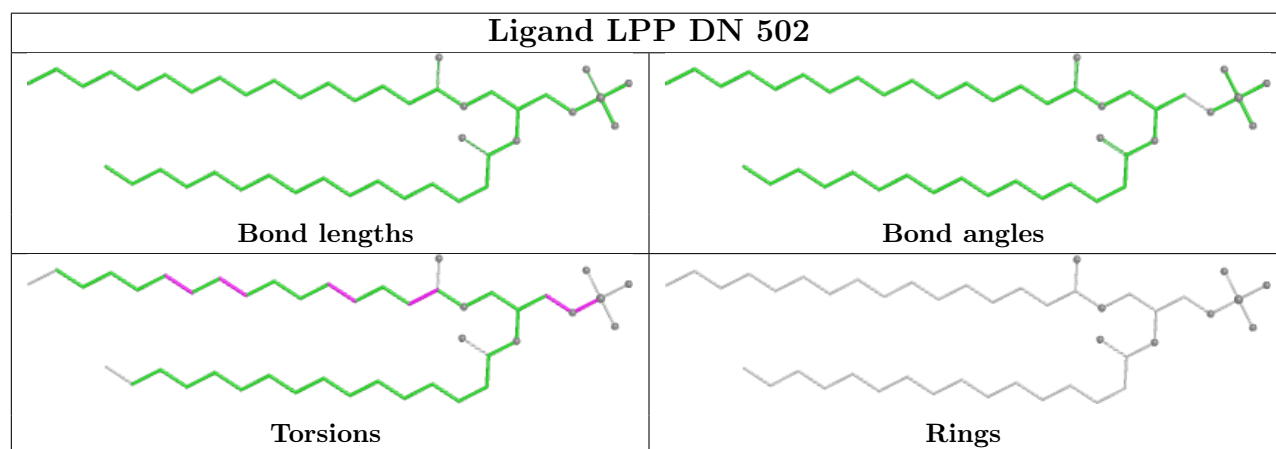
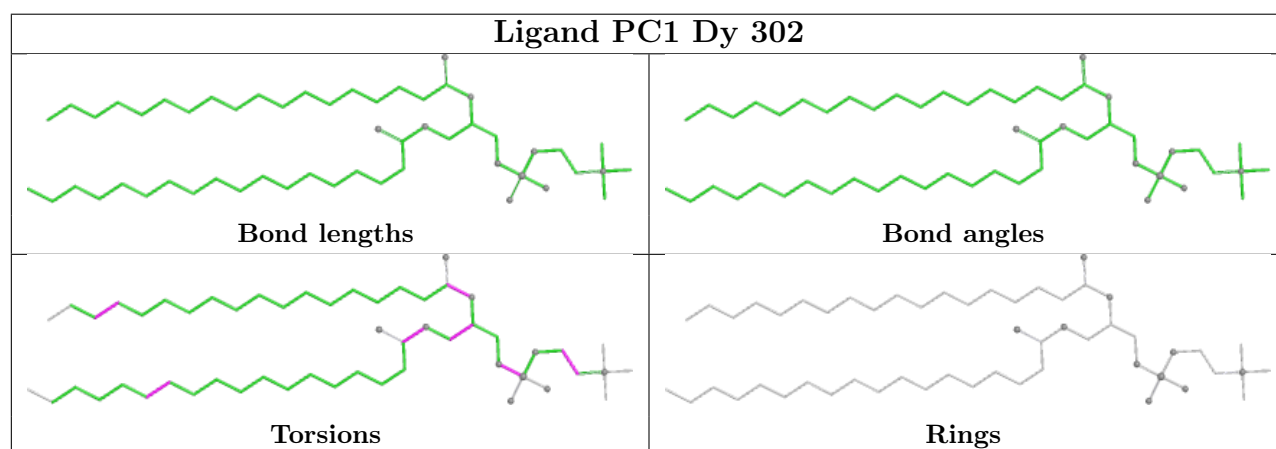
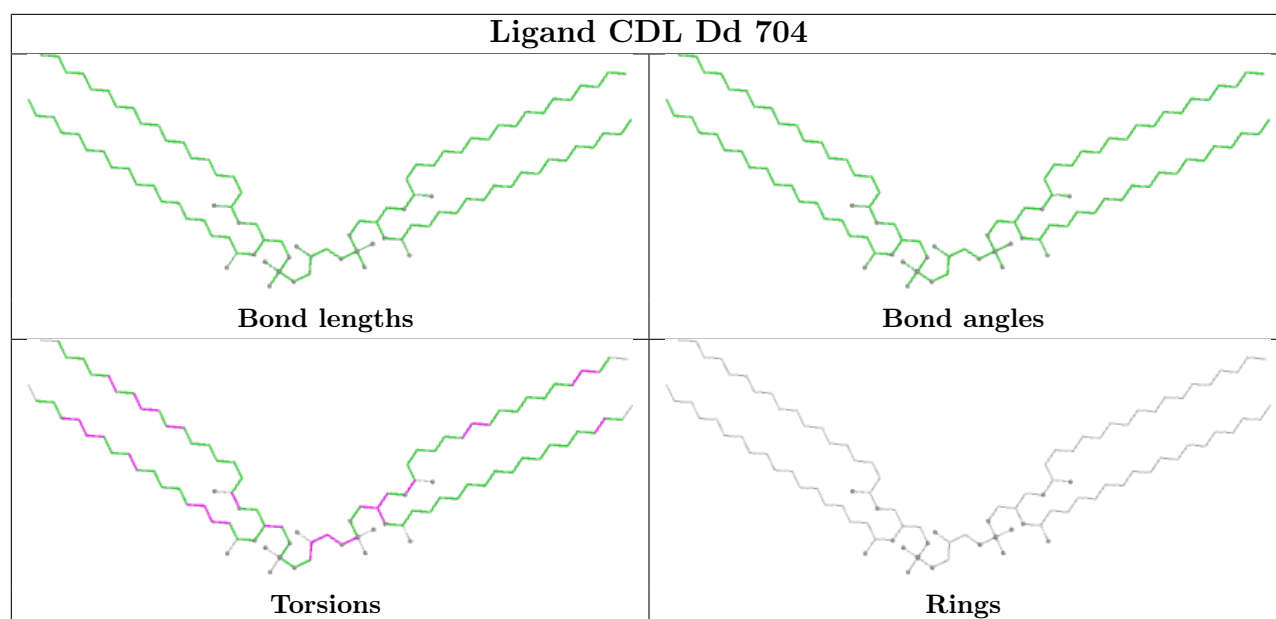


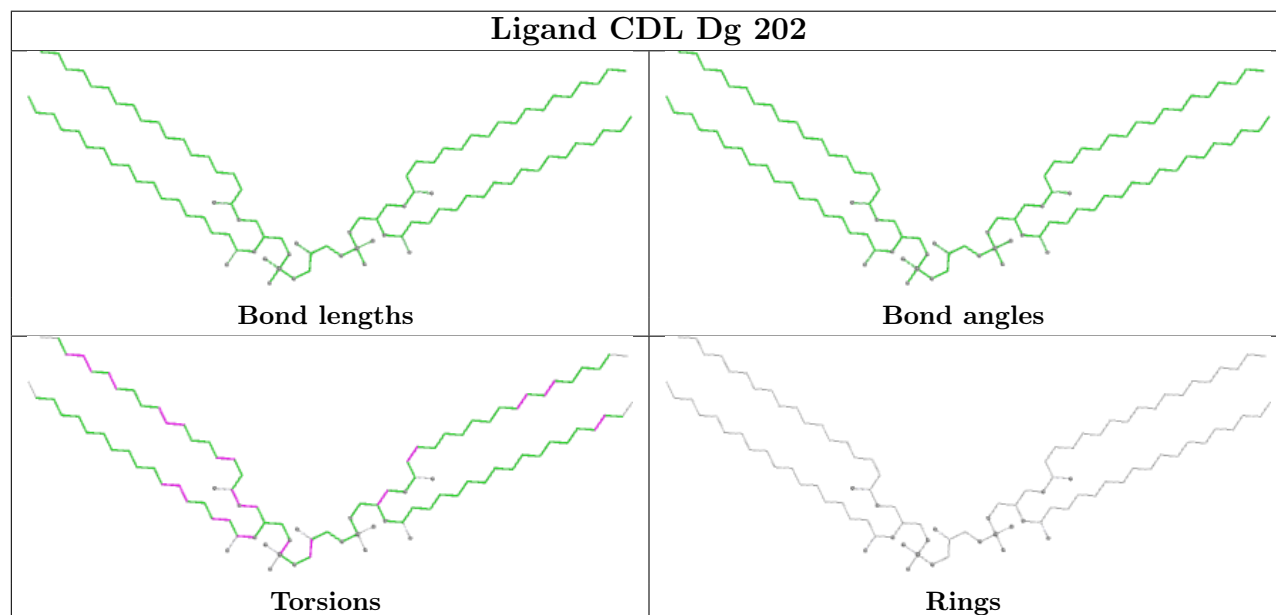
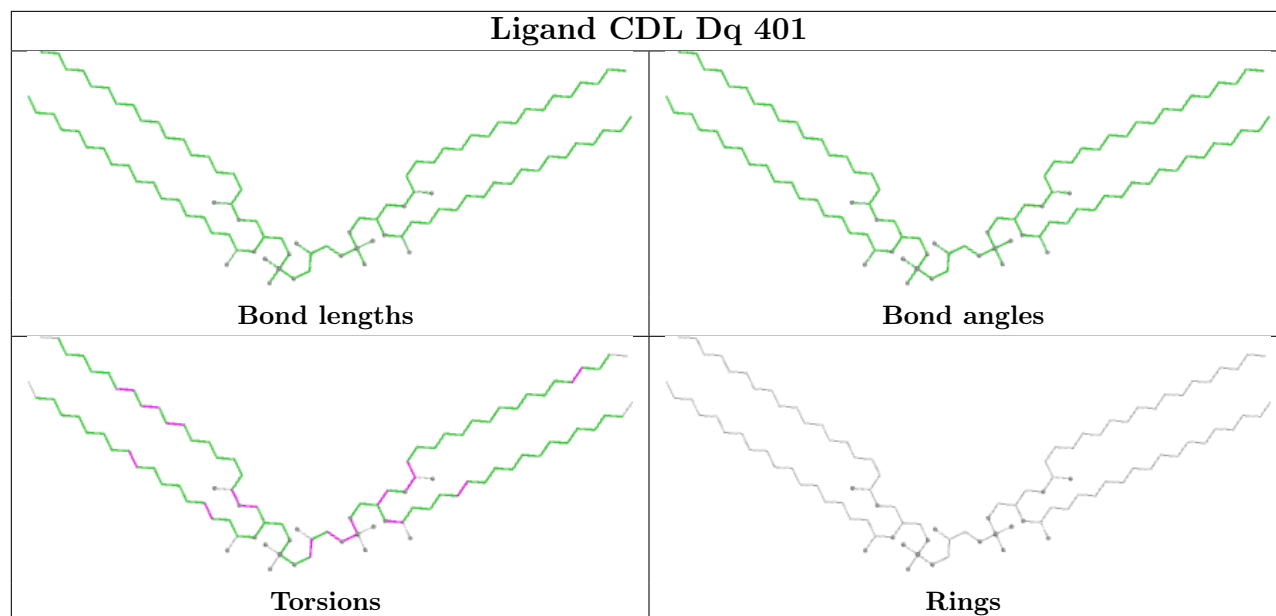


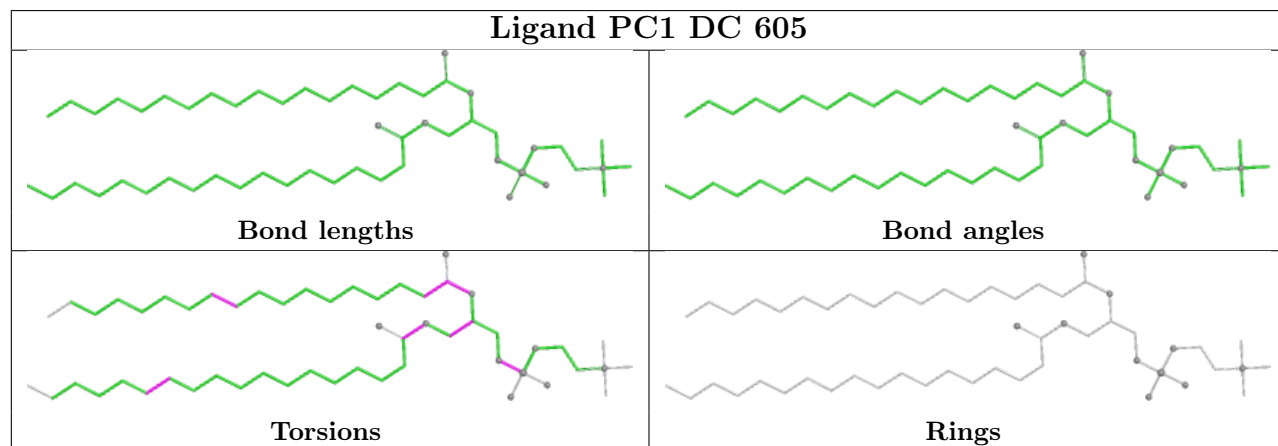
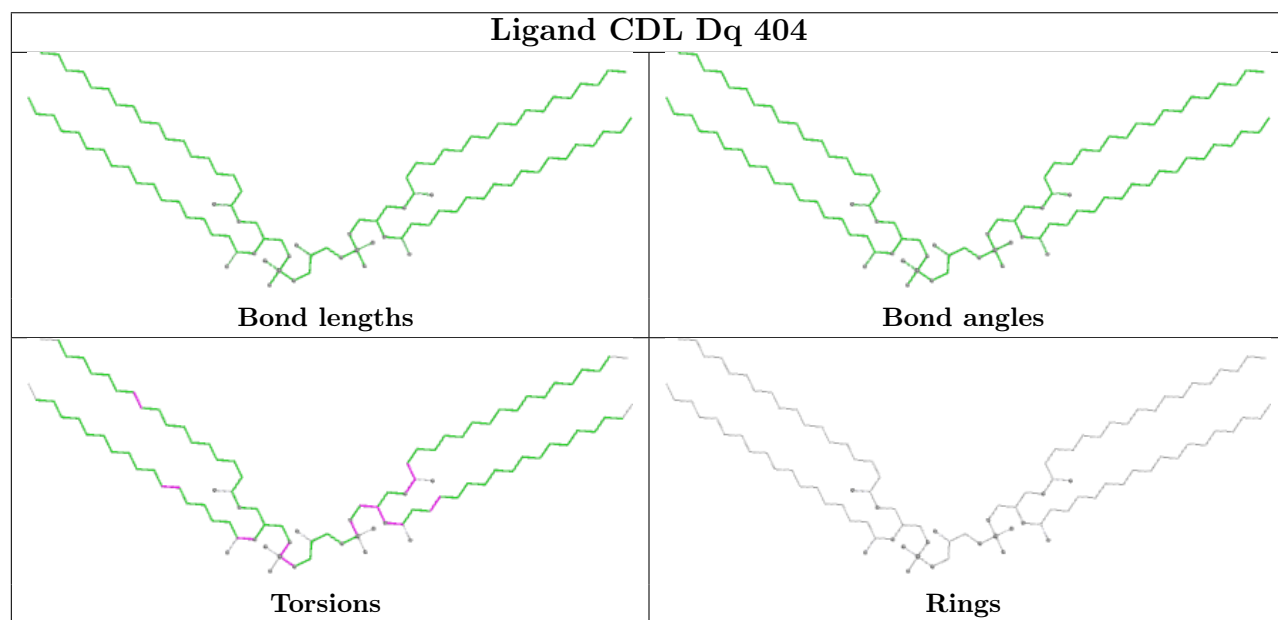
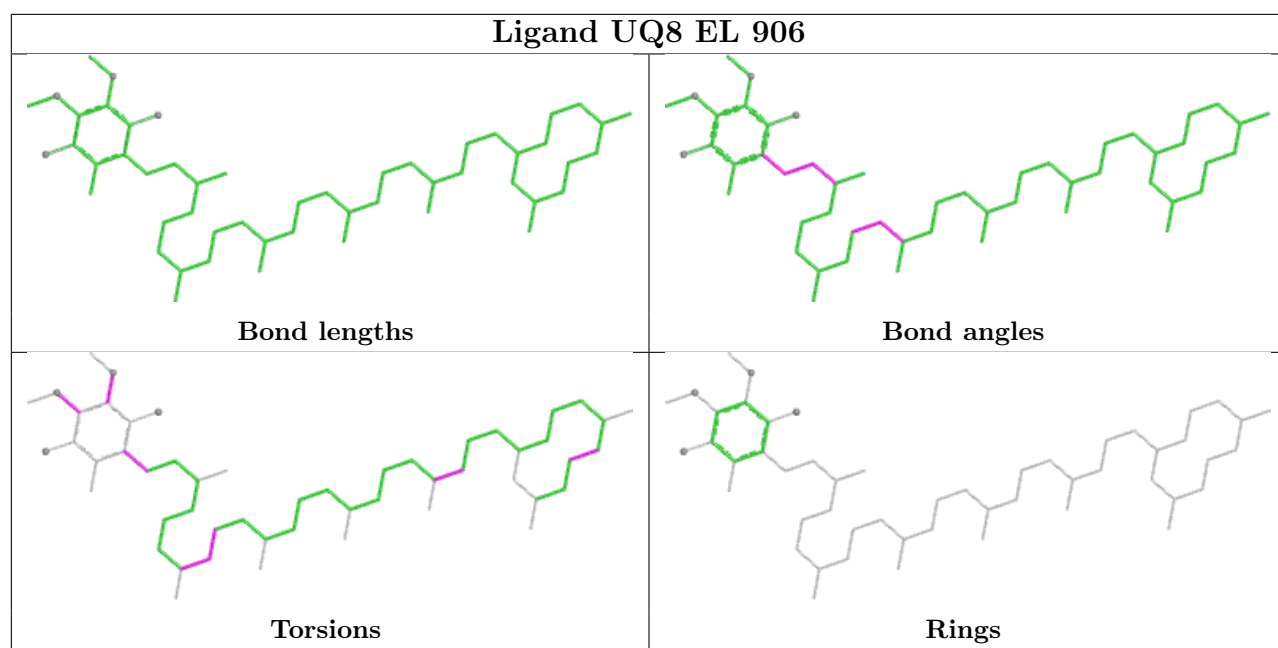


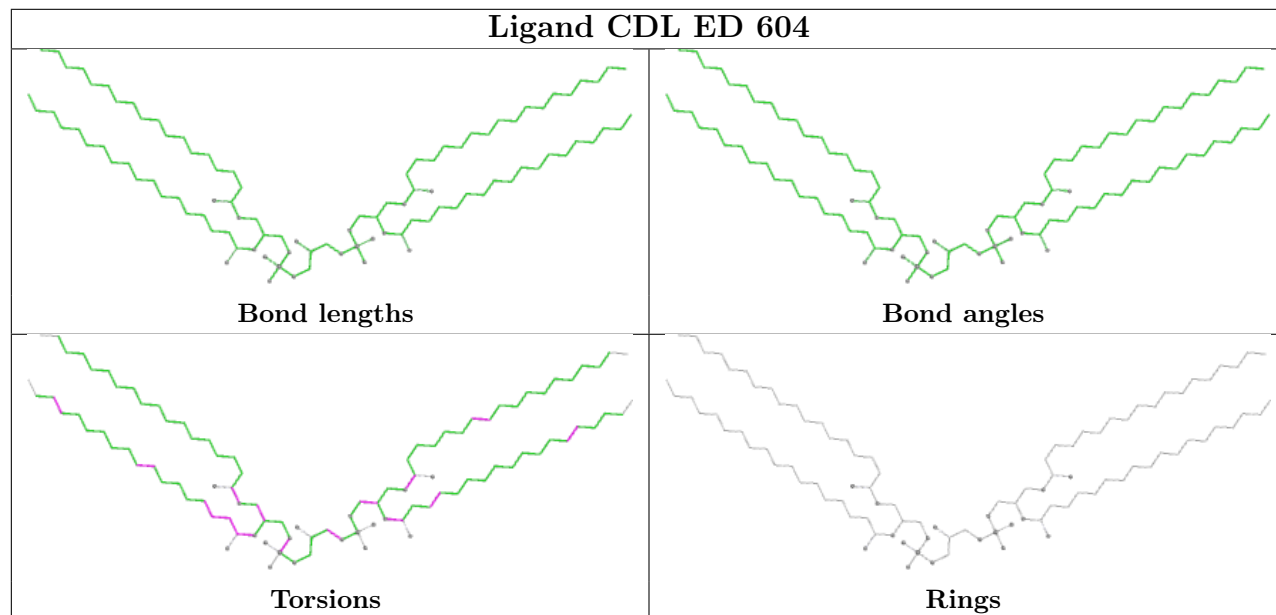
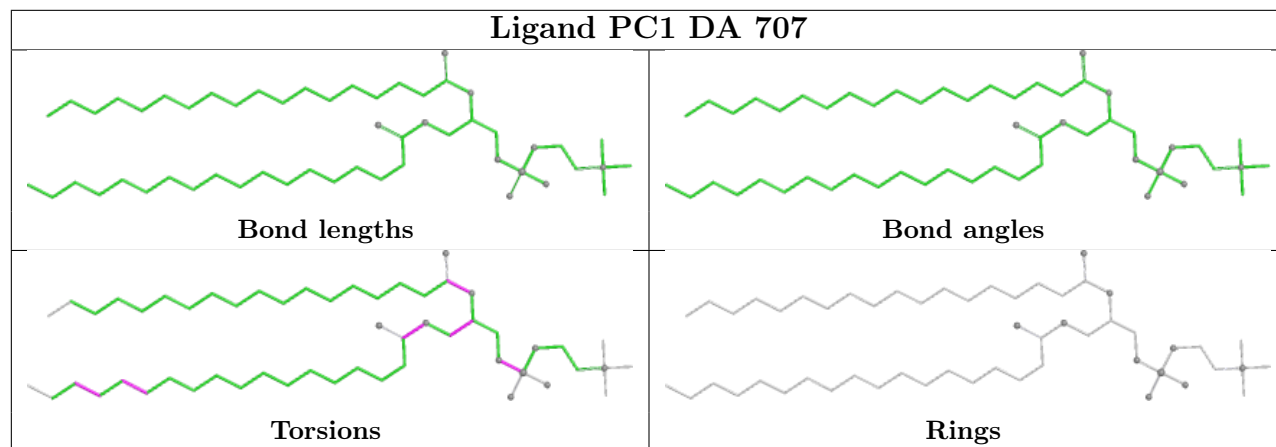
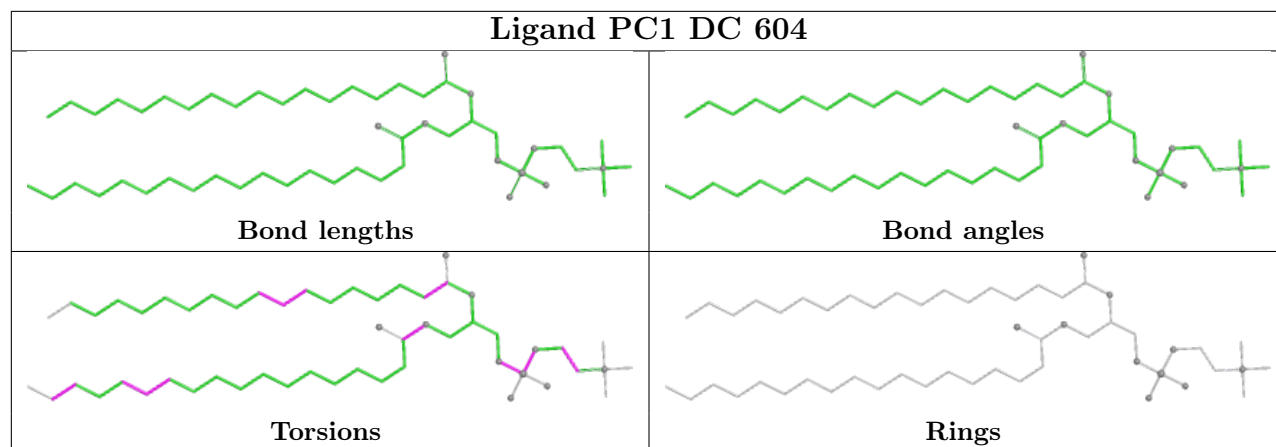


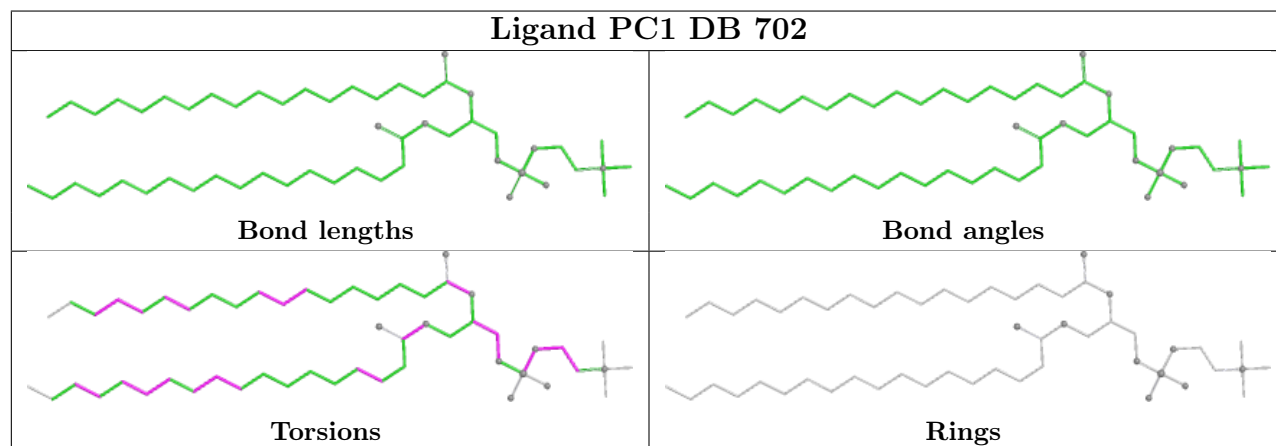
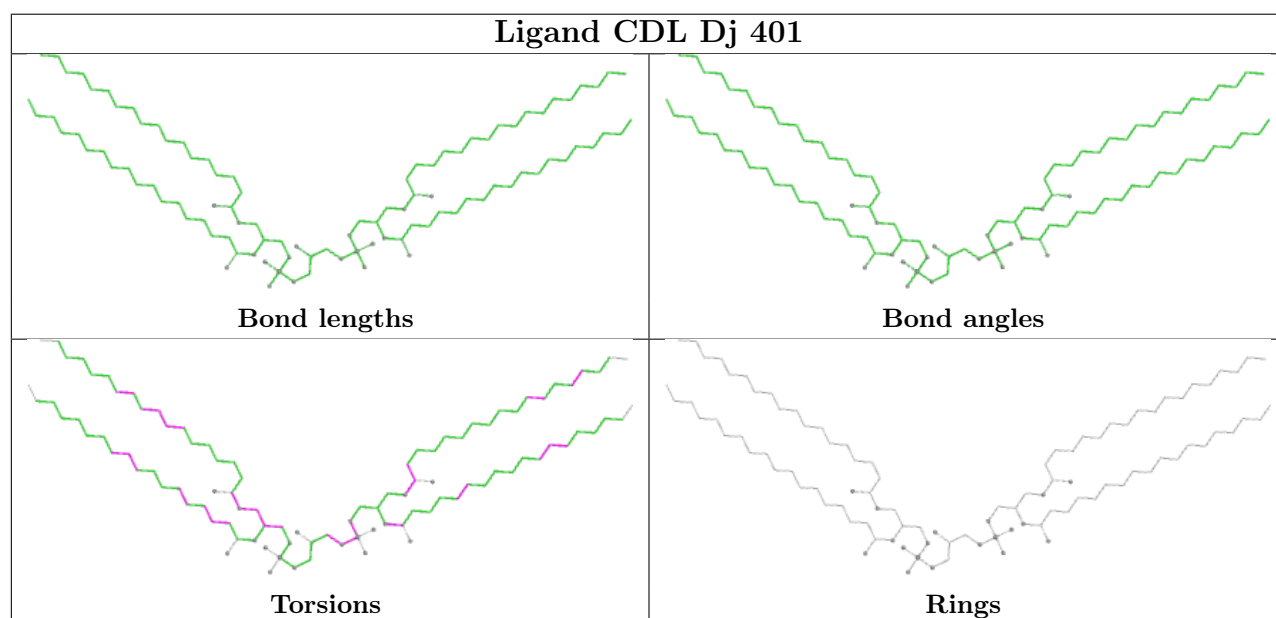
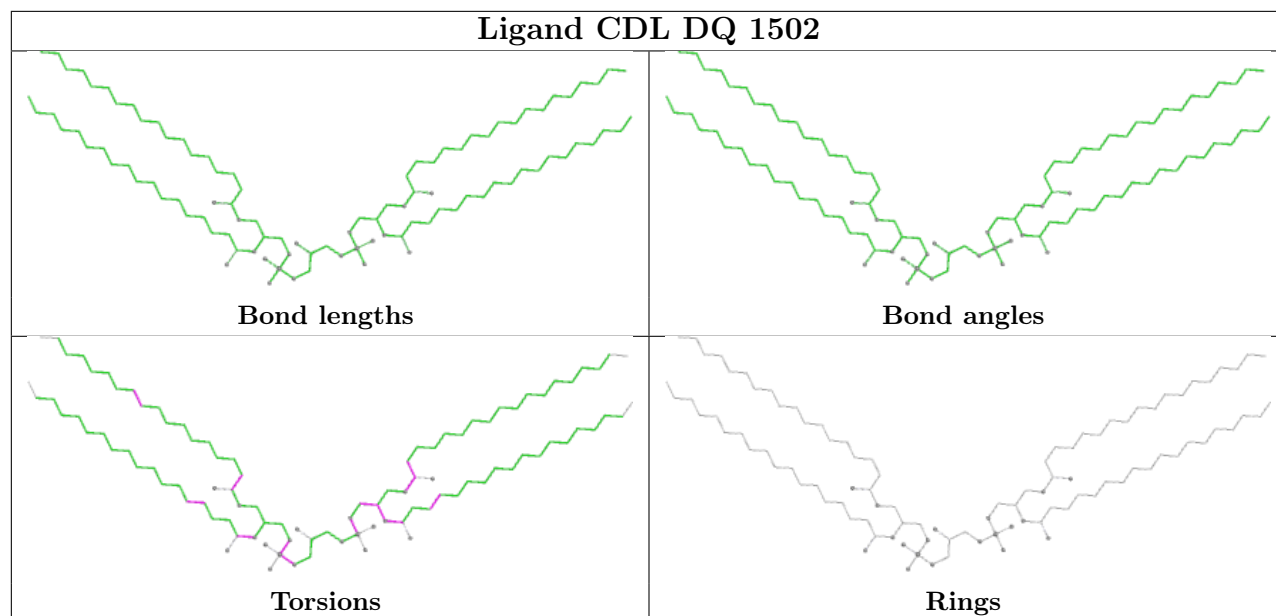


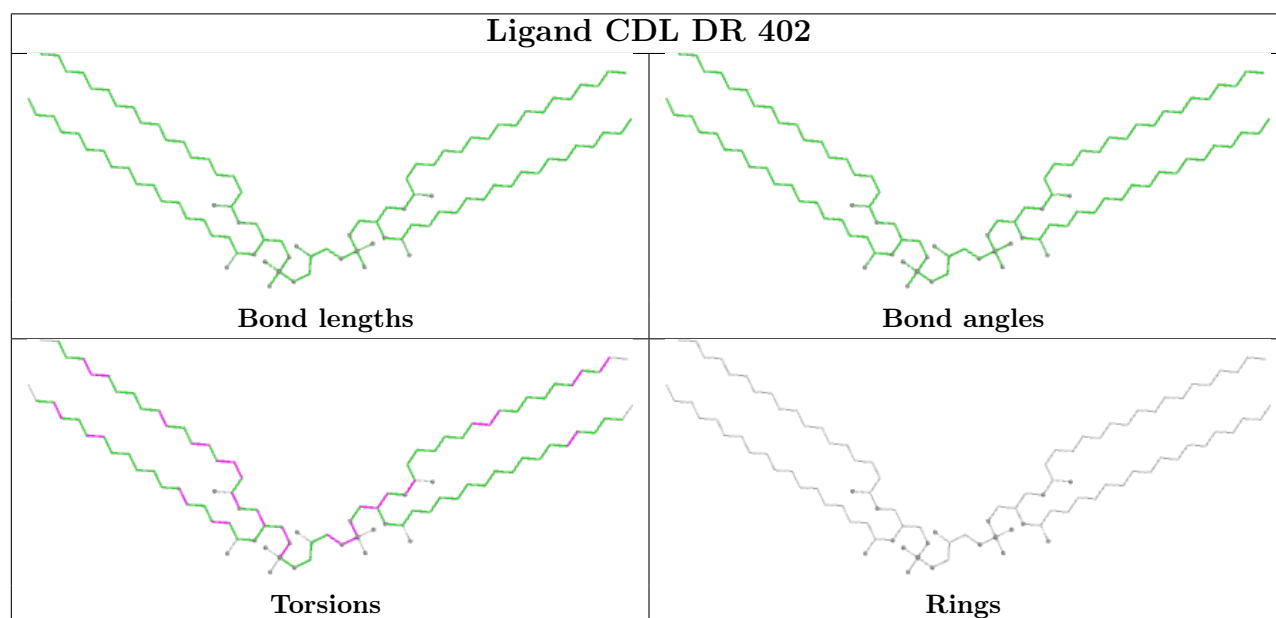
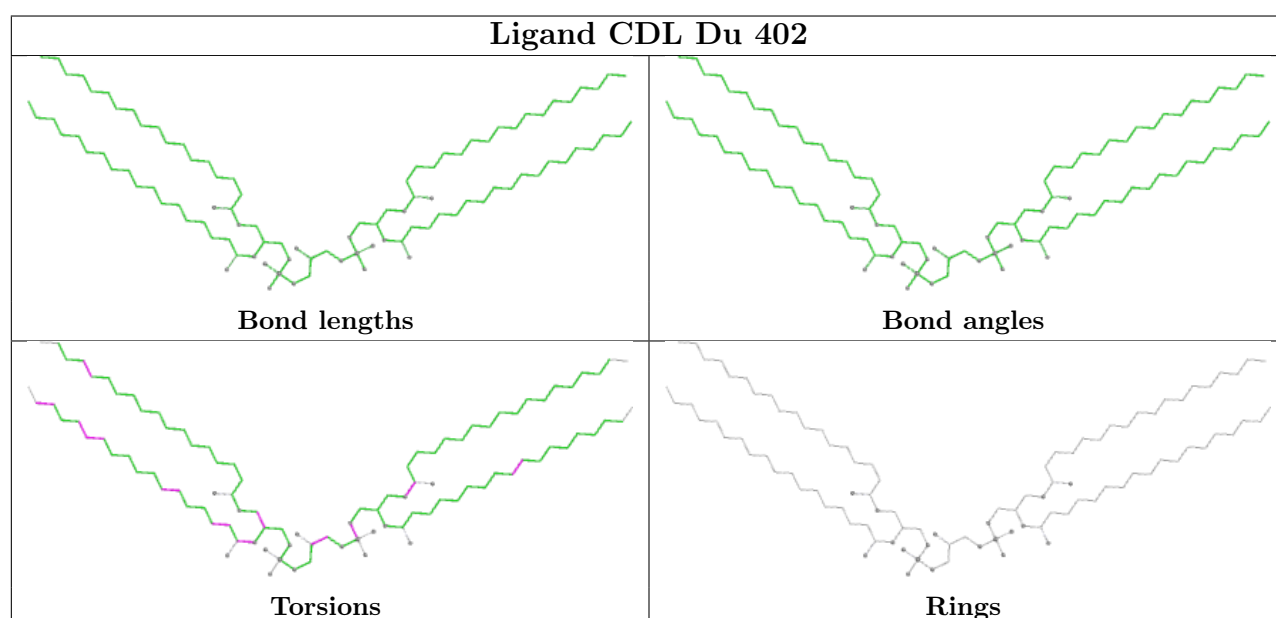
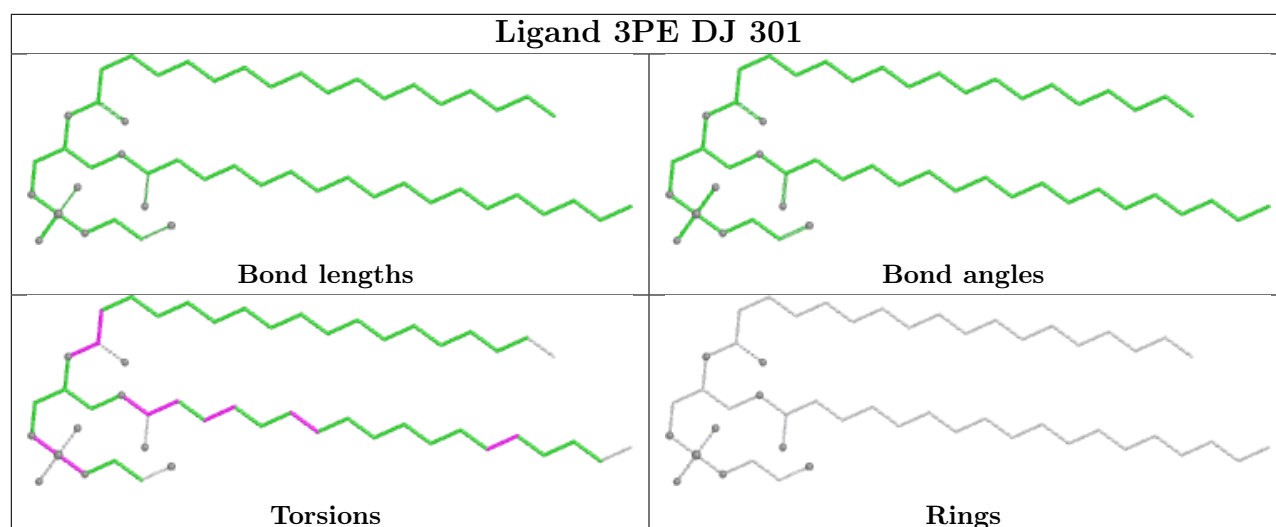


