wwPDB EM Validation Summary Report (i)

Feb 20, 2025 – 05:13 PM EST

PDB ID	:	8BQS
EMDB ID	:	EMD-16184
Title	:	Cryo-EM structure of the I-II-III2-IV2 respiratory supercomplex from Tetrahymena thermophila
Authors	:	Muhleip, A.; Kock Flygaard, R.; Baradaran, R.; Amunts, A.
Deposited on	:	2022-11-21
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

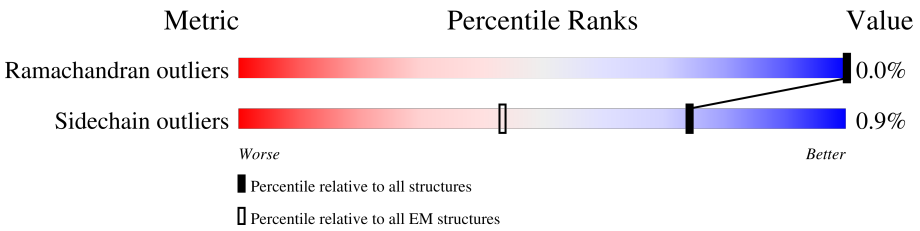
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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 <=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	A0	516	20% 97%
2	A1	362	93% 7%
3	A2	317	6% 84% 15%
4	A3	333	58% 87% 13%
5	A4	311	39% 100%
6	A5	282	10% 100%
7	A6	251	10% 91% 8%
8	A7	238	6% 55% 44%
9	A8	217	12% 100%

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Mol	Chain	Length	Quality of chain
10	A9	231	6% 98%
11	AA	750	6% 93% 5%
12	AB	718	25% 96%
13	AC	505	99%
14	AD	474	39% 93% 7%
15	AE	442	99%
16	AF	360	100%
17	AG	346	100%
18	AH	284	98%
19	AI	274	36% 84% 16%
20	AJ	255	99%
21	AK	257	89% 11%
22	AL	236	91% 8%
23	AM	233	99%
24	AN	206	9% 76% 24%
25	AO	198	99%
26	AP	194	11% 98%
27	AQ	189	5% 98%
28	AR	185	14% 97%
29	AS	172	99%
30	AT	162	97%
31	AU	150	7% 99%
32	AV	138	81% 19%
33	AW	133	74% 26%
34	AX	121	98%

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Mol	Chain	Length	Quality of chain
35	AY	116	99%
36	AZ	103	35%, 91%, 9%
37	B0	94	99%
38	B1	93	9%, 98%
39	B2	94	16%, 99%
40	B3	83	12%, 88%, 12%
41	B4	73	19%, 100%
42	B5	71	6%, 76%, 24%
43	B6	59	98%
44	BA	212	17%, 93%, 6%
45	BB	214	8%, 78%, 22%
46	BC	207	84%, 16%
47	BD	205	6%, 72%, 28%
48	BE	189	14%, 88%, 11%
49	BF	188	94%, 6%
50	BG	175	6%, 91%, 9%
51	BH	178	100%
52	BI	172	87%, 13%
53	BJ	166	86%, 13%
54	BK	144	5%, 76%, 24%
55	BL	143	9%, 98%
56	BM	135	94%, 5%
57	BN	135	7%, 99%
58	BO	136	8%, 100%
59	BP	129	56%, 44%

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Mol	Chain	Length	Quality of chain
60	BQ	127	80% 20%
61	BR	132	5% 68% 31%
62	BS	126	5% 95% 5%
63	BT	125	94% 6%
64	BU	134	13% 100%
65	BV	125	10% 100%
66	BW	120	7% 98%
67	BX	113	85% 15%
68	BY	100	100%
69	BZ	102	5% 100%
70	CH	195	32% 56% 44%
71	CM	76	51% 97%
72	CL	89	36% 99%
73	CA	636	92% 93% 6%
74	CI	114	39% 100%
75	CB	312	76% 90% 9%
76	CF	296	35% 74% 26%
77	CG	198	82% 98%
78	CK	93	59% 98%
79	CE	322	92% 98%
80	CJ	103	68% 100%
81	CN	62	71% 100%
82	CC	60	70% 98%
83	CO	46	59% 93% 7%
84	CD	44	77% 100%

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Mol	Chain	Length	Quality of chain
85	A	513	6% 93% 6%
85	a	513	37% 93% 6%
86	B	482	22% 95% 5%
86	b	482	26% 95% 5%
87	C	426	15% 99%
87	c	426	97%
88	D	319	92% 8%
88	d	319	21% 91% 8%
89	E	269	33% 90% 9%
89	e	269	60% 90% 9%
90	F	86	13% 100%
90	f	86	56% 98%
91	G	328	33% 99%
91	g	328	12% 99%
92	H	130	22% 99%
92	h	130	98%
93	I	119	8% 96%
93	i	119	34% 97%
94	J	66	74% 100%
94	j	66	76% 100%
95	K	62	16% 94% 6%
95	k	62	29% 94% 6%
96	L	41	22% 76% 22%
96	l	41	7% 78% 22%
97	DA	688	96%

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Mol	Chain	Length	Quality of chain
97	Da	688	96%
98	DB	604	9%, 98%
98	Db	604	12%, 98%
99	DC	594	7%, 97%
99	Dc	594	12%, 98%
100	DD	637	86%, 12%
100	Dd	637	87%, 12%
101	DE	130	97%
101	De	130	96%
102	DF	230	5%, 95%
102	Df	230	6%, 95%
103	DG	103	6%, 94%, 5%
103	Dg	103	95%, 5%
104	DH	134	99%
104	Dh	134	99%
105	DI	236	86%, 13%
105	Di	236	85%, 13%
106	DJ	220	98%
106	Dj	220	98%
107	DK	990	13%, 87%
107	Dk	990	13%, 87%
108	DM	490	92%, 7%
108	Dm	490	92%, 7%
109	DN	453	10%, 99%
109	Dn	453	13%, 99%

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Mol	Chain	Length	Quality of chain
110	DO	473	19% 92% 8%
110	Do	473	41% 92% 8%
111	DP	402	7% 72% 28%
111	Dp	402	13% 72% 28%
112	DQ	386	98%
112	Dq	386	99%
113	DR	348	69% 30%
113	Dr	348	70% 30%
114	DS	347	99%
114	Ds	347	99%
115	DT	318	92% 8%
115	Dt	318	92% 8%
116	DU	330	5% 99%
116	Du	330	9% 99%
117	DV	319	99%
117	Dv	319	99%
118	DW	318	13% 93% 5%
118	Dw	318	9% 93% 5%
119	DX	252	9% 99%
119	Dx	252	7% 98%
120	DY	234	79% 20%
120	Dy	234	6% 79% 20%
121	DZ	231	90% 10%
121	Dz	231	6% 90% 10%
122	EA	215	89% 10%

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Mol	Chain	Length	Quality of chain
122	Ea	215	6% 89% 10%
123	EB	210	99%
123	Eb	210	6% 98%
124	EC	212	35% 99%
124	Ec	212	50% 99%
125	ED	190	10% 99%
125	Ed	190	18% 99%
126	EE	193	5% 65% 35%
126	Ee	193	6% 65% 35%
127	EF	188	99%
127	Ef	188	99%
128	EG	100	98%
128	Eg	100	98%
129	EH	174	99%
129	Eh	174	100%
130	EI	173	97%
130	Ei	173	5% 97%
131	EV	89	7% 89% 11%
131	Ev	89	12% 89% 11%
132	EK	170	6% 99%
132	Ek	170	98%
133	EL	158	96%
133	El	158	96%
134	EM	154	99%
134	Em	154	99%

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Mol	Chain	Length	Quality of chain
135	EN	149	5% 97%
135	En	149	7% 97%
136	EO	124	10% 98%
136	Eo	124	7% 98%
137	EP	127	78% 21%
137	Ep	127	78% 21%
138	EQ	123	98%
138	Eq	123	98%
139	ER	105	98%
139	Er	105	99%
140	ES	89	100%
140	Es	89	100%
141	ET	93	30% 85% 12%
141	Et	93	38% 86% 12%
142	EU	90	8% 98%
142	Eu	90	8% 98%
143	EJ	175	8% 98%
143	Ej	175	14% 99%
144	EW	81	22% 78% 22%
144	Ew	81	35% 78% 22%
145	EX	72	19% 94%
145	Ex	72	26% 94%
146	EY	72	24% 96%
146	Ey	72	19% 96%
147	EZ	68	12% 82% 15%

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Mol	Chain	Length	Quality of chain
147	Ez	68	15% 84% 15%
148	FA	72	15% 96%
148	Fa	72	21% 96%
149	DL	462	82% 18%
149	Dl	462	7% 82% 18%

2 Entry composition (i)

There are 173 unique types of molecules in this entry. The entry contains 805862 atoms, of which 406234 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 Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A0	503	8090	2609	4019	699	750	13	0	0

- Molecule 2 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A1	338	5368	1737	2650	475	494	12	0	0

- Molecule 3 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	A2	269	4362	1392	2163	408	396	3	0	0

- Molecule 4 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	A3	291	4523	1438	2260	390	434	1	0	0

- Molecule 5 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	A4	311	4985	1583	2491	434	469	8	0	0

- Molecule 6 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	A5	282	4596	1478	2249	413	453	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	A6	230	3770	1241	1862	322	340	5	0	0

- Molecule 8 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	A7	133	2124	682	1040	182	209	11	0	0

- Molecule 9 is a protein called ND5a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	A8	217	3597	1153	1803	305	328	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	A9	231	3697	1219	1818	317	336	7	0	0

- Molecule 11 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	AA	713	11919	4066	5978	855	1004	16	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AB	688	10762	3410	5359	935	1030	28	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AC	505	8393	2859	4223	601	692	18	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AD	441	6744	2140	3345	596	639	24	0	0

- Molecule 15 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	AE	441	7126	2285	3539	620	658	24	0	0

- Molecule 16 is a protein called Ymf65.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	AF	359	6216	2132	3148	435	494	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	208	VAL	GLY	conflict	UNP Q951A3

- Molecule 17 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	AG	346	5531	1766	2727	481	549	8	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	AH	283	4656	1581	2350	334	379	12	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	AI	231	3710	1173	1848	321	358	10	0	0

- Molecule 20 is a protein called Ymf62.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AJ	254	4316	1478	2156	305	373	4	0	0

- Molecule 21 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AK	230	3519	1117	1740	306	351	5	0	0

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AL	218	3501	1155	1689	299	347	11	0	0

- Molecule 23 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AM	231	3558	1112	1788	316	335	7	0	0

- Molecule 24 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	AN	157	2651	846	1329	221	249	6	0	0

- Molecule 25 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AO	198	3363	1097	1680	268	312	6	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	AP	191	3104	1013	1505	301	280	5	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	AQ	187	3084	1027	1496	254	303	4	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	AR	181	2937	948	1445	267	269	8	0	0

- Molecule 29 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	AS	172	2802	903	1382	253	256	8	0	0

- Molecule 30 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	AT	161	2549	822	1272	220	225	10	0	0

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
31	AU	149	2436	800	1209	213	214	0	0

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
32	AV	112	1829	586	904	158	181	0	0

- Molecule 33 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	AW	98	1584	512	781	133	157	1	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	AX	121	2047	710	1020	143	170	4	0	0

- Molecule 35 is a protein called Ymf58.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	AY	116	1944	648	987	142	163	4	0	0

- Molecule 36 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	AZ	94	1552	491	775	140	144	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
37	B0	93	1607	531	802	139	135	0	0

- Molecule 38 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	B1	92	1536	497	746	146	146	1	0	0

- Molecule 39 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	B2	93	1485	480	728	129	142	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	B3	73	1251	414	618	113	105	1	0	0

- Molecule 41 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	B4	73	1247	408	623	111	104	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	B5	54	917	305	464	71	75	2	0	0

- Molecule 43 is a protein called NADH dehydrogenase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	B6	59	1043	362	528	78	72	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B6	49	VAL	LEU	conflict	UNP Q09FB0
B6	56	THR	SER	conflict	UNP Q09FB0

- Molecule 44 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	BA	199	3289	1071	1638	285	292	3	0	0

- Molecule 45 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	BB	167	2626	848	1280	228	265	5	0	0

- Molecule 46 is a protein called NDUB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	BC	173	2848	928	1406	244	264	6	0	0

- Molecule 47 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	BD	148	2414	764	1223	211	214	2	0	0

- Molecule 48 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	BE	168	2807	930	1385	227	260	5	0	0

- Molecule 49 is a protein called NDUB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	BF	177	2961	934	1486	267	270	4	0	0

- Molecule 50 is a protein called NDUA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	BG	160	2725	858	1376	256	227	8	0	0

- Molecule 51 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	BH	178	3036	1015	1554	215	247	5	0	0

- Molecule 52 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	BI	149	2318	731	1139	211	227	10	0	0

- Molecule 53 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	BJ	144	2361	767	1156	205	226	7	0	0

- Molecule 54 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	BK	109	1757	562	854	161	174	6	0	0

- Molecule 55 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	BL	142	2325	770	1138	202	209	6	0	0

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	BM	128	2074	695	1002	194	180	3	0	0

- Molecule 57 is a protein called PH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
57	BN	133	2229	716	1126	196	191	0	0

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	BO	136	2156	690	1058	190	208	10	0	0

- Molecule 59 is a protein called NDUB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	BP	72	1194	404	590	100	96	4	0	0

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	BQ	101	1674	547	829	140	153	5	0	0

- Molecule 61 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	BR	91	1449	460	719	129	137	4	0	0

- Molecule 62 is a protein called NDUB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	BS	120	1907	621	941	167	175	3	0	0

- Molecule 63 is a protein called NDUTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	BT	125	2016	696	953	172	190	5	0	0

- Molecule 64 is a protein called NDUTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
64	BU	134	2176	683	1094	194	204	1	0	0

- Molecule 65 is a protein called NDUTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
65	BV	125	2001	632	1014	177	177	1	0	0

- Molecule 66 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
66	BW	118	1848	603	893	167	179	6	0	0

- Molecule 67 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
67	BX	96	1552	512	755	139	146	0	0

- Molecule 68 is a protein called Ymf57.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
68	BY	100	1806	620	917	128	138	3	0	0

- Molecule 69 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	BZ	102	1690	553	840	139	150	8	0	0

- Molecule 70 is a protein called Diphthamide synthesis protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
70	CH	110	1700	529	845	147	171	8	0	0

- Molecule 71 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
71	CM	74	1232	403	603	115	109	2	0	0

- Molecule 72 is a protein called Transposase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
72	CL	88	1522	499	752	125	144	2	0	0

- Molecule 73 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	CA	599	9198	2907	4574	825	866	26	0	0

- Molecule 74 is a protein called DUF4885 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
74	CI	114	1805	580	890	153	180	2	0	0

- Molecule 75 is a protein called succinate dehydrogenase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
75	CB	285	4561	1457	2261	392	430	21	0	0

- Molecule 76 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
76	CF	218	3598	1171	1786	306	331	4	0	0

- Molecule 77 is a protein called chain 77.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
77	CG	196	3247	1072	1593	273	305	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
78	CK	93	1577	530	782	129	134	2	0	0

- Molecule 79 is a protein called NmrA domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
79	CE	321	5115	1623	2554	449	488	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
80	CJ	103	1663	554	815	140	151	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
81	CN	62	1029	345	515	80	87	2	0	0

- Molecule 82 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
82	CC	59	976	319	487	86	83	1	0	0

- Molecule 83 is a protein called SDHTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
83	CO	43	740	245	376	60	57	2	0	0

- Molecule 84 is a protein called succinate dehydrogenase complex iron-sulfur subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
84	CD	44	807	271	412	61	62	1	0	0

- Molecule 85 is a protein called Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
85	A	482	7587	2437	3740	671	734	5	0	0
			Total	C	H	N	O	S		
85	a	482	7587	2437	3740	671	734	5	0	0

- Molecule 86 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
86	B	460	7118	2240	3555	609	708	6	0	0
			Total	C	H	N	O	S		
86	b	460	7118	2240	3555	609	708	6	0	0

- Molecule 87 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
87	C	426	7075	2417	3485	541	610	22	0	0
			Total	C	H	N	O	S		
87	c	426	7074	2417	3484	541	610	22	0	0

- Molecule 88 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
88	D	295	4832	1627	2343	418	431	13	0	0
88	d	295	4832	1627	2343	418	431	13	0	0

- Molecule 89 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
89	E	245	3893	1251	1927	344	362	9	0	0
89	e	245	3891	1251	1925	344	362	9	0	0

- Molecule 90 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
90	F	86	1372	432	686	116	128	10	0	0
90	f	85	1352	427	674	115	127	9	0	0

- Molecule 91 is a protein called UQCRTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
91	G	327	5474	1789	2706	482	491	6	0	0
91	g	327	5474	1789	2706	482	491	6	0	0

- Molecule 92 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
92	H	129	2138	708	1040	195	187	8	0	0
92	h	129	2138	708	1040	195	187	8	0	0

- Molecule 93 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
93	I	117	1998	664	1003	164	166	1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
93	i	117	1998	664	1003	164	166	1	0	0

- Molecule 94 is a protein called UQCRTT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
94	J	66	596	198	266	66	66	0	0
94	j	66	596	198	266	66	66	0	0

- Molecule 95 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
95	K	58	1004	341	503	79	79	2	0	0
95	k	58	1004	341	503	79	79	2	0	0

- Molecule 96 is a protein called UQCRTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
96	L	32	535	178	273	41	42	1	0	0
96	l	32	535	178	273	41	42	1	0	0

- Molecule 97 is a protein called Cytochrome c oxidase subunit 1.

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

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 98 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 99 is a protein called Ymf68.

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

- Molecule 100 is a protein called Cytochrome C oxidase subunit Vb protein.

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

- Molecule 101 is a protein called Transmembrane protein, putative.

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

- Molecule 102 is a protein called Structural protein.

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

- Molecule 103 is a protein called Transmembrane protein, putative.

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

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

- Molecule 104 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
104	DH	134	2299	771	1129	197	201	1	0	0
			Total	C	H	N	O	S		
104	Dh	134	2299	771	1129	197	201	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	0	ACE	-	acetylation	UNP I7MGF9
Dh	0	ACE	-	acetylation	UNP I7MGF9

- Molecule 105 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 106 is a protein called Transmembrane protein, putative.

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

- Molecule 107 is a protein called CTF/NF-I domain-containing protein.

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

- Molecule 108 is a protein called Transmembrane protein, putative.

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

- Molecule 109 is a protein called Ymf67.

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

- Molecule 110 is a protein called Protein phosphatase 2C, putative.

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

- Molecule 111 is a protein called SURF1-like protein.

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

- Molecule 112 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
112	DQ	384	6271	2041	3102	546	575	7	0	0
112	Dq	384	6271	2041	3102	546	575	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DQ	0	ACE	-	acetylation	UNP Q23DP7

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Chain	Residue	Modelled	Actual	Comment	Reference
Dq	0	ACE	-	acetylation	UNP Q23DP7

- Molecule 113 is a protein called Transmembrane protein, putative.

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

- Molecule 114 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
114	DS	347	5636	1892	2770	469	492	13	0	0
114	Ds	347	5636	1892	2770	469	492	13	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DS	0	ACE	-	acetylation	UNP A4VDV3
Ds	0	ACE	-	acetylation	UNP A4VDV3

- Molecule 115 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

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

- Molecule 116 is a protein called Carrier protein.

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

- Molecule 117 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
117	DV	319	5114	1667	2552	440	451	4	0	0
117	Dv	319	5114	1667	2552	440	451	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	0	ACE	-	acetylation	UNP Q23M99
Dv	0	ACE	-	acetylation	UNP Q23M99

- Molecule 118 is a protein called SURF1-like protein.

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

- Molecule 119 is a protein called COXTT9.

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

- Molecule 120 is a protein called COXTT10.

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

- Molecule 121 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
121	DZ	208	3382	1089	1671	302	317	3	0	0
121	Dz	208	3383	1089	1672	302	317	3	0	0

- Molecule 122 is a protein called COXTT12,Transmembrane protein,Transmembrane protei n,Transmembrane protein.

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

- Molecule 123 is a protein called Transmembrane protein, putative.

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

- Molecule 124 is a protein called COXTT27.

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

- Molecule 125 is a protein called Ymf75.

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

- Molecule 126 is a protein called Mobilization protein.

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

- Molecule 127 is a protein called Iron-binding zinc finger CDGSH type protein.

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

- Molecule 128 is a protein called COXTT28.

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

- Molecule 129 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
129	EH	174	2820	929	1382	243	257	9	0	0
129	Eh	174	2820	929	1382	243	257	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EH	0	ACE	-	acetylation	UNP Q23D87
Eh	0	ACE	-	acetylation	UNP Q23D87

- Molecule 130 is a protein called Transmembrane protein.

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

- Molecule 131 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
131	EV	79	1276	411	633	109	117	6	0	0
131	Ev	79	1276	411	633	109	117	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EV	0	ACE	-	acetylation	UNP I7LVX0
Ev	0	ACE	-	acetylation	UNP I7LVX0

- Molecule 132 is a protein called Complex III subunit VII.

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

- Molecule 133 is a protein called Transmembrane protein, putative.

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

- Molecule 134 is a protein called Transmembrane protein, putative.

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

- Molecule 135 is a protein called COXTT22.

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

- Molecule 136 is a protein called Transmembrane protein, putative.

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

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

- Molecule 137 is a protein called Phage protein.

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

- Molecule 138 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
138	EQ	123	2004	667	989	171	173	4	0	0
138	Eq	123	2004	667	989	171	173	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EQ	0	ACE	-	acetylation	UNP Q22W32
Eq	0	ACE	-	acetylation	UNP Q22W32

- Molecule 139 is a protein called Lysozyme.

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

- Molecule 140 is a protein called Ymf70.

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

- Molecule 141 is a protein called Zf-Tim10_DDP domain-containing protein.

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

- Molecule 142 is a protein called ABC transporter.

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

- Molecule 143 is a protein called YflT domain-containing protein.

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

- Molecule 144 is a protein called Cullin domain-containing protein.

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

- Molecule 145 is a protein called Zf-Tim10_DDP domain-containing protein.

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

- Molecule 146 is a protein called Annexin.

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

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

- Molecule 147 is a protein called Transposase.

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

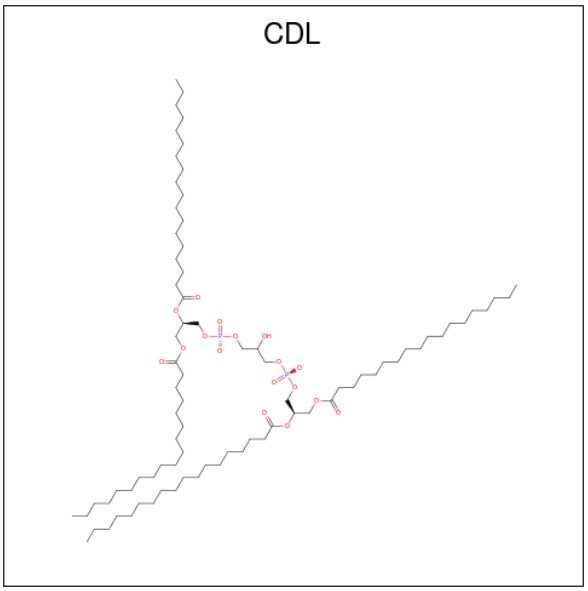
- Molecule 148 is a protein called Tim10/DDP family zinc finger protein.

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

- Molecule 149 is a protein called Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150.

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

- Molecule 150 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
			Total	C	H	O	P	
150	A0	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	A0	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	A1	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AA	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AA	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AF	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AF	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AM	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	AP	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	B0	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	B0	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	B1	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	BC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BE	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BL	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BT	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BT	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BV	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BY	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	E	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	H	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	H	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	c	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	c	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	c	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	c	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	g	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	h	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DA	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DA	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DH	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DH	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DI	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	DJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DM	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DM	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DN	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DN	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DN	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DN	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DO	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DQ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DQ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DQ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DR	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DR	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DS	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DS	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DS	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DU	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	DU	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DU	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DU	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DV	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DV	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DV	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DX	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DX	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DX	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DY	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	DZ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EA	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EB	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	ED	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	ED	1	255	81	155	17	2	0
			Total	C	H	O	P	
150	ED	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EH	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EI	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EK	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EL	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EL	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	EL	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EN	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EN	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	EO	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	ES	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Da	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dc	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dc	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dd	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dd	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dd	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dd	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dg	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dg	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dh	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dh	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Di	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Di	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dj	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dj	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dj	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	Dj	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dj	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dj	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dm	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dm	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dn	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dn	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dn	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dn	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Do	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dq	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dq	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dq	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dr	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dr	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ds	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ds	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ds	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ds	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Du	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Du	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	Du	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dv	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dv	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dv	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dx	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dx	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Dy	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ea	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ea	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Eb	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ed	1	255	81	155	17	2	0
			Total	C	H	O	P	
150	Ed	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Eg	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Eh	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ei	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ek	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	El	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	El	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	El	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	En	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	Ep	1	256	81	156	17	2	0

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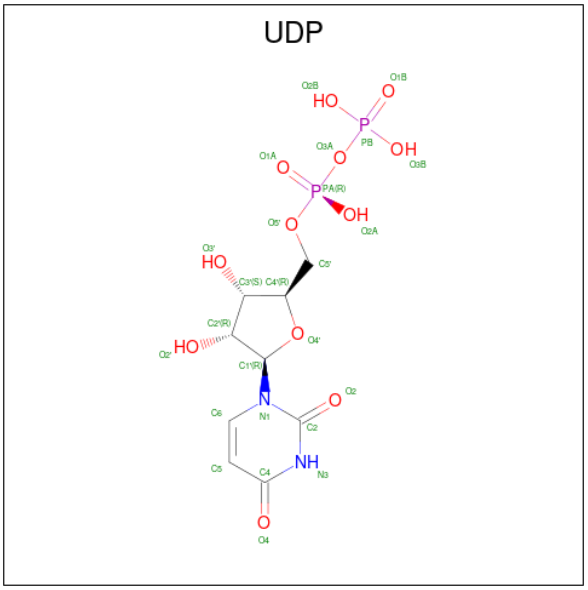
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	Eu	1	256	81	156	17	2	0

- Molecule 151 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

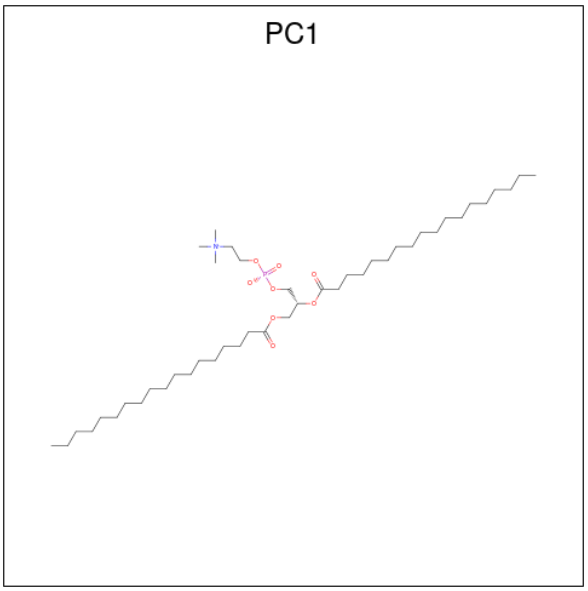


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
151	A0	1	36	9	11	2	12	2	0

- Molecule 152 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
152	A0	1	1	1	0
152	A8	1	1	1	0
152	DA	1	1	1	0
152	Da	1	1	1	0

- Molecule 153 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
			Total	C	H	N	O	P	
153	A0	1	142	44	88	1	8	1	0
153	A1	1	142	44	88	1	8	1	0
153	A2	1	142	44	88	1	8	1	0
153	A6	1	142	44	88	1	8	1	0
153	A6	1	142	44	88	1	8	1	0
153	A9	1	142	44	88	1	8	1	0
153	A9	1	142	44	88	1	8	1	0
153	AA	1	142	44	88	1	8	1	0
153	AA	1	142	44	88	1	8	1	0
153	AA	1	142	44	88	1	8	1	0
153	AA	1	142	44	88	1	8	1	0
153	AA	1	142	44	88	1	8	1	0
153	AC	1	142	44	88	1	8	1	0
153	AH	1	142	44	88	1	8	1	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
153	AJ	1	142	44	88	1	8	1	0
153	AL	1	142	44	88	1	8	1	0
153	AM	1	142	44	88	1	8	1	0
153	AQ	1	142	44	88	1	8	1	0
153	AU	1	142	44	88	1	8	1	0
153	AU	1	142	44	88	1	8	1	0
153	AX	1	142	44	88	1	8	1	0
153	B1	1	142	44	88	1	8	1	0
153	B1	1	142	44	88	1	8	1	0
153	BG	1	142	44	88	1	8	1	0
153	BS	1	142	44	88	1	8	1	0
153	BS	1	142	44	88	1	8	1	0
153	BT	1	142	44	88	1	8	1	0
153	CC	1	142	44	88	1	8	1	0
153	A	1	142	44	88	1	8	1	0
153	C	1	142	44	88	1	8	1	0
153	C	1	142	44	88	1	8	1	0
153	C	1	142	44	88	1	8	1	0
153	D	1	142	44	88	1	8	1	0
153	E	1	142	44	88	1	8	1	0
153	K	1	142	44	88	1	8	1	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
153	K	1	142	44	88	1	8	1	0
153	c	1	142	44	88	1	8	1	0
153	c	1	142	44	88	1	8	1	0
153	c	1	142	44	88	1	8	1	0
153	d	1	142	44	88	1	8	1	0
153	e	1	142	44	88	1	8	1	0
153	g	1	142	44	88	1	8	1	0
153	k	1	142	44	88	1	8	1	0
153	DA	1	141	44	87	1	8	1	0
153	DA	1	142	44	88	1	8	1	0
153	DB	1	142	44	88	1	8	1	0
153	DC	1	142	44	88	1	8	1	0
153	DC	1	142	44	88	1	8	1	0
153	DC	1	142	44	88	1	8	1	0
153	DC	1	142	44	88	1	8	1	0
153	DC	1	141	44	87	1	8	1	0
153	DG	1	142	44	88	1	8	1	0
153	DI	1	142	44	88	1	8	1	0
153	DJ	1	142	44	88	1	8	1	0
153	DQ	1	142	44	88	1	8	1	0
153	DS	1	142	44	88	1	8	1	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
153	DV	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	DV	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	DV	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	DX	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	DX	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	DY	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EB	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EB	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EN	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EO	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EO	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EO	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	EO	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Da	1	141	44	87	1	8	1	0
			Total	C	H	N	O	P	
153	Da	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Db	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dc	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dc	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dc	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dc	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dc	1	141	44	87	1	8	1	0

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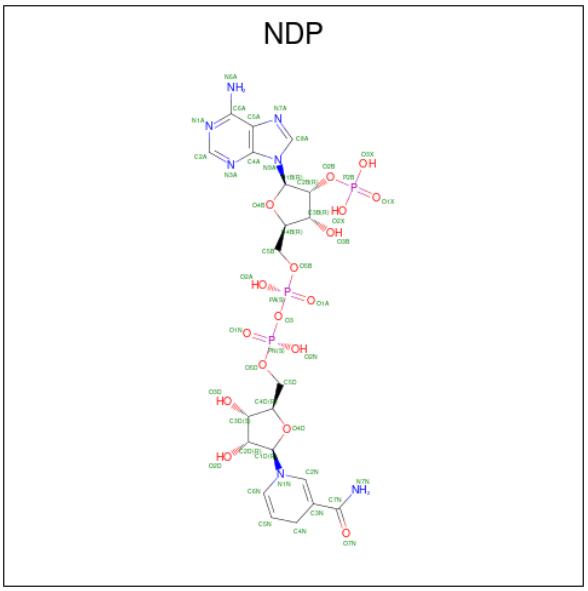
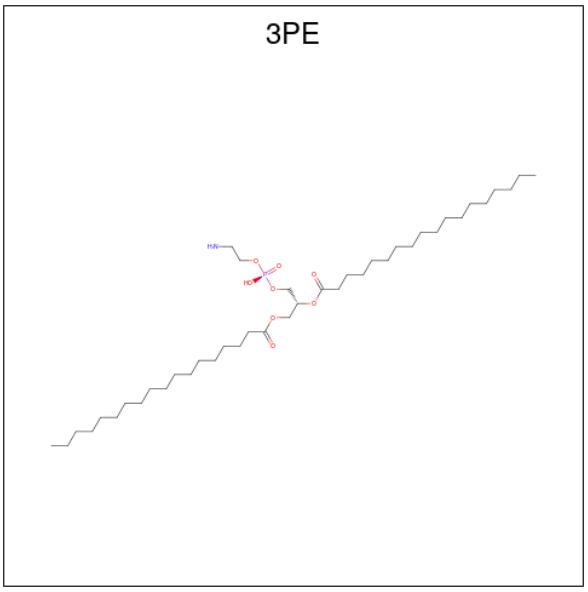
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
153	Dg	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Di	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dj	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dq	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Ds	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dv	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dv	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dv	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dv	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dx	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dx	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dx	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dy	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Eb	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Eb	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Ef	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	El	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Eo	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Eo	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Eo	1	142	44	88	1	8	1	0

- Molecule 154 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
154	A1	1	74	21	26	7	17	3	0

- Molecule 155 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
			Total	C	H	N	O	P	
155	A2	1	133	41	82	1	8	1	0
155	A9	1	133	41	82	1	8	1	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
155	AJ	1	133	41	82	1	8	1	0
155	BA	1	133	41	82	1	8	1	0
155	BP	1	133	41	82	1	8	1	0
155	BT	1	133	41	82	1	8	1	0
155	CK	1	133	41	82	1	8	1	0
155	CC	1	133	41	82	1	8	1	0
155	CD	1	133	41	82	1	8	1	0
155	C	1	133	41	82	1	8	1	0
155	G	1	133	41	82	1	8	1	0
155	DC	1	133	41	82	1	8	1	0
155	DC	1	133	41	82	1	8	1	0
155	DG	1	133	41	82	1	8	1	0
155	DG	1	133	41	82	1	8	1	0
155	DI	1	133	41	82	1	8	1	0
155	DJ	1	133	41	82	1	8	1	0
155	DN	1	133	41	82	1	8	1	0
155	DR	1	133	41	82	1	8	1	0
155	DS	1	133	41	82	1	8	1	0
155	DX	1	133	41	82	1	8	1	0
155	DX	1	133	41	82	1	8	1	0
155	DX	1	133	41	82	1	8	1	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
155	EL	1	133	41	82	1	8	1	0
155	EM	1	133	41	82	1	8	1	0
155	EN	1	133	41	82	1	8	1	0
155	EO	1	133	41	82	1	8	1	0
155	Da	1	133	41	82	1	8	1	0
155	Dc	1	133	41	82	1	8	1	0
155	Dc	1	133	41	82	1	8	1	0
155	Dd	1	133	41	82	1	8	1	0
155	Dg	1	133	41	82	1	8	1	0
155	Di	1	133	41	82	1	8	1	0
155	Dr	1	133	41	82	1	8	1	0
155	Dr	1	133	41	82	1	8	1	0
155	Ds	1	133	41	82	1	8	1	0
155	Ds	1	133	41	82	1	8	1	0
155	Dx	1	133	41	82	1	8	1	0
155	Dx	1	133	41	82	1	8	1	0
155	Dx	1	133	41	82	1	8	1	0
155	Dx	1	133	41	82	1	8	1	0
155	El	1	133	41	82	1	8	1	0
155	Em	1	133	41	82	1	8	1	0
155	Eo	1	133	41	82	1	8	1	0

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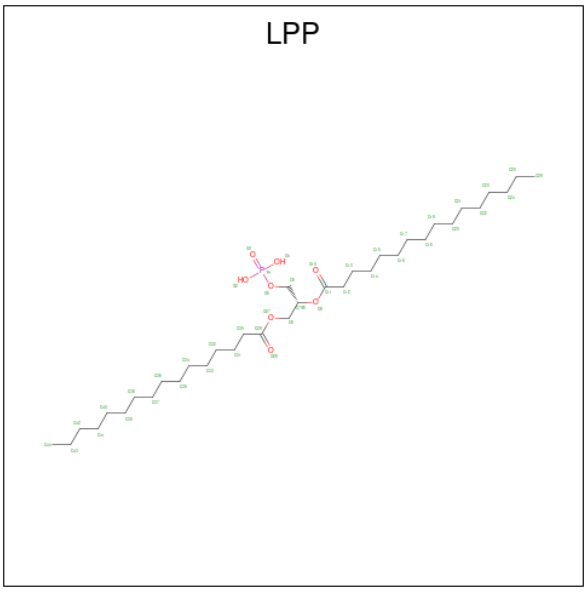
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
155	Eo	1	133	41	82	1	8	1	0

- Molecule 156 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
156	A6	1	111	35	67	8	1	0
156	AA	1	111	35	67	8	1	0
156	AC	1	111	35	67	8	1	0
156	AL	1	111	35	67	8	1	0
156	DA	1	111	35	67	8	1	0
156	DN	1	111	35	67	8	1	0
156	DN	1	111	35	67	8	1	0
156	EI	1	111	35	67	8	1	0
156	Dn	1	111	35	67	8	1	0

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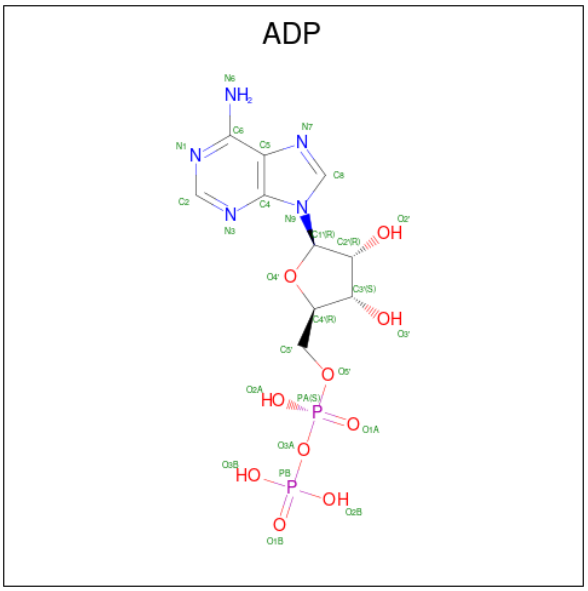
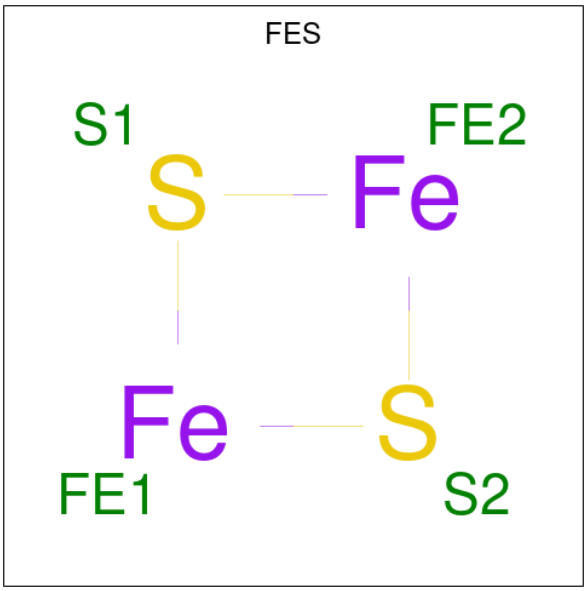
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
156	Dn	1	111	35	67	8	1	0
			Total	C	H	O	P	
156	Ed	1	111	35	67	8	1	0
			Total	C	H	O	P	
156	Dl	1	111	35	67	8	1	0

- Molecule 157 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



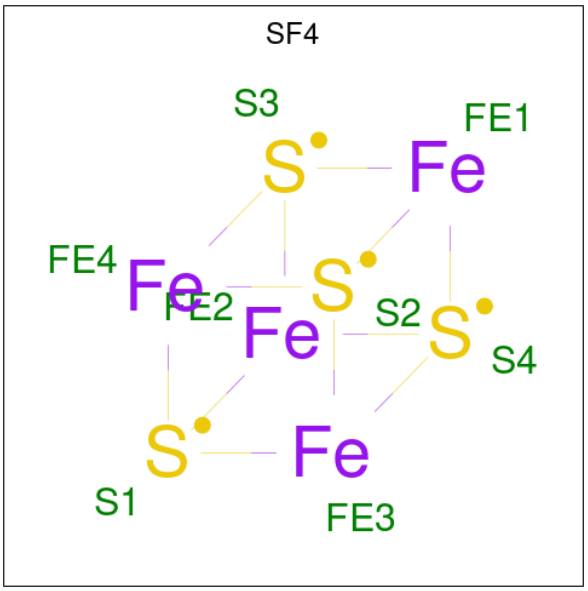
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
157	A8	1	39	10	12	5	10	2	0
			Total	C	H	N	O	P	
157	AQ	1	39	10	12	5	10	2	0

- Molecule 158 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



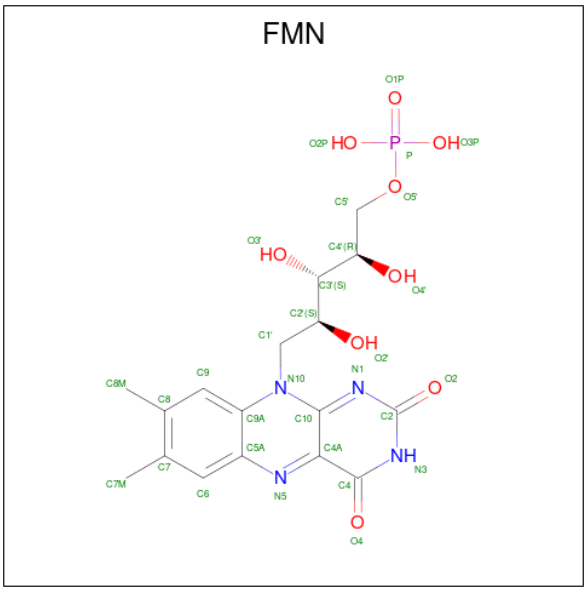
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
158	AB	1	4	2	2	0
158	AI	1	4	2	2	0
158	BI	1	4	2	2	0
158	CB	1	4	2	2	0
158	E	1	4	2	2	0
158	e	1	4	2	2	0
158	EF	1	4	2	2	0
158	EF	1	4	2	2	0
158	Ef	1	4	2	2	0
158	Ef	1	4	2	2	0

- Molecule 159 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



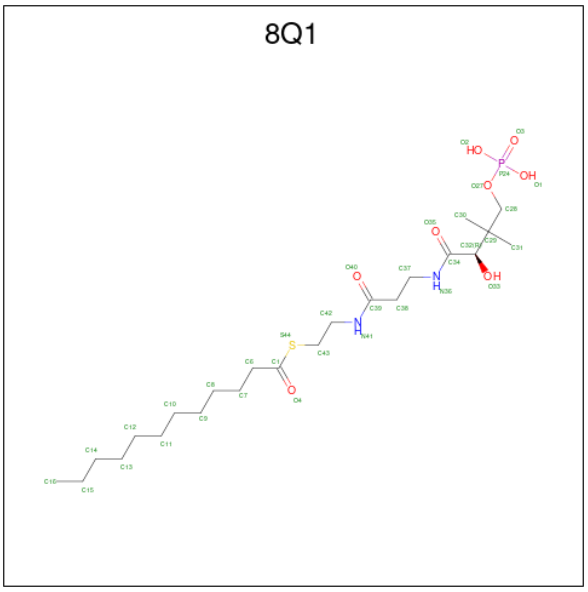
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
159	AB	1	8	4	4	0
159	AB	1	8	4	4	0
159	AD	1	8	4	4	0
159	AL	1	8	4	4	0
159	AL	1	8	4	4	0
159	AT	1	8	4	4	0
159	CB	1	8	4	4	0

- Molecule 160 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
160	AD	1	49	17	18	4	9	1	0

- Molecule 161 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
161	AS	1	77	23	43	2	7	1	1	0

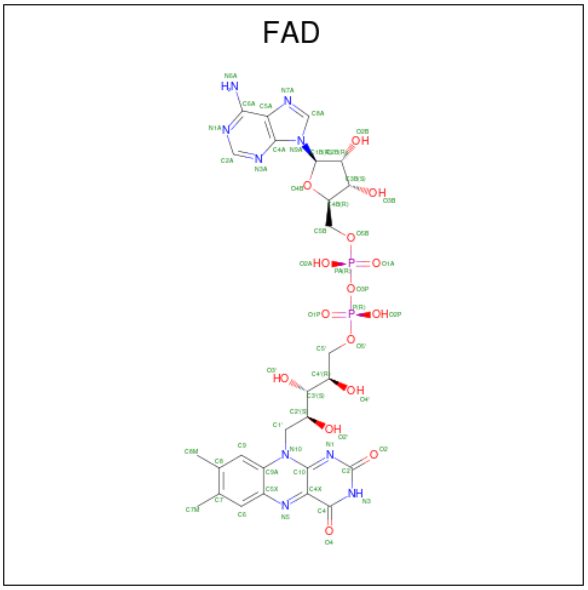
- Molecule 162 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
162	BR	1	1	1	0
162	DD	1	1	1	0
162	Dd	1	1	1	0

- Molecule 163 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
163	CA	1	1	1	0
163	CB	1	1	1	0
163	DA	1	1	1	0
163	Da	1	1	1	0

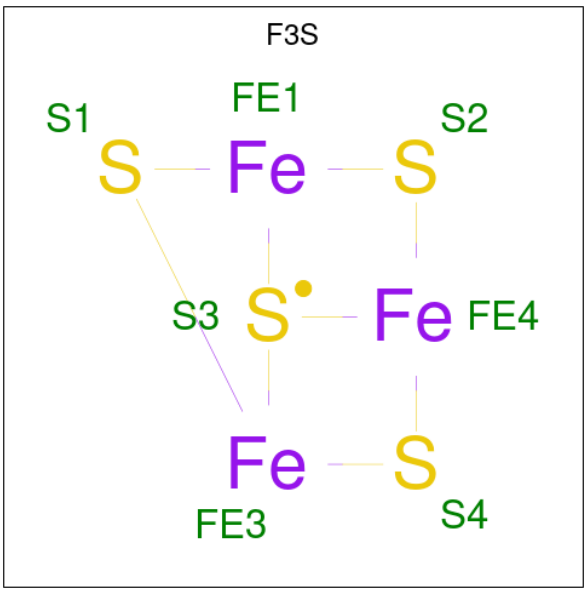
- Molecule 164 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
164	CA	1	84	27	31	9	15	2	0

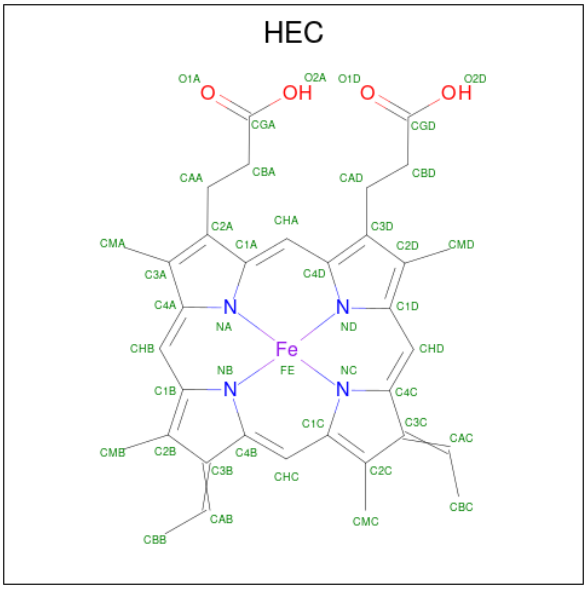
- Molecule 165 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
165	CB	1	7	3	4	0

- Molecule 166 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
166	CE	1	75	34	1	32	4	4	0

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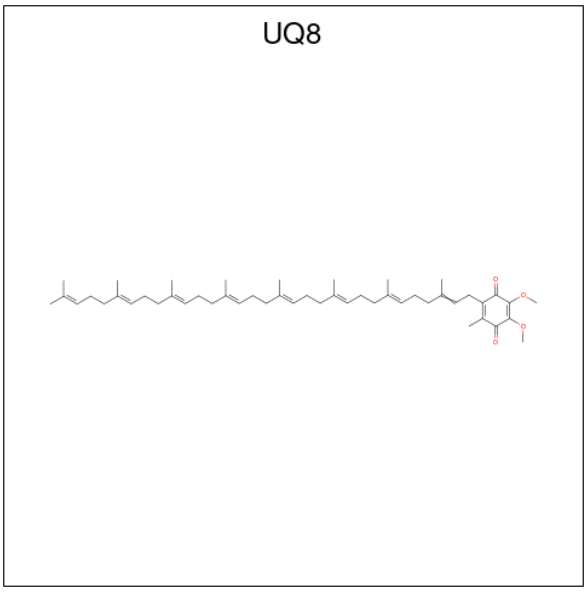
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
166	D	1	73	34	1	30	4	4	0
166	d	1	73	34	1	30	4	4	0

- Molecule 167 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
167	CC	1	127	49	74	4	0
			Total	C	O		
167	C	1	53	49	4		0
			Total	C	O		
167	C	1	53	49	4		0
			Total	C	O		
167	c	1	53	49	4		0
			Total	C	H	O	
167	DS	1	127	49	74	4	0
			Total	C	H	O	
167	ED	1	127	49	74	4	0
			Total	C	H	O	
167	EL	1	127	49	74	4	0
			Total	C	H	O	
167	EN	1	127	49	74	4	0
			Total	C	H	O	
167	Ds	1	127	49	74	4	0

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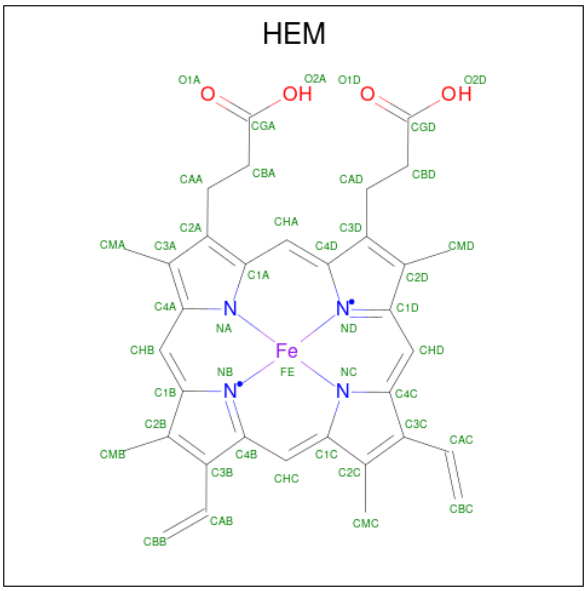
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
167	Ed	1	127	49	74	4	0
			Total	C	H	O	
167	El	1	127	49	74	4	0
			Total	C	H	O	
167	En	1	127	49	74	4	0

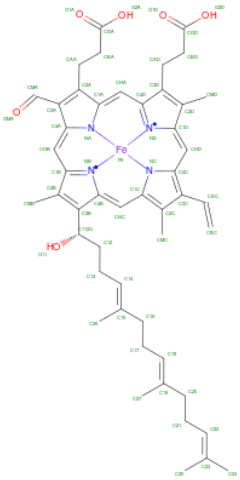
- Molecule 168 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
168	C	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
168	C	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
168	c	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
168	c	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
168	ED	1	65	34	1	22	4	4	0
			Total	C	Fe	H	N	O	
168	Ed	1	67	34	1	24	4	4	0

- Molecule 169 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

HEA

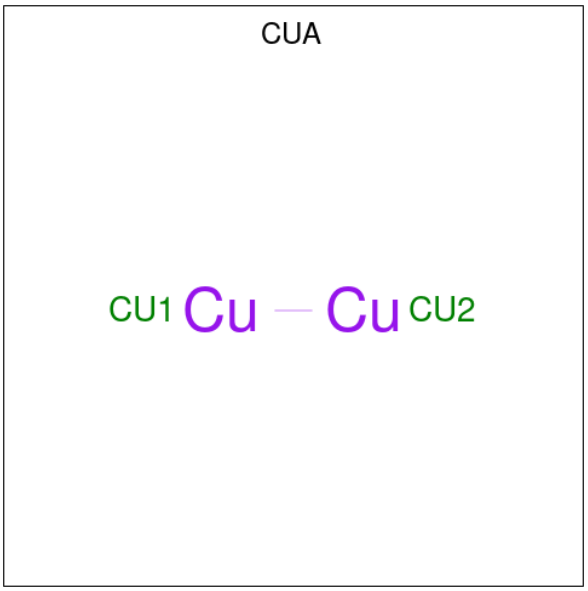


Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
169	DA	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
169	DA	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
169	Da	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
169	Da	1	114	49	1	54	4	6	0

- Molecule 170 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 171 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).

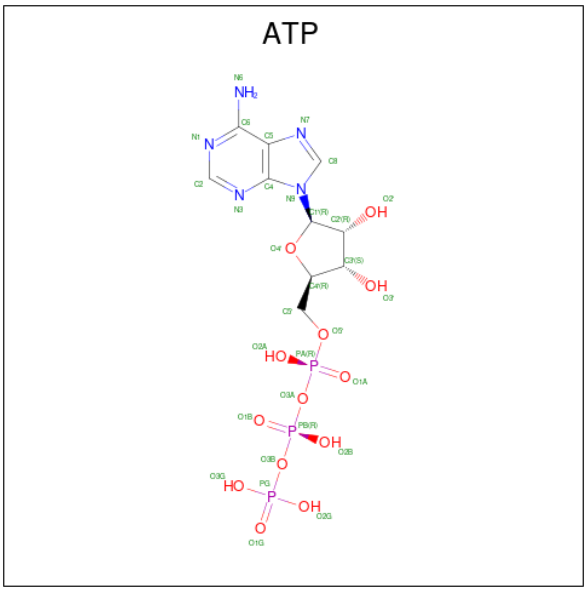


Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
171	DB	1	2	2	0
171	Db	1	2	2	0

- Molecule 172 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 173 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



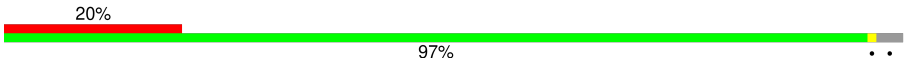
Mol	Chain	Residues	Atoms						AltConf
173	ER	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
173	Er	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

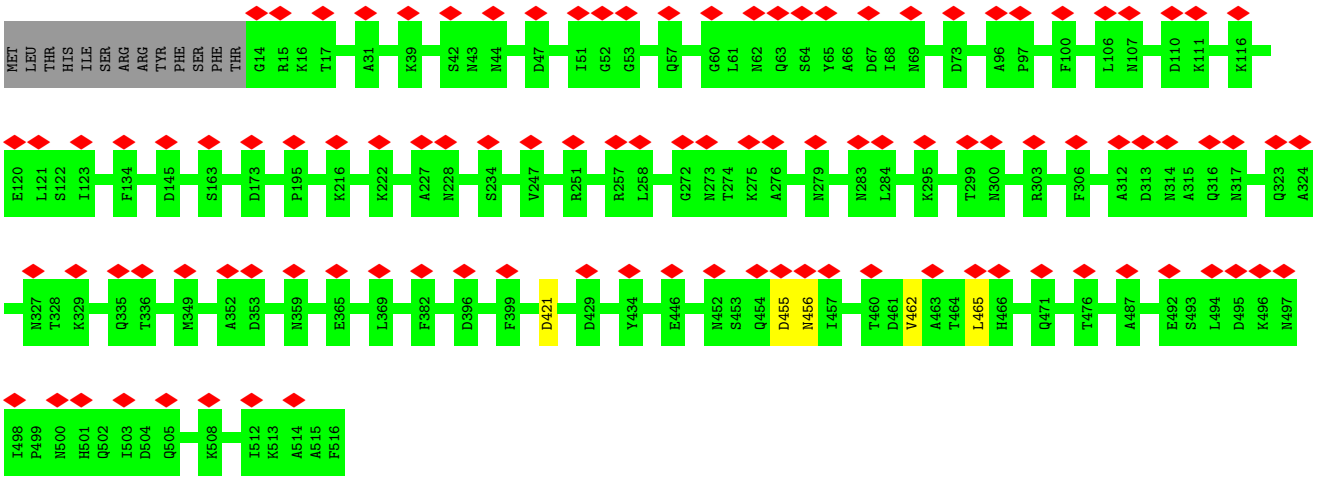
3 Residue-property plots (i)

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

• Molecule 1: Lipid-A-disaccharide synthase

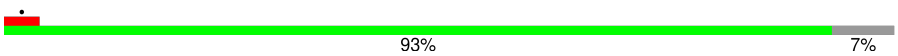
Chain A0:

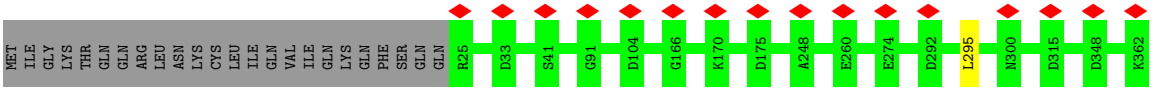




• Molecule 2: NAD-dependent epimerase/dehydratase family protein

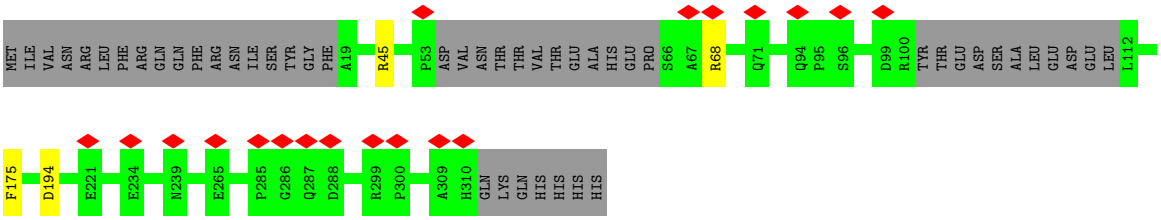
Chain A1:





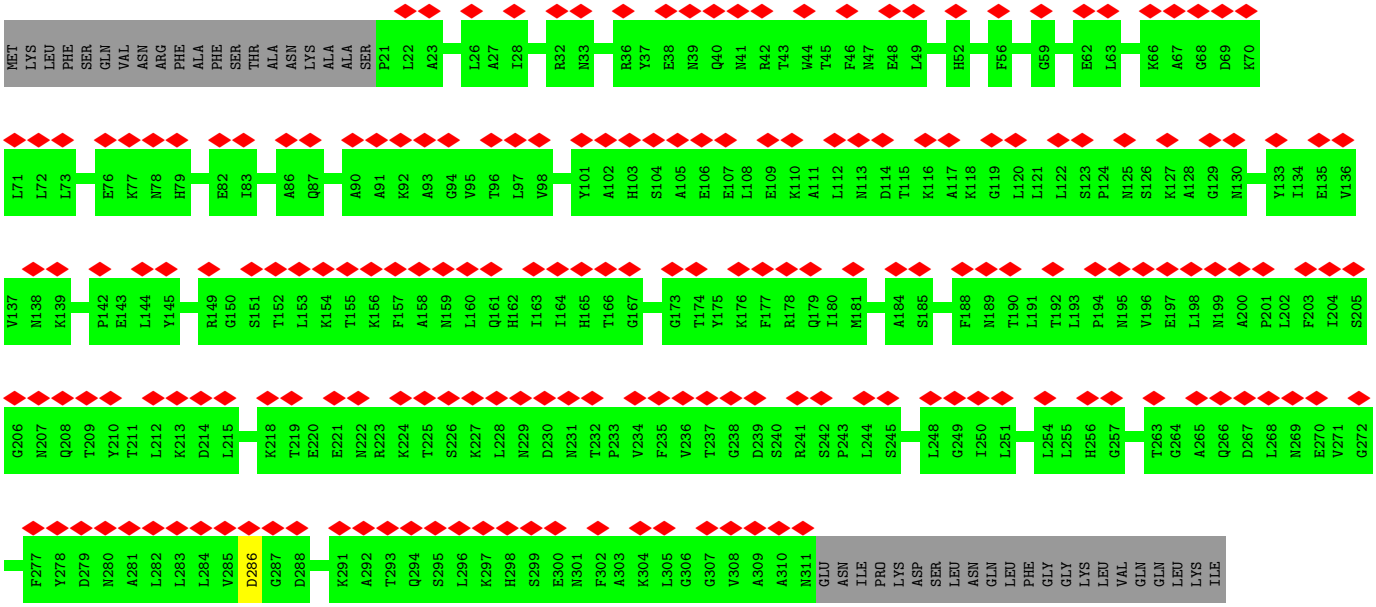
• Molecule 3: DnaJ domain protein

Chain A2:



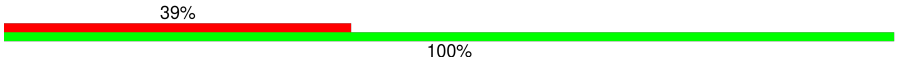
- Molecule 4: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

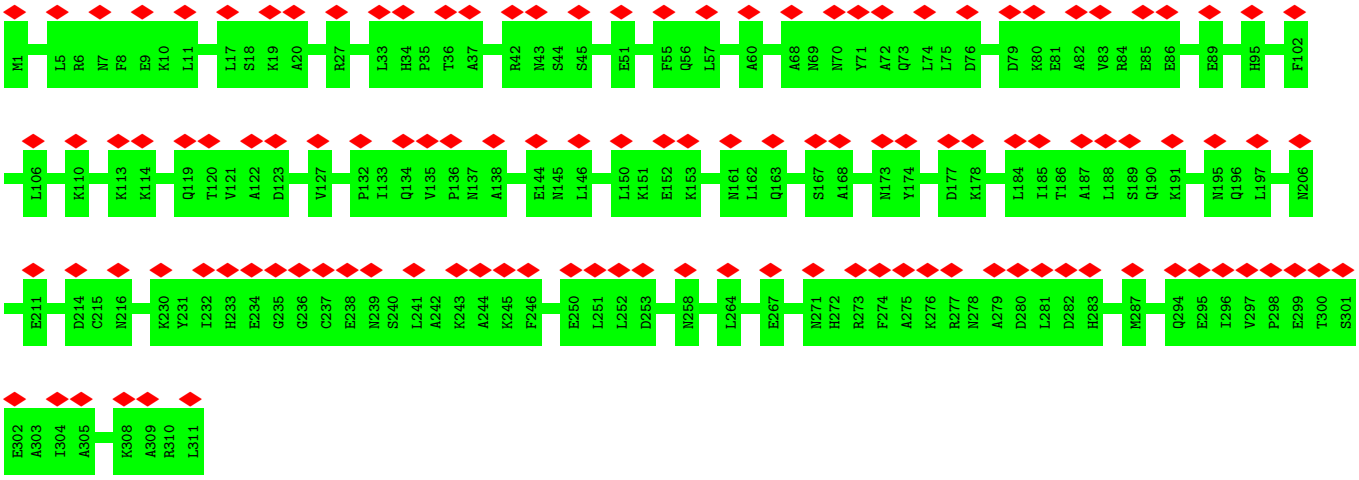
Chain A3:



- Molecule 5: RNase III domain-containing protein

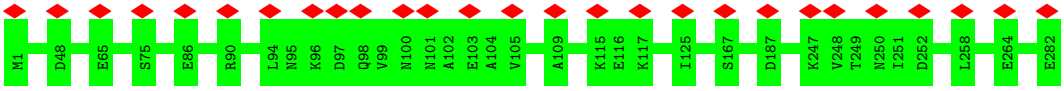
Chain A4:





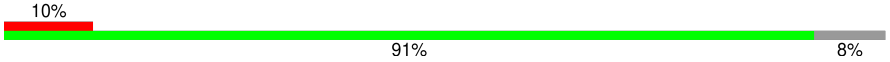
- Molecule 6: 37S ribosomal protein S25, mitochondrial

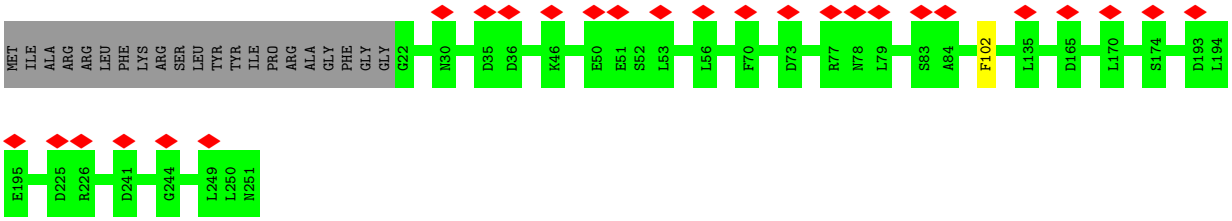
Chain A5:



- Molecule 7: Transmembrane protein, putative

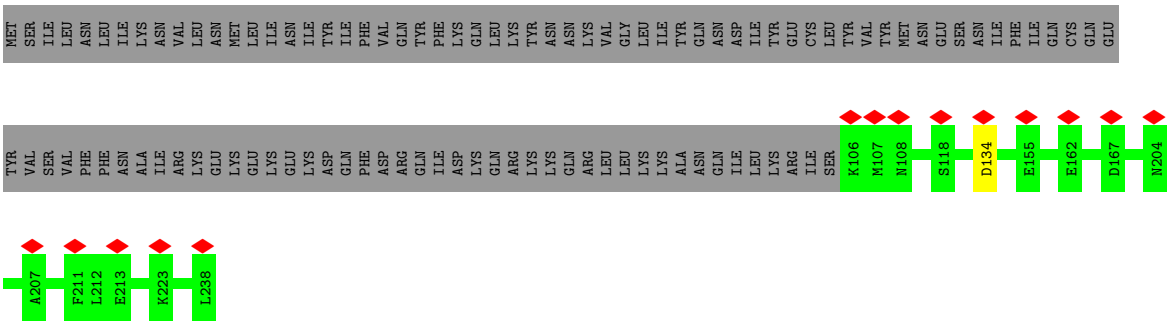
Chain A6:





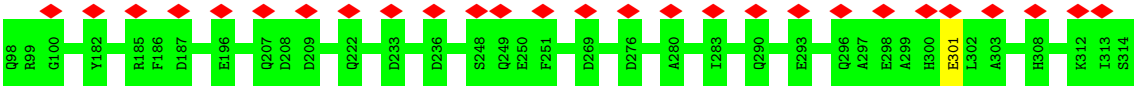
- Molecule 8: CX9C domain-containing protein

Chain A7:



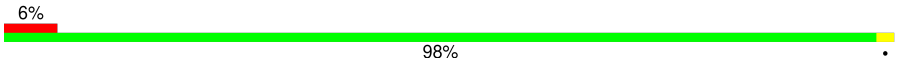
- Molecule 9: ND5a

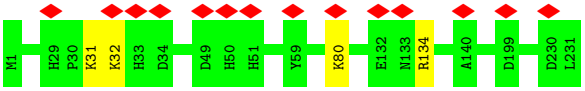
Chain A8:



- Molecule 10: Transmembrane protein, putative

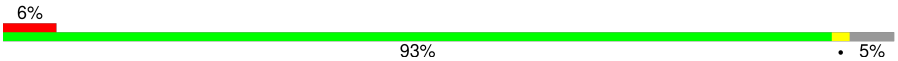
Chain A9:

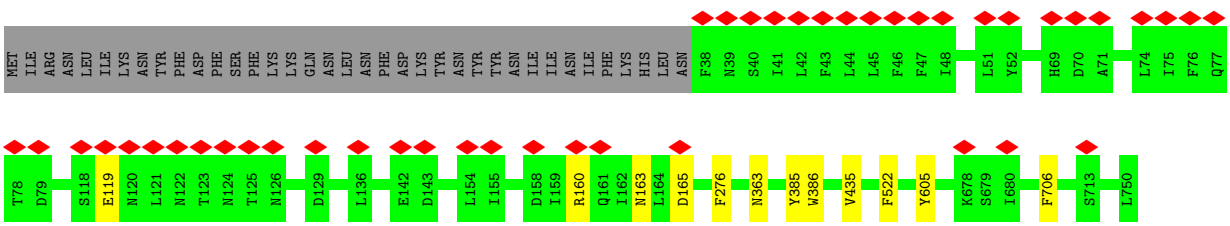




- Molecule 11: NADH dehydrogenase subunit 5

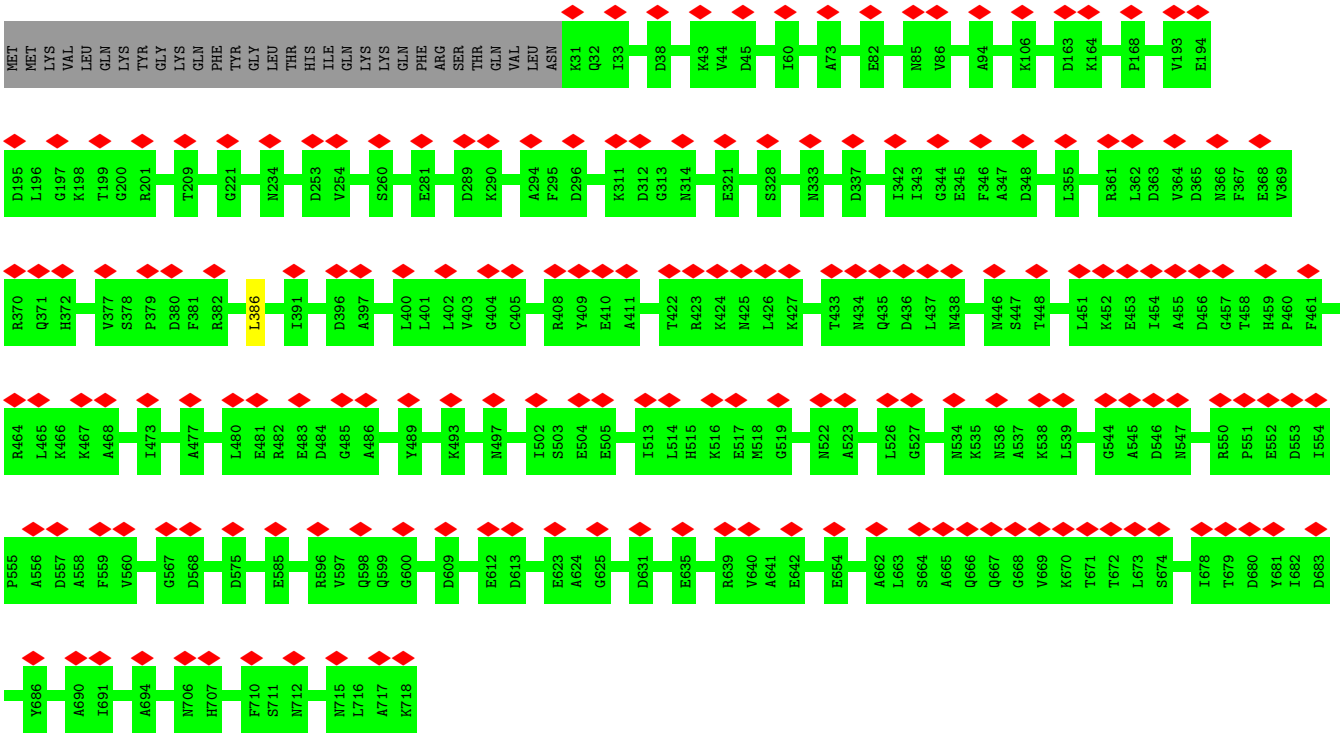
Chain AA:





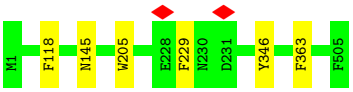
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain AB: 25% 96%



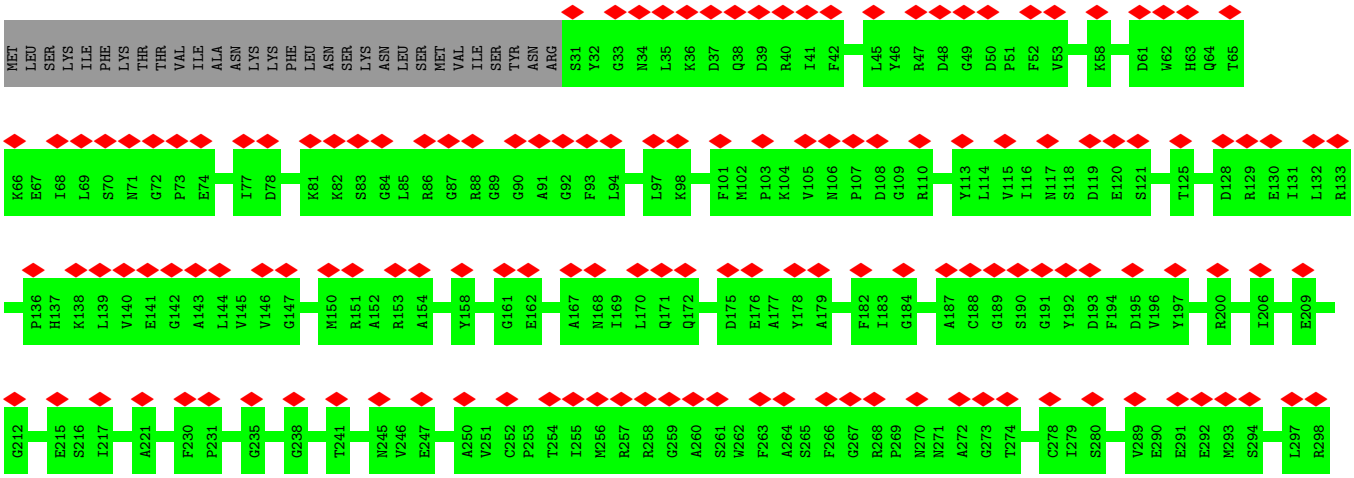
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

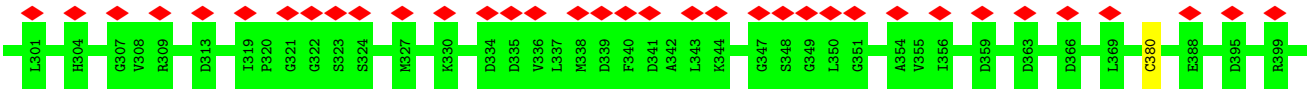
Chain AC: 99%

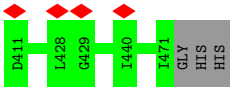


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain AD: 39% 93% 7%

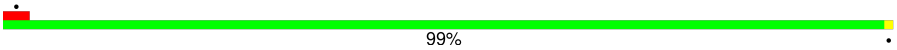


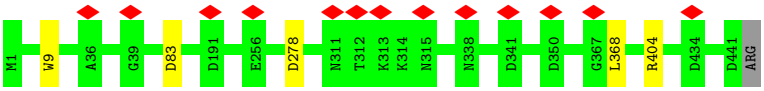




• Molecule 15: NADH dehydrogenase subunit 7

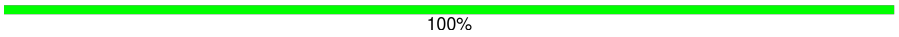
Chain AE:

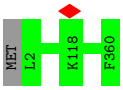




• Molecule 16: Ymf65

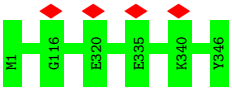
Chain AF:





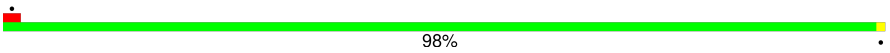
• Molecule 17: Transcription factor apfi protein, putative

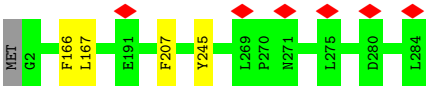
Chain AG:



• Molecule 18: NADH-ubiquinone oxidoreductase chain 1

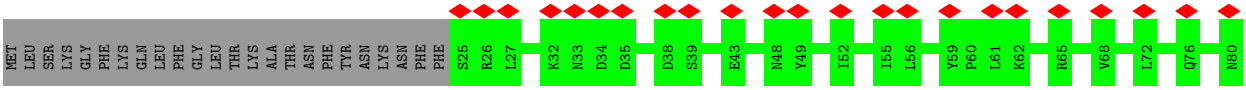
Chain AH:

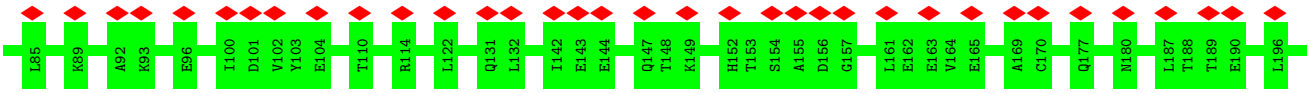


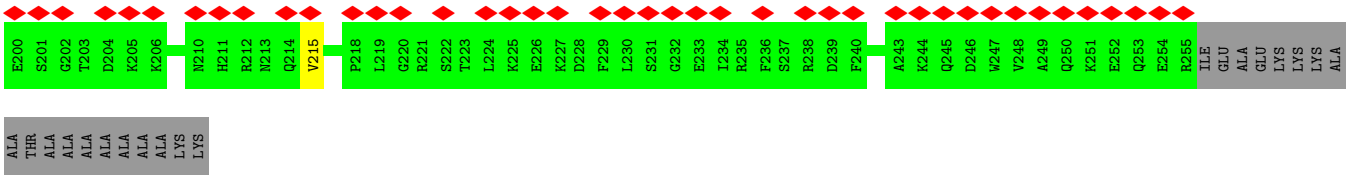


• Molecule 19: NADH-ubiquinone oxidoreductase 24 kDa subunit

Chain AI:

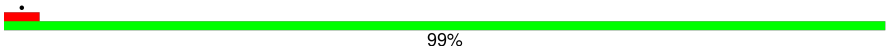


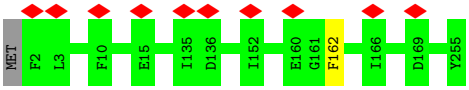




- Molecule 20: Ymf62

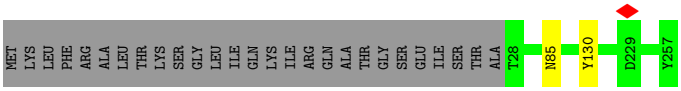
Chain AJ:





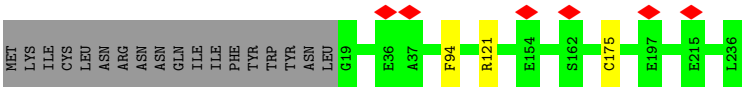
- Molecule 21: Gamma-carbonic anhydrase

Chain AK:



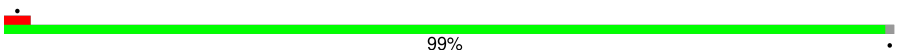
- Molecule 22: NADH-ubiquinone oxidoreductase 1, chain, putative

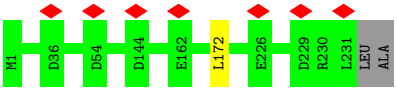
Chain AL:



- Molecule 23: Gamma-carbonic anhydrase

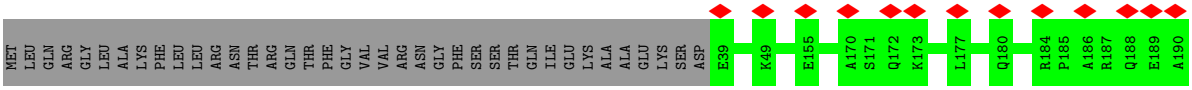
Chain AM:

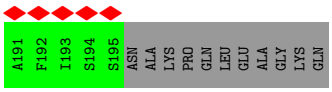




- Molecule 24: ETC complex I subunit motif protein

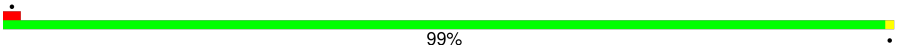
Chain AN:

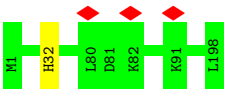




- Molecule 25: NADH dehydrogenase subunit 9

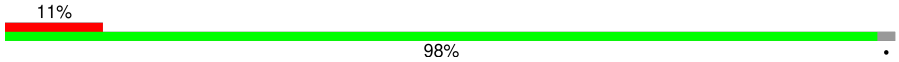
Chain AO:

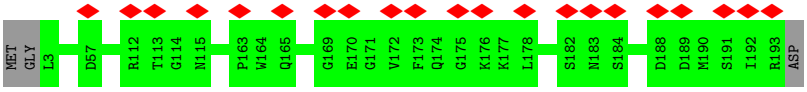




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

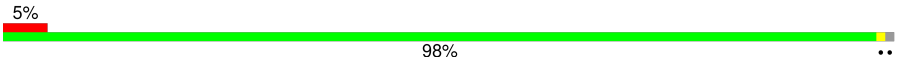
Chain AP:

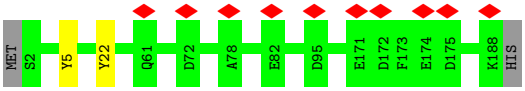




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

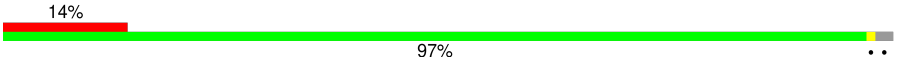
Chain AQ:

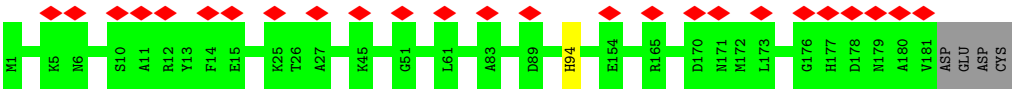




• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

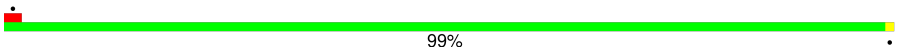
Chain AR:

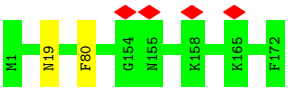




• Molecule 29: NADH dehydrogenase, putative

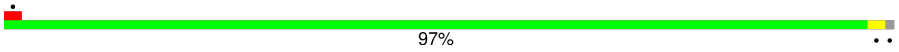
Chain AS:

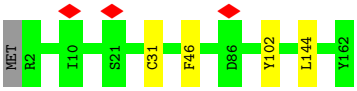




• Molecule 30: NADH dehydrogenase subunit 10

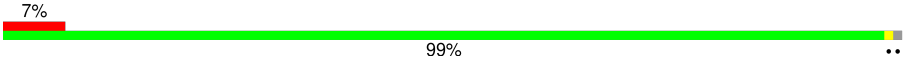
Chain AT:

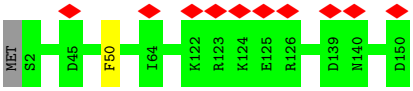




• Molecule 31: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

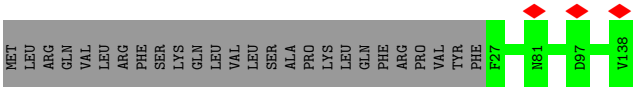
Chain AU:





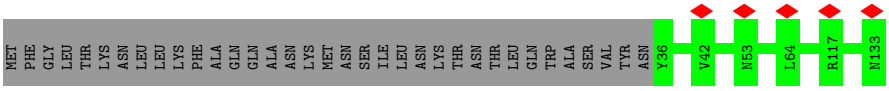
- Molecule 32: Acyl carrier protein

Chain AV:



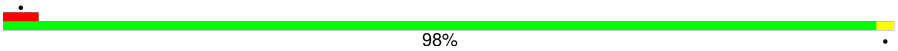
- Molecule 33: Acyl carrier protein

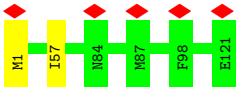
Chain AW:



- Molecule 34: NADH-ubiquinone oxidoreductase chain 3

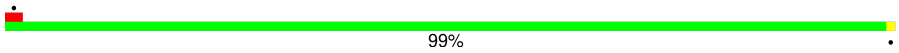
Chain AX:

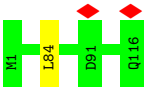




- Molecule 35: Ymf58

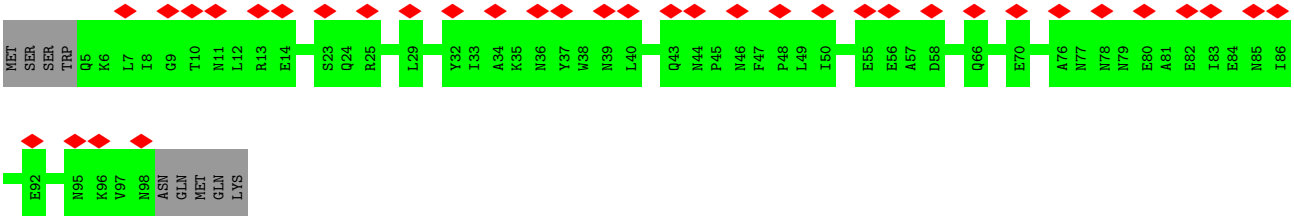
Chain AY:





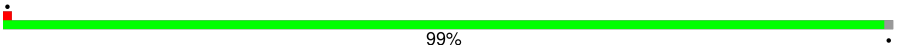
- Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein

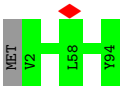
Chain AZ:



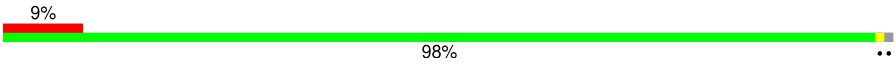
- Molecule 37: Transmembrane protein, putative

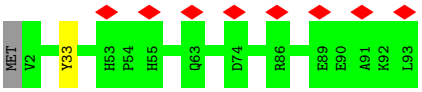
Chain B0:



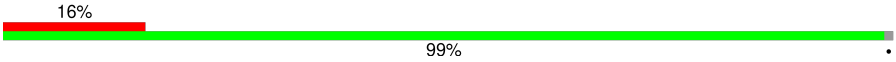


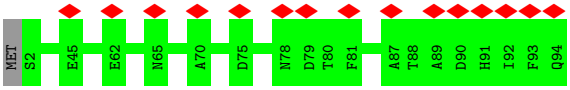
- Molecule 38: ATP synthase subunit e, mitochondrial

Chain B1: 



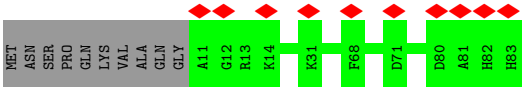
• Molecule 39: GRAM domain protein

Chain B2: 



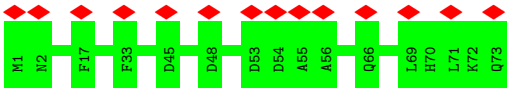
• Molecule 40: Transmembrane protein, putative

Chain B3:



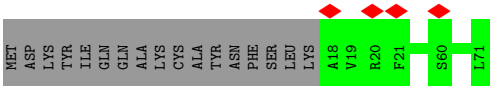
• Molecule 41: Transmembrane protein, putative

Chain B4:

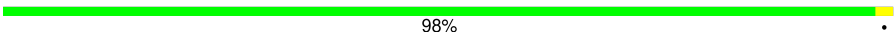


• Molecule 42: Transmembrane protein, putative

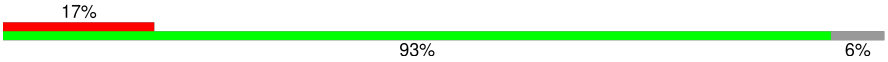
Chain B5:

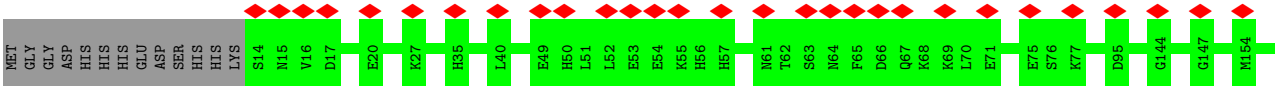


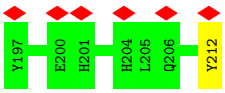
• Molecule 43: NADH dehydrogenase subunit 1

Chain B6: 

• Molecule 44: Transmembrane protein

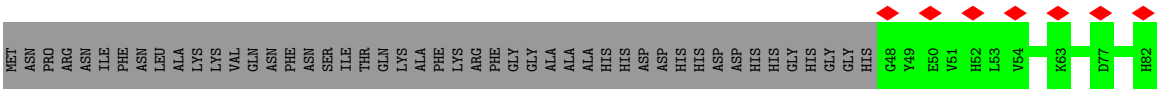
Chain BA: 

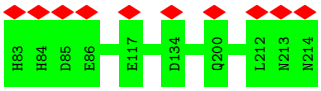




• Molecule 45: Transmembrane protein, putative

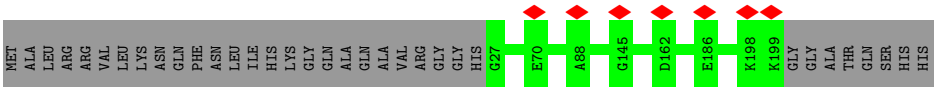
Chain BB:





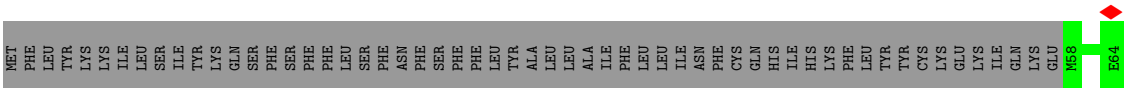
• Molecule 46: NDUB8

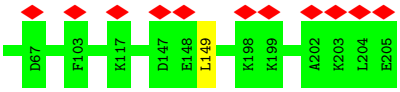
Chain BC:



• Molecule 47: Transmembrane protein, putative

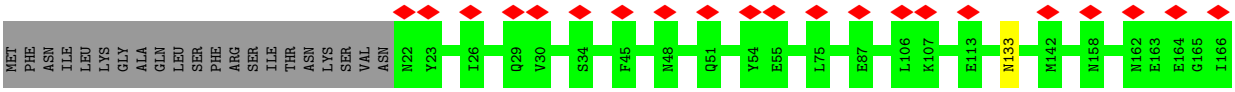
Chain BD:

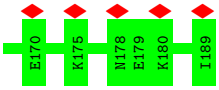




• Molecule 48: NDUPH2

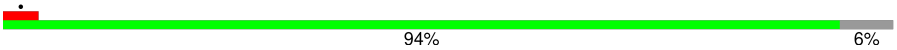
Chain BE:

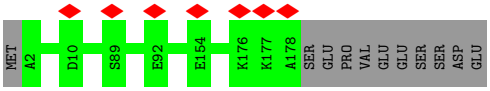




• Molecule 49: NDUB10

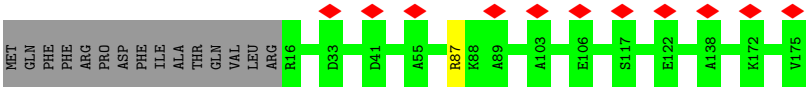
Chain BF:





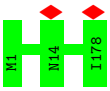
• Molecule 50: NDUA13

Chain BG:



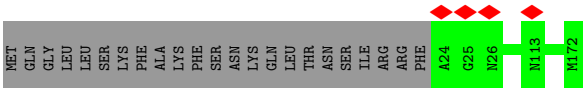
• Molecule 51: NADH dehydrogenase subunit 2

Chain BH:



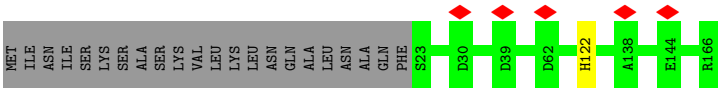
• Molecule 52: 2 iron, 2 sulfur cluster-binding protein

Chain BI:



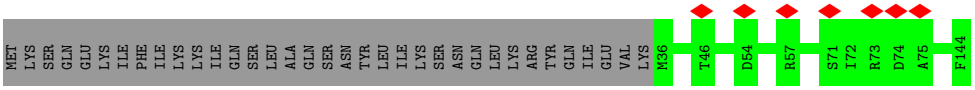
• Molecule 53: Thioredoxin

Chain BJ:



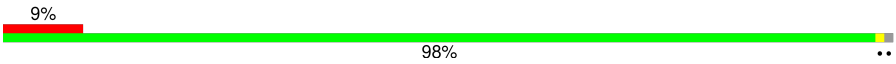
• Molecule 54: COX assembly mitochondrial protein

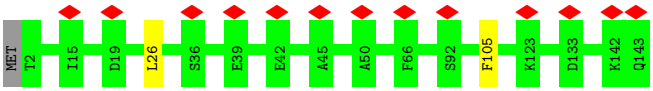
Chain BK:



• Molecule 55: Transmembrane protein, putative

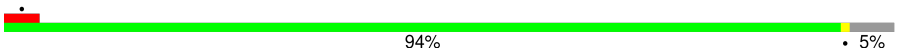
Chain BL:

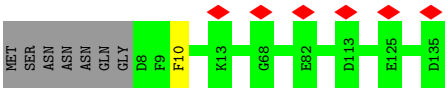




• Molecule 56: Transmembrane protein, putative

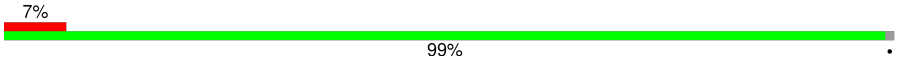
Chain BM:

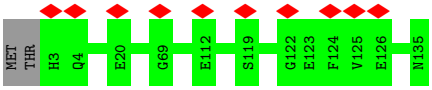




• Molecule 57: PH domain-containing protein

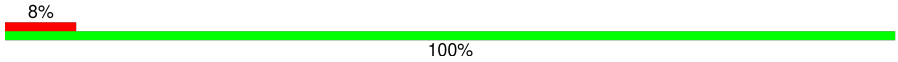
Chain BN:

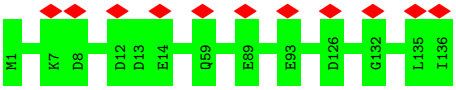




• Molecule 58: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

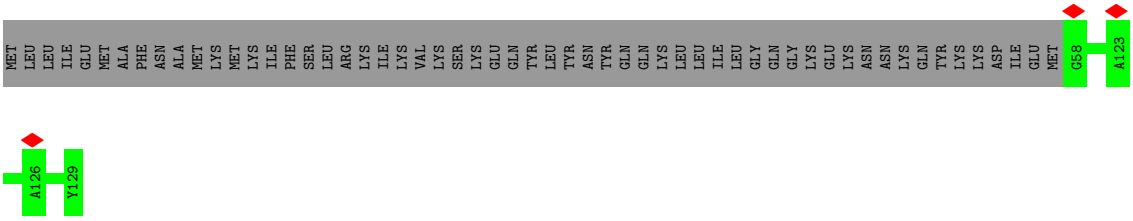
Chain BO:





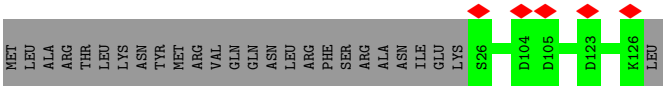
• Molecule 59: NDUB6

Chain BP:



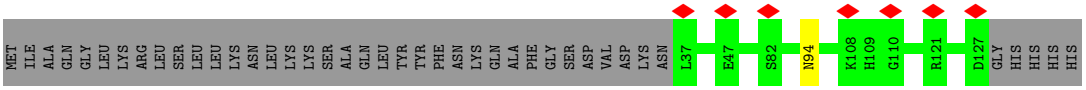
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain BQ:



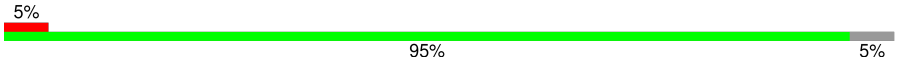
• Molecule 61: Zinc-finger protein

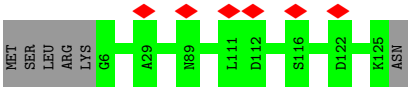
Chain BR:



• Molecule 62: NDUB4

Chain BS:



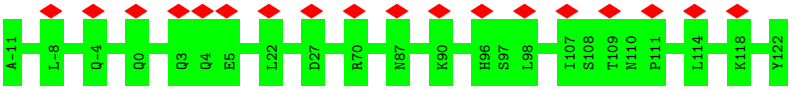


• Molecule 63: NDUTT10

Chain BT: 94% 6%

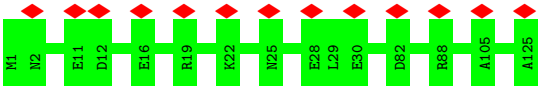
• Molecule 64: NDUTT11

Chain BU: 13% 100%



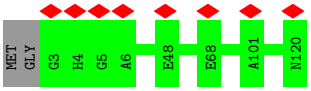
• Molecule 65: NDUTT12

Chain BV: 10% 100%



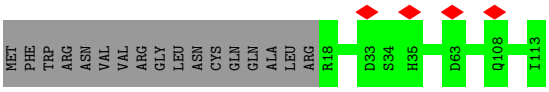
• Molecule 66: CHCH domain-containing protein

Chain BW: 7% 98%



• Molecule 67: Transmembrane protein, putative

Chain BX: 85% 15%

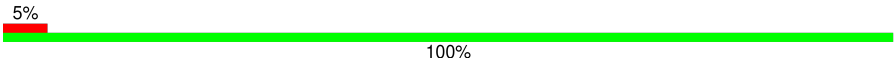


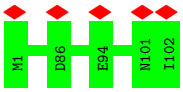
• Molecule 68: Ymf57

Chain BY: 100%

• Molecule 69: Complex I-MNLL

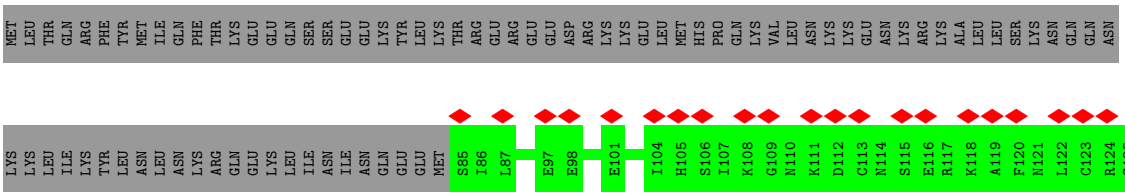
Chain BZ:

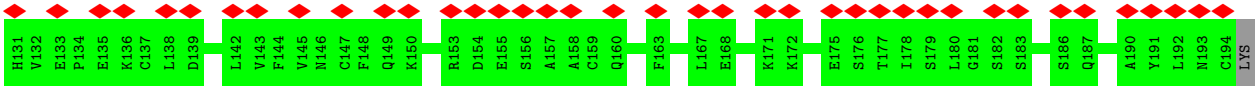




• Molecule 70: Diphthamide synthesis protein

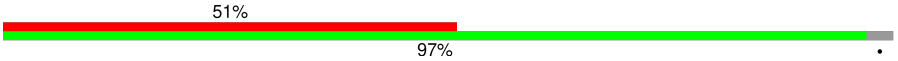
Chain CH:

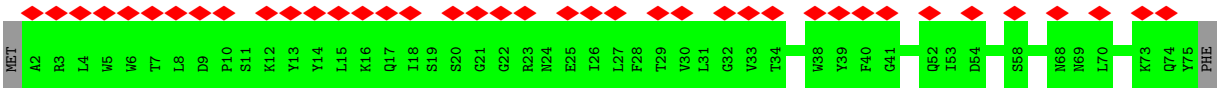




• Molecule 71: Transmembrane protein, putative

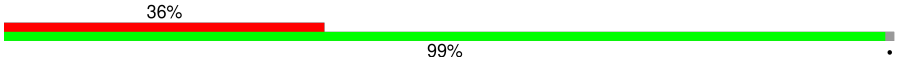
Chain CM:

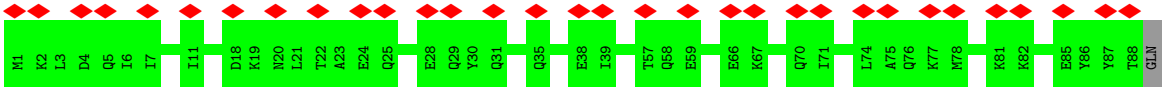




• Molecule 72: Transposase

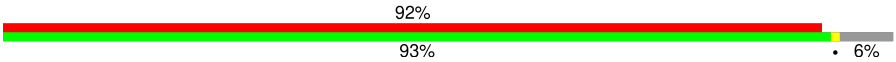
Chain CL:

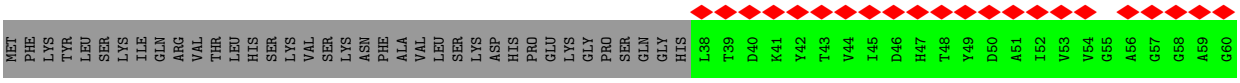


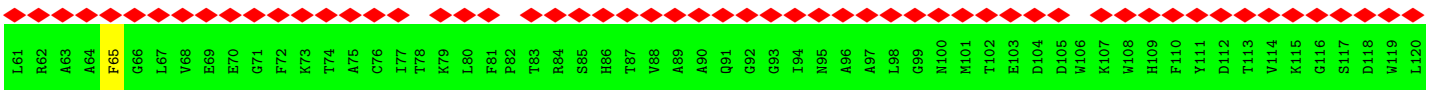


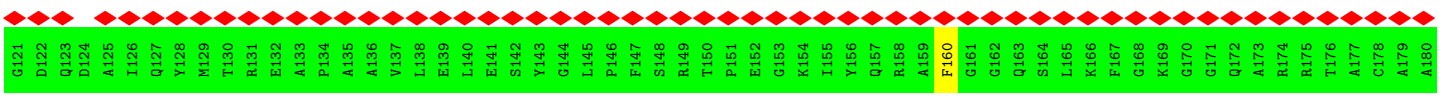
• Molecule 73: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain CA:









D181 R182 T183 G184 H185 A186 M187 L188 H189 T190 L191 F192 G193 R194 S195 L196 A197 Y198 N199 C200 N201 F202 F203 I204 E205 Y206 F207 V208 I209 D210 L211 I212 M213 D214 E215 E216 G217 A218 C219 R220 G221 V222 I223 C224 M225 S226 M227 A228 D229 G230 S231 I232 H233 R234 I235 R236 A237 H238 Y239 T240

V241 L242 A243 A244 G245 G246 Y247 G248 R249 S250 Y251 L252 S253 C254 T255 A256 A257 H258 T259 C260 T261 G262 D263 G264 M265 A266 L267 A268 T269 R270 A271 G272 L273 P274 L275 E276 D277 P278 E279 F280 V281 Q282 F283 H284 P285 T286 G287 I288 Y289 G290 S291 G292 C293 L294 M295 T296 E297 G298 C299 R300

G301 E302 G303 G304 I305 L306 V307 N308 S309 N310 G311 E312 A313 F314 M315 E316 K317 Y318 A319 P320 T321 A322 K323 D324 L325 A326 S327 R328 D329 V330 V331 S332 R333 A334 M335 T336 I337 E338 I339 L340 E341 G342 R343 G344 V345 G346 P347 K348 K349 D350 H351 I352 F353 L354 Q355 L356 H357 H358 L359 S360

P361 E362 T363 L364 H365 Q366 R367 L368 P369 G370 I371 S372 E373 T374 A375 R376 I377 F378 A379 G380 V381 D382 V383 T384 K385 E386 P387 A388 P389 V390 V391 P392 T393 V394 H395 Y396 N397 M398 G399 G400 V401 P402 T403 N404 W405 K406 T407 E408 V409 I410 T411 Q412 D413 K414 N415 G416 K417 D418 K419 I420

V421 P422 G423 L424 L425 A426 A427 G428 E429 N430 A431 C432 A433 S434 V435 H436 G437 A438 N439 R440 L441 G442 A443 N444 S445 L446 L447 D448 I449 V450 V451 F452 G453 R454 A455 A456 A457 K458 L459 V460 K461 E462 K463 L464 K465 P466 G467 T468 P469 H470 K471 D472 L473 P474 K475 M476 A477 G478 E479 Q480

A481 L482 A483 R484 L485 D486 K487 Y488 R489 F490 A491 N492 G493 E494 Y495 T496 T497 H498 H499 V500 R501 T502 A503 M504 Q505 E506 T507 M508 Q509 R510 H511 A512 A513 V514 F515 R516 I517 E518 K519 L520 M521 A522 E523 G524 V525 Q526 K527 L528 D529 H530 I531 Y532 E533 Q534 S535 K536 S537 L538 K539 T540

F541 D542 R543 G544 L545 V546 W547 N548 T549 D550 L551 I552 E553 T554 L555 E556 L557 E558 N559 L560 I561 L562 C563 S564 K565 Q566 T567 L568 L569 A570 G571 L572 L573 R574 K575 E576 S577 R578 G579 A580 H581 A582 R583 D584 D585 F586 K587 E588 R589 D590 D591 K592 N593 W594 M595 K596 H597 S598 L599 T600

W601 I602 K603 D604 V605 N606 T607 G608 K609 T610 E611 V612 T613 Y614 R615 D616 V617 I618 N619 H620 T621 L622 D623 S624 E625 V626 T627 P628 V629 P630 P631 A632 K633 R634 S635 Y636

- Molecule 74: DUF4885 domain-containing protein

Chain CI: 39% 100%

M1 F2 M6 M7 Y8 E9 A10 L14 V17 A20 F24 R25 L34 A35 R36 Y37 E38 S39 Q42 S43 G47 S48 T49 S50 G51 A52 I55 D58 R64 N65 F66 K67 A68 L69 K70 K73 Y77 E80 I81 K84 A87 D95 Y96

T97 A98 F102 L103 N104 E105 K108 K109 Q112 D113 A114

- Molecule 75: succinate dehydrogenase

Chain CB: 76% 90% 9%

MET LEU ARG THR ILE PHE LYS THR ARG SER LEU PHE ASN ALA SER VAL SER ARG PHE GLY SER GLY PHE ASP ARG ILE A27 E28 S29 N30 D31 A32 T33 S34 I35 C36 L37 I40 S41 G42 T43 I44 L47 Q48 K49 A50 N51 Y52 V53 V54 E55 H56 N57 P58 N59 L60 T61 S62

E63 E64 K65 K66 H67 L68 K69 Q70 F71 L72 V73 Y74 R75 Y76 N77 P78 A79 D80 P81 H82 D83 Q84 P85 K86 Y87 V88 S89 Y90 D93 I94 K95 K96 F97 P98 P99 M100 F101 L102 D103 A104 I105 L106 Y107 I108 K109 N110 E111 L112 D113 P114 T115 L116 S117 I118 R119 R120 S121 C122 R123

E124 G125 I126 C127 G128 S129 C130 A131 V132 N133 C134 D135 G136 L137 H138 T139 L140 A141 C142 I143 S144 G145 F146 N147 R148 D149 L150 S151 K152 P153 T154 I155 K156 T157 P158 L159 G160 H161 M162 F163 I164 L165 K166 D167 L168 V169 V170 D171 M172 T173 N174 F175 Y176 A177 Q178 Y179 K180 M181 I182 E183

P184 Y185 L186 K187 R188 K189 T190 P191 K192 P193 D194 A195 N196 K197 E198 Y199 P200 P203 E204 Q205 R206 A207 L208 L209 D210 G211 L212 Y213 E214 C215 V216 L217 C218 A219 A220 C221 S224 C225 P226 W229 W230 H231 P232 D233 R234 Y235 L236 G237 P238 A239 I240 L241 Q242 Q243 A244 Y245 R246

W247 I248 V249 D250 S251 R252 D253 E254 Y255 T256 Q257 E258 R259 I260 E261 R262 I263 A264 E265 D266 V267 R268 L269 D270 D271 C272 Q273 Q274 I275 G276 M277 C278 S279 F280 T281 C282 P283 K284 G285 L286 N287 P288 Q289 L290 S291 L292 K293 N294 L295 M296 D297 M298 V299 K300 D301 F302 R303 Q304 K305 R306

I307 E308 Q309 E310 V311 LEU

- Molecule 76: Transmembrane protein, putative

Chain CF: 35% 74% 26%

MET ILE LYS TYR LEU LEU HIS GLN LEU PHE ILE TYR ILE TYR VAL ALA GLU VAL LEU LEU GLY CYS ILE PHE ALA PHE ALA GLU THR VAL PHE PHE HIS SER ASP GLN ASP GLU ASP TYR PHE LEU GLN ILE LYS GLN ILE GLN ILE LYS ASN GLN LYS ARG PHE ARG ASN ASN GLN LYS

LYS SER ARG SER PHE LYS LYS LYS ILE ILE ASN GLN GLN LEU VAL SER LYS MET V79 R80 L81 N82 L83 K84 S85 N86 V87 D88 Q89 N90 E91 L95 A96 D99 K100 D101 M102 R103 Q104 N105 Y106 E107 E108 Y109 Q110 N111 R112 I113 D114 T117 Y118 R122 S123 Q124 R125

A128 V129 F130 G131 E132 R137 Y138 F139 D142 I143 L146 E147 R150 L155 G156 K157 I158 Y159 P160 E161 E162 I173 A174 N175 D176 N182 A183 K184 V189 M192 T193 V194 G195 A196 G197 F198 F199 A200 F201 A202 H203 L204 F205 N206 L207 P208 Y209 S210 F211 R212 L213

G214 L215 F216 V217 A221 L224 A225 F226 T227 W228 G229 N230 K231 E239 D242 L245 Q246 Y247 S250 L253 L254 E255 K256 N257 A258 K259 H260 F261 A262 E263 K264 A267 K270 E271 I272 N273 S274 S275 Q276 Q279 D280 L281 Y282 N283 Q284 L285 I286 S290

E296

- Molecule 77: chain 77

Chain CG: 82% 98%

MET S2 L3 V4 F7 K8 N9 T10 F11 L12 K13 S14 R15 V16 I17 G18 L19 S20 F21 Q22 A23 Q24 R25 V26 M27 A28 Q29 M30 A31 K32 T33 D34 F35 E36 N37 P38 D39 E40 H41 F42 L43 L44 N45 D46 A47 M48 K49 Y50 N51 E52 L53 V54 F55 R58 L59 A60 E61 N62

W63 S64 I65 N66 P67 E68 L69 F70 G71 K72 A73 E74 L75 A76 K77 Y78 N79 E80 A81 K82 Q83 T84 L85 I86 D87 F88 N89 Q90 Y91 H92 A93 L94 V95 Q96 H99 E100 W103 E104 L105 K106 T107 L110 E111 L112 S113 R114 G115 T118 S119 N120 F121 H122 N123 K124 R125 E126

V127 T128 H129 S130 I131 I132 E133 S134 D135 I136 K137 N138 S139 I140 H141 K142 Y143 I144 Q145 L146 I147 D148 D149 L150 K151 D152 Y153 P154 E155 W156 Q157 H158 K159 V160 R161 E162 E163 I164 G165 Y166 Y167 A168 H169 M170 I171 Y172 T173 S174 V175 N176 H177 D178 G179 N180 F181 P182 E183 I184 F185 K186

E187 F188 N189 K190 V191 D192 S193 L194 Y195 Y196 F197 LYS

- Molecule 78: Transmembrane protein, putative

Chain CK: 59% 98%

M1 L2 D3 D4 T5 K6 Y7 I8 Q9 M10 A11 Q12 K13 F14 P15 R16 N17 V18 S19 V20 Q21 L22 N23 K24 K25 L26 F27 V28 R34 N35 Y36 Y37 F38 V39 G40 V41 F42 G43 I44 F45 A46 Y47 F48 I49 Y50 N51 Q52 I55 F59 Y62 K69 A70 Q71 F72

D77 Q78 V79 I80 Q87 N88 T89 L90 K91 N92 F93

- Molecule 79: NmrA domain-containing protein

Chain CE: 92% 98%

MET S2 L3 L4 V5 V6 S7 G8 A9 N10 K11 V12 G13 Q14 G15 I16 I17 R18 G19 L20 H21 S22 S23 G24 K25 Y26 E27 K28 I29 V30 V31 A32 D33 V34 F35 P36 K37 Y38 Y39 E42 R43 Y44 L45 R46 F47 K48 D49 T50 L51 T52 Q53 N54 K55 T56 K57 L58 E59 E60 V61

K62 L63 T64 D65 K66 T67 D68 L69 E70 S71 A72 I73 K74 K75 A76 S77 H78 V79 V80 Y81 V82 T83 H84 D85 Y86 Y87 Y88 N89 V90 P91 S92 K93 L94 N95 L96 I97 K98 H99 T100 A101 T102 L103 S104 R105 S106 A107 G108 V109 K110 R111 L112 V113 N114 V115 T116 P117 V118 E119 N120 D121

H122 Y123 G124 E125 S126 Q127 A128 V129 L130 A131 A132 T133 Q134 S135 E136 N137 E138 A139 R140 V141 A142 F143 P144 G145 L146 V147 E148 L149 K150 T151 D152 L153 T154 F155 G156 Q157 D158 S159 T160 V161 V162 S163 E164 L165 L166 T167 R168 L169 A170 Y171 G172 K173 S174 I175 Y176 F177 K178 P179 S180 A181

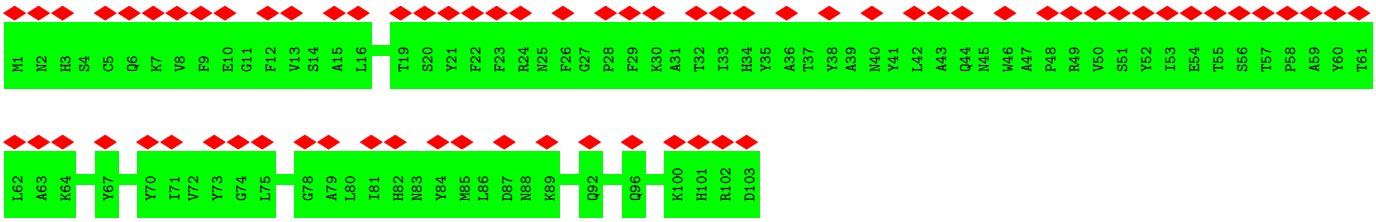
H182 R183 I184 S185 P186 V187 H188 T189 L190 N191 V192 A193 E194 A195 T196 Q197 R198 I199 L200 E201 N202 N203 S204 L205 Q206 N207 L208 R209 Y210 V211 A212 R213 G214 T215 E216 S217 F218 D219 W220 N221 T222 I223 I224 S225 T226 L227 A228 A229 A230 I231 G232 K233 N234 A235 N236 L237 N238 Q239 N240 P241

L242 E243 N244 I245 I246 S247 P248 L249 S250 D251 N252 I253 V254 S255 Q256 T257 V258 H259 H260 H261 H262 Y263 L264 N265 L266 T267 R268 F269 I270 N271 Q272 Y273 Q274 E275 P276 K277 Q278 T279 E280 H281 H282 E283 L284 T285 N286 L287 G288 V289 N290 N291 L292 V293 K294 F295 S296 E297 F298 Y299 K300 P301

N302 S303 V304 S305 T306 Q307 D308 Y309 Q310 I311 K312 T313 G314 L315 S316 H317 W318 A319 H320 C321 L322

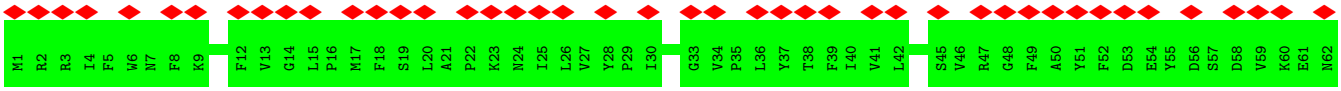
- Molecule 80: Transmembrane protein, putative

Chain CJ: 68% 100%



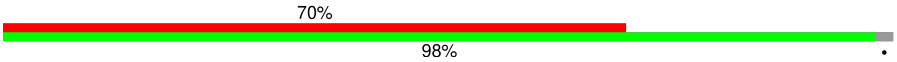
- Molecule 81: Transmembrane protein, putative

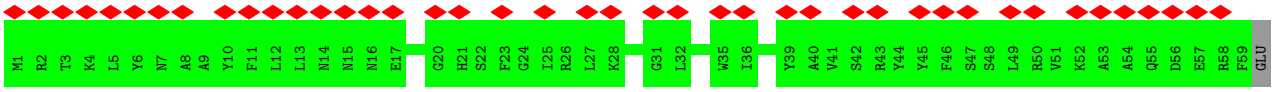
Chain CN:



- Molecule 82: Transmembrane protein

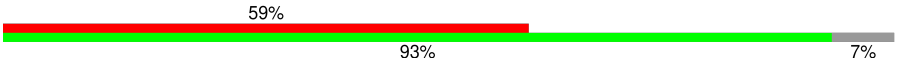
Chain CC:

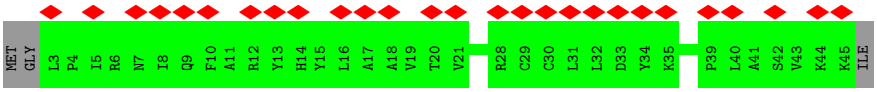




- Molecule 83: SDHTT11

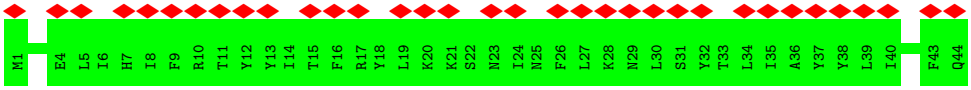
Chain CO:





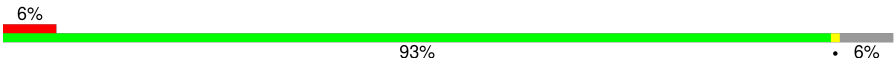
- Molecule 84: succinate dehydrogenase complex iron-sulfur subunit D

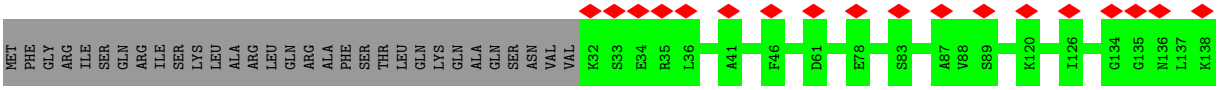
Chain CD:

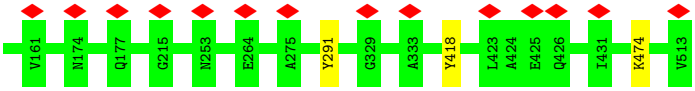


- Molecule 85: Peptidase M16 inactive domain protein

Chain A:

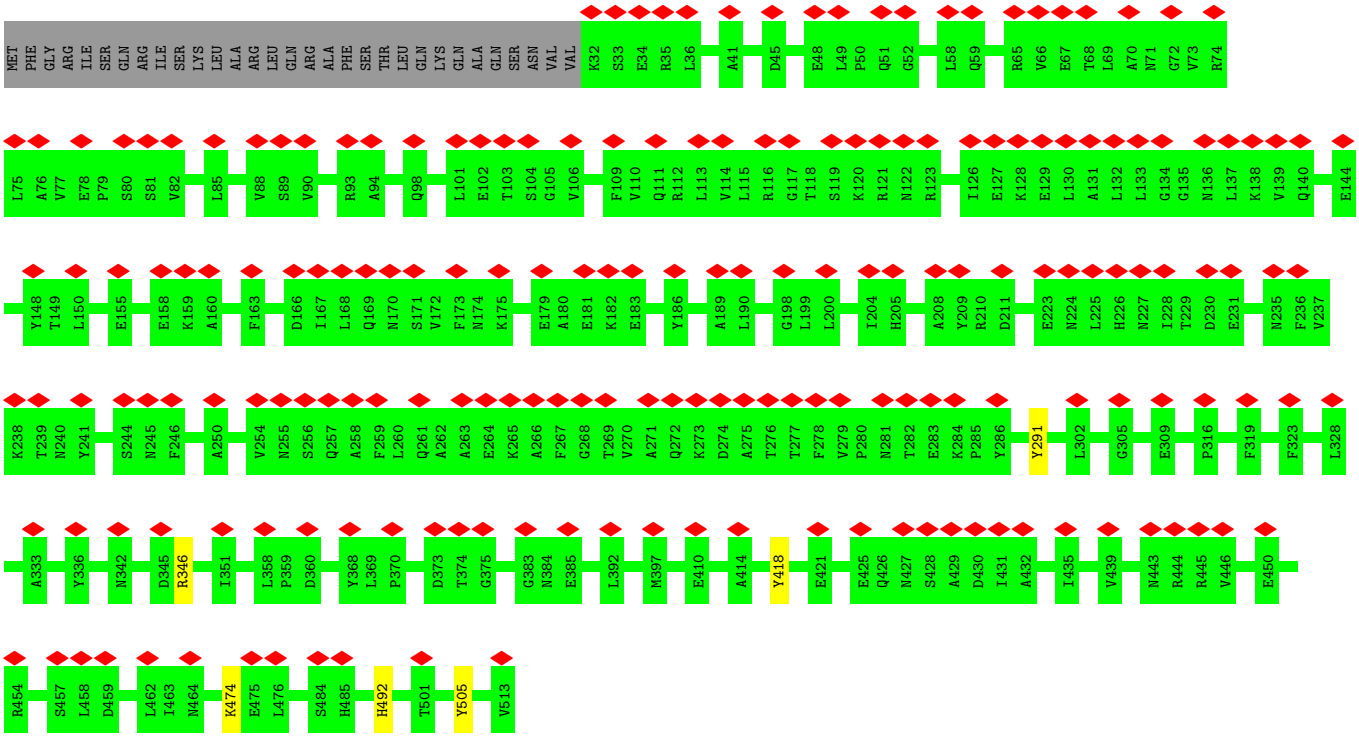






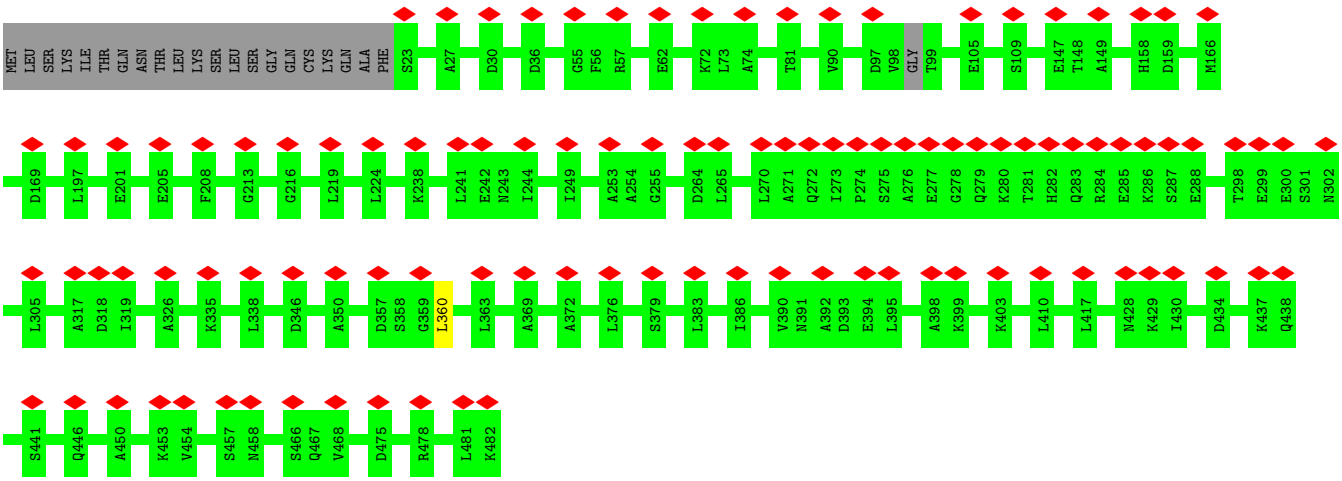
- Molecule 85: Peptidase M16 inactive domain protein

Chain a: 37% 93% • 6%



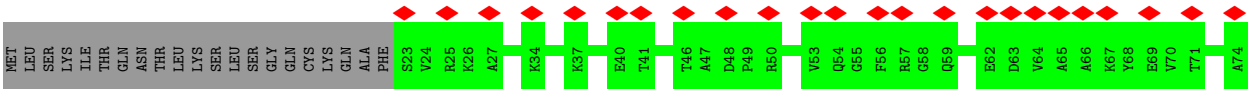
• Molecule 86: M16 family peptidase, putative

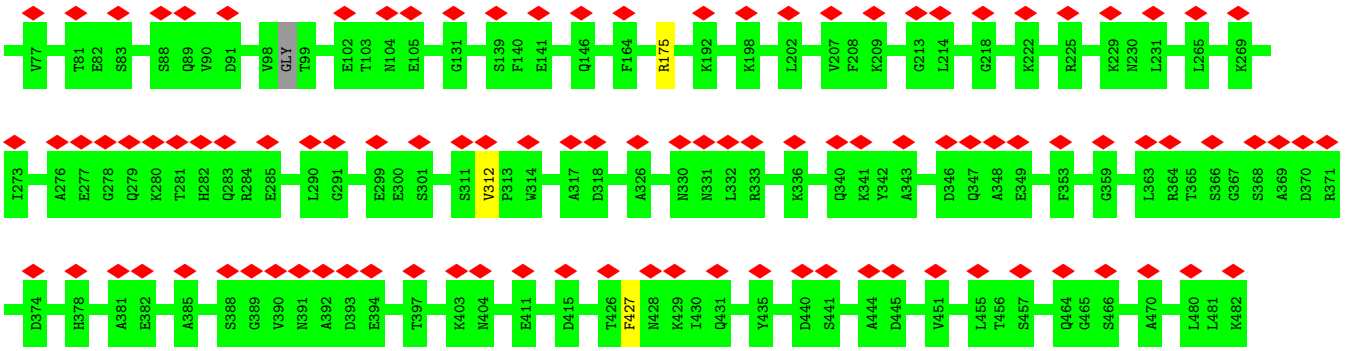
Chain B: 22% 95% 5%



• Molecule 86: M16 family peptidase, putative

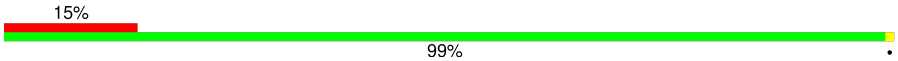
Chain b: 26% 95% • 5%

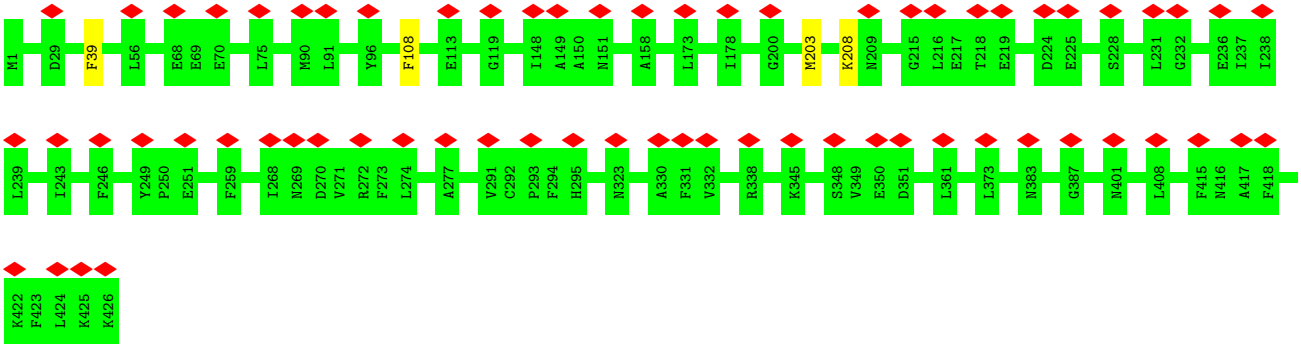




- Molecule 87: Apocytochrome b

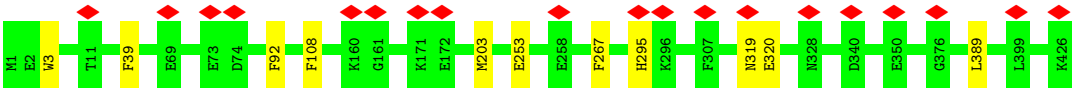
Chain C:





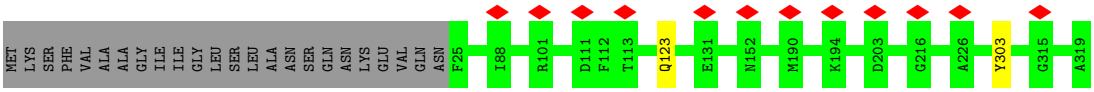
- Molecule 87: Apocytochrome b

Chain c:



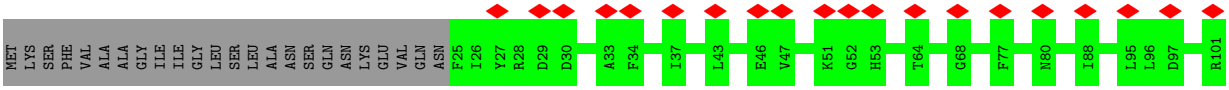
- Molecule 88: Cytochrome protein c1

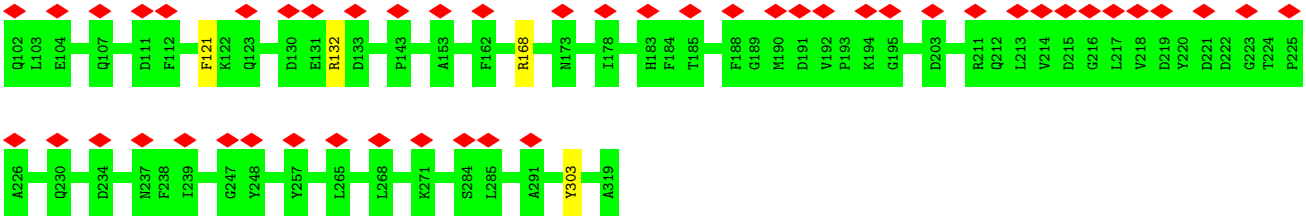
Chain D:



- Molecule 88: Cytochrome protein c1

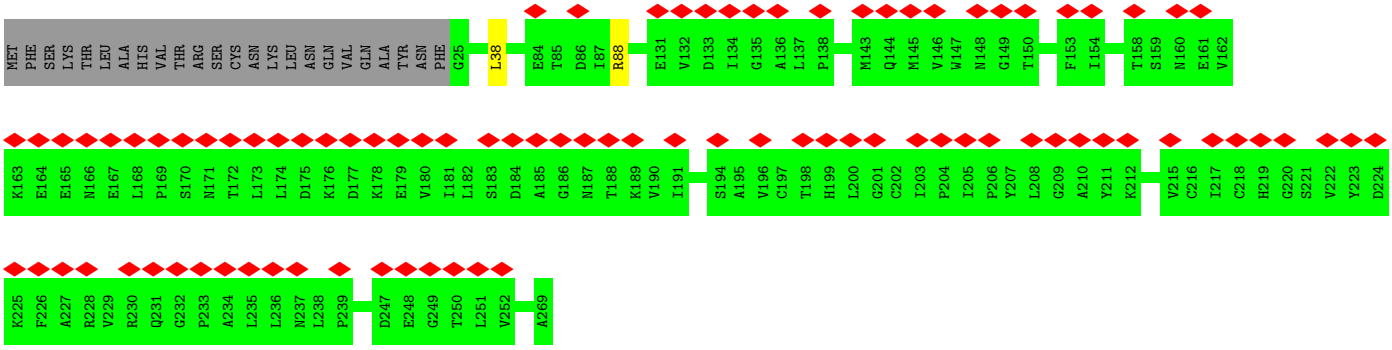
Chain d:





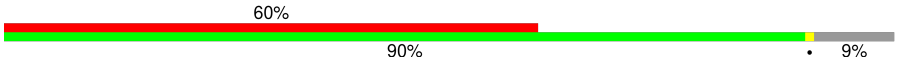
• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

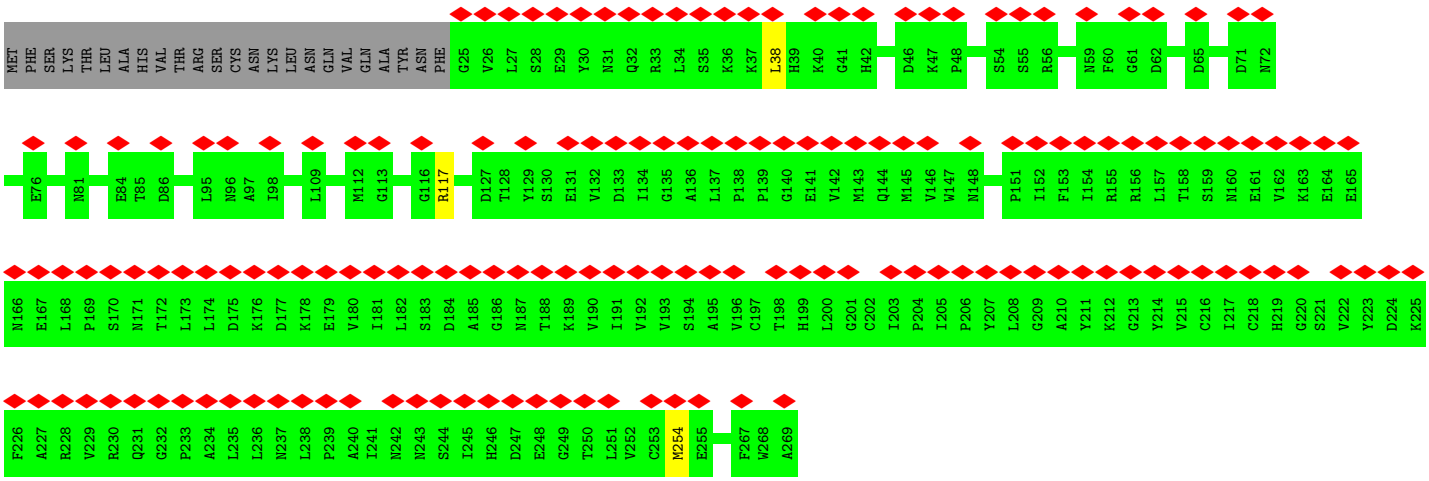
Chain E:



• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

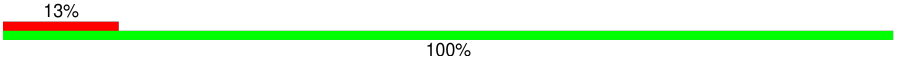
Chain e:

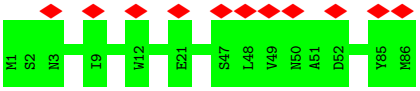




• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

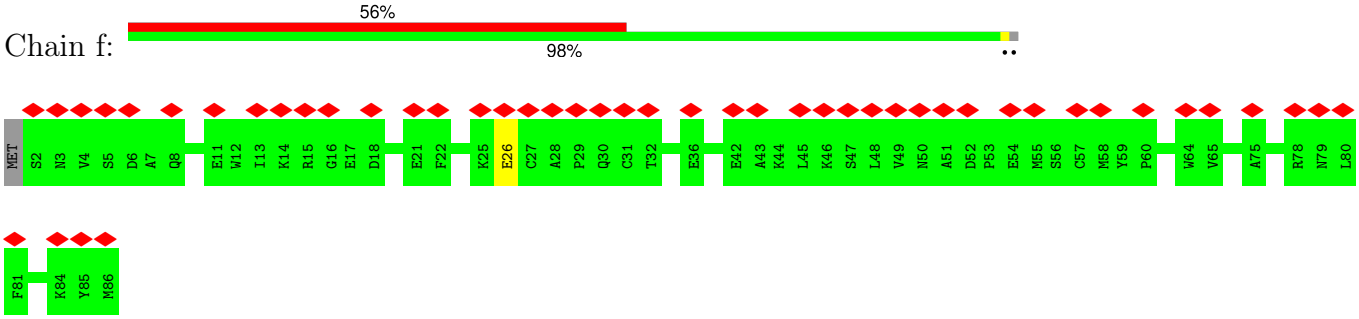
Chain F:





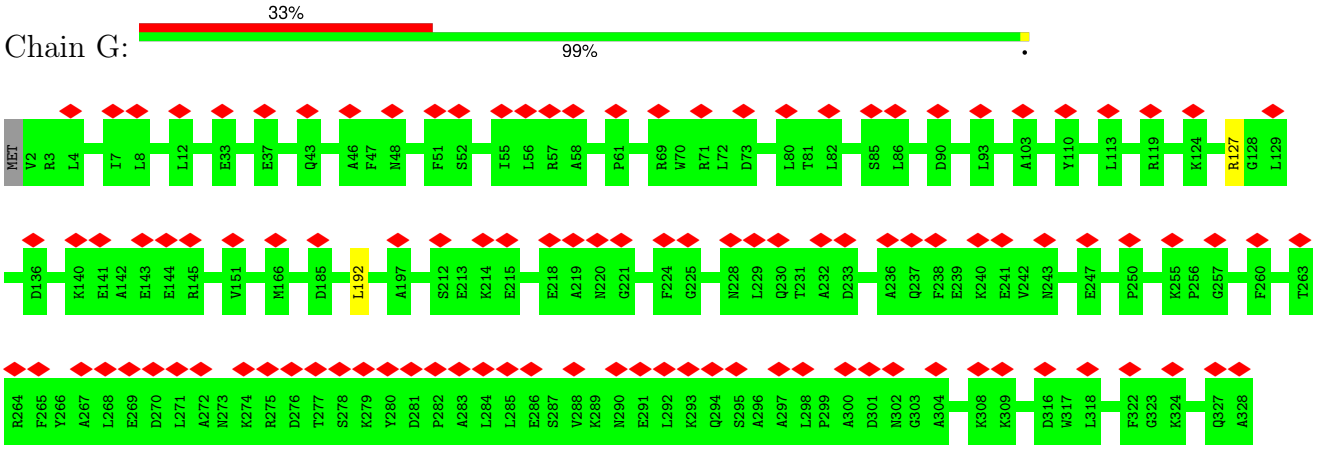
- Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

Chain f:



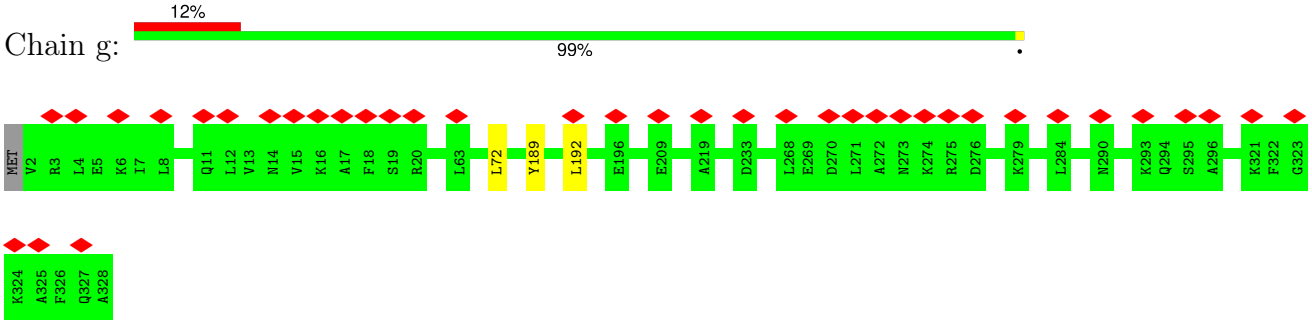
- Molecule 91: UQCRTT1

Chain G:



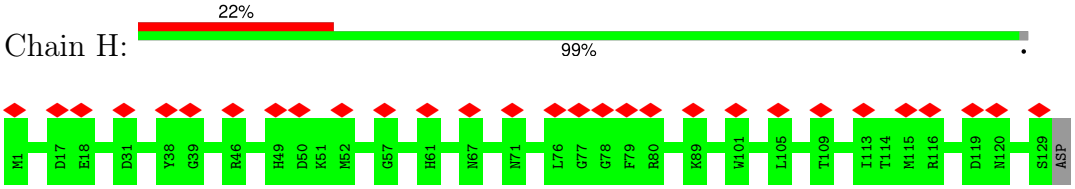
- Molecule 91: UQCRTT1

Chain g:



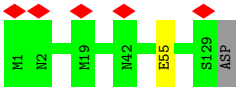
- Molecule 92: Transmembrane protein, putative

Chain H:



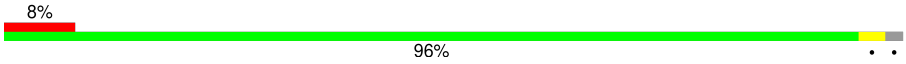
- Molecule 92: Transmembrane protein, putative

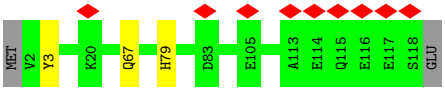
Chain h:



• Molecule 93: Transmembrane protein, putative

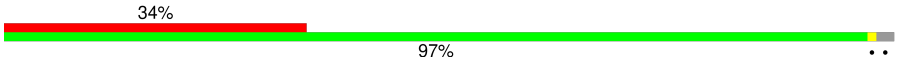
Chain I:

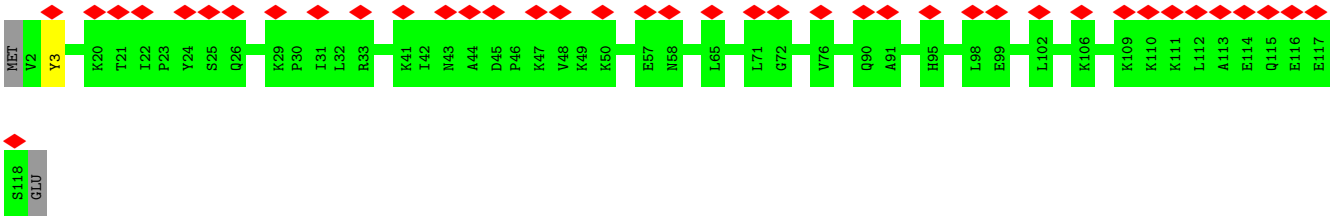




• Molecule 93: Transmembrane protein, putative

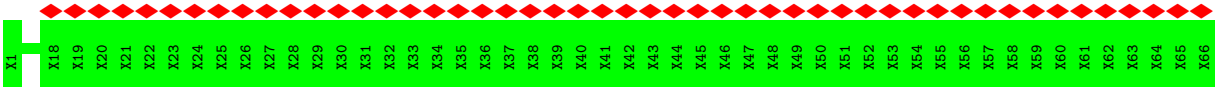
Chain i:





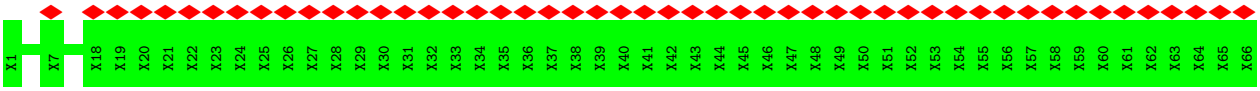
• Molecule 94: UQCRTT3

Chain J:



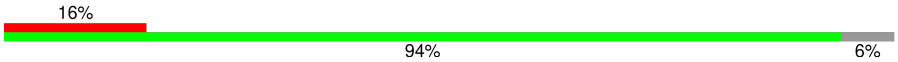
• Molecule 94: UQCRTT3

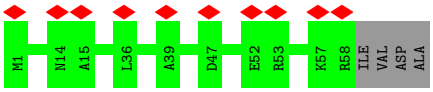
Chain j:



• Molecule 95: Transmembrane protein, putative

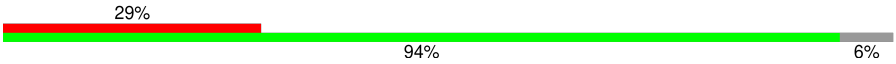
Chain K:

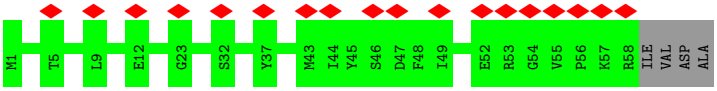




• Molecule 95: Transmembrane protein, putative

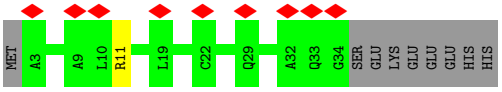
Chain k:





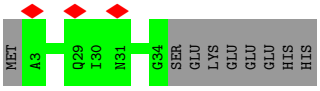
• Molecule 96: UQCRTT2

Chain L:



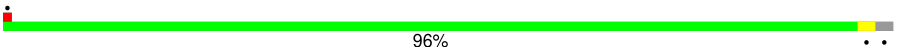
• Molecule 96: UQCRTT2

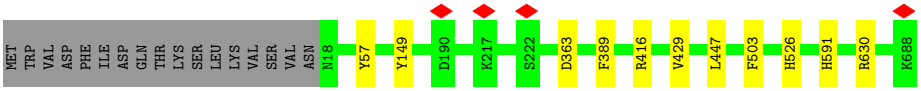
Chain l:



• Molecule 97: Cytochrome c oxidase subunit 1

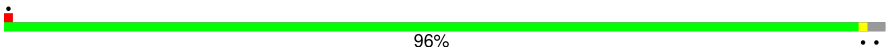
Chain DA:

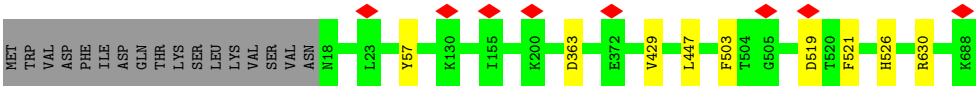




• Molecule 97: Cytochrome c oxidase subunit 1

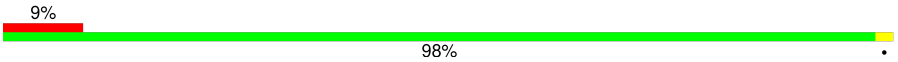
Chain Da:

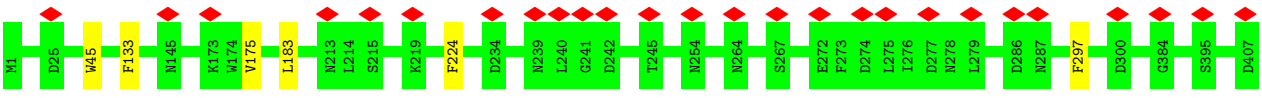




• Molecule 98: Cytochrome c oxidase subunit 2

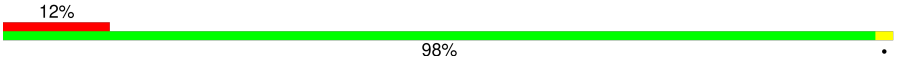
Chain DB:

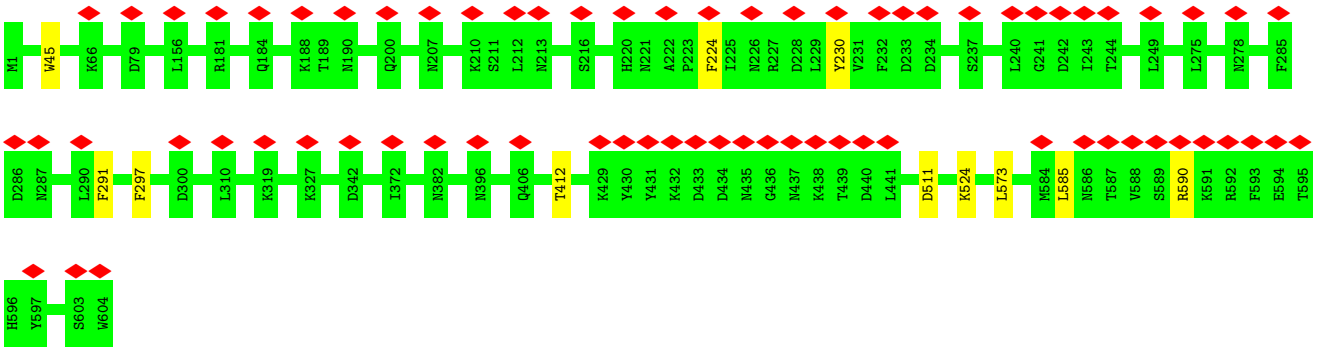




• Molecule 98: Cytochrome c oxidase subunit 2

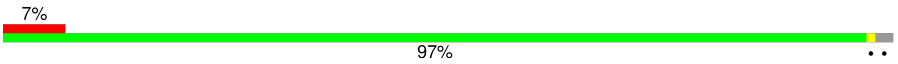
Chain Db:

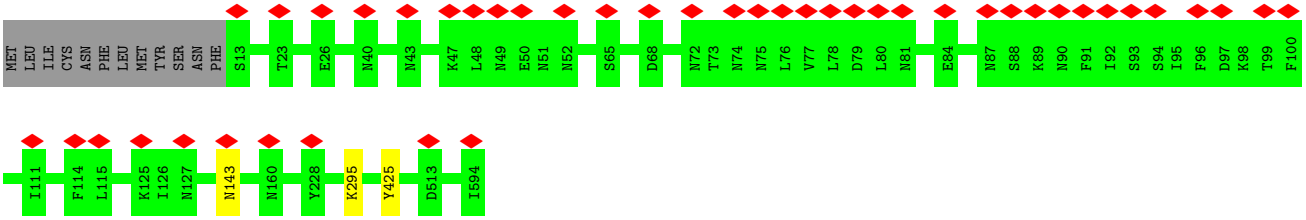




- Molecule 99: Ymf68

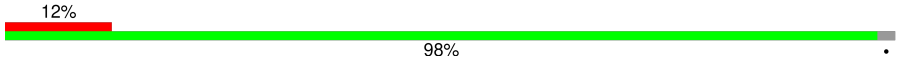
Chain DC:

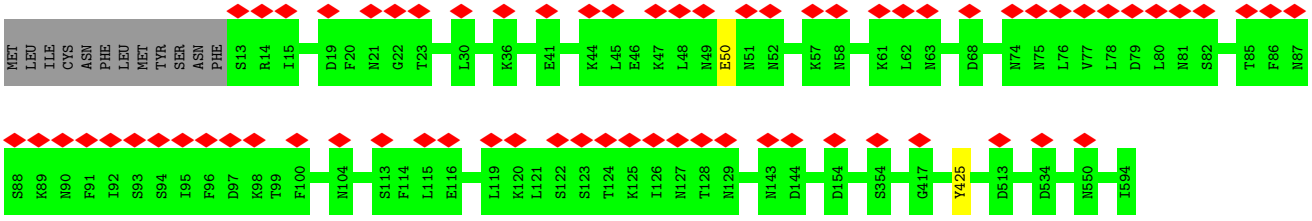




- Molecule 99: Ymf68

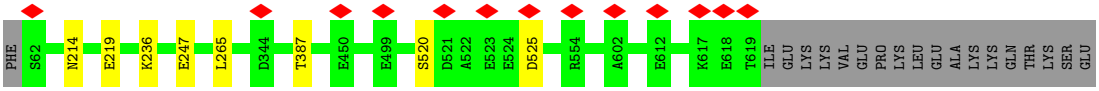
Chain Dc:





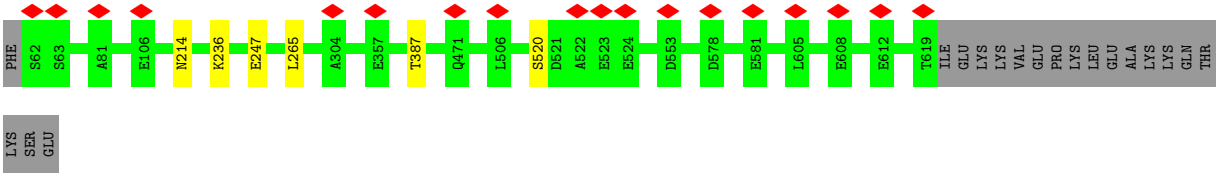
- Molecule 100: Cytochrome C oxidase subunit Vb protein

Chain DD:



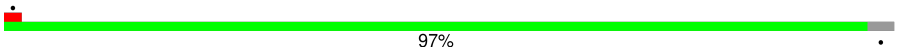
- Molecule 100: Cytochrome C oxidase subunit Vb protein

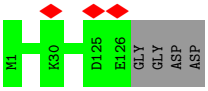
Chain Dd:



• Molecule 101: Transmembrane protein, putative

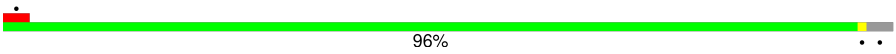
Chain DE:

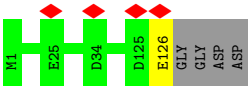




• Molecule 101: Transmembrane protein, putative

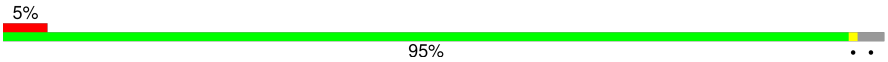
Chain De:

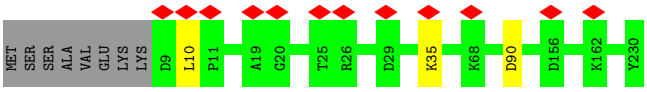




• Molecule 102: Structural protein

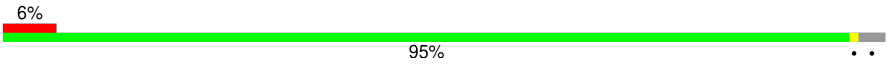
Chain DF:





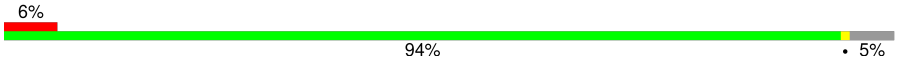
• Molecule 102: Structural protein

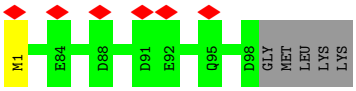
Chain Df:



• Molecule 103: Transmembrane protein, putative

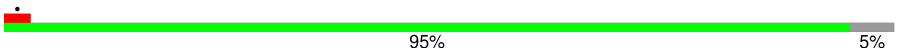
Chain DG:

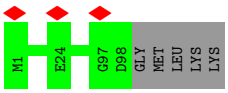




• Molecule 103: Transmembrane protein, putative

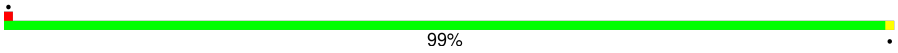
Chain Dg:

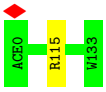




• Molecule 104: Transmembrane protein, putative

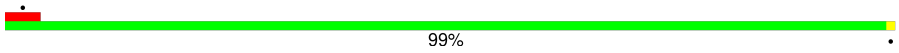
Chain DH:

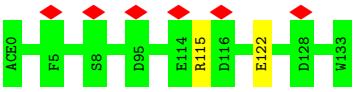




• Molecule 104: Transmembrane protein, putative

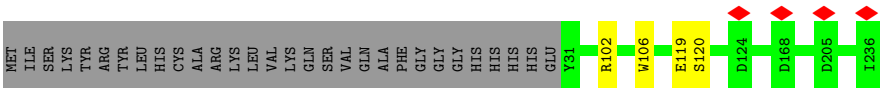
Chain Dh:





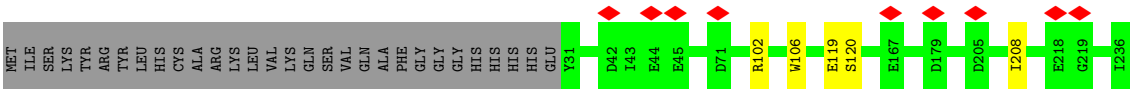
• Molecule 105: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain DI:



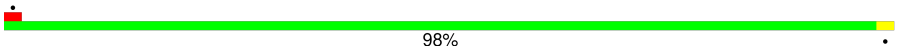
• Molecule 105: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

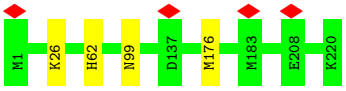
Chain Di:



• Molecule 106: Transmembrane protein, putative

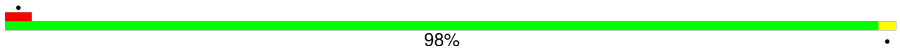
Chain DJ:

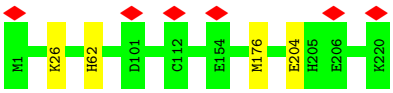




• Molecule 106: Transmembrane protein, putative

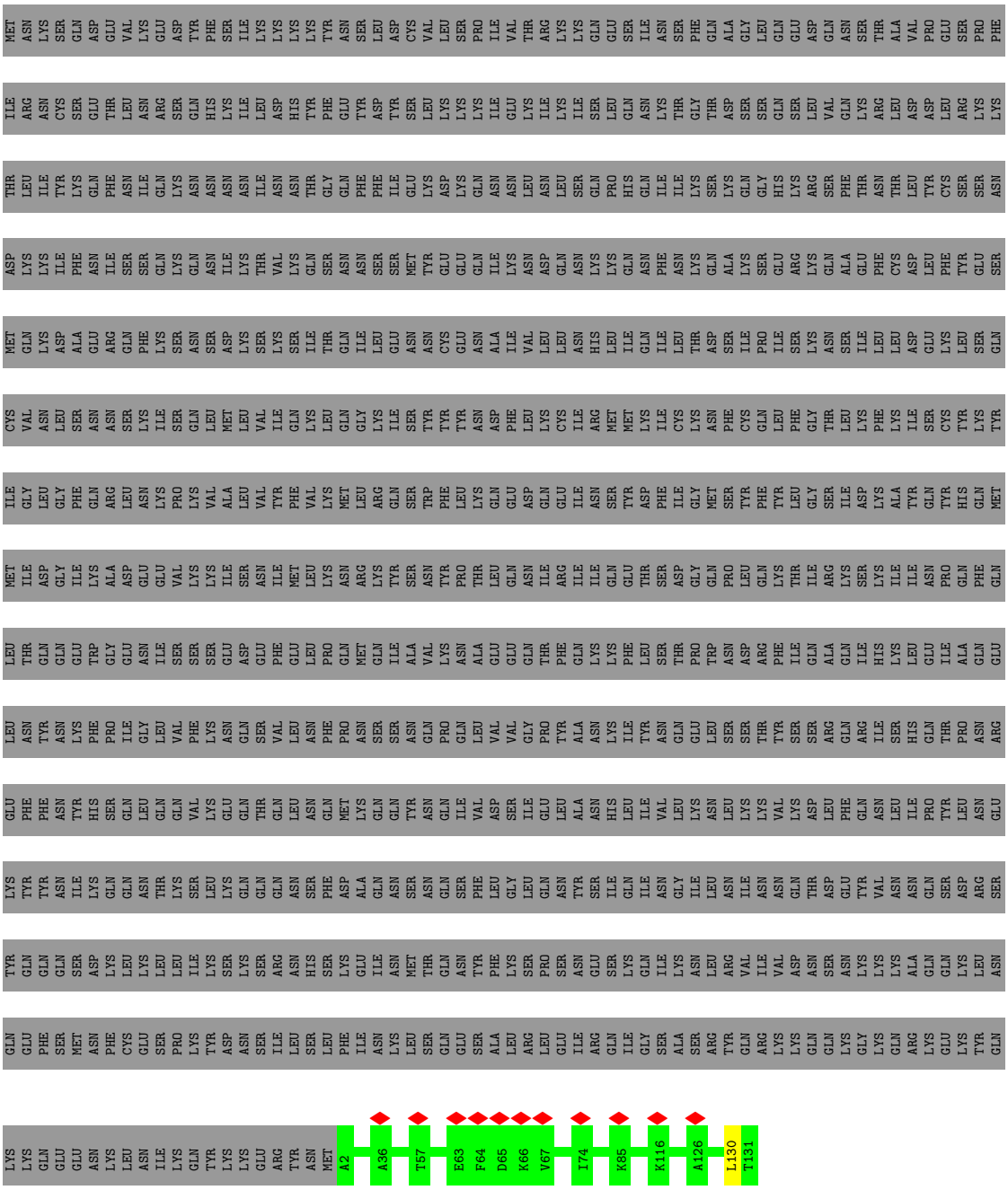
Chain Dj:





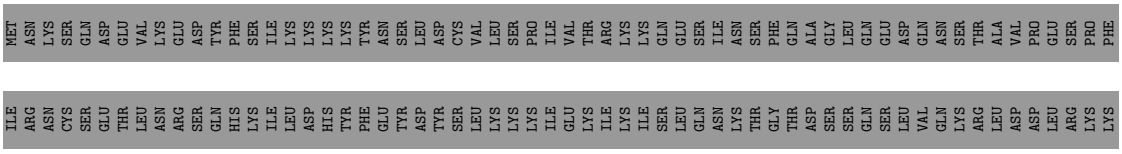
- Molecule 107: CTF/NF-I domain-containing protein

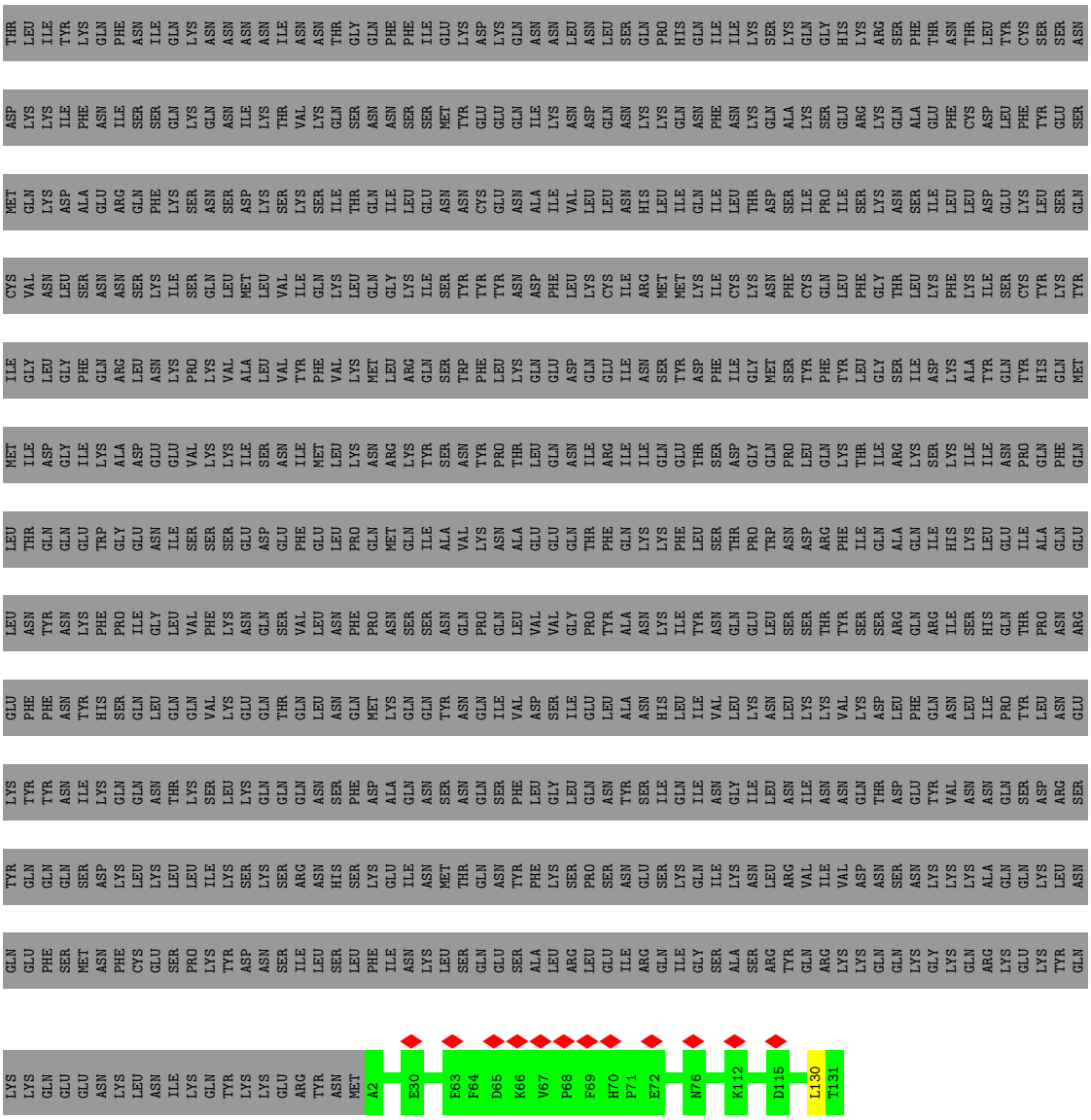
Chain DK:



- Molecule 107: CTF/NF-I domain-containing protein

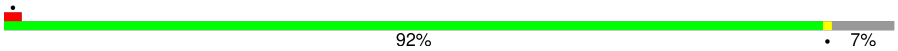
Chain Dk:

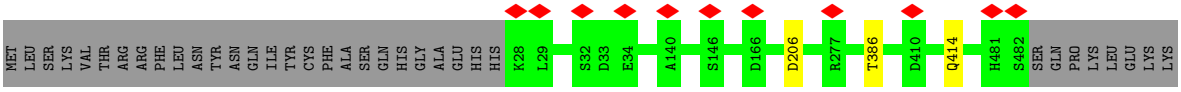




• Molecule 108: Transmembrane protein, putative

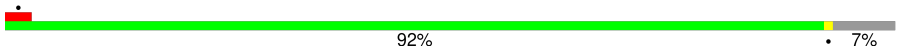
Chain DM:

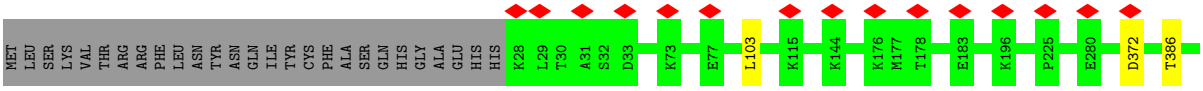


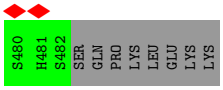


• Molecule 108: Transmembrane protein, putative

Chain Dm:

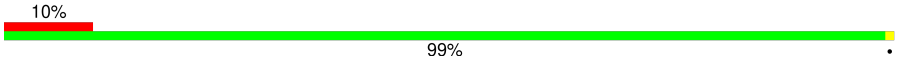


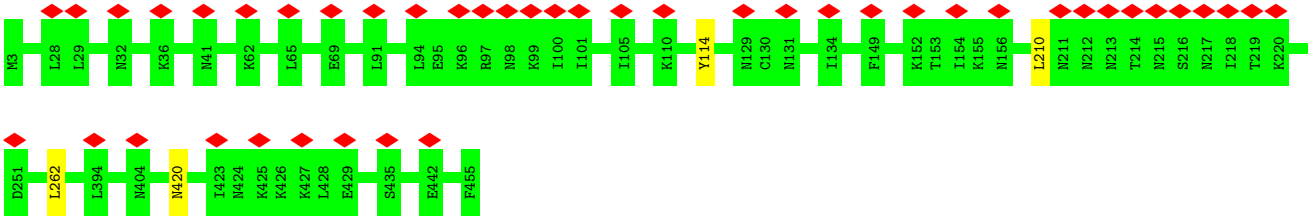




• Molecule 109: Ymf67

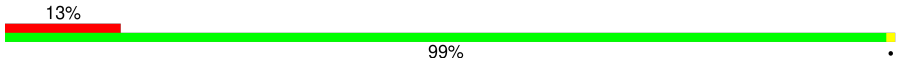
Chain DN:

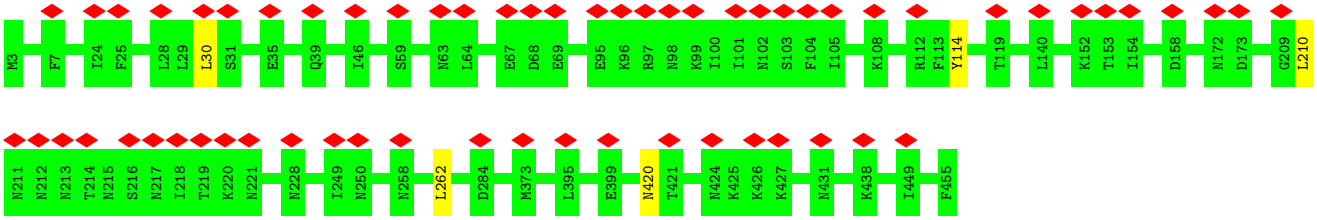




• Molecule 109: Ymf67

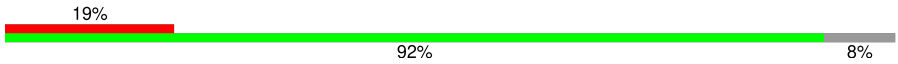
Chain Dn:

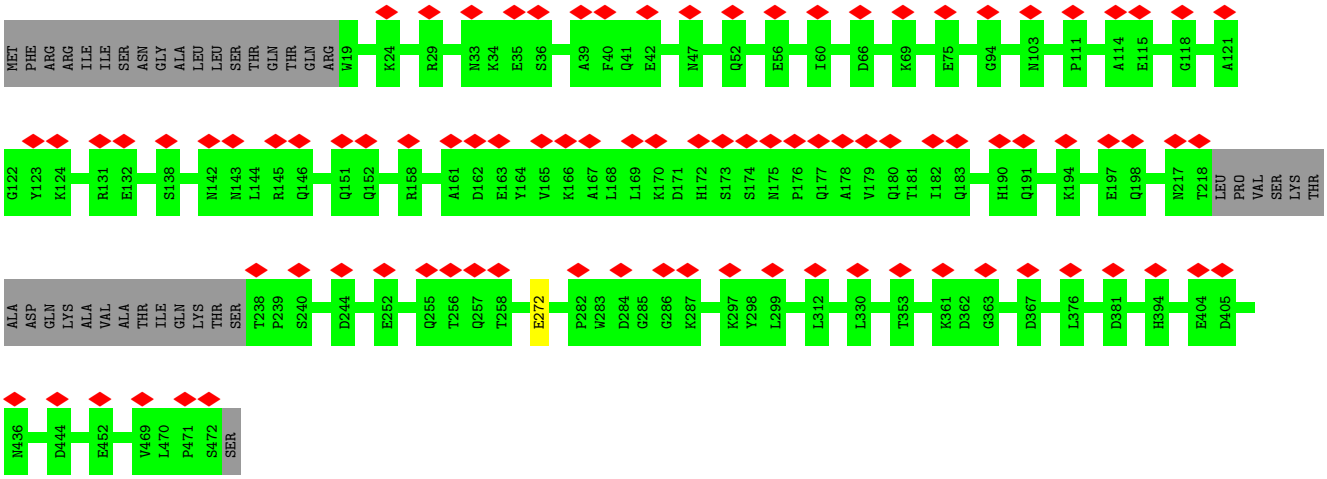




• Molecule 110: Protein phosphatase 2C, putative

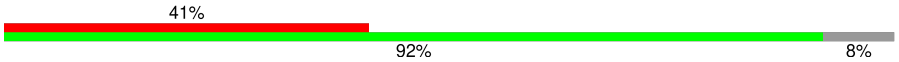
Chain DO:

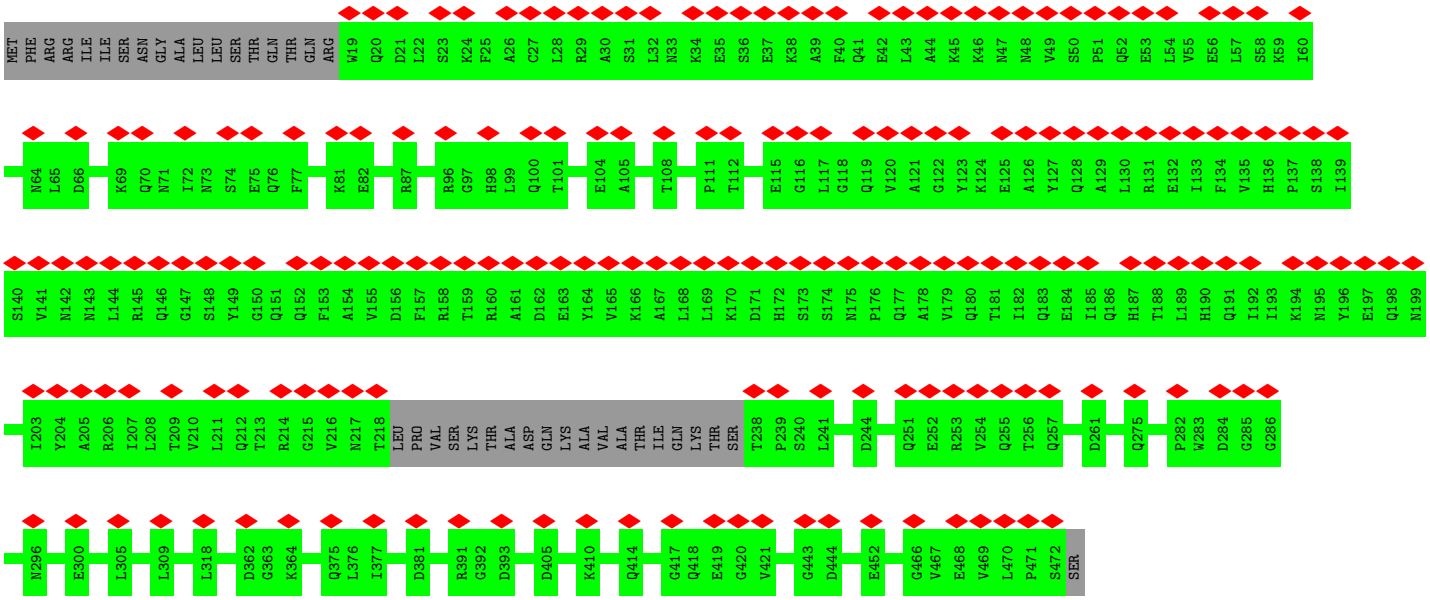




• Molecule 110: Protein phosphatase 2C, putative

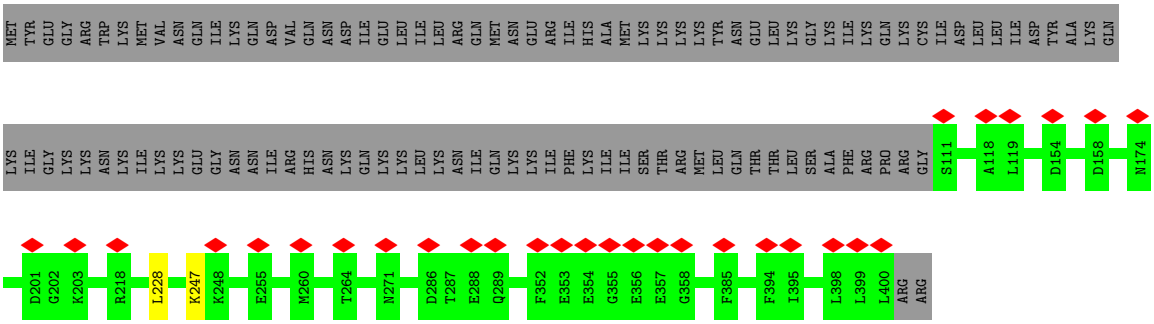
Chain Do:





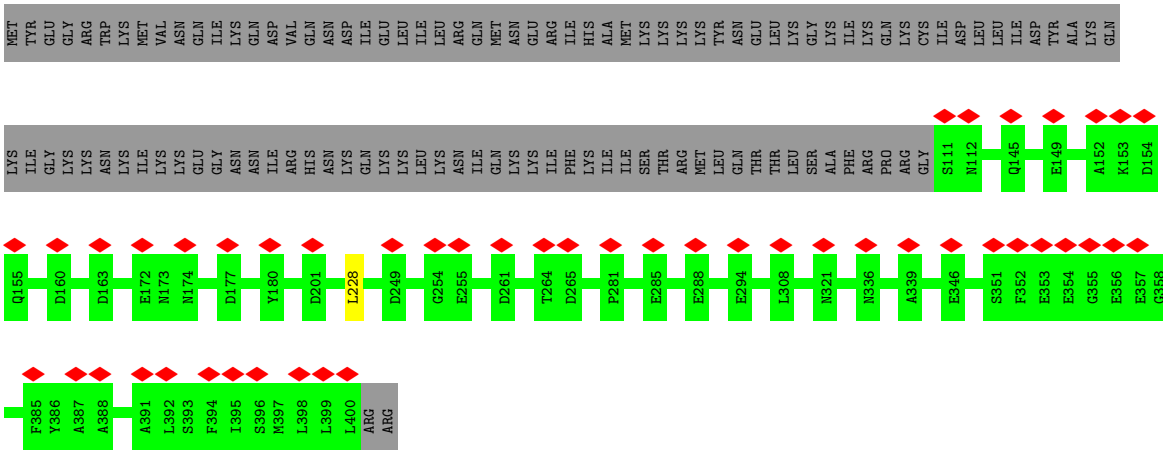
- Molecule 111: SURF1-like protein

Chain DP:



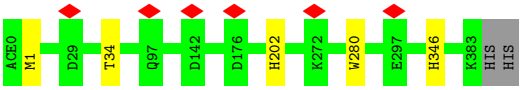
- Molecule 111: SURF1-like protein

Chain Dp:



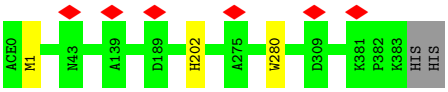
- Molecule 112: TraB family protein

Chain DQ: 98%



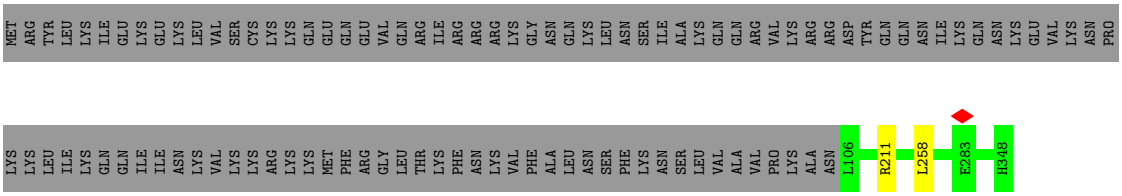
• Molecule 112: TraB family protein

Chain Dq: 99%



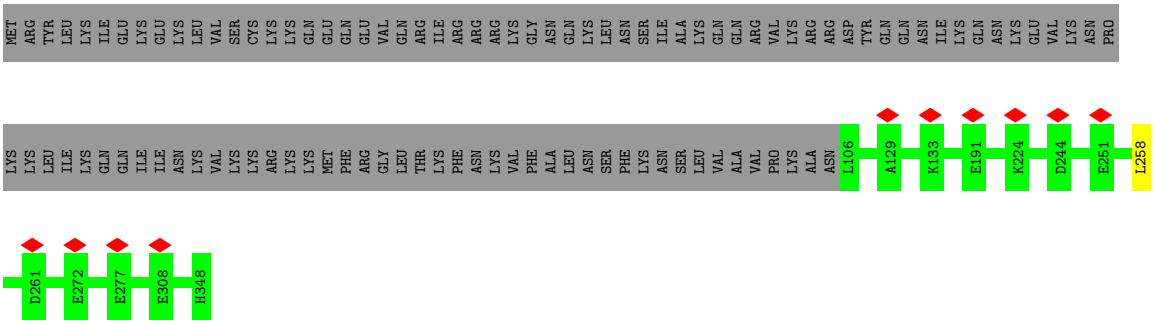
• Molecule 113: Transmembrane protein, putative

Chain DR: 69% 30%



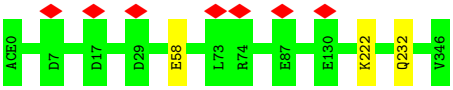
• Molecule 113: Transmembrane protein, putative

Chain Dr: 70% 30%



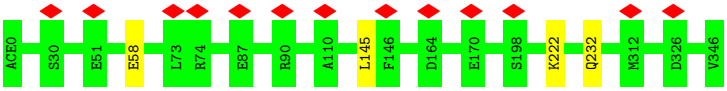
• Molecule 114: Oxoglutarate/malate translocator protein, putative

Chain DS: 99%



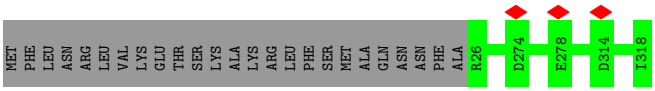
• Molecule 114: Oxoglutarate/malate translocator protein, putative

Chain Ds: 99%



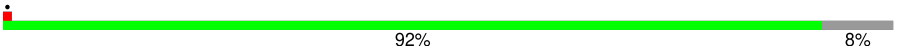
• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

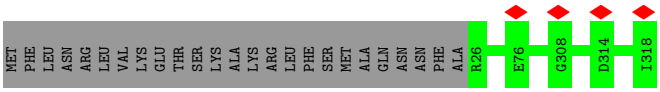
Chain DT:



• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

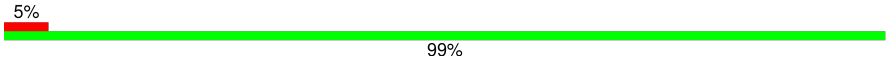
Chain Dt:

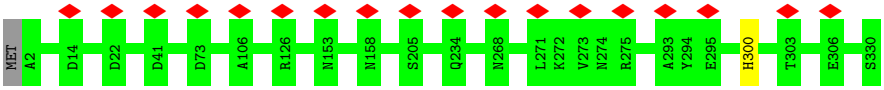




• Molecule 116: Carrier protein

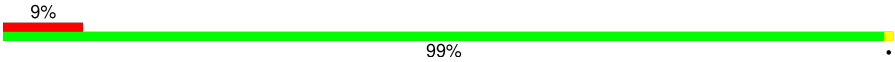
Chain DU:

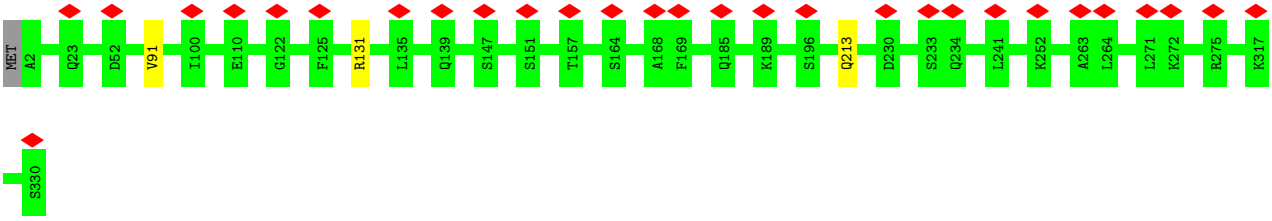




• Molecule 116: Carrier protein

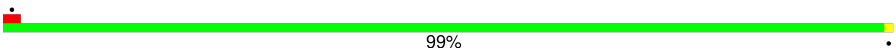
Chain Du:

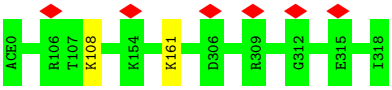




• Molecule 117: 2-oxoglutarate/malate carrier protein

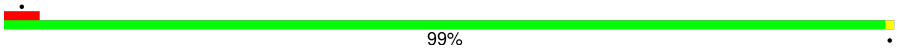
Chain DV:

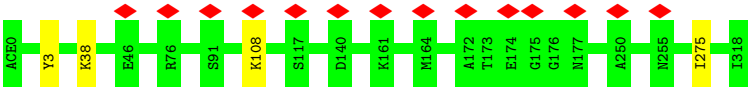




• Molecule 117: 2-oxoglutarate/malate carrier protein

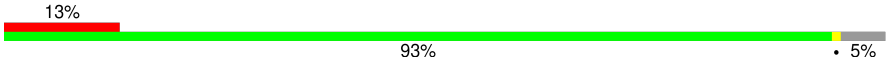
Chain Dv:

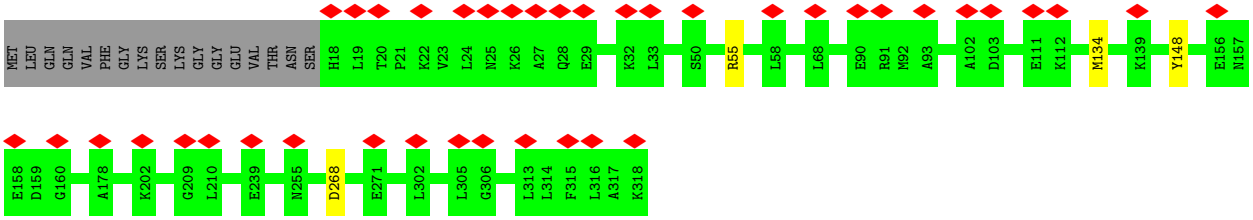




• Molecule 118: SURF1-like protein

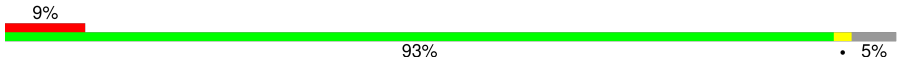
Chain DW:

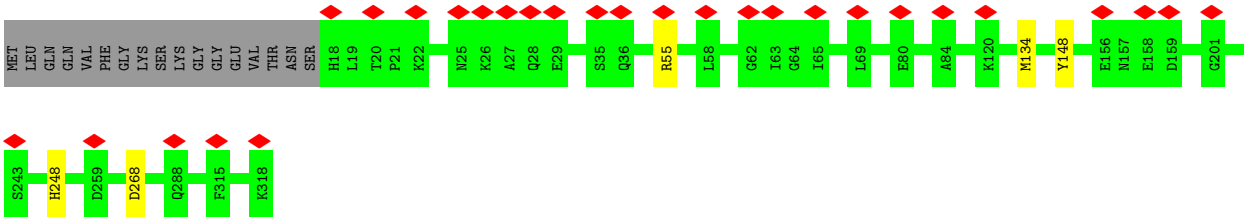




• Molecule 118: SURF1-like protein

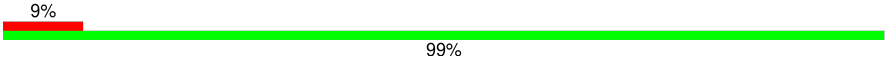
Chain Dw:

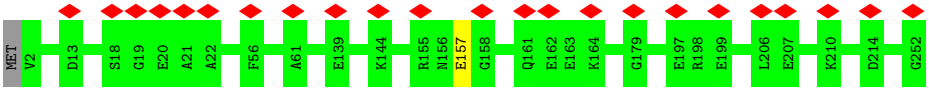




• Molecule 119: COXTT9

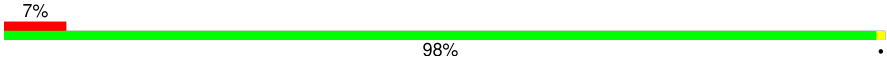
Chain DX:

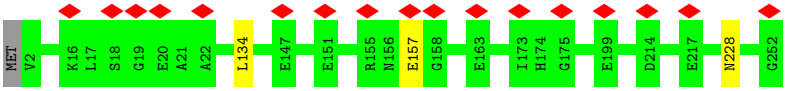




• Molecule 119: COXTT9

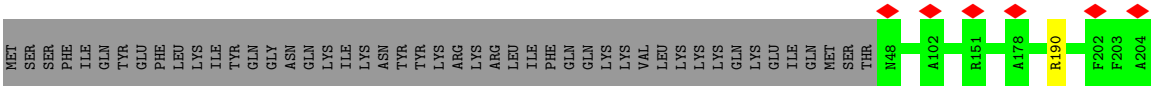
Chain Dx:

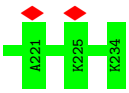




• Molecule 120: COXTT10

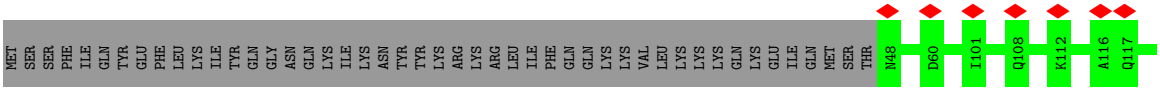
Chain DY:

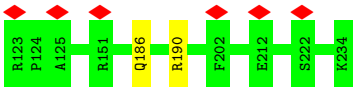




• Molecule 120: COXTT10

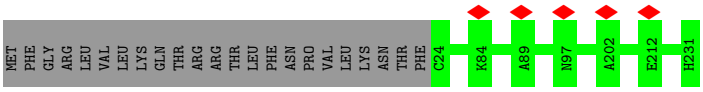
Chain Dy:





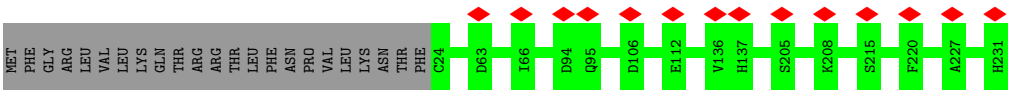
• Molecule 121: 39S ribosomal protein L9, mitochondrial

Chain DZ:



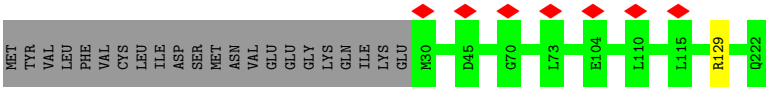
• Molecule 121: 39S ribosomal protein L9, mitochondrial

Chain Dz:



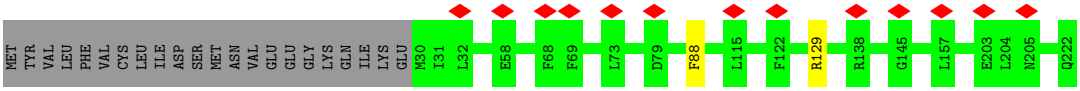
• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein,Transmembrane protein

Chain EA:



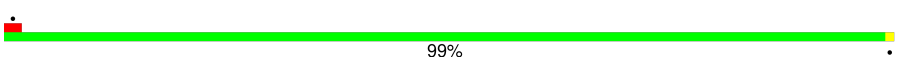
• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein,Transmembrane protein

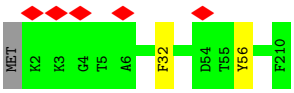
Chain Ea:



• Molecule 123: Transmembrane protein, putative

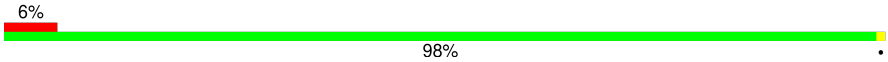
Chain EB:

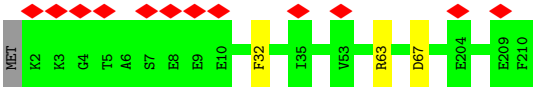




- Molecule 123: Transmembrane protein, putative

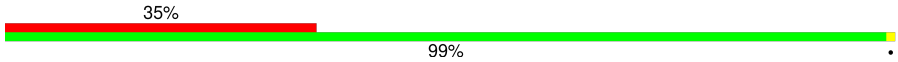
Chain Eb:

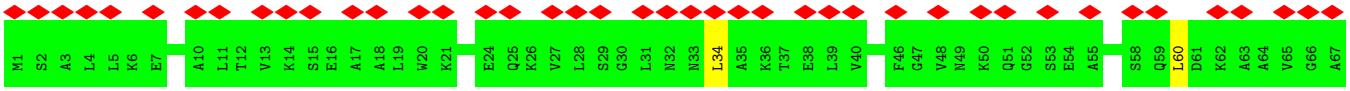


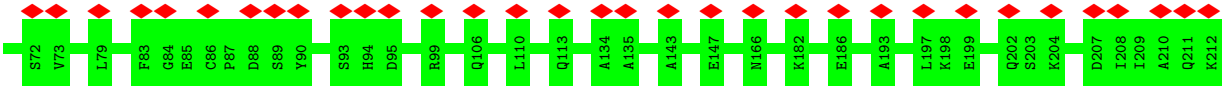


- Molecule 124: COXTT27

Chain EC:

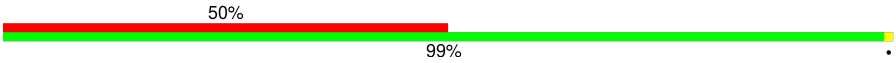


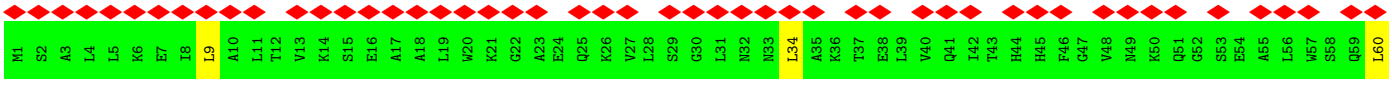


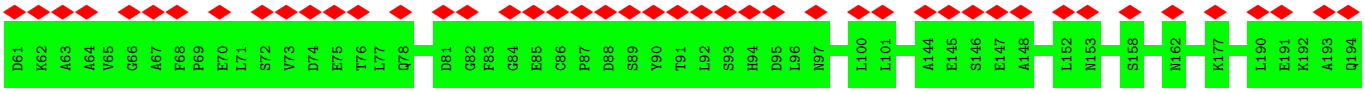


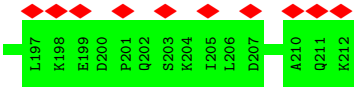
- Molecule 124: COXTT27

Chain Ec:



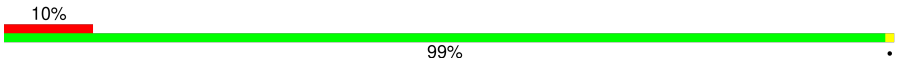


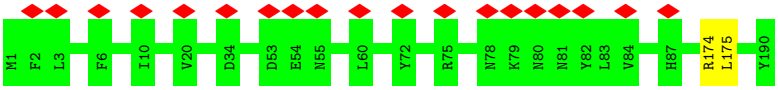




- Molecule 125: Ymf75

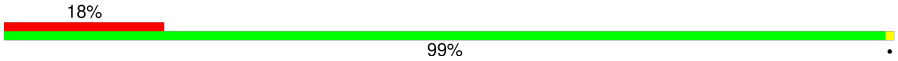
Chain ED:

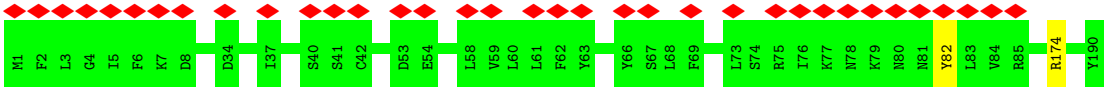




- Molecule 125: Ymf75

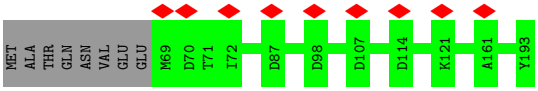
Chain Ed:





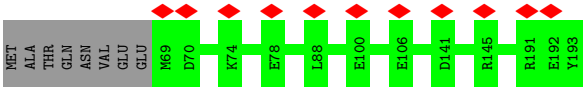
• Molecule 126: Mobilization protein

Chain EE:



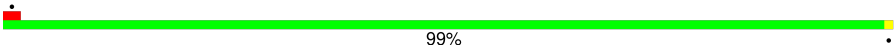
• Molecule 126: Mobilization protein

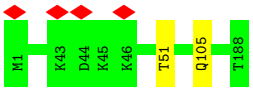
Chain Ee:



• Molecule 127: Iron-binding zinc finger CDGSH type protein

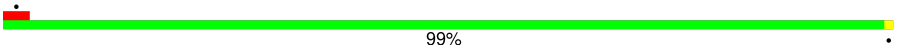
Chain EF:

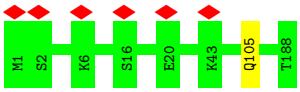




• Molecule 127: Iron-binding zinc finger CDGSH type protein

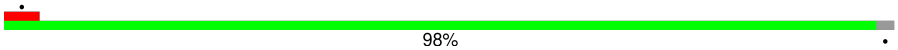
Chain Ef:

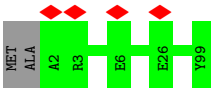




• Molecule 128: COXTT28

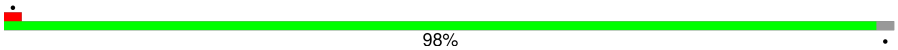
Chain EG:

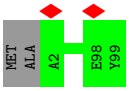




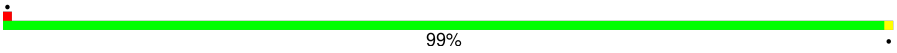
• Molecule 128: COXTT28

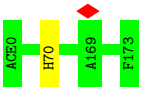
Chain Eg:





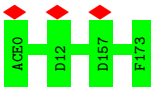
• Molecule 129: Transmembrane protein, putative

Chain EH: 

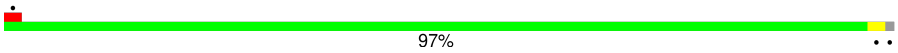


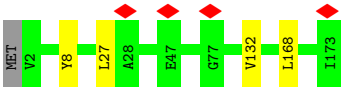
• Molecule 129: Transmembrane protein, putative

Chain Eh:

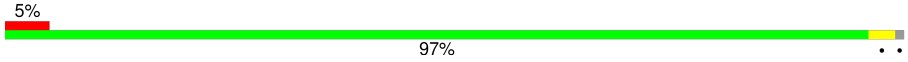


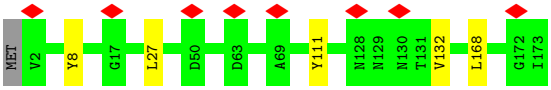
• Molecule 130: Transmembrane protein

Chain EI: 



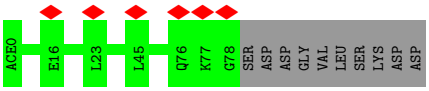
• Molecule 130: Transmembrane protein

Chain Ei: 



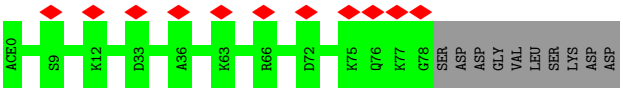
• Molecule 131: Decapping nuclease

Chain EV:

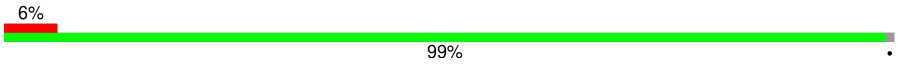


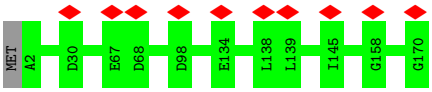
• Molecule 131: Decapping nuclease

Chain Ev:

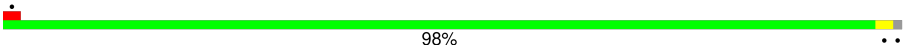


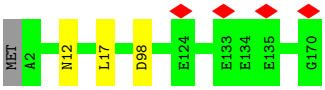
• Molecule 132: Complex III subunit VII

Chain EK: 

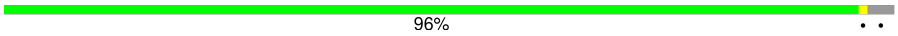


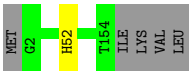
• Molecule 132: Complex III subunit VII

Chain Ek: 

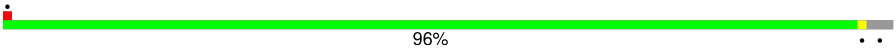


• Molecule 133: Transmembrane protein, putative

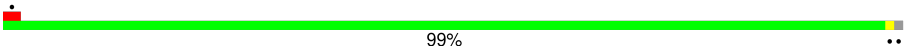
Chain EL: 

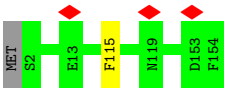


• Molecule 133: Transmembrane protein, putative

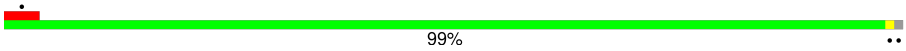
Chain El: 

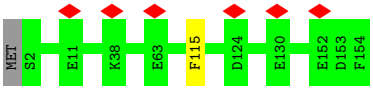
• Molecule 134: Transmembrane protein, putative

Chain EM: 

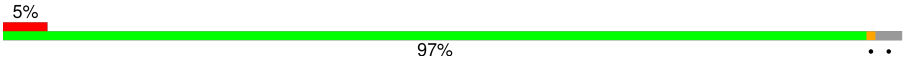


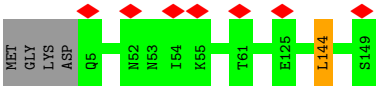
• Molecule 134: Transmembrane protein, putative

Chain Em: 



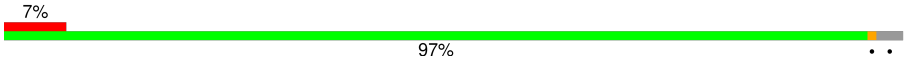
• Molecule 135: COXTT22

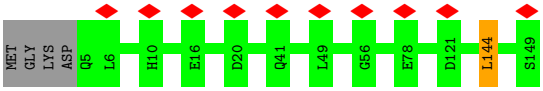
Chain EN: 



• Molecule 135: COXTT22

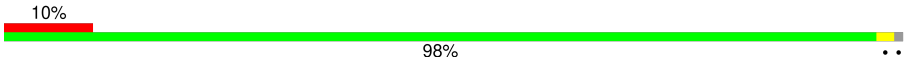
Chain En:

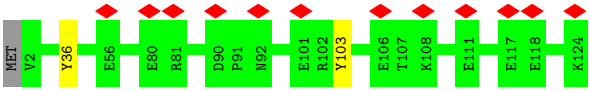




• Molecule 136: Transmembrane protein, putative

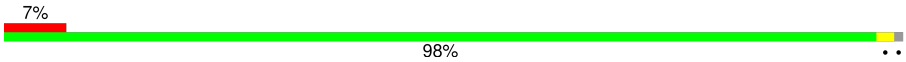
Chain EO:

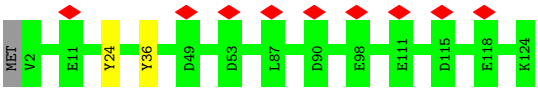




• Molecule 136: Transmembrane protein, putative

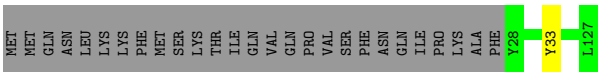
Chain Eo:





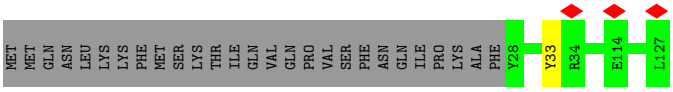
• Molecule 137: Phage protein

Chain EP:



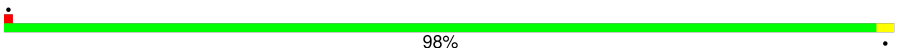
• Molecule 137: Phage protein

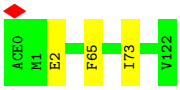
Chain Ep:



• Molecule 138: Transmembrane protein, putative

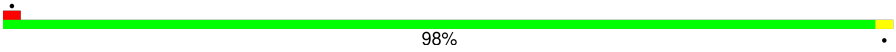
Chain EQ:

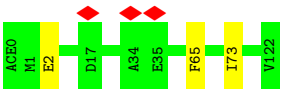




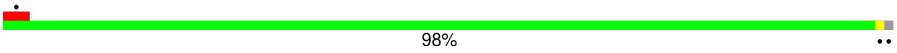
• Molecule 138: Transmembrane protein, putative

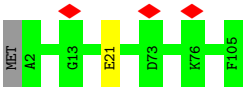
Chain Eq:



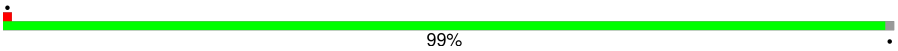


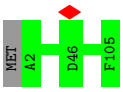
• Molecule 139: Lysozyme

Chain ER: 



• Molecule 139: Lysozyme

Chain Er: 



• Molecule 140: Ymf70

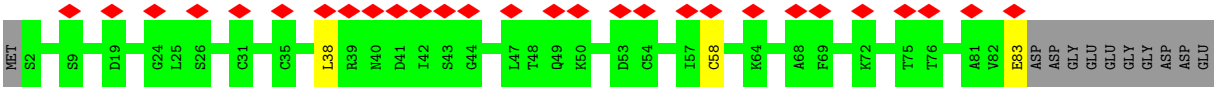
Chain ES:

• Molecule 140: Ymf70

Chain Es:

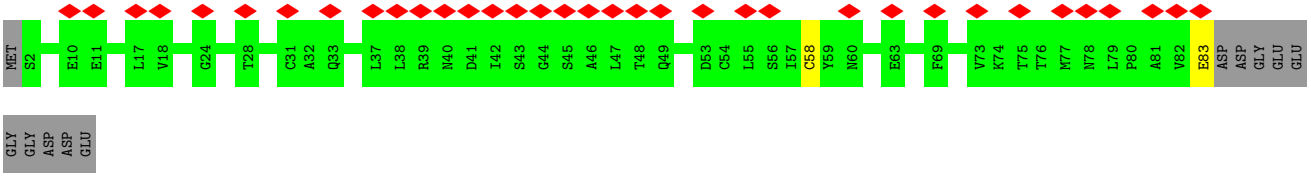
• Molecule 141: Zf-Tim10_DDP domain-containing protein