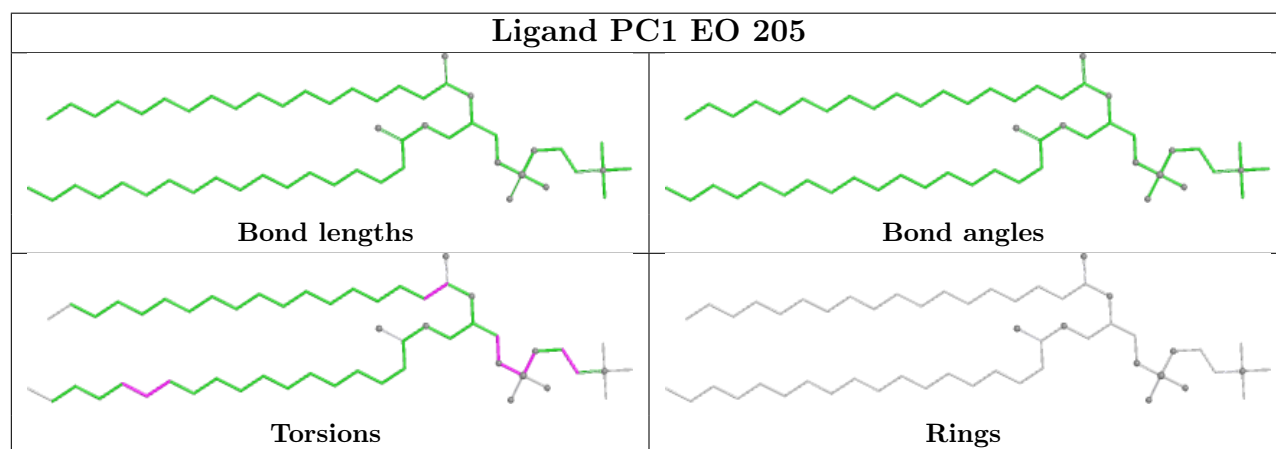
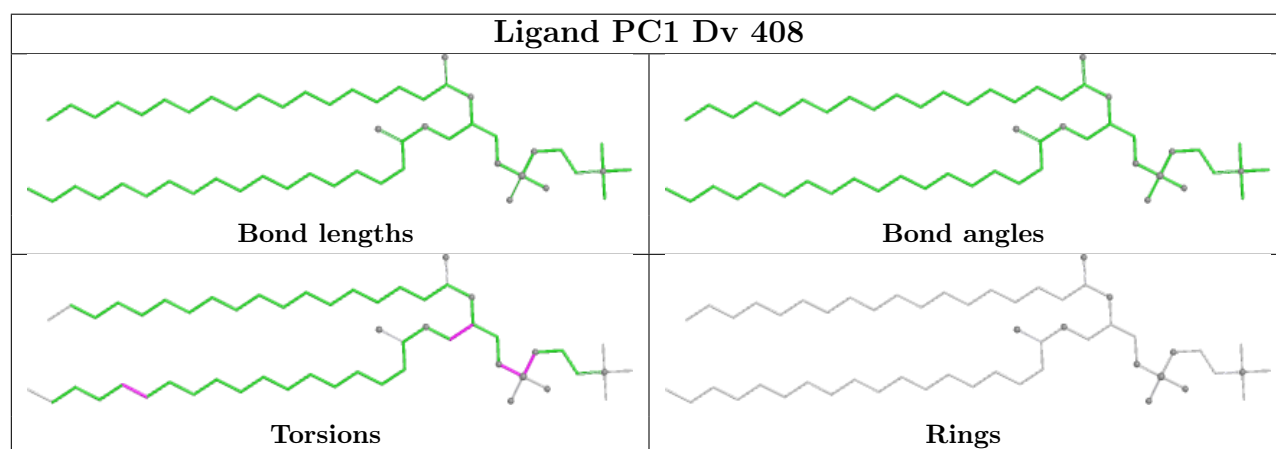
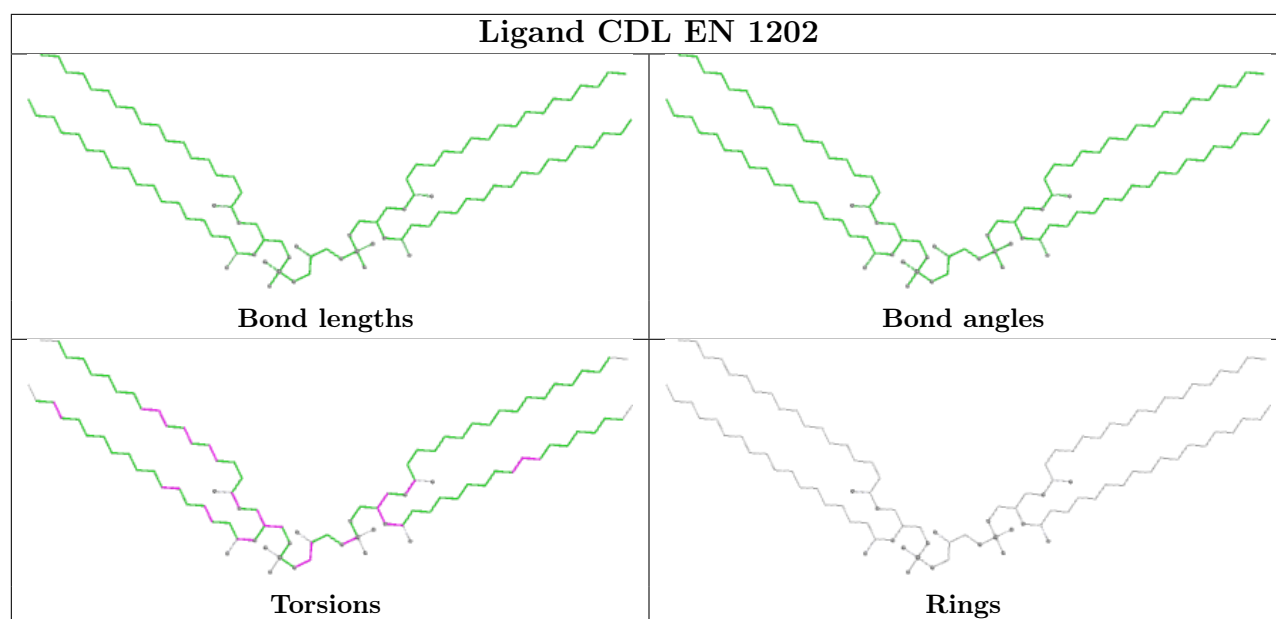


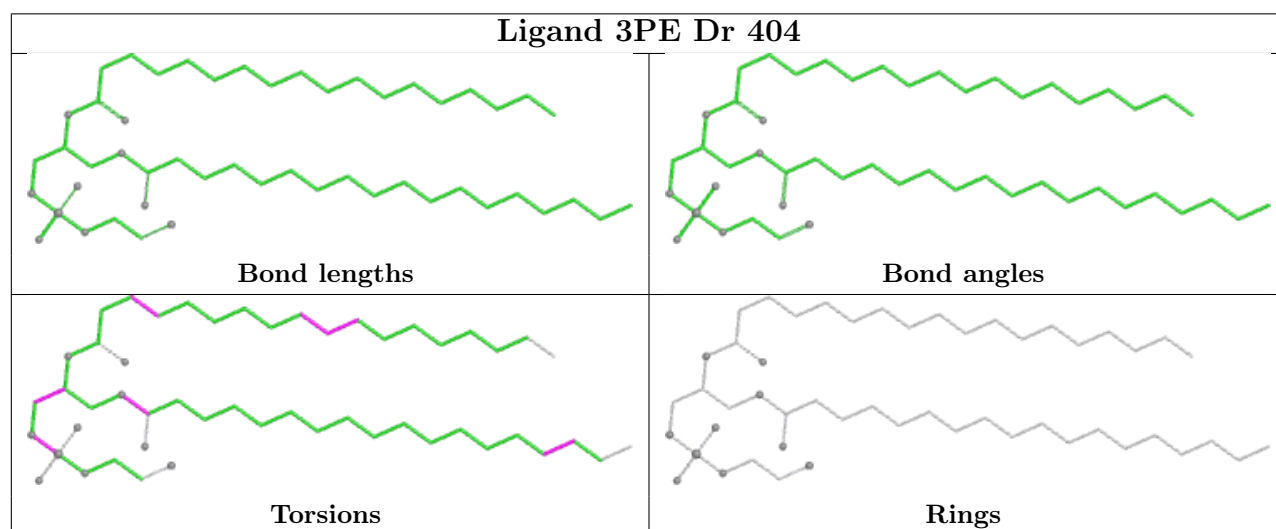
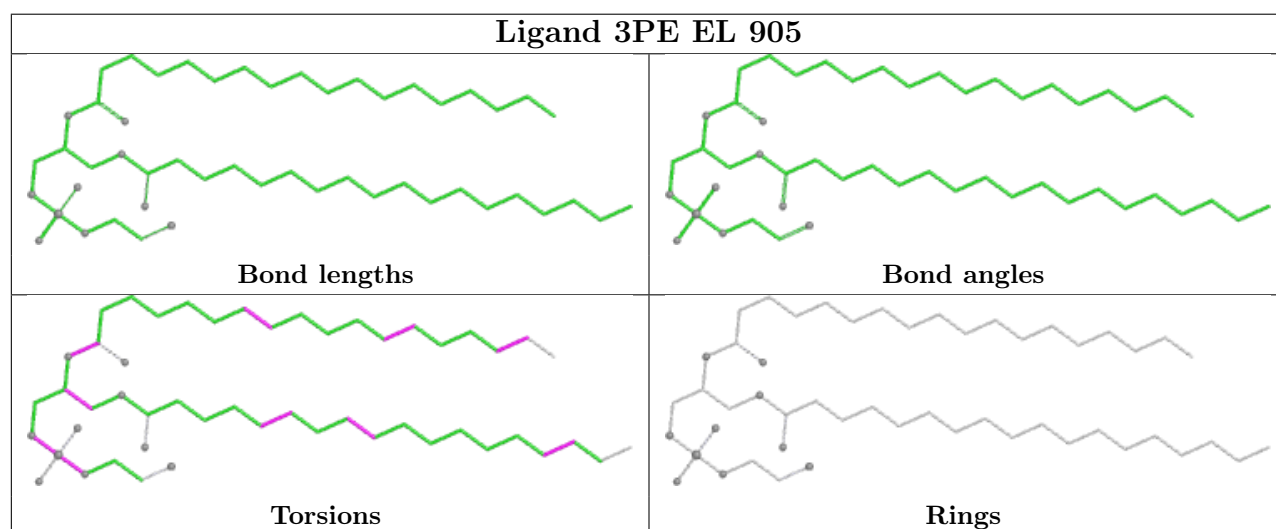
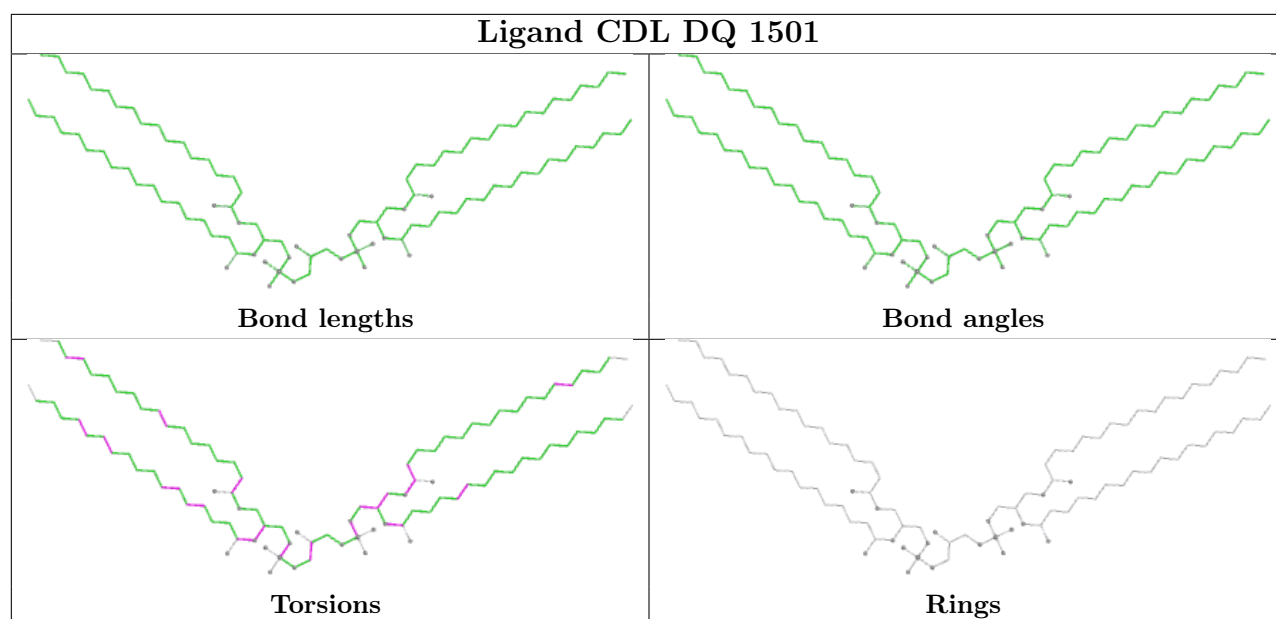


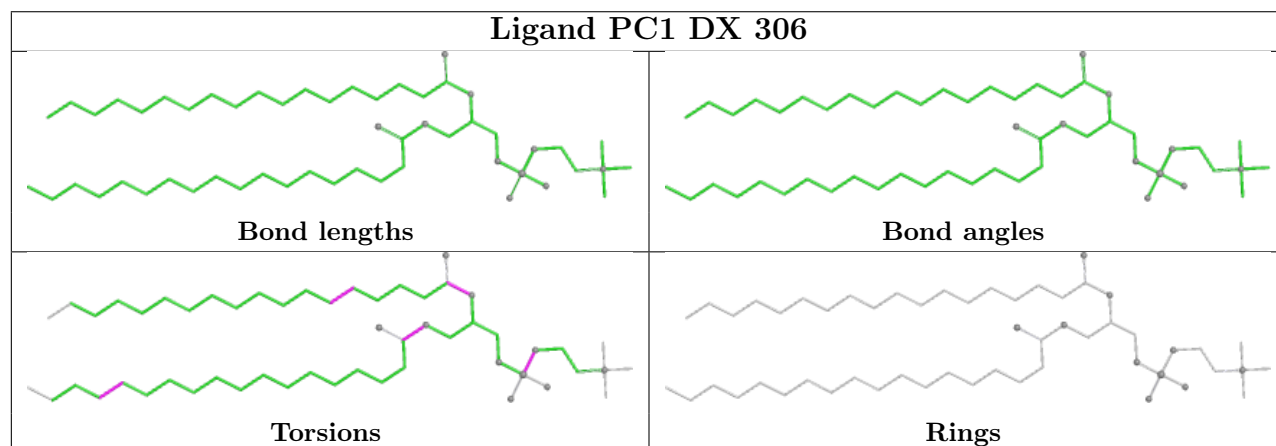
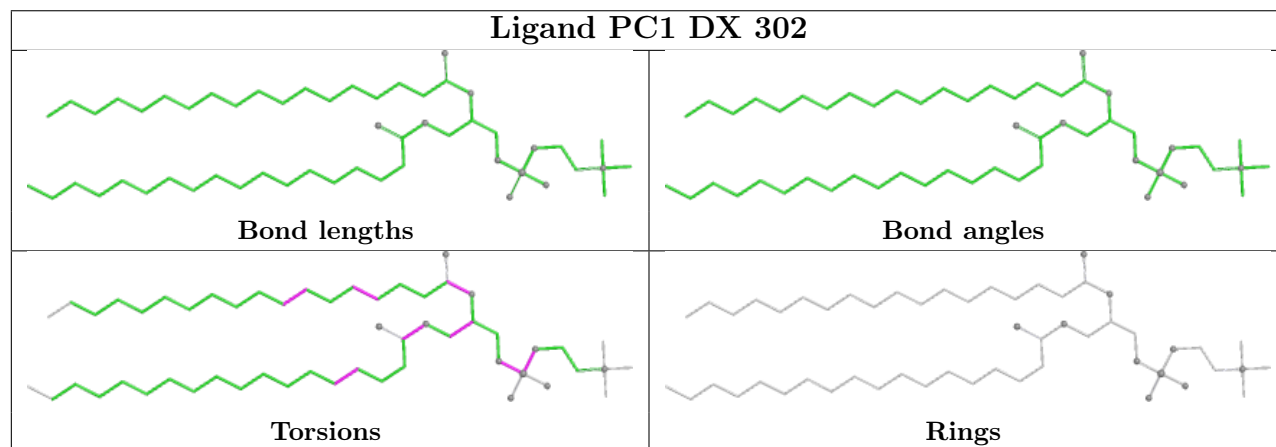
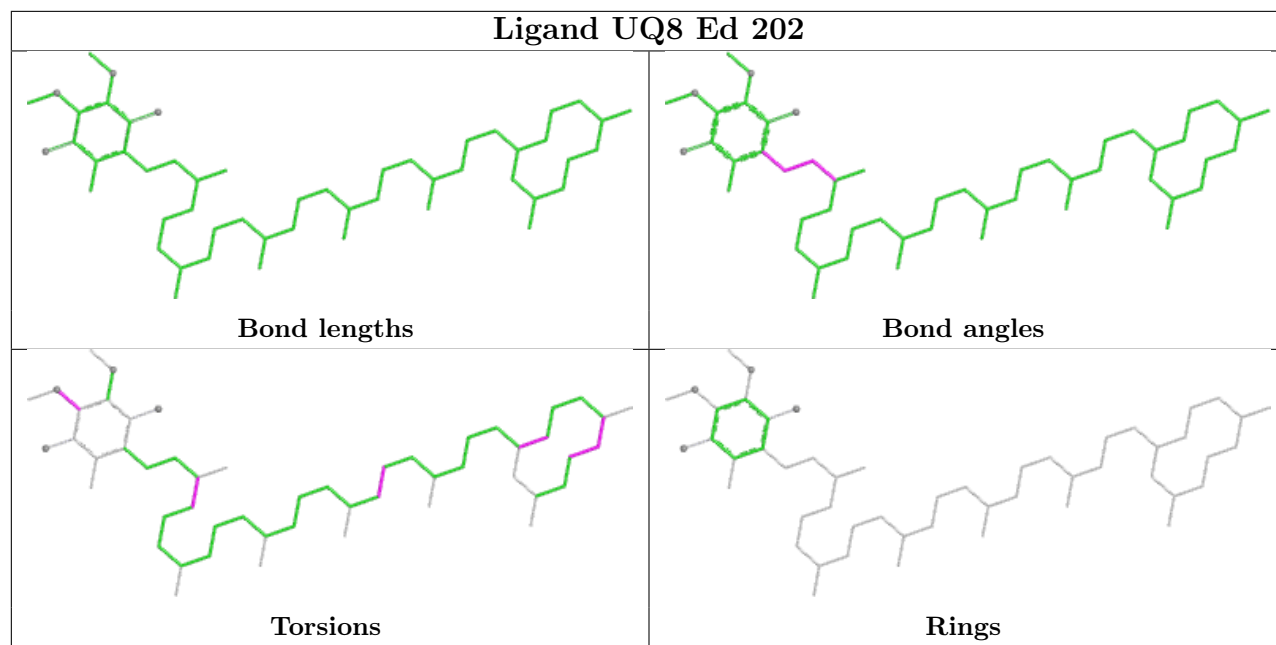


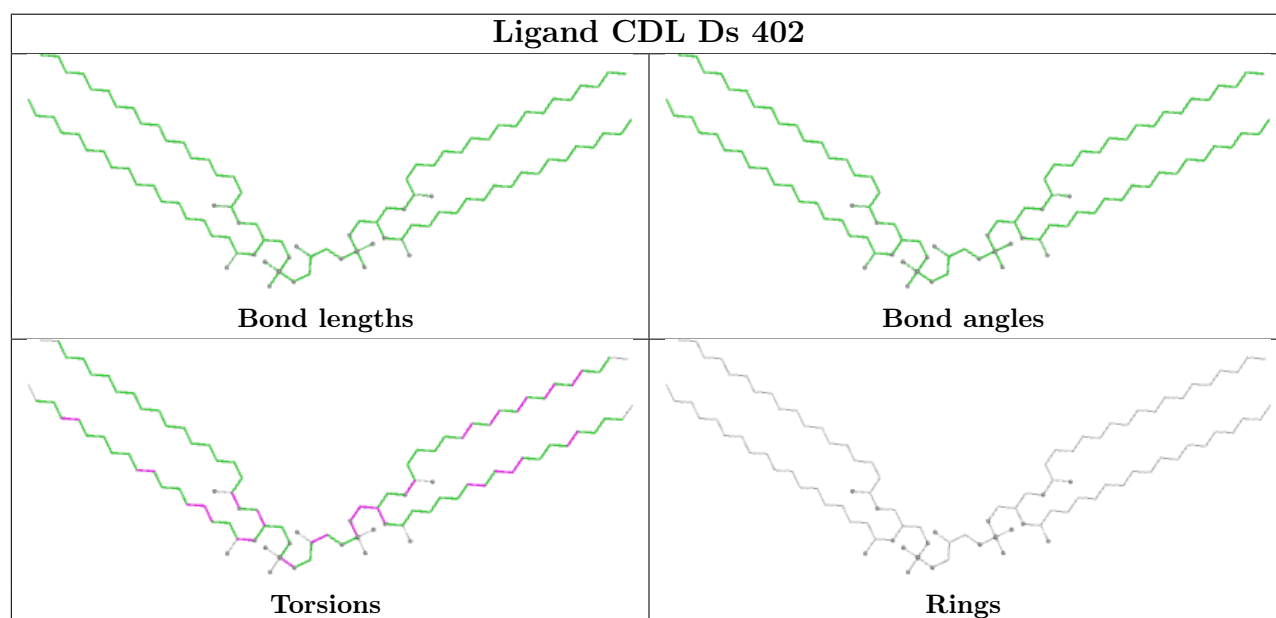
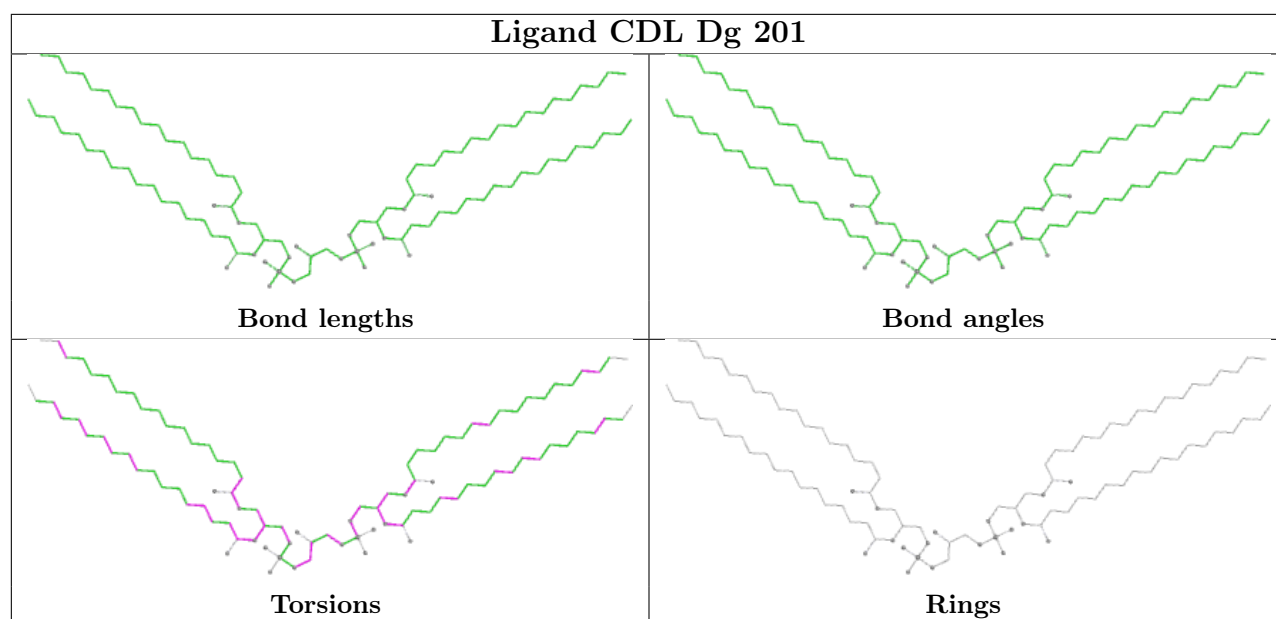


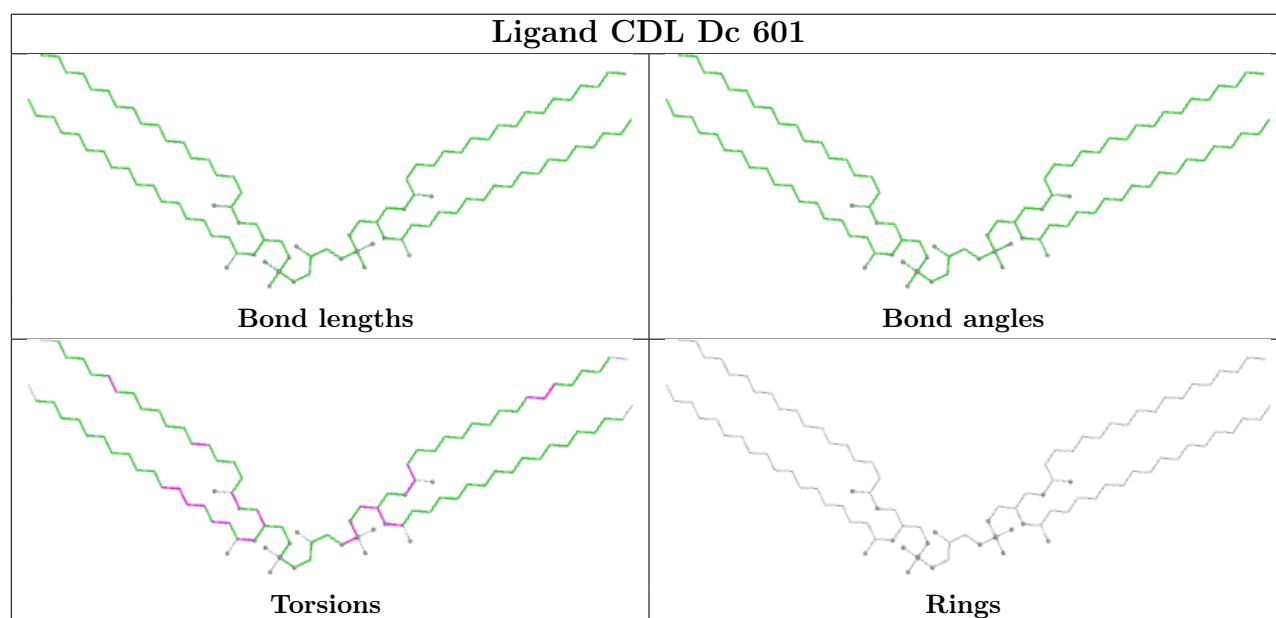
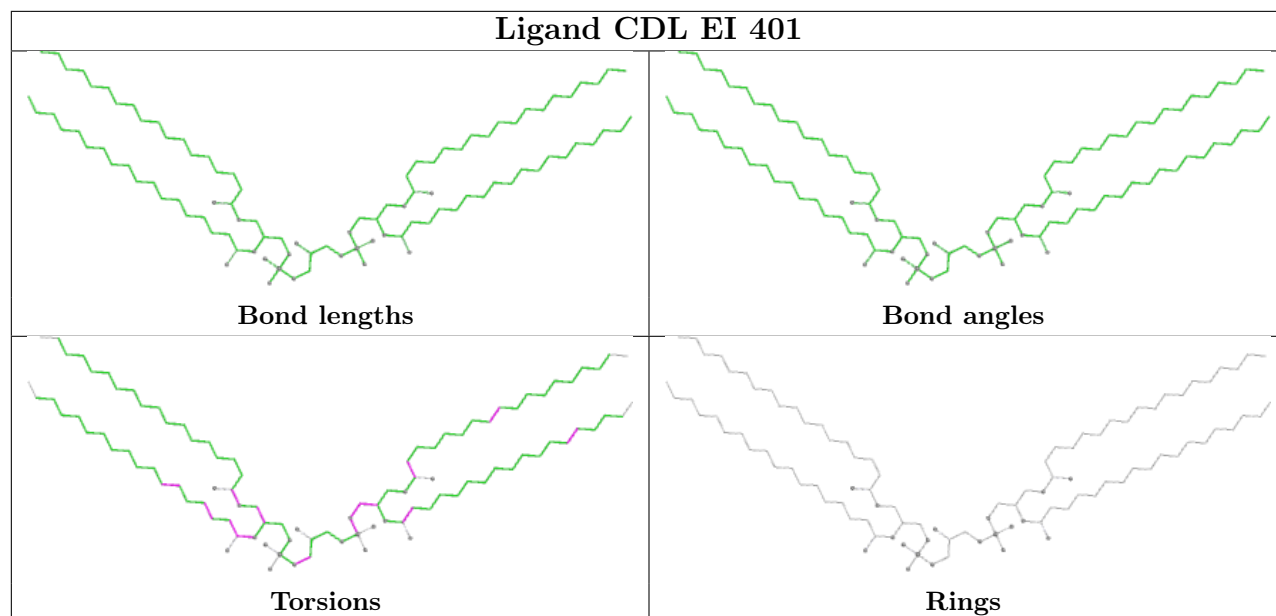


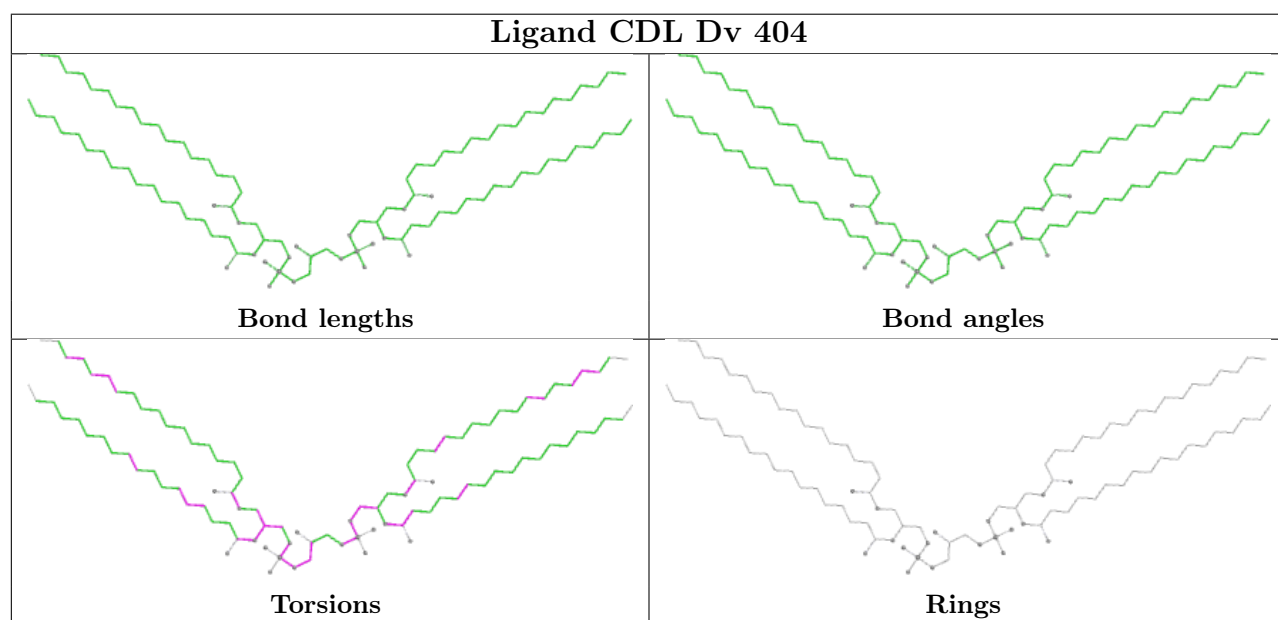
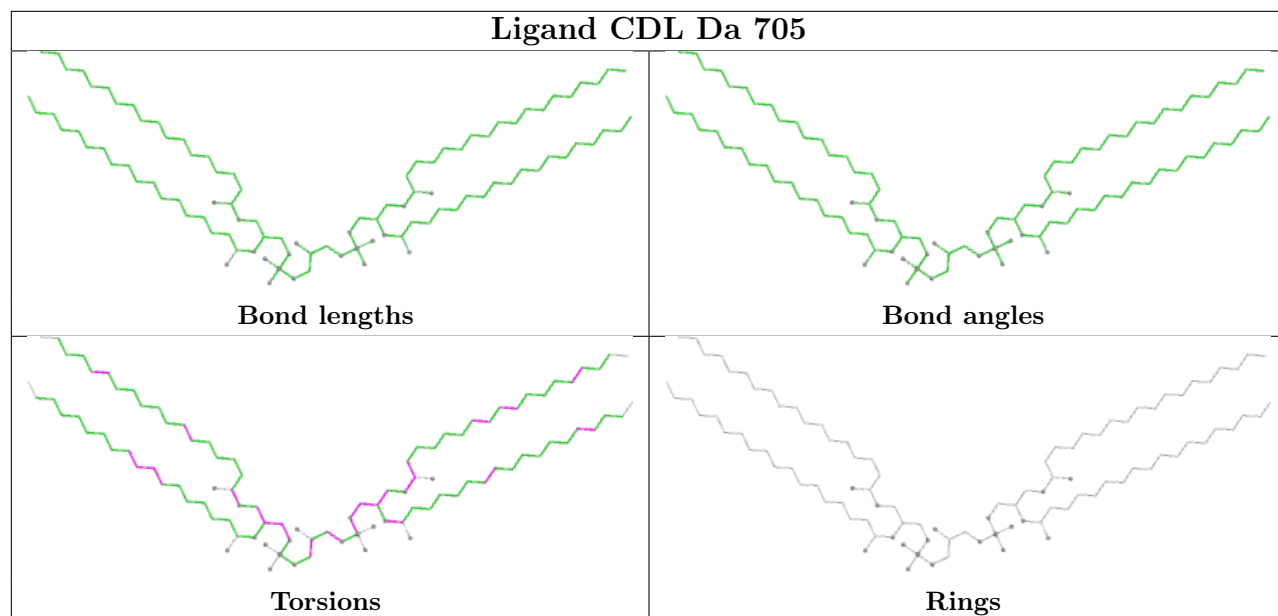


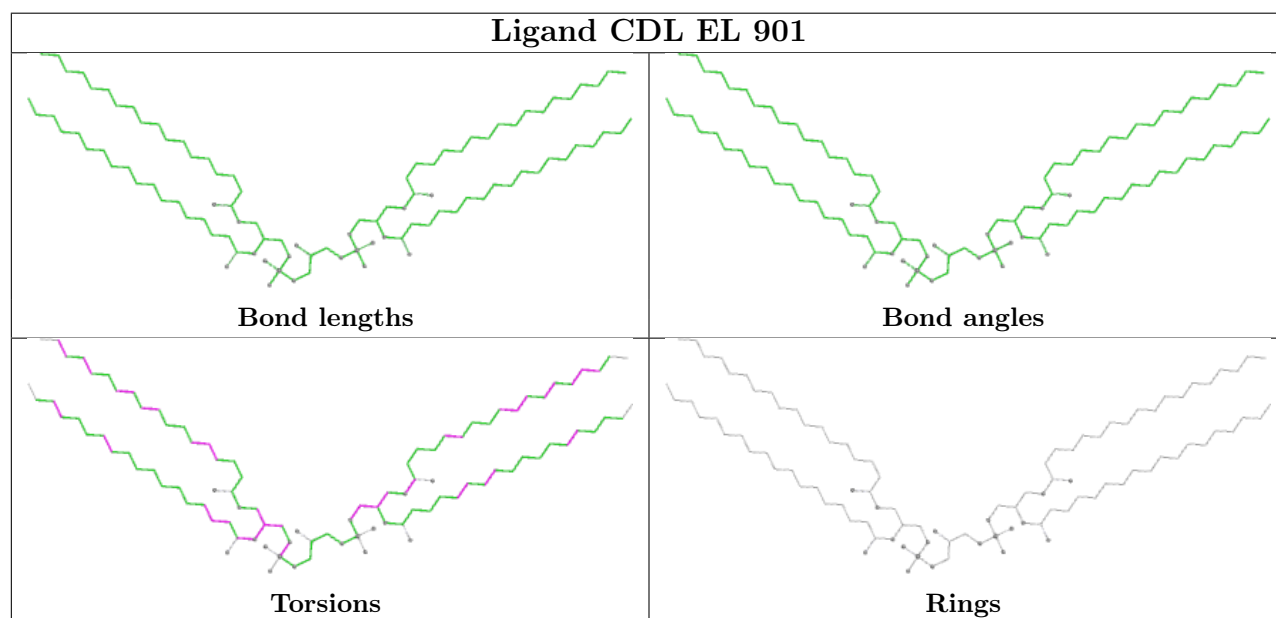
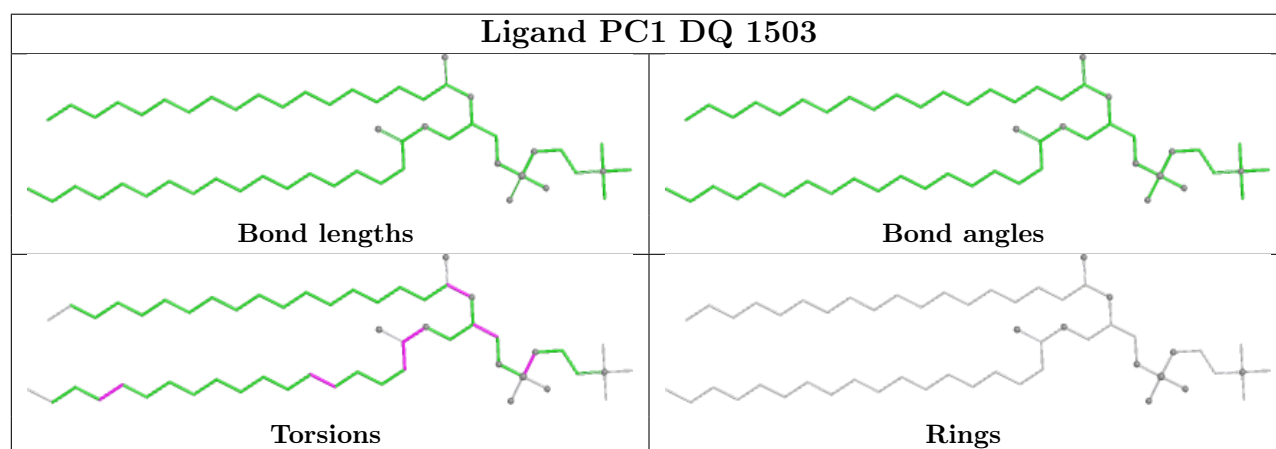
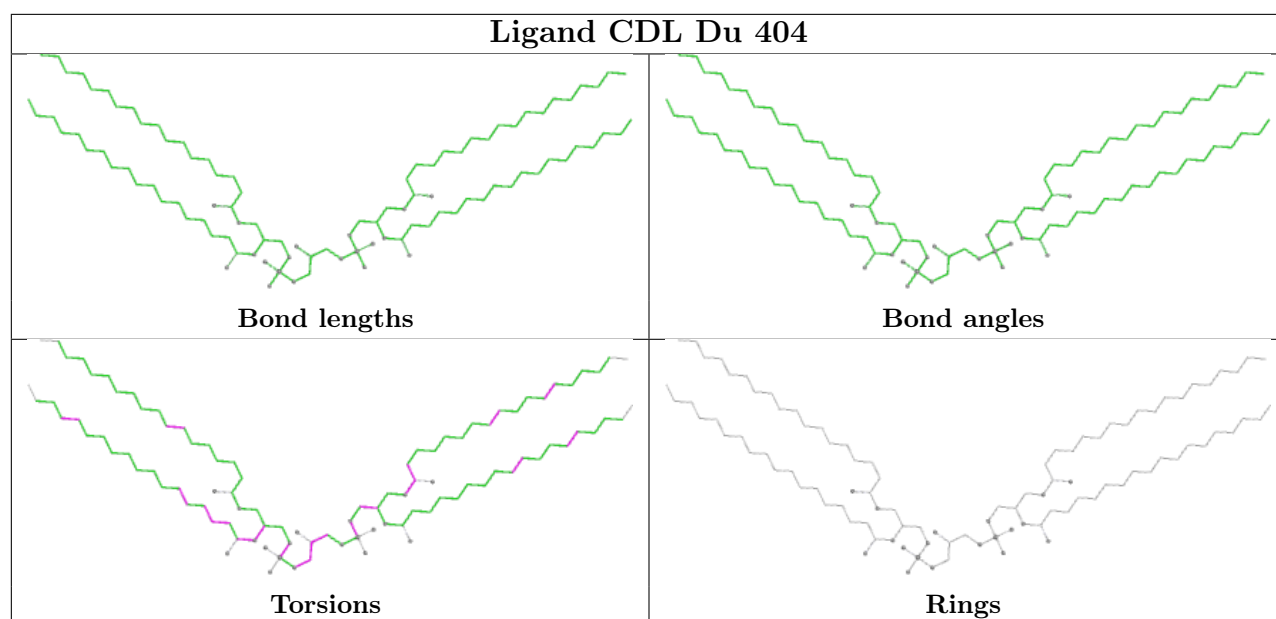


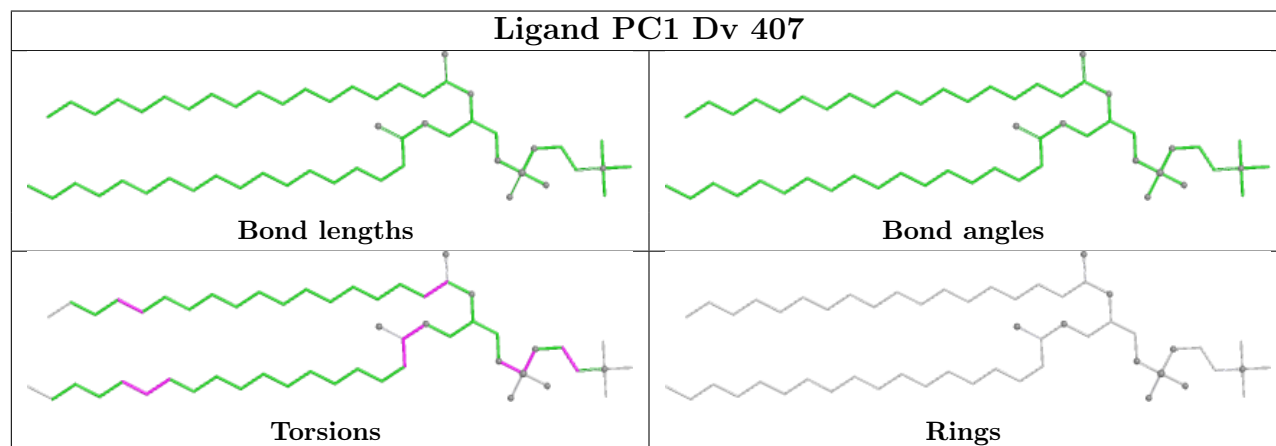
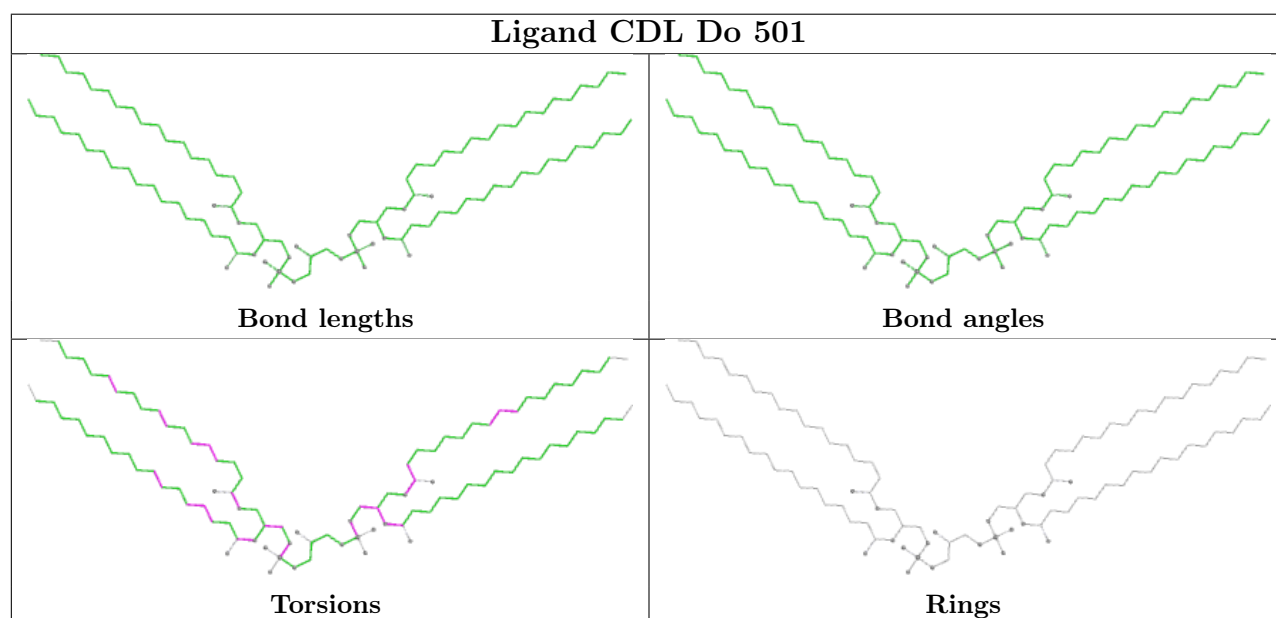
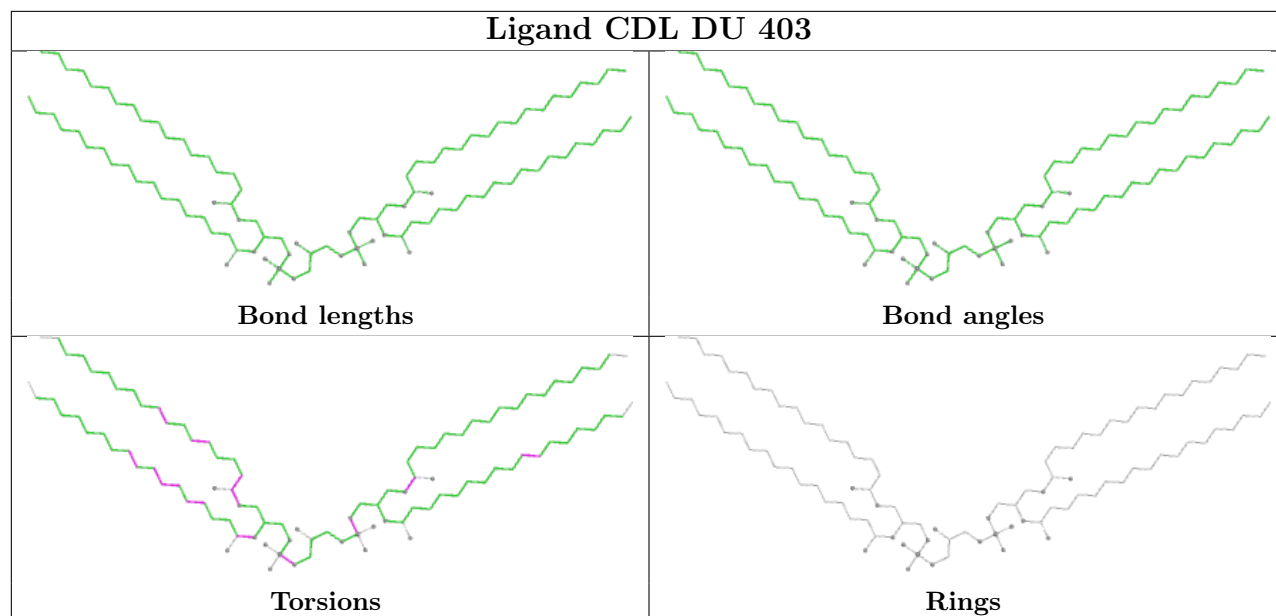


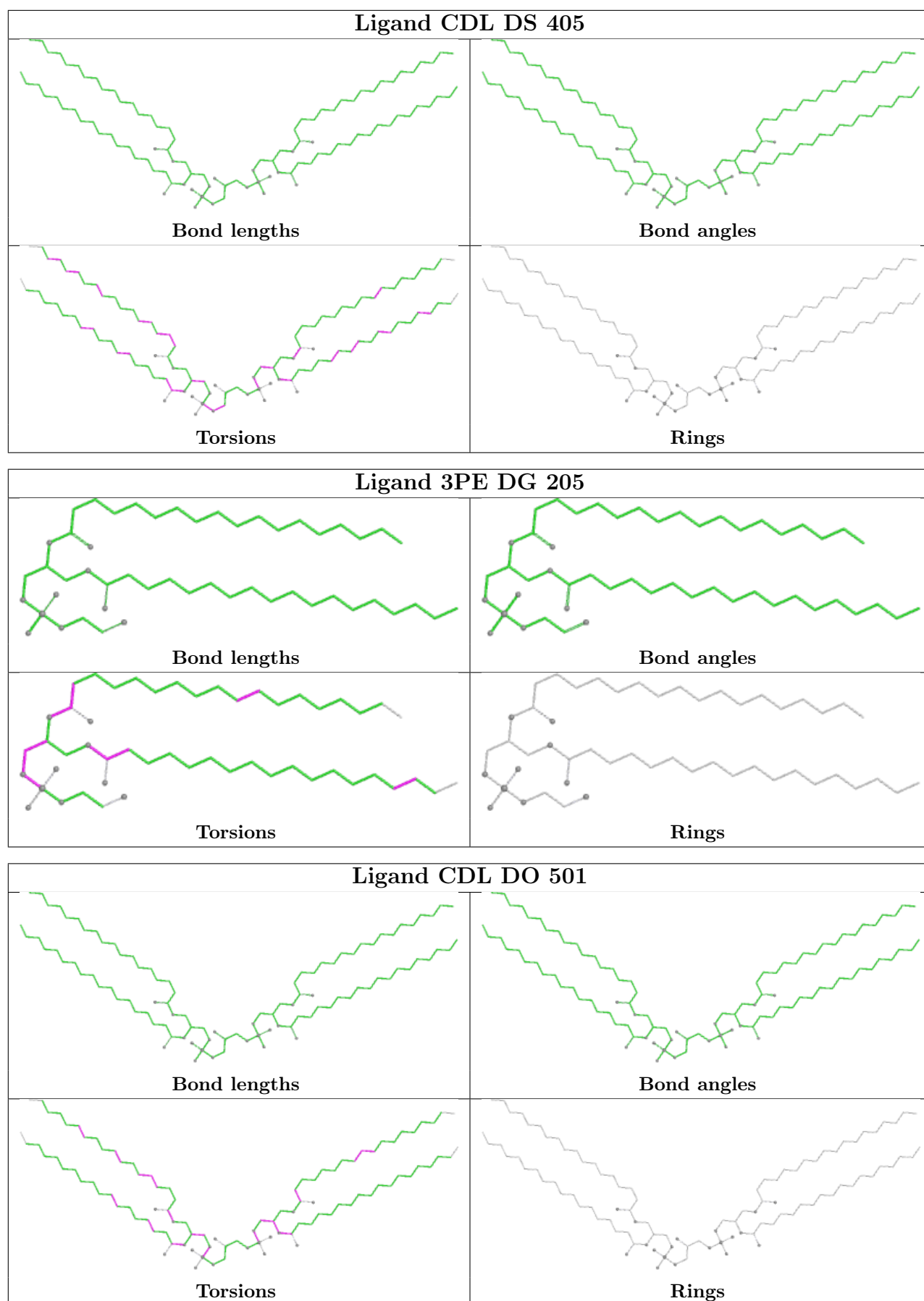




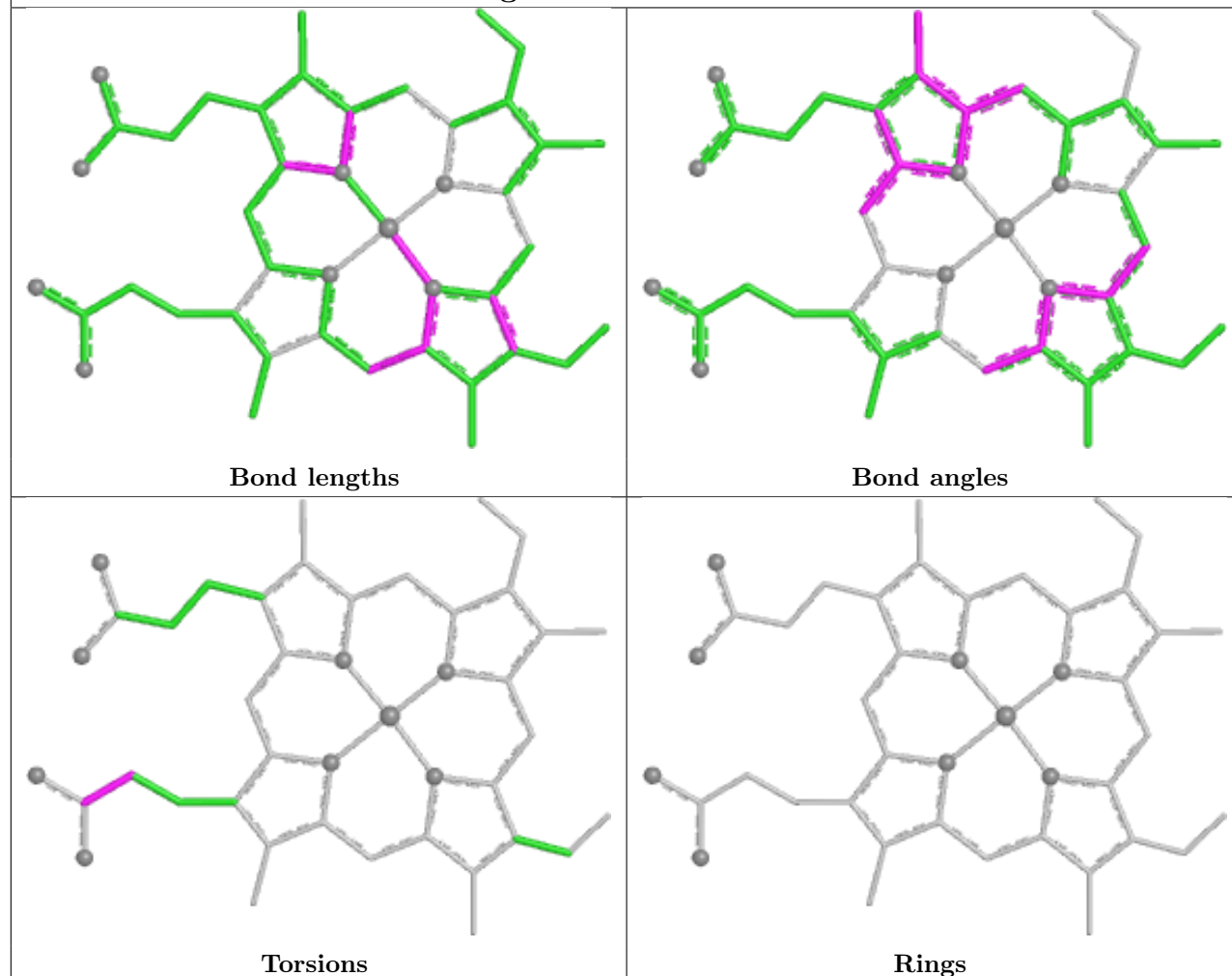




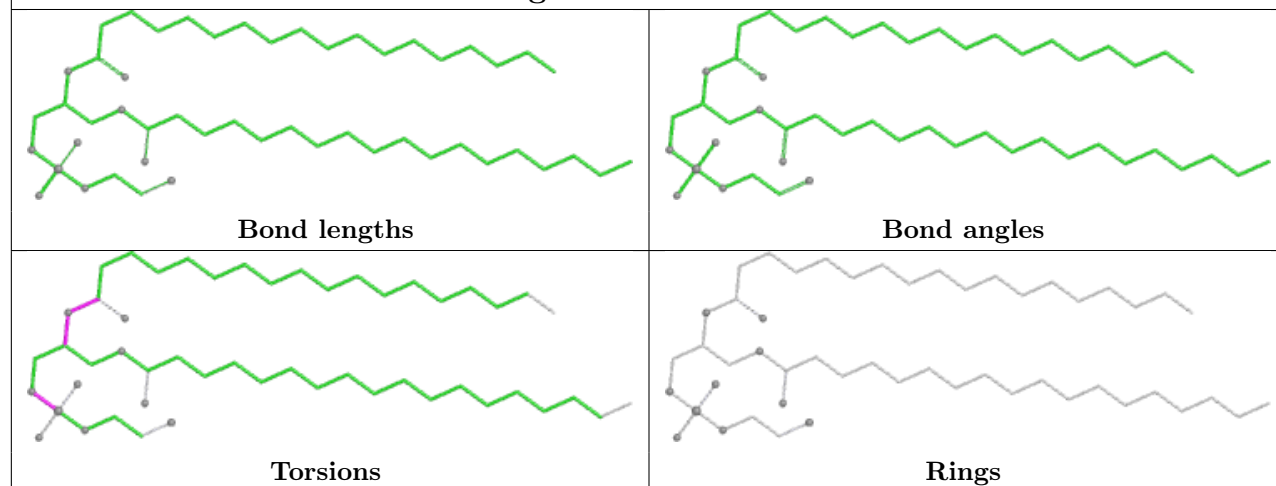


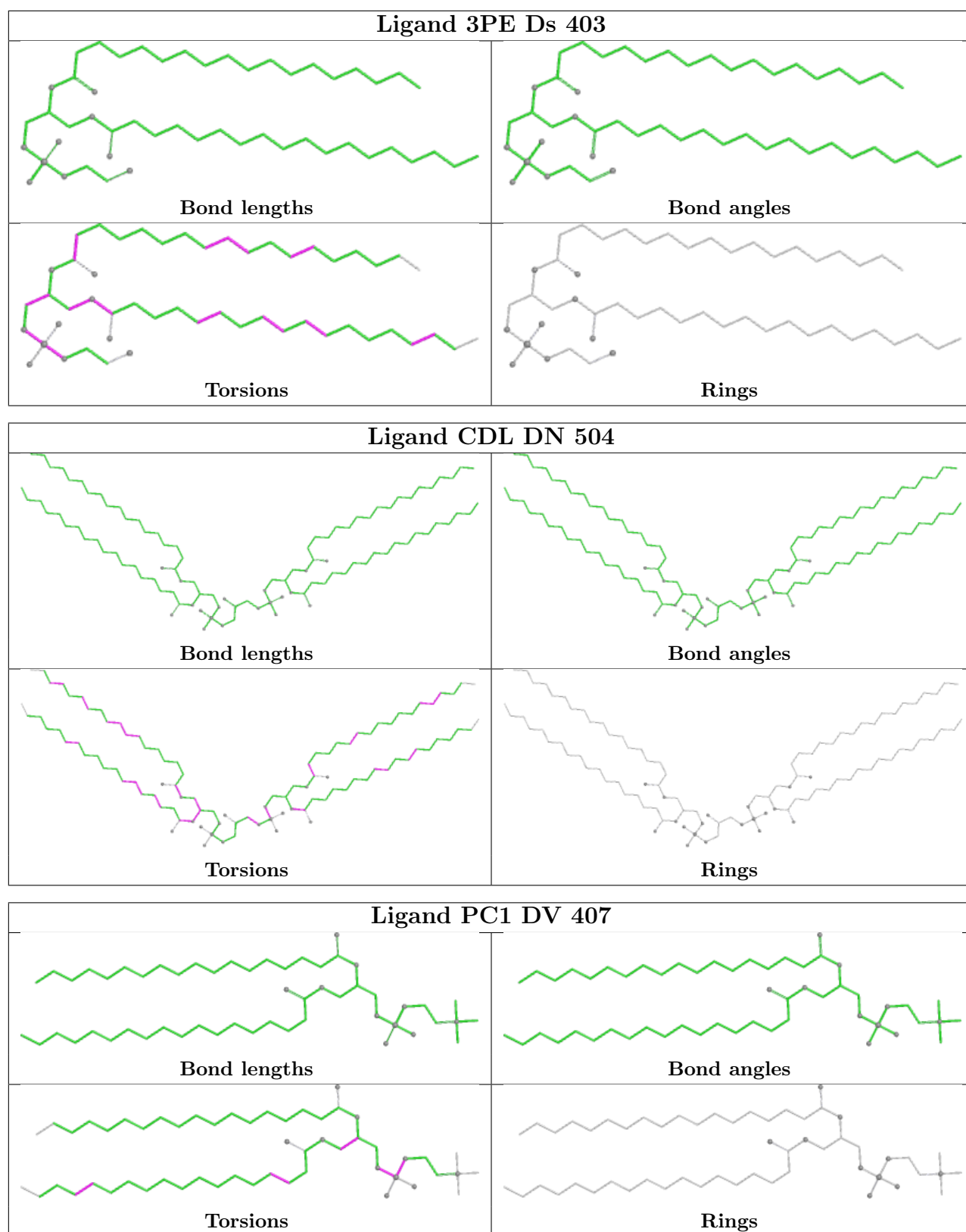


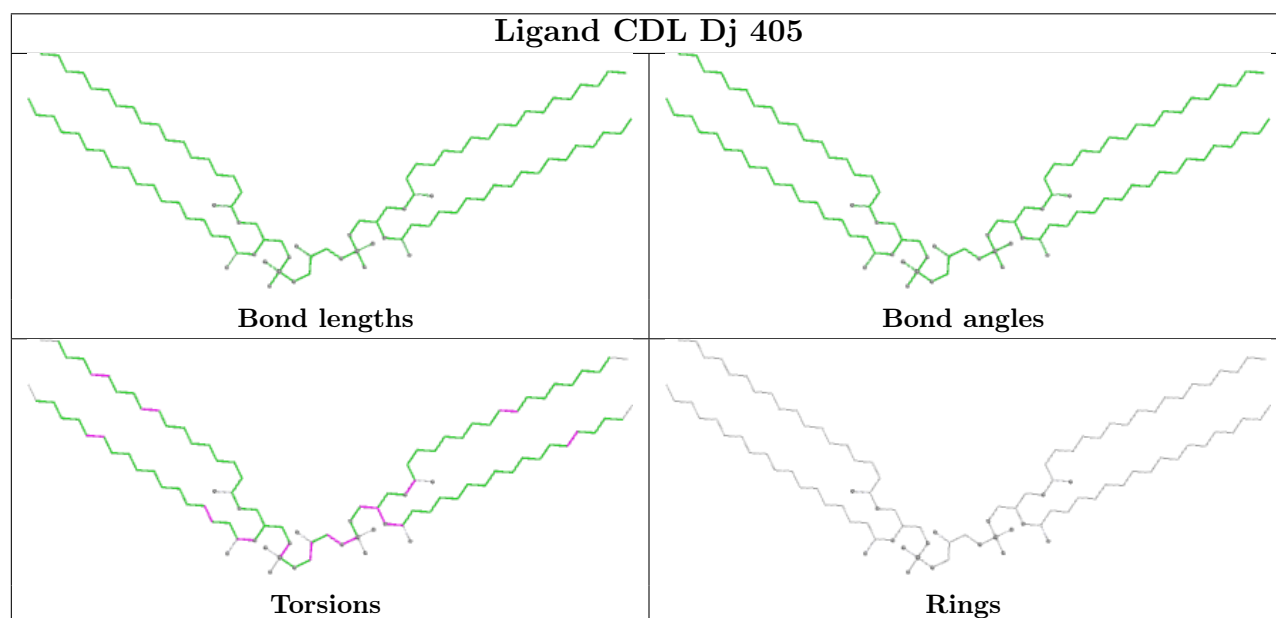
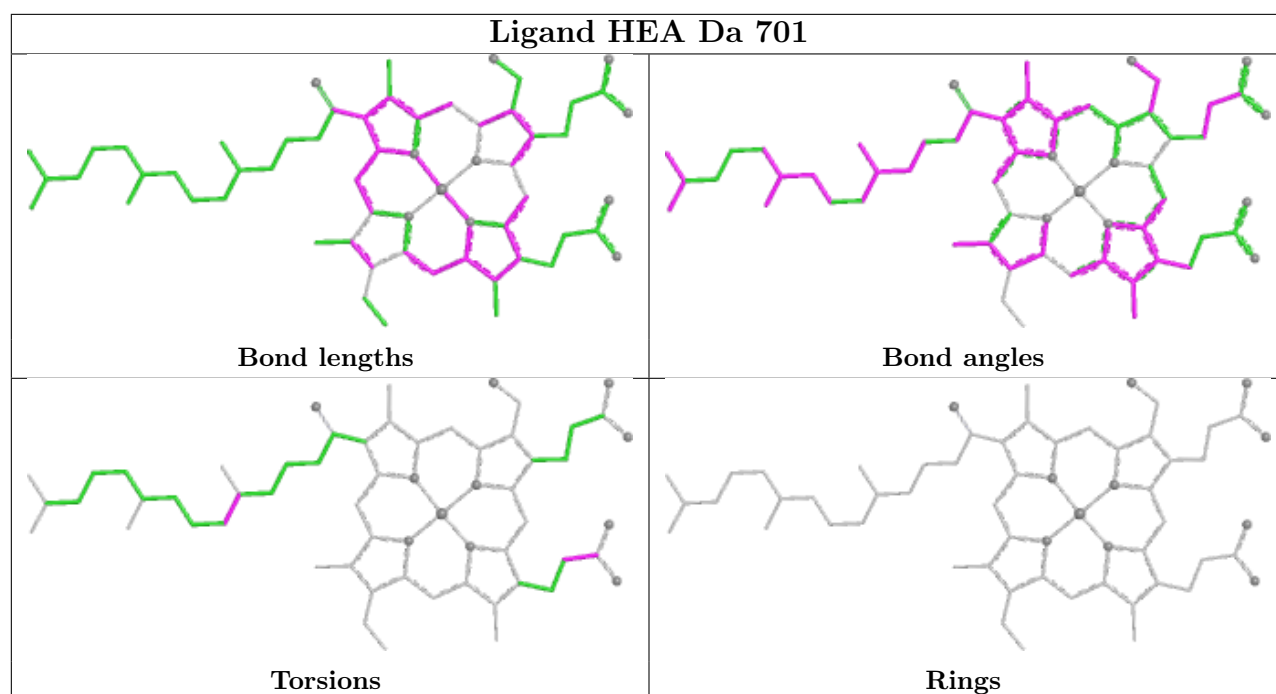
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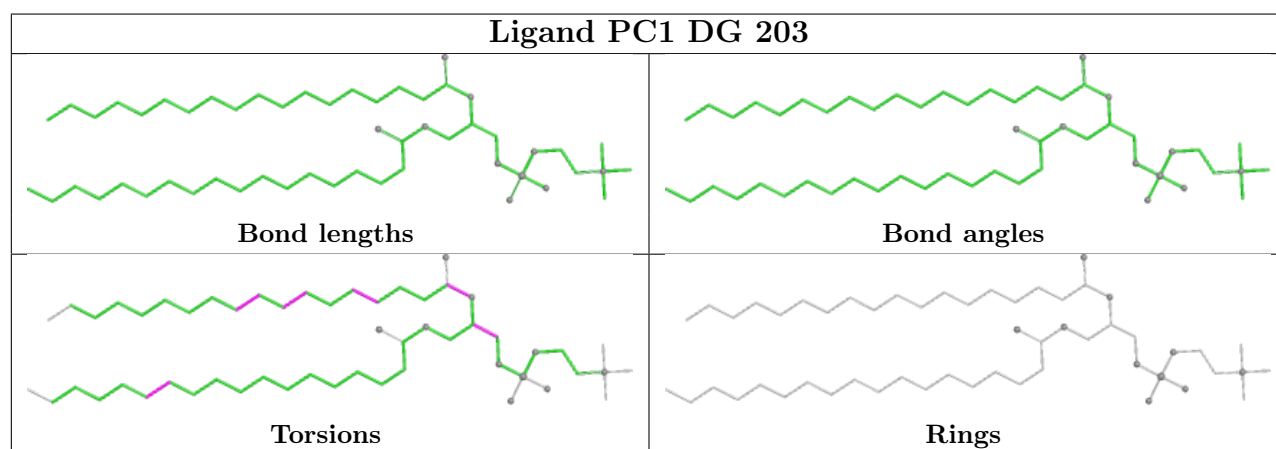
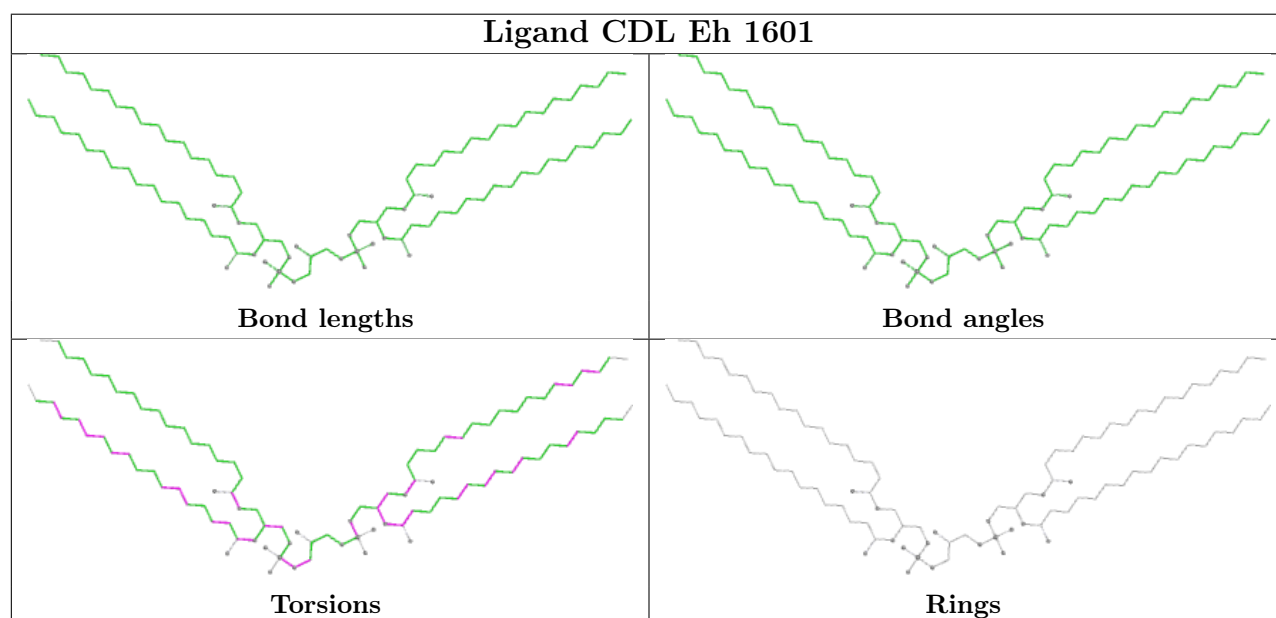
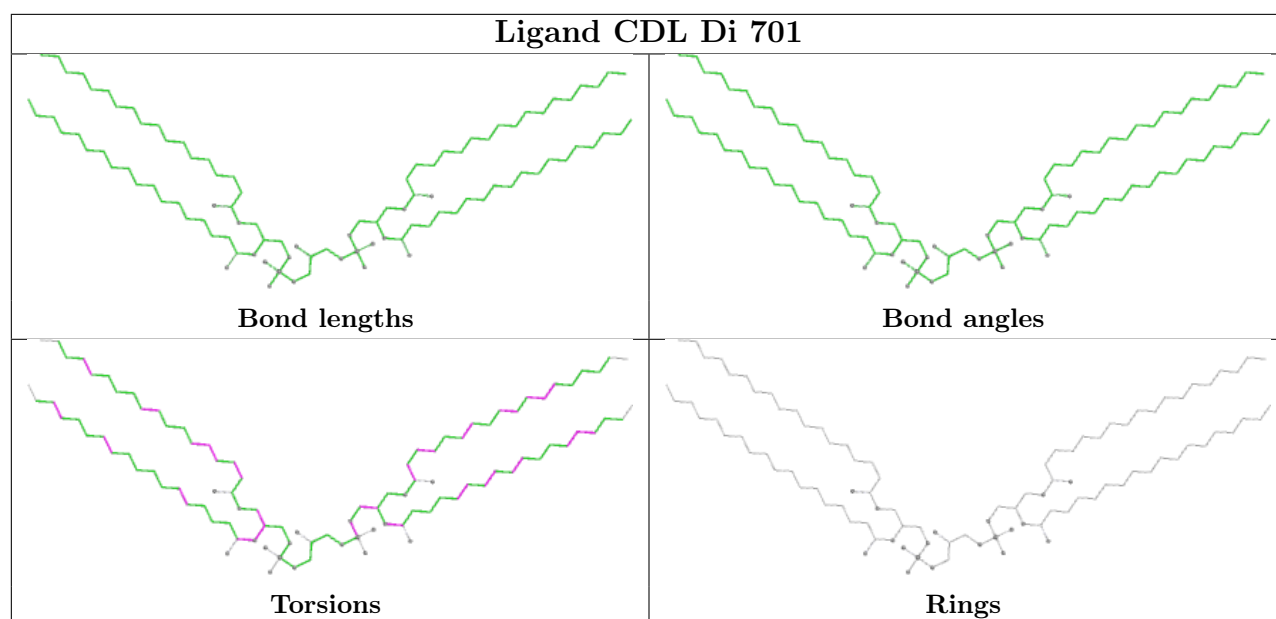