Chain ET:



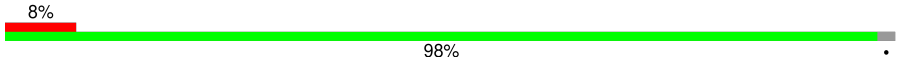
• Molecule 141: Zf-Tim10_DDP domain-containing protein

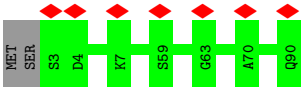
Chain Et:



- Molecule 142: ABC transporter

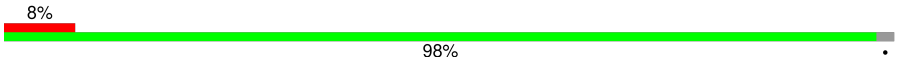
Chain EU:

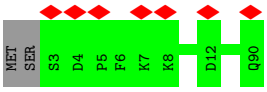




- Molecule 142: ABC transporter

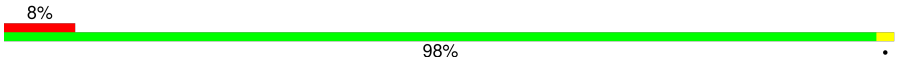
Chain Eu:

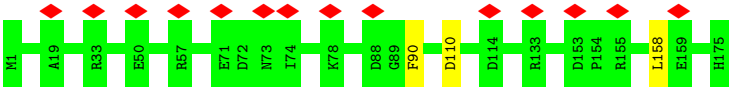




- Molecule 143: YflT domain-containing protein

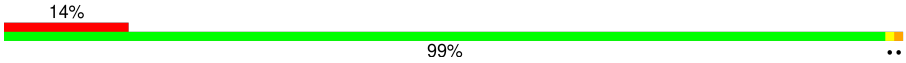
Chain EJ:

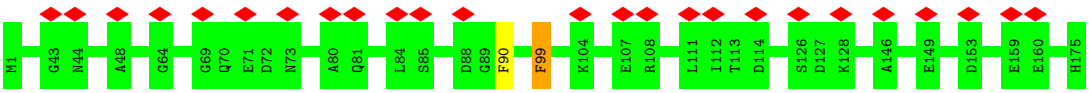




- Molecule 143: YflT domain-containing protein

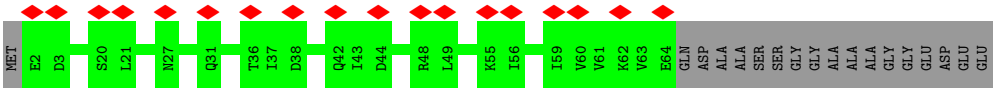
Chain Ej:





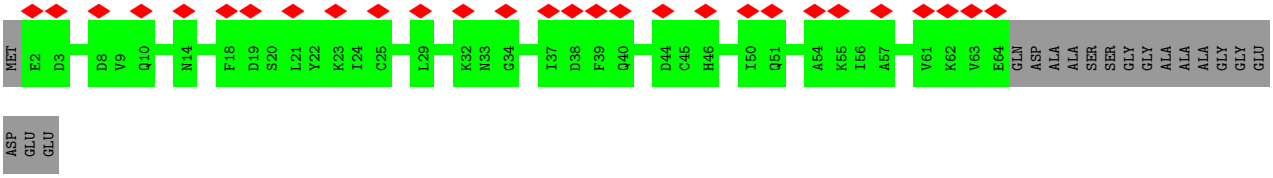
- Molecule 144: Cullin domain-containing protein

Chain EW:



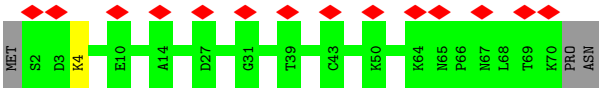
- Molecule 144: Cullin domain-containing protein

Chain Ew:



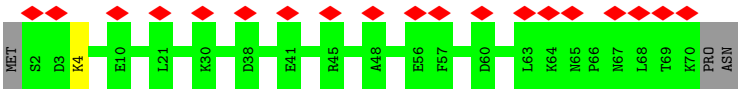
- Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain EX: 19% 94%



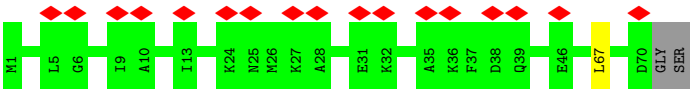
• Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain Ex: 26% 94%



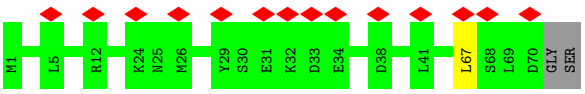
• Molecule 146: Annexin

Chain EY: 24% 96%



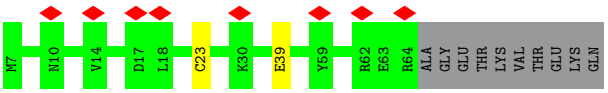
• Molecule 146: Annexin

Chain Ey: 19% 96%



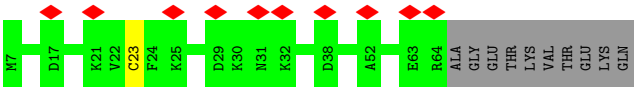
• Molecule 147: Transposase

Chain EZ: 12% 82% 15%



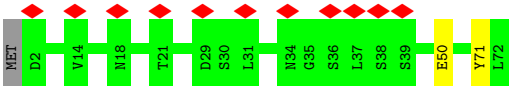
• Molecule 147: Transposase

Chain Ez: 15% 84% 15%



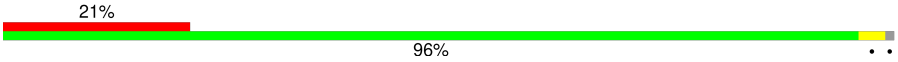
• Molecule 148: Tim10/DDP family zinc finger protein

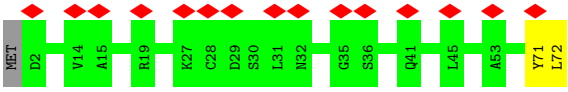
Chain FA: 15% 96%



• Molecule 148: Tim10/DDP family zinc finger protein

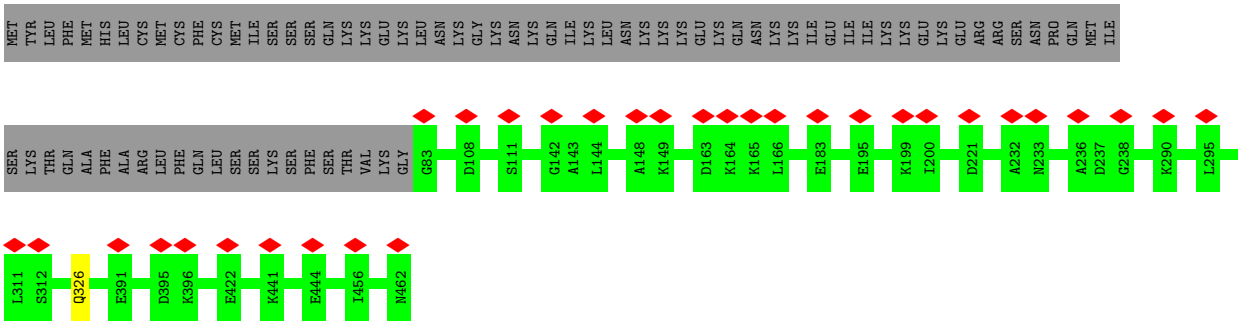
Chain Fa:





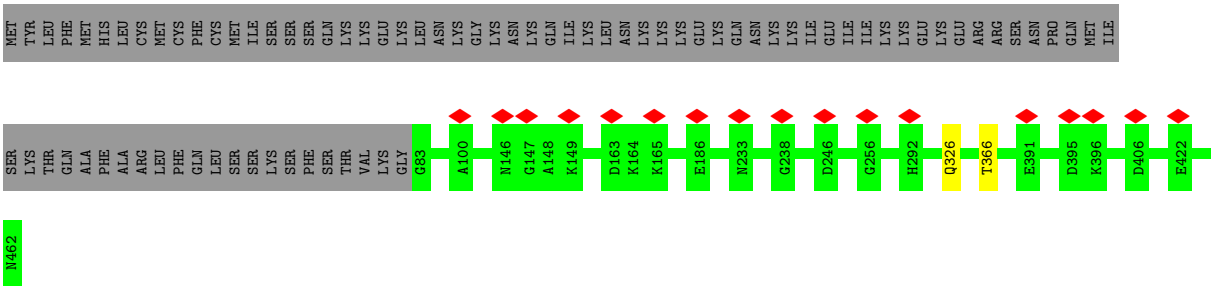
• Molecule 149: Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150

Chain Dl:



• Molecule 149: Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150

Chain DL:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
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 ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	6.348	Depositor
Minimum map value	-3.280	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.240	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, CUA, ADP, UQ8, ATP, 3PE, UDP, CA, HEC, F3S, TPO, SEP, ZN, K, LPP, CDL, HEA, PC1, CU, NDP, FMN, ACE, FAD, SF4, 8Q1, MG

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	A0	0.25	0/4166	0.43	0/5634
2	A1	0.24	0/2789	0.45	0/3777
3	A2	0.25	0/2248	0.47	0/3027
4	A3	0.24	0/2308	0.43	0/3134
5	A4	0.24	0/2542	0.42	0/3441
6	A5	0.24	0/2408	0.45	0/3269
7	A6	0.25	0/1963	0.46	0/2658
8	A7	0.25	0/1108	0.40	0/1488
9	A8	0.24	0/1833	0.43	0/2479
10	A9	0.25	0/1935	0.43	0/2616
11	AA	0.26	0/6132	0.39	0/8343
12	AB	0.24	0/5511	0.47	0/7465
13	AC	0.26	0/4303	0.39	0/5844
14	AD	0.25	0/3474	0.47	0/4699
15	AE	0.25	0/3669	0.46	0/4955
16	AF	0.26	0/3168	0.37	0/4307
17	AG	0.24	0/2865	0.46	0/3877
18	AH	0.26	0/2377	0.40	0/3234
19	AI	0.24	0/1899	0.43	0/2563
20	AJ	0.26	0/2224	0.39	0/3025
21	AK	0.25	0/1816	0.46	0/2475
22	AL	0.25	0/1867	0.46	0/2538
23	AM	0.24	0/1801	0.48	0/2449
24	AN	0.24	0/1351	0.44	0/1817
25	AO	0.24	0/1720	0.43	0/2322
26	AP	0.24	0/1654	0.48	0/2240
27	AQ	0.25	0/1636	0.42	0/2214
28	AR	0.25	0/1535	0.47	0/2077
29	AS	0.25	0/1458	0.47	0/1965
30	AT	0.24	0/1310	0.48	0/1779
31	AU	0.26	0/1261	0.47	0/1698

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	AV	0.24	0/941	0.42	0/1272
33	AW	0.24	0/819	0.46	0/1110
34	AX	0.26	0/1061	0.38	0/1441
35	AY	0.24	0/982	0.37	0/1335
36	AZ	0.25	0/790	0.46	0/1066
37	B0	0.25	0/833	0.50	0/1132
38	B1	0.24	0/812	0.44	0/1093
39	B2	0.25	0/776	0.43	0/1048
40	B3	0.25	0/654	0.45	0/884
41	B4	0.25	0/642	0.47	0/865
42	B5	0.26	0/466	0.41	0/630
43	B6	0.26	0/535	0.42	0/727
44	BA	0.24	0/1696	0.41	0/2292
45	BB	0.25	0/1376	0.42	0/1862
46	BC	0.25	0/1479	0.44	0/1996
47	BD	0.24	0/1216	0.44	0/1643
48	BE	0.25	0/1462	0.42	0/1981
49	BF	0.24	0/1503	0.48	0/2018
50	BG	0.24	0/1379	0.48	0/1841
51	BH	0.26	0/1519	0.38	0/2058
52	BI	0.24	0/1203	0.47	0/1630
53	BJ	0.25	0/1234	0.44	0/1662
54	BK	0.25	0/923	0.43	0/1239
55	BL	0.26	0/1223	0.45	0/1648
56	BM	0.25	0/1110	0.46	0/1502
57	BN	0.24	0/1132	0.43	0/1534
58	BO	0.25	0/1120	0.46	0/1500
59	BP	0.26	0/631	0.40	0/860
60	BQ	0.26	0/868	0.43	0/1170
61	BR	0.24	0/747	0.44	0/1011
62	BS	0.26	0/991	0.41	0/1333
63	BT	0.27	0/1106	0.42	0/1504
64	BU	0.24	0/1102	0.46	0/1486
65	BV	0.24	0/1003	0.45	0/1353
66	BW	0.25	0/983	0.40	0/1327
67	BX	0.26	0/821	0.44	0/1111
68	BY	0.27	0/916	0.41	0/1224
69	BZ	0.26	0/873	0.44	0/1175
70	CH	0.24	0/867	0.40	0/1166
71	CM	0.24	0/648	0.49	0/879
72	CL	0.25	0/788	0.42	0/1058
73	CA	0.24	0/4722	0.49	0/6385
74	CI	0.27	0/930	0.39	0/1244

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	CB	0.24	0/2355	0.44	0/3191
76	CF	0.26	0/1857	0.44	0/2512
77	CG	0.25	0/1699	0.40	0/2296
78	CK	0.26	0/821	0.45	0/1112
79	CE	0.24	0/2615	0.44	0/3553
80	CJ	0.26	0/875	0.39	0/1186
81	CN	0.26	0/530	0.45	0/719
82	CC	0.26	0/501	0.47	0/674
83	CO	0.26	0/375	0.45	0/508
84	CD	0.25	0/406	0.40	0/546
85	A	0.25	0/3933	0.49	0/5338
85	a	0.24	0/3933	0.48	0/5338
86	B	0.24	0/3616	0.45	0/4897
86	b	0.24	0/3616	0.45	0/4897
87	C	0.25	0/3716	0.41	0/5046
87	c	0.25	0/3716	0.41	0/5046
88	D	0.26	0/2580	0.47	0/3491
88	d	0.25	0/2580	0.46	0/3491
89	E	0.24	0/2015	0.47	0/2732
89	e	0.24	0/2015	0.47	0/2732
90	F	0.25	0/700	0.44	0/942
90	f	0.24	0/692	0.43	0/932
91	G	0.24	0/2846	0.47	0/3839
91	g	0.25	0/2846	0.48	0/3839
92	H	0.25	0/1133	0.48	0/1524
92	h	0.27	0/1133	0.51	0/1524
93	I	0.25	0/1029	0.41	0/1397
93	i	0.25	0/1029	0.40	0/1397
95	K	0.26	0/522	0.43	0/712
95	k	0.26	0/522	0.43	0/712
96	L	0.27	0/269	0.41	0/366
96	l	0.27	0/269	0.42	0/366
97	DA	0.24	0/5748	0.43	0/7793
97	Da	0.25	0/5748	0.45	0/7793
98	DB	0.24	0/5282	0.46	2/7159 (0.0%)
98	Db	0.24	0/5282	0.46	2/7159 (0.0%)
99	DC	0.25	0/5256	0.41	0/7142
99	Dc	0.25	0/5256	0.42	0/7142
100	DD	0.24	0/4734	0.46	2/6387 (0.0%)
100	Dd	0.25	0/4734	0.46	2/6387 (0.0%)
101	DE	0.25	0/1116	0.42	0/1512
101	De	0.25	0/1116	0.41	0/1512
102	DF	0.25	0/1977	0.48	2/2673 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
102	Df	0.25	0/1977	0.49	2/2673 (0.1%)
103	DG	0.24	0/906	0.45	0/1230
103	Dg	0.25	0/906	0.46	0/1230
104	DH	0.24	0/1208	0.46	0/1633
104	Dh	0.24	0/1208	0.46	0/1633
105	DI	0.24	0/1829	0.42	0/2486
105	Di	0.24	0/1829	0.42	0/2486
106	DJ	0.24	0/1950	0.44	0/2647
106	Dj	0.24	0/1950	0.44	0/2647
107	DK	0.24	0/1100	0.47	2/1495 (0.1%)
107	Dk	0.25	0/1100	0.47	2/1495 (0.1%)
108	DM	0.24	0/3910	0.44	0/5320
108	Dm	0.24	0/3910	0.44	0/5320
109	DN	0.24	0/3963	0.39	0/5359
109	Dn	0.25	0/3963	0.40	0/5359
110	DO	0.24	0/3505	0.42	0/4745
110	Do	0.24	0/3505	0.42	0/4745
111	DP	0.24	0/2433	0.46	0/3307
111	Dp	0.24	0/2433	0.46	0/3307
112	DQ	0.24	0/3256	0.44	0/4422
112	Dq	0.24	0/3256	0.45	0/4422
113	DR	0.24	0/2077	0.45	2/2824 (0.1%)
113	Dr	0.24	0/2077	0.46	2/2824 (0.1%)
114	DS	0.25	0/2959	0.44	0/4015
114	Ds	0.25	0/2959	0.44	0/4015
115	DT	0.24	0/2518	0.45	0/3433
115	Dt	0.24	0/2518	0.45	0/3433
116	DU	0.24	0/2689	0.42	0/3657
116	Du	0.24	0/2689	0.42	0/3657
117	DV	0.24	0/2631	0.44	0/3566
117	Dv	0.24	0/2631	0.45	0/3566
118	DW	0.24	0/2449	0.44	0/3312
118	Dw	0.24	0/2449	0.45	0/3312
119	DX	0.24	0/2171	0.44	0/2930
119	Dx	0.25	0/2171	0.44	0/2930
120	DY	0.23	0/1619	0.44	0/2198
120	Dy	0.23	0/1619	0.45	0/2198
121	DZ	0.23	0/1752	0.41	0/2372
121	Dz	0.23	0/1752	0.41	0/2372
122	EA	0.24	0/1709	0.43	0/2321
122	Ea	0.24	0/1709	0.44	0/2321
123	EB	0.24	0/1793	0.42	0/2418
123	Eb	0.25	0/1793	0.42	0/2418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
124	EC	0.24	0/1673	0.45	4/2258 (0.2%)
124	Ec	0.24	0/1673	0.46	4/2258 (0.2%)
125	ED	0.25	0/1708	0.38	0/2306
125	Ed	0.26	0/1708	0.38	0/2306
126	EE	0.23	0/1066	0.44	0/1432
126	Ee	0.24	0/1066	0.45	0/1432
127	EF	0.26	0/1562	0.45	0/2123
127	Ef	0.26	0/1562	0.46	0/2123
128	EG	0.24	0/786	0.43	0/1060
128	Eg	0.25	0/786	0.44	0/1060
129	EH	0.24	0/1480	0.43	0/2007
129	Eh	0.25	0/1480	0.44	0/2007
130	EI	0.25	0/1442	0.49	4/1952 (0.2%)
130	Ei	0.25	0/1442	0.50	4/1952 (0.2%)
131	EV	0.24	0/654	0.41	0/878
131	Ev	0.24	0/654	0.42	0/878
132	EK	0.23	0/1410	0.42	0/1900
132	Ek	0.24	0/1410	0.43	0/1900
133	EL	0.24	0/1335	0.44	0/1810
133	El	0.25	0/1335	0.45	0/1810
134	EM	0.24	0/1335	0.46	0/1794
134	Em	0.24	0/1335	0.47	0/1794
135	EN	0.24	0/1270	0.50	2/1724 (0.1%)
135	En	0.24	0/1270	0.51	2/1724 (0.1%)
136	EO	0.24	0/1137	0.45	0/1545
136	Eo	0.24	0/1137	0.45	0/1545
137	EP	0.23	0/837	0.49	0/1133
137	Ep	0.24	0/837	0.49	0/1133
138	EQ	0.24	0/1044	0.42	0/1415
138	Eq	0.24	0/1044	0.43	0/1415
139	ER	0.24	0/874	0.46	0/1182
139	Er	0.24	0/874	0.46	0/1182
140	ES	0.26	0/802	0.40	0/1087
140	Es	0.26	0/802	0.41	0/1087
141	ET	0.24	0/654	0.42	0/878
141	Et	0.24	0/654	0.43	0/878
142	EU	0.24	0/744	0.44	0/1003
142	Eu	0.24	0/744	0.45	0/1003
143	EJ	0.24	0/1437	0.42	0/1941
143	Ej	0.25	0/1437	0.43	0/1941
144	EW	0.24	0/523	0.41	0/705
144	Ew	0.24	0/523	0.41	0/705
145	EX	0.23	0/564	0.41	0/757

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
145	Ex	0.23	0/564	0.42	0/757
146	EY	0.25	0/573	0.48	2/770 (0.3%)
146	Ey	0.25	0/573	0.50	2/770 (0.3%)
147	EZ	0.24	0/502	0.44	0/676
147	Ez	0.25	0/502	0.43	0/676
148	FA	0.22	0/554	0.39	0/746
148	Fa	0.23	0/554	0.40	0/746
149	DL	0.25	0/2984	0.45	0/4047
149	Dl	0.25	0/2984	0.44	0/4047
All	All	0.25	0/382937	0.44	44/518529 (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
143	Ej	0	1

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
146	EY	67	LEU	CB-CG-CD2	6.21	121.56	111.00
146	Ey	67	LEU	CB-CG-CD2	6.17	121.49	111.00
130	Ei	168	LEU	CB-CG-CD2	6.15	121.45	111.00
100	Dd	265	LEU	CB-CG-CD2	6.11	121.38	111.00
130	EI	168	LEU	CB-CG-CD2	6.07	121.31	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
143	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	A0	501/516 (97%)	487 (97%)	14 (3%)	0	100	100
2	A1	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
3	A2	263/317 (83%)	257 (98%)	6 (2%)	0	100	100
4	A3	289/333 (87%)	287 (99%)	2 (1%)	0	100	100
5	A4	309/311 (99%)	305 (99%)	4 (1%)	0	100	100
6	A5	280/282 (99%)	279 (100%)	1 (0%)	0	100	100
7	A6	228/251 (91%)	224 (98%)	4 (2%)	0	100	100
8	A7	131/238 (55%)	129 (98%)	2 (2%)	0	100	100
9	A8	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
10	A9	229/231 (99%)	226 (99%)	3 (1%)	0	100	100
11	AA	711/750 (95%)	694 (98%)	16 (2%)	1 (0%)	48	77
12	AB	686/718 (96%)	674 (98%)	12 (2%)	0	100	100
13	AC	503/505 (100%)	489 (97%)	14 (3%)	0	100	100
14	AD	439/474 (93%)	427 (97%)	12 (3%)	0	100	100
15	AE	439/442 (99%)	431 (98%)	8 (2%)	0	100	100
16	AF	357/360 (99%)	349 (98%)	8 (2%)	0	100	100
17	AG	344/346 (99%)	340 (99%)	4 (1%)	0	100	100
18	AH	281/284 (99%)	273 (97%)	8 (3%)	0	100	100
19	AI	229/274 (84%)	227 (99%)	2 (1%)	0	100	100
20	AJ	252/255 (99%)	245 (97%)	7 (3%)	0	100	100
21	AK	228/257 (89%)	219 (96%)	9 (4%)	0	100	100
22	AL	216/236 (92%)	209 (97%)	7 (3%)	0	100	100
23	AM	229/233 (98%)	223 (97%)	6 (3%)	0	100	100
24	AN	155/206 (75%)	154 (99%)	1 (1%)	0	100	100
25	AO	196/198 (99%)	192 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AP	189/194 (97%)	182 (96%)	7 (4%)	0	100	100
27	AQ	185/189 (98%)	181 (98%)	4 (2%)	0	100	100
28	AR	179/185 (97%)	178 (99%)	1 (1%)	0	100	100
29	AS	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
30	AT	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
31	AU	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
32	AV	110/138 (80%)	108 (98%)	2 (2%)	0	100	100
33	AW	96/133 (72%)	95 (99%)	1 (1%)	0	100	100
34	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
35	AY	114/116 (98%)	114 (100%)	0	0	100	100
36	AZ	92/103 (89%)	89 (97%)	3 (3%)	0	100	100
37	B0	91/94 (97%)	91 (100%)	0	0	100	100
38	B1	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
39	B2	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
40	B3	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
41	B4	71/73 (97%)	71 (100%)	0	0	100	100
42	B5	52/71 (73%)	52 (100%)	0	0	100	100
43	B6	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
44	BA	197/212 (93%)	192 (98%)	5 (2%)	0	100	100
45	BB	165/214 (77%)	164 (99%)	1 (1%)	0	100	100
46	BC	171/207 (83%)	168 (98%)	3 (2%)	0	100	100
47	BD	146/205 (71%)	145 (99%)	1 (1%)	0	100	100
48	BE	166/189 (88%)	159 (96%)	7 (4%)	0	100	100
49	BF	175/188 (93%)	166 (95%)	9 (5%)	0	100	100
50	BG	158/175 (90%)	153 (97%)	5 (3%)	0	100	100
51	BH	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
52	BI	147/172 (86%)	146 (99%)	1 (1%)	0	100	100
53	BJ	142/166 (86%)	142 (100%)	0	0	100	100
54	BK	107/144 (74%)	105 (98%)	2 (2%)	0	100	100
55	BL	140/143 (98%)	139 (99%)	1 (1%)	0	100	100
56	BM	126/135 (93%)	119 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	BN	131/135 (97%)	129 (98%)	2 (2%)	0	100	100
58	BO	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
59	BP	70/129 (54%)	69 (99%)	1 (1%)	0	100	100
60	BQ	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
61	BR	89/132 (67%)	88 (99%)	1 (1%)	0	100	100
62	BS	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
63	BT	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
64	BU	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
65	BV	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
66	BW	116/120 (97%)	112 (97%)	4 (3%)	0	100	100
67	BX	94/113 (83%)	94 (100%)	0	0	100	100
68	BY	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
69	BZ	100/102 (98%)	100 (100%)	0	0	100	100
70	CH	108/195 (55%)	108 (100%)	0	0	100	100
71	CM	72/76 (95%)	72 (100%)	0	0	100	100
72	CL	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
73	CA	597/636 (94%)	580 (97%)	16 (3%)	1 (0%)	44	73
74	CI	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
75	CB	283/312 (91%)	277 (98%)	6 (2%)	0	100	100
76	CF	216/296 (73%)	212 (98%)	4 (2%)	0	100	100
77	CG	194/198 (98%)	191 (98%)	3 (2%)	0	100	100
78	CK	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
79	CE	319/322 (99%)	301 (94%)	16 (5%)	2 (1%)	22	52
80	CJ	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
81	CN	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
82	CC	57/60 (95%)	57 (100%)	0	0	100	100
83	CO	41/46 (89%)	41 (100%)	0	0	100	100
84	CD	42/44 (96%)	42 (100%)	0	0	100	100
85	A	480/513 (94%)	464 (97%)	16 (3%)	0	100	100
85	a	480/513 (94%)	469 (98%)	11 (2%)	0	100	100
86	B	456/482 (95%)	449 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	b	456/482 (95%)	451 (99%)	5 (1%)	0	100	100
87	C	424/426 (100%)	416 (98%)	8 (2%)	0	100	100
87	c	424/426 (100%)	415 (98%)	9 (2%)	0	100	100
88	D	293/319 (92%)	288 (98%)	5 (2%)	0	100	100
88	d	293/319 (92%)	288 (98%)	5 (2%)	0	100	100
89	E	243/269 (90%)	237 (98%)	6 (2%)	0	100	100
89	e	243/269 (90%)	240 (99%)	3 (1%)	0	100	100
90	F	84/86 (98%)	84 (100%)	0	0	100	100
90	f	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
91	G	325/328 (99%)	317 (98%)	8 (2%)	0	100	100
91	g	325/328 (99%)	322 (99%)	3 (1%)	0	100	100
92	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
92	h	127/130 (98%)	127 (100%)	0	0	100	100
93	I	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
93	i	115/119 (97%)	115 (100%)	0	0	100	100
95	K	56/62 (90%)	55 (98%)	1 (2%)	0	100	100
95	k	56/62 (90%)	56 (100%)	0	0	100	100
96	L	30/41 (73%)	30 (100%)	0	0	100	100
96	l	30/41 (73%)	30 (100%)	0	0	100	100
97	DA	669/688 (97%)	655 (98%)	14 (2%)	0	100	100
97	Da	669/688 (97%)	655 (98%)	14 (2%)	0	100	100
98	DB	602/604 (100%)	589 (98%)	13 (2%)	0	100	100
98	Db	602/604 (100%)	591 (98%)	11 (2%)	0	100	100
99	DC	580/594 (98%)	569 (98%)	10 (2%)	1 (0%)	44	73
99	Dc	580/594 (98%)	568 (98%)	12 (2%)	0	100	100
100	DD	554/637 (87%)	551 (100%)	3 (0%)	0	100	100
100	Dd	554/637 (87%)	550 (99%)	4 (1%)	0	100	100
101	DE	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
101	De	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
102	DF	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
102	Df	220/230 (96%)	215 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
103	DG	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
103	Dg	96/103 (93%)	93 (97%)	3 (3%)	0	100	100
104	DH	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
104	Dh	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
105	DI	203/236 (86%)	198 (98%)	4 (2%)	1 (0%)	25	56
105	Di	203/236 (86%)	196 (97%)	6 (3%)	1 (0%)	25	56
106	DJ	218/220 (99%)	217 (100%)	1 (0%)	0	100	100
106	Dj	218/220 (99%)	216 (99%)	2 (1%)	0	100	100
107	DK	128/990 (13%)	121 (94%)	7 (6%)	0	100	100
107	Dk	128/990 (13%)	121 (94%)	7 (6%)	0	100	100
108	DM	453/490 (92%)	449 (99%)	4 (1%)	0	100	100
108	Dm	453/490 (92%)	448 (99%)	5 (1%)	0	100	100
109	DN	451/453 (100%)	443 (98%)	8 (2%)	0	100	100
109	Dn	451/453 (100%)	442 (98%)	9 (2%)	0	100	100
110	DO	431/473 (91%)	428 (99%)	3 (1%)	0	100	100
110	Do	431/473 (91%)	428 (99%)	3 (1%)	0	100	100
111	DP	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
111	Dp	288/402 (72%)	279 (97%)	9 (3%)	0	100	100
112	DQ	382/386 (99%)	376 (98%)	6 (2%)	0	100	100
112	Dq	382/386 (99%)	369 (97%)	13 (3%)	0	100	100
113	DR	241/348 (69%)	234 (97%)	7 (3%)	0	100	100
113	Dr	241/348 (69%)	238 (99%)	3 (1%)	0	100	100
114	DS	345/347 (99%)	344 (100%)	1 (0%)	0	100	100
114	Ds	345/347 (99%)	343 (99%)	2 (1%)	0	100	100
115	DT	291/318 (92%)	287 (99%)	4 (1%)	0	100	100
115	Dt	291/318 (92%)	288 (99%)	3 (1%)	0	100	100
116	DU	327/330 (99%)	322 (98%)	5 (2%)	0	100	100
116	Du	327/330 (99%)	321 (98%)	6 (2%)	0	100	100
117	DV	317/319 (99%)	315 (99%)	2 (1%)	0	100	100
117	Dv	317/319 (99%)	312 (98%)	5 (2%)	0	100	100
118	DW	299/318 (94%)	297 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
118	Dw	299/318 (94%)	297 (99%)	2 (1%)	0	100	100
119	DX	249/252 (99%)	248 (100%)	1 (0%)	0	100	100
119	Dx	249/252 (99%)	248 (100%)	1 (0%)	0	100	100
120	DY	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
120	Dy	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
121	DZ	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
121	Dz	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
122	EA	191/215 (89%)	189 (99%)	2 (1%)	0	100	100
122	Ea	191/215 (89%)	187 (98%)	4 (2%)	0	100	100
123	EB	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
123	Eb	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
124	EC	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
124	Ec	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
125	ED	188/190 (99%)	186 (99%)	2 (1%)	0	100	100
125	Ed	188/190 (99%)	185 (98%)	3 (2%)	0	100	100
126	EE	123/193 (64%)	122 (99%)	1 (1%)	0	100	100
126	Ee	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
127	EF	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
127	Ef	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
128	EG	96/100 (96%)	96 (100%)	0	0	100	100
128	Eg	96/100 (96%)	96 (100%)	0	0	100	100
129	EH	172/174 (99%)	171 (99%)	1 (1%)	0	100	100
129	Eh	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
130	EI	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
130	Ei	170/173 (98%)	165 (97%)	5 (3%)	0	100	100
131	EV	77/89 (86%)	76 (99%)	1 (1%)	0	100	100
131	Ev	77/89 (86%)	76 (99%)	1 (1%)	0	100	100
132	EK	167/170 (98%)	167 (100%)	0	0	100	100
132	Ek	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
133	EL	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
133	El	151/158 (96%)	149 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
134	EM	151/154 (98%)	147 (97%)	4 (3%)	0	100	100
134	Em	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
135	EN	143/149 (96%)	140 (98%)	3 (2%)	0	100	100
135	En	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
136	EO	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
136	Eo	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
137	EP	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
137	Ep	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
138	EQ	121/123 (98%)	121 (100%)	0	0	100	100
138	Eq	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
139	ER	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
139	Er	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
140	ES	87/89 (98%)	87 (100%)	0	0	100	100
140	Es	87/89 (98%)	87 (100%)	0	0	100	100
141	ET	80/93 (86%)	80 (100%)	0	0	100	100
141	Et	80/93 (86%)	80 (100%)	0	0	100	100
142	EU	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
142	Eu	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
143	EJ	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
143	Ej	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
144	EW	61/81 (75%)	61 (100%)	0	0	100	100
144	Ew	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
145	EX	67/72 (93%)	67 (100%)	0	0	100	100
145	Ex	67/72 (93%)	67 (100%)	0	0	100	100
146	EY	68/72 (94%)	68 (100%)	0	0	100	100
146	Ey	68/72 (94%)	68 (100%)	0	0	100	100
147	EZ	56/68 (82%)	55 (98%)	1 (2%)	0	100	100
147	Ez	56/68 (82%)	56 (100%)	0	0	100	100
148	FA	69/72 (96%)	69 (100%)	0	0	100	100
148	Fa	69/72 (96%)	69 (100%)	0	0	100	100
149	DL	378/462 (82%)	362 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
149	Dl	378/462 (82%)	370 (98%)	8 (2%)	0	100	100
All	All	44796/50144 (89%)	44009 (98%)	780 (2%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
73	CA	405	TRP
79	CE	83	THR
105	Di	119	GLU
79	CE	153	LEU
99	DC	143	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	441/454 (97%)	436 (99%)	5 (1%)	70	90
2	A1	288/311 (93%)	287 (100%)	1 (0%)	91	97
3	A2	225/270 (83%)	221 (98%)	4 (2%)	54	82
4	A3	244/280 (87%)	243 (100%)	1 (0%)	89	97
5	A4	275/275 (100%)	275 (100%)	0	100	100
6	A5	257/257 (100%)	257 (100%)	0	100	100
7	A6	207/223 (93%)	206 (100%)	1 (0%)	86	96
8	A7	122/224 (54%)	121 (99%)	1 (1%)	79	93
9	A8	195/195 (100%)	194 (100%)	1 (0%)	86	96
10	A9	199/199 (100%)	195 (98%)	4 (2%)	50	79
11	AA	657/694 (95%)	646 (98%)	11 (2%)	56	83
12	AB	589/617 (96%)	588 (100%)	1 (0%)	92	98
13	AC	463/463 (100%)	457 (99%)	6 (1%)	65	88
14	AD	361/392 (92%)	360 (100%)	1 (0%)	91	97
15	AE	398/399 (100%)	393 (99%)	5 (1%)	65	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AF	346/347 (100%)	346 (100%)	0	100	100
17	AG	309/309 (100%)	309 (100%)	0	100	100
18	AH	249/250 (100%)	245 (98%)	4 (2%)	58	84
19	AI	206/236 (87%)	205 (100%)	1 (0%)	86	96
20	AJ	243/244 (100%)	242 (100%)	1 (0%)	89	97
21	AK	196/218 (90%)	194 (99%)	2 (1%)	73	91
22	AL	197/215 (92%)	194 (98%)	3 (2%)	60	85
23	AM	196/197 (100%)	195 (100%)	1 (0%)	86	96
24	AN	146/186 (78%)	146 (100%)	0	100	100
25	AO	191/191 (100%)	190 (100%)	1 (0%)	86	96
26	AP	168/170 (99%)	168 (100%)	0	100	100
27	AQ	170/172 (99%)	168 (99%)	2 (1%)	67	89
28	AR	159/163 (98%)	158 (99%)	1 (1%)	84	95
29	AS	154/154 (100%)	152 (99%)	2 (1%)	65	88
30	AT	136/137 (99%)	132 (97%)	4 (3%)	37	72
31	AU	132/133 (99%)	131 (99%)	1 (1%)	79	93
32	AV	104/129 (81%)	104 (100%)	0	100	100
33	AW	87/119 (73%)	87 (100%)	0	100	100
34	AX	112/112 (100%)	110 (98%)	2 (2%)	54	82
35	AY	108/108 (100%)	107 (99%)	1 (1%)	75	92
36	AZ	84/93 (90%)	84 (100%)	0	100	100
37	B0	88/89 (99%)	88 (100%)	0	100	100
38	B1	83/84 (99%)	82 (99%)	1 (1%)	67	89
39	B2	82/83 (99%)	82 (100%)	0	100	100
40	B3	66/74 (89%)	66 (100%)	0	100	100
41	B4	65/65 (100%)	65 (100%)	0	100	100
42	B5	48/63 (76%)	48 (100%)	0	100	100
43	B6	55/55 (100%)	54 (98%)	1 (2%)	54	82
44	BA	179/190 (94%)	178 (99%)	1 (1%)	84	95
45	BB	145/182 (80%)	145 (100%)	0	100	100
46	BC	155/180 (86%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	BD	124/179 (69%)	123 (99%)	1 (1%)	79	93
48	BE	159/178 (89%)	158 (99%)	1 (1%)	84	95
49	BF	161/172 (94%)	161 (100%)	0	100	100
50	BG	142/156 (91%)	141 (99%)	1 (1%)	81	94
51	BH	170/170 (100%)	170 (100%)	0	100	100
52	BI	131/152 (86%)	131 (100%)	0	100	100
53	BJ	128/147 (87%)	127 (99%)	1 (1%)	79	93
54	BK	97/131 (74%)	97 (100%)	0	100	100
55	BL	124/125 (99%)	122 (98%)	2 (2%)	58	84
56	BM	108/114 (95%)	107 (99%)	1 (1%)	75	92
57	BN	120/122 (98%)	120 (100%)	0	100	100
58	BO	122/122 (100%)	122 (100%)	0	100	100
59	BP	64/117 (55%)	64 (100%)	0	100	100
60	BQ	93/117 (80%)	93 (100%)	0	100	100
61	BR	81/116 (70%)	80 (99%)	1 (1%)	67	89
62	BS	103/109 (94%)	103 (100%)	0	100	100
63	BT	110/110 (100%)	103 (94%)	7 (6%)	14	41
64	BU	121/121 (100%)	121 (100%)	0	100	100
65	BV	102/102 (100%)	102 (100%)	0	100	100
66	BW	98/99 (99%)	98 (100%)	0	100	100
67	BX	81/97 (84%)	81 (100%)	0	100	100
68	BY	98/98 (100%)	98 (100%)	0	100	100
69	BZ	89/89 (100%)	89 (100%)	0	100	100
70	CH	100/184 (54%)	100 (100%)	0	100	100
71	CM	65/67 (97%)	65 (100%)	0	100	100
72	CL	82/83 (99%)	82 (100%)	0	100	100
73	CA	481/515 (93%)	477 (99%)	4 (1%)	79	93
74	CI	97/97 (100%)	97 (100%)	0	100	100
75	CB	259/283 (92%)	255 (98%)	4 (2%)	60	85
76	CF	194/268 (72%)	194 (100%)	0	100	100
77	CG	179/181 (99%)	177 (99%)	2 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	CK	85/85 (100%)	83 (98%)	2 (2%)	44	76
79	CE	286/287 (100%)	281 (98%)	5 (2%)	56	83
80	CJ	86/86 (100%)	86 (100%)	0	100	100
81	CN	56/56 (100%)	56 (100%)	0	100	100
82	CC	50/51 (98%)	50 (100%)	0	100	100
83	CO	38/40 (95%)	38 (100%)	0	100	100
84	CD	43/43 (100%)	43 (100%)	0	100	100
85	A	411/440 (93%)	408 (99%)	3 (1%)	81	94
85	a	411/440 (93%)	405 (98%)	6 (2%)	60	85
86	B	389/409 (95%)	388 (100%)	1 (0%)	91	97
86	b	389/409 (95%)	386 (99%)	3 (1%)	79	93
87	C	386/386 (100%)	382 (99%)	4 (1%)	73	91
87	c	386/386 (100%)	375 (97%)	11 (3%)	38	73
88	D	255/274 (93%)	253 (99%)	2 (1%)	79	93
88	d	255/274 (93%)	251 (98%)	4 (2%)	58	84
89	E	215/237 (91%)	213 (99%)	2 (1%)	75	92
89	e	215/237 (91%)	212 (99%)	3 (1%)	62	86
90	F	76/76 (100%)	76 (100%)	0	100	100
90	f	75/76 (99%)	74 (99%)	1 (1%)	65	88
91	G	288/289 (100%)	286 (99%)	2 (1%)	81	94
91	g	288/289 (100%)	285 (99%)	3 (1%)	73	91
92	H	117/118 (99%)	117 (100%)	0	100	100
92	h	117/118 (99%)	116 (99%)	1 (1%)	75	92
93	I	107/109 (98%)	104 (97%)	3 (3%)	38	73
93	i	107/109 (98%)	106 (99%)	1 (1%)	75	92
95	K	53/56 (95%)	53 (100%)	0	100	100
95	k	53/56 (95%)	53 (100%)	0	100	100
96	L	27/36 (75%)	26 (96%)	1 (4%)	29	64
96	l	27/36 (75%)	27 (100%)	0	100	100
97	DA	596/613 (97%)	585 (98%)	11 (2%)	54	82
97	Da	596/613 (97%)	587 (98%)	9 (2%)	60	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
98	DB	569/569 (100%)	560 (98%)	9 (2%)	58	84
98	Db	569/569 (100%)	559 (98%)	10 (2%)	54	82
99	DC	553/565 (98%)	551 (100%)	2 (0%)	89	97
99	Dc	553/565 (98%)	551 (100%)	2 (0%)	89	97
100	DD	506/579 (87%)	501 (99%)	5 (1%)	73	91
100	Dd	506/579 (87%)	503 (99%)	3 (1%)	84	95
101	DE	114/116 (98%)	114 (100%)	0	100	100
101	De	114/116 (98%)	113 (99%)	1 (1%)	75	92
102	DF	200/207 (97%)	198 (99%)	2 (1%)	73	91
102	Df	200/207 (97%)	198 (99%)	2 (1%)	73	91
103	DG	84/88 (96%)	83 (99%)	1 (1%)	67	89
103	Dg	84/88 (96%)	84 (100%)	0	100	100
104	DH	120/120 (100%)	119 (99%)	1 (1%)	79	93
104	Dh	120/120 (100%)	118 (98%)	2 (2%)	56	83
105	DI	193/218 (88%)	191 (99%)	2 (1%)	73	91
105	Di	193/218 (88%)	190 (98%)	3 (2%)	58	84
106	DJ	199/199 (100%)	195 (98%)	4 (2%)	50	79
106	Dj	199/199 (100%)	195 (98%)	4 (2%)	50	79
107	DK	121/943 (13%)	121 (100%)	0	100	100
107	Dk	121/943 (13%)	121 (100%)	0	100	100
108	DM	413/447 (92%)	410 (99%)	3 (1%)	81	94
108	Dm	413/447 (92%)	410 (99%)	3 (1%)	81	94
109	DN	442/442 (100%)	438 (99%)	4 (1%)	75	92
109	Dn	442/442 (100%)	437 (99%)	5 (1%)	70	90
110	DO	380/413 (92%)	379 (100%)	1 (0%)	91	97
110	Do	380/413 (92%)	380 (100%)	0	100	100
111	DP	253/358 (71%)	251 (99%)	2 (1%)	79	93
111	Dp	253/358 (71%)	252 (100%)	1 (0%)	89	97
112	DQ	341/343 (99%)	336 (98%)	5 (2%)	60	85
112	Dq	341/343 (99%)	338 (99%)	3 (1%)	75	92
113	DR	219/318 (69%)	218 (100%)	1 (0%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
113	Dr	219/318 (69%)	219 (100%)	0	100	100
114	DS	294/294 (100%)	291 (99%)	3 (1%)	73	91
114	Ds	294/294 (100%)	290 (99%)	4 (1%)	62	86
115	DT	267/289 (92%)	267 (100%)	0	100	100
115	Dt	267/289 (92%)	267 (100%)	0	100	100
116	DU	275/276 (100%)	274 (100%)	1 (0%)	89	97
116	Du	275/276 (100%)	272 (99%)	3 (1%)	70	90
117	DV	260/260 (100%)	258 (99%)	2 (1%)	79	93
117	Dv	260/260 (100%)	256 (98%)	4 (2%)	60	85
118	DW	258/272 (95%)	254 (98%)	4 (2%)	58	84
118	Dw	258/272 (95%)	253 (98%)	5 (2%)	52	81
119	DX	218/219 (100%)	217 (100%)	1 (0%)	86	96
119	Dx	218/219 (100%)	215 (99%)	3 (1%)	62	86
120	DY	169/216 (78%)	168 (99%)	1 (1%)	84	95
120	Dy	169/216 (78%)	167 (99%)	2 (1%)	67	89
121	DZ	189/213 (89%)	189 (100%)	0	100	100
121	Dz	189/213 (89%)	189 (100%)	0	100	100
122	EA	180/201 (90%)	179 (99%)	1 (1%)	84	95
122	Ea	180/201 (90%)	178 (99%)	2 (1%)	70	90
123	EB	180/181 (99%)	178 (99%)	2 (1%)	70	90
123	Eb	180/181 (99%)	177 (98%)	3 (2%)	56	83
124	EC	178/178 (100%)	178 (100%)	0	100	100
124	Ec	178/178 (100%)	177 (99%)	1 (1%)	84	95
125	ED	185/185 (100%)	183 (99%)	2 (1%)	70	90
125	Ed	185/185 (100%)	183 (99%)	2 (1%)	70	90
126	EE	116/180 (64%)	116 (100%)	0	100	100
126	Ee	116/180 (64%)	116 (100%)	0	100	100
127	EF	164/164 (100%)	162 (99%)	2 (1%)	67	89
127	Ef	164/164 (100%)	163 (99%)	1 (1%)	84	95
128	EG	77/78 (99%)	77 (100%)	0	100	100
128	Eg	77/78 (99%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
129	EH	157/157 (100%)	156 (99%)	1 (1%)	84	95
129	Eh	157/157 (100%)	157 (100%)	0	100	100
130	EI	156/157 (99%)	154 (99%)	2 (1%)	65	88
130	Ei	156/157 (99%)	153 (98%)	3 (2%)	52	81
131	EV	72/81 (89%)	72 (100%)	0	100	100
131	Ev	72/81 (89%)	72 (100%)	0	100	100
132	EK	153/154 (99%)	153 (100%)	0	100	100
132	Ek	153/154 (99%)	150 (98%)	3 (2%)	50	79
133	EL	134/139 (96%)	133 (99%)	1 (1%)	81	94
133	El	134/139 (96%)	133 (99%)	1 (1%)	81	94
134	EM	137/138 (99%)	136 (99%)	1 (1%)	81	94
134	Em	137/138 (99%)	136 (99%)	1 (1%)	81	94
135	EN	132/135 (98%)	131 (99%)	1 (1%)	79	93
135	En	132/135 (98%)	131 (99%)	1 (1%)	79	93
136	EO	112/113 (99%)	110 (98%)	2 (2%)	54	82
136	Eo	112/113 (99%)	110 (98%)	2 (2%)	54	82
137	EP	87/113 (77%)	86 (99%)	1 (1%)	70	90
137	Ep	87/113 (77%)	86 (99%)	1 (1%)	70	90
138	EQ	105/105 (100%)	102 (97%)	3 (3%)	37	72
138	Eq	105/105 (100%)	102 (97%)	3 (3%)	37	72
139	ER	87/88 (99%)	86 (99%)	1 (1%)	70	90
139	Er	87/88 (99%)	87 (100%)	0	100	100
140	ES	84/84 (100%)	84 (100%)	0	100	100
140	Es	84/84 (100%)	84 (100%)	0	100	100
141	ET	75/83 (90%)	72 (96%)	3 (4%)	27	61
141	Et	75/83 (90%)	73 (97%)	2 (3%)	40	73
142	EU	78/80 (98%)	78 (100%)	0	100	100
142	Eu	78/80 (98%)	78 (100%)	0	100	100
143	EJ	157/157 (100%)	154 (98%)	3 (2%)	52	81
143	Ej	157/157 (100%)	155 (99%)	2 (1%)	65	88
144	EW	57/66 (86%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
144	Ew	57/66 (86%)	57 (100%)	0	100	100
145	EX	64/67 (96%)	63 (98%)	1 (2%)	58	84
145	Ex	64/67 (96%)	63 (98%)	1 (2%)	58	84
146	EY	62/63 (98%)	62 (100%)	0	100	100
146	Ey	62/63 (98%)	62 (100%)	0	100	100
147	EZ	55/63 (87%)	53 (96%)	2 (4%)	30	65
147	Ez	55/63 (87%)	54 (98%)	1 (2%)	54	82
148	FA	62/63 (98%)	60 (97%)	2 (3%)	34	69
148	Fa	62/63 (98%)	60 (97%)	2 (3%)	34	69
149	DL	308/386 (80%)	306 (99%)	2 (1%)	84	95
149	Dl	308/386 (80%)	307 (100%)	1 (0%)	91	97
All	All	40248/44802 (90%)	39894 (99%)	354 (1%)	74	92

5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
135	EN	144	LEU
108	Dm	103	LEU
139	ER	21	GLU
98	Db	224	PHE
114	Ds	222	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
119	DX	228	ASN
100	Dd	85	HIS
123	EB	121	GLN
98	Db	198	GLN
108	Dm	451	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	$\#\|Z\| > 2$
100	SEP	DD	520	100	8,9,10	1.60	1 (12%)	7,12,14	1.34	1 (14%)
100	TPO	DD	387	100	8,10,11	1.63	1 (12%)	10,14,16	2.11	1 (10%)
100	SEP	Dd	520	100	8,9,10	1.60	1 (12%)	7,12,14	1.33	1 (14%)
100	TPO	Dd	387	100	8,10,11	1.62	1 (12%)	10,14,16	2.03	1 (10%)
105	SEP	Di	120	105	8,9,10	1.59	1 (12%)	7,12,14	1.32	1 (14%)
105	SEP	DI	120	105	8,9,10	1.59	1 (12%)	7,12,14	1.20	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
100	SEP	DD	520	100	-	0/6/8/10	-
100	TPO	DD	387	100	-	2/9/11/13	-
100	SEP	Dd	520	100	-	0/6/8/10	-
100	TPO	Dd	387	100	-	3/9/11/13	-
105	SEP	Di	120	105	-	0/6/8/10	-
105	SEP	DI	120	105	-	0/6/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
100	Dd	520	SEP	P-O1P	3.51	1.61	1.50
100	DD	520	SEP	P-O1P	3.49	1.61	1.50
100	DD	387	TPO	P-O1P	3.48	1.61	1.50
105	Di	120	SEP	P-O1P	3.48	1.61	1.50
105	DI	120	SEP	P-O1P	3.47	1.61	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
100	DD	387	TPO	P-OG1-CB	-6.12	106.71	123.33
100	Dd	387	TPO	P-OG1-CB	-5.90	107.29	123.33
100	DD	520	SEP	OG-CB-CA	2.96	111.03	108.14
105	Di	120	SEP	OG-CB-CA	2.90	110.97	108.14
100	Dd	520	SEP	OG-CB-CA	2.88	110.95	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
100	Dd	387	TPO	C-CA-CB-CG2
100	DD	387	TPO	C-CA-CB-CG2
100	DD	387	TPO	O-C-CA-CB
100	Dd	387	TPO	O-C-CA-CB
100	Dd	387	TPO	N-CA-CB-CG2