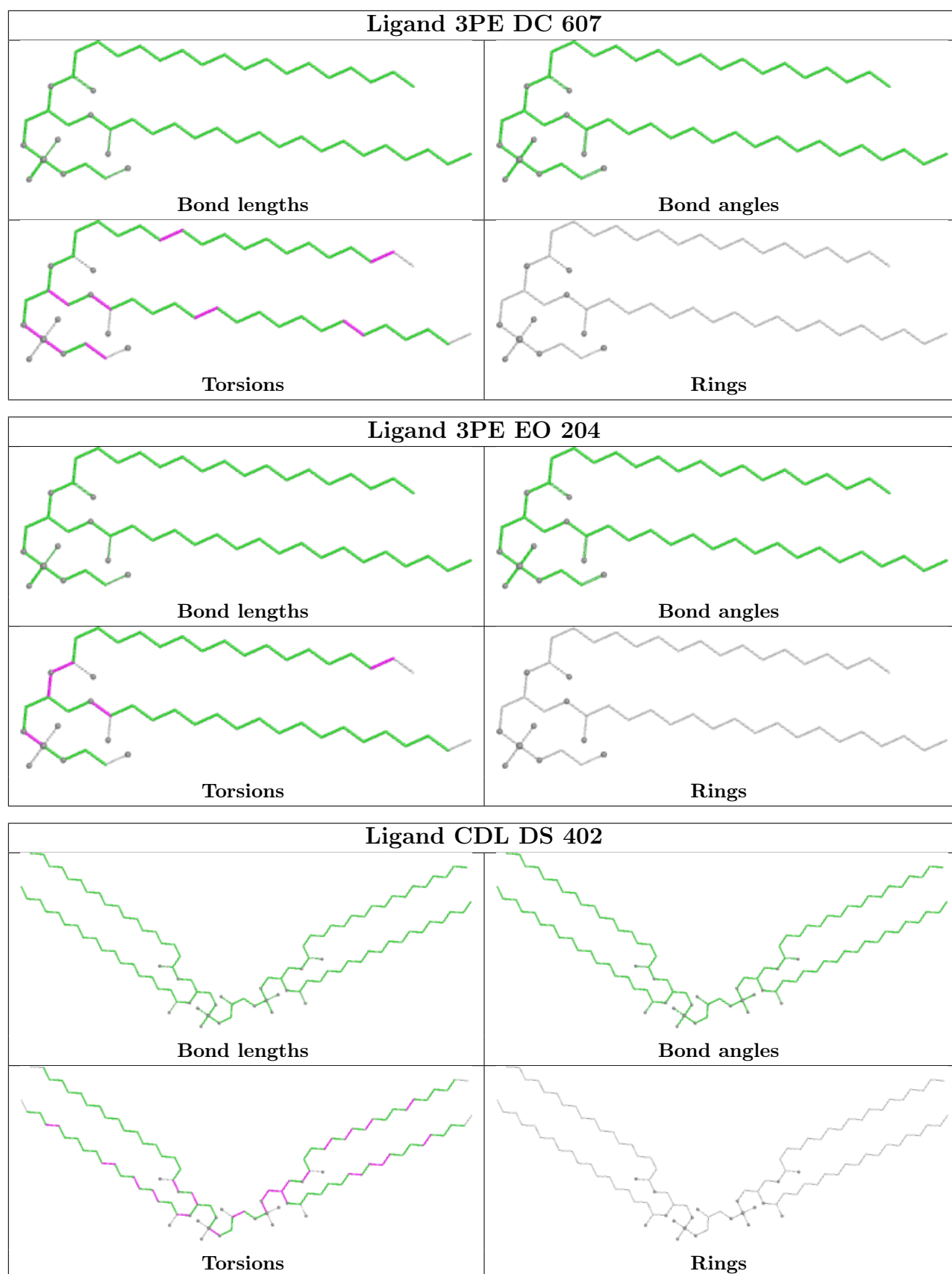
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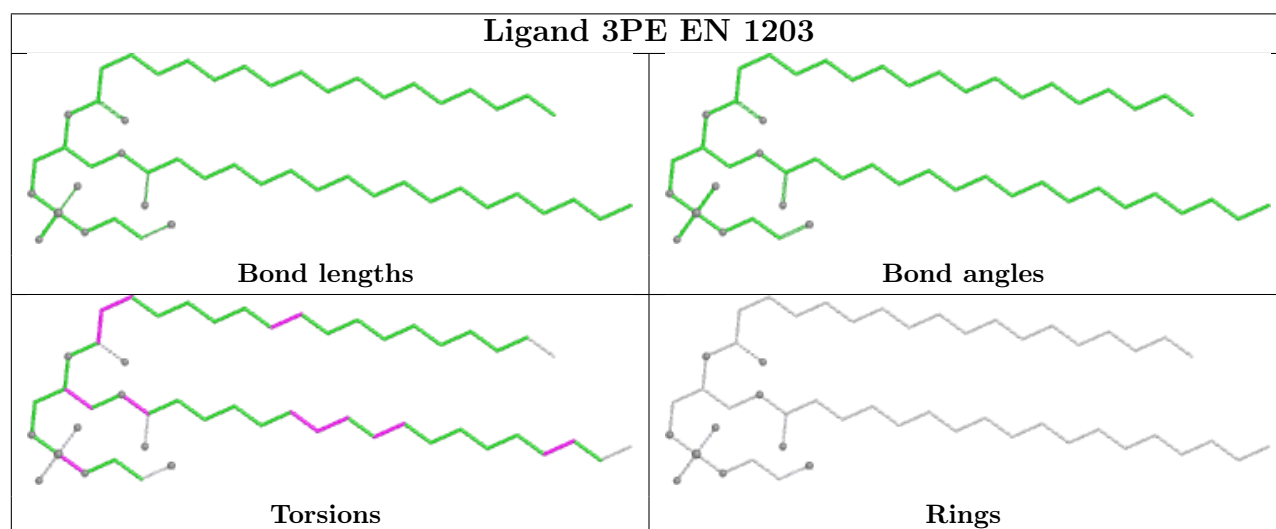
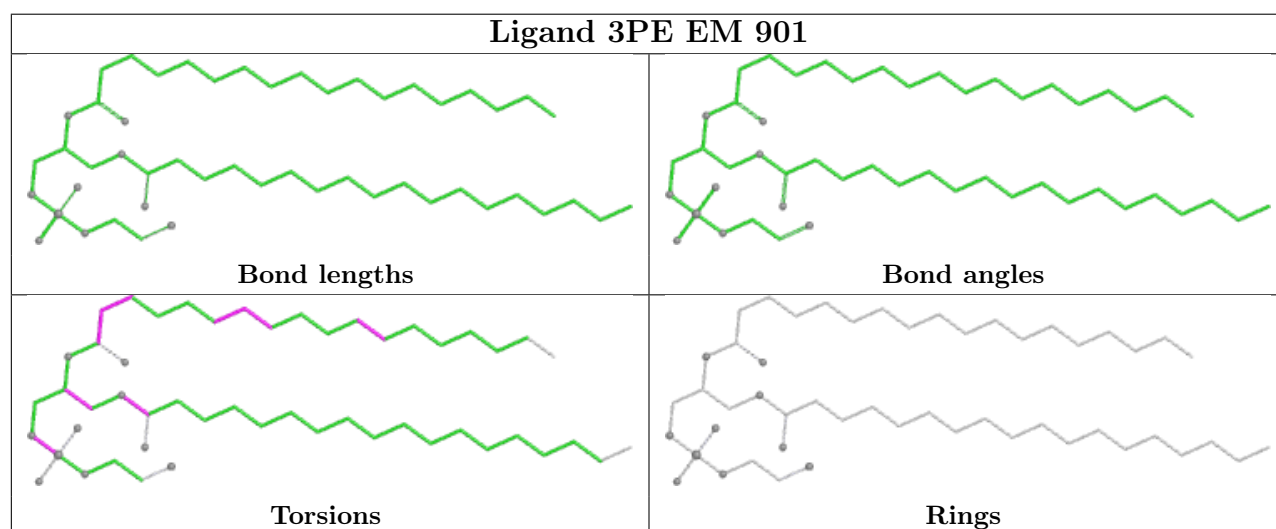
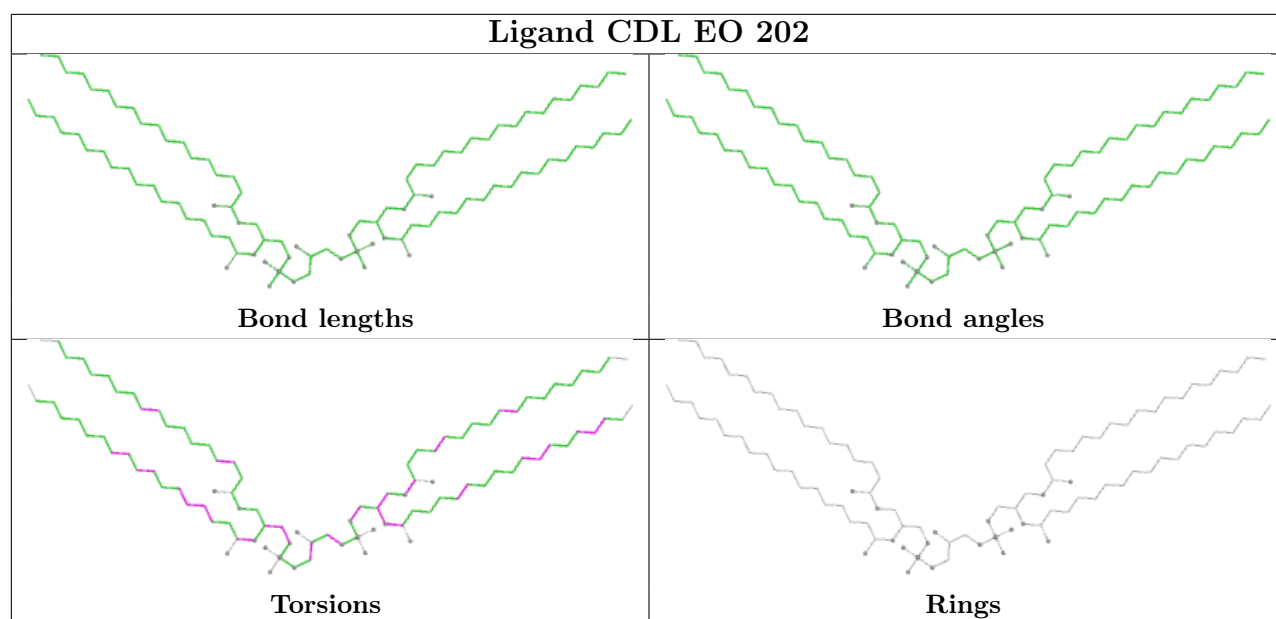


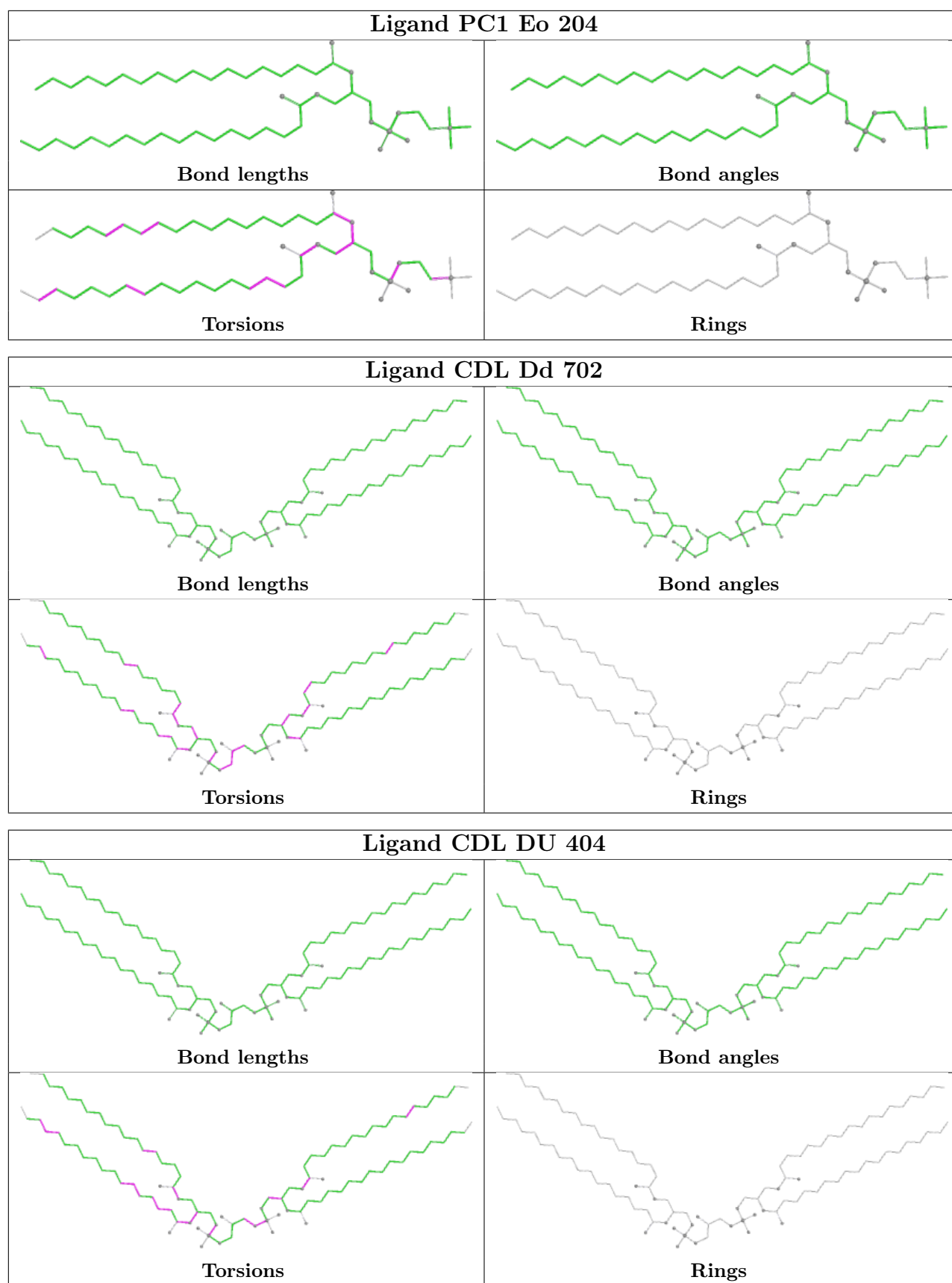


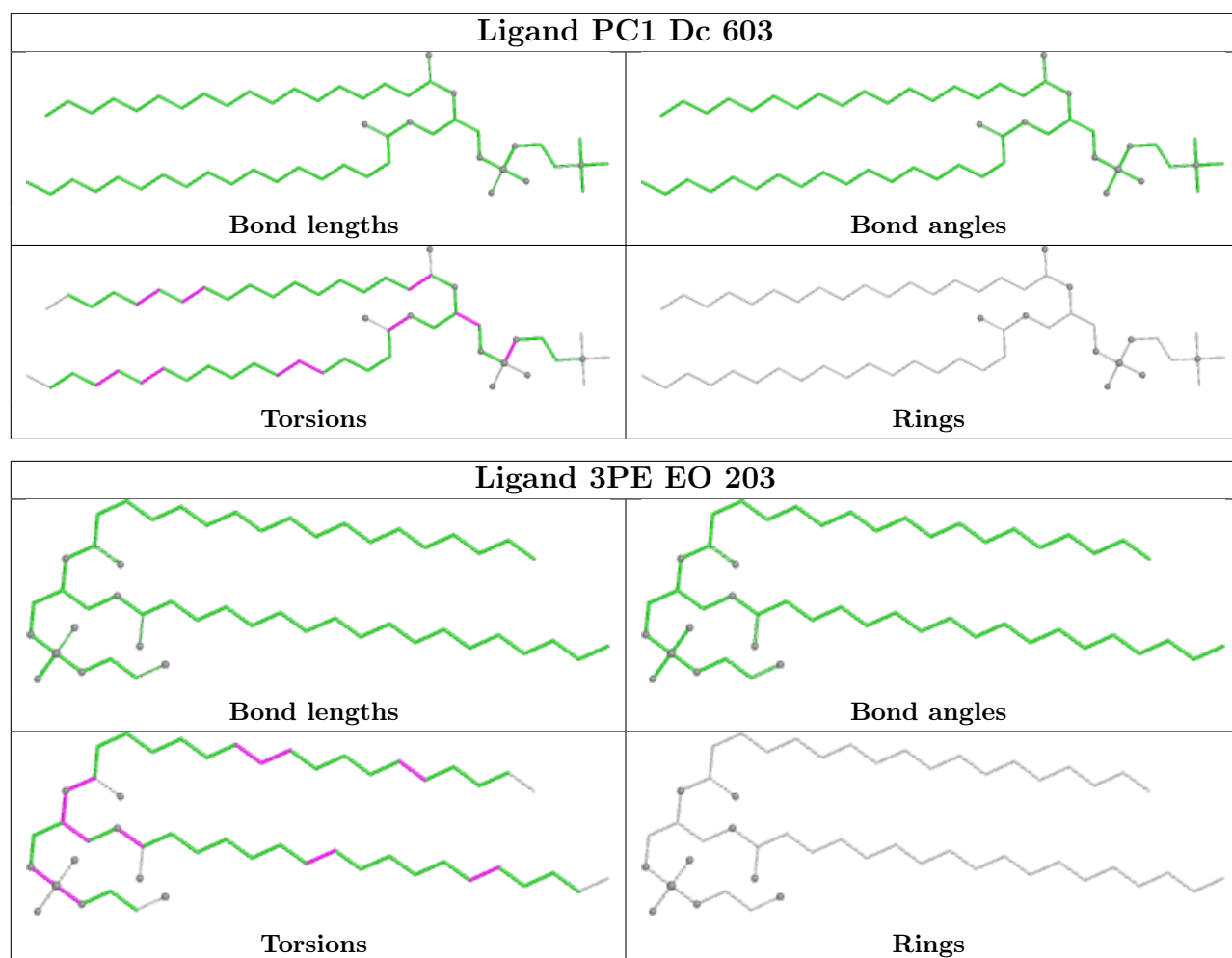


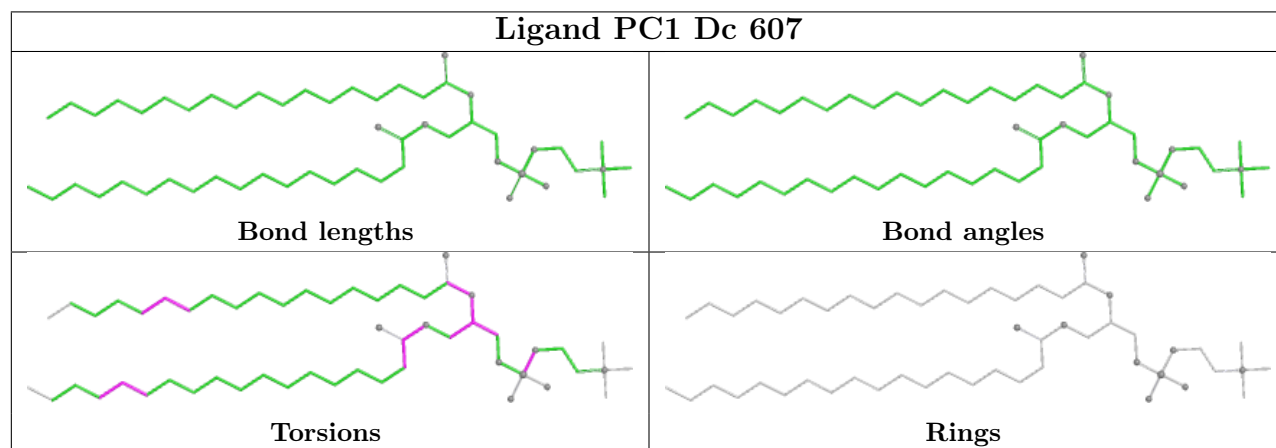
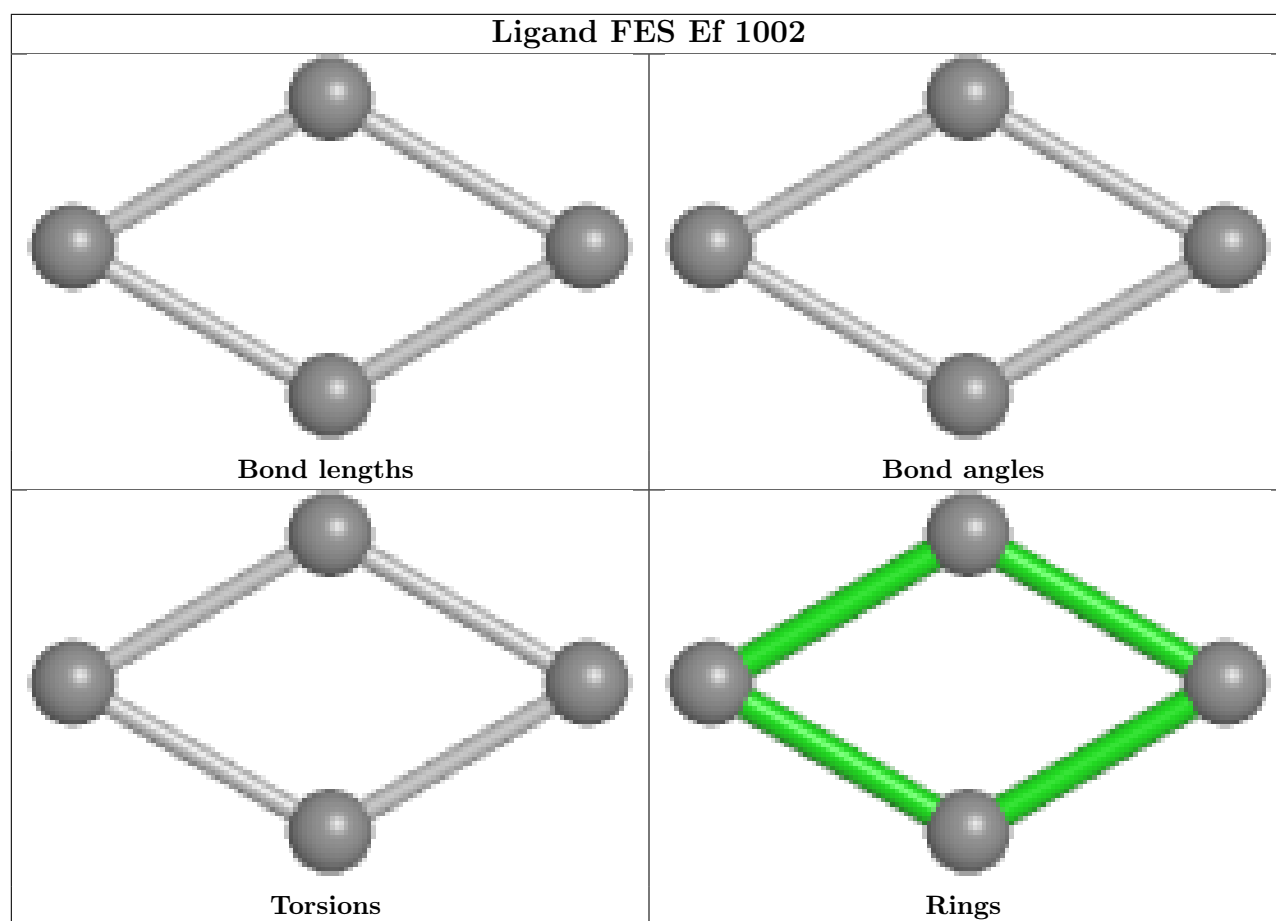


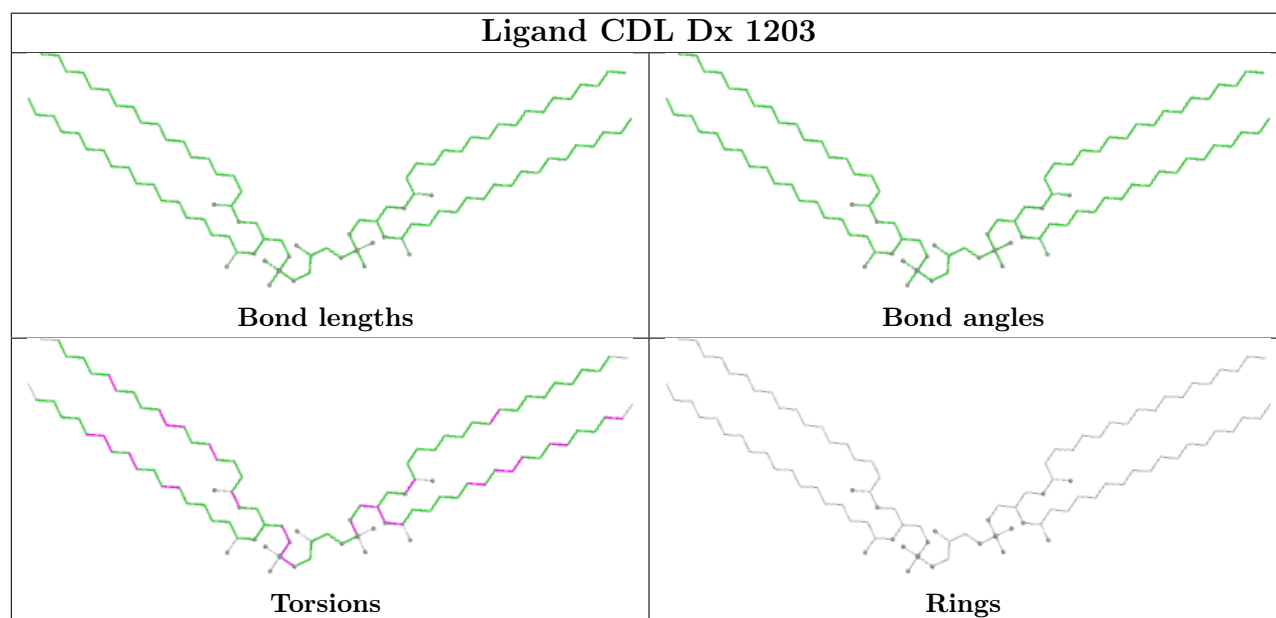
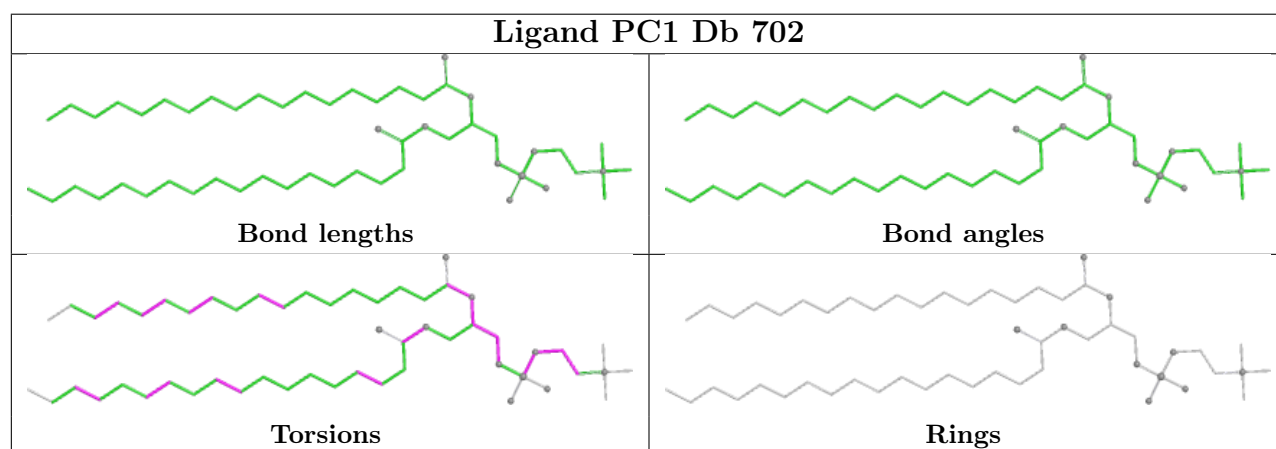
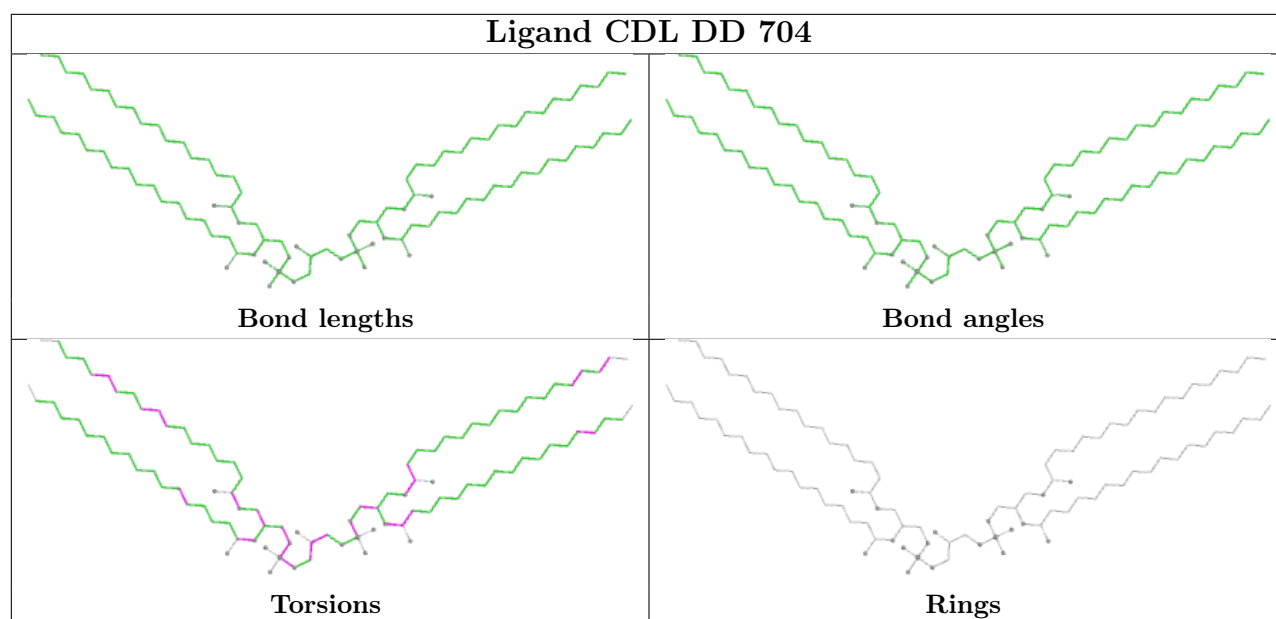


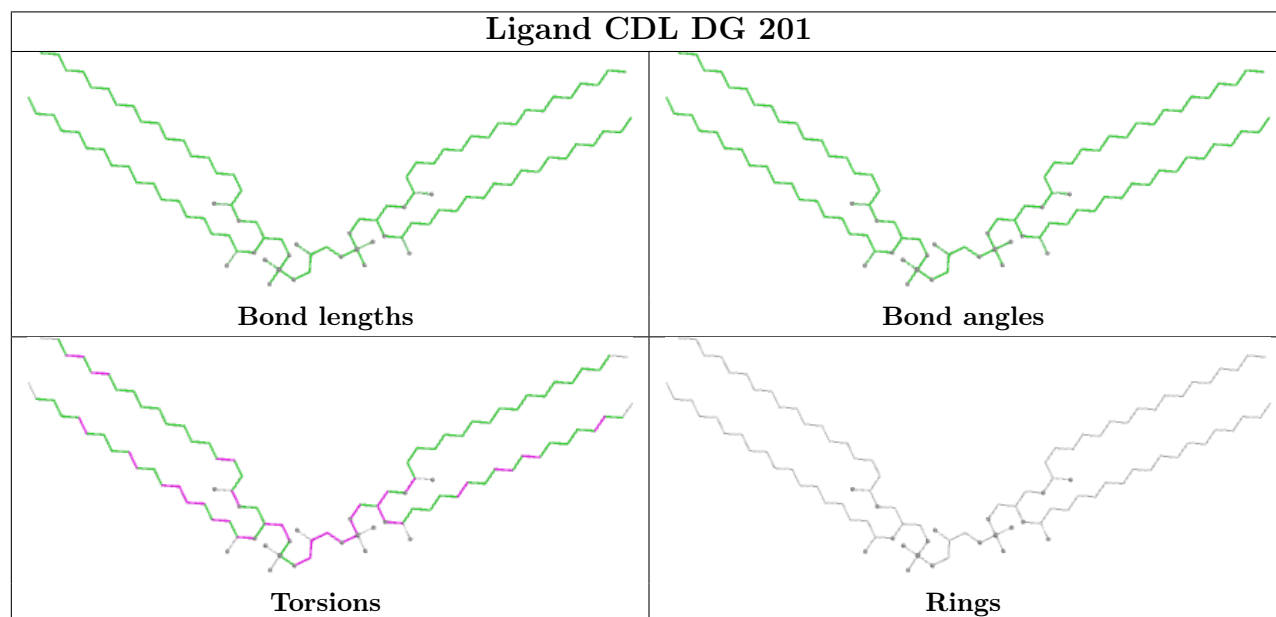
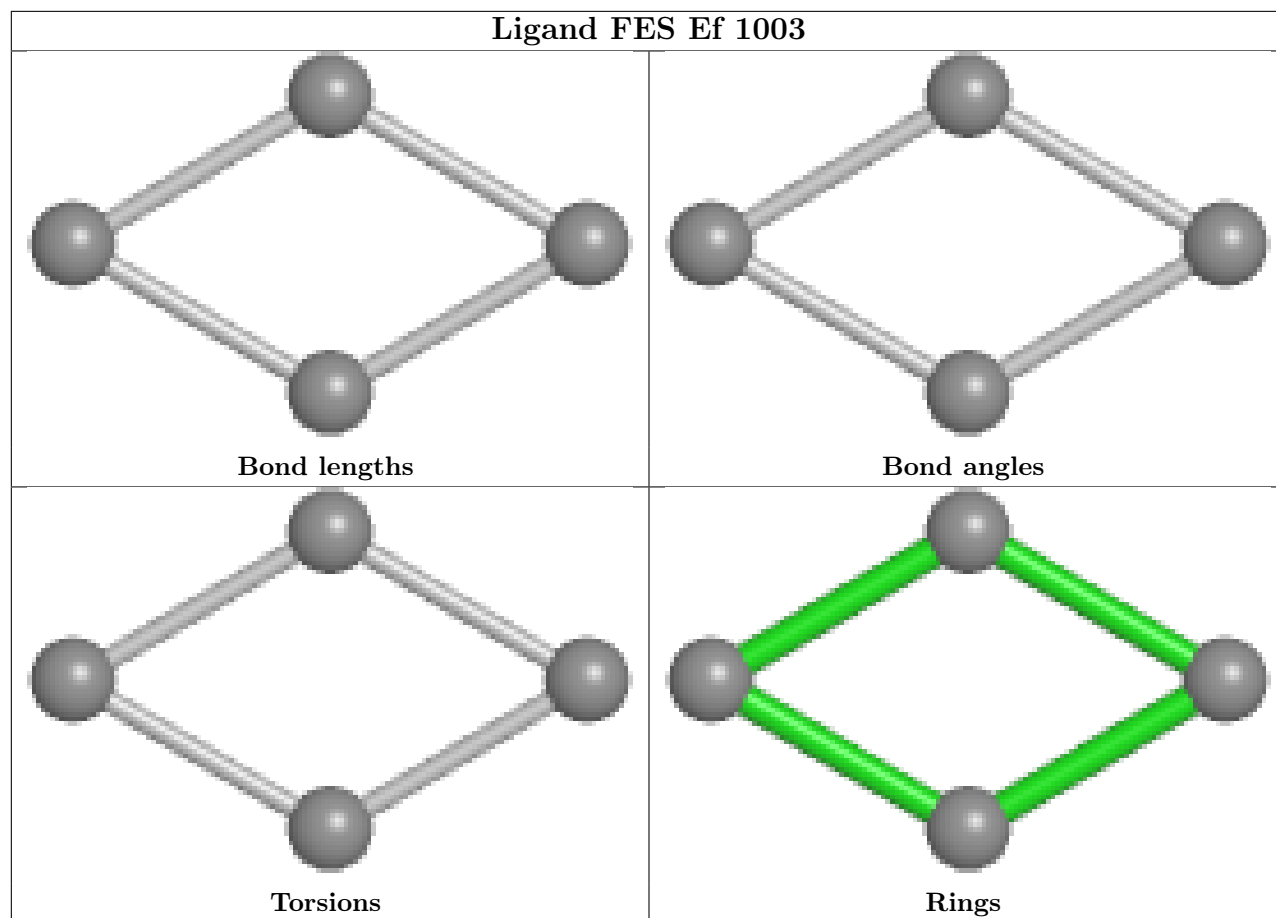


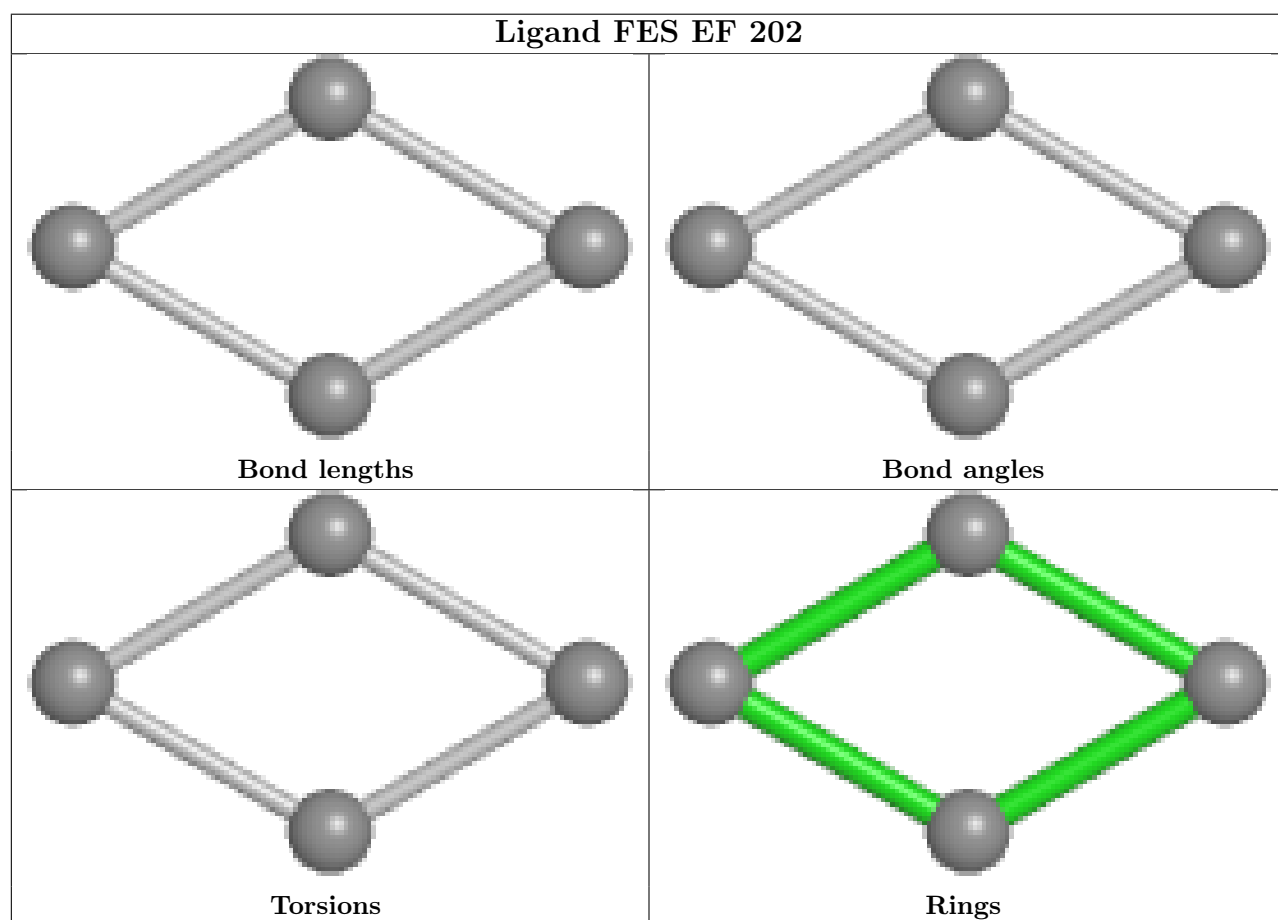
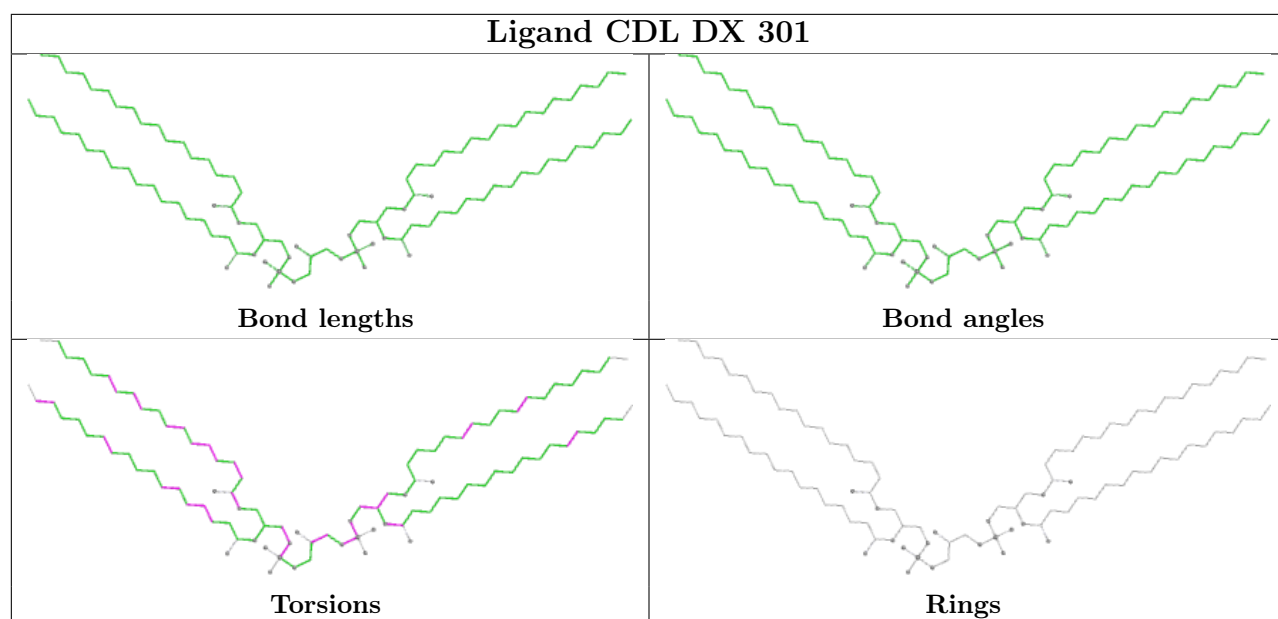


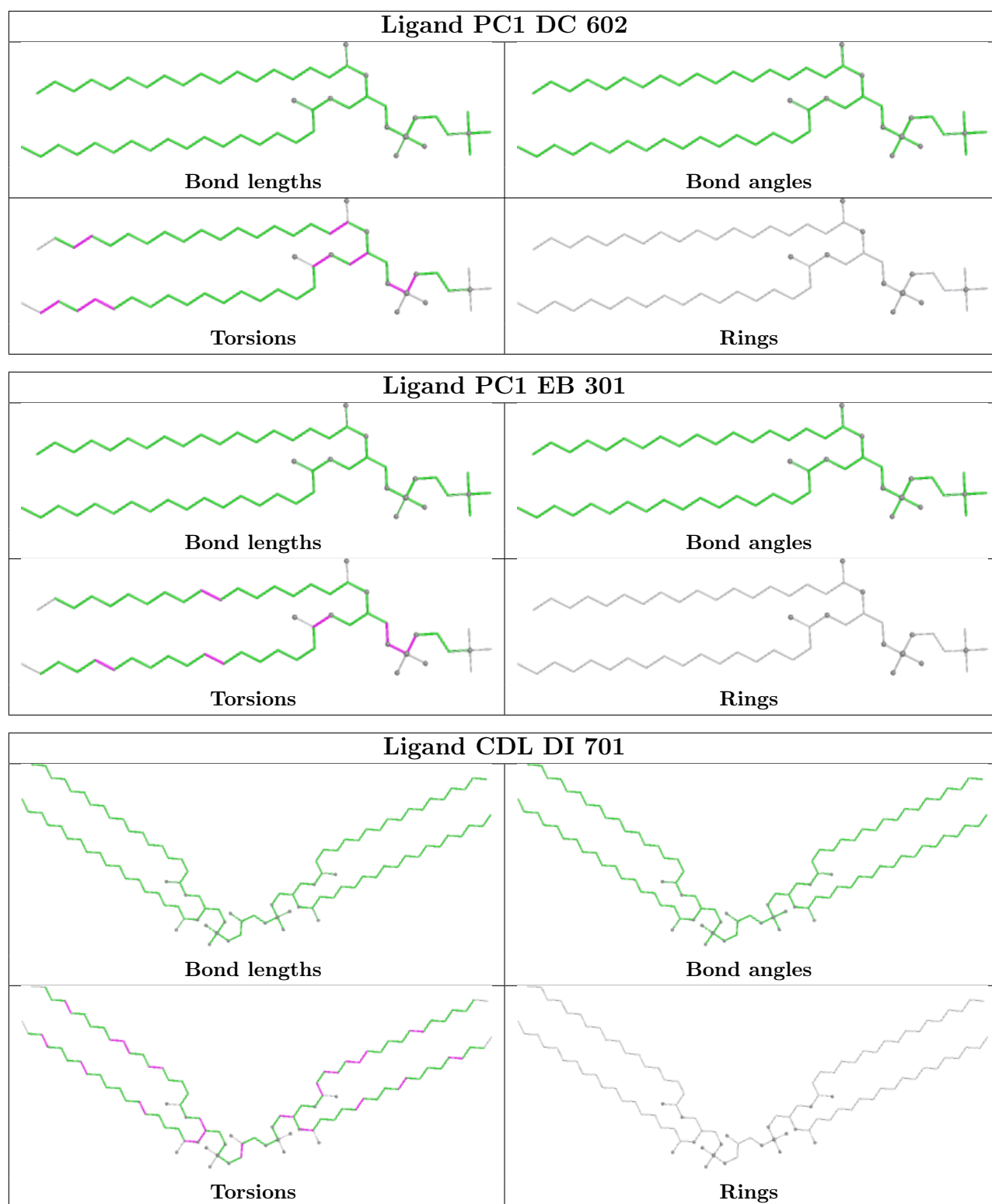


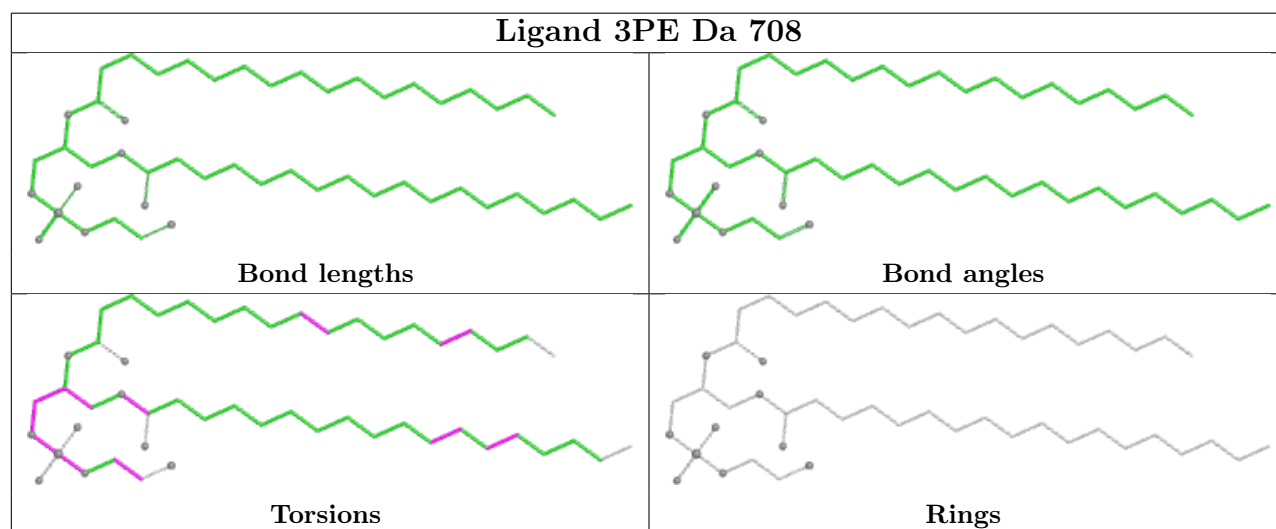
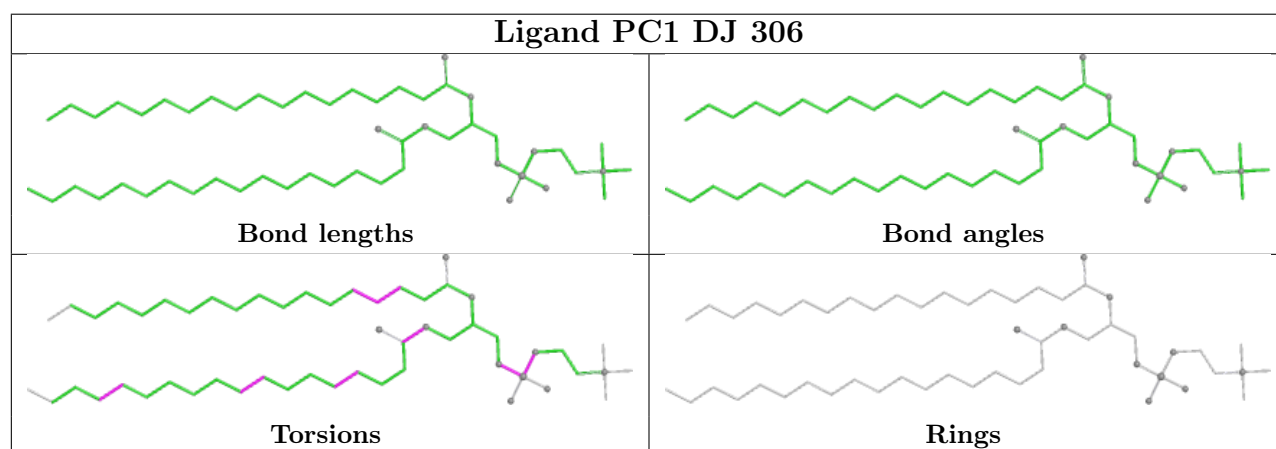
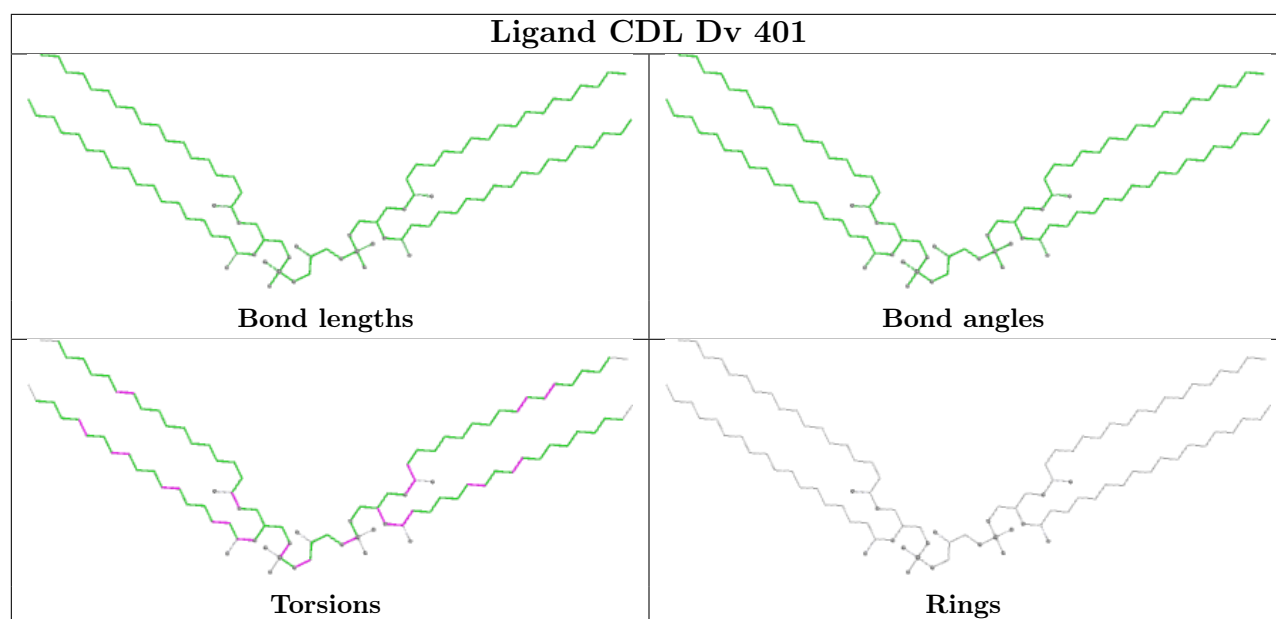


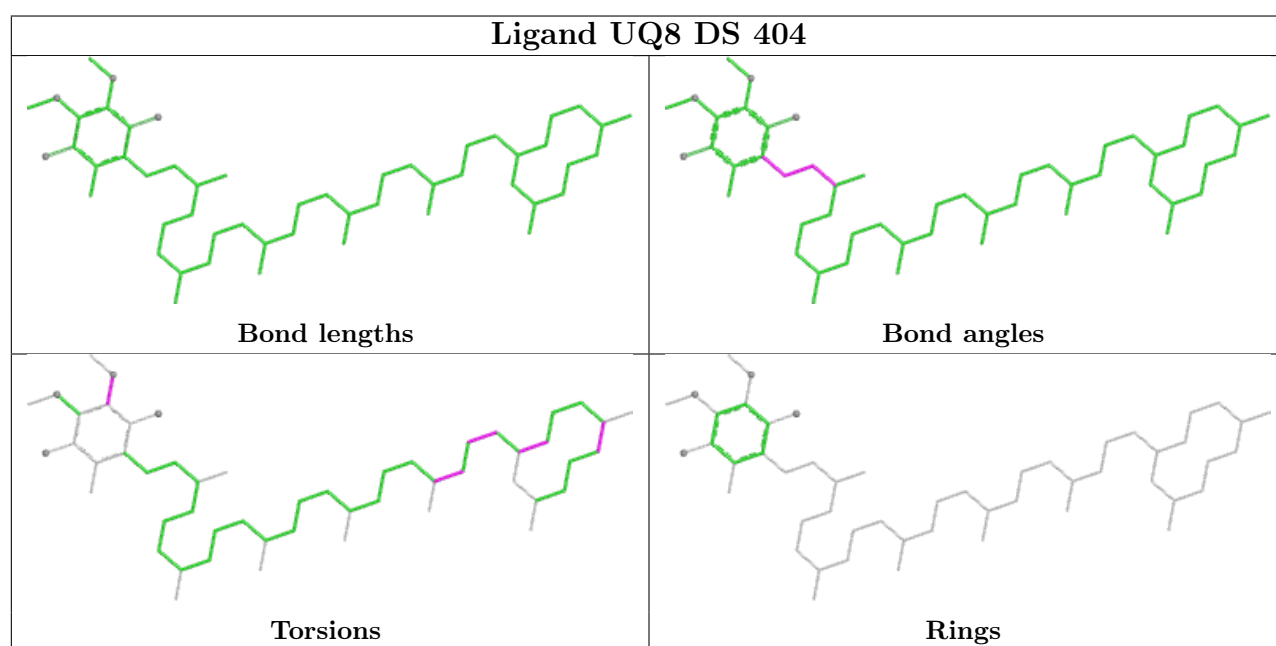
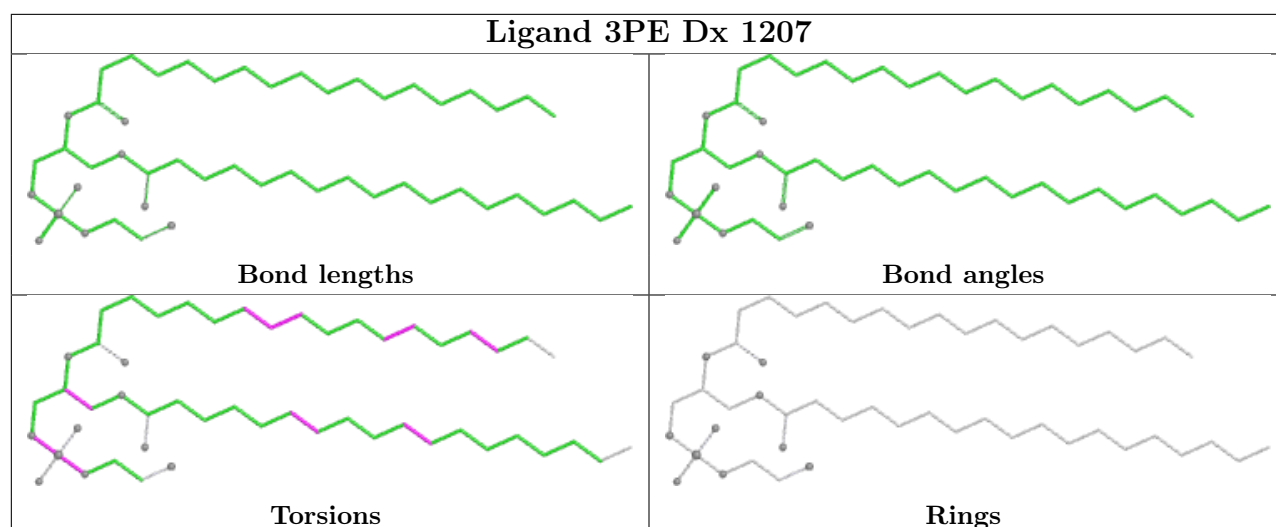


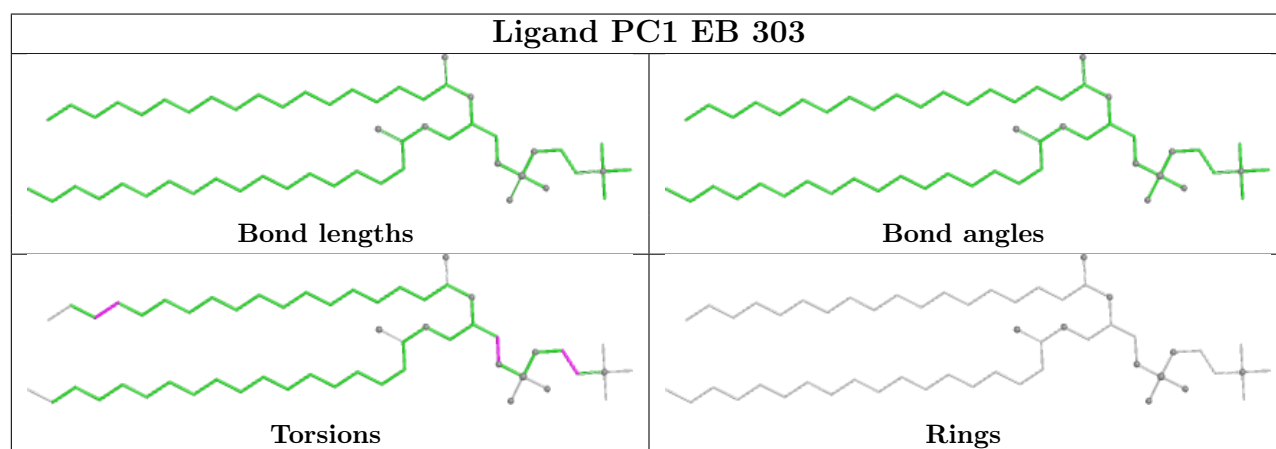
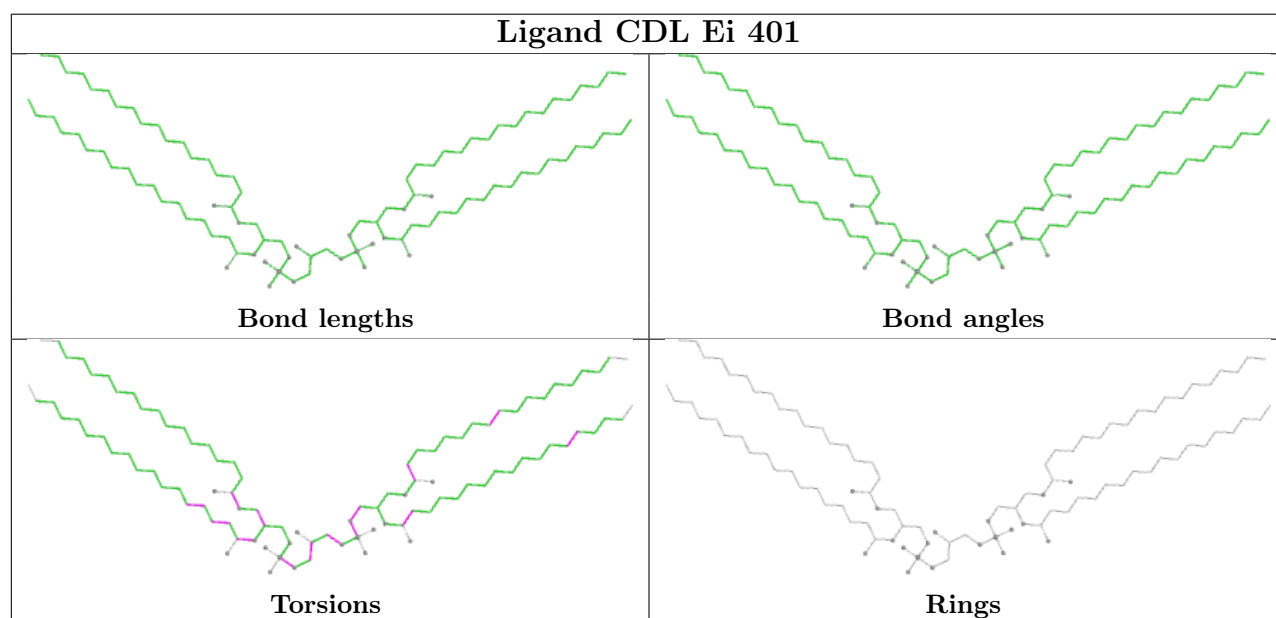
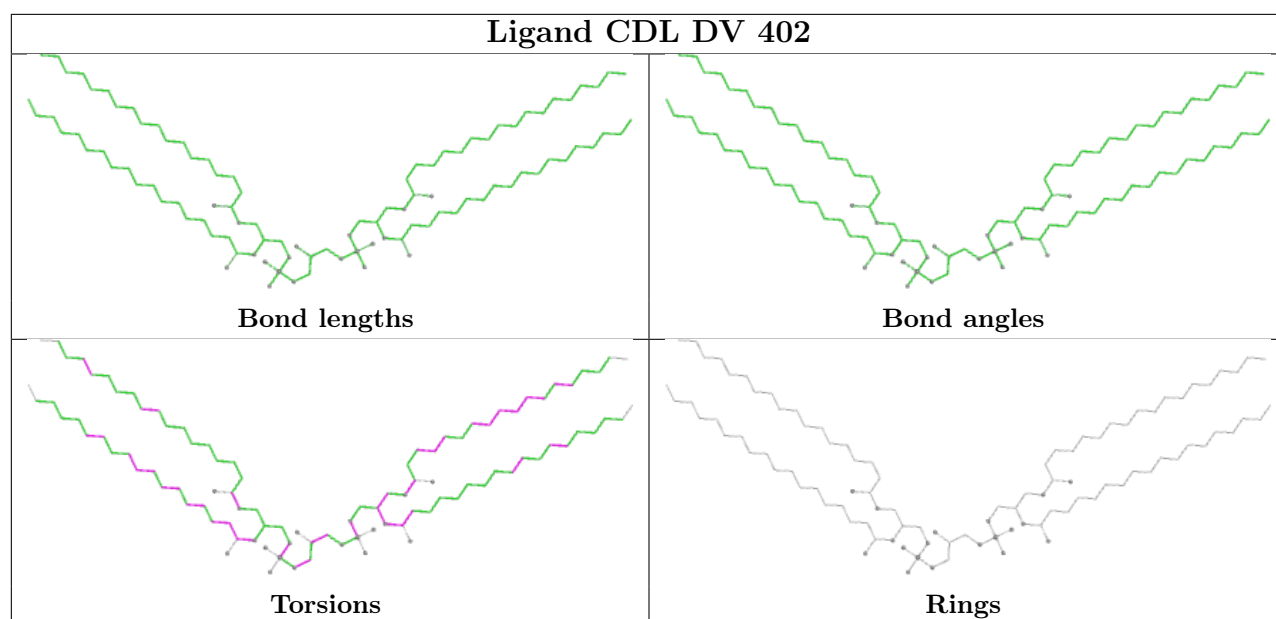