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 384 ligands modelled in this entry, 14 are monoatomic - leaving 370 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	$\#\|Z\| > 2$
153	PC1	Dc	609	-	53,53,53	0.27	0	59,61,61	0.28	0
150	CDL	DU	403	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
150	CDL	Dq	1403	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	A2	402	-	53,53,53	0.27	0	59,61,61	0.27	0
155	3PE	DX	302	-	50,50,50	0.25	0	53,55,55	0.18	0
153	PC1	El	904	-	53,53,53	0.27	0	59,61,61	0.30	0
168	HEM	Ed	201	125	42,50,50	1.49	6 (14%)	46,82,82	1.45	7 (15%)
155	3PE	EN	1204	-	50,50,50	0.27	0	53,55,55	0.19	0
150	CDL	BG	201	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	C	505	-	99,99,99	0.29	0	105,111,111	0.56	1 (0%)
150	CDL	C	503	-	99,99,99	0.30	0	105,111,111	0.53	0
153	PC1	EB	301	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	Dg	204	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	DN	503	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
155	3PE	Dx	1207	-	50,50,50	0.26	0	53,55,55	0.20	0
153	PC1	B1	403	-	53,53,53	0.28	0	59,61,61	0.28	0
155	3PE	DX	304	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	DJ	305	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
166	HEC	D	401	88	32,50,50	2.35	12 (37%)	30,82,82	2.10	5 (16%)
153	PC1	Dy	302	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	BA	301	-	50,50,50	0.27	0	53,55,55	0.21	0
153	PC1	Dv	406	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	ES	1101	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
171	CUA	DB	701	98	0,1,1	-	-	-		
153	PC1	Da	707	-	53,53,53	0.29	0	59,61,61	0.29	0
150	CDL	CC	304	-	99,99,99	0.29	0	105,111,111	0.55	1 (0%)
155	3PE	A2	401	-	50,50,50	0.26	0	53,55,55	0.21	0
153	PC1	A6	302	-	53,53,53	0.28	0	59,61,61	0.30	0
150	CDL	AA	901	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	BC	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DG	202	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
150	CDL	DC	601	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
165	F3S	CB	1002	75	0,9,9	-	-	-		
167	UQ8	c	510	-	53,53,53	0.52	0	66,67,67	0.73	2 (3%)
150	CDL	BY	201	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	EB	303	-	53,53,53	0.29	0	59,61,61	0.28	0
153	PC1	DC	602	-	53,53,53	0.27	0	59,61,61	0.28	0
150	CDL	DU	402	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
153	PC1	EO	205	-	53,53,53	0.29	0	59,61,61	0.28	0
166	HEC	CE	401	79	32,50,50	2.79	10 (31%)	30,82,82	1.93	6 (20%)
169	HEA	DA	702	97	58,67,67	2.31	21 (36%)	63,103,103	2.26	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
156	LPP	Dl	1101	-	43,43,43	0.22	0	46,48,48	0.26	0
150	CDL	DV	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
156	LPP	DN	504	-	43,43,43	0.22	0	46,48,48	0.29	0
150	CDL	DM	502	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Dn	502	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dd	706	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
153	PC1	AC	804	-	53,53,53	0.29	0	59,61,61	0.28	0
155	3PE	DG	205	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	BT	203	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	DV	404	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	Dx	1205	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	d	801	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	AJ	502	-	50,50,50	0.26	0	53,55,55	0.23	0
150	CDL	Dj	403	-	99,99,99	0.31	0	105,111,111	0.58	1 (0%)
159	SF4	CB	1001	75	0,12,12	-	-	-		
150	CDL	DN	506	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	DJ	301	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	H	1302	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	DR	401	-	50,50,50	0.26	0	53,55,55	0.22	0
164	FAD	CA	702	73	54,58,58	0.66	0	71,89,89	0.64	1 (1%)
150	CDL	DX	301	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
153	PC1	DY	302	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Ed	205	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
167	UQ8	ED	603	-	53,53,53	0.52	0	66,67,67	0.70	2 (3%)
150	CDL	Dc	601	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	DC	608	-	53,53,53	0.27	0	59,61,61	0.27	0
153	PC1	Dc	604	-	53,53,53	0.27	0	59,61,61	0.29	0
150	CDL	Ds	406	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
171	CUA	Db	701	98	0,1,1	-	-	-		
150	CDL	Dv	403	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
155	3PE	CD	303	-	50,50,50	0.26	0	53,55,55	0.22	0
150	CDL	DS	404	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Dh	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	Di	1102	-	50,50,50	0.25	0	53,55,55	0.23	0
155	3PE	Dr	401	-	50,50,50	0.26	0	53,55,55	0.22	0
150	CDL	DX	306	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	Eu	101	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	Dc	606	-	50,50,50	0.27	0	53,55,55	0.20	0
156	LPP	DN	505	-	43,43,43	0.21	0	46,48,48	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
150	CDL	Dx	1204	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
153	PC1	EN	1203	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	Dc	607	-	50,50,50	0.27	0	53,55,55	0.20	0
168	HEM	c	505	87	42,50,50	1.47	6 (14%)	46,82,82	1.32	4 (8%)
168	HEM	C	502	87	42,50,50	1.46	6 (14%)	46,82,82	1.24	4 (8%)
153	PC1	Di	1104	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	DQ	1503	-	53,53,53	0.28	0	59,61,61	0.28	0
155	3PE	EM	901	-	50,50,50	0.26	0	53,55,55	0.20	0
168	HEM	ED	602	125	42,50,50	1.48	6 (14%)	46,82,82	1.41	8 (17%)
150	CDL	En	1201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
158	FES	EF	202	127	0,4,4	-	-	-		
150	CDL	Dg	201	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
150	CDL	Dv	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	EI	401	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	EN	1201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	EO	206	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	DV	406	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	A6	303	-	53,53,53	0.28	0	59,61,61	0.27	0
158	FES	Ef	502	127	0,4,4	-	-	-		
150	CDL	DG	201	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	DG	203	-	53,53,53	0.28	0	59,61,61	0.29	0
150	CDL	Ds	405	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	AU	202	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	Dg	203	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	Dr	403	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
166	HEC	d	802	88	32,50,50	2.32	12 (37%)	30,82,82	2.08	5 (16%)
150	CDL	Ed	204	-	99,99,99	0.30	0	105,111,111	0.47	1 (0%)
155	3PE	Dx	1208	-	50,50,50	0.27	0	53,55,55	0.19	0
150	CDL	BV	201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	AF	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DC	605	-	53,53,53	0.28	0	59,61,61	0.27	0
159	SF4	AB	803	12	0,12,12	-	-	-		
151	UDP	A0	603	152	25,26,26	0.40	0	38,40,40	0.60	1 (2%)
150	CDL	DQ	1504	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
153	PC1	Eb	303	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	Dn	503	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	Eo	202	-	50,50,50	0.26	0	53,55,55	0.20	0
153	PC1	DC	603	-	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	$\#\|Z\| > 2$
156	LPP	AC	803	-	43,43,43	0.22	0	46,48,48	0.26	0
153	PC1	K	501	-	53,53,53	0.29	0	59,61,61	0.29	0
153	PC1	Dq	1404	-	53,53,53	0.28	0	59,61,61	0.27	0
169	HEA	Da	703	97	58,67,67	2.29	21 (36%)	63,103,103	2.30	25 (39%)
173	ATP	Er	201	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
155	3PE	El	905	-	50,50,50	0.27	0	53,55,55	0.21	0
150	CDL	c	502	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Dn	506	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Ds	401	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
161	8Q1	AS	200	-	28,33,34	0.11	0	32,40,43	0.33	0
155	3PE	DC	606	-	50,50,50	0.27	0	53,55,55	0.22	0
150	CDL	Dj	401	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
167	UQ8	Ed	202	-	53,53,53	0.53	0	66,67,67	0.71	2 (3%)
150	CDL	Dx	1201	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
150	CDL	Dj	404	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
159	SF4	AB	802	12	0,12,12	-	-	-		
153	PC1	CC	302	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	c	507	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DD	706	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
153	PC1	AH	301	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	c	508	-	53,53,53	0.27	0	59,61,61	0.28	0
150	CDL	EB	302	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	EL	903	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	CK	101	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	Dn	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	DA	708	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	Dg	202	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Da	709	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
168	HEM	c	504	87	42,50,50	1.49	5 (11%)	46,82,82	1.31	7 (15%)
150	CDL	Dm	502	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	Di	1101	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
150	CDL	Dd	702	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
153	PC1	Db	702	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	DN	502	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
153	PC1	K	502	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	AA	905	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	Di	1103	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
153	PC1	BS	1302	-	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	$\#\|Z\| > 2$
158	FES	BI	201	52	0,4,4	-	-	-		
167	UQ8	C	512	-	53,53,53	0.51	0	66,67,67	0.70	3 (4%)
158	FES	e	1102	89	0,4,4	-	-	-		
150	CDL	DU	404	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
150	CDL	ED	605	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
158	FES	Ef	503	127	0,4,4	-	-	-		
153	PC1	A1	403	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	AA	908	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Eo	204	-	53,53,53	0.29	0	59,61,61	0.27	0
155	3PE	G	401	-	50,50,50	0.26	0	53,55,55	0.22	0
154	NDP	A1	401	-	47,52,52	0.52	0	61,80,80	0.55	1 (1%)
160	FMN	AD	502	-	33,33,33	0.19	0	48,50,50	0.30	0
150	CDL	DQ	1501	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
159	SF4	AT	201	30	0,12,12	-	-	-		
155	3PE	CC	301	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	CG	301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
156	LPP	EI	402	-	43,43,43	0.21	0	46,48,48	0.26	0
150	CDL	ED	601	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Eb	302	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
155	3PE	A9	602	-	50,50,50	0.27	0	53,55,55	0.22	0
159	SF4	AL	302	22	0,12,12	-	-	-		
156	LPP	Ed	203	-	43,43,43	0.21	0	46,48,48	0.26	0
158	FES	E	302	89	0,4,4	-	-	-		
150	CDL	Dj	407	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DX	305	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	k	301	-	53,53,53	0.27	0	59,61,61	0.29	0
150	CDL	Dc	608	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	EL	902	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Du	402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	AX	401	-	53,53,53	0.28	0	59,61,61	0.27	0
167	UQ8	C	511	-	53,53,53	0.52	0	66,67,67	0.77	3 (4%)
155	3PE	C	513	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	Dh	202	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	DN	501	-	50,50,50	0.26	0	53,55,55	0.19	0
168	HEM	C	501	87	42,50,50	1.47	5 (11%)	46,82,82	1.32	7 (15%)
153	PC1	AL	303	-	53,53,53	0.27	0	59,61,61	0.29	0
153	PC1	DA	707	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	Dy	301	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	B0	102	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
150	CDL	DR	403	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	D	402	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	AA	903	-	53,53,53	0.28	0	59,61,61	0.27	0
157	ADP	AQ	201	-	24,29,29	0.66	0	29,45,45	0.63	1 (3%)
153	PC1	AA	906	-	53,53,53	0.27	0	59,61,61	0.29	0
153	PC1	AQ	202	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	AC	802	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
153	PC1	EO	204	-	53,53,53	0.27	0	59,61,61	0.29	0
153	PC1	Dv	407	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Dj	405	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	BS	1301	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	AF	402	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	A	1201	-	53,53,53	0.28	0	59,61,61	0.28	0
158	FES	AB	801	12	0,4,4	-	-	-		
150	CDL	CG	302	-	99,99,99	0.29	0	105,111,111	0.51	1 (0%)
153	PC1	c	503	-	53,53,53	0.28	0	59,61,61	0.31	0
150	CDL	AC	801	-	99,99,99	0.30	0	105,111,111	0.58	1 (0%)
155	3PE	Em	901	-	50,50,50	0.26	0	53,55,55	0.19	0
153	PC1	AM	302	-	53,53,53	0.27	0	59,61,61	0.27	0
150	CDL	DH	202	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
156	LPP	AL	304	-	43,43,43	0.21	0	46,48,48	0.28	0
150	CDL	DJ	304	-	99,99,99	0.30	0	105,111,111	0.49	1 (0%)
150	CDL	EA	301	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	DV	402	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	E	303	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Ds	402	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
153	PC1	DB	702	-	53,53,53	0.29	0	59,61,61	0.27	0
155	3PE	Ds	408	-	50,50,50	0.27	0	53,55,55	0.20	0
167	UQ8	EL	905	-	53,53,53	0.53	0	66,67,67	0.81	3 (4%)
150	CDL	C	507	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	El	901	-	99,99,99	0.31	0	105,111,111	0.58	1 (0%)
153	PC1	B1	401	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	EN	1202	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DO	501	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
153	PC1	g	802	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	Dd	705	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	AP	301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	A1	402	-	99,99,99	0.30	0	105,111,111	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
150	CDL	DS	405	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
167	UQ8	EN	1205	-	53,53,53	0.53	0	66,67,67	0.69	2 (3%)
153	PC1	EO	201	-	53,53,53	0.28	0	59,61,61	0.29	0
150	CDL	c	509	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	H	1301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	CD	302	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	Dq	1401	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	E	301	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	Dr	402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	A0	601	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	BG	202	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	Da	708	-	50,50,50	0.25	0	53,55,55	0.21	0
153	PC1	Eb	301	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	Dx	1209	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	DS	406	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	EO	202	-	99,99,99	0.32	0	105,111,111	0.53	1 (0%)
150	CDL	DD	705	-	99,99,99	0.31	0	105,111,111	0.53	0
150	CDL	B1	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	DN	507	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
153	PC1	DJ	306	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	Dn	505	-	43,43,43	0.21	0	46,48,48	0.28	0
158	FES	AI	301	19	0,4,4	-	-	-		
159	SF4	AD	501	14	0,12,12	-	-	-		
150	CDL	A0	602	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	C	510	-	53,53,53	0.28	0	59,61,61	0.28	0
155	3PE	DX	303	-	50,50,50	0.26	0	53,55,55	0.21	0
153	PC1	C	508	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	Eo	203	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	Dx	1203	-	53,53,53	0.28	0	59,61,61	0.28	0
167	UQ8	El	906	-	53,53,53	0.54	0	66,67,67	0.85	4 (6%)
153	PC1	A9	603	-	53,53,53	0.28	0	59,61,61	0.28	0
169	HEA	DA	703	97	58,67,67	2.29	20 (34%)	63,103,103	2.32	25 (39%)
153	PC1	Dj	406	-	53,53,53	0.28	0	59,61,61	0.27	0
173	ATP	ER	201	-	28,33,33	0.67	0	34,52,52	0.91	1 (2%)
169	HEA	Da	702	97	58,67,67	2.30	21 (36%)	63,103,103	2.27	27 (42%)
150	CDL	DA	709	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
155	3PE	Ds	403	-	50,50,50	0.26	0	53,55,55	0.19	0
150	CDL	DS	401	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
167	UQ8	DS	403	-	53,53,53	0.51	0	66,67,67	0.68	2 (3%)
150	CDL	CC	305	-	99,99,99	0.29	0	105,111,111	0.53	1 (0%)
150	CDL	ED	604	-	99,99,99	0.30	0	105,111,111	0.48	1 (0%)
153	PC1	Eo	201	-	53,53,53	0.28	0	59,61,61	0.29	0
150	CDL	CJ	201	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	EL	904	-	50,50,50	0.27	0	53,55,55	0.22	0
150	CDL	DX	307	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
150	CDL	Ep	701	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	h	501	-	99,99,99	0.30	0	105,111,111	0.55	2 (1%)
150	CDL	AM	301	-	99,99,99	0.30	0	105,111,111	0.51	0
153	PC1	A9	601	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DU	401	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	DX	308	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	EO	203	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	BC	302	-	99,99,99	0.30	0	105,111,111	0.58	2 (1%)
155	3PE	Dd	703	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	Ea	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Ek	201	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	BE	201	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Du	401	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	Eo	205	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	Dx	1206	-	50,50,50	0.27	0	53,55,55	0.21	0
153	PC1	AA	904	-	53,53,53	0.27	0	59,61,61	0.30	0
155	3PE	Dr	404	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	DJ	303	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	Dx	1202	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	El	903	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
157	ADP	A8	401	152	24,29,29	0.65	0	29,45,45	0.61	1 (3%)
153	PC1	DC	604	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	Dv	405	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Eg	101	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
158	FES	CB	1000	75	0,4,4	-	-	-		
153	PC1	Dv	404	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	DA	706	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
150	CDL	g	801	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	A0	605	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	A6	301	-	43,43,43	0.30	0	46,48,48	0.29	0
150	CDL	EK	201	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
150	CDL	DD	703	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	BP	201	-	50,50,50	0.26	0	53,55,55	0.22	0
155	3PE	DS	402	-	50,50,50	0.27	0	53,55,55	0.19	0
150	CDL	BT	204	-	99,99,99	0.34	0	105,111,111	0.60	1 (0%)
155	3PE	BT	201	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	Do	501	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dq	1402	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	c	506	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	AA	907	-	53,53,53	0.28	0	59,61,61	0.28	0
156	LPP	DA	710	-	43,43,43	0.22	0	46,48,48	0.27	0
155	3PE	DC	607	-	50,50,50	0.26	0	53,55,55	0.20	0
153	PC1	Dc	602	-	53,53,53	0.27	0	59,61,61	0.28	0
155	3PE	DG	204	-	50,50,50	0.26	0	53,55,55	0.19	0
167	UQ8	Ds	404	-	53,53,53	0.52	0	66,67,67	0.67	1 (1%)
150	CDL	DY	301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Eh	1601	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
158	FES	EF	201	127	0,4,4	-	-	-		
150	CDL	c	501	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dj	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
159	SF4	AL	301	22	0,12,12	-	-	-		
153	PC1	Ds	407	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	C	506	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	DI	301	-	50,50,50	0.26	0	53,55,55	0.23	0
150	CDL	EL	901	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
150	CDL	DM	501	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
167	UQ8	En	1202	-	53,53,53	0.52	0	66,67,67	0.65	3 (4%)
150	CDL	BL	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DD	704	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
153	PC1	AJ	501	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	Dn	504	-	43,43,43	0.22	0	46,48,48	0.29	0
150	CDL	DR	402	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	DJ	307	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	DZ	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
167	UQ8	CC	303	-	53,53,53	0.52	0	66,67,67	0.71	4 (6%)
150	CDL	DI	302	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	Dv	401	-	99,99,99	0.30	0	105,111,111	0.53	2 (1%)
153	PC1	Ef	501	-	53,53,53	0.27	0	59,61,61	0.29	0
153	PC1	C	509	-	53,53,53	0.27	0	59,61,61	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
150	CDL	BT	202	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	CD	301	-	99,99,99	0.29	0	105,111,111	0.52	1 (0%)
150	CDL	B0	101	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	DQ	1502	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	EH	1601	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Du	403	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Dm	501	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	DI	303	-	53,53,53	0.29	0	59,61,61	0.27	0
156	LPP	AA	902	-	43,43,43	0.21	0	46,48,48	0.27	0
153	PC1	e	1101	-	53,53,53	0.28	0	59,61,61	0.29	0
150	CDL	DJ	302	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
153	PC1	Dc	603	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Ei	401	-	99,99,99	0.29	0	105,111,111	0.55	1 (0%)
150	CDL	DV	403	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
153	PC1	AU	201	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	El	902	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Da	706	-	53,53,53	0.28	0	59,61,61	0.29	0
153	PC1	DV	405	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	Dc	605	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DH	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Ea	502	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	C	504	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dd	704	-	99,99,99	0.31	0	105,111,111	0.48	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
153	PC1	Dc	609	-	-	16/57/57/57	-
150	CDL	DU	403	-	-	31/110/110/110	-
150	CDL	Dq	1403	-	-	32/110/110/110	-
153	PC1	A2	402	-	-	8/57/57/57	-
155	3PE	DX	302	-	-	13/54/54/54	-
153	PC1	El	904	-	-	10/57/57/57	-
168	HEM	Ed	201	125	-	0/12/54/54	-
155	3PE	EN	1204	-	-	15/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	BG	201	-	-	33/110/110/110	-
150	CDL	C	505	-	-	34/110/110/110	-
150	CDL	C	503	-	-	33/110/110/110	-
153	PC1	EB	301	-	-	12/57/57/57	-
155	3PE	Dg	204	-	-	13/54/54/54	-
150	CDL	DN	503	-	-	25/110/110/110	-
155	3PE	Dx	1207	-	-	19/54/54/54	-
153	PC1	B1	403	-	-	16/57/57/57	-
155	3PE	DX	304	-	-	14/54/54/54	-
150	CDL	DJ	305	-	-	25/110/110/110	-
166	HEC	D	401	88	-	1/10/54/54	-
153	PC1	Dy	302	-	-	11/57/57/57	-
155	3PE	BA	301	-	-	18/54/54/54	-
153	PC1	Dv	406	-	-	12/57/57/57	-
150	CDL	ES	1101	-	-	38/110/110/110	-
153	PC1	Da	707	-	-	12/57/57/57	-
150	CDL	CC	304	-	-	20/110/110/110	-
155	3PE	A2	401	-	-	9/54/54/54	-
153	PC1	A6	302	-	-	10/57/57/57	-
150	CDL	AA	901	-	-	32/110/110/110	-
150	CDL	BC	301	-	-	20/110/110/110	-
150	CDL	DG	202	-	-	29/110/110/110	-
150	CDL	DC	601	-	-	37/110/110/110	-
167	UQ8	c	510	-	-	11/51/75/75	0/1/1/1
165	F3S	CB	1002	75	-	-	0/3/3/3
150	CDL	BY	201	-	-	23/110/110/110	-
153	PC1	EB	303	-	-	5/57/57/57	-
153	PC1	DC	602	-	-	15/57/57/57	-
150	CDL	DU	402	-	-	29/110/110/110	-
153	PC1	EO	205	-	-	24/57/57/57	-
166	HEC	CE	401	79	-	5/10/54/54	-
169	HEA	DA	702	97	-	4/32/76/76	-
156	LPP	Dl	1101	-	-	8/45/45/45	-
150	CDL	DV	401	-	-	29/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
156	LPP	DN	504	-	-	9/45/45/45	-
150	CDL	DM	502	-	-	24/110/110/110	-
150	CDL	Dn	502	-	-	40/110/110/110	-
150	CDL	Dd	706	-	-	28/110/110/110	-
153	PC1	AC	804	-	-	11/57/57/57	-
155	3PE	DG	205	-	-	13/54/54/54	-
153	PC1	BT	203	-	-	15/57/57/57	-
153	PC1	DV	404	-	-	13/57/57/57	-
153	PC1	Dx	1205	-	-	14/57/57/57	-
153	PC1	d	801	-	-	16/57/57/57	-
155	3PE	AJ	502	-	-	13/54/54/54	-
150	CDL	Dj	403	-	-	33/110/110/110	-
159	SF4	CB	1001	75	-	-	0/6/5/5
150	CDL	DN	506	-	-	35/110/110/110	-
155	3PE	DJ	301	-	-	14/54/54/54	-
150	CDL	H	1302	-	-	28/110/110/110	-
155	3PE	DR	401	-	-	8/54/54/54	-
164	FAD	CA	702	73	-	16/30/50/50	0/6/6/6
150	CDL	DX	301	-	-	32/110/110/110	-
153	PC1	DY	302	-	-	9/57/57/57	-
150	CDL	Ed	205	-	-	28/110/110/110	-
167	UQ8	ED	603	-	-	10/51/75/75	0/1/1/1
150	CDL	Dc	601	-	-	37/110/110/110	-
153	PC1	DC	608	-	-	16/57/57/57	-
153	PC1	Dc	604	-	-	11/57/57/57	-
150	CDL	Ds	406	-	-	34/110/110/110	-
150	CDL	Dv	403	-	-	41/110/110/110	-
155	3PE	CD	303	-	-	12/54/54/54	-
150	CDL	DS	404	-	-	36/110/110/110	-
150	CDL	Dh	201	-	-	33/110/110/110	-
155	3PE	Di	1102	-	-	16/54/54/54	-
155	3PE	Dr	401	-	-	15/54/54/54	-
150	CDL	DX	306	-	-	33/110/110/110	-
150	CDL	Eu	101	-	-	32/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
155	3PE	Dc	606	-	-	5/54/54/54	-
156	LPP	DN	505	-	-	1/45/45/45	-
150	CDL	Dx	1204	-	-	46/110/110/110	-
153	PC1	EN	1203	-	-	15/57/57/57	-
155	3PE	Dc	607	-	-	18/54/54/54	-
168	HEM	c	505	87	-	1/12/54/54	-
168	HEM	C	502	87	-	5/12/54/54	-
153	PC1	Di	1104	-	-	19/57/57/57	-
153	PC1	DQ	1503	-	-	11/57/57/57	-
155	3PE	EM	901	-	-	13/54/54/54	-
168	HEM	ED	602	125	-	0/12/54/54	-
150	CDL	En	1201	-	-	31/110/110/110	-
158	FES	EF	202	127	-	-	0/1/1/1
150	CDL	Dg	201	-	-	44/110/110/110	-
150	CDL	Dv	402	-	-	34/110/110/110	-
150	CDL	EI	401	-	-	20/110/110/110	-
150	CDL	EN	1201	-	-	28/110/110/110	-
153	PC1	EO	206	-	-	17/57/57/57	-
153	PC1	DV	406	-	-	9/57/57/57	-
153	PC1	A6	303	-	-	10/57/57/57	-
158	FES	Ef	502	127	-	-	0/1/1/1
150	CDL	DG	201	-	-	35/110/110/110	-
153	PC1	DG	203	-	-	8/57/57/57	-
150	CDL	Ds	405	-	-	39/110/110/110	-
153	PC1	AU	202	-	-	12/57/57/57	-
153	PC1	Dg	203	-	-	13/57/57/57	-
150	CDL	Dr	403	-	-	29/110/110/110	-
166	HEC	d	802	88	-	2/10/54/54	-
150	CDL	Ed	204	-	-	27/110/110/110	-
155	3PE	Dx	1208	-	-	14/54/54/54	-
150	CDL	BV	201	-	-	22/110/110/110	-
150	CDL	AF	401	-	-	21/110/110/110	-
153	PC1	DC	605	-	-	12/57/57/57	-
159	SF4	AB	803	12	-	-	0/6/5/5
151	UDP	A0	603	152	-	5/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	DQ	1504	-	-	35/110/110/110	-
153	PC1	Eb	303	-	-	4/57/57/57	-
150	CDL	Dn	503	-	-	30/110/110/110	-
155	3PE	Eo	202	-	-	13/54/54/54	-
153	PC1	DC	603	-	-	14/57/57/57	-
156	LPP	AC	803	-	-	11/45/45/45	-
153	PC1	K	501	-	-	15/57/57/57	-
153	PC1	Dq	1404	-	-	10/57/57/57	-
169	HEA	Da	703	97	-	9/32/76/76	-
173	ATP	Er	201	-	-	2/18/38/38	0/3/3/3
155	3PE	El	905	-	-	17/54/54/54	-
150	CDL	c	502	-	-	29/110/110/110	-
150	CDL	Dn	506	-	-	33/110/110/110	-
150	CDL	Ds	401	-	-	26/110/110/110	-
161	8Q1	AS	200	-	-	11/38/40/41	-
155	3PE	DC	606	-	-	10/54/54/54	-
150	CDL	Dj	401	-	-	38/110/110/110	-
167	UQ8	Ed	202	-	-	8/51/75/75	0/1/1/1
150	CDL	Dx	1201	-	-	37/110/110/110	-
150	CDL	Dj	404	-	-	35/110/110/110	-
159	SF4	AB	802	12	-	-	0/6/5/5
153	PC1	CC	302	-	-	15/57/57/57	-
153	PC1	c	507	-	-	17/57/57/57	-
150	CDL	DD	706	-	-	30/110/110/110	-
153	PC1	AH	301	-	-	8/57/57/57	-
153	PC1	c	508	-	-	8/57/57/57	-
150	CDL	EB	302	-	-	31/110/110/110	-
150	CDL	EL	903	-	-	36/110/110/110	-
155	3PE	CK	101	-	-	2/54/54/54	-
150	CDL	Dn	501	-	-	37/110/110/110	-
153	PC1	DA	708	-	-	10/57/57/57	-
150	CDL	Dg	202	-	-	31/110/110/110	-
150	CDL	Da	709	-	-	41/110/110/110	-
168	HEM	c	504	87	-	1/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Dm	502	-	-	23/110/110/110	-
150	CDL	Di	1101	-	-	38/110/110/110	-
150	CDL	Dd	702	-	-	29/110/110/110	-
153	PC1	Db	702	-	-	22/57/57/57	-
150	CDL	DN	502	-	-	39/110/110/110	-
153	PC1	K	502	-	-	12/57/57/57	-
153	PC1	AA	905	-	-	15/57/57/57	-
150	CDL	Di	1103	-	-	33/110/110/110	-
153	PC1	BS	1302	-	-	10/57/57/57	-
158	FES	BI	201	52	-	-	0/1/1/1
167	UQ8	C	512	-	-	9/51/75/75	0/1/1/1
158	FES	e	1102	89	-	-	0/1/1/1
150	CDL	DU	404	-	-	25/110/110/110	-
150	CDL	ED	605	-	-	34/110/110/110	-
158	FES	Ef	503	127	-	-	0/1/1/1
153	PC1	A1	403	-	-	14/57/57/57	-
150	CDL	AA	908	-	-	29/110/110/110	-
153	PC1	Eo	204	-	-	18/57/57/57	-
155	3PE	G	401	-	-	7/54/54/54	-
154	NDP	A1	401	-	-	4/30/77/77	0/5/5/5
160	FMN	AD	502	-	-	1/18/18/18	0/3/3/3
150	CDL	DQ	1501	-	-	30/110/110/110	-
159	SF4	AT	201	30	-	-	0/6/5/5
155	3PE	CC	301	-	-	5/54/54/54	-
150	CDL	CG	301	-	-	27/110/110/110	-
156	LPP	EI	402	-	-	8/45/45/45	-
150	CDL	ED	601	-	-	29/110/110/110	-
150	CDL	Eb	302	-	-	36/110/110/110	-
155	3PE	A9	602	-	-	7/54/54/54	-
159	SF4	AL	302	22	-	-	0/6/5/5
156	LPP	Ed	203	-	-	2/45/45/45	-
158	FES	E	302	89	-	-	0/1/1/1
150	CDL	Dj	407	-	-	32/110/110/110	-
153	PC1	DX	305	-	-	10/57/57/57	-
153	PC1	k	301	-	-	17/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Dc	608	-	-	25/110/110/110	-
150	CDL	EL	902	-	-	45/110/110/110	-
150	CDL	Du	402	-	-	32/110/110/110	-
153	PC1	AX	401	-	-	8/57/57/57	-
167	UQ8	C	511	-	-	15/51/75/75	0/1/1/1
155	3PE	C	513	-	-	11/54/54/54	-
150	CDL	Dh	202	-	-	38/110/110/110	-
155	3PE	DN	501	-	-	11/54/54/54	-
168	HEM	C	501	87	-	4/12/54/54	-
153	PC1	AL	303	-	-	9/57/57/57	-
153	PC1	DA	707	-	-	18/57/57/57	-
150	CDL	Dy	301	-	-	36/110/110/110	-
150	CDL	B0	102	-	-	22/110/110/110	-
150	CDL	DR	403	-	-	28/110/110/110	-
153	PC1	D	402	-	-	18/57/57/57	-
153	PC1	AA	903	-	-	12/57/57/57	-
157	ADP	AQ	201	-	-	2/12/32/32	0/3/3/3
153	PC1	AA	906	-	-	17/57/57/57	-
153	PC1	AQ	202	-	-	15/57/57/57	-
150	CDL	AC	802	-	-	34/110/110/110	-
153	PC1	EO	204	-	-	10/57/57/57	-
153	PC1	Dv	407	-	-	9/57/57/57	-
150	CDL	Dj	405	-	-	26/110/110/110	-
153	PC1	BS	1301	-	-	16/57/57/57	-
150	CDL	AF	402	-	-	28/110/110/110	-
153	PC1	A	1201	-	-	13/57/57/57	-
158	FES	AB	801	12	-	-	0/1/1/1
150	CDL	CG	302	-	-	34/110/110/110	-
153	PC1	c	503	-	-	16/57/57/57	-
150	CDL	AC	801	-	-	38/110/110/110	-
155	3PE	Em	901	-	-	14/54/54/54	-
153	PC1	AM	302	-	-	19/57/57/57	-
150	CDL	DH	202	-	-	40/110/110/110	-
156	LPP	AL	304	-	-	3/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	DJ	304	-	-	38/110/110/110	-
150	CDL	EA	301	-	-	28/110/110/110	-
150	CDL	DV	402	-	-	29/110/110/110	-
153	PC1	E	303	-	-	10/57/57/57	-
150	CDL	Ds	402	-	-	31/110/110/110	-
153	PC1	DB	702	-	-	22/57/57/57	-
155	3PE	Ds	408	-	-	10/54/54/54	-
167	UQ8	EL	905	-	-	10/51/75/75	0/1/1/1
150	CDL	C	507	-	-	32/110/110/110	-
150	CDL	El	901	-	-	41/110/110/110	-
153	PC1	B1	401	-	-	18/57/57/57	-
150	CDL	EN	1202	-	-	27/110/110/110	-
150	CDL	DO	501	-	-	28/110/110/110	-
153	PC1	g	802	-	-	11/57/57/57	-
150	CDL	Dd	705	-	-	28/110/110/110	-
150	CDL	AP	301	-	-	25/110/110/110	-
150	CDL	A1	402	-	-	40/110/110/110	-
150	CDL	DS	405	-	-	33/110/110/110	-
167	UQ8	EN	1205	-	-	15/51/75/75	0/1/1/1
153	PC1	EO	201	-	-	12/57/57/57	-
150	CDL	c	509	-	-	33/110/110/110	-
150	CDL	H	1301	-	-	30/110/110/110	-
150	CDL	CD	302	-	-	28/110/110/110	-
150	CDL	Dq	1401	-	-	38/110/110/110	-
150	CDL	E	301	-	-	28/110/110/110	-
150	CDL	Dr	402	-	-	35/110/110/110	-
150	CDL	A0	601	-	-	23/110/110/110	-
153	PC1	BG	202	-	-	21/57/57/57	-
155	3PE	Da	708	-	-	16/54/54/54	-
153	PC1	Eb	301	-	-	10/57/57/57	-
153	PC1	Dx	1209	-	-	5/57/57/57	-
153	PC1	DS	406	-	-	19/57/57/57	-
150	CDL	EO	202	-	-	33/110/110/110	-
150	CDL	DD	705	-	-	31/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	B1	402	-	-	32/110/110/110	-
150	CDL	DN	507	-	-	38/110/110/110	-
153	PC1	DJ	306	-	-	12/57/57/57	-
156	LPP	Dn	505	-	-	7/45/45/45	-
158	FES	AI	301	19	-	-	0/1/1/1
159	SF4	AD	501	14	-	-	0/6/5/5
150	CDL	A0	602	-	-	35/110/110/110	-
153	PC1	C	510	-	-	11/57/57/57	-
155	3PE	DX	303	-	-	18/54/54/54	-
153	PC1	C	508	-	-	19/57/57/57	-
155	3PE	Eo	203	-	-	8/54/54/54	-
153	PC1	Dx	1203	-	-	15/57/57/57	-
167	UQ8	El	906	-	-	13/51/75/75	0/1/1/1
153	PC1	A9	603	-	-	17/57/57/57	-
169	HEA	DA	703	97	-	10/32/76/76	-
153	PC1	Dj	406	-	-	10/57/57/57	-
173	ATP	ER	201	-	-	6/18/38/38	0/3/3/3
169	HEA	Da	702	97	-	4/32/76/76	-
150	CDL	DA	709	-	-	22/110/110/110	-
155	3PE	Ds	403	-	-	20/54/54/54	-
150	CDL	DS	401	-	-	27/110/110/110	-
167	UQ8	DS	403	-	-	8/51/75/75	0/1/1/1
150	CDL	CC	305	-	-	26/110/110/110	-
150	CDL	ED	604	-	-	26/110/110/110	-
153	PC1	Eo	201	-	-	15/57/57/57	-
150	CDL	CJ	201	-	-	22/110/110/110	-
155	3PE	EL	904	-	-	17/54/54/54	-
150	CDL	DX	307	-	-	28/110/110/110	-
150	CDL	Ep	701	-	-	31/110/110/110	-
150	CDL	h	501	-	-	25/110/110/110	-
150	CDL	AM	301	-	-	31/110/110/110	-
153	PC1	A9	601	-	-	12/57/57/57	-
150	CDL	DU	401	-	-	34/110/110/110	-
153	PC1	DX	308	-	-	17/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
155	3PE	EO	203	-	-	9/54/54/54	-
150	CDL	BC	302	-	-	31/110/110/110	-
155	3PE	Dd	703	-	-	16/54/54/54	-
150	CDL	Ea	501	-	-	35/110/110/110	-
150	CDL	Ek	201	-	-	30/110/110/110	-
150	CDL	BE	201	-	-	29/110/110/110	-
150	CDL	Du	401	-	-	37/110/110/110	-
153	PC1	Eo	205	-	-	14/57/57/57	-
155	3PE	Dx	1206	-	-	15/54/54/54	-
153	PC1	AA	904	-	-	13/57/57/57	-
155	3PE	Dr	404	-	-	10/54/54/54	-
150	CDL	DJ	303	-	-	31/110/110/110	-
155	3PE	Dx	1202	-	-	17/54/54/54	-
150	CDL	El	903	-	-	38/110/110/110	-
157	ADP	A8	401	152	-	2/12/32/32	0/3/3/3
153	PC1	DC	604	-	-	15/57/57/57	-
153	PC1	Dv	405	-	-	19/57/57/57	-
150	CDL	Eg	101	-	-	31/110/110/110	-
158	FES	CB	1000	75	-	-	0/1/1/1
153	PC1	Dv	404	-	-	9/57/57/57	-
150	CDL	DA	706	-	-	33/110/110/110	-
150	CDL	g	801	-	-	31/110/110/110	-
153	PC1	A0	605	-	-	13/57/57/57	-
156	LPP	A6	301	-	-	2/45/45/45	-
150	CDL	EK	201	-	-	29/110/110/110	-
150	CDL	DD	703	-	-	29/110/110/110	-
155	3PE	BP	201	-	-	14/54/54/54	-
155	3PE	DS	402	-	-	20/54/54/54	-
150	CDL	BT	204	-	-	37/110/110/110	-
155	3PE	BT	201	-	-	20/54/54/54	-
150	CDL	Do	501	-	-	34/110/110/110	-
150	CDL	Dq	1402	-	-	28/110/110/110	-
150	CDL	c	506	-	-	37/110/110/110	-
153	PC1	AA	907	-	-	18/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
156	LPP	DA	710	-	-	7/45/45/45	-
155	3PE	DC	607	-	-	12/54/54/54	-
153	PC1	Dc	602	-	-	16/57/57/57	-
155	3PE	DG	204	-	-	14/54/54/54	-
167	UQ8	Ds	404	-	-	12/51/75/75	0/1/1/1
150	CDL	DY	301	-	-	31/110/110/110	-
150	CDL	Eh	1601	-	-	40/110/110/110	-
158	FES	EF	201	127	-	-	0/1/1/1
150	CDL	c	501	-	-	35/110/110/110	-
150	CDL	Dj	402	-	-	34/110/110/110	-
159	SF4	AL	301	22	-	-	0/6/5/5
153	PC1	Ds	407	-	-	8/57/57/57	-
150	CDL	C	506	-	-	31/110/110/110	-
155	3PE	DI	301	-	-	17/54/54/54	-
150	CDL	EL	901	-	-	41/110/110/110	-
150	CDL	DM	501	-	-	40/110/110/110	-
167	UQ8	En	1202	-	-	11/51/75/75	0/1/1/1
150	CDL	BL	301	-	-	20/110/110/110	-
150	CDL	DD	704	-	-	29/110/110/110	-
153	PC1	AJ	501	-	-	16/57/57/57	-
156	LPP	Dn	504	-	-	9/45/45/45	-
150	CDL	DR	402	-	-	33/110/110/110	-
150	CDL	DJ	307	-	-	33/110/110/110	-
150	CDL	DZ	501	-	-	37/110/110/110	-
167	UQ8	CC	303	-	-	9/51/75/75	0/1/1/1
150	CDL	DI	302	-	-	39/110/110/110	-
150	CDL	Dv	401	-	-	36/110/110/110	-
153	PC1	Ef	501	-	-	13/57/57/57	-
153	PC1	C	509	-	-	22/57/57/57	-
150	CDL	BT	202	-	-	34/110/110/110	-
150	CDL	CD	301	-	-	37/110/110/110	-
150	CDL	B0	101	-	-	33/110/110/110	-
150	CDL	DQ	1502	-	-	32/110/110/110	-
150	CDL	EH	1601	-	-	32/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Du	403	-	-	28/110/110/110	-
150	CDL	Dm	501	-	-	38/110/110/110	-
153	PC1	DI	303	-	-	17/57/57/57	-
156	LPP	AA	902	-	-	10/45/45/45	-
153	PC1	e	1101	-	-	12/57/57/57	-
150	CDL	DJ	302	-	-	28/110/110/110	-
153	PC1	Dc	603	-	-	15/57/57/57	-
150	CDL	Ei	401	-	-	25/110/110/110	-
150	CDL	DV	403	-	-	35/110/110/110	-
153	PC1	AU	201	-	-	13/57/57/57	-
150	CDL	El	902	-	-	39/110/110/110	-
153	PC1	Da	706	-	-	15/57/57/57	-
153	PC1	DV	405	-	-	9/57/57/57	-
153	PC1	Dc	605	-	-	16/57/57/57	-
150	CDL	DH	201	-	-	24/110/110/110	-
150	CDL	Ea	502	-	-	26/110/110/110	-
150	CDL	C	504	-	-	38/110/110/110	-
150	CDL	Dd	704	-	-	35/110/110/110	-

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	CE	401	HEC	C2B-C3B	9.88	1.51	1.40
169	Da	702	HEA	C3A-C2A	6.66	1.49	1.40
166	D	401	HEC	C3C-C2C	6.64	1.48	1.40
169	DA	702	HEA	C3A-C2A	6.55	1.49	1.40
169	Da	703	HEA	C3A-C2A	6.43	1.49	1.40

The worst 5 of 353 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	D	401	HEC	CMB-C2B-C3B	6.11	133.00	125.82
169	DA	702	HEA	C3D-C4D-ND	6.06	116.21	110.35
169	DA	703	HEA	C3D-C4D-ND	6.02	116.17	110.35
169	Da	702	HEA	C3D-C4D-ND	5.93	116.08	110.35
169	Da	703	HEA	C3D-C4D-ND	5.90	116.06	110.35

There are no chirality outliers.

5 of 7363 torsion outliers are listed below:

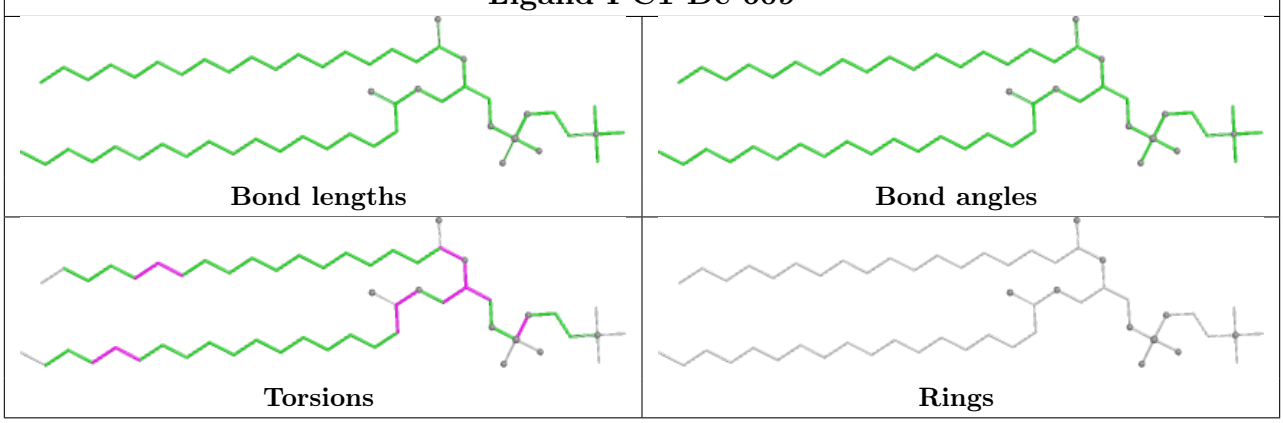
Mol	Chain	Res	Type	Atoms
150	A0	601	CDL	C11-CA5-OA6-CA4
150	A0	601	CDL	CB2-OB2-PB2-OB4
150	A0	601	CDL	CB2-OB2-PB2-OB5
150	A0	601	CDL	CB3-OB5-PB2-OB2
150	A0	601	CDL	CB3-OB5-PB2-OB3

There are no ring outliers.

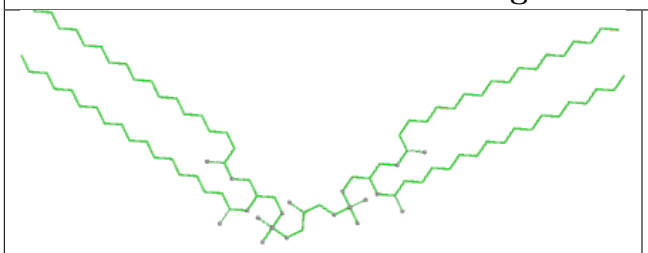
No monomer is involved in short contacts.

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 then 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.

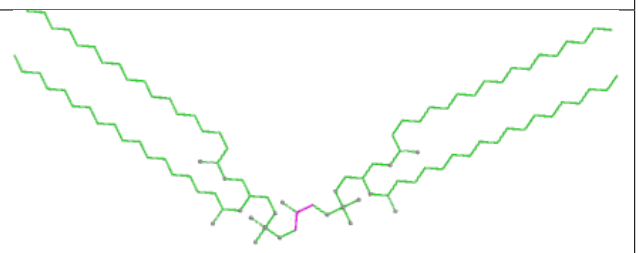
Ligand PC1 Dc 609



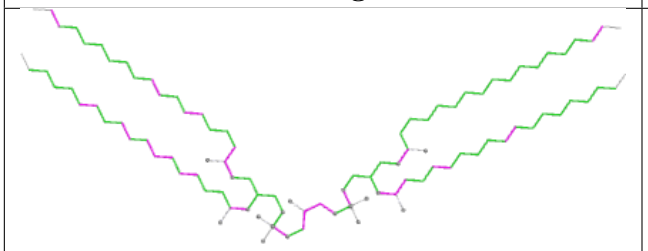
Ligand CDL DU 403



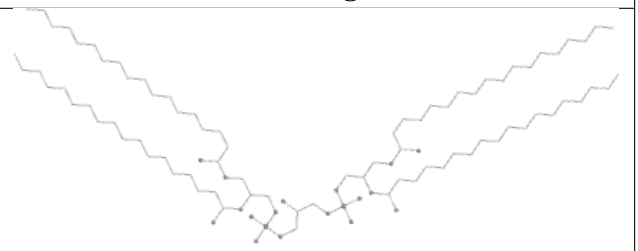
Bond lengths



Bond angles

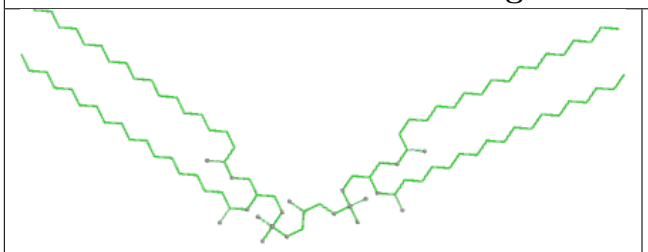


Torsions

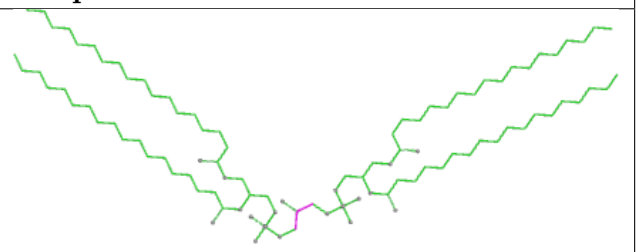


Rings

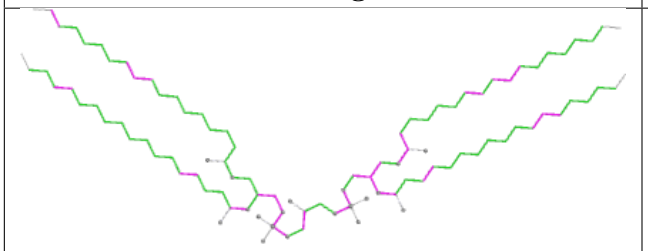
Ligand CDL Dq 1403



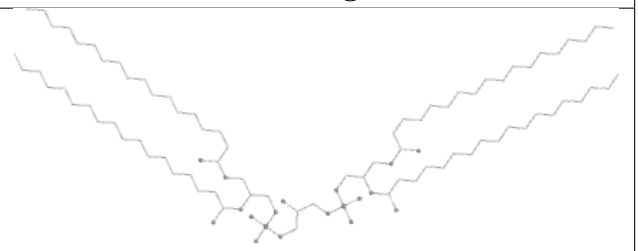
Bond lengths



Bond angles

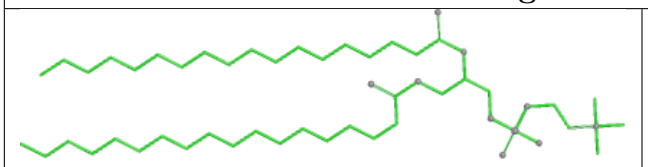


Torsions

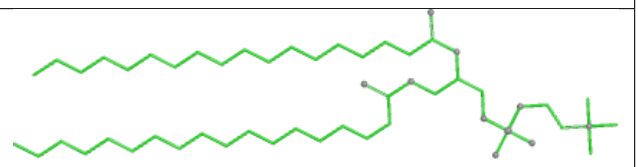


Rings

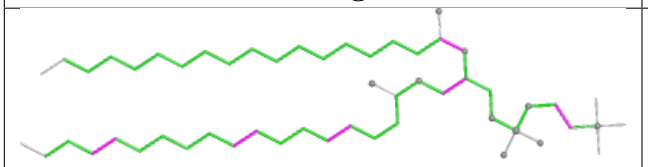
Ligand PC1 A2 402



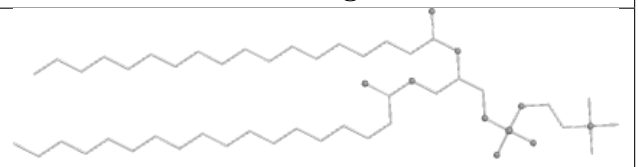
Bond lengths



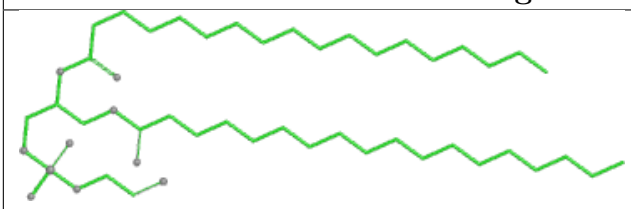
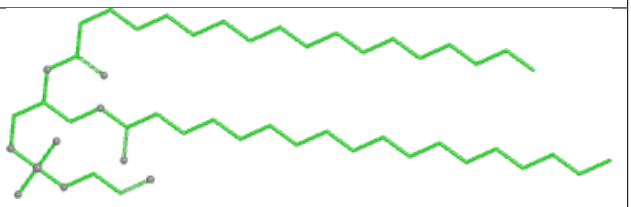
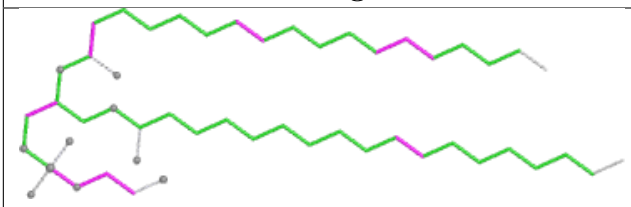
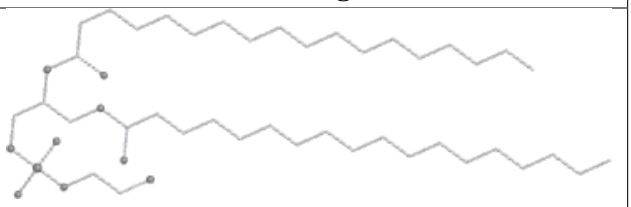
Bond angles

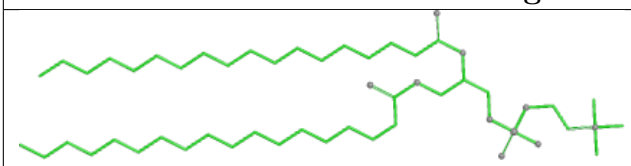
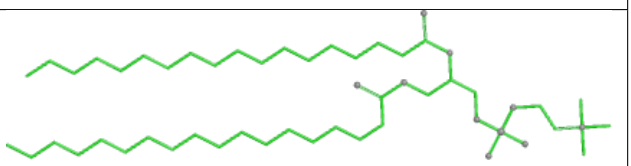
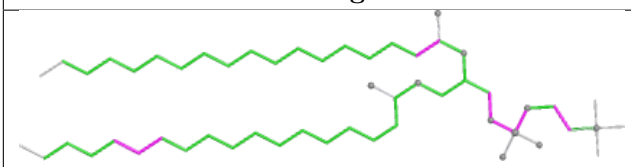
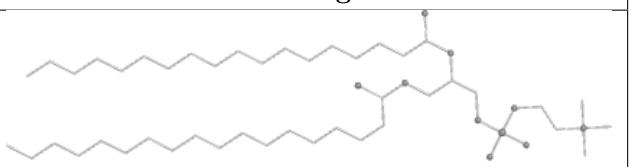


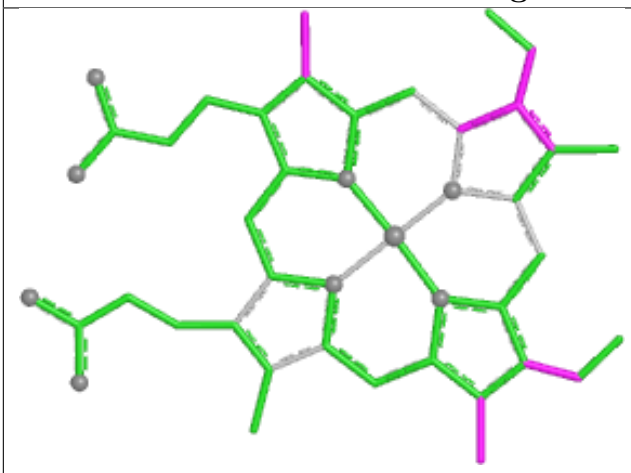
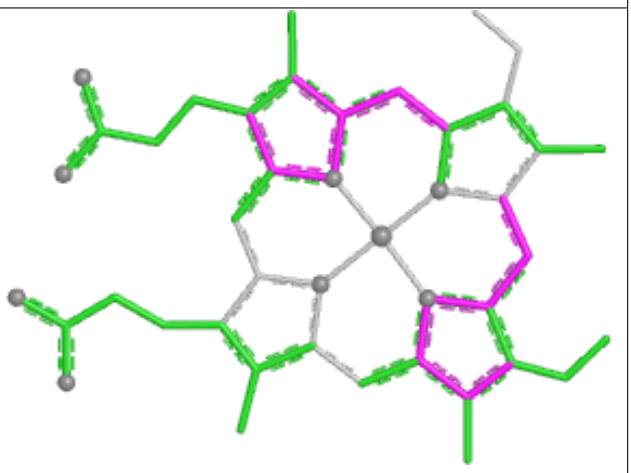
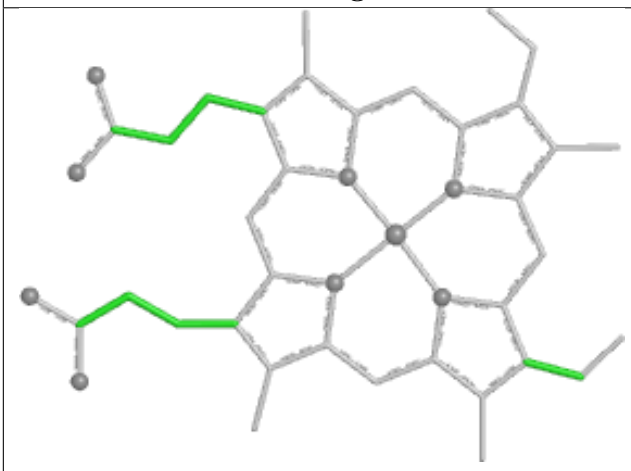
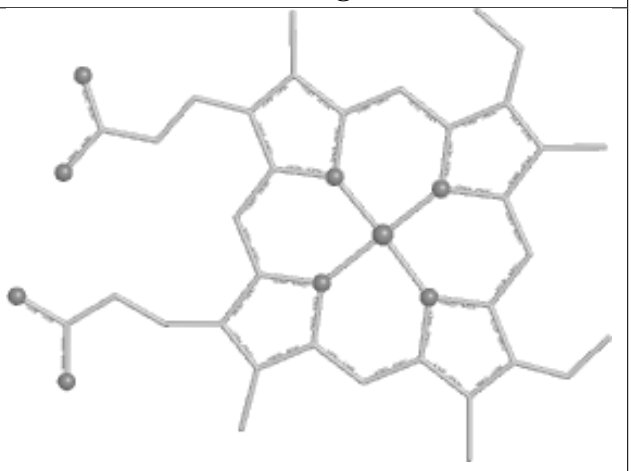
Torsions

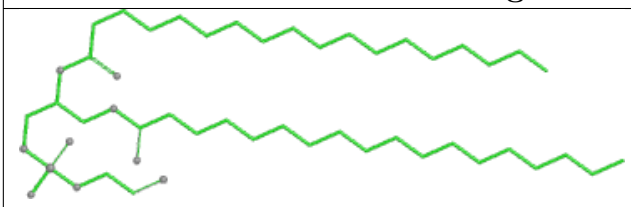
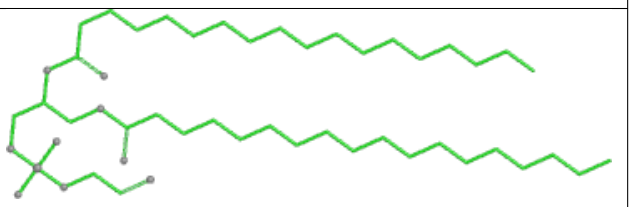
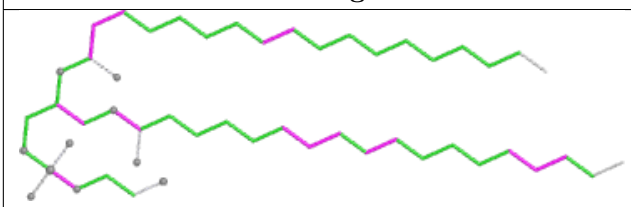
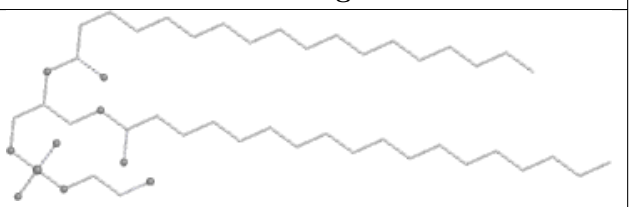


Rings

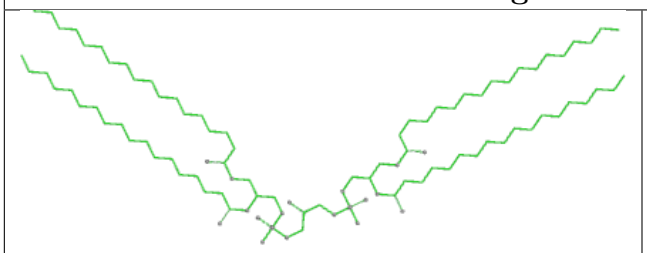
Ligand 3PE DX 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 El 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

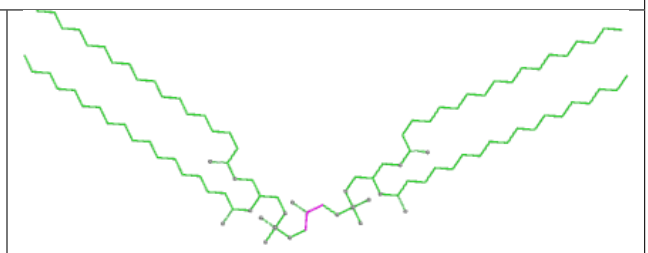
Ligand HEM Ed 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE EN 1204	
 Bond lengths	 Bond angles
 Torsions	 Rings

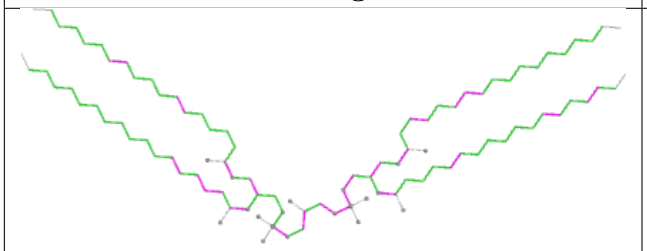
Ligand CDL BG 201



Bond lengths



Bond angles



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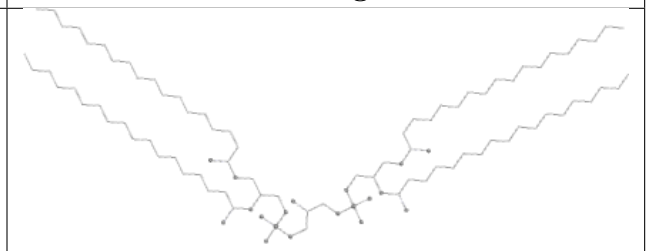
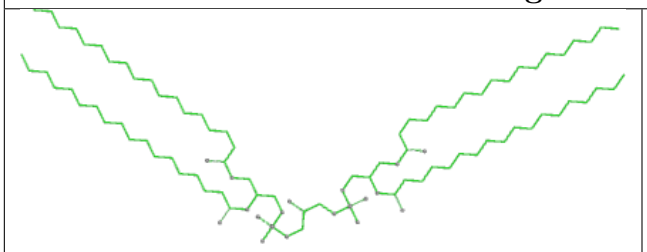
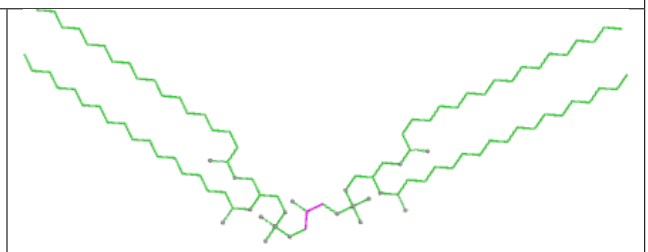


Rings

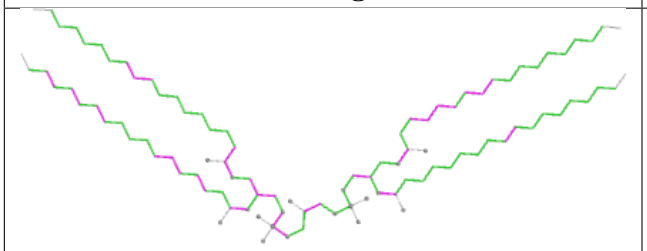
Ligand CDL C 505



Bond lengths



Bond angles



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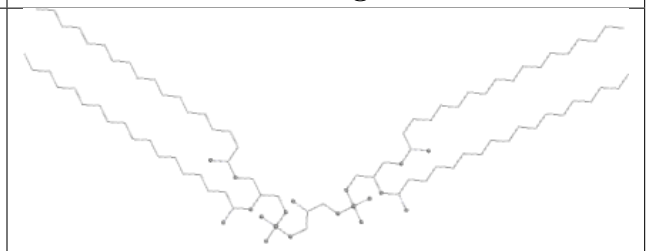
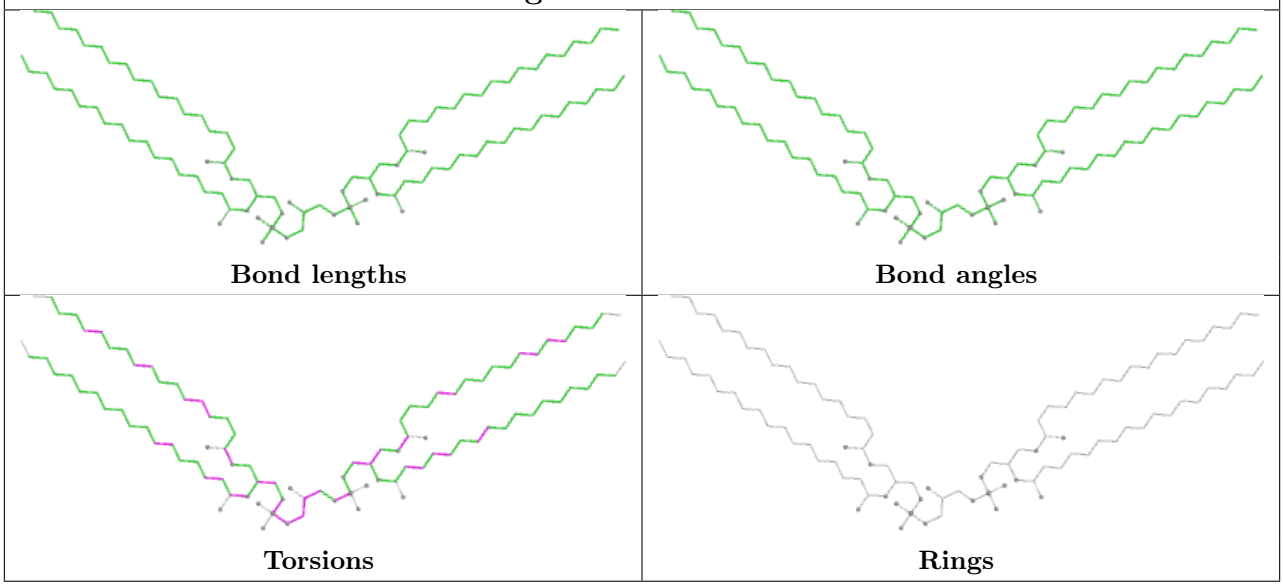
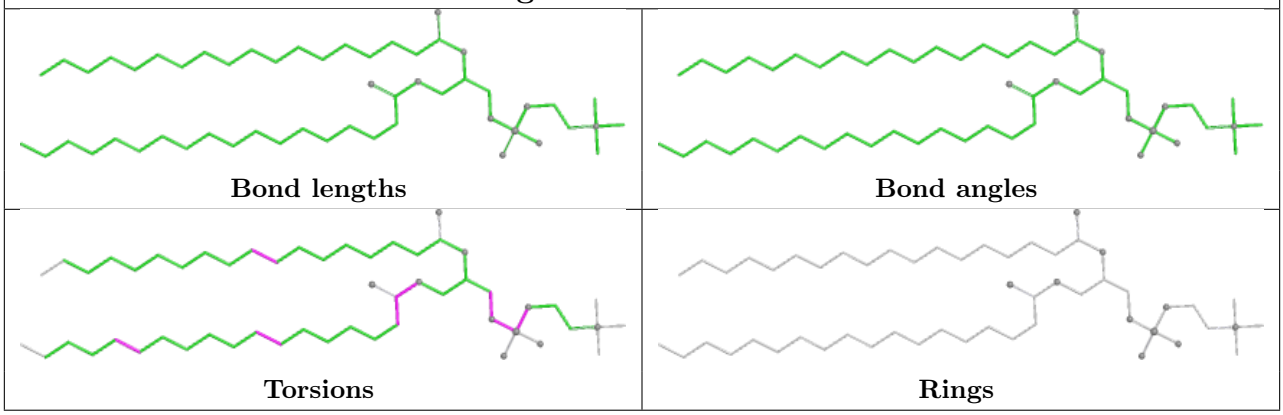


Rings

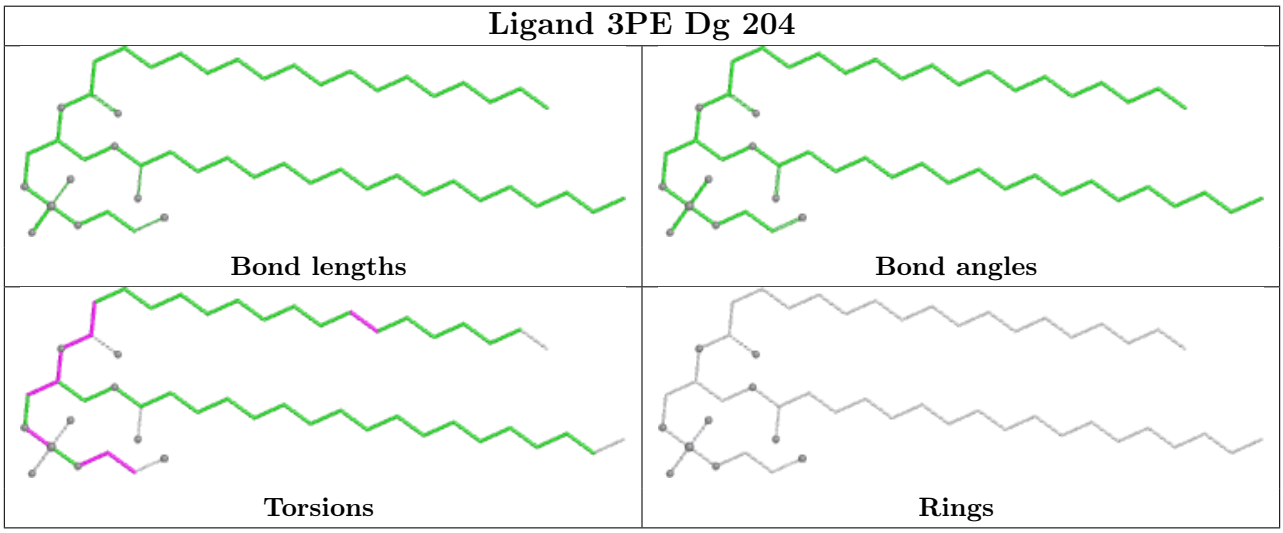
Ligand CDL C 503



Ligand PC1 EB 301



Ligand 3PE Dg 204



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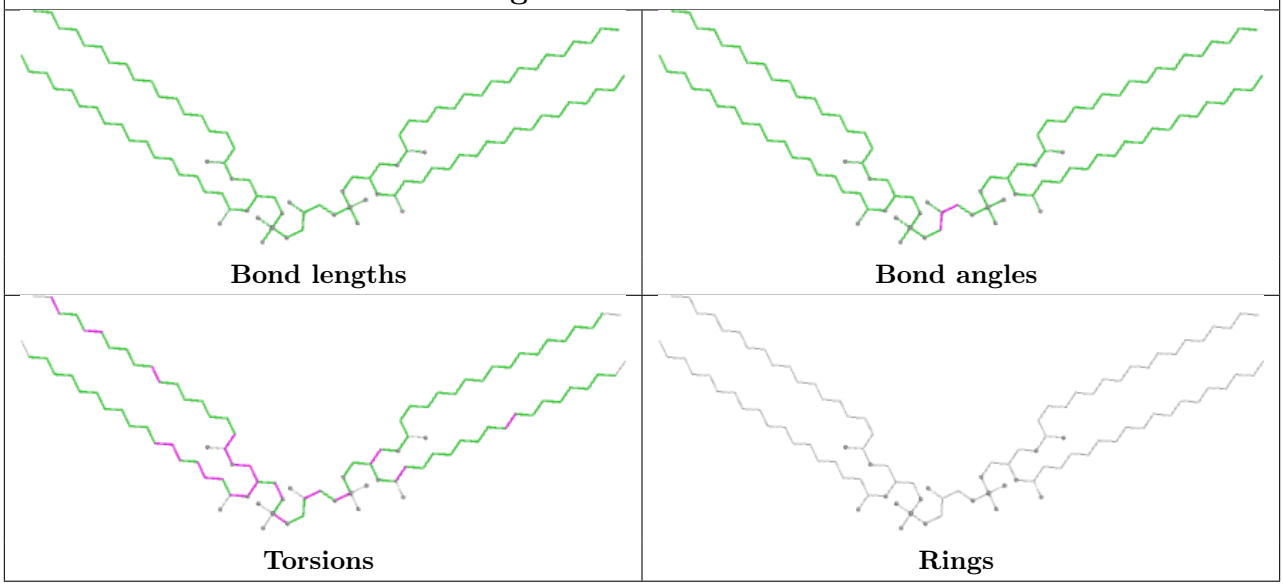

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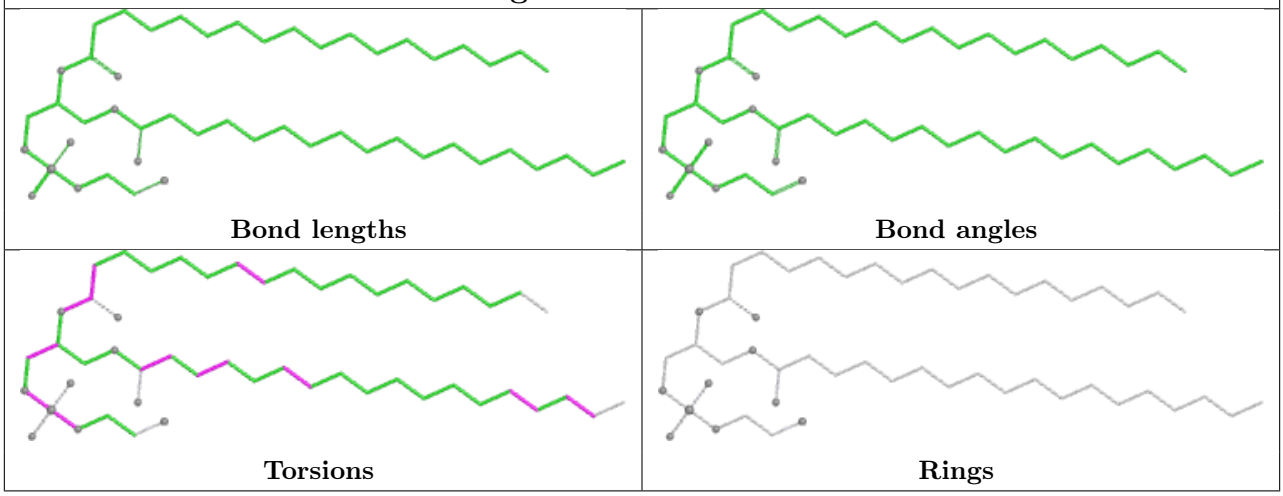

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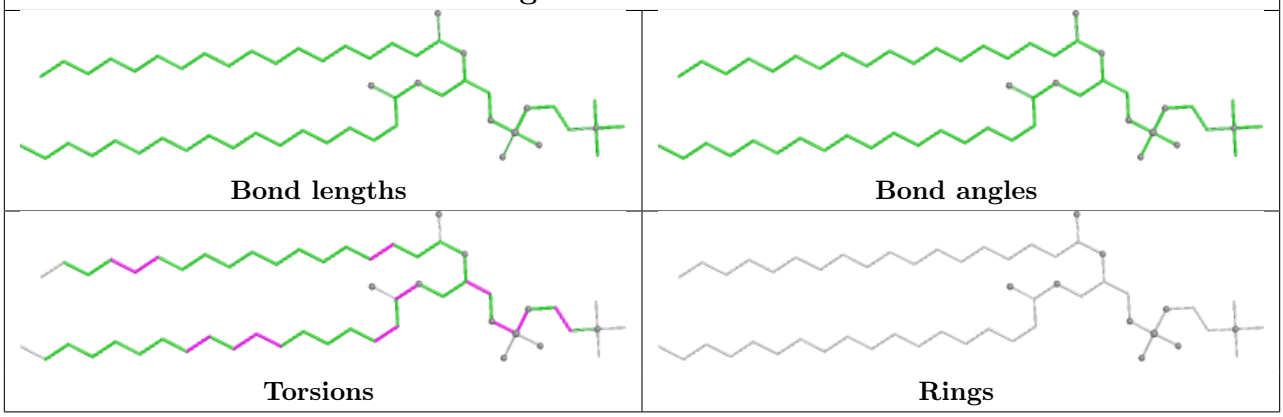

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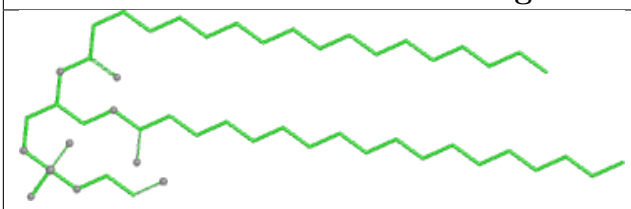
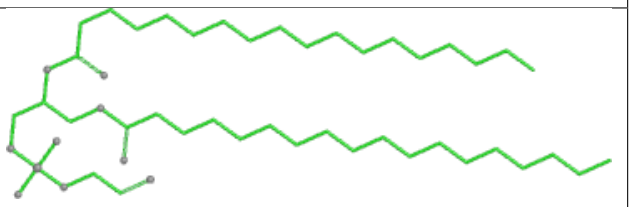
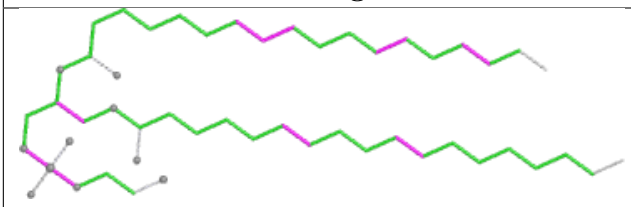
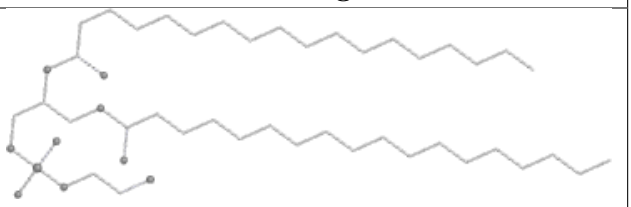
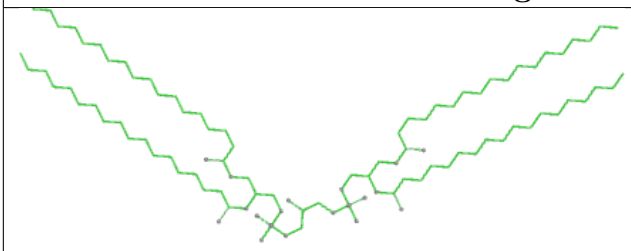
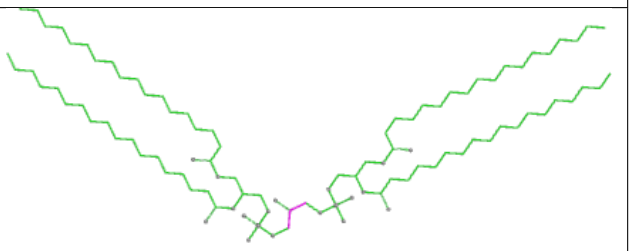
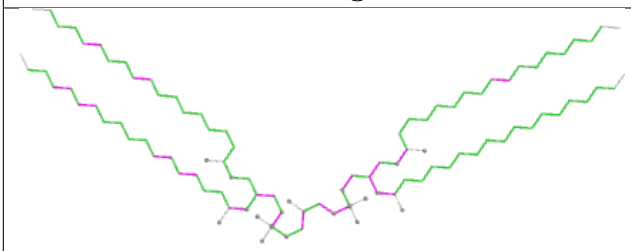
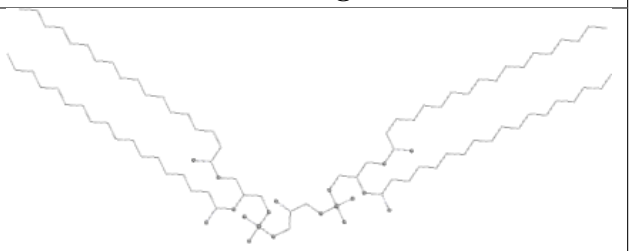
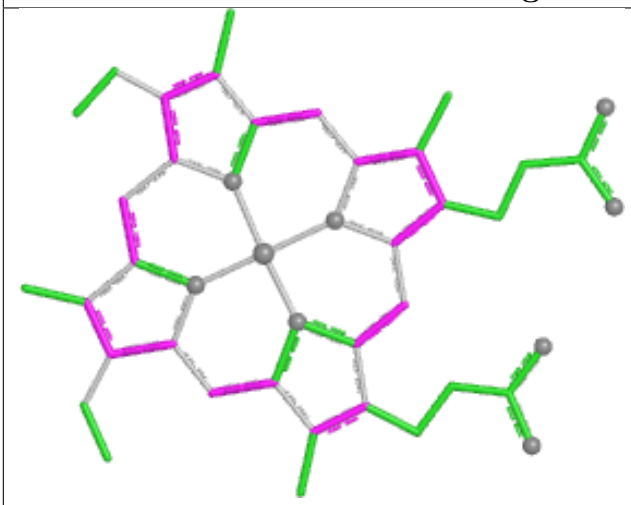
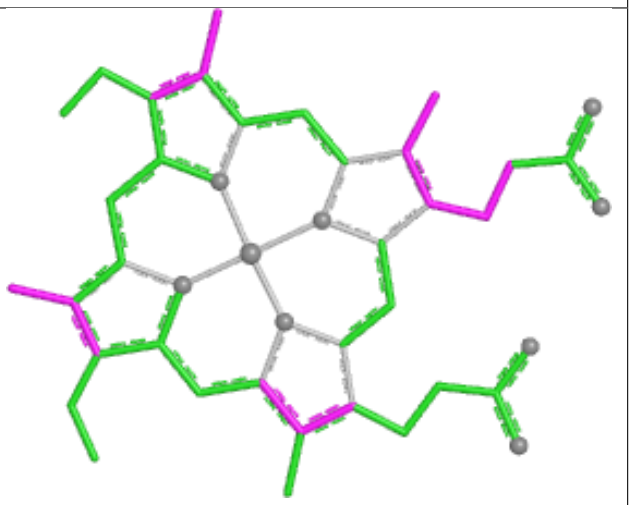
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL DJ 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

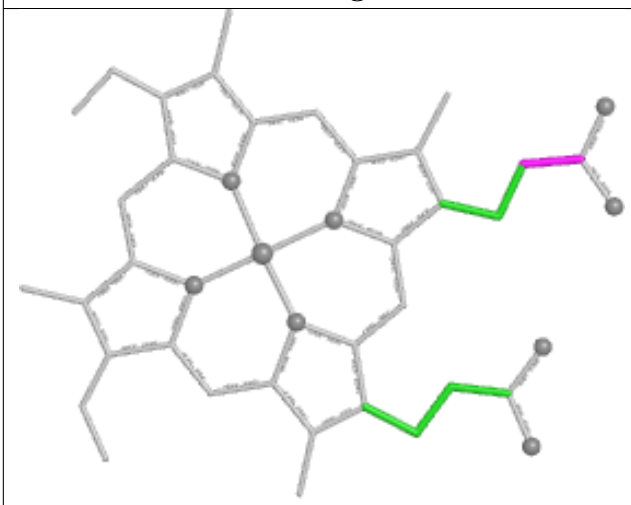
Ligand HEC D 401



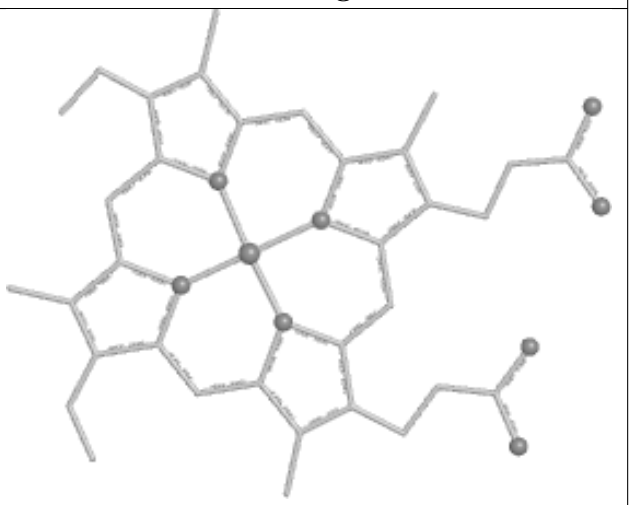
Bond lengths



Bond angles

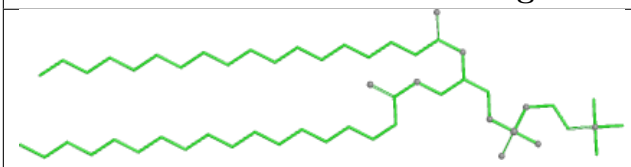


Torsions



Rings

Ligand PC1 Dy 302



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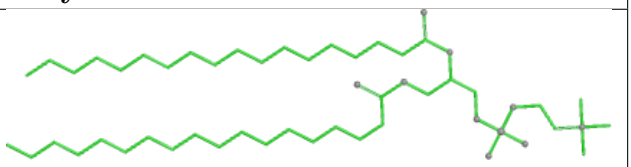
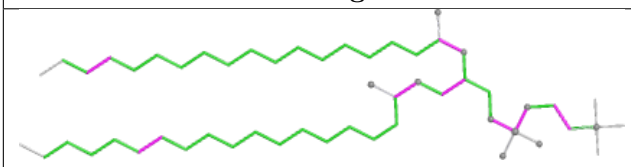
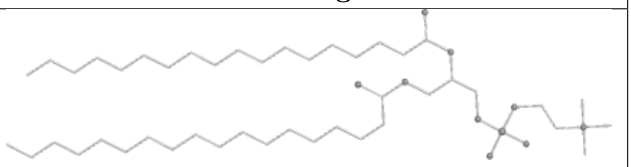


Bond angles

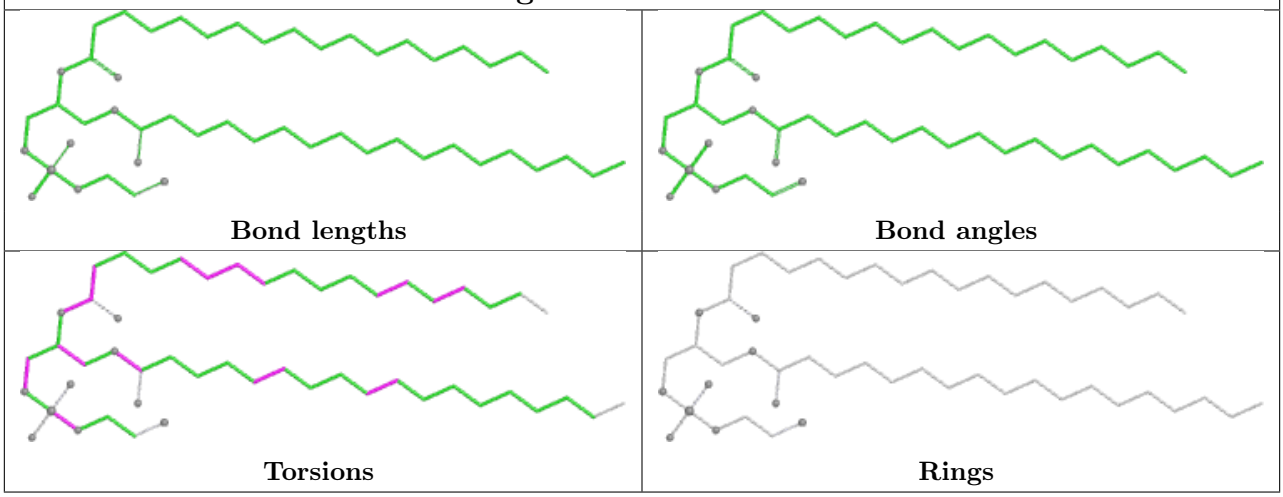


Torsions



Rings

Ligand 3PE BA 301



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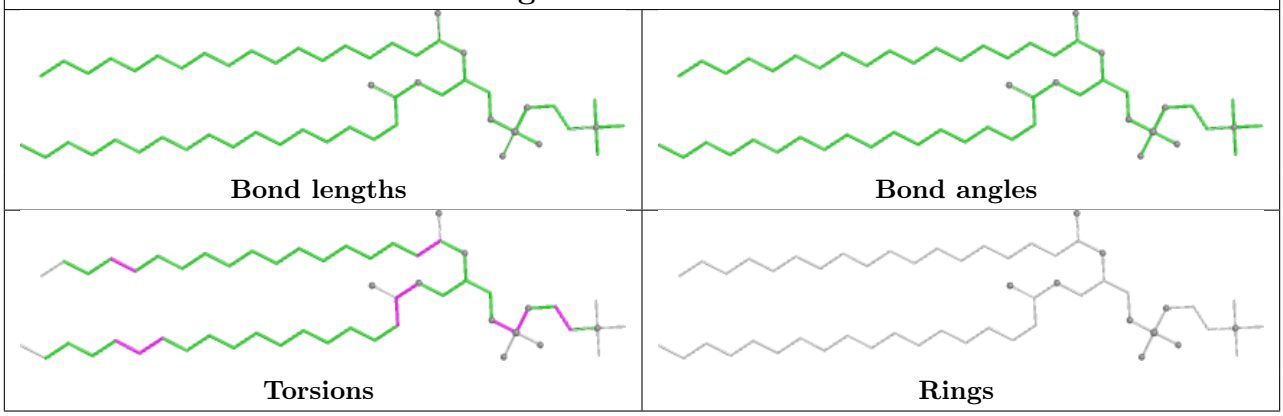
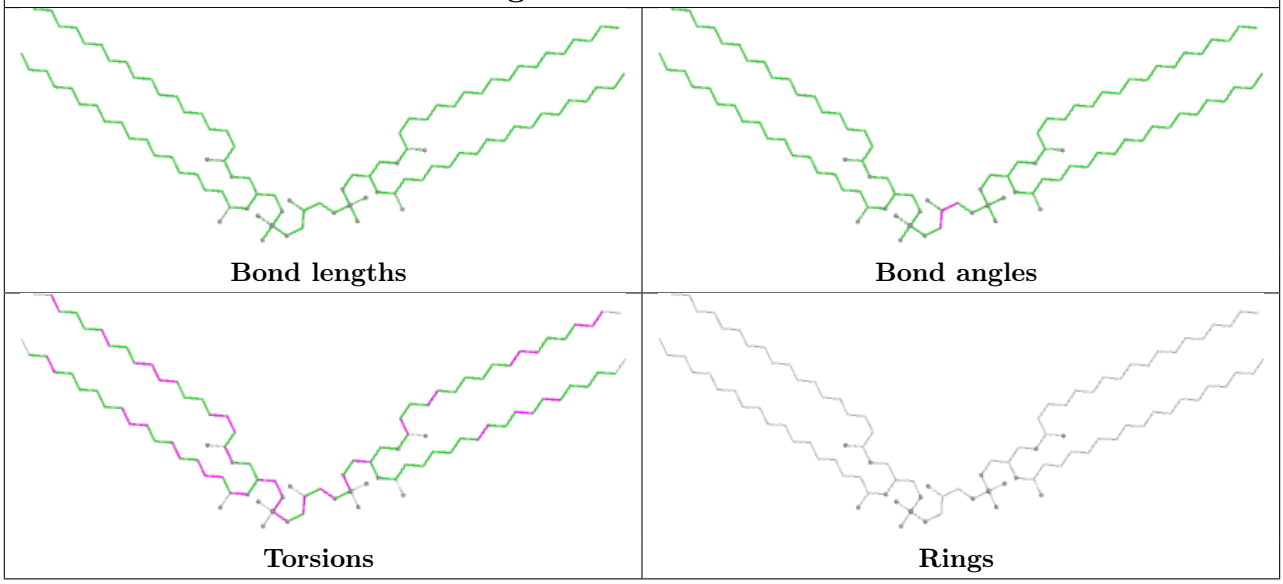
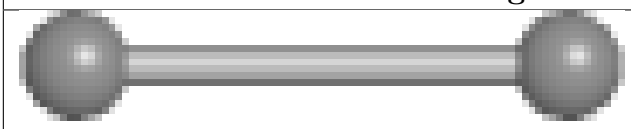


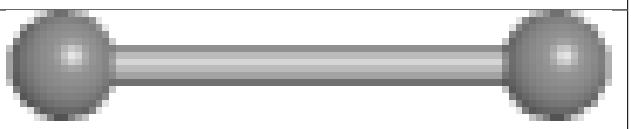
Ligand CDL ES 1101



Ligand CUA DB 701



Bond lengths

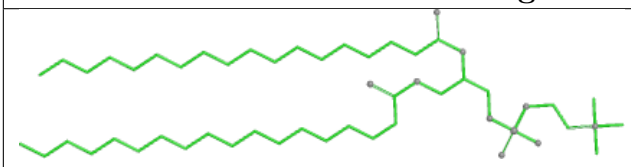


Bond angles

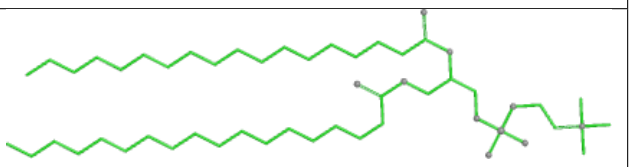
Torsions

Rings

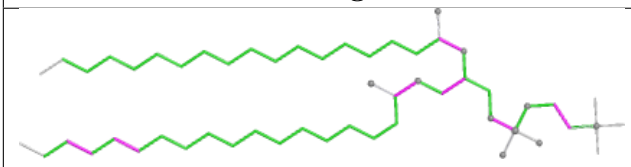
Ligand PC1 Da 707



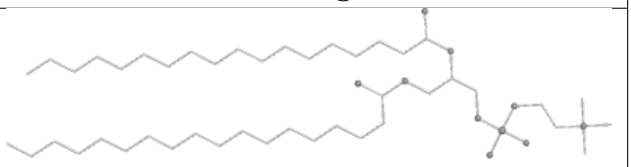
Bond lengths



Bond angles

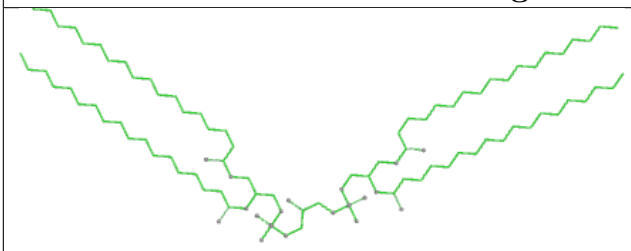


Torsions



Rings

Ligand CDL CC 304



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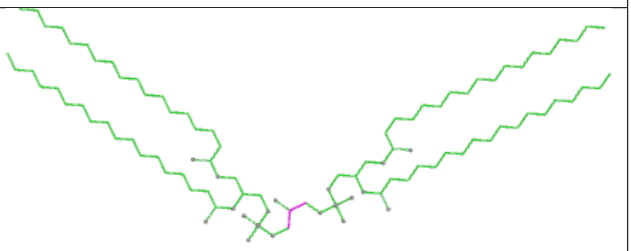
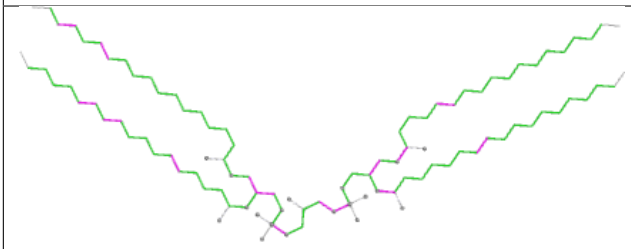
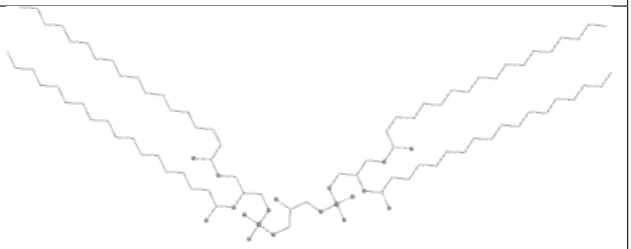


Bond angles

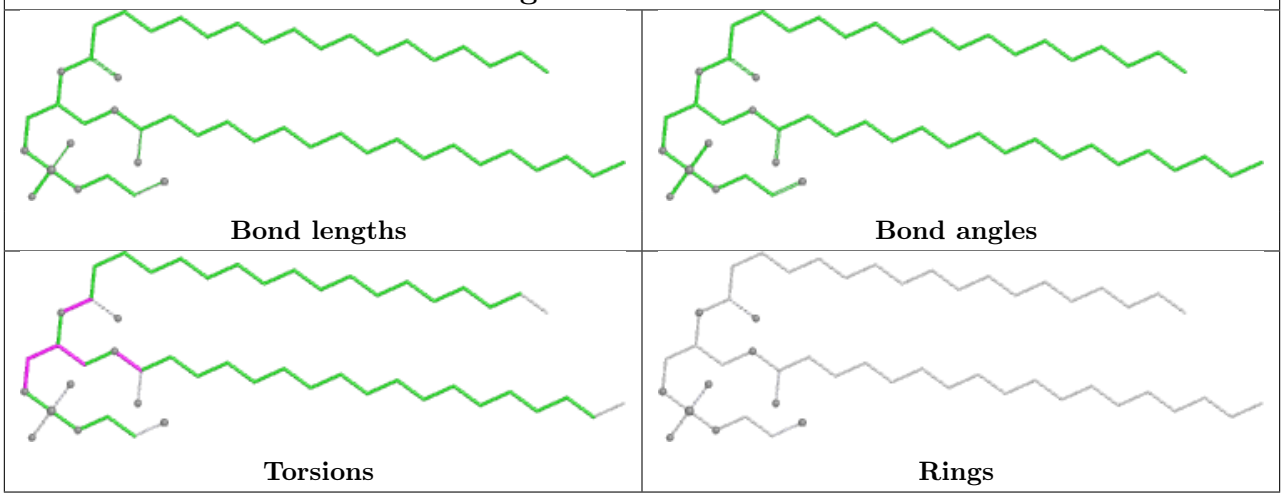


Torsions

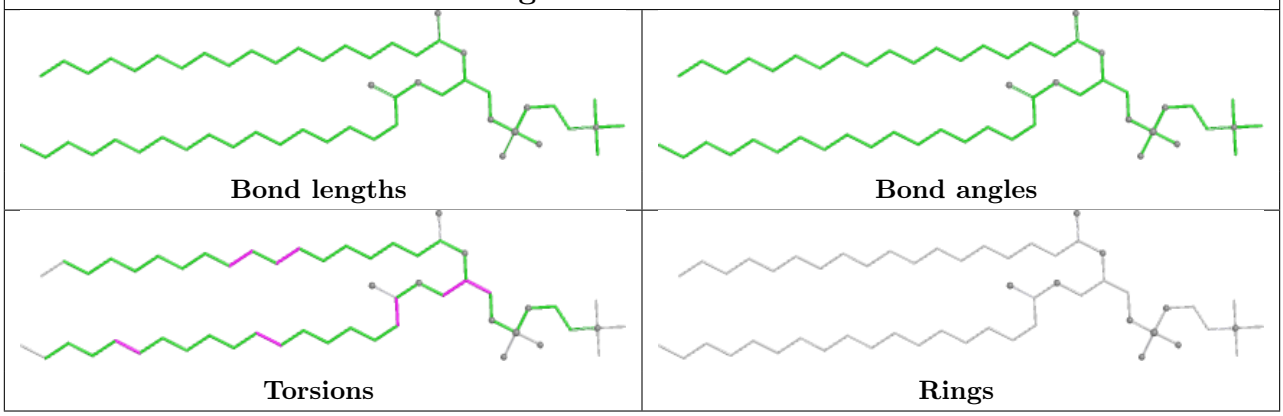


Rings

Ligand 3PE A2 401



Ligand PC1 A6 302



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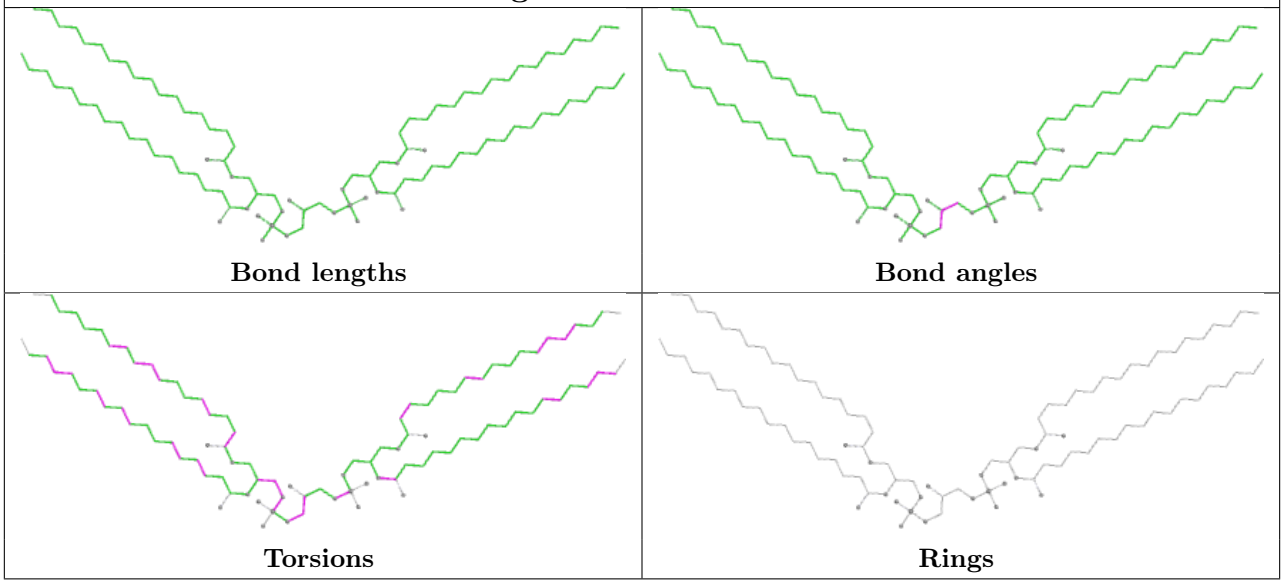
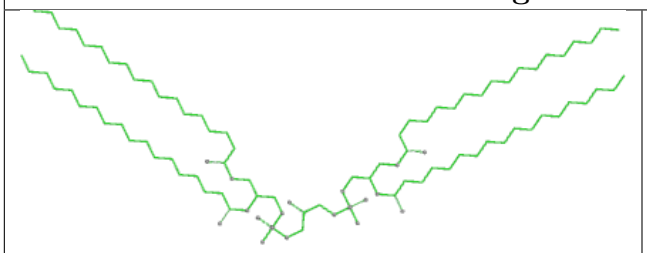
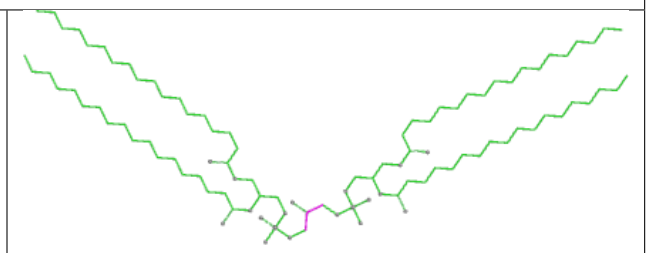


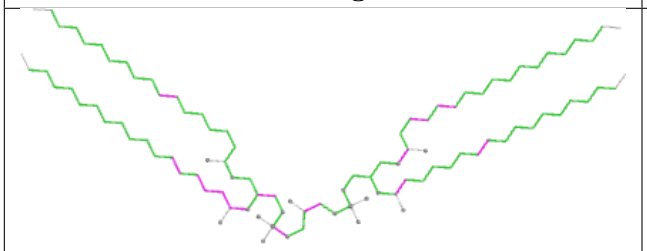
Ligand CDL BC 301



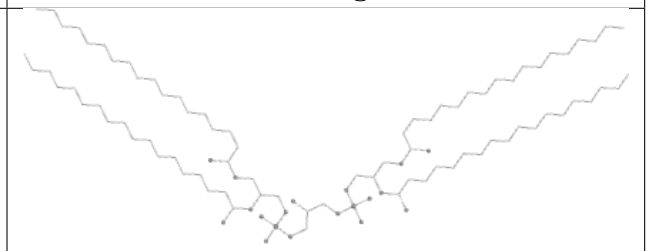
Bond lengths



Bond angles

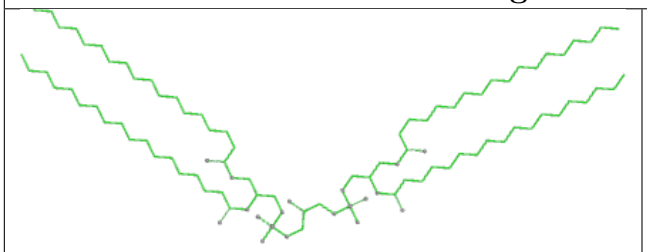


Torsions

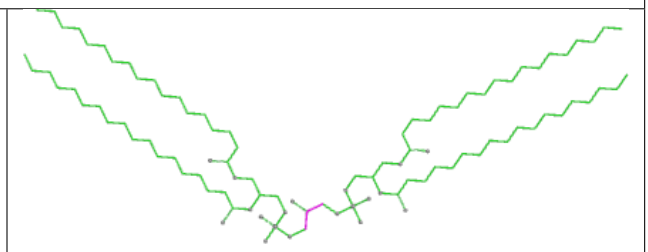


Rings

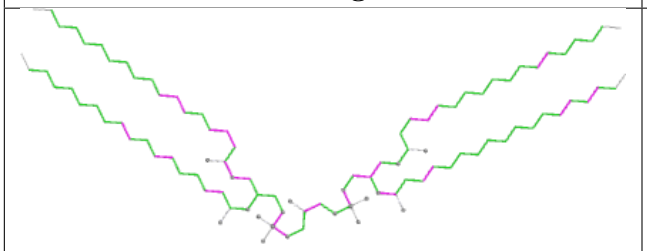
Ligand CDL DG 202



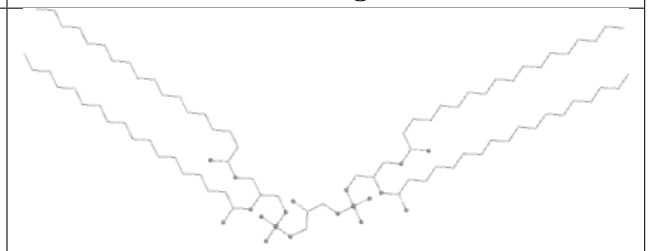
Bond lengths



Bond angles

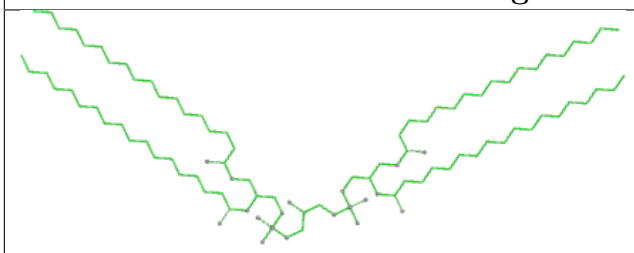


Torsions

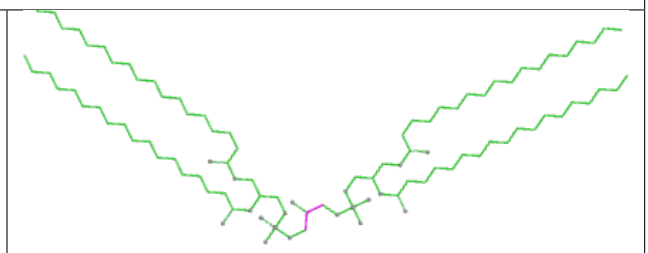


Rings

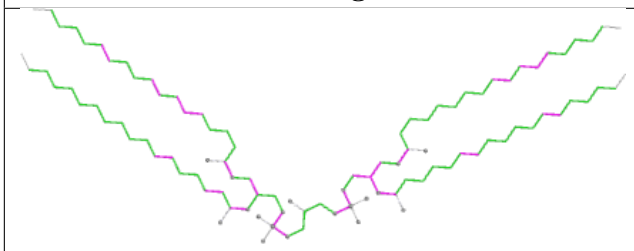
Ligand CDL DC 601



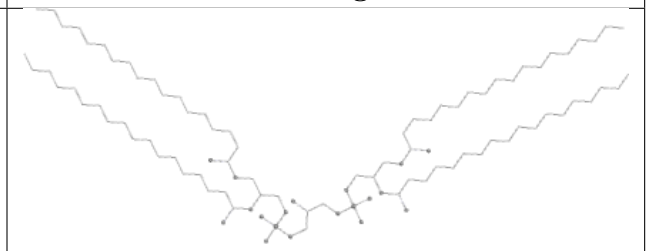
Bond lengths



Bond angles

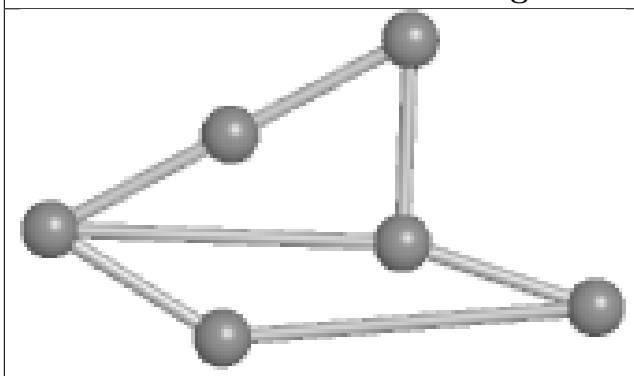


Torsions

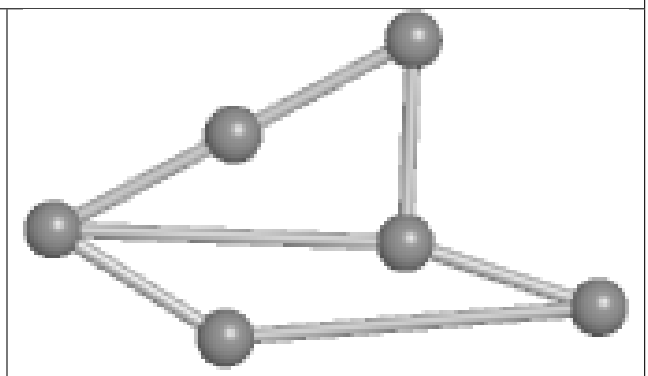


Rings

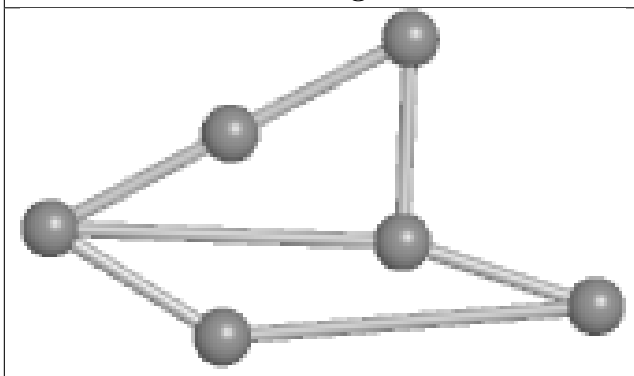
Ligand F3S CB 1002



Bond lengths



Bond angles



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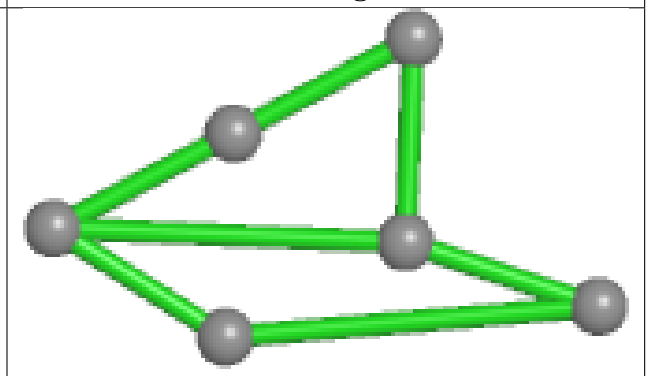
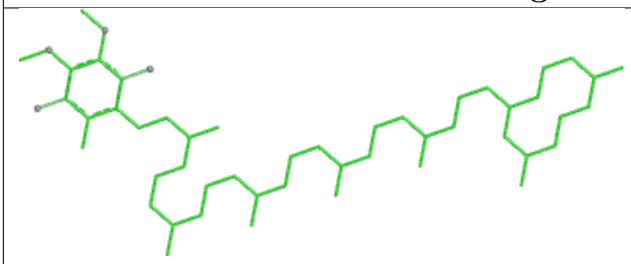


Rings

Ligand UQ8 c 510



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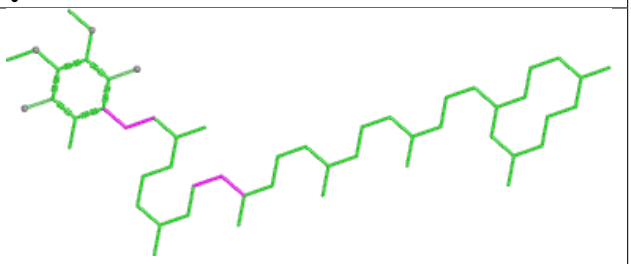
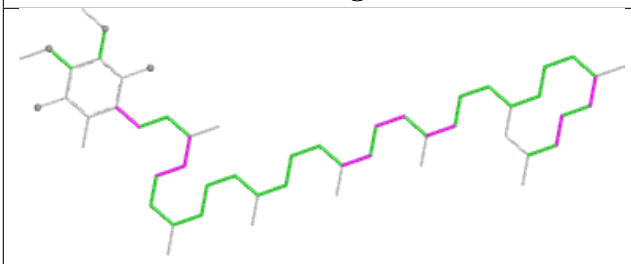


Bond angles



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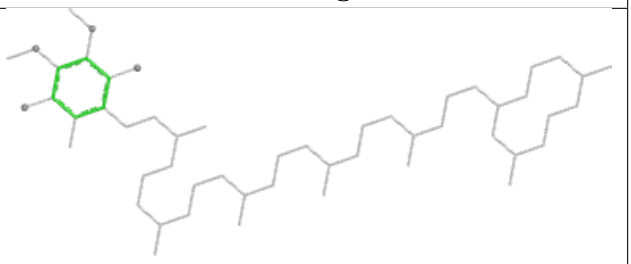
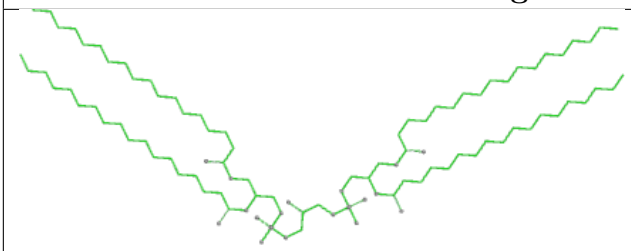


Rings

Ligand CDL BY 201



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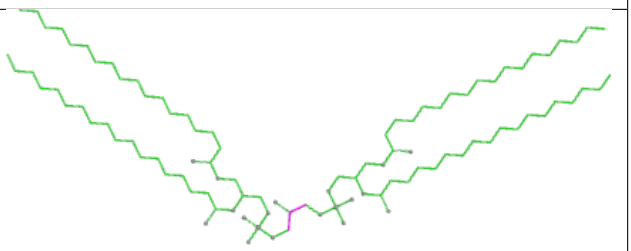
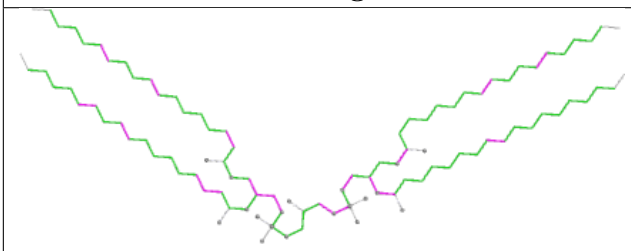


Bond angles



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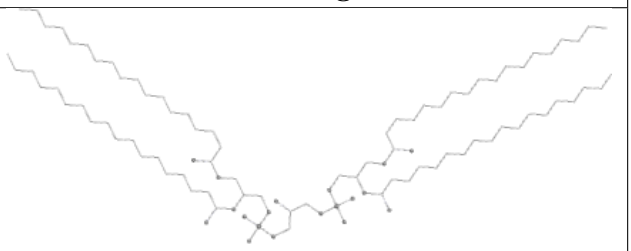
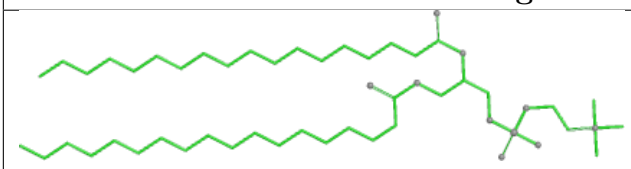
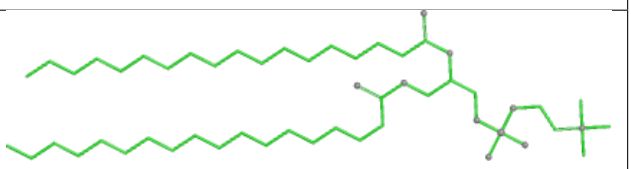


Rings

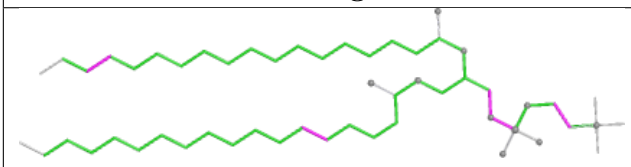
Ligand PC1 EB 303



Bond lengths



Bond angles



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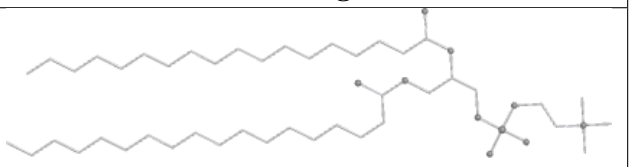
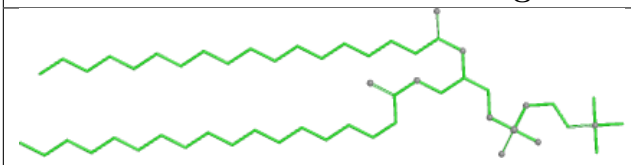


Rings

Ligand PC1 DC 602



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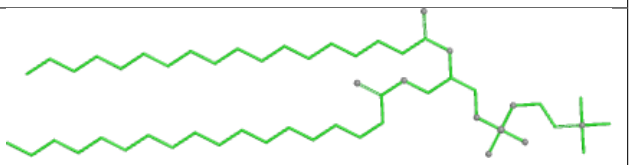
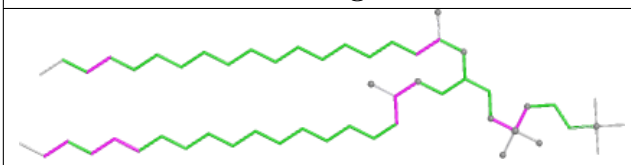


Bond angles



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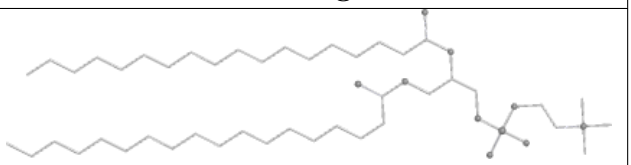
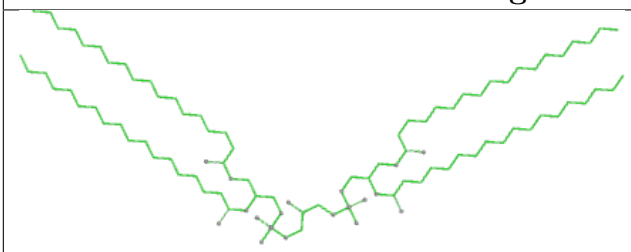


Rings

Ligand CDL DU 402



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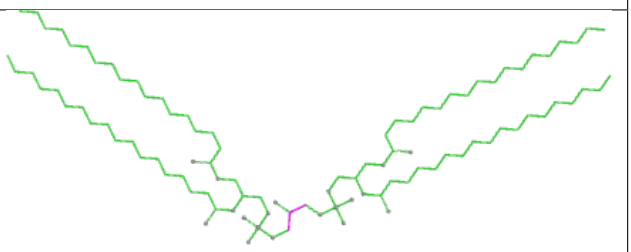
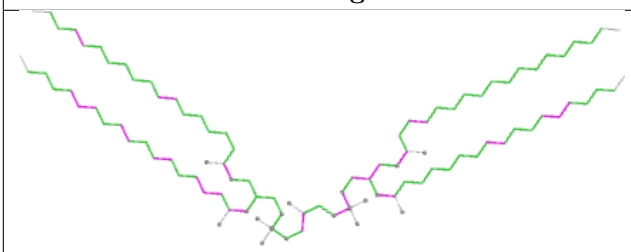
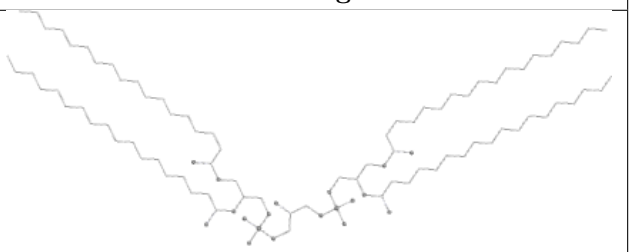


Bond angles

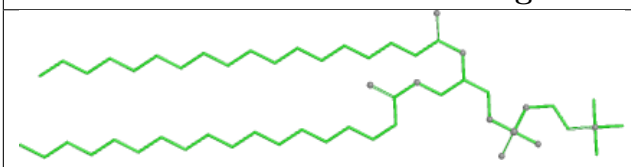


Torsions



Rings

Ligand PC1 EO 205



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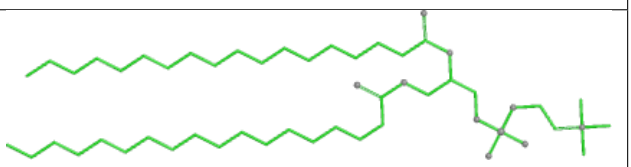
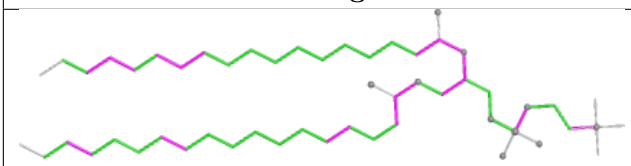


Bond angles



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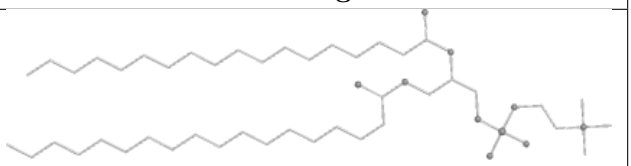
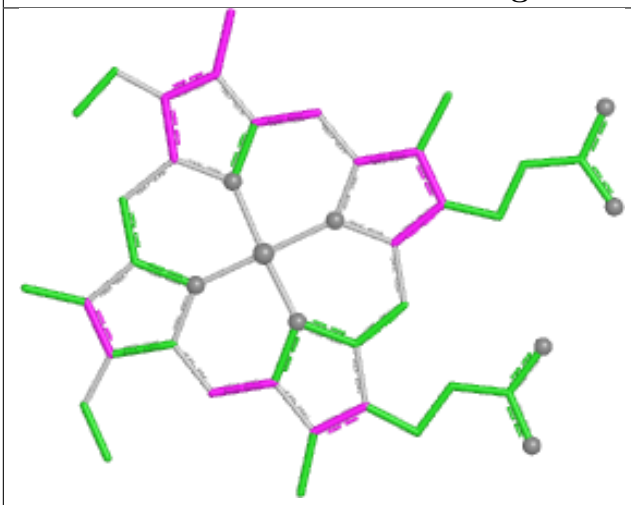
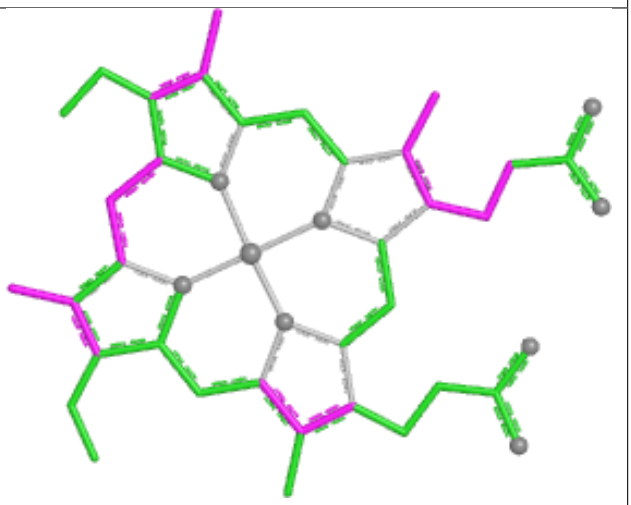
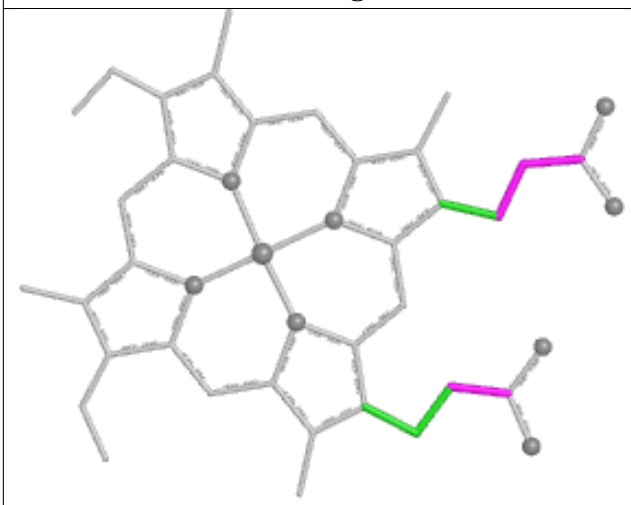
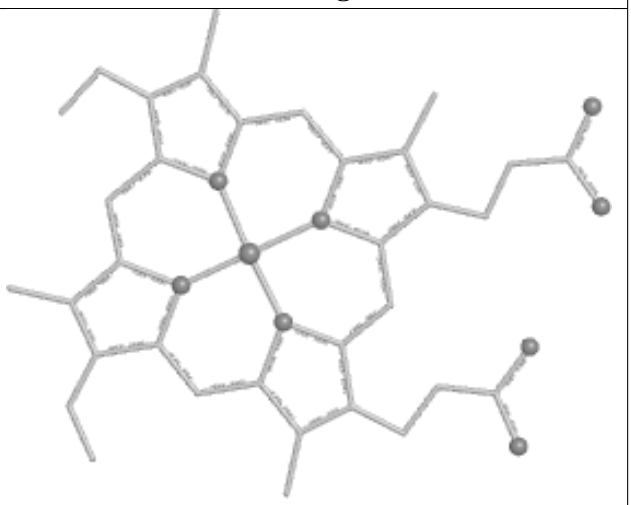
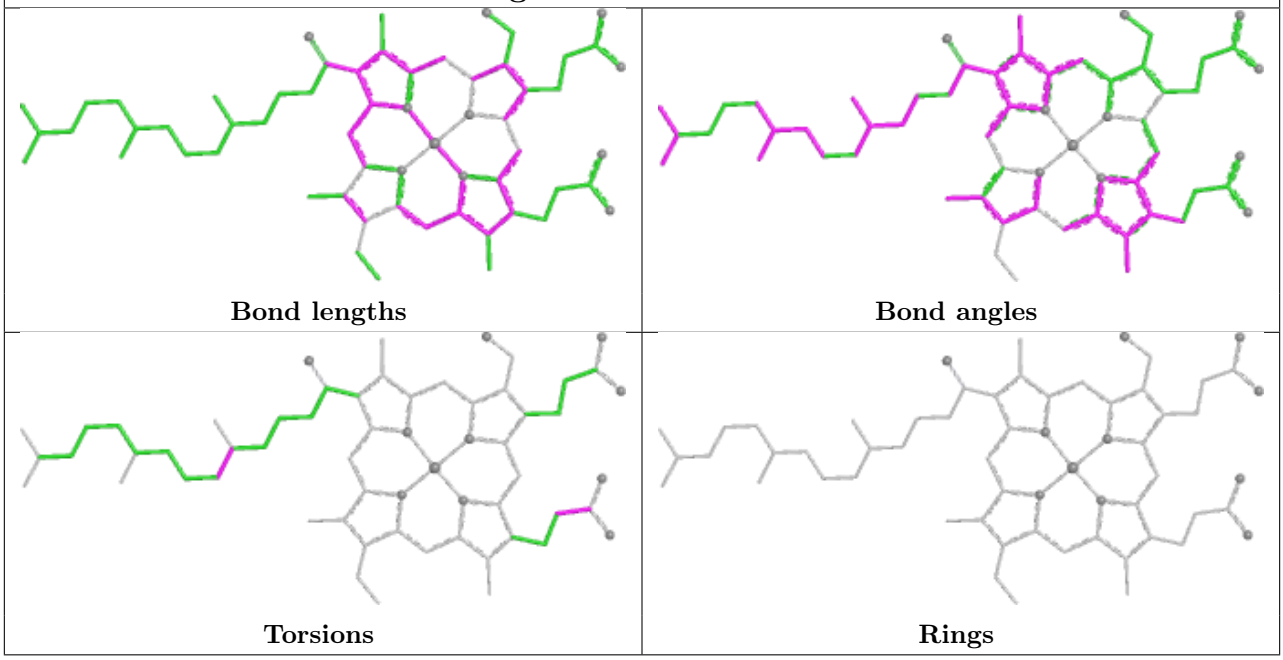


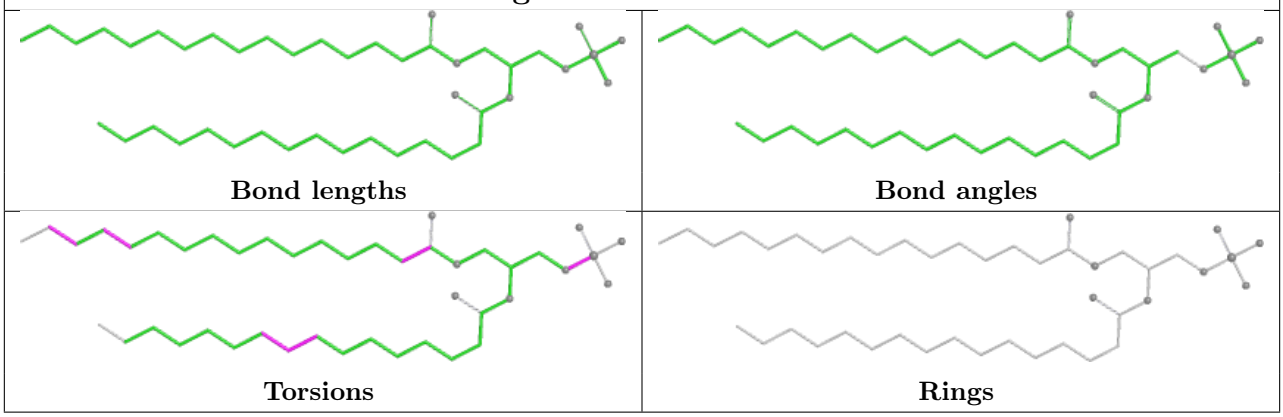
Rings

Ligand HEC CE 401	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand HEA DA 702



Ligand LPP Dl 1101



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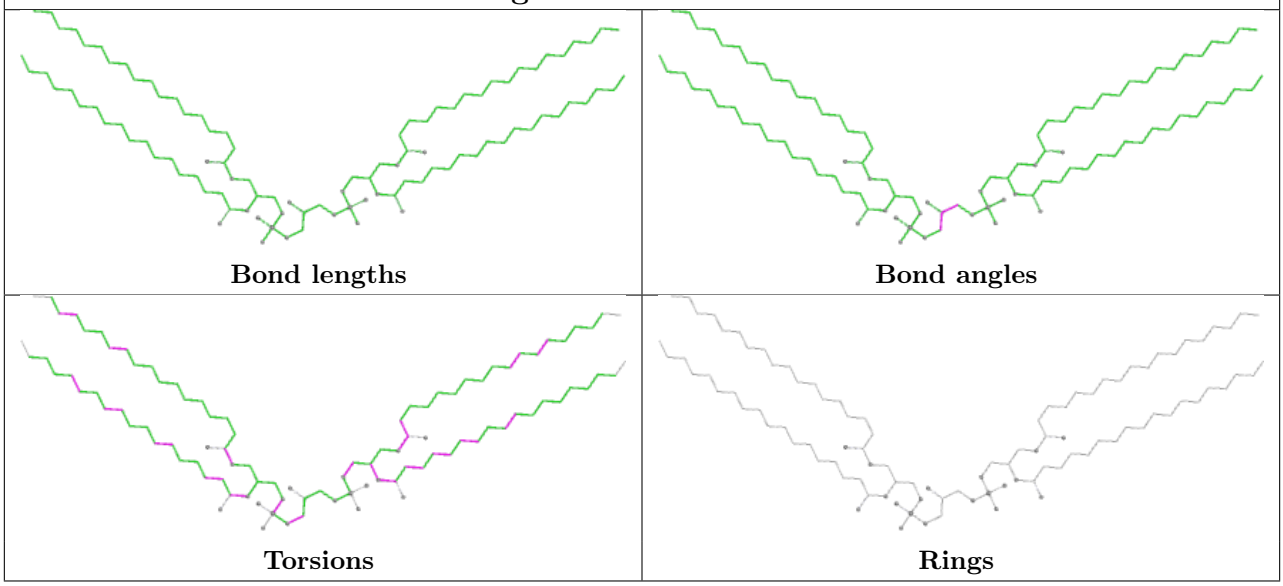
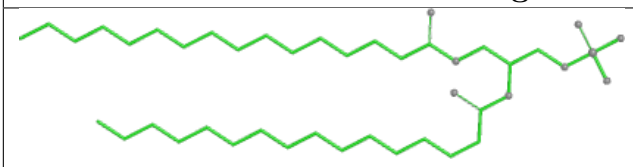
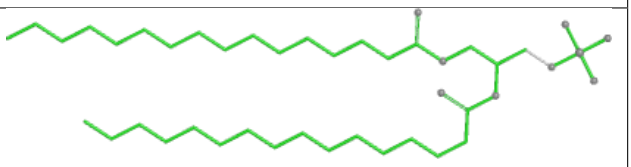


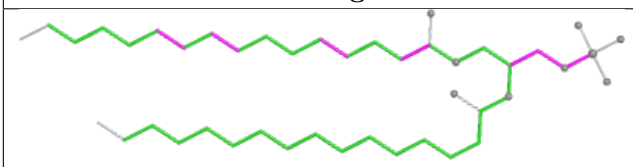
Ligand LPP DN 504



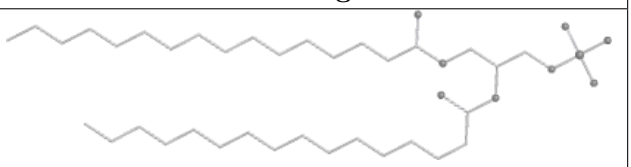
Bond lengths



Bond angles

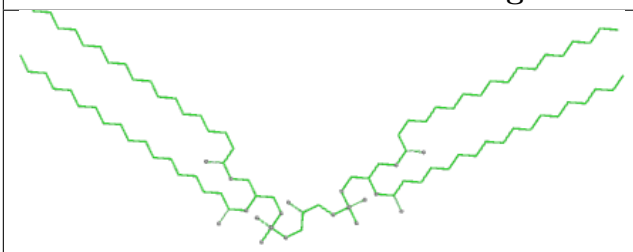


Torsions

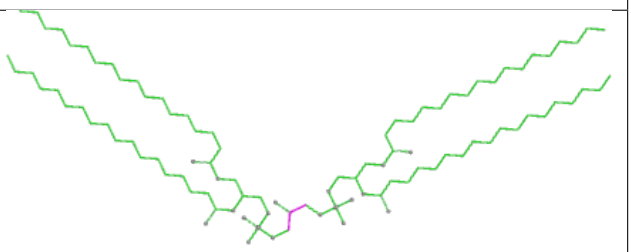


Rings

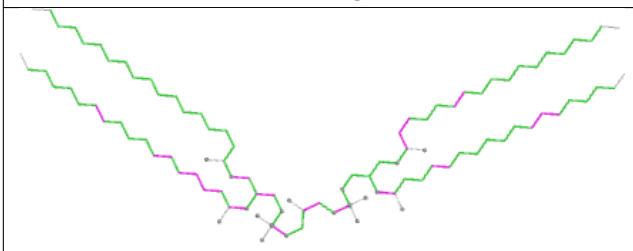
Ligand CDL DM 502



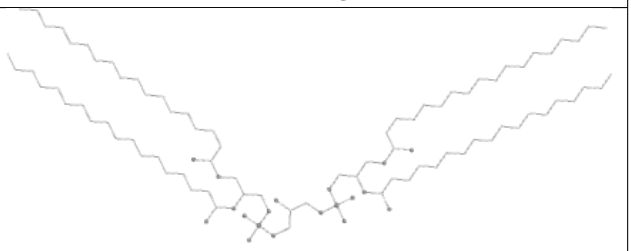
Bond lengths



Bond angles

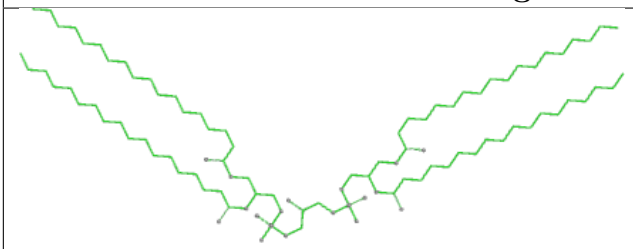


Torsions

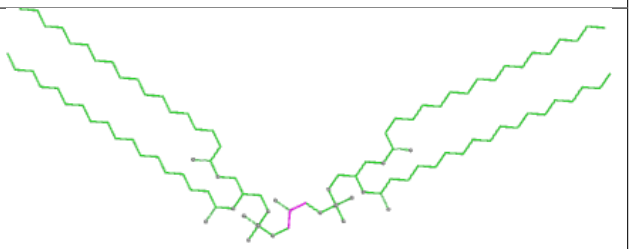


Rings

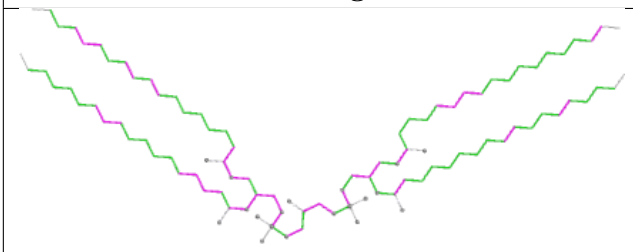
Ligand CDL Dn 502



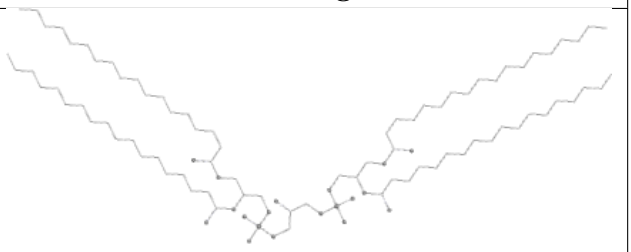
Bond lengths



Bond angles

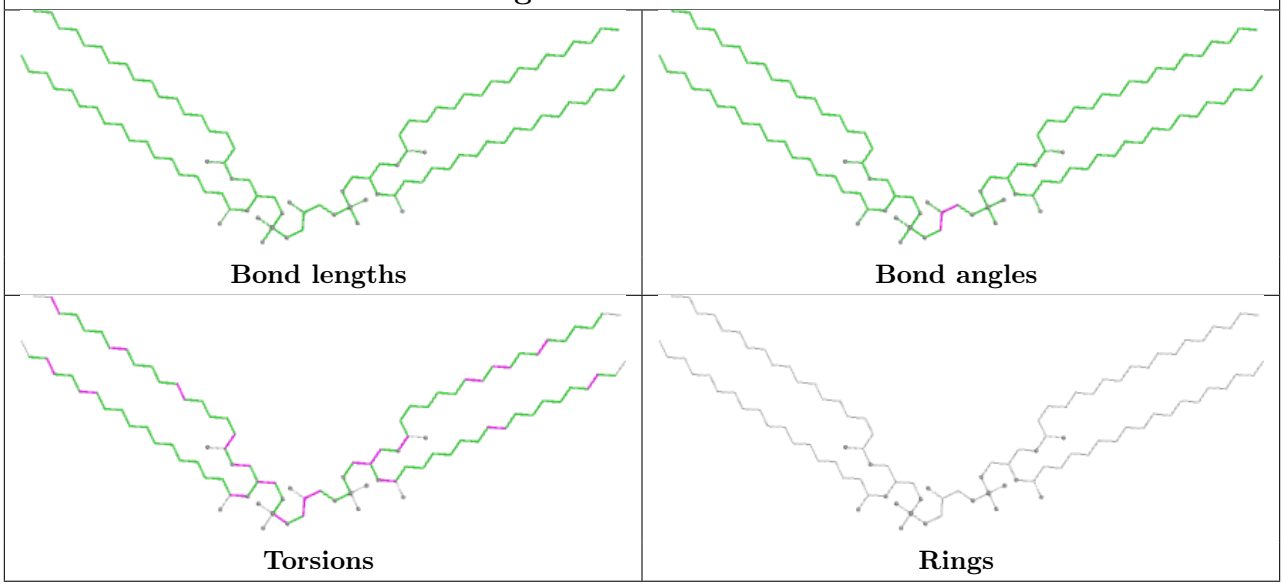


Torsions

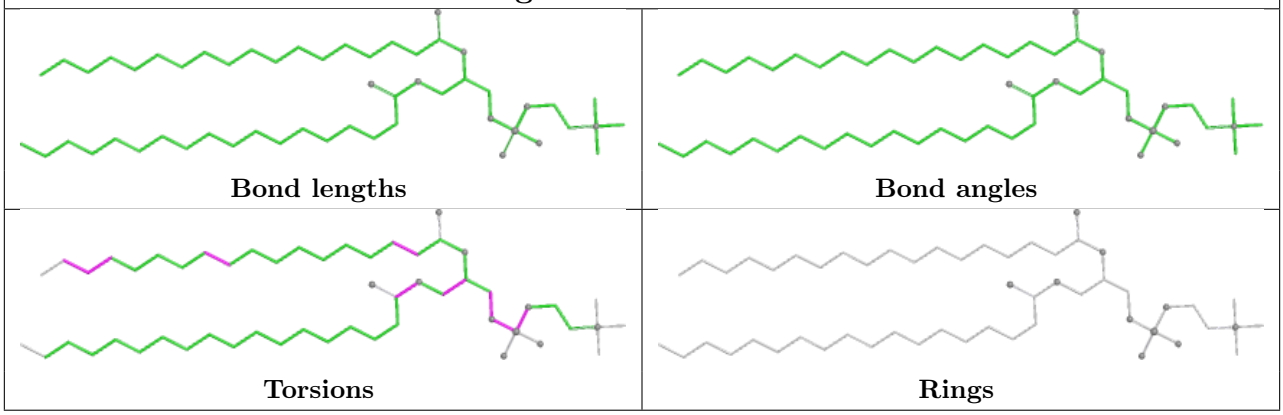


Rings

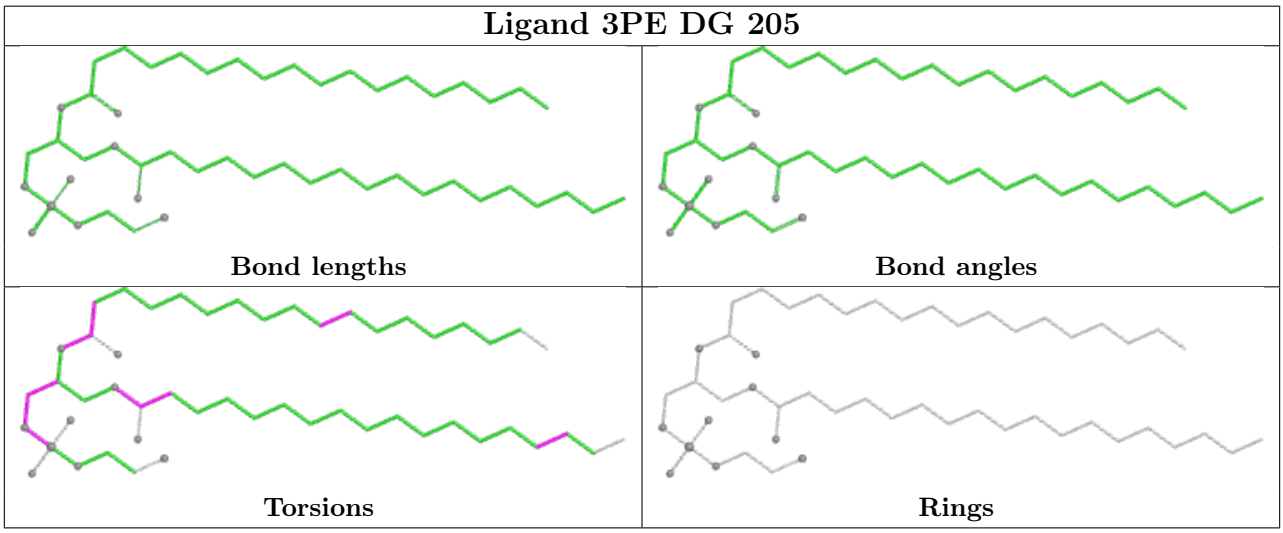
Ligand CDL Dd 706

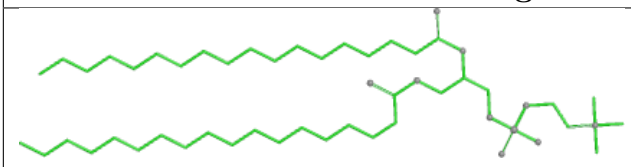
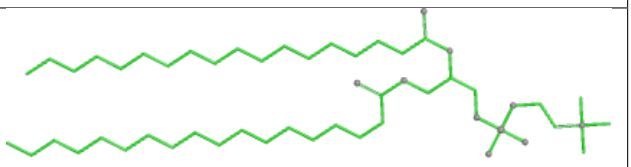
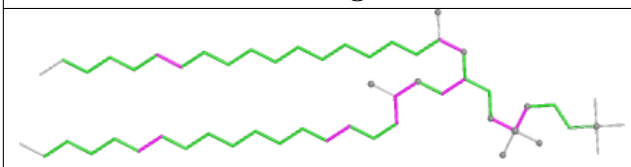
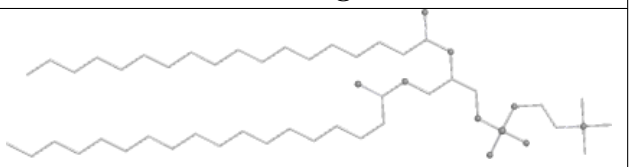


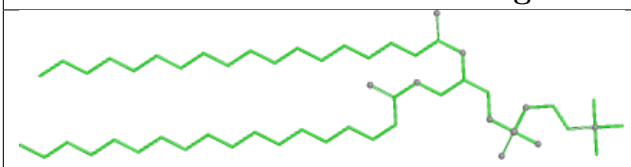
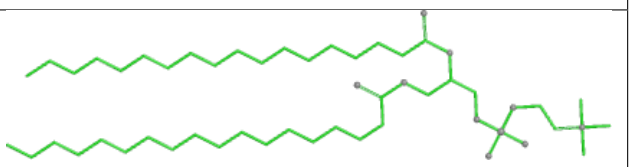
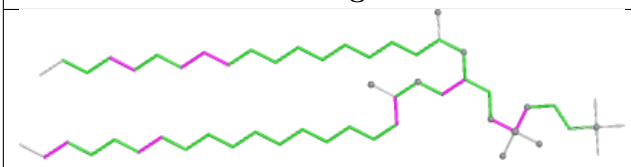
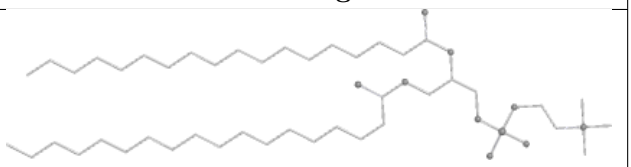
Ligand PC1 AC 804

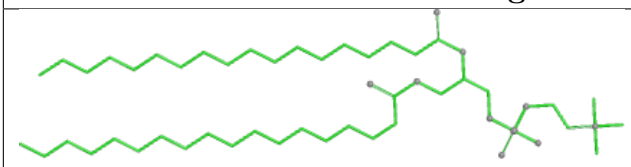
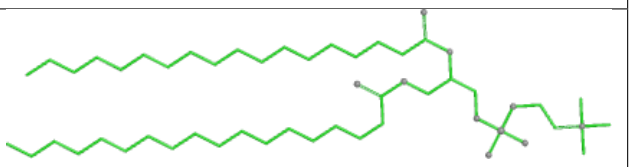
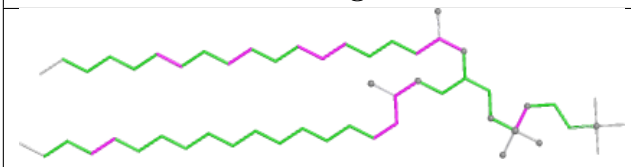
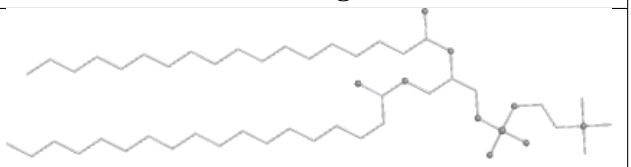


Ligand 3PE DG 205

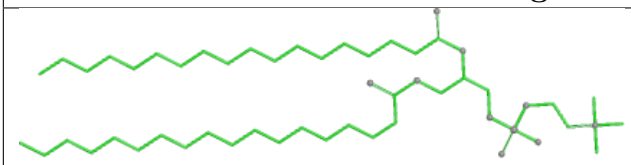


Ligand PC1 BT 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

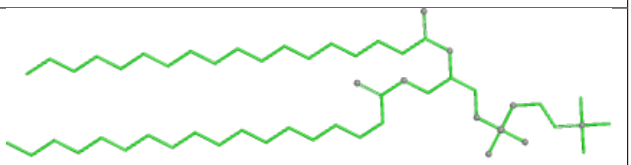
Ligand PC1 DV 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 Dx 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings

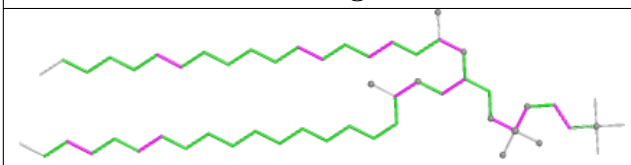
Ligand PC1 d 801



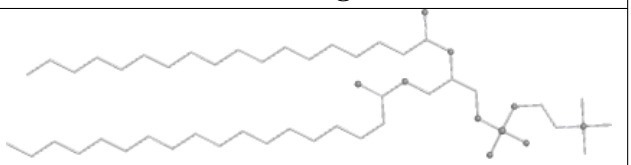
Bond lengths



Bond angles

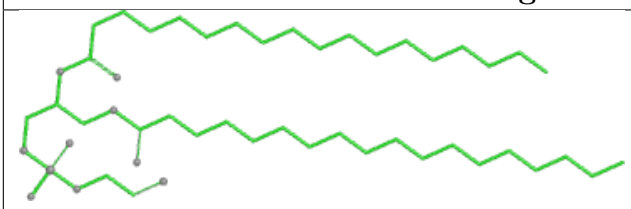


Torsions

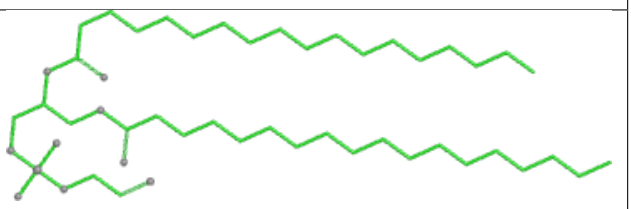


Rings

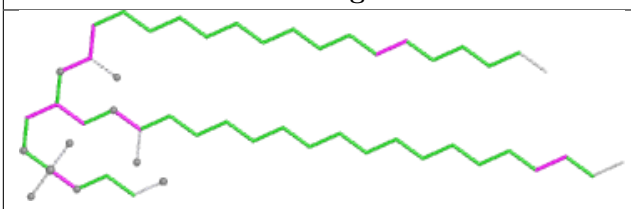
Ligand 3PE AJ 502



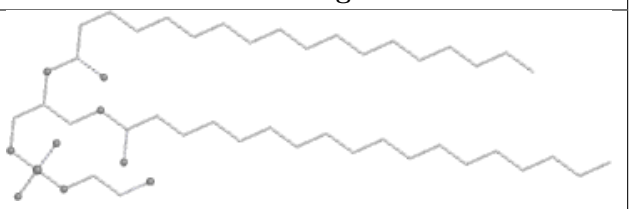
Bond lengths



Bond angles

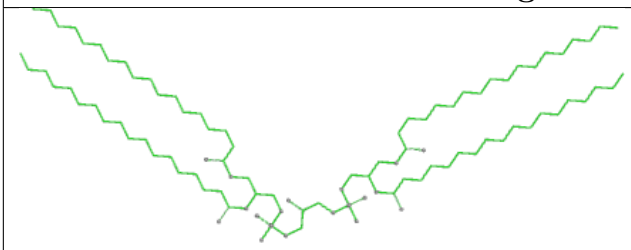


Torsions

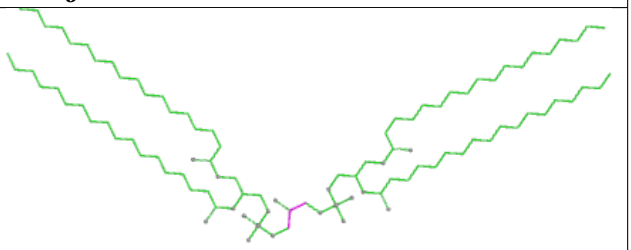


Rings

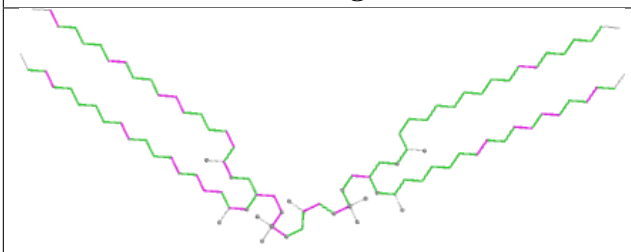
Ligand CDL Dj 403



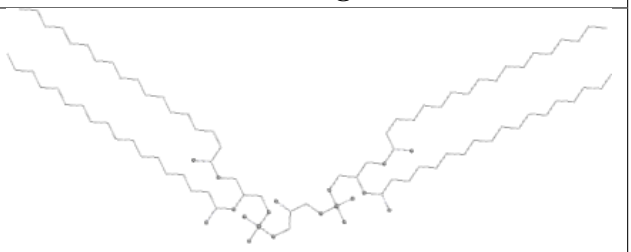
Bond lengths



Bond angles

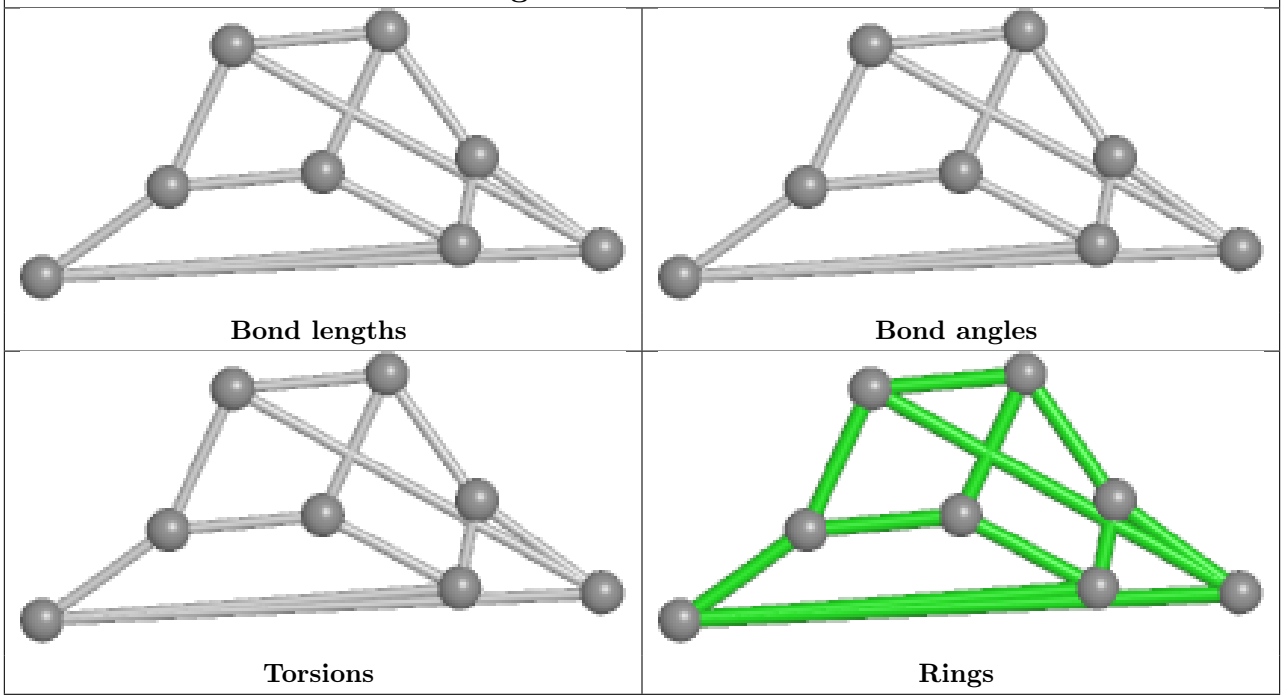


Torsions

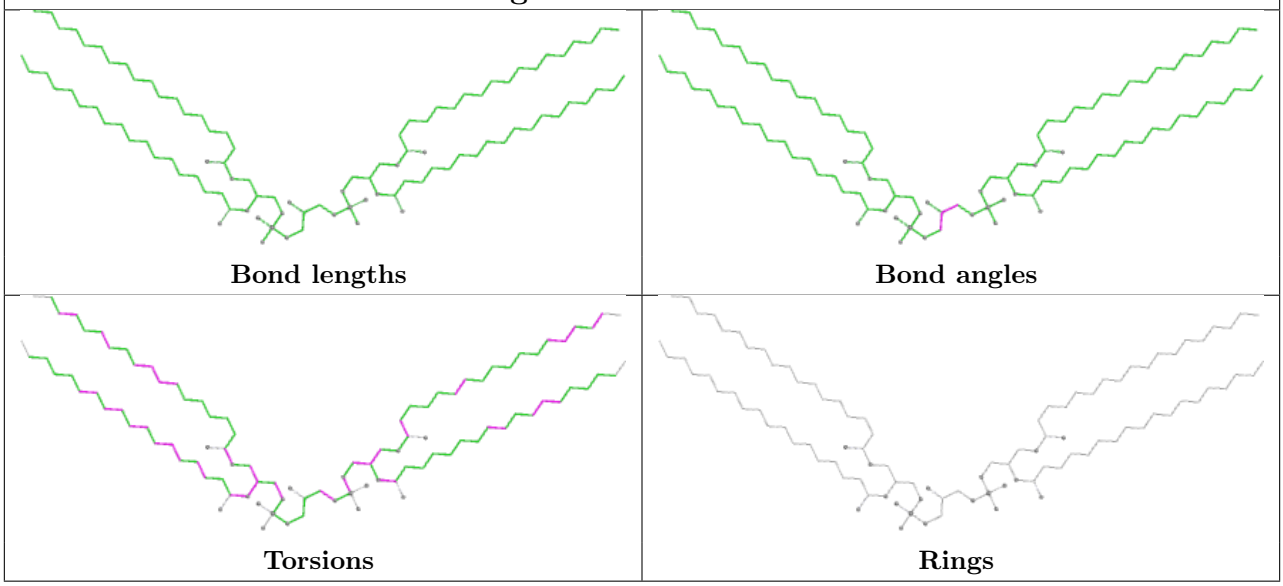


Rings

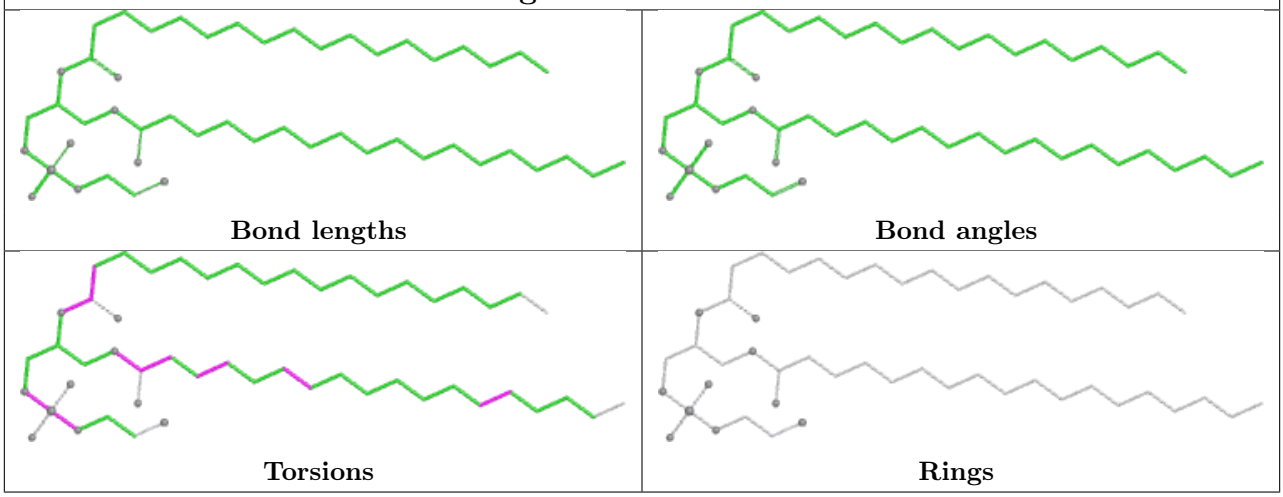
Ligand SF4 CB 1001



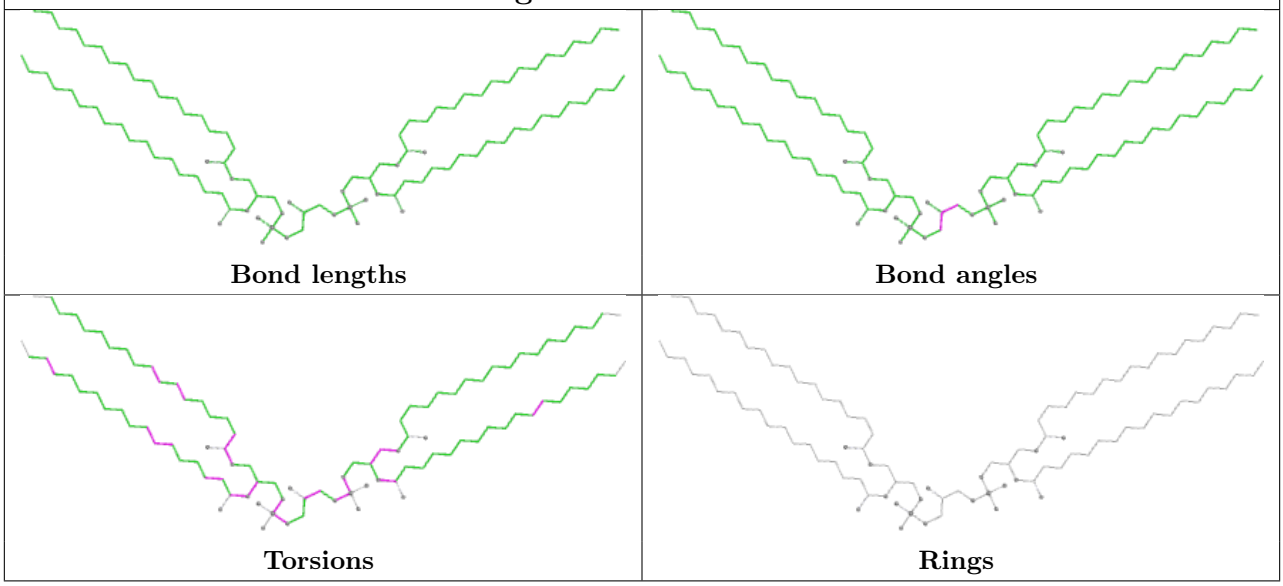
Ligand CDL DN 506



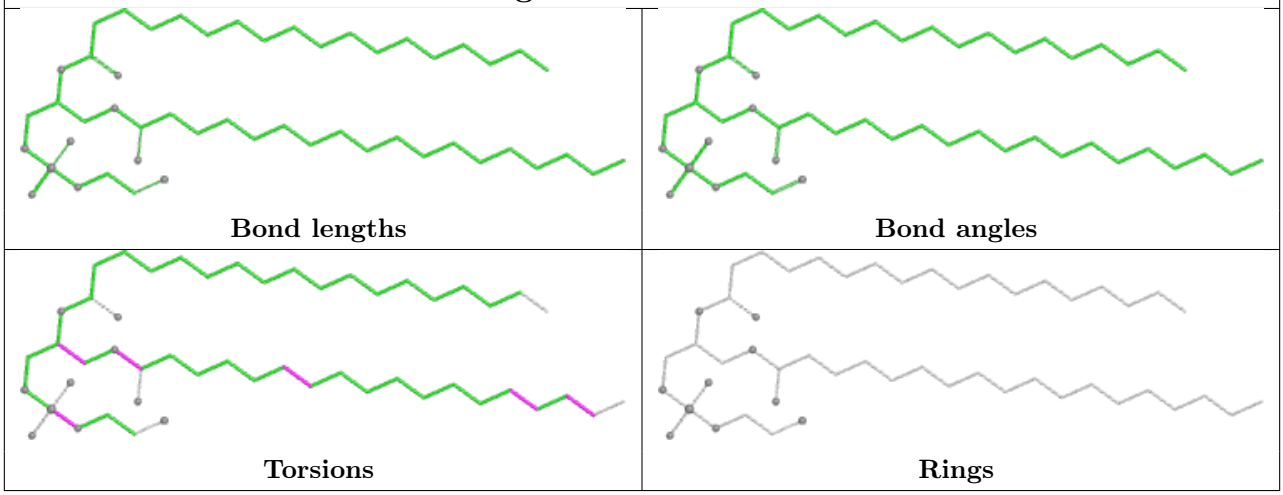
Ligand 3PE DJ 301



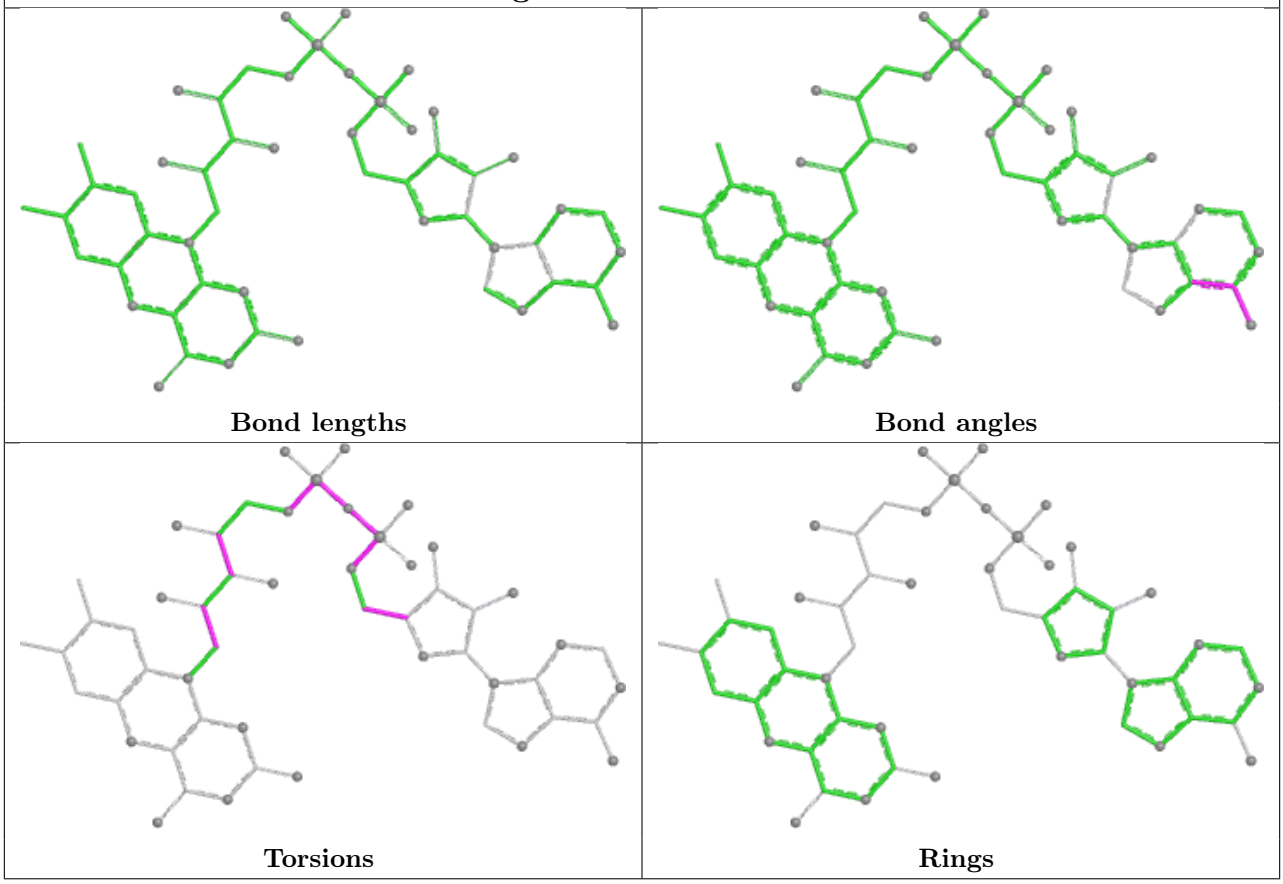
Ligand CDL H 1302



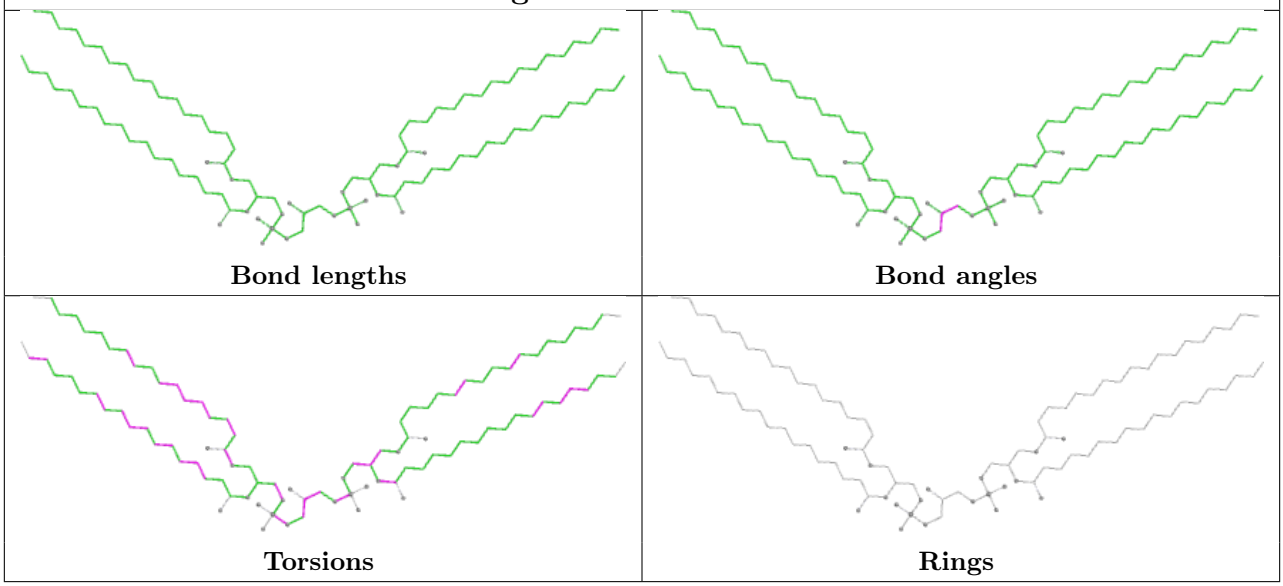
Ligand 3PE DR 401



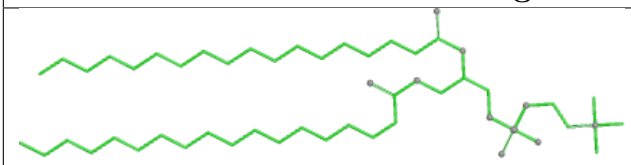
Ligand FAD CA 702



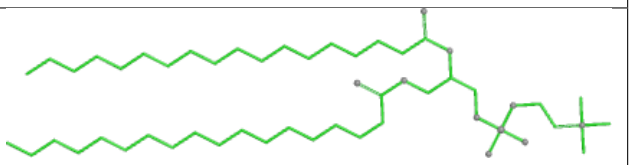
Ligand CDL DX 301



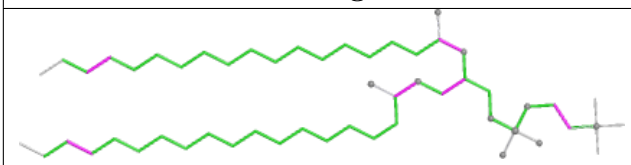
Ligand PC1 DY 302



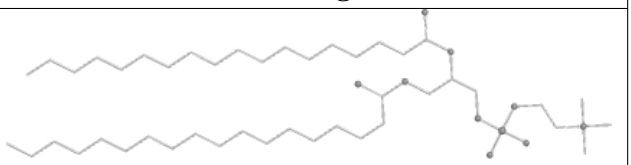
Bond lengths



Bond angles

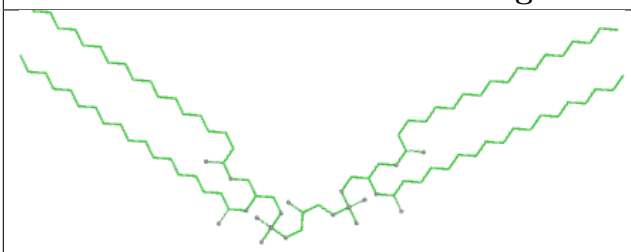


Torsions

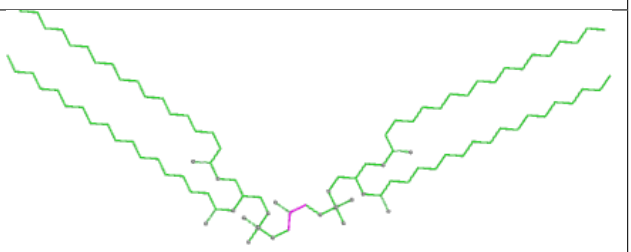


Rings

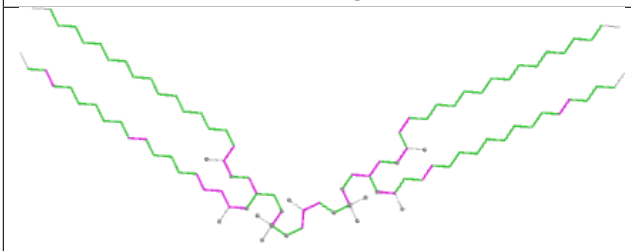
Ligand CDL Ed 205



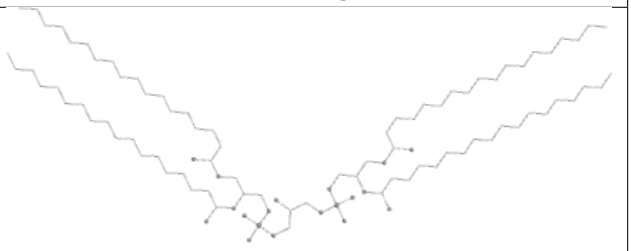
Bond lengths



Bond angles

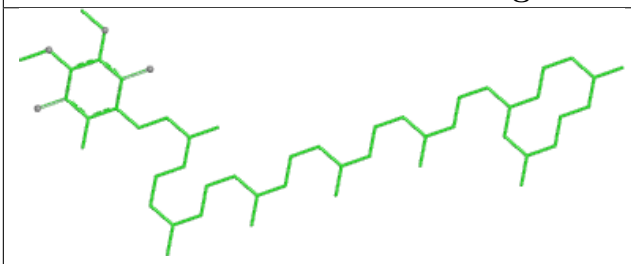


Torsions

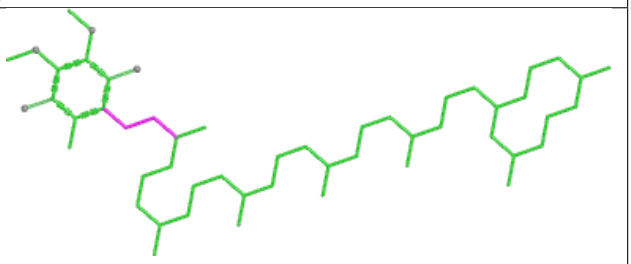


Rings

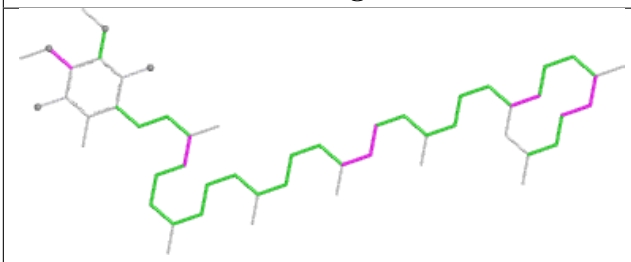
Ligand UQ8 ED 603



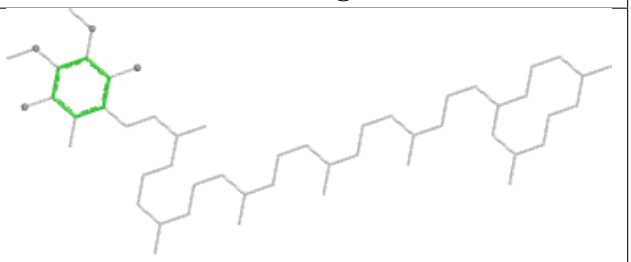
Bond lengths



Bond angles

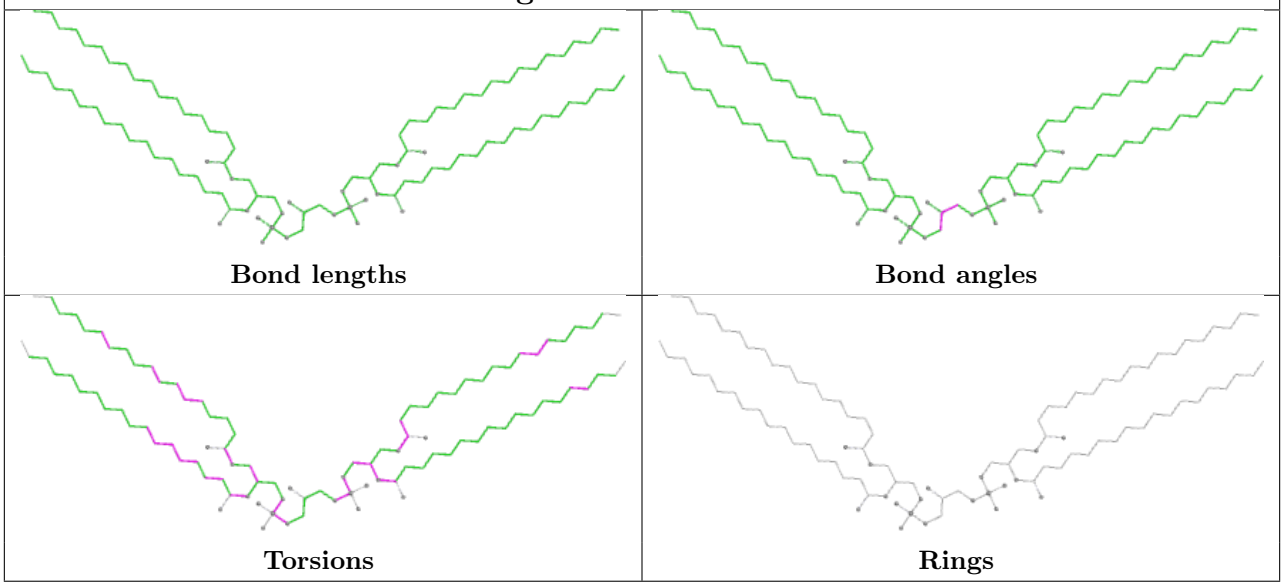


Torsions

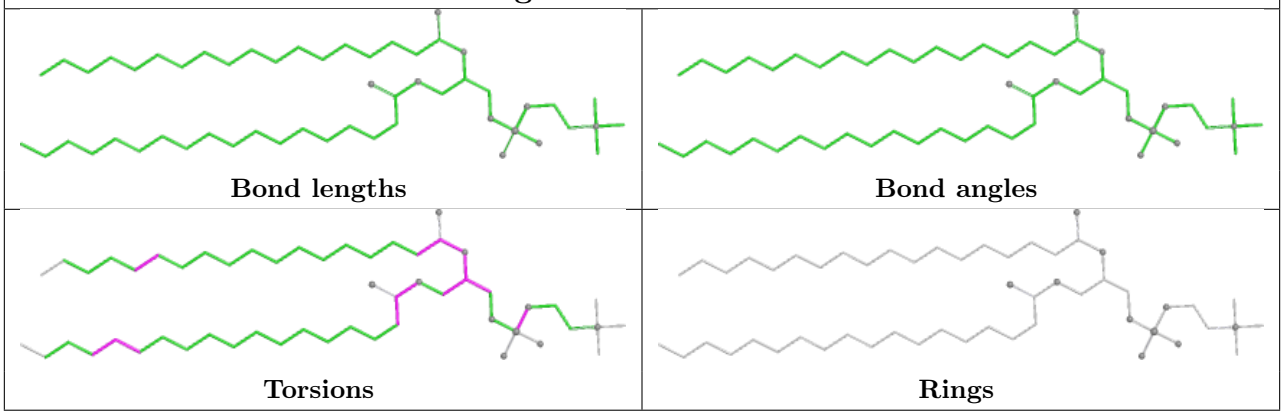


Rings

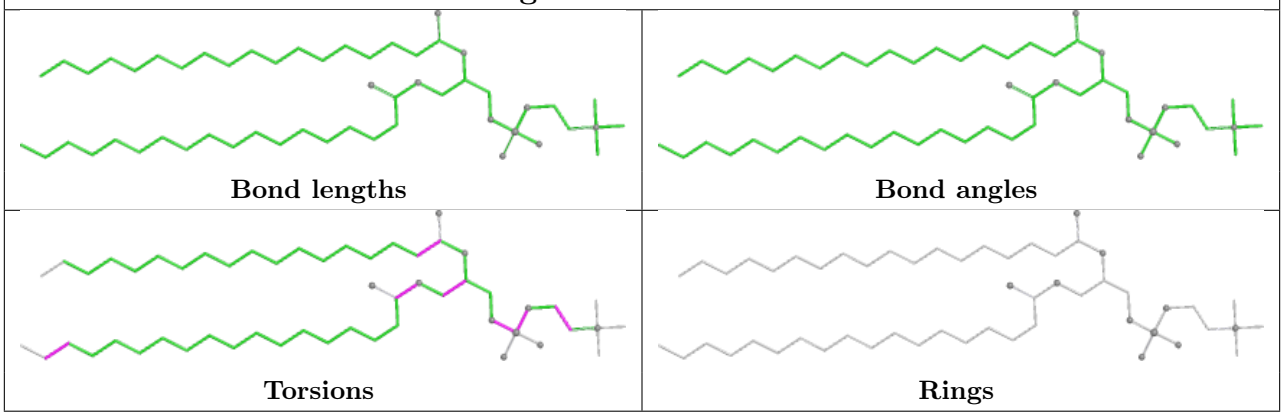
Ligand CDL Dc 601



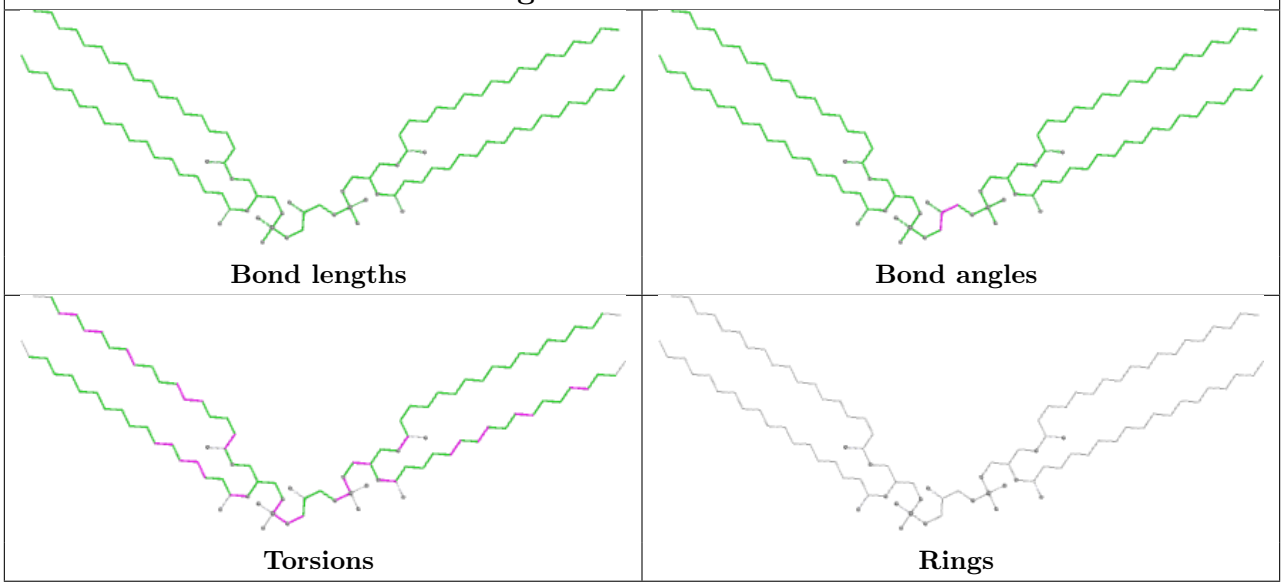
Ligand PC1 DC 608



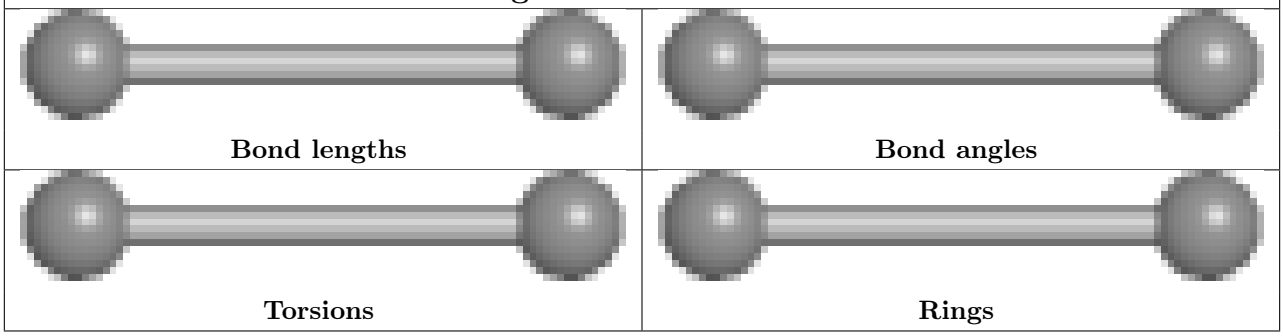
Ligand PC1 Dc 604



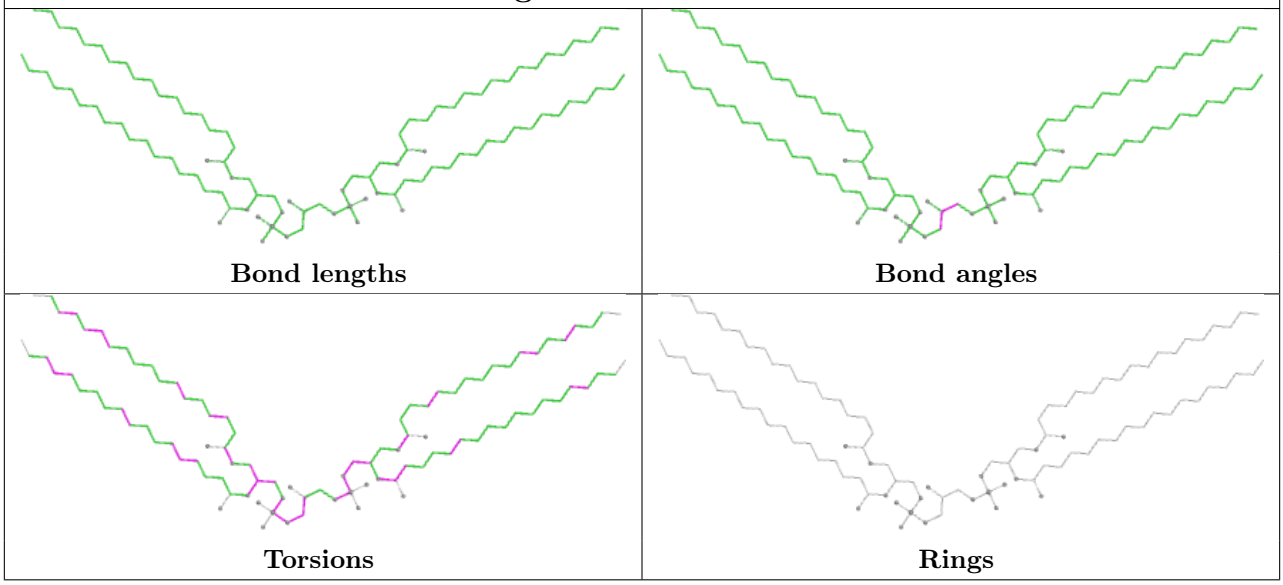
Ligand CDL Ds 406



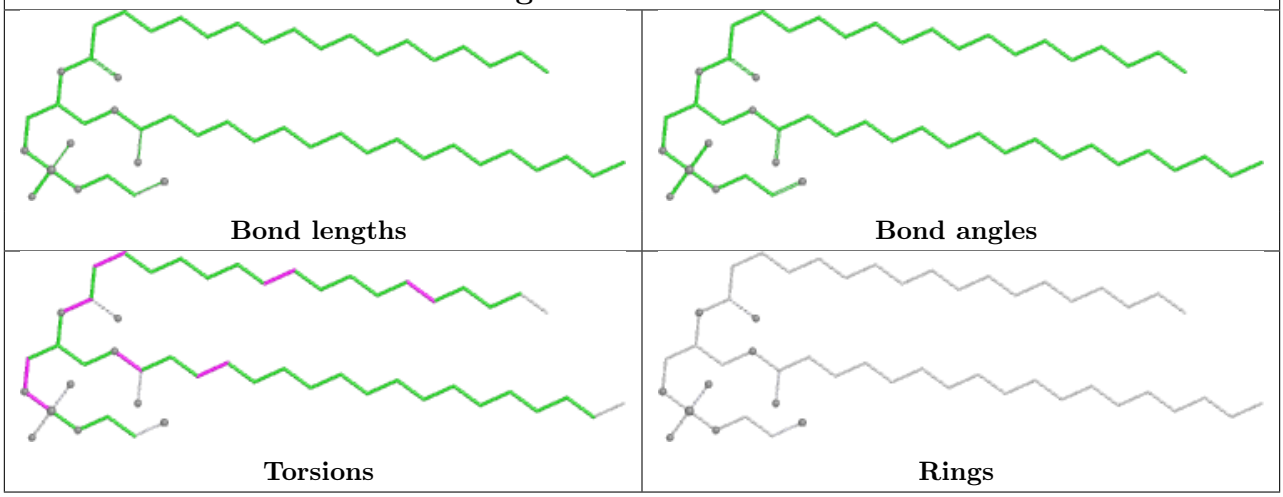
Ligand CUA Db 701



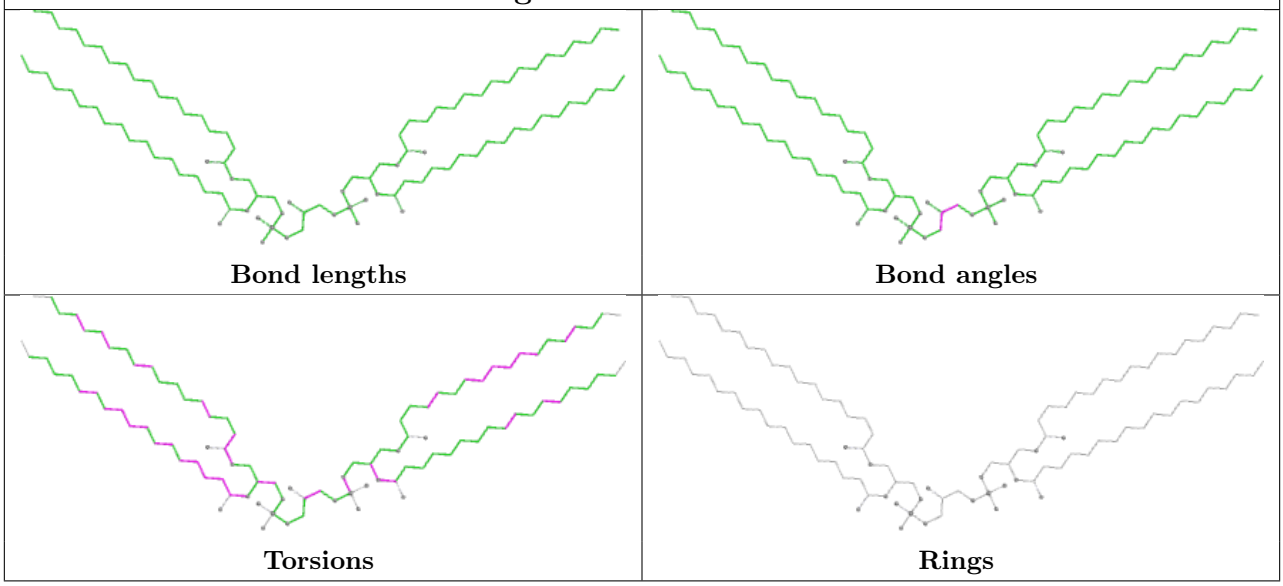
Ligand CDL Dv 403



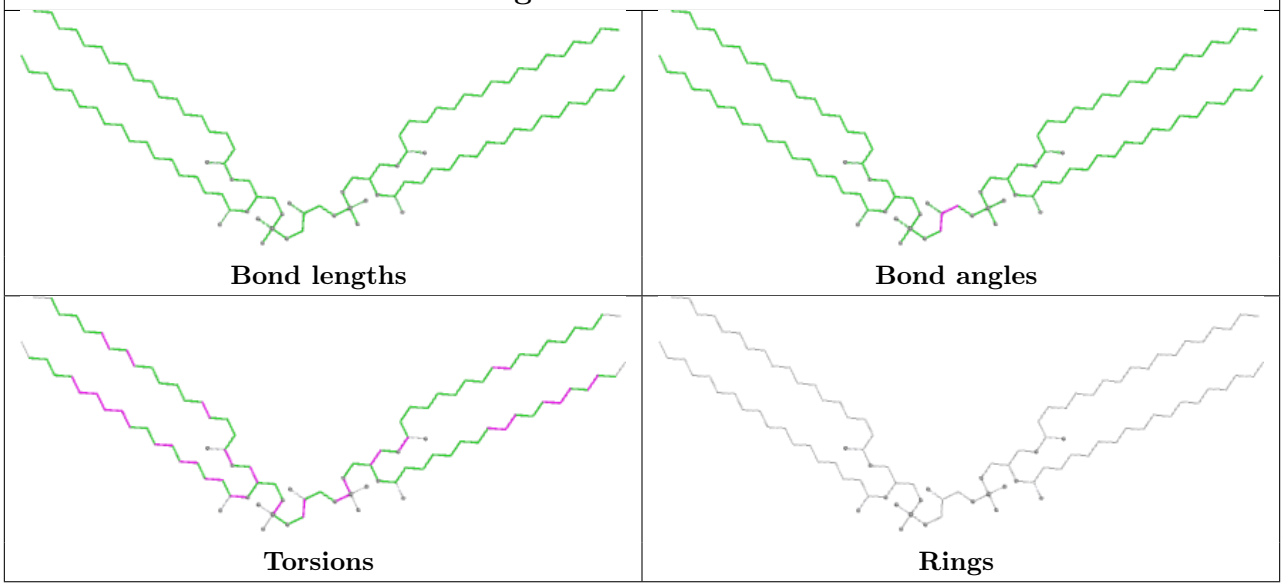
Ligand 3PE CD 303



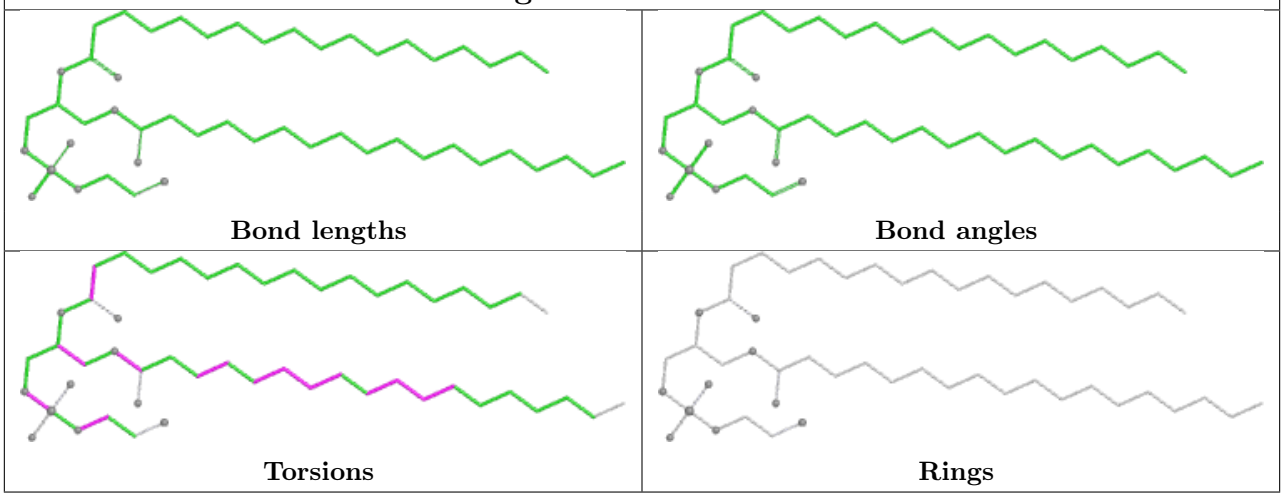
Ligand CDL DS 404



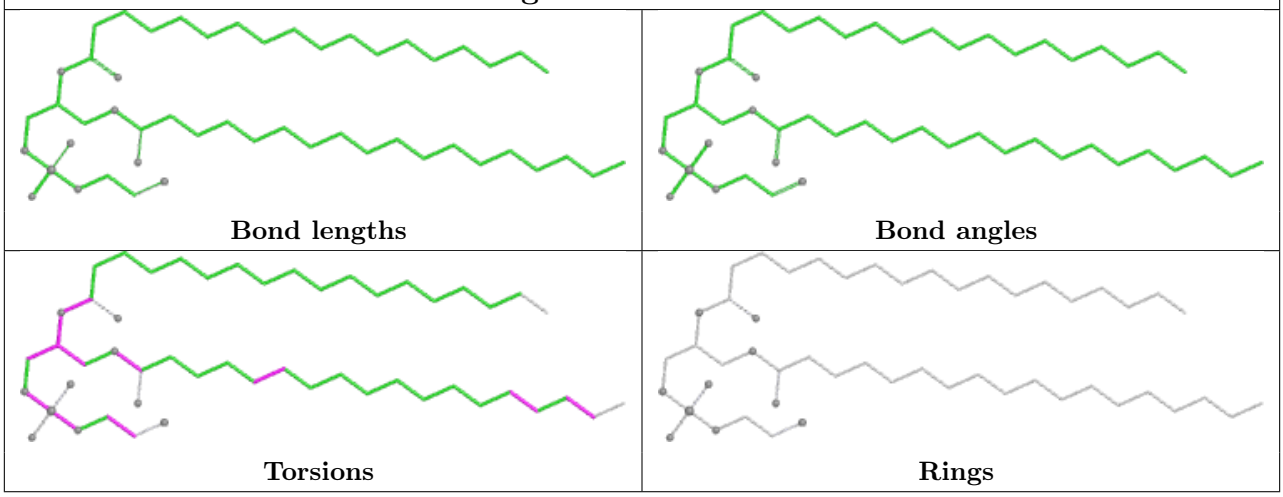
Ligand CDL Dh 201



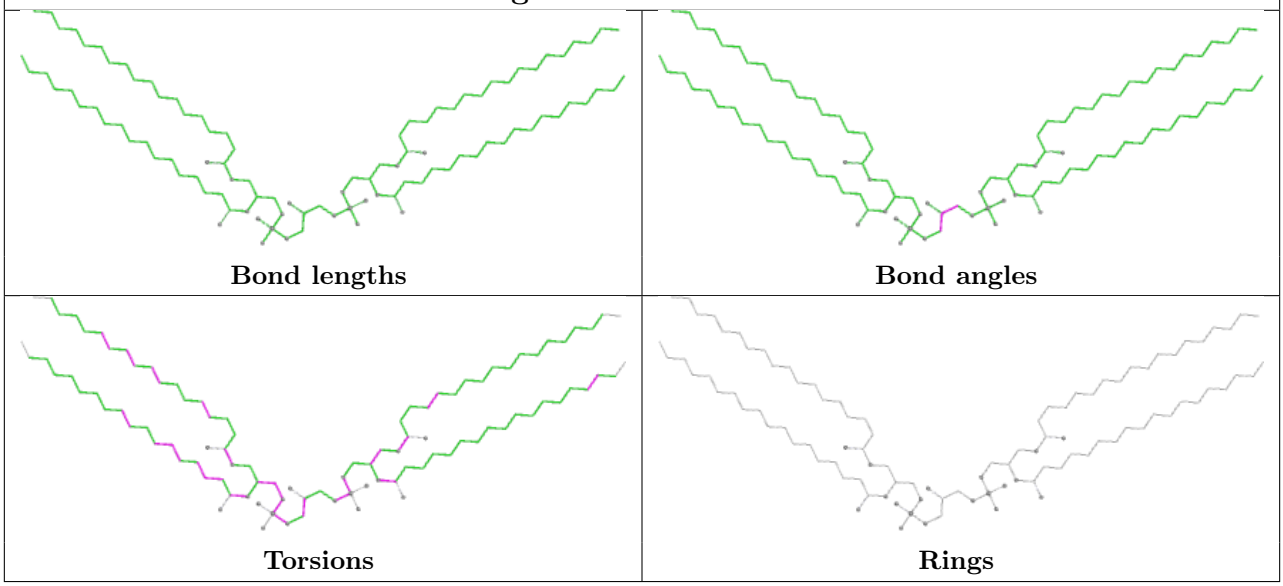
Ligand 3PE Di 1102



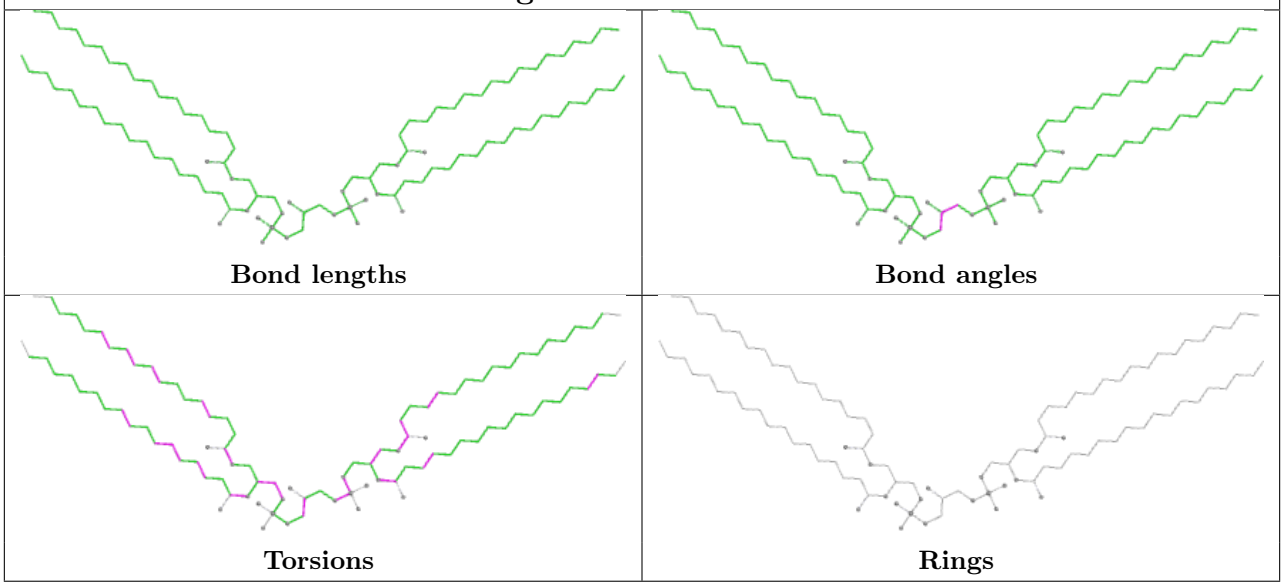
Ligand 3PE Dr 401



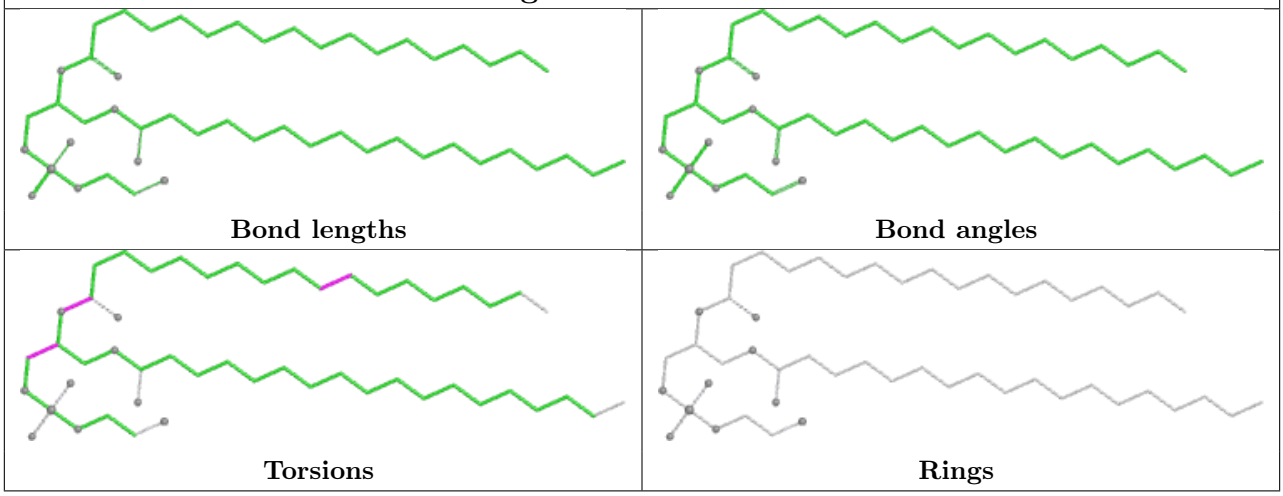
Ligand CDL DX 306



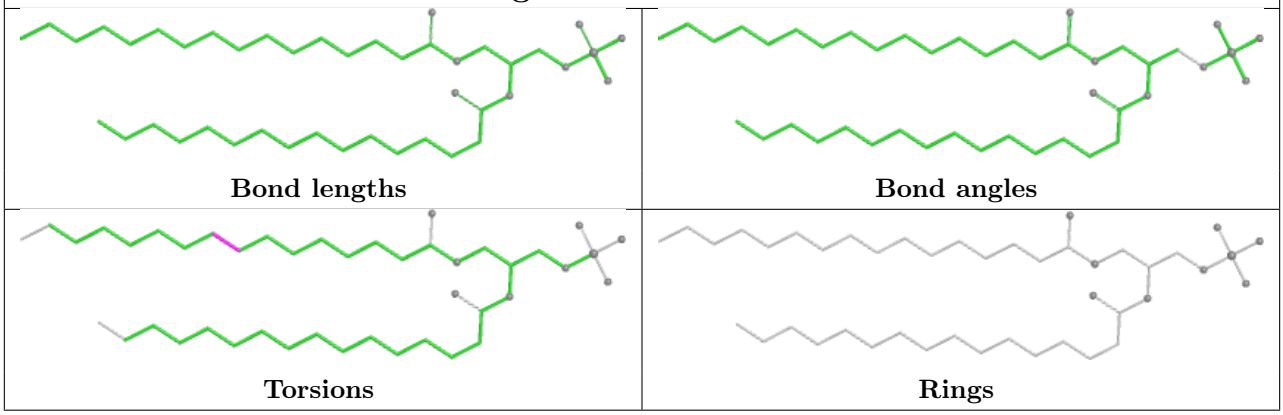
Ligand CDL Eu 101



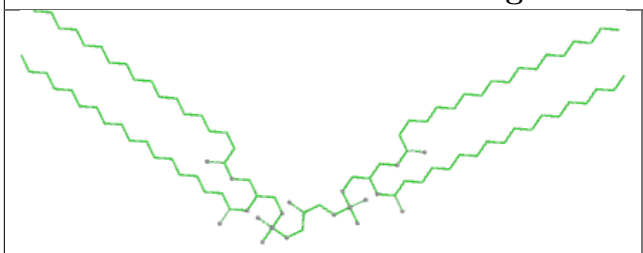
Ligand 3PE Dc 606



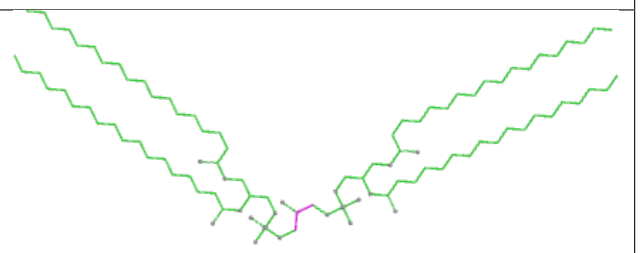
Ligand LPP DN 505



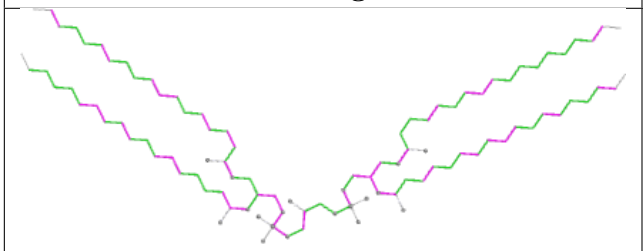
Ligand CDL Dx 1204



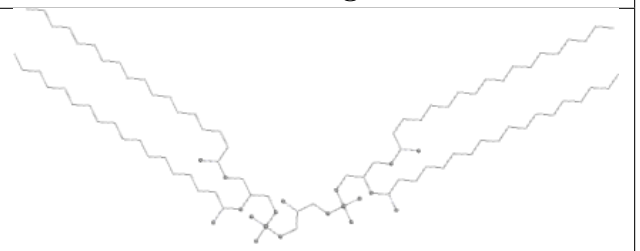
Bond lengths



Bond angles

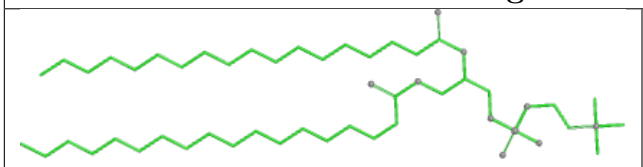


Torsions

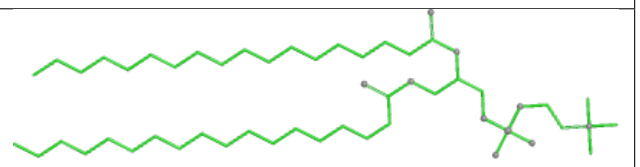


Rings

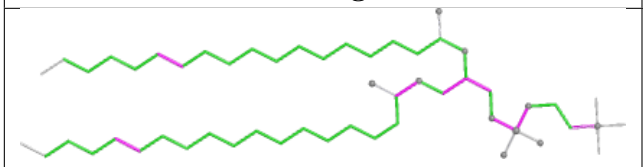
Ligand PC1 EN 1203



Bond lengths



Bond angles



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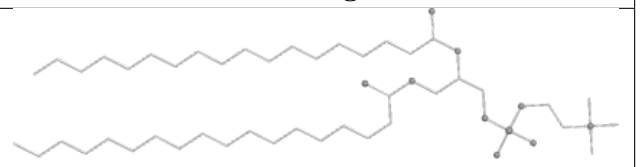
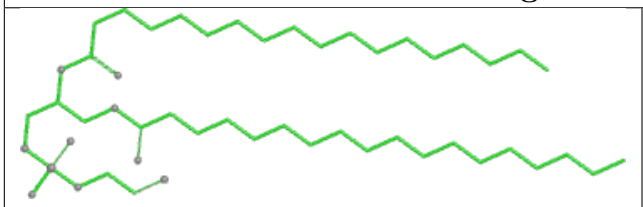
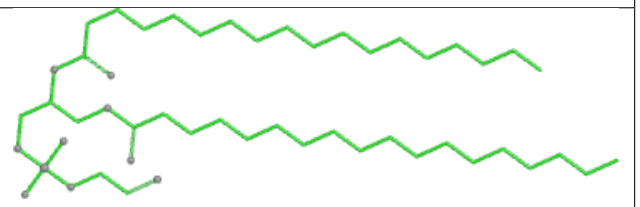


Rings

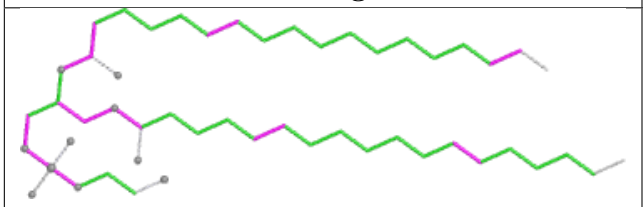
Ligand 3PE Dc 607



Bond lengths



Bond angles



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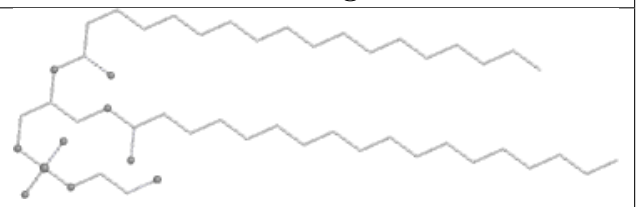
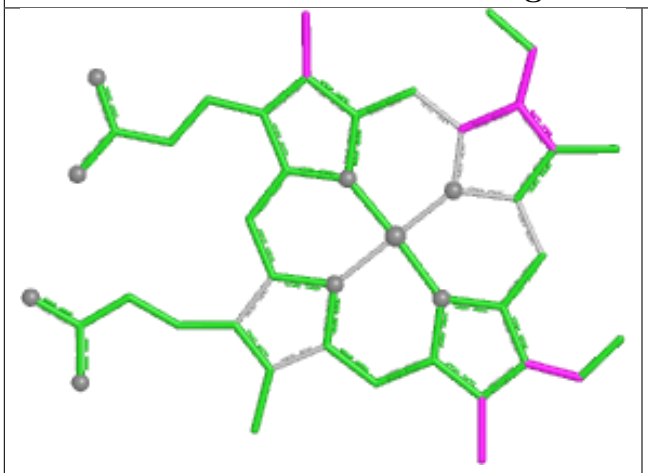
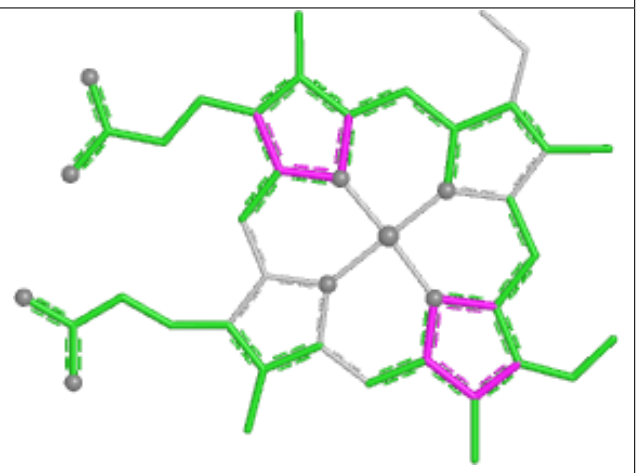


Rings

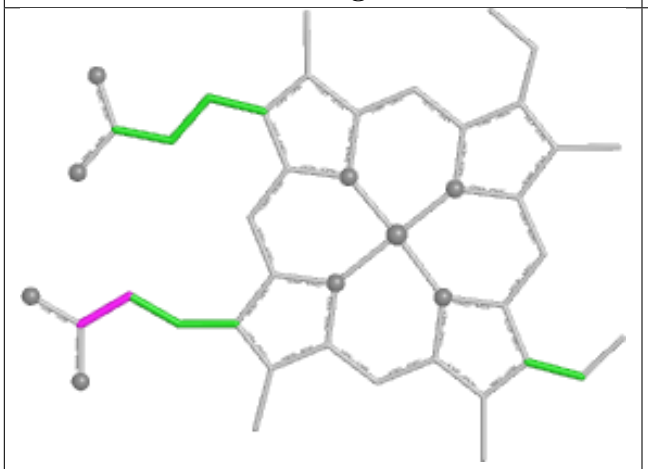
Ligand HEM c 505



Bond lengths



Bond angles



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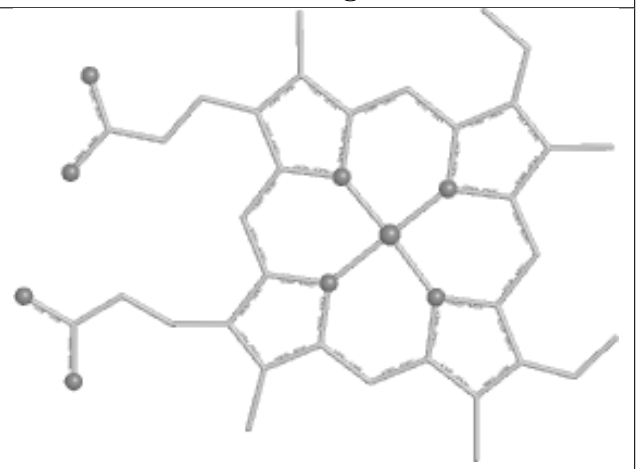
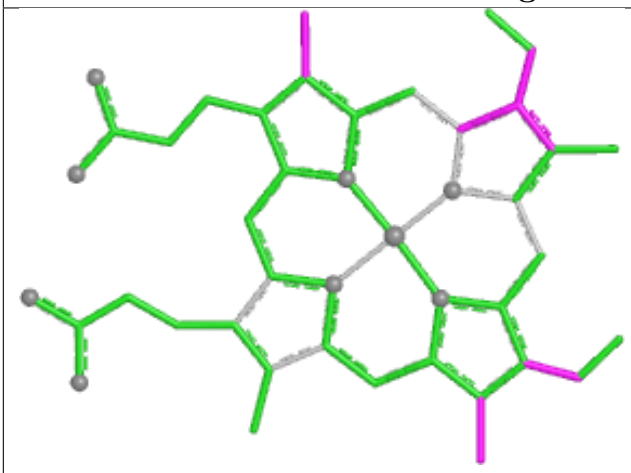


Rings

Ligand HEM C 502



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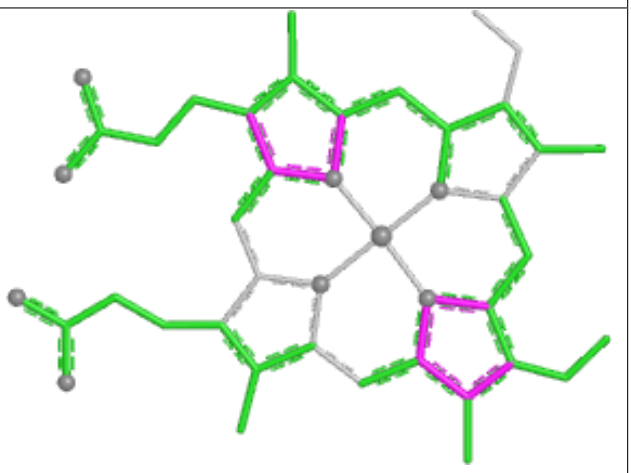
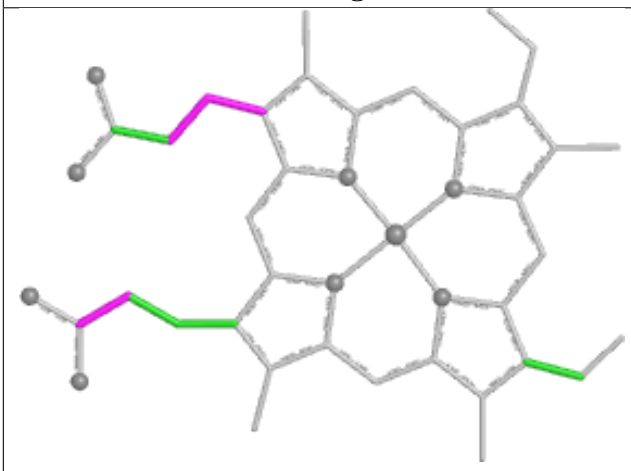


Bond angles



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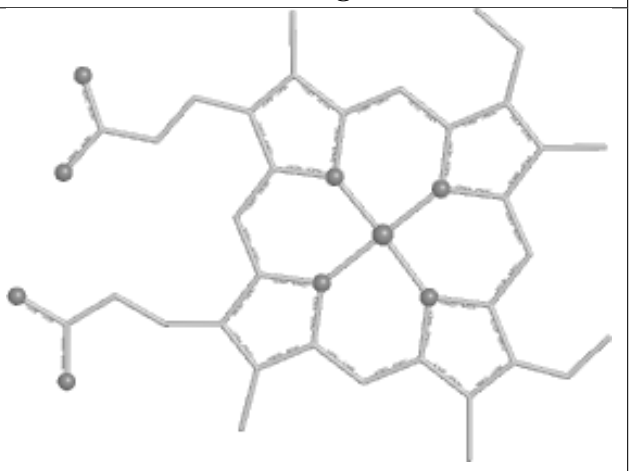
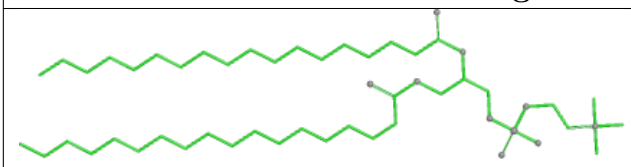
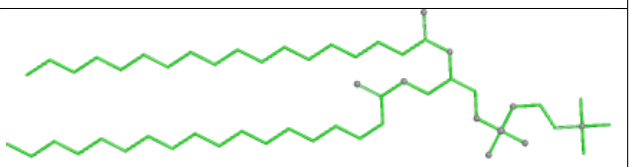


Rings

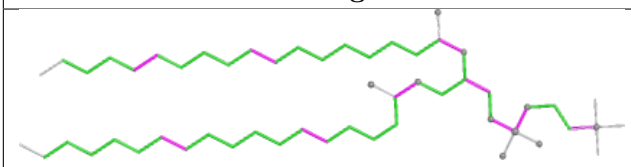
Ligand PC1 Di 1104



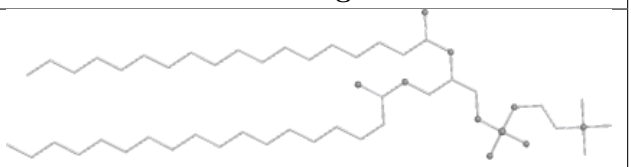
Bond lengths



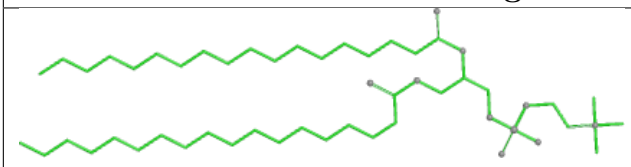
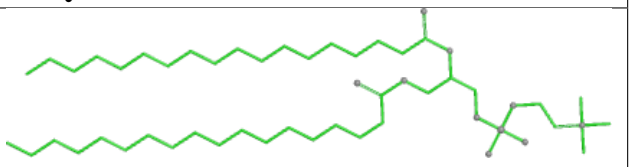
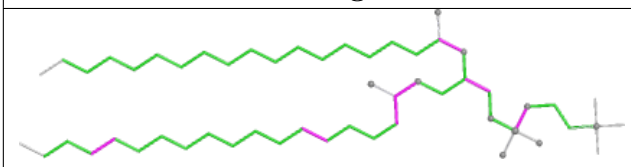
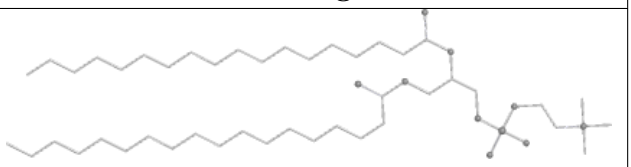
Bond angles

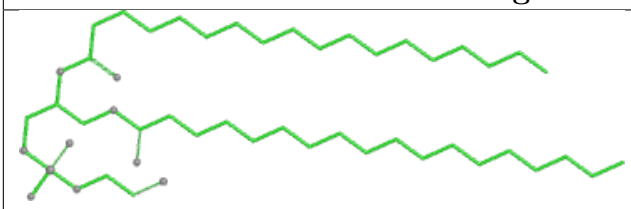
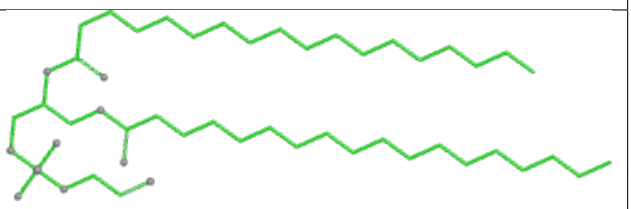
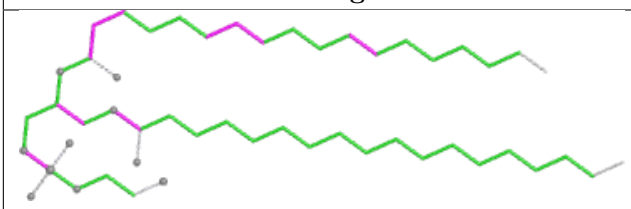
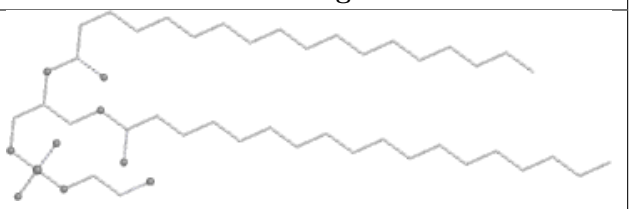


Torsions

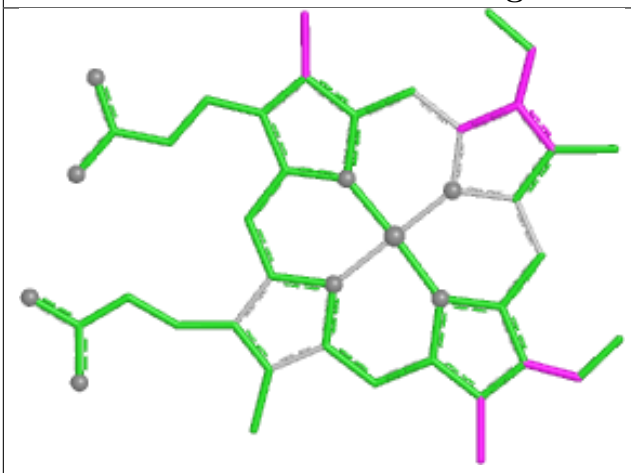


Rings

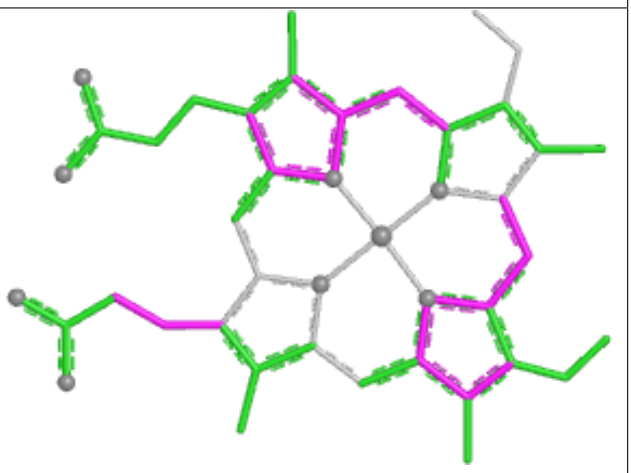
Ligand PC1 DQ 1503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE EM 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

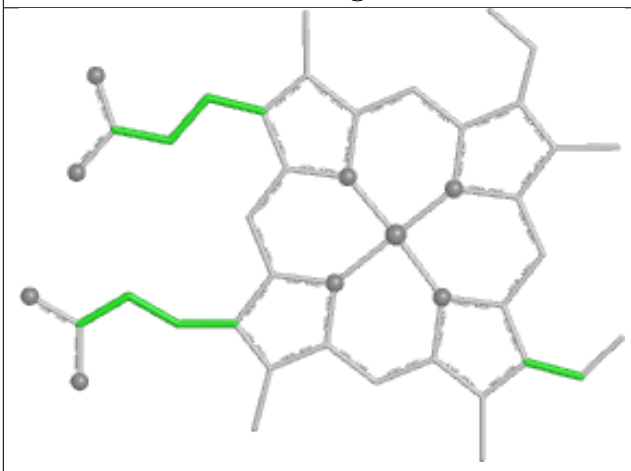
Ligand HEM ED 602



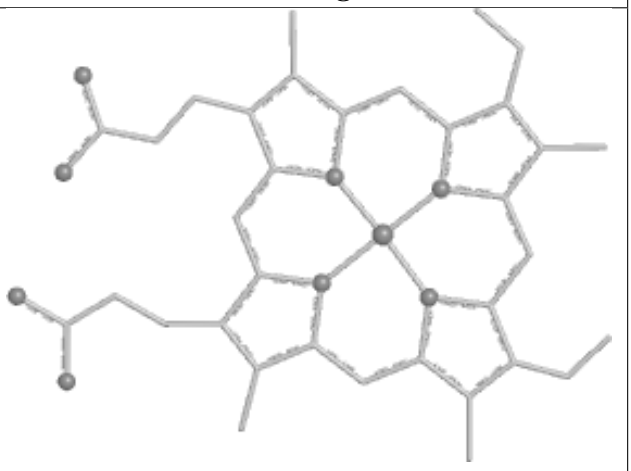
Bond lengths



Bond angles

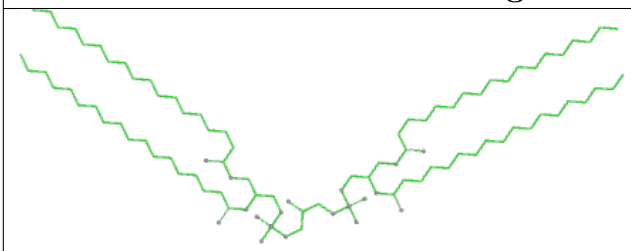


Torsions

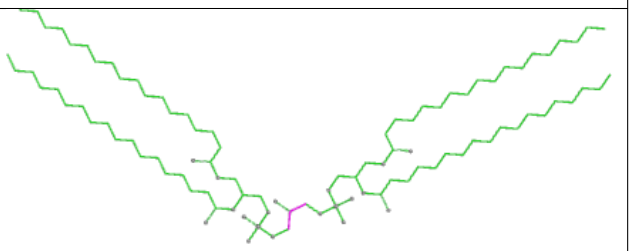


Rings

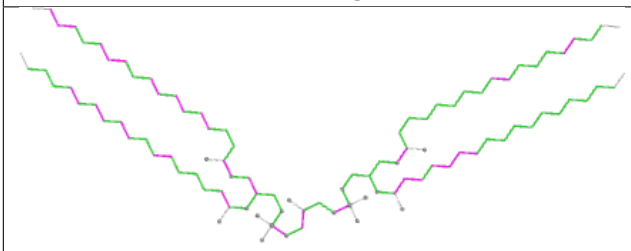
Ligand CDL En 1201



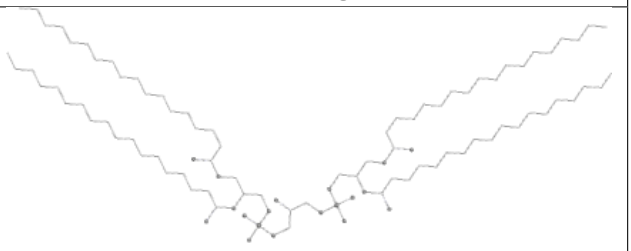
Bond lengths



Bond angles

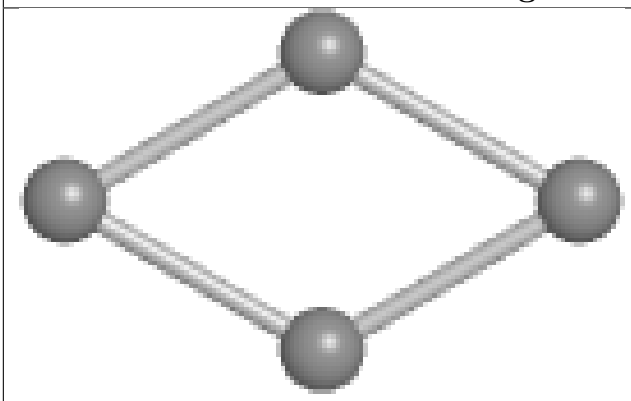


Torsions

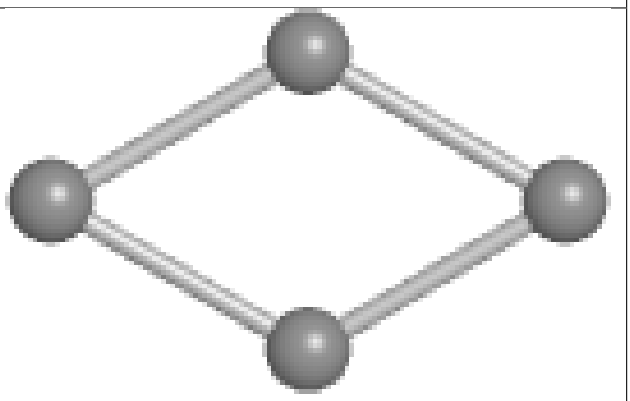


Rings

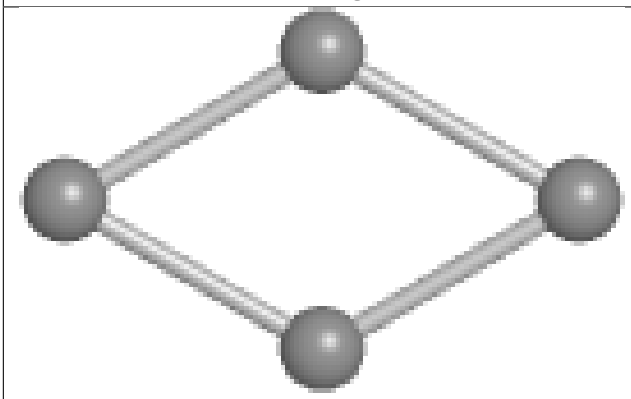
Ligand FES EF 202



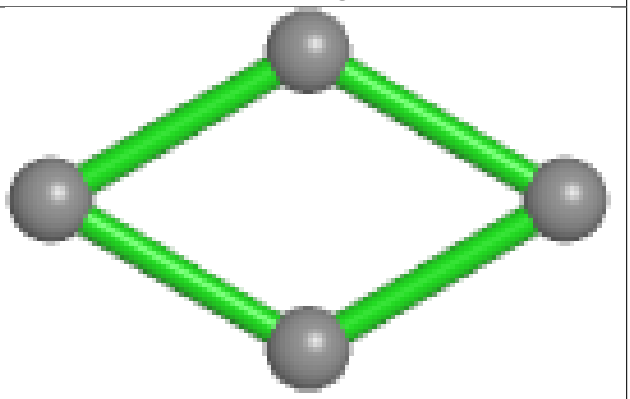
Bond lengths



Bond angles

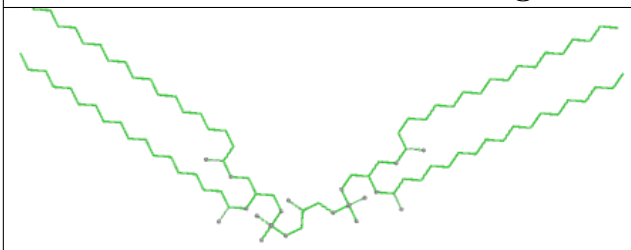


Torsions

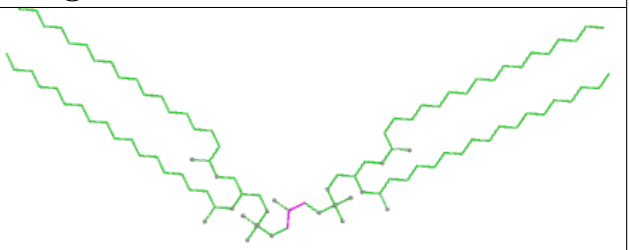


Rings

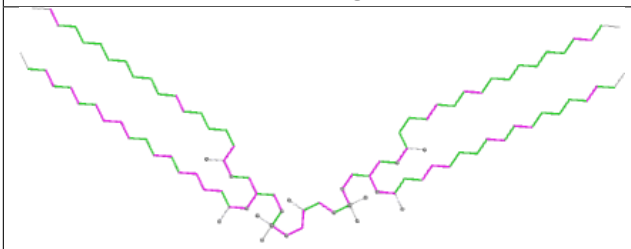
Ligand CDL Dg 201



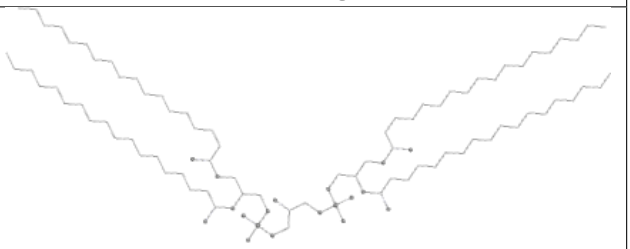
Bond lengths



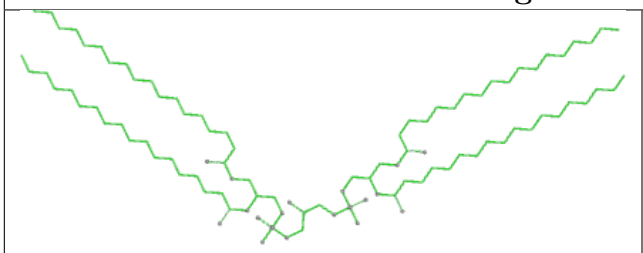
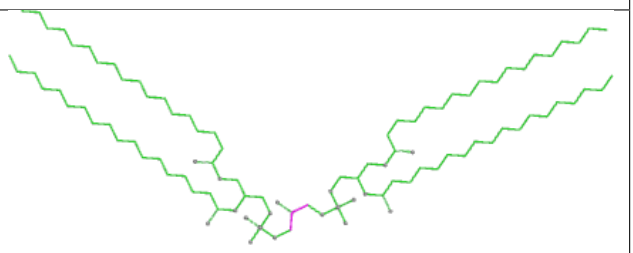
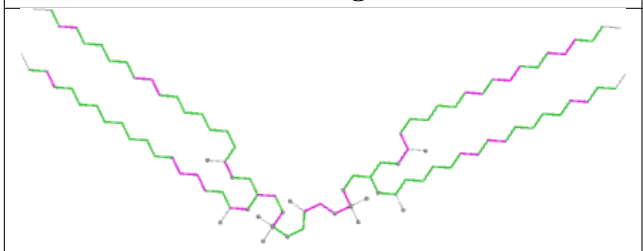
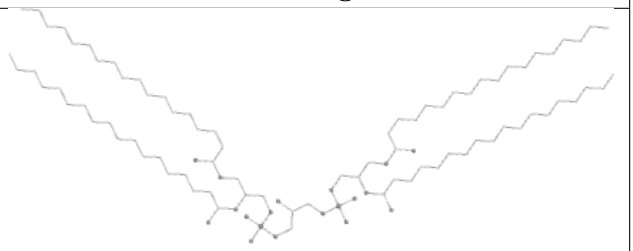
Bond angles

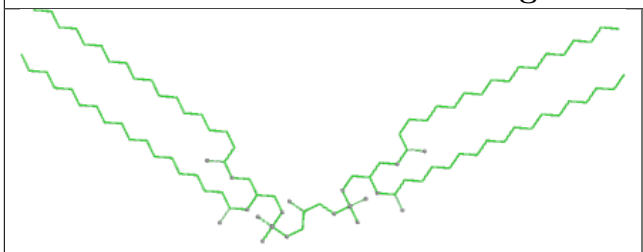
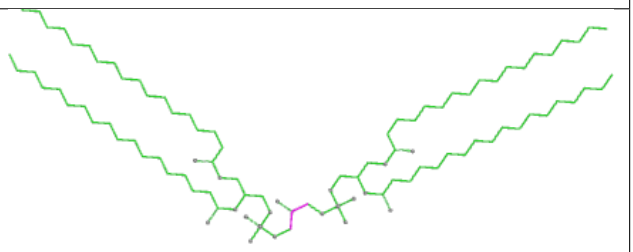
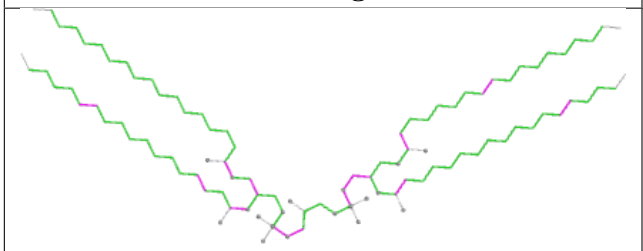
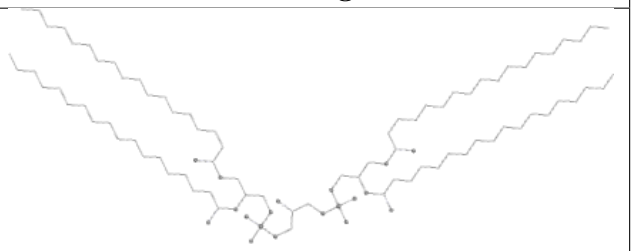


Torsions

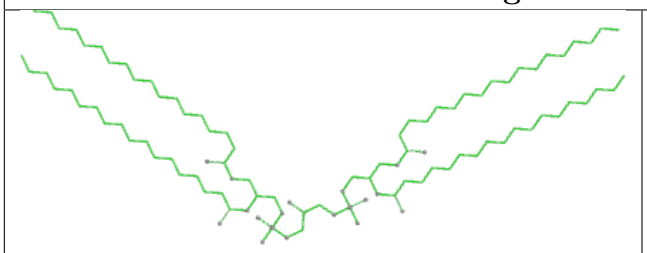


Rings

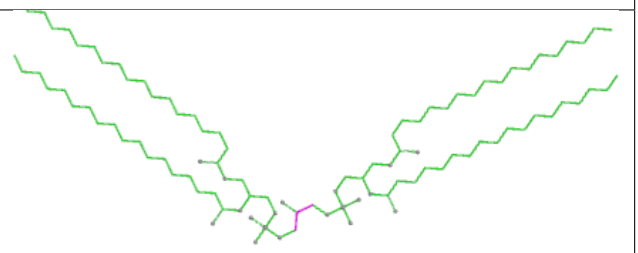
Ligand CDL Dv 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL EI 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

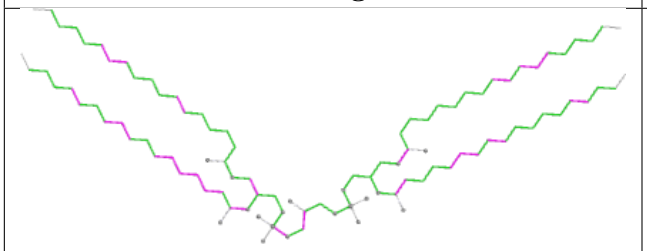
Ligand CDL EN 1201



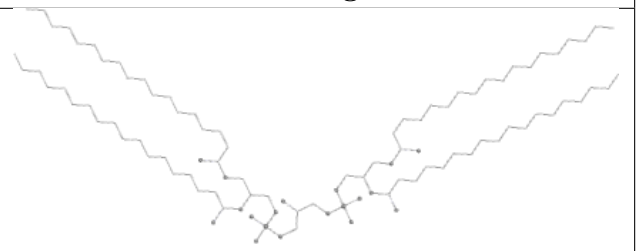
Bond lengths



Bond angles

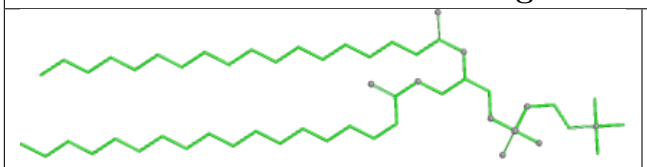


Torsions

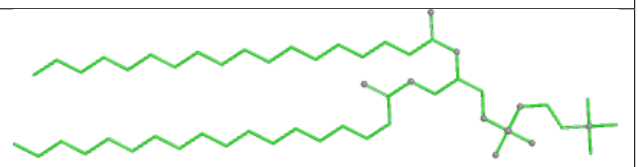


Rings

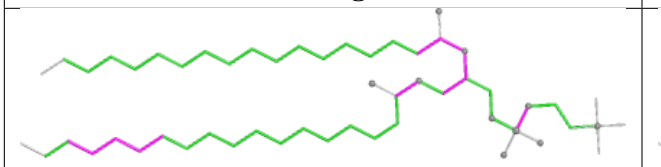
Ligand PC1 EO 206



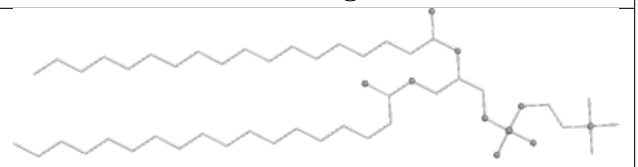
Bond lengths



Bond angles

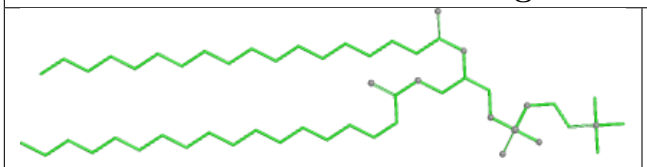


Torsions

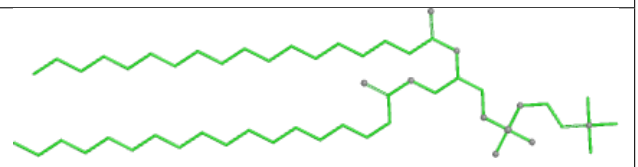


Rings

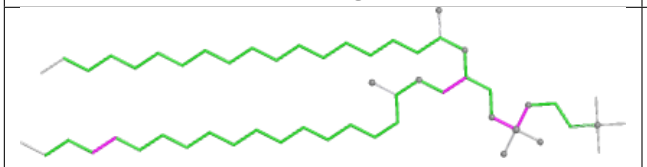
Ligand PC1 DV 406



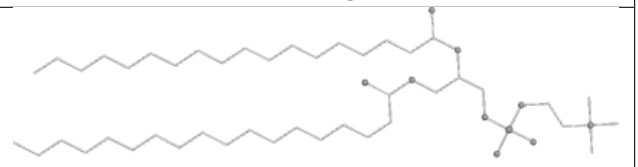
Bond lengths



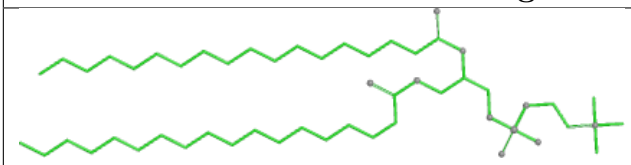
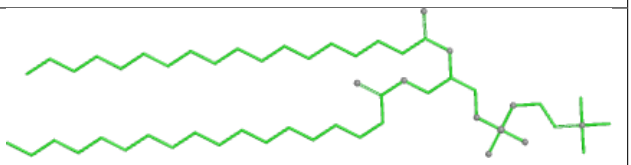
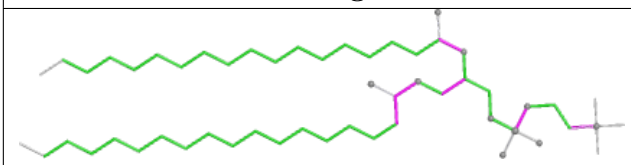
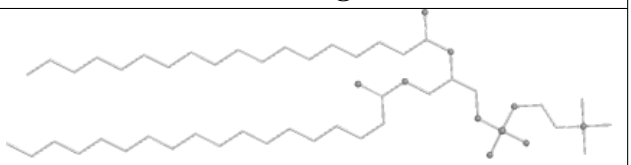
Bond angles

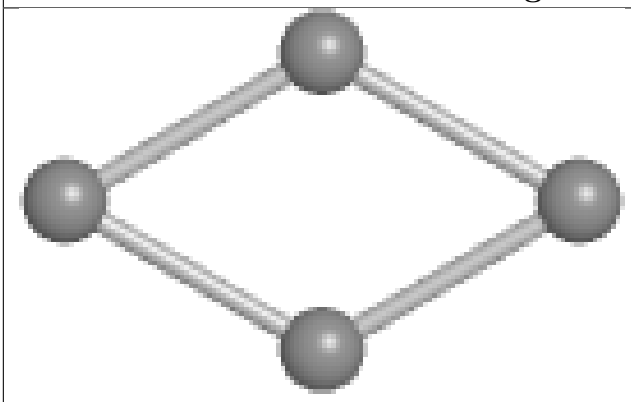
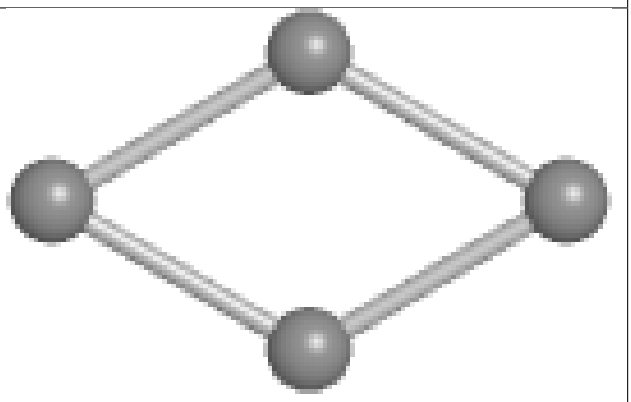
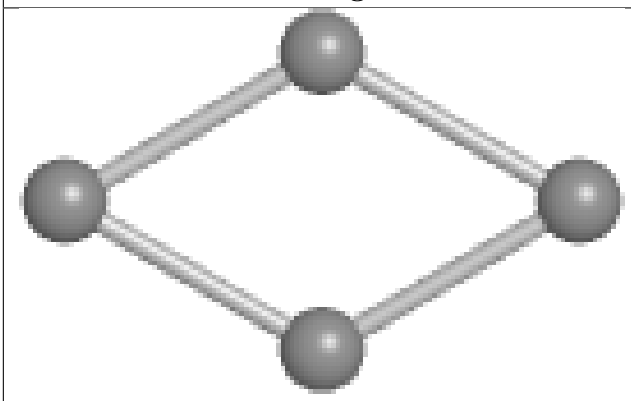
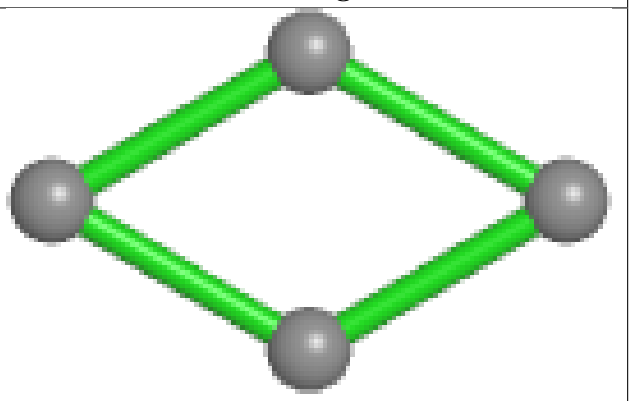


Torsions

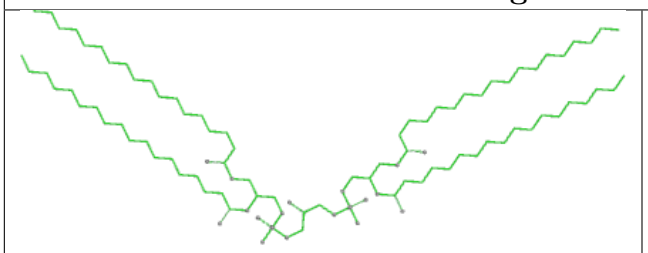


Rings

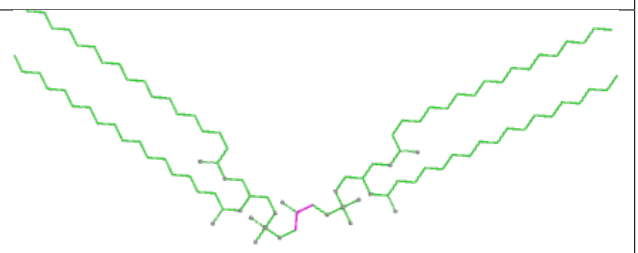
Ligand PC1 A6 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES Ef 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

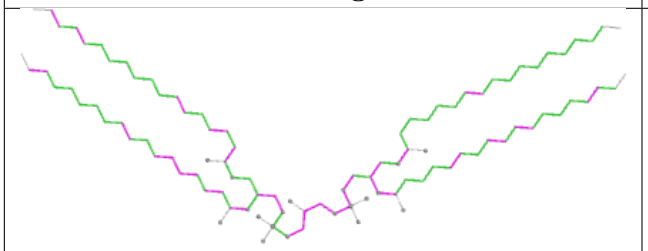
Ligand CDL DG 201



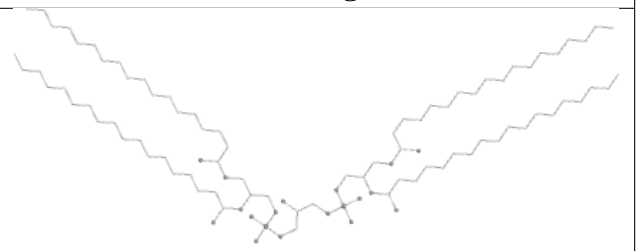
Bond lengths



Bond angles

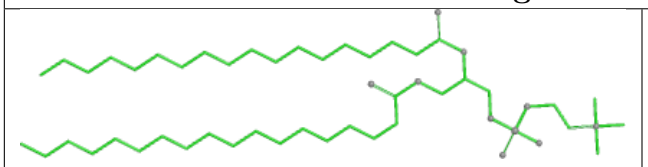


Torsions



Rings

Ligand PC1 DG 203



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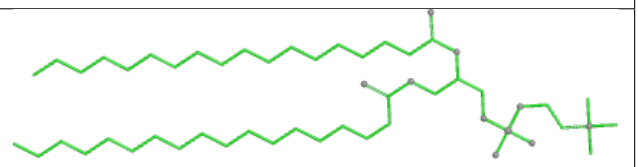
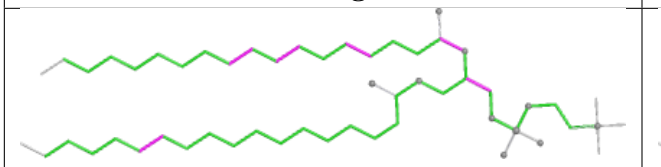
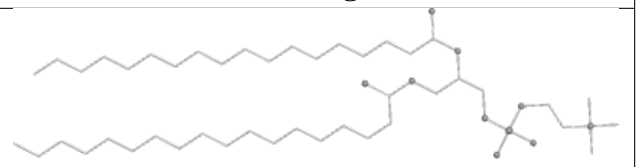


Bond angles

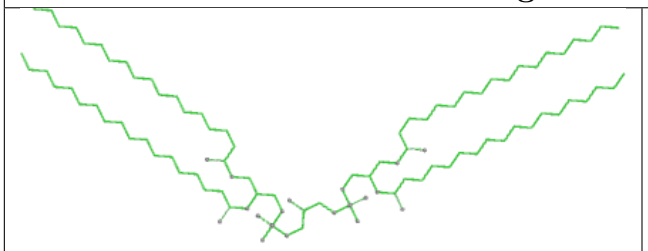


Torsions

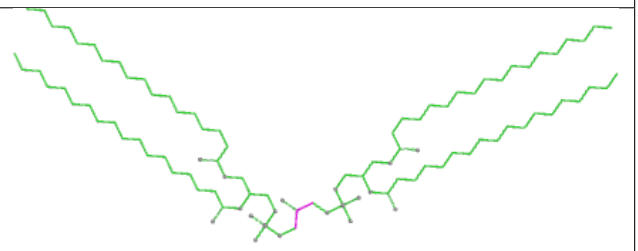


Rings

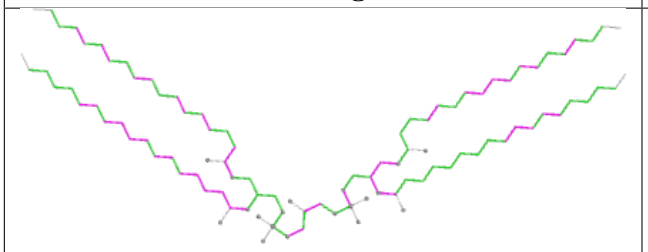
Ligand CDL Ds 405



Bond lengths



Bond angles



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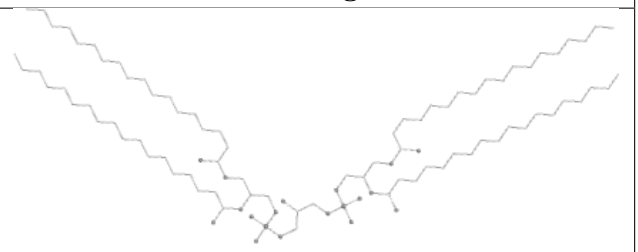
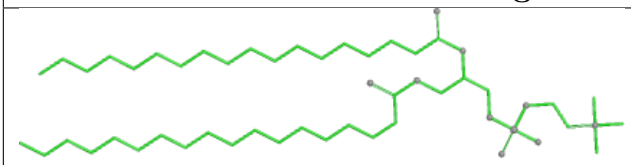
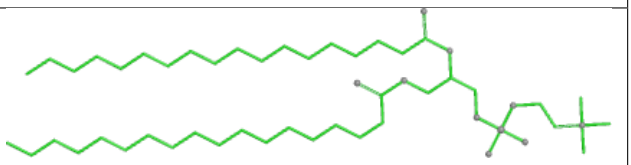


Rings

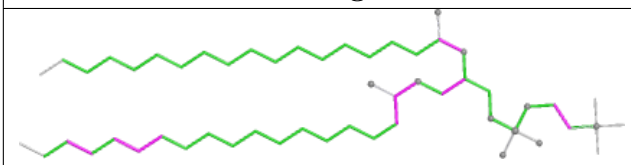
Ligand PC1 AU 202



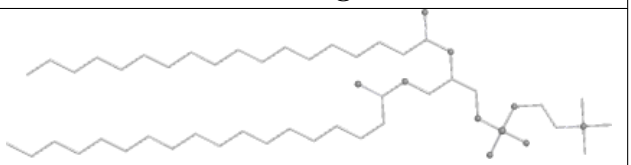
Bond lengths



Bond angles

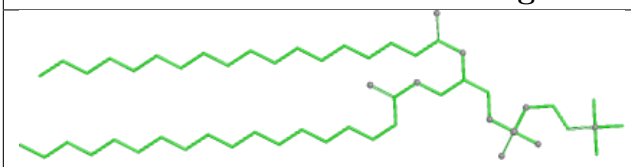


Torsions

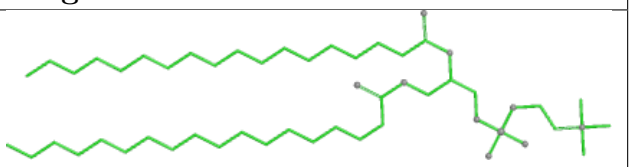


Rings

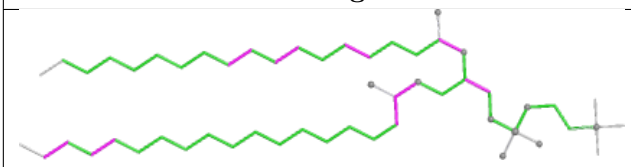
Ligand PC1 Dg 203



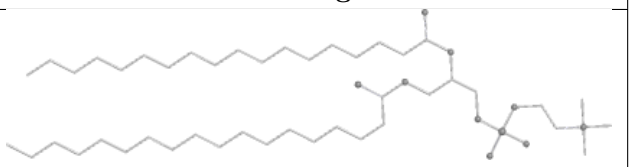
Bond lengths



Bond angles

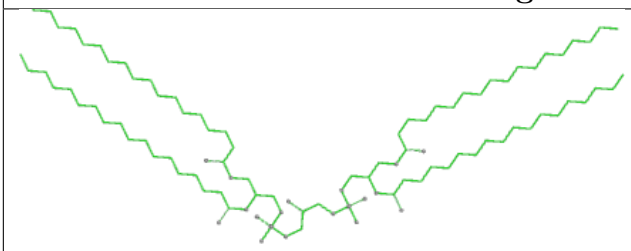


Torsions

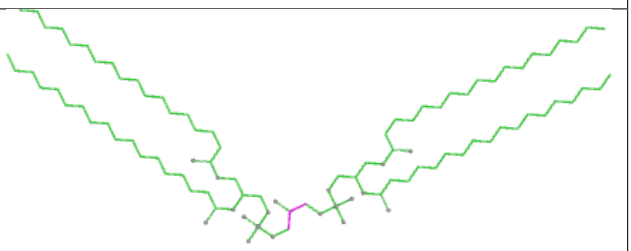


Rings

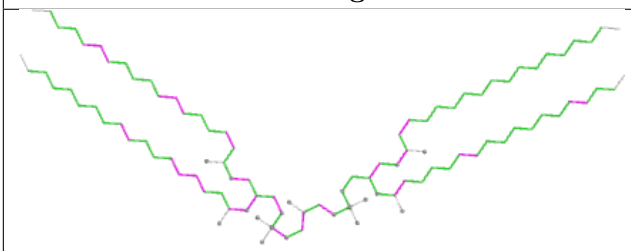
Ligand CDL Dr 403



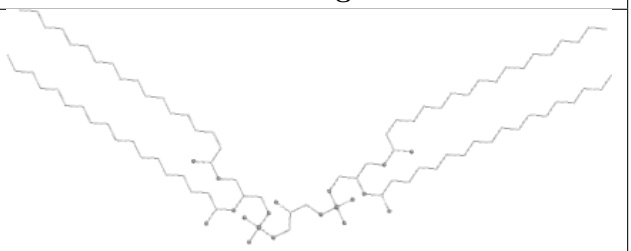
Bond lengths



Bond angles

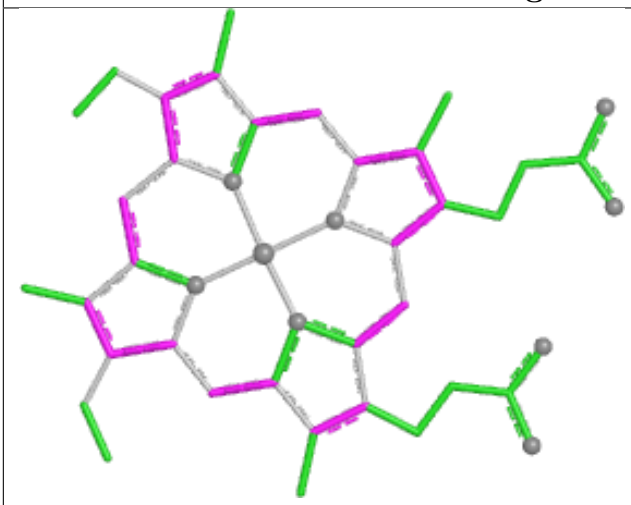


Torsions

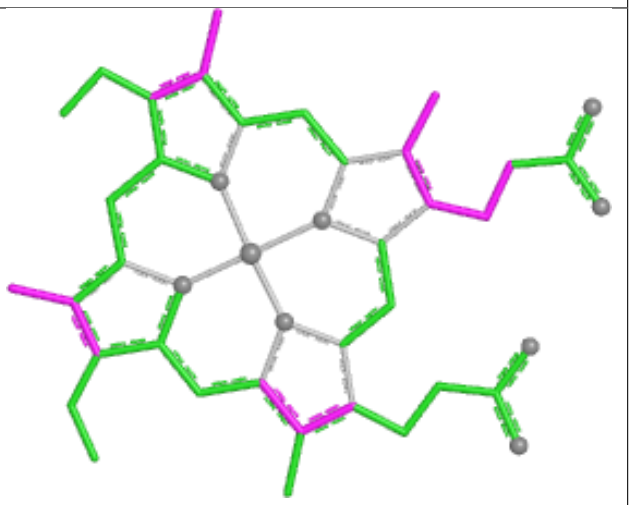


Rings

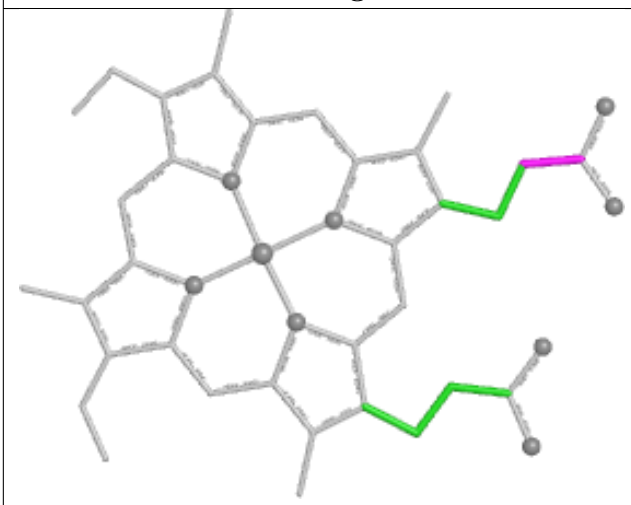
Ligand HEC d 802



Bond lengths



Bond angles



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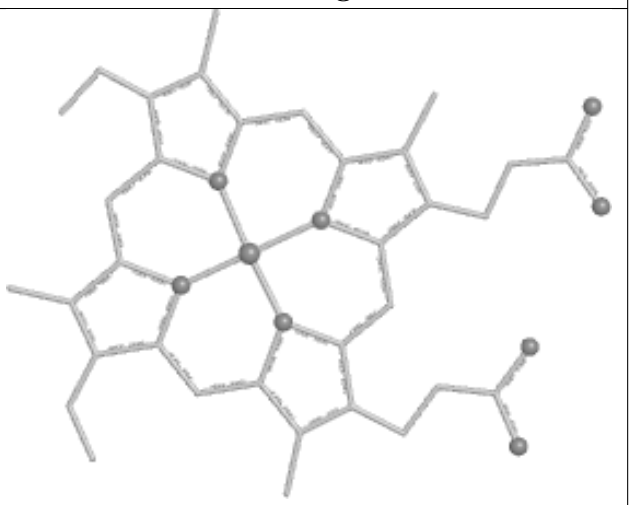
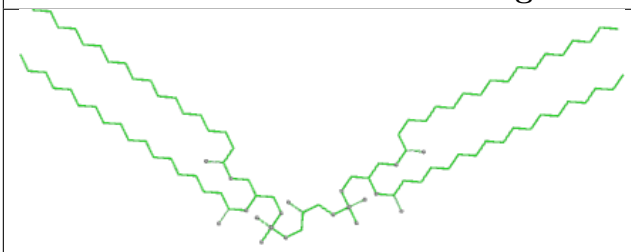


Rings

Ligand CDL Ed 204



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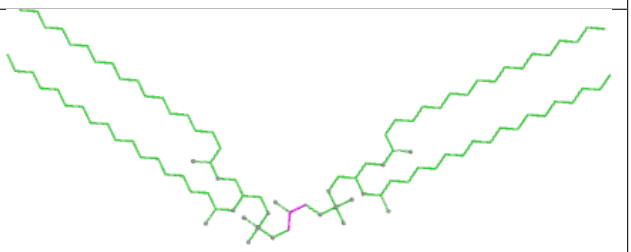
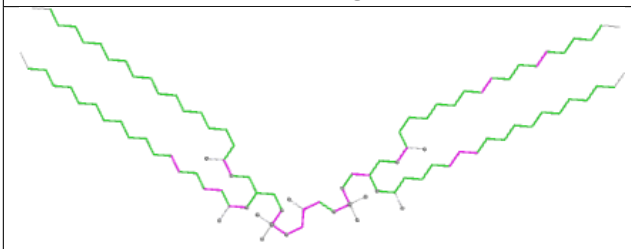
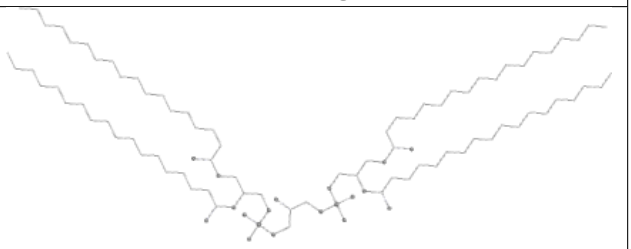


Bond angles

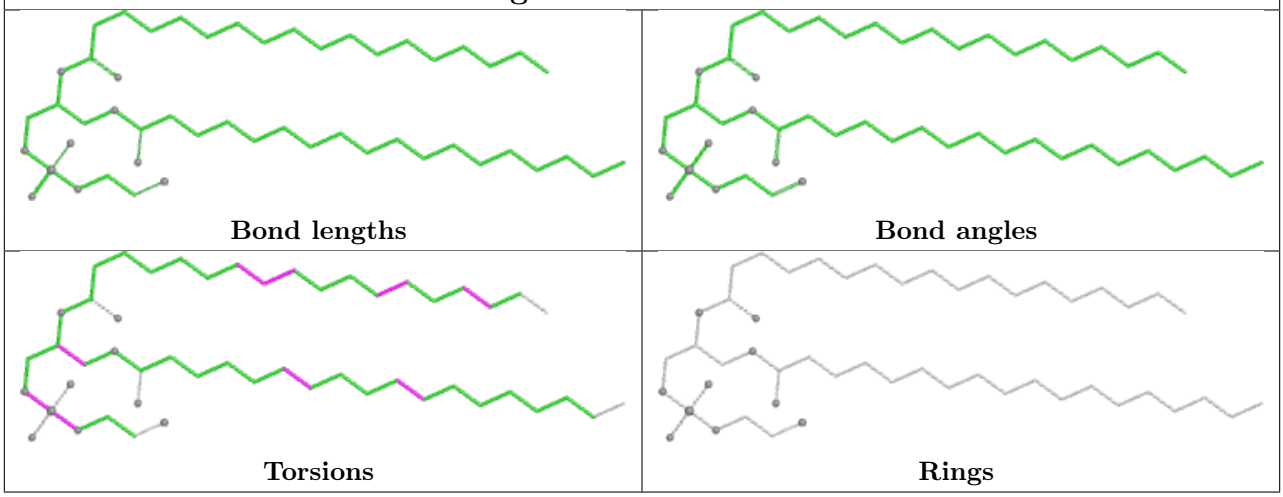


Torsions

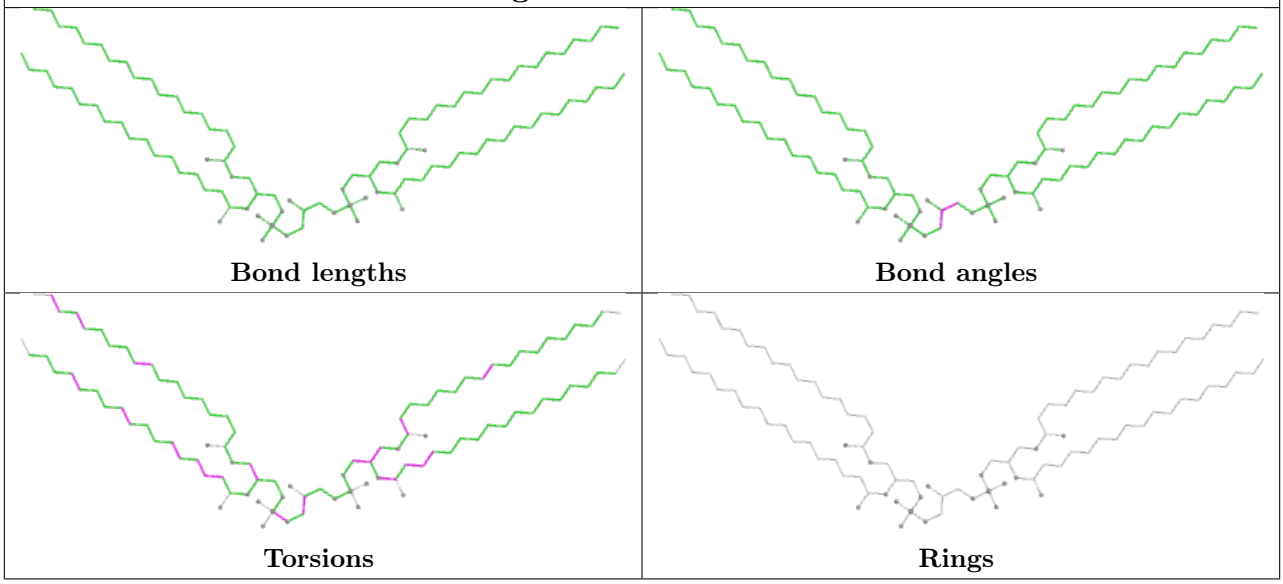


Rings

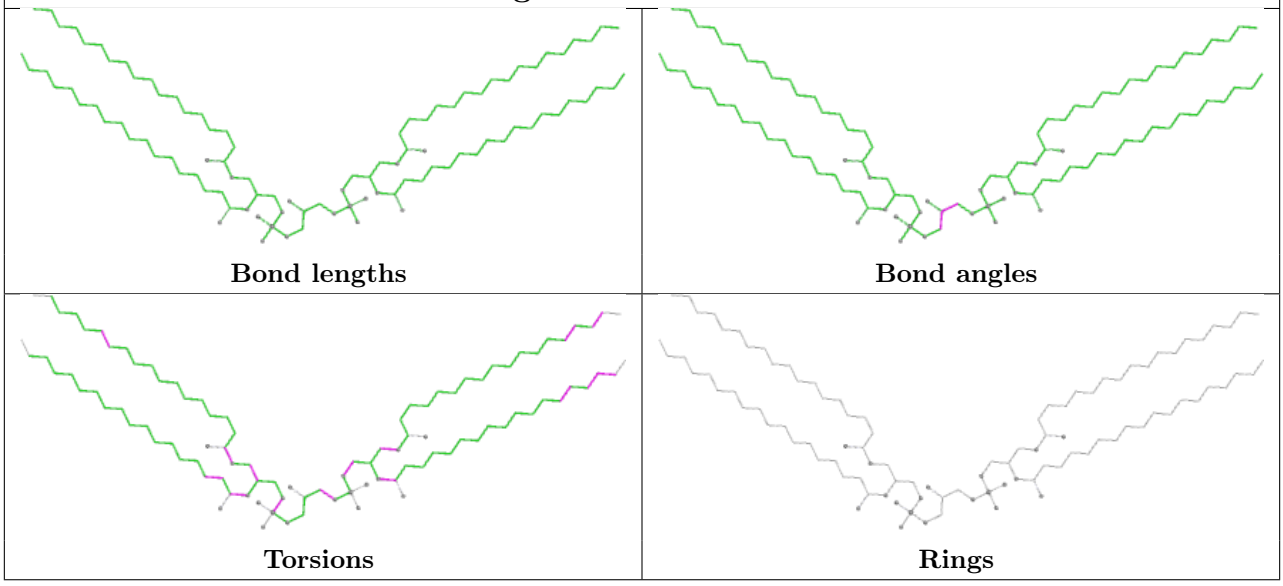
Ligand 3PE Dx 1208



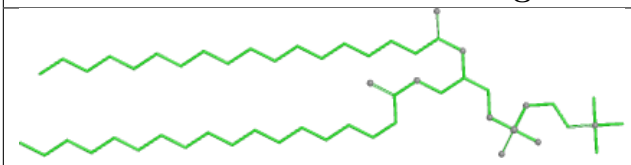
Ligand CDL BV 201



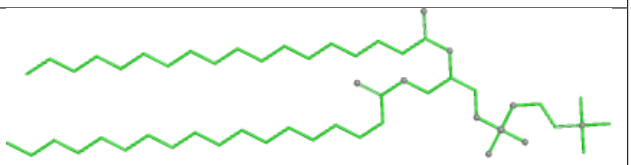
Ligand CDL AF 401



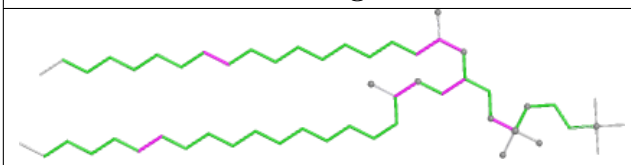
Ligand PC1 DC 605



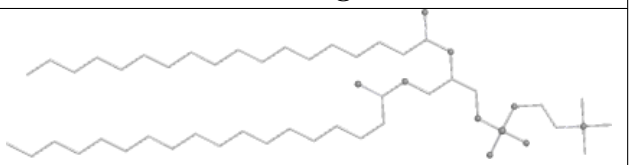
Bond lengths



Bond angles

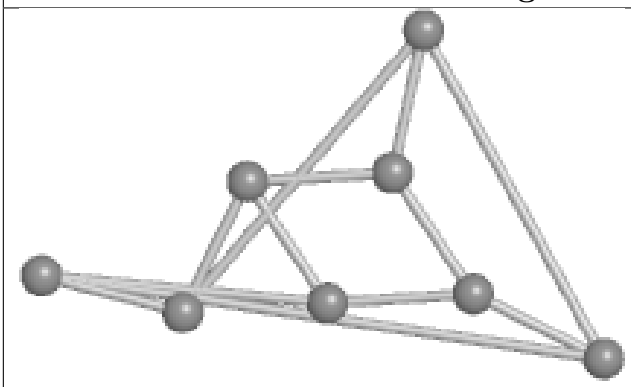


Torsions



Rings

Ligand SF4 AB 803



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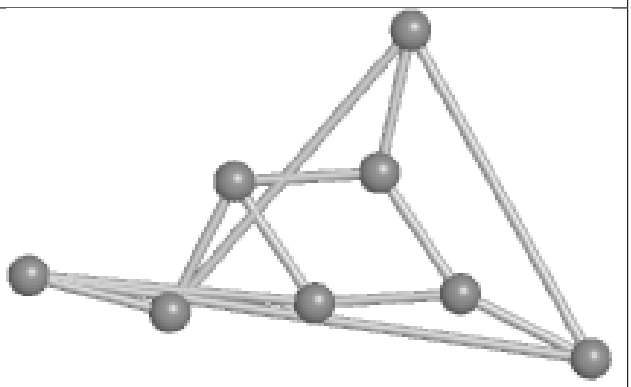
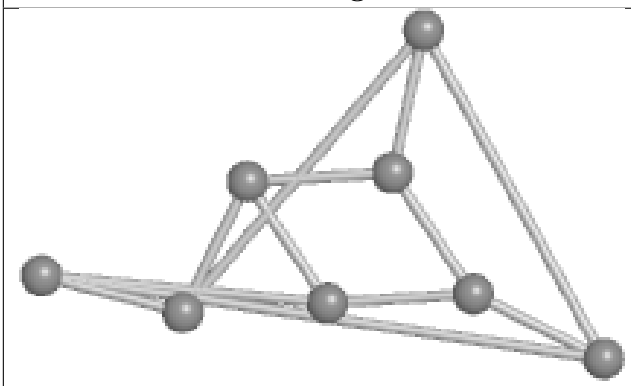


Bond angles



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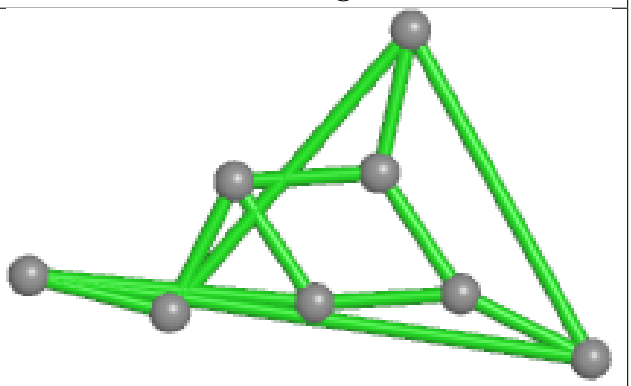
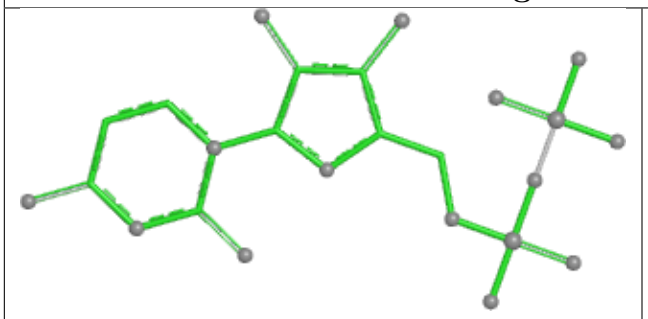


Rings

Ligand UDP A0 603



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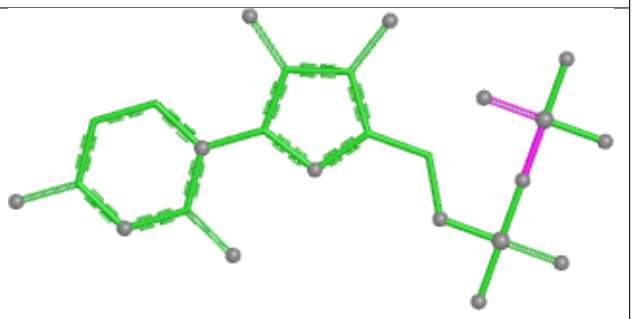
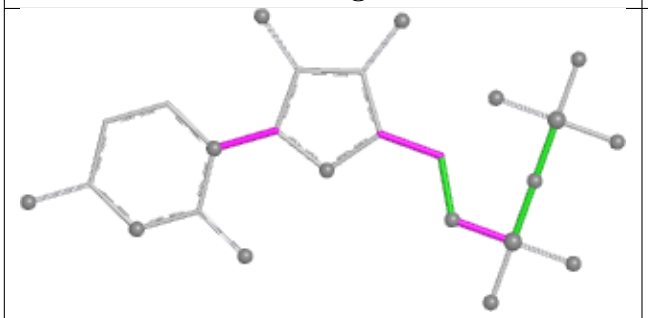


Bond angles



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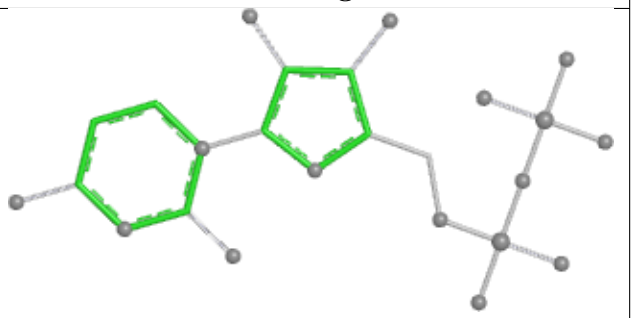
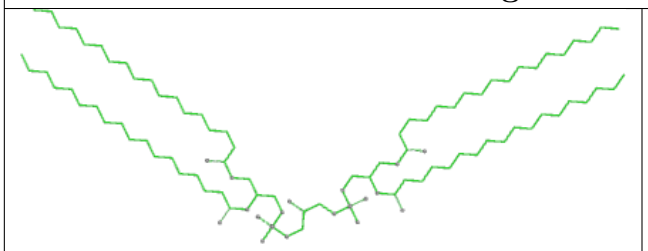


Rings

Ligand CDL DQ 1504



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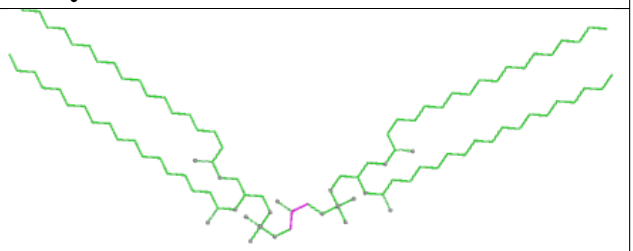
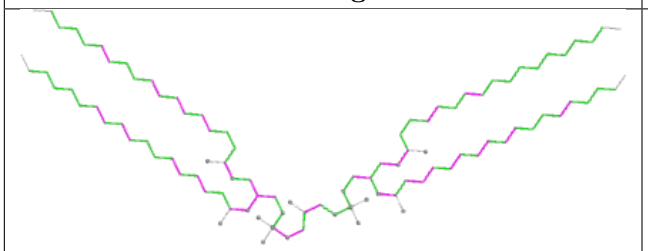


Bond angles



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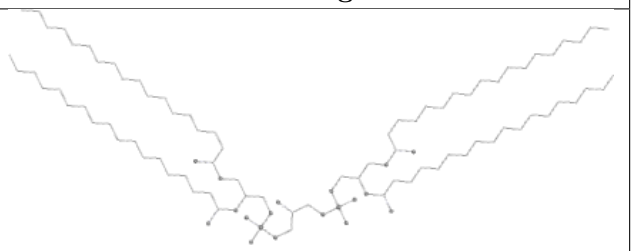
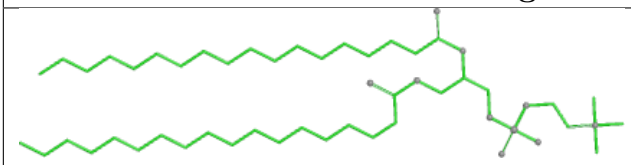
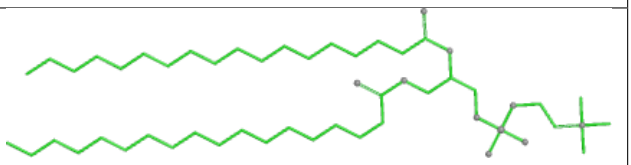


Rings

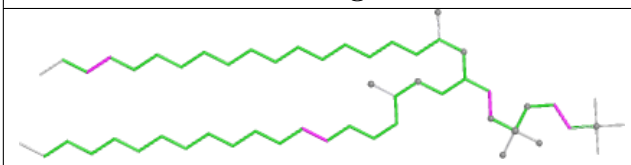
Ligand PC1 Eb 303



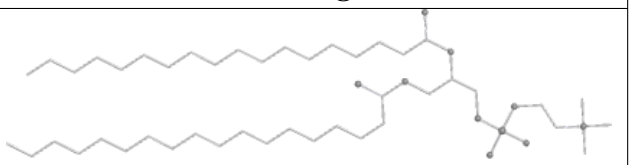
Bond lengths



Bond angles

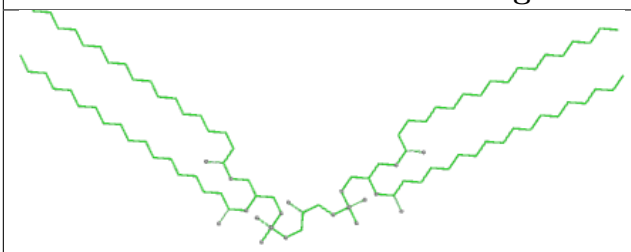


Torsions



Rings

Ligand CDL Dn 503



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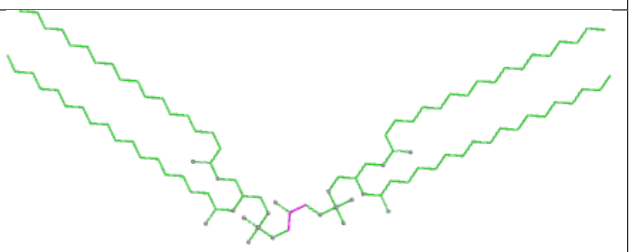
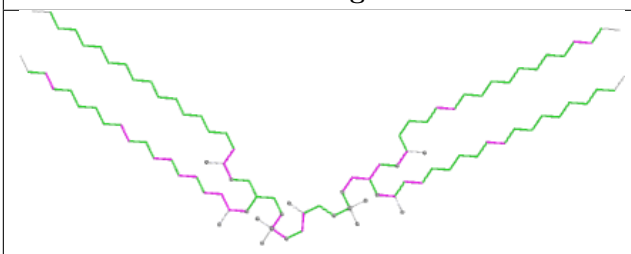