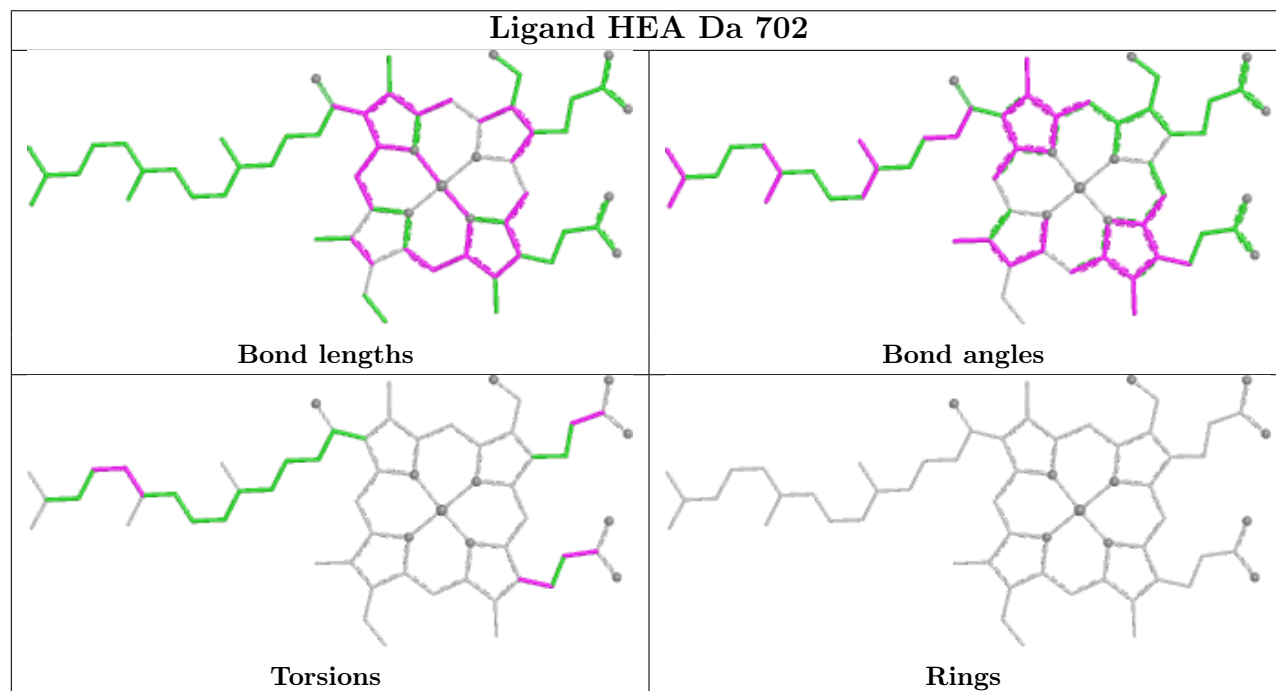
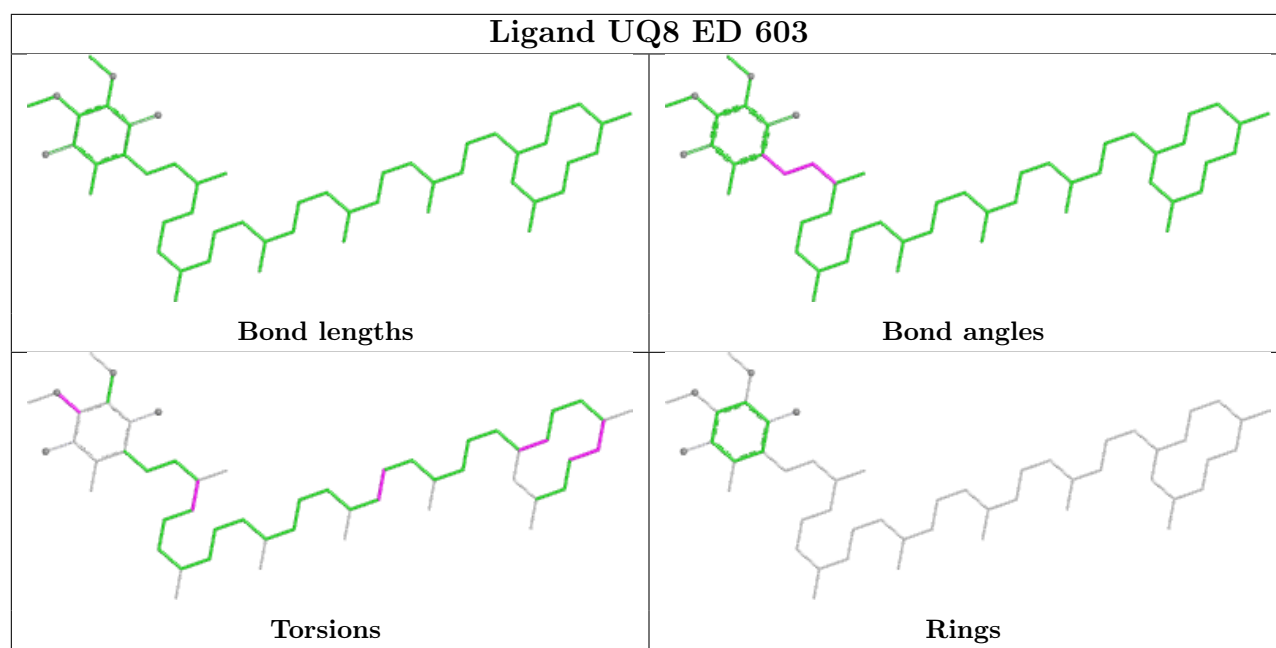


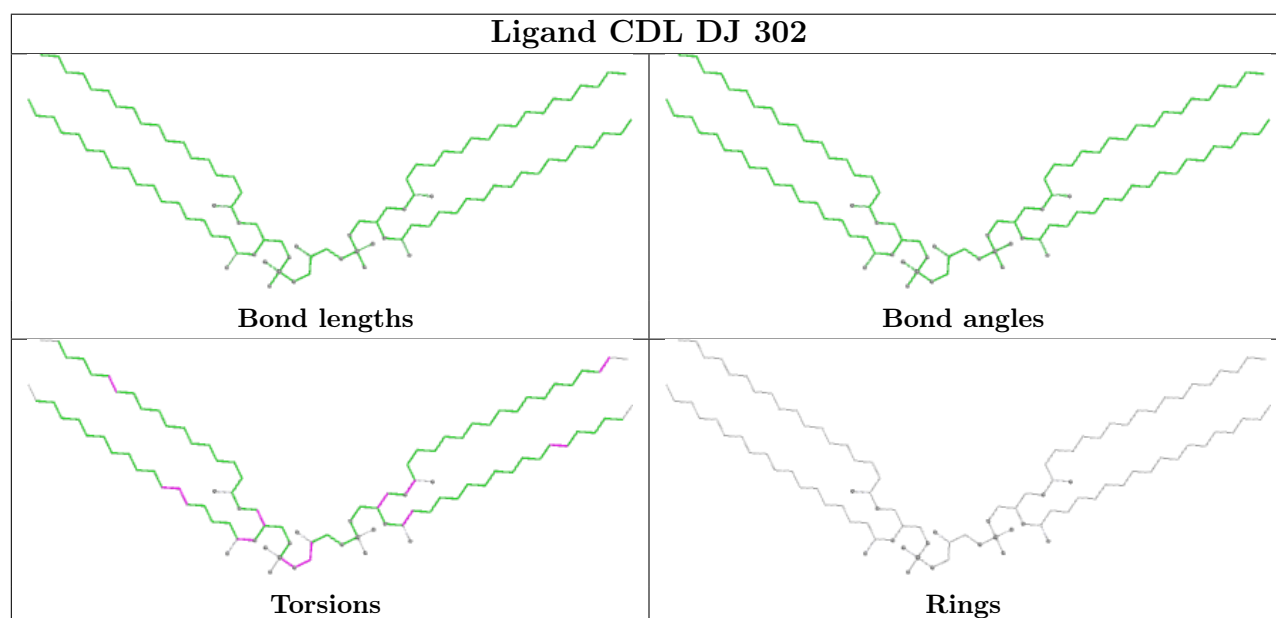
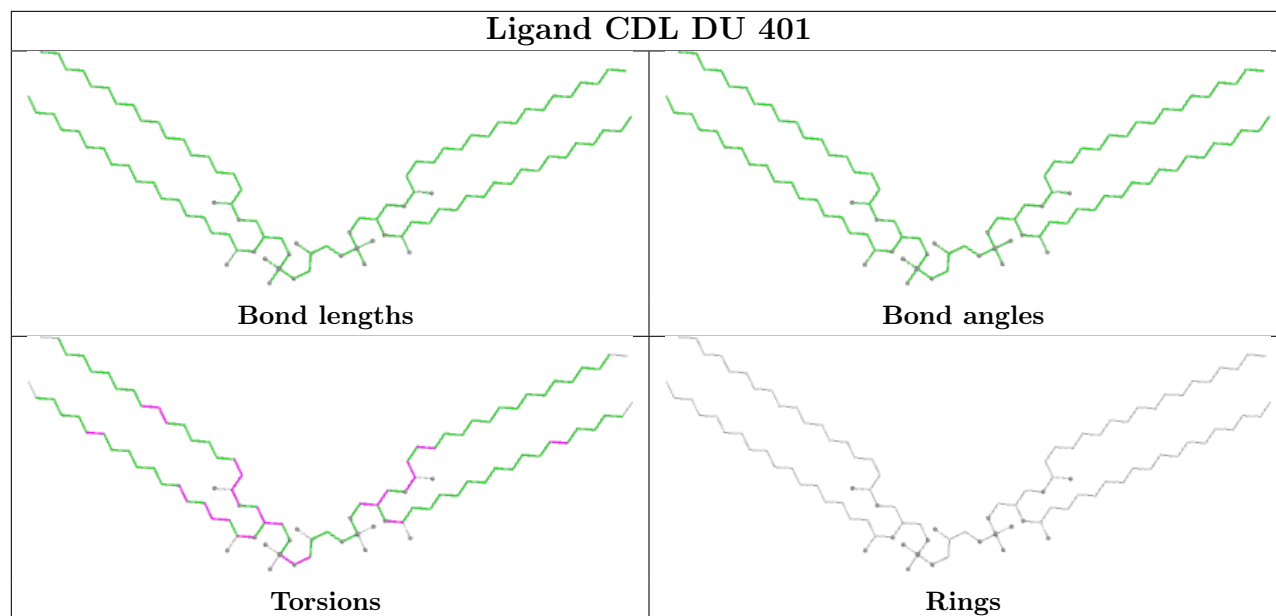


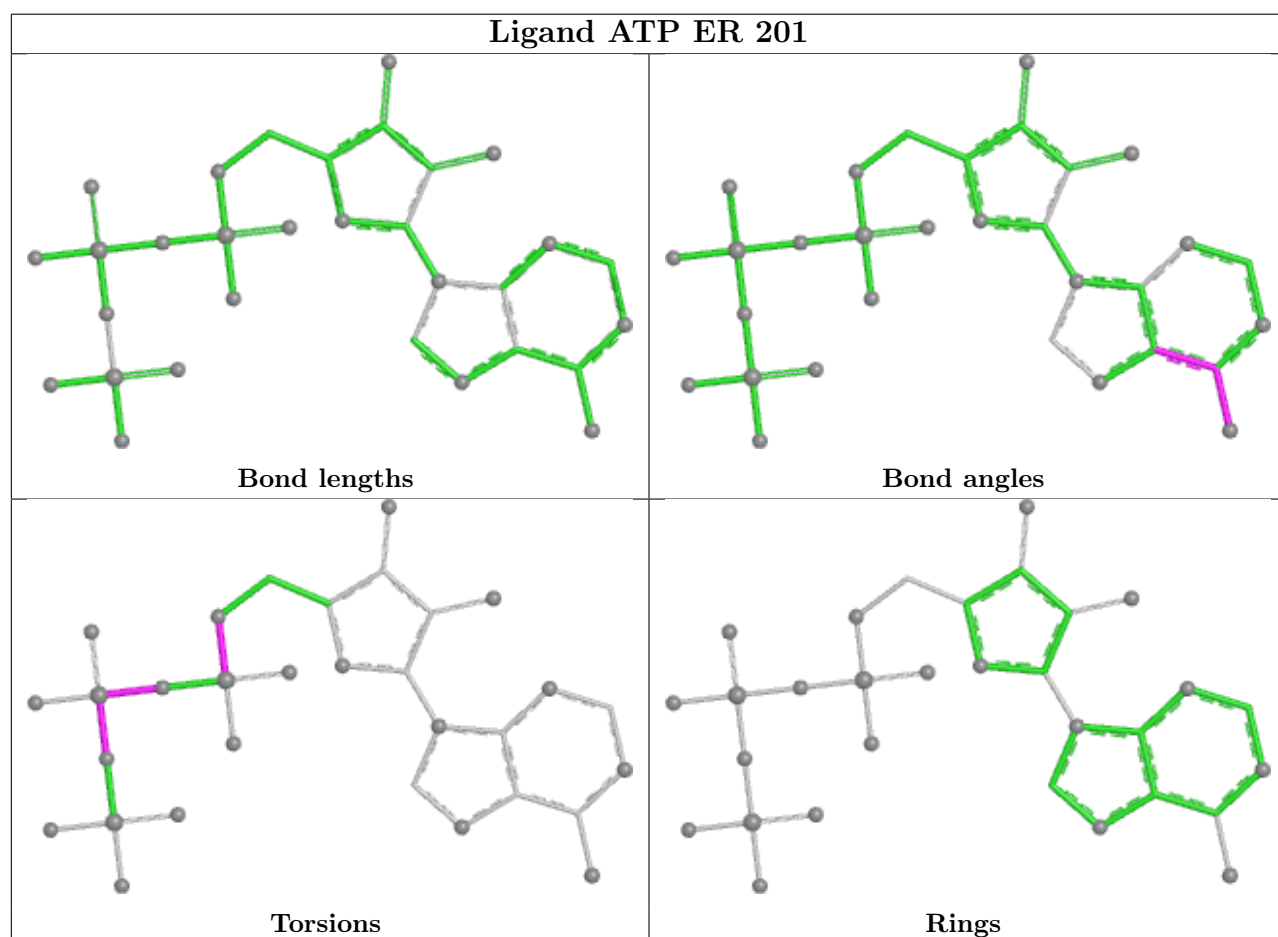
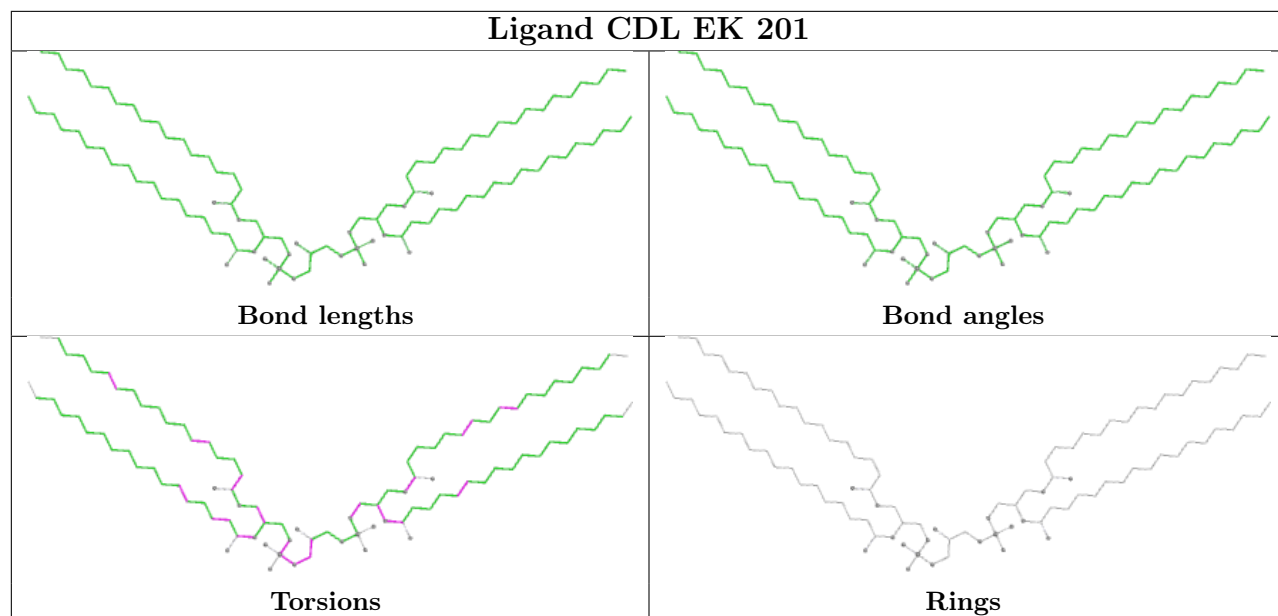


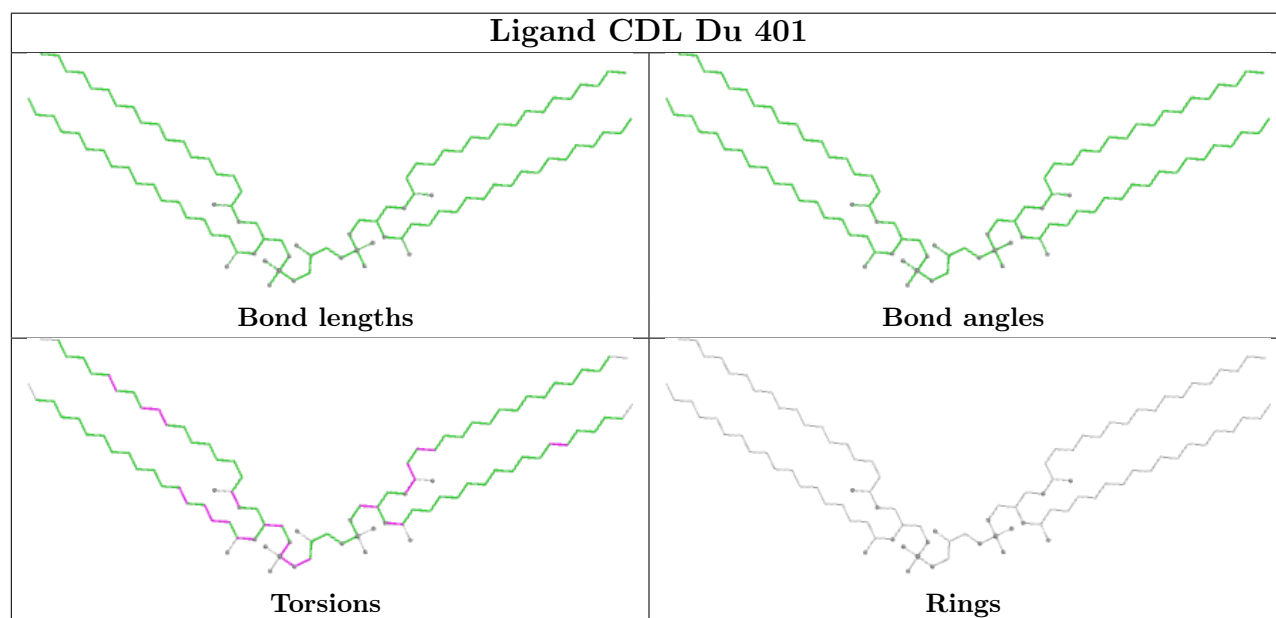
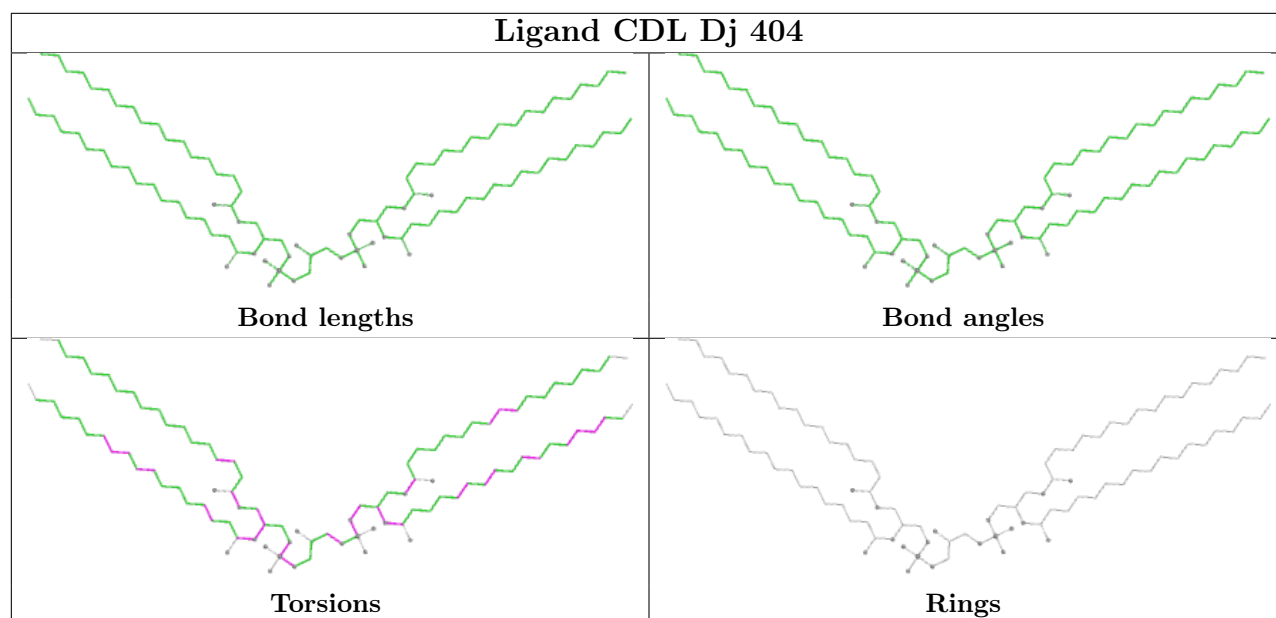
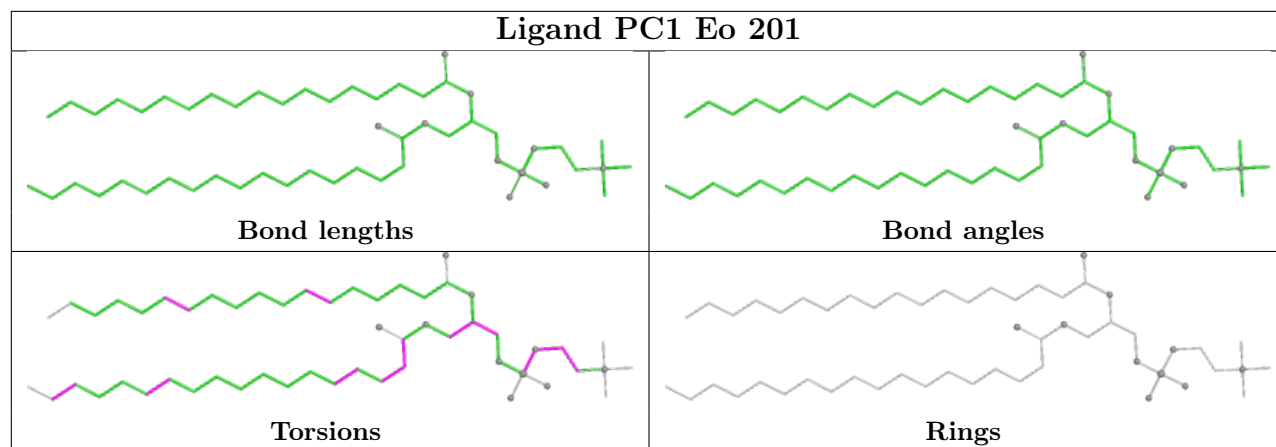


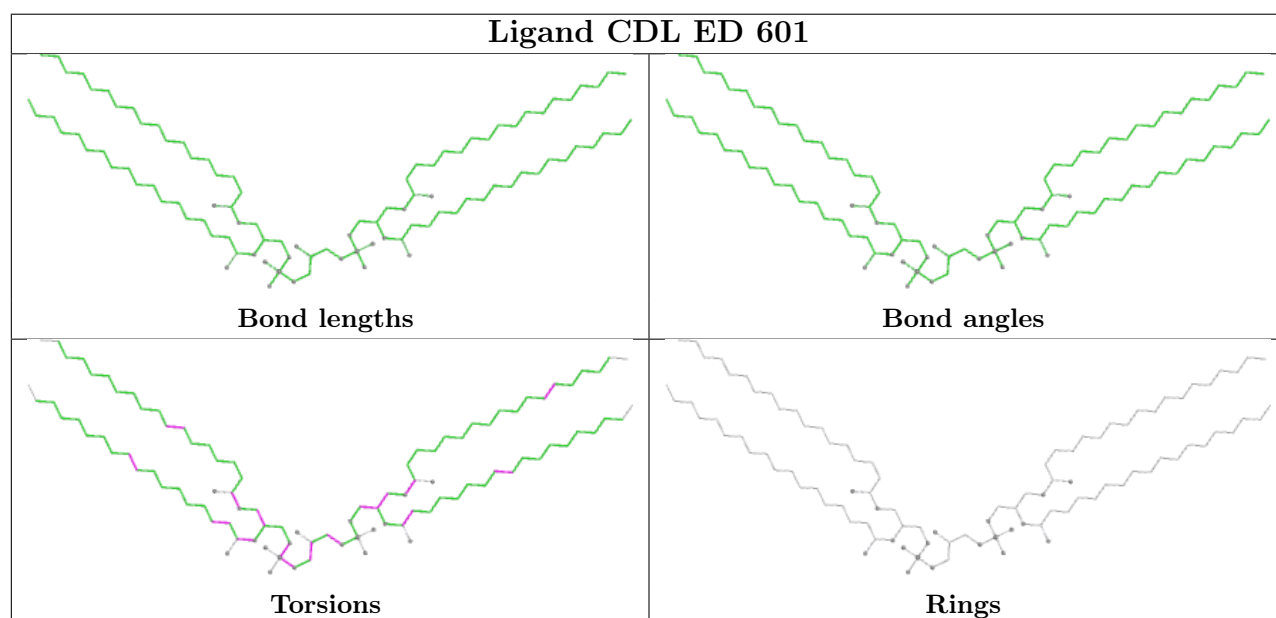
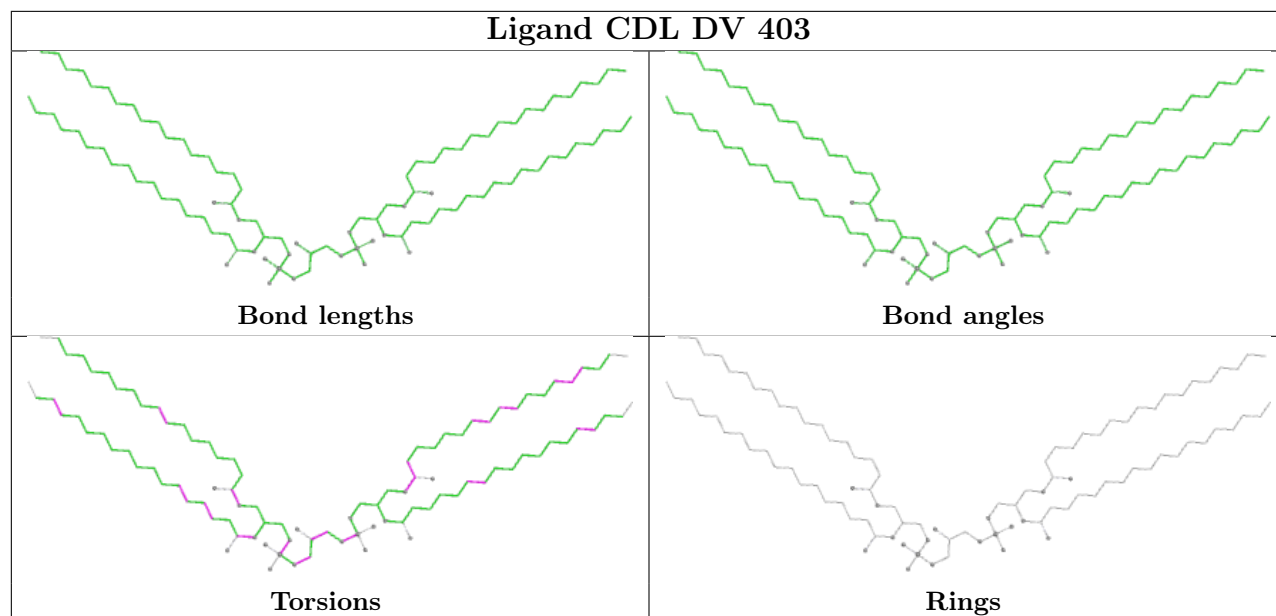


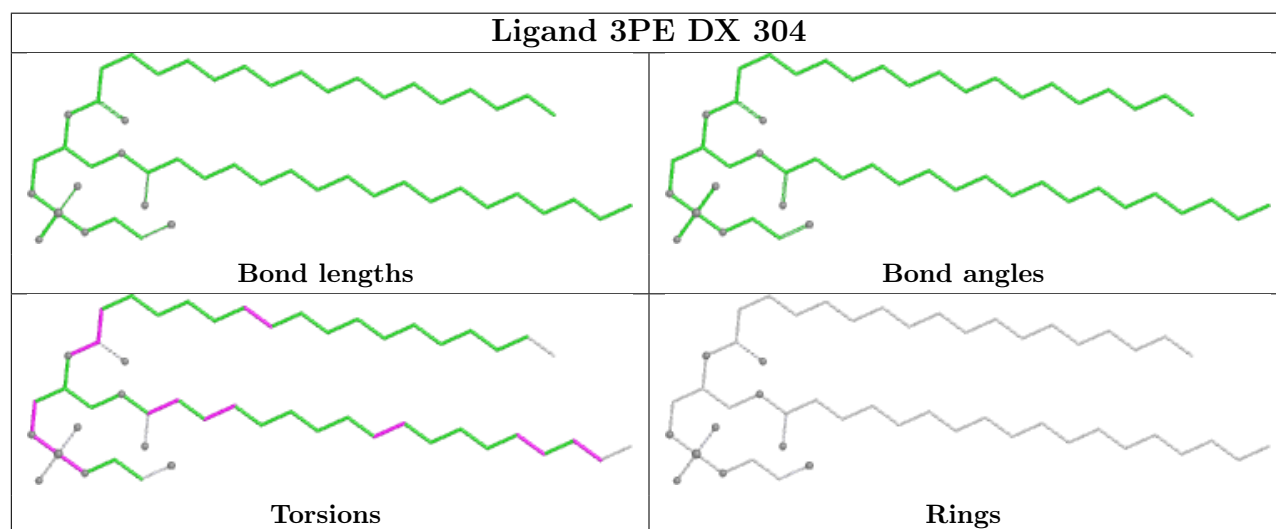
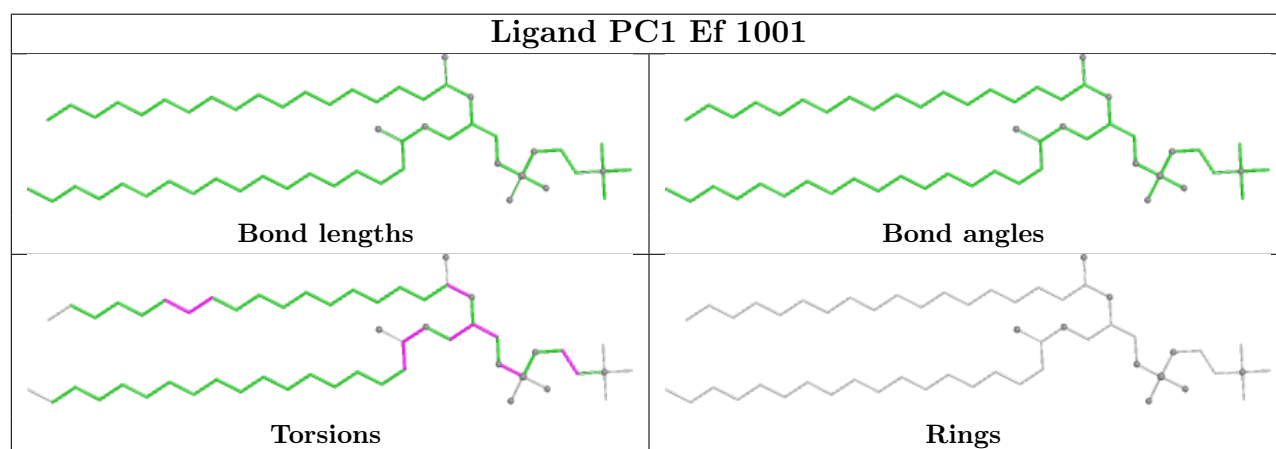
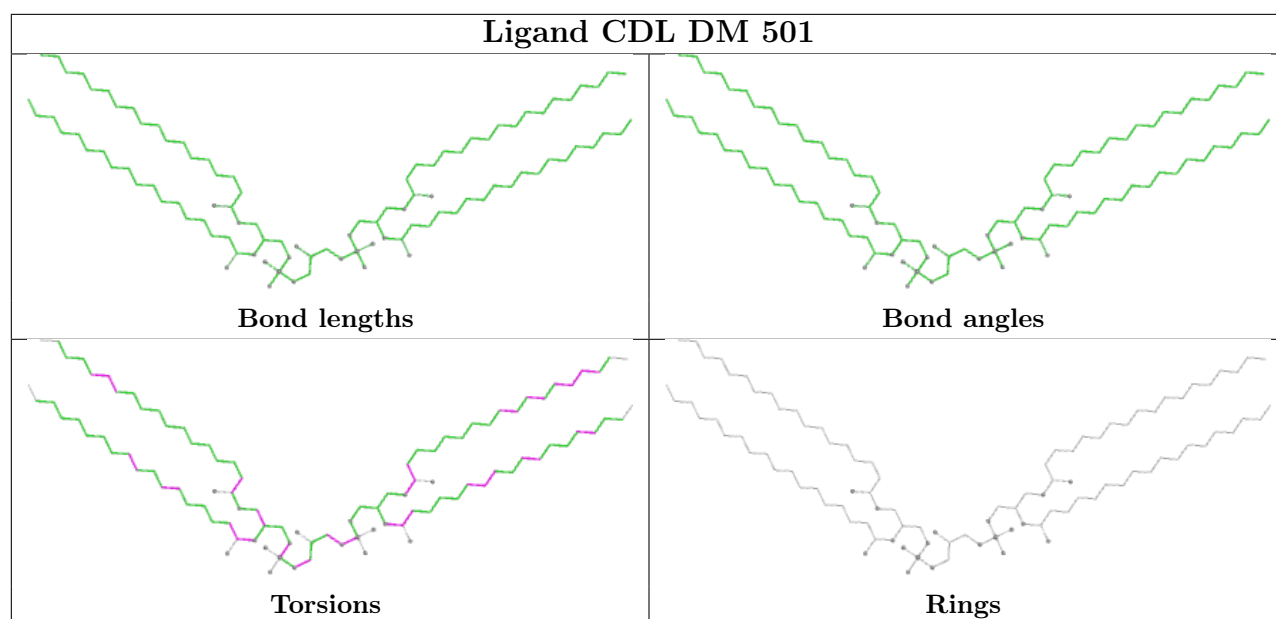


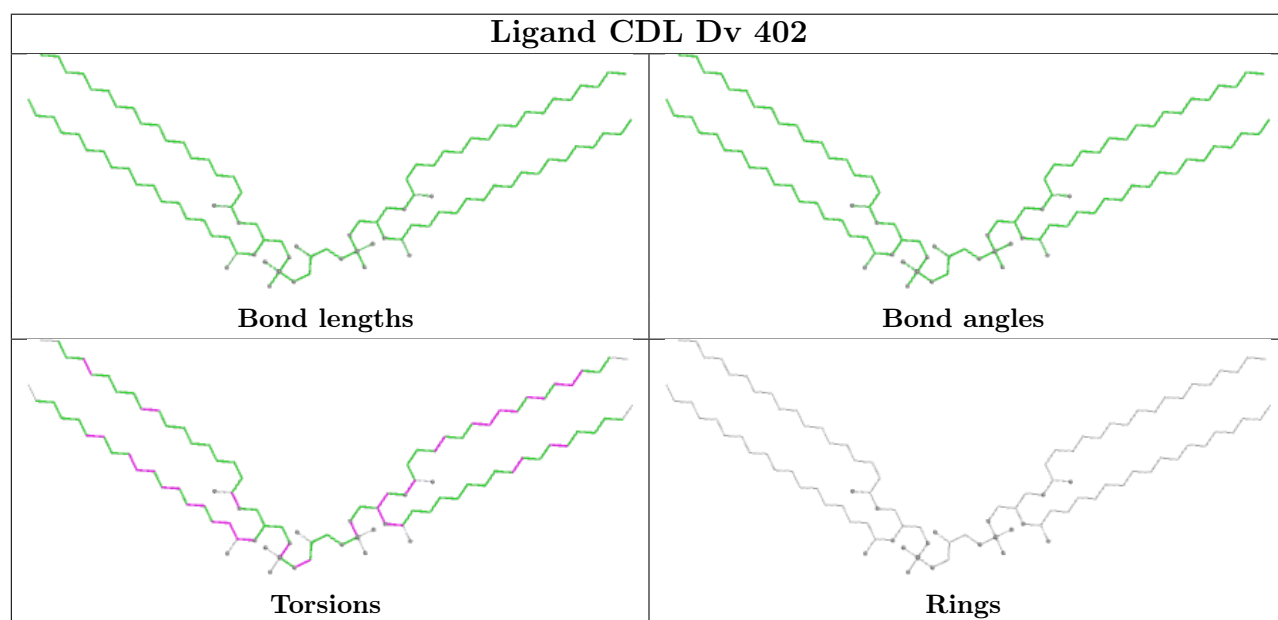
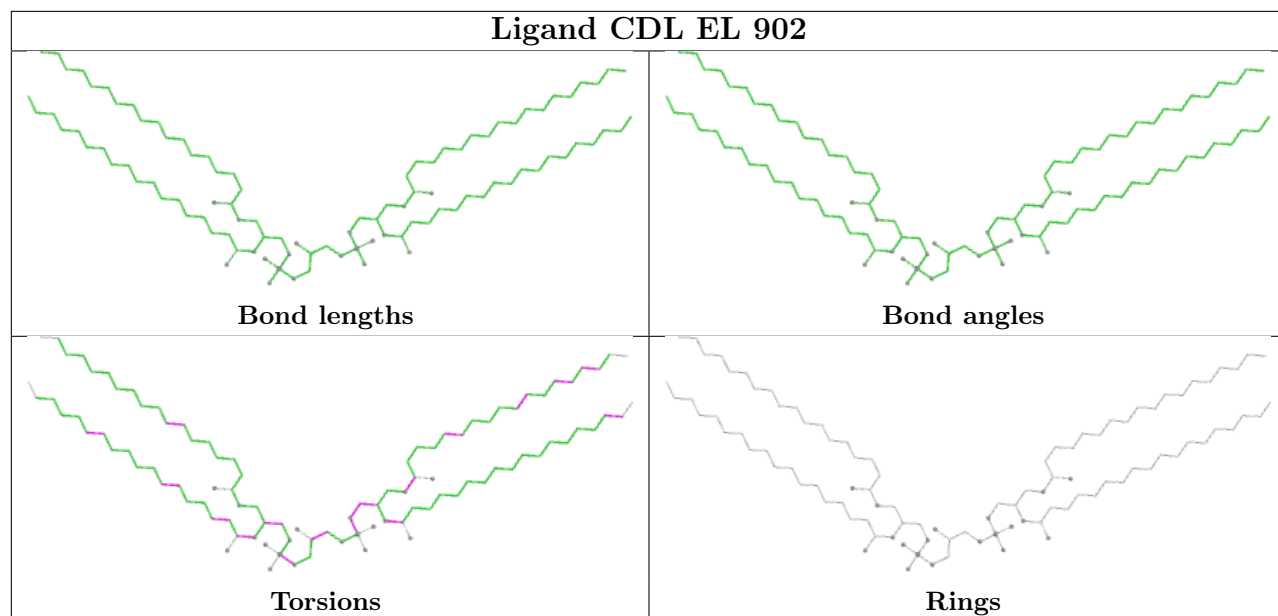


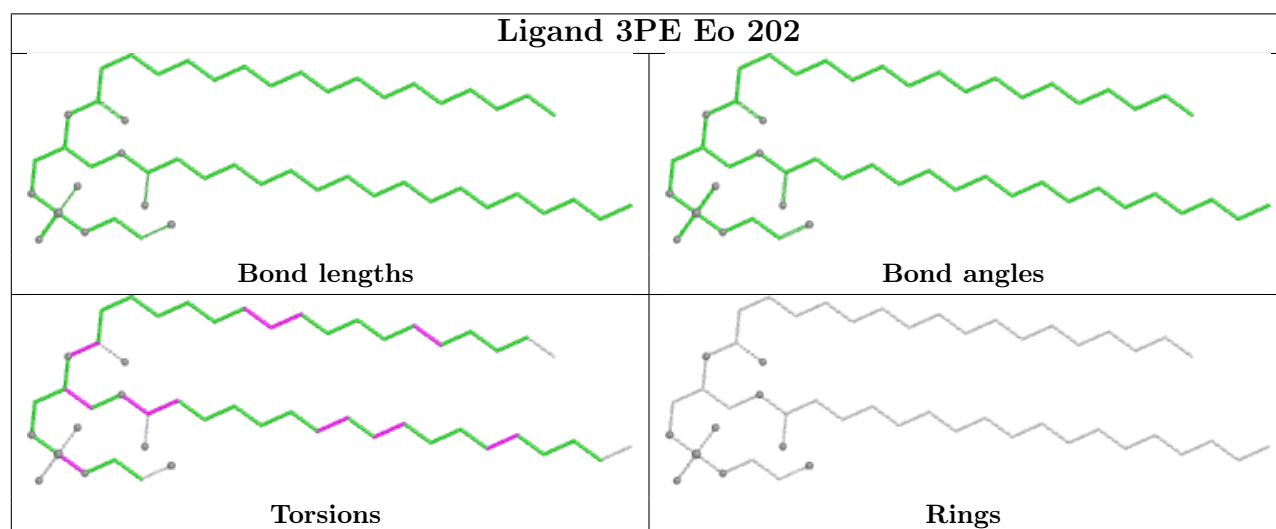
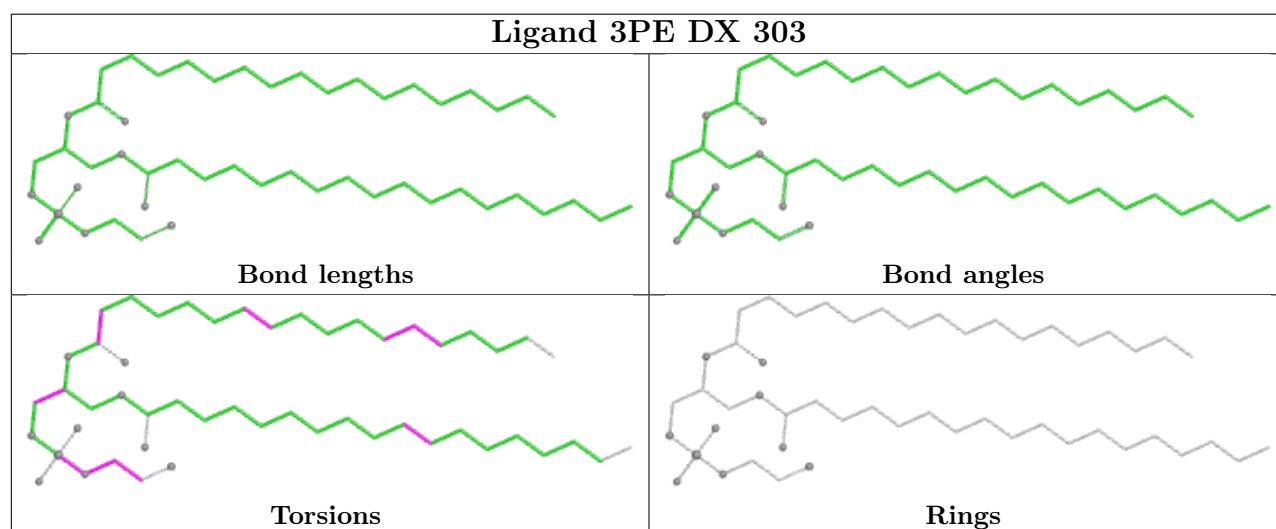
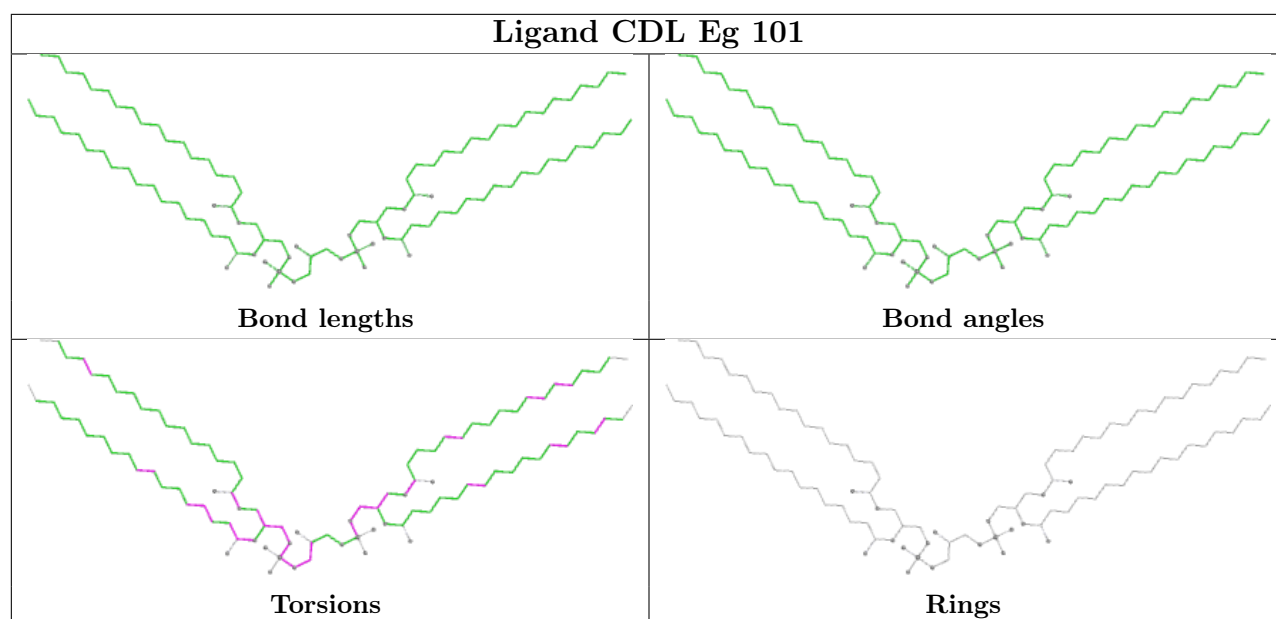


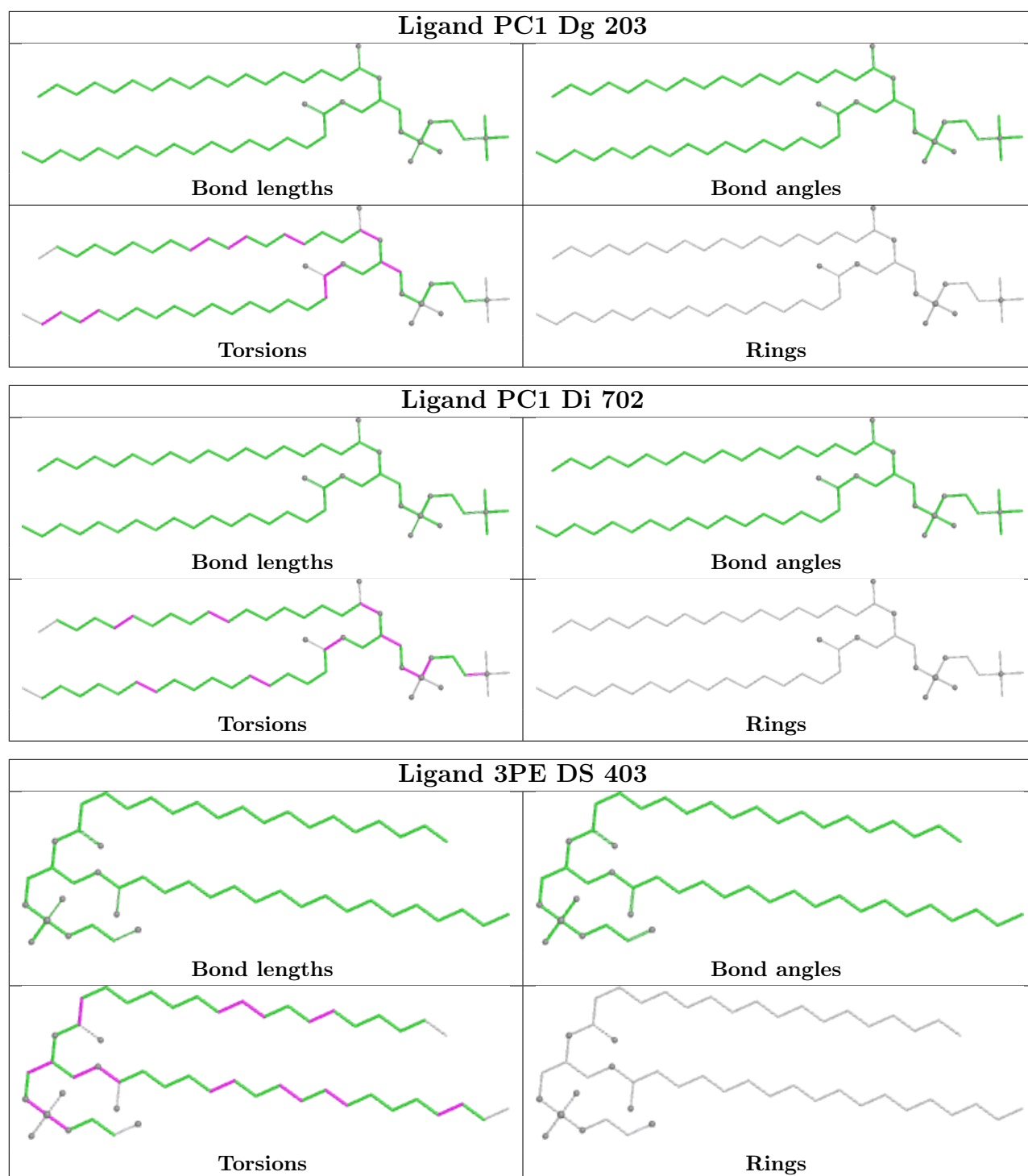


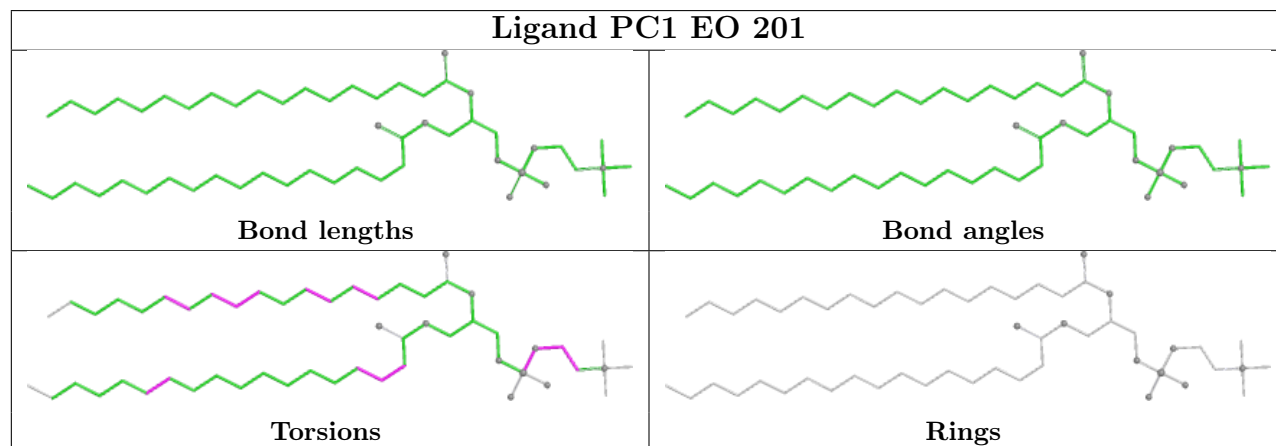
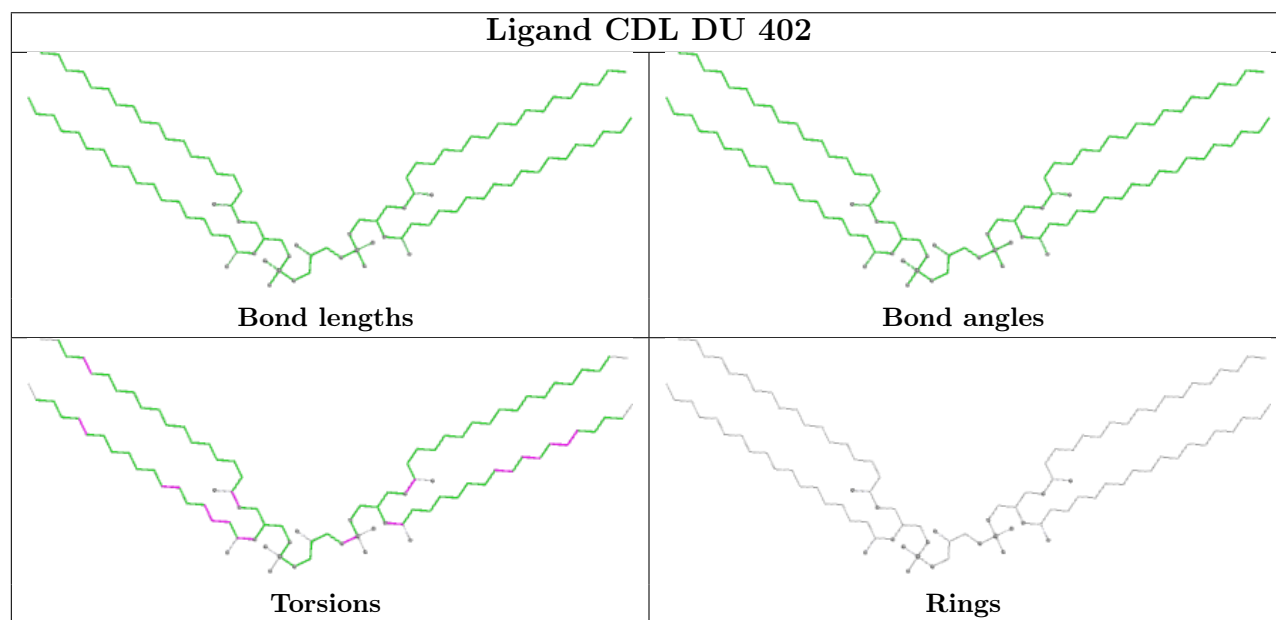
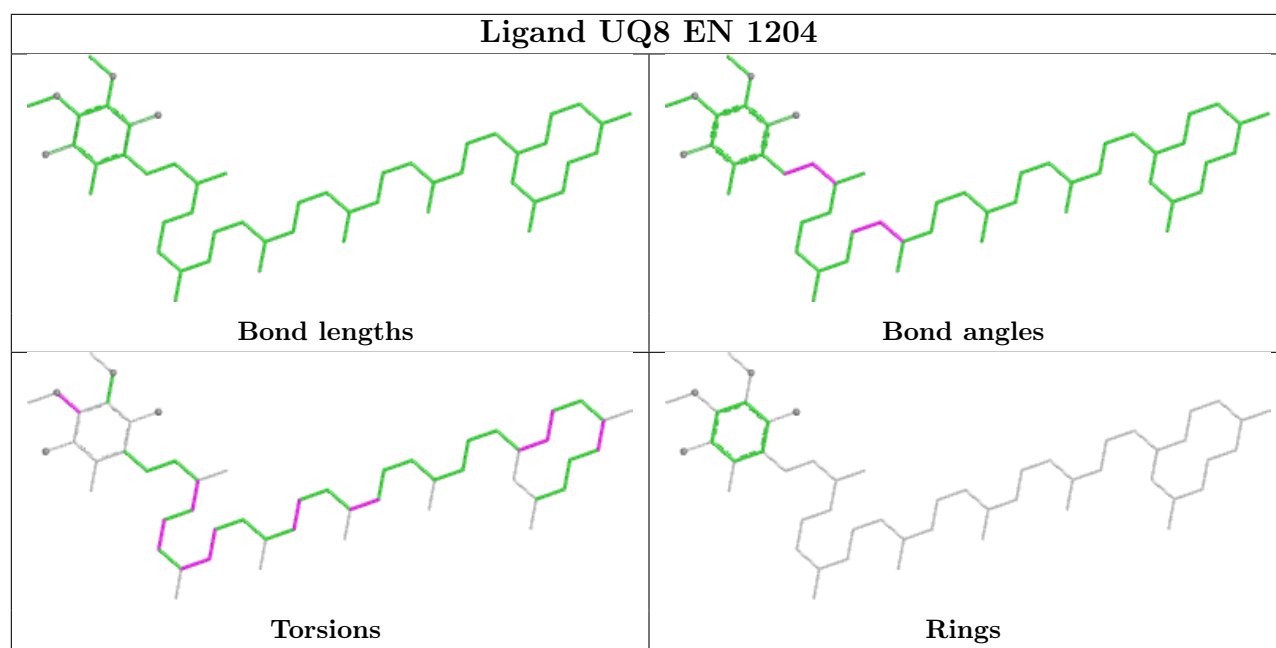


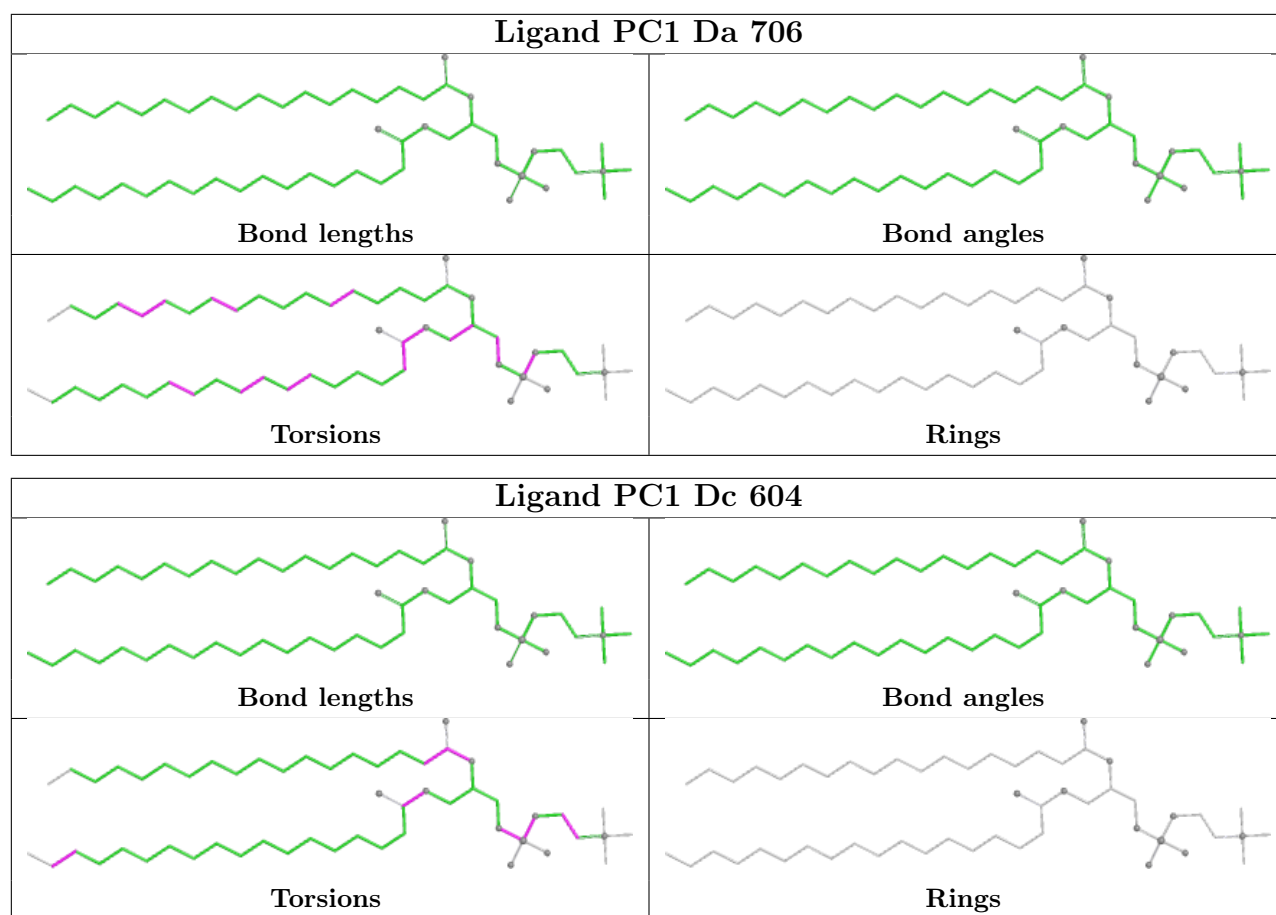












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

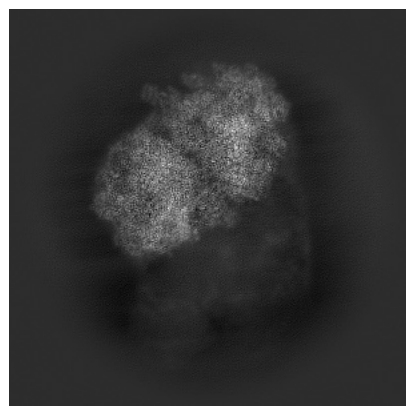
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15867. These allow visual inspection of the internal detail of the map and identification of artifacts.

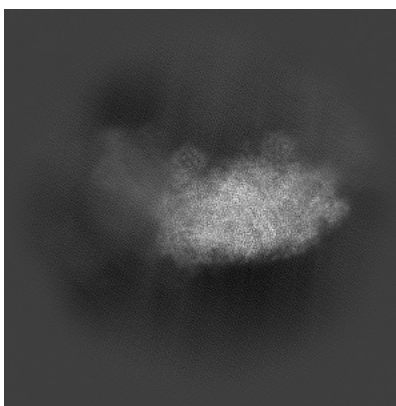
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

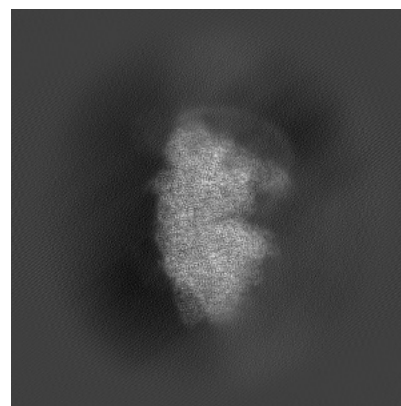
6.1.1 Primary map



X

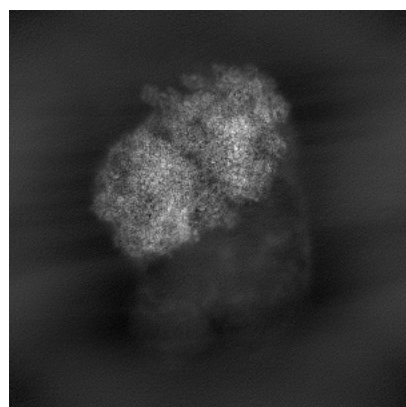


Y

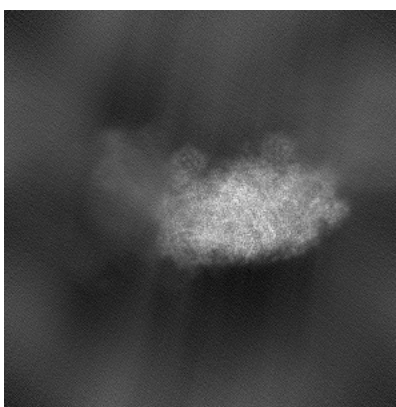


Z

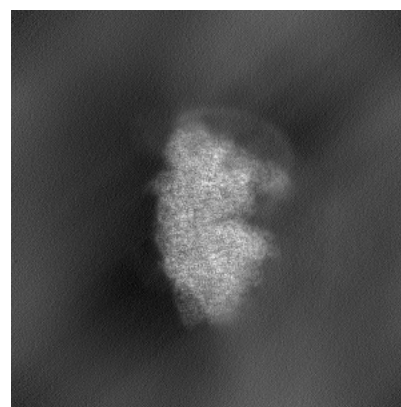
6.1.2 Raw map



X



Y

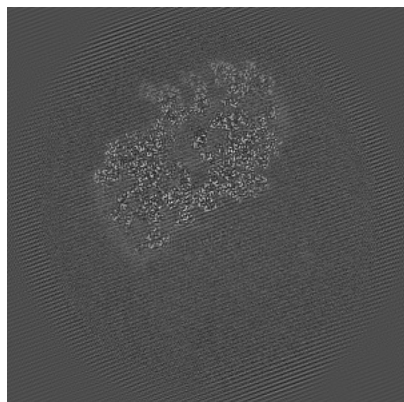


Z

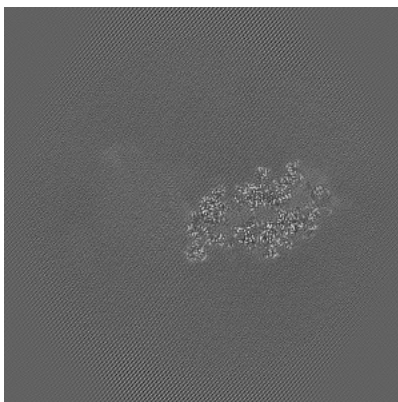
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

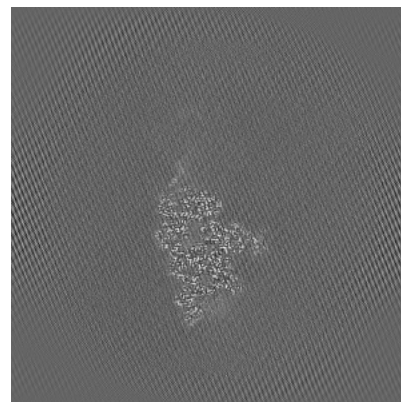
6.2.1 Primary map



X Index: 240

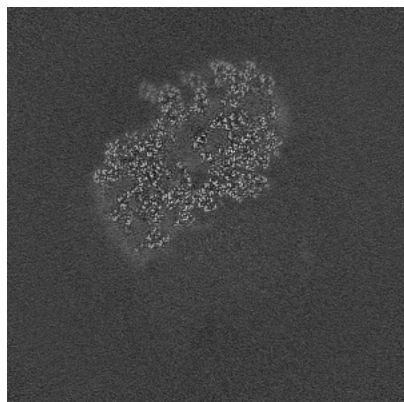


Y Index: 240

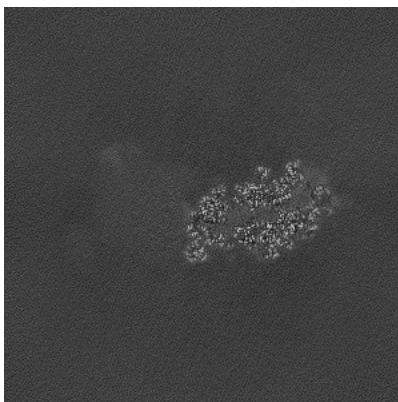


Z Index: 240

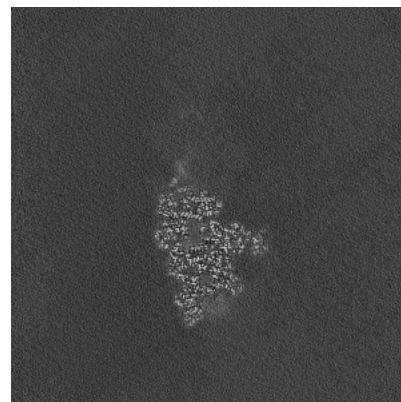
6.2.2 Raw map



X Index: 240



Y Index: 240

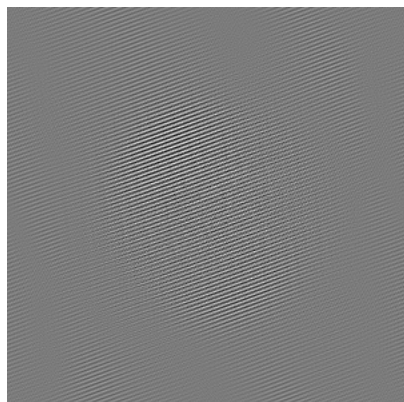


Z Index: 240

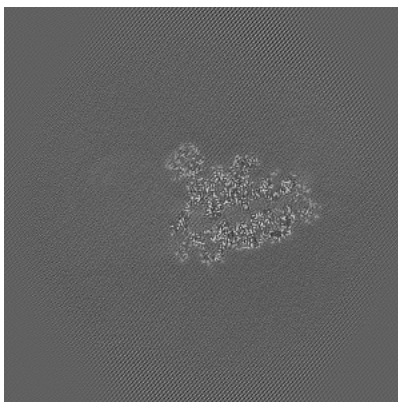
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

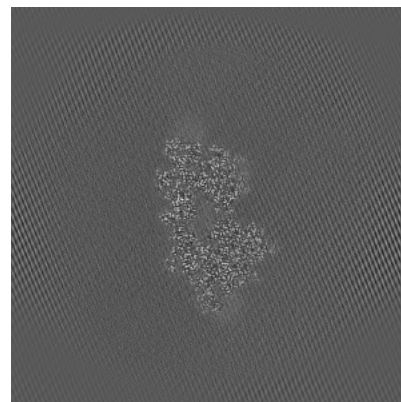
6.3.1 Primary map



X Index: 444

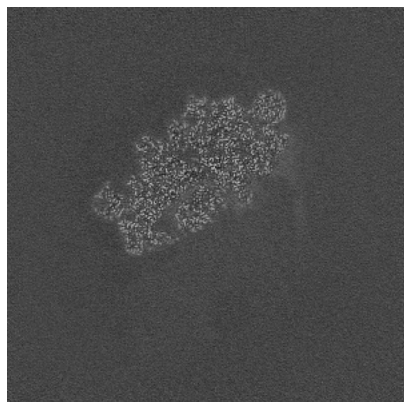


Y Index: 204

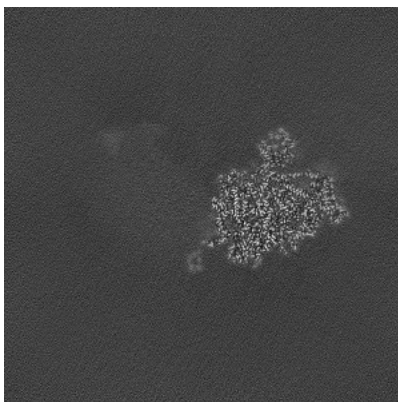


Z Index: 287

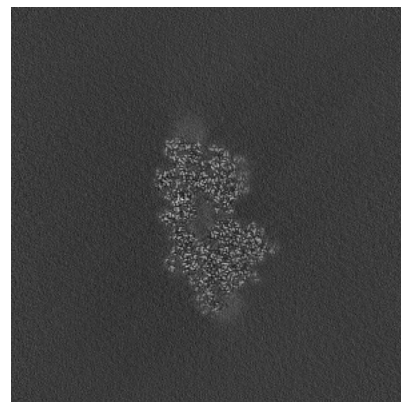
6.3.2 Raw map



X Index: 206



Y Index: 271

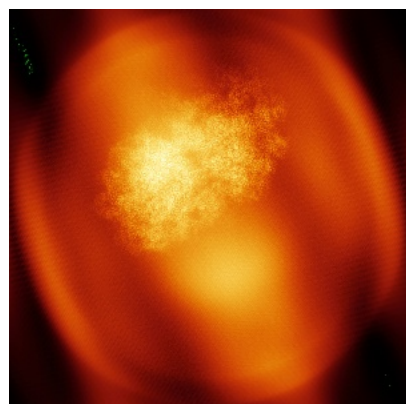


Z Index: 287

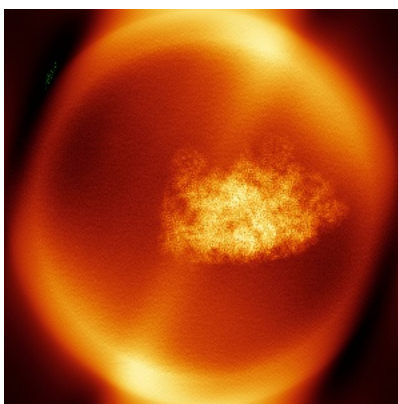
The images above show the largest variance slices of the map in three orthogonal directions.

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

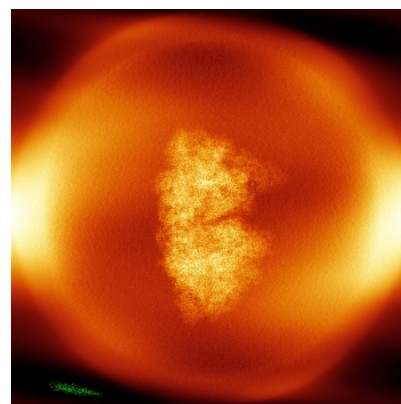
6.4.1 Primary map



X

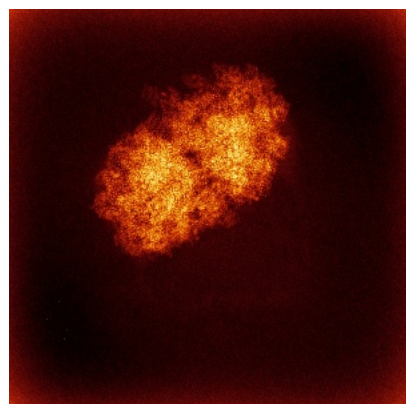


Y

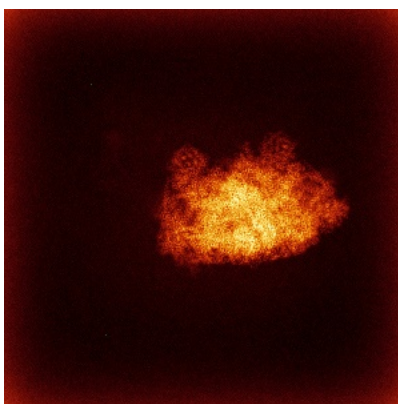


Z

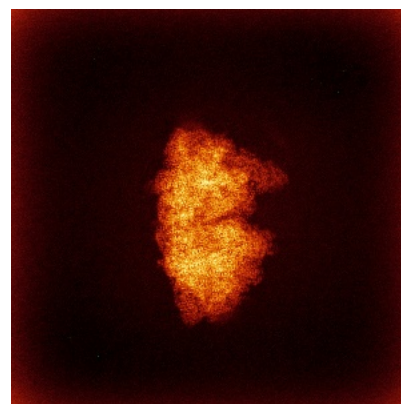
6.4.2 Raw map



X



Y

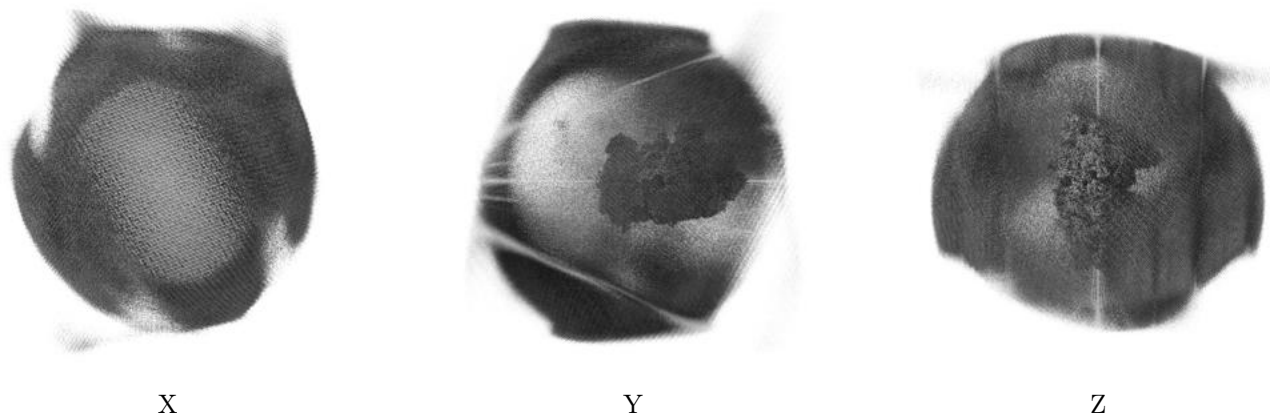


Z

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

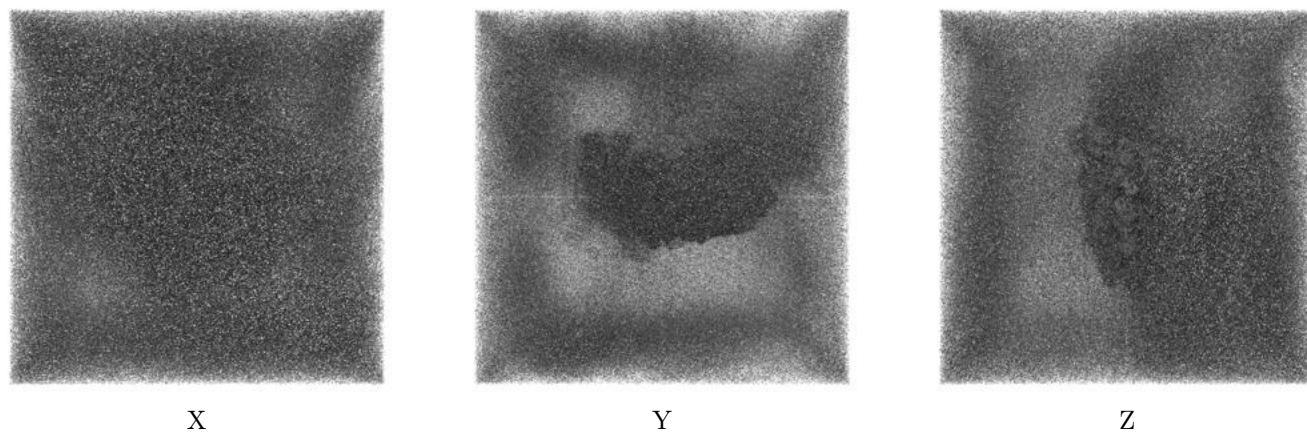
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

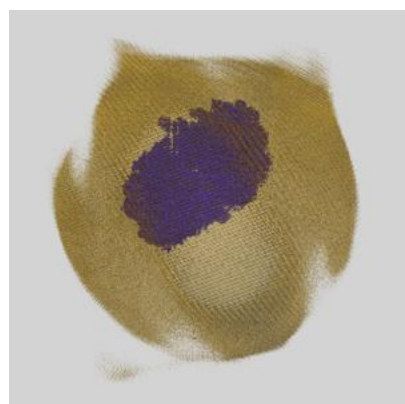
6.6 Mask visualisation [i](#)

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

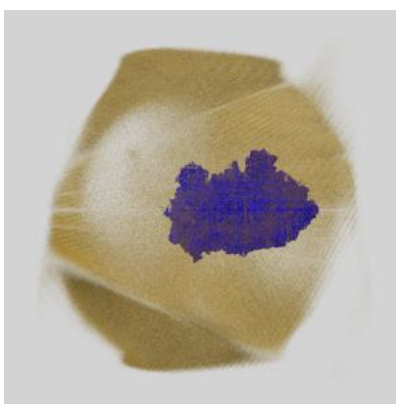
A mask typically either:

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

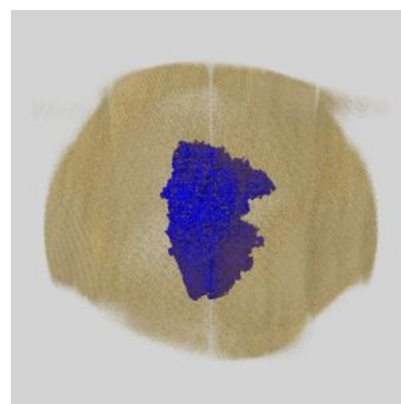
6.6.1 emd_15867_msk_1.map [i](#)



X



Y

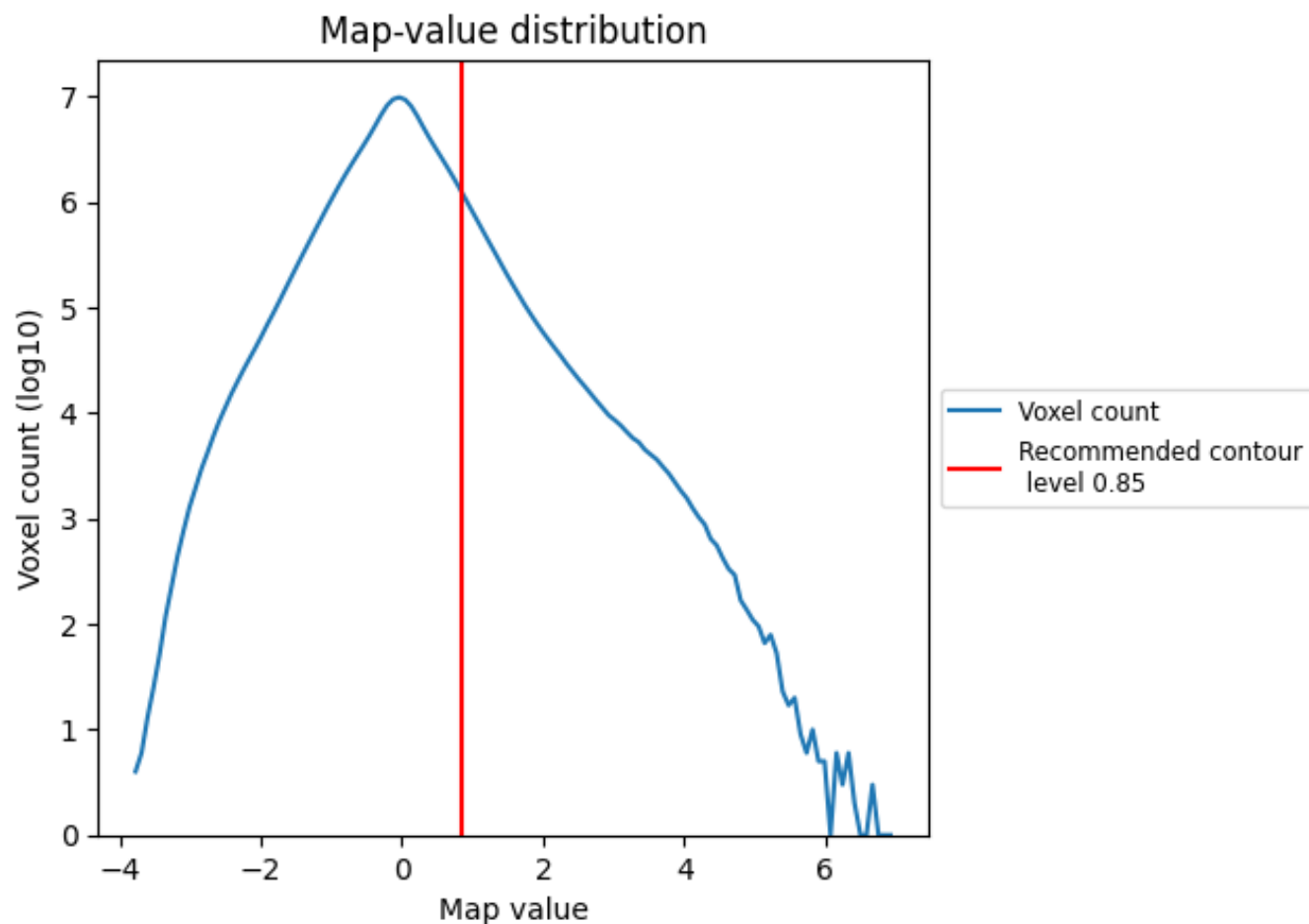


Z

7 Map analysis [i](#)

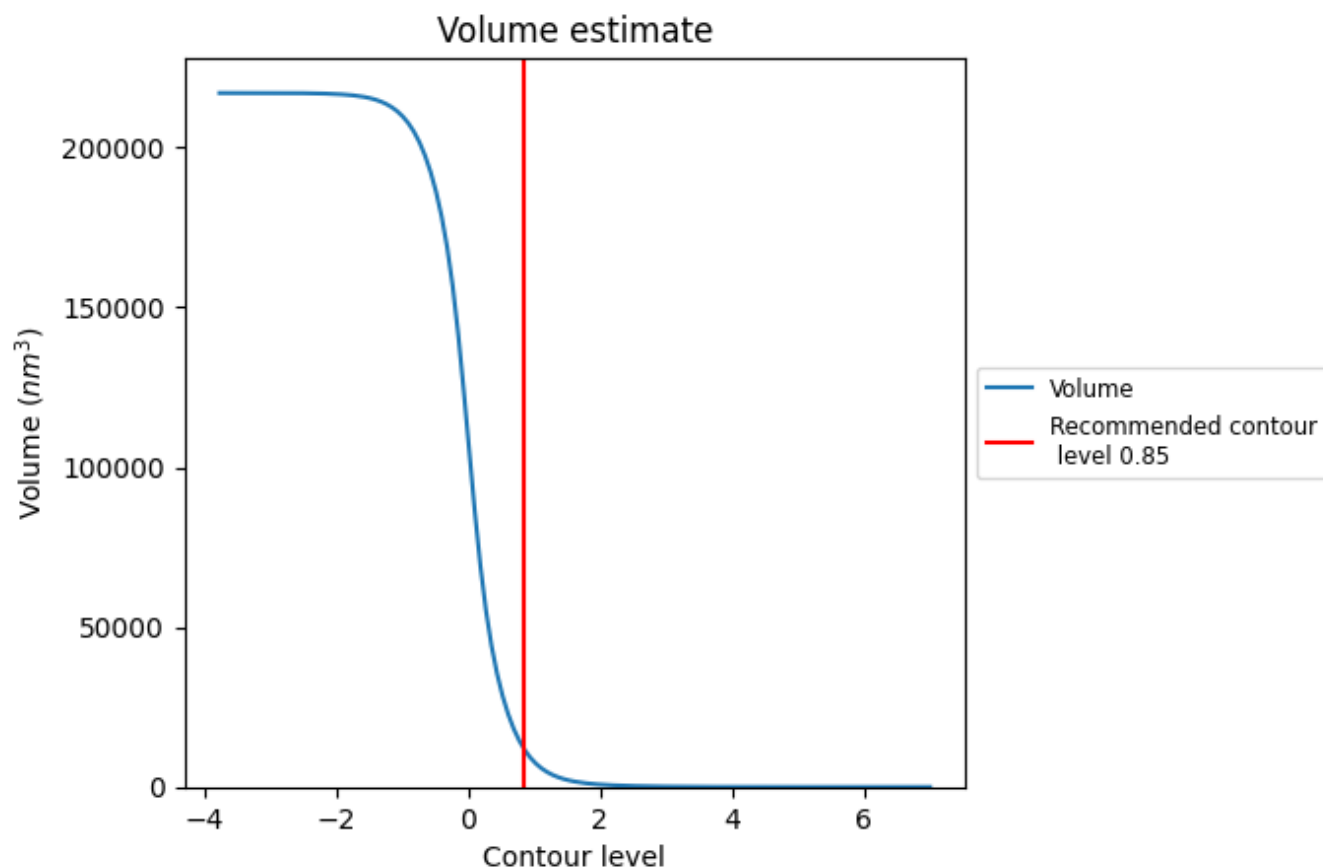
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

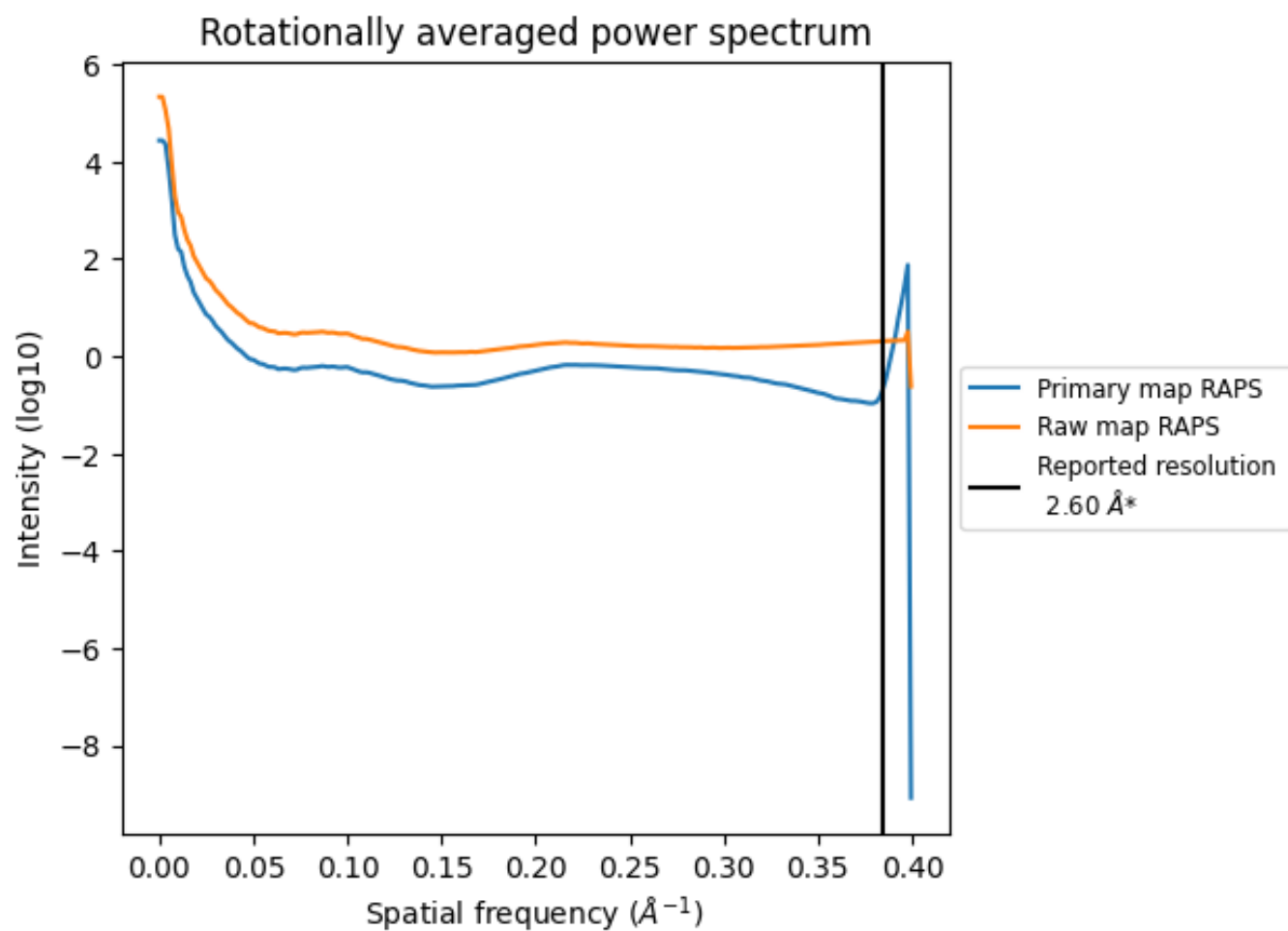
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11769 nm^3 ; this corresponds to an approximate mass of 10631 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 ⓘ

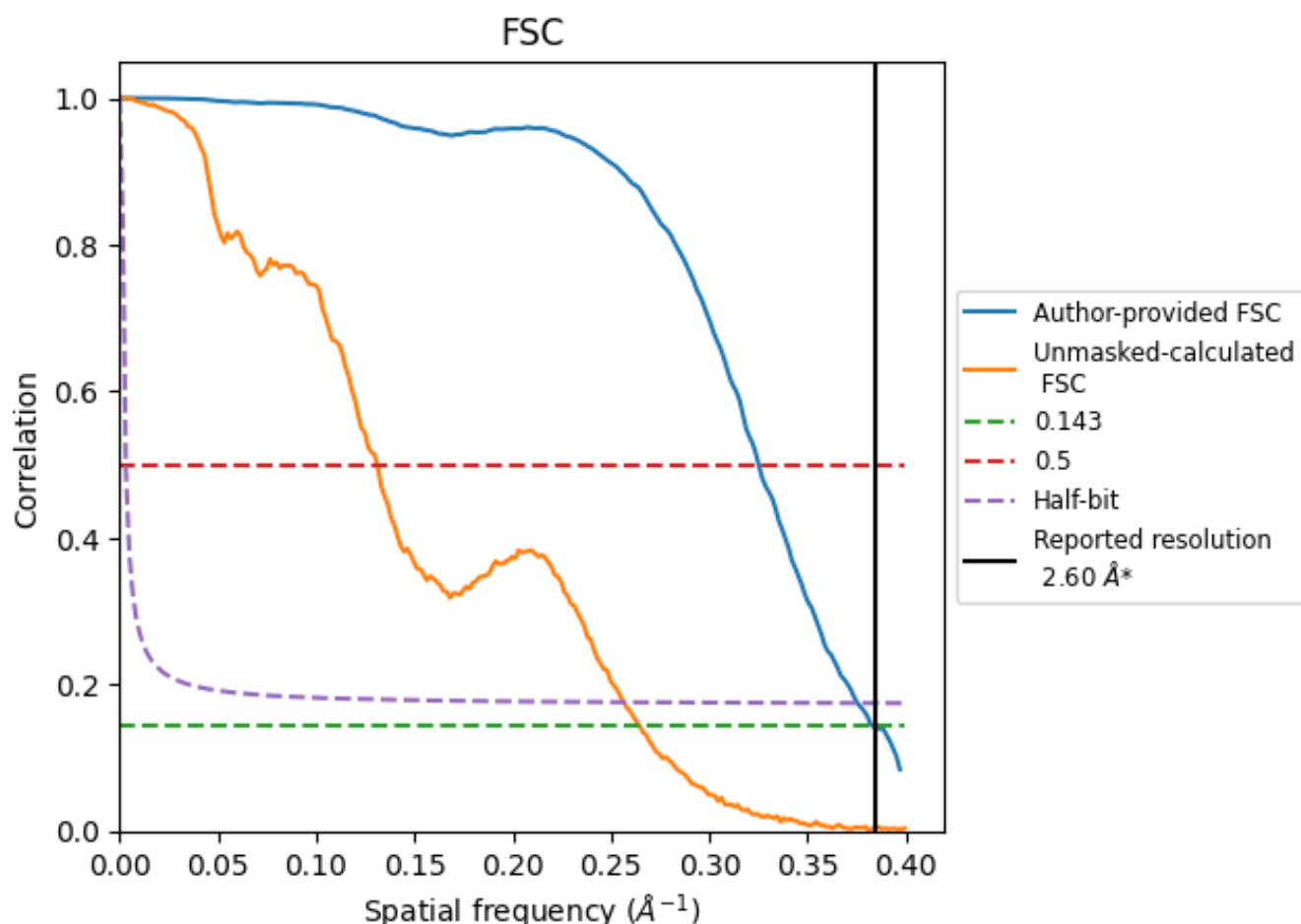


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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](#)

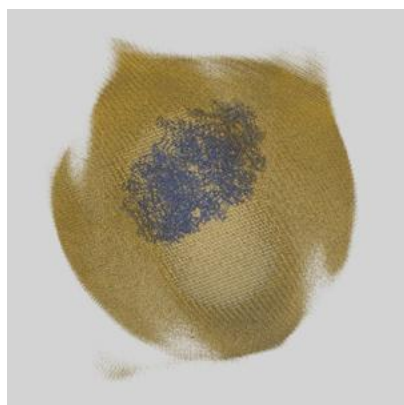
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	3.08	2.66
Unmasked-calculated*	3.78	7.63	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.6 by more than 10 %

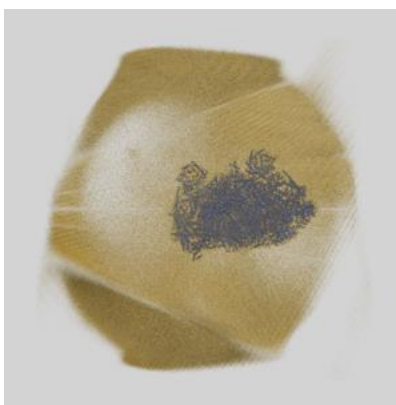
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15867 and PDB model 8B6H. Per-residue inclusion information can be found in section [3](#) on page [35](#).

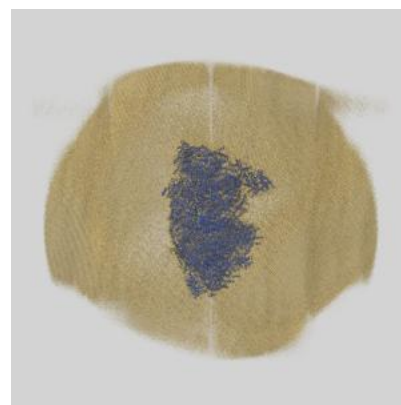
9.1 Map-model overlay [i](#)



X



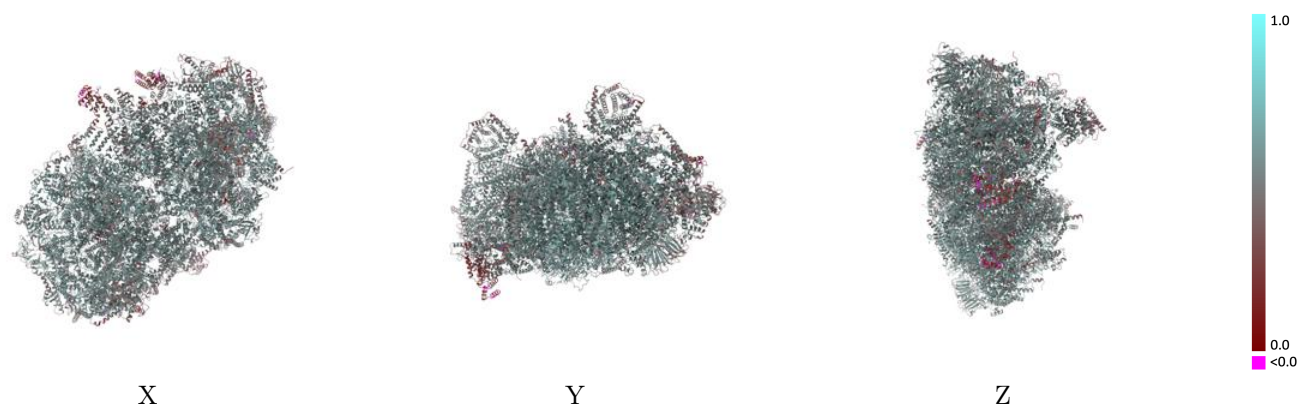
Y



Z

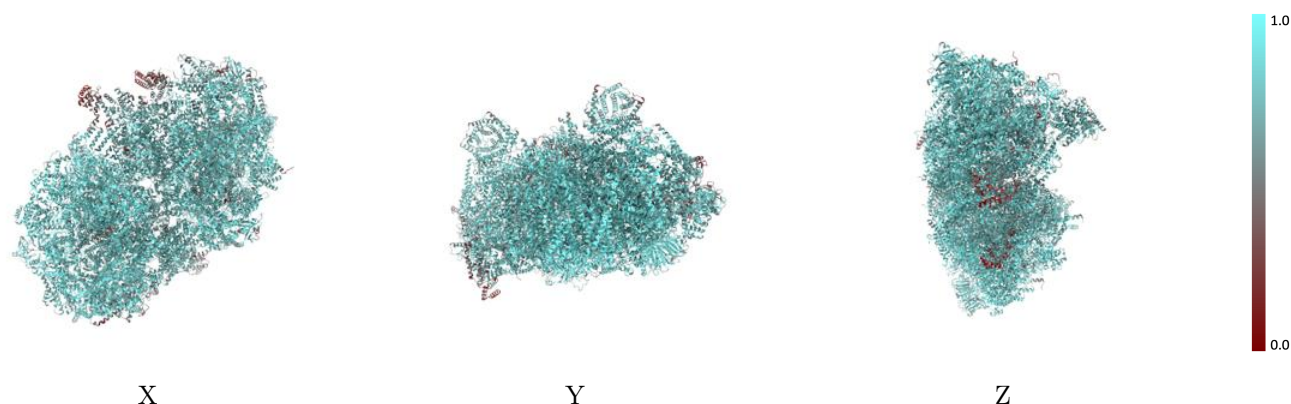
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



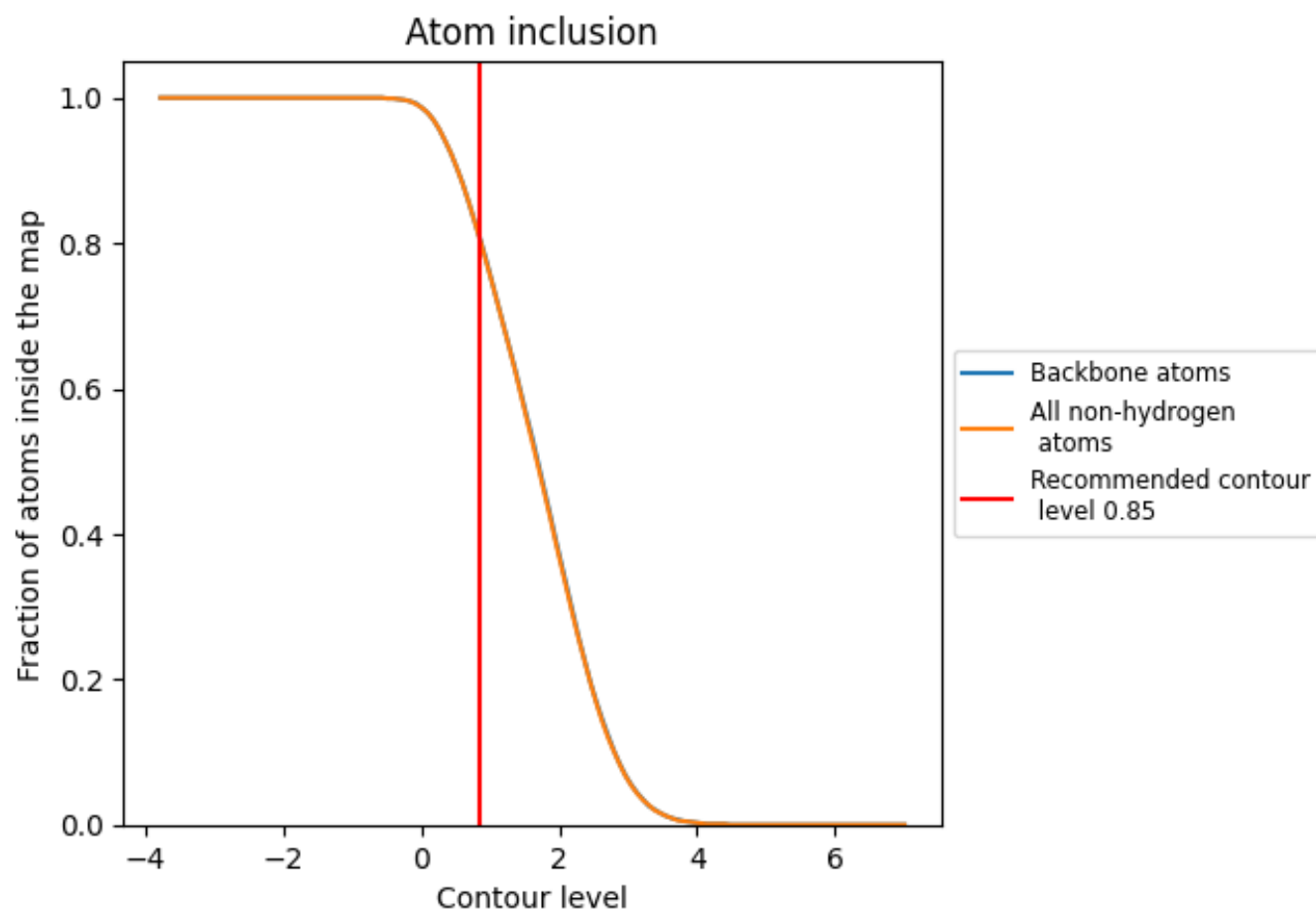
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.5310
DA	 0.8810	 0.5710
DB	 0.8500	 0.5430
DC	 0.8300	 0.5390
DD	 0.8510	 0.5550
DE	 0.8880	 0.5740
DF	 0.8890	 0.5670
DG	 0.7980	 0.5330
DH	 0.8850	 0.5740
DI	 0.8520	 0.5570
DJ	 0.7770	 0.5310
DK	 0.8630	 0.5500
DL	 0.8360	 0.5440
DM	 0.8640	 0.5680
DN	 0.7760	 0.5020
DO	 0.6980	 0.4450
DP	 0.8050	 0.5130
DQ	 0.8430	 0.5560
DR	 0.8460	 0.5530
DS	 0.8390	 0.5470
DT	 0.9000	 0.5850
DU	 0.8200	 0.5360
DV	 0.8040	 0.5240
DW	 0.7730	 0.4920
DX	 0.7740	 0.5200
DY	 0.8330	 0.5420
DZ	 0.8440	 0.5570
Da	 0.8890	 0.5800
Db	 0.8280	 0.5440
Dc	 0.8030	 0.5240
Dd	 0.8080	 0.5320
De	 0.8870	 0.5650
Df	 0.8780	 0.5640
Dg	 0.8040	 0.5350
Dh	 0.8330	 0.5540































































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Chain	Atom inclusion	Q-score
Di	 0.8280	 0.5500
Dj	 0.7660	 0.5300
Dk	 0.8440	 0.5420
Dl	 0.8090	 0.5110
Dm	 0.8380	 0.5440
Dn	 0.7040	 0.4610
Do	 0.5570	 0.3840
Dp	 0.7700	 0.4890
Dq	 0.8230	 0.5440
Dr	 0.8630	 0.5640
Ds	 0.8650	 0.5640
Dt	 0.8970	 0.5890
Du	 0.7640	 0.5150
Dv	 0.7940	 0.5110
Dw	 0.7680	 0.5000
Dx	 0.7520	 0.5130
Dy	 0.8110	 0.5200
Dz	 0.8030	 0.5230
EA	 0.8070	 0.5260
EB	 0.8090	 0.5290
EC	 0.6260	 0.3840
ED	 0.7530	 0.5100
EE	 0.8440	 0.5340
EF	 0.9090	 0.5870
EG	 0.8710	 0.5720
EH	 0.8430	 0.5530
EI	 0.8310	 0.5470
EJ	 0.8560	 0.5500
EK	 0.8080	 0.5280
EL	 0.7890	 0.5330
EM	 0.8530	 0.5510
EN	 0.8270	 0.5410
EO	 0.7610	 0.5170
EP	 0.8910	 0.5920
EQ	 0.9210	 0.5850
ER	 0.9190	 0.5840
ES	 0.9060	 0.5920
ET	 0.6820	 0.4310
EU	 0.7770	 0.5170
EV	 0.8080	 0.5100
EW	 0.7410	 0.4740
EX	 0.7180	 0.4750

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Chain	Atom inclusion	Q-score
EY	 0.7590	 0.4680
EZ	 0.8090	 0.5170
Ea	 0.7830	 0.5220
Eb	 0.8310	 0.5440
Ec	 0.4840	 0.3370
Ed	 0.6940	 0.4880
Ee	 0.8170	 0.5240
Ef	 0.8900	 0.5800
Eg	 0.7810	 0.5430
Eh	 0.8540	 0.5680
Ei	 0.7960	 0.5310
Ej	 0.7740	 0.4980
Ek	 0.7820	 0.5210
El	 0.7810	 0.5470
Em	 0.8570	 0.5550
En	 0.8240	 0.5480
Eo	 0.7860	 0.5290
Ep	 0.8270	 0.5520
Eq	 0.8960	 0.5810
Er	 0.9110	 0.6000
Es	 0.8860	 0.5860
Et	 0.6830	 0.4060
Eu	 0.7390	 0.5030
Ev	 0.8100	 0.5100
Ew	 0.7000	 0.4350
Ex	 0.6710	 0.4530
Ey	 0.7090	 0.4490
Ez	 0.7880	 0.5110
FA	 0.8150	 0.5050
Fa	 0.7740	 0.4920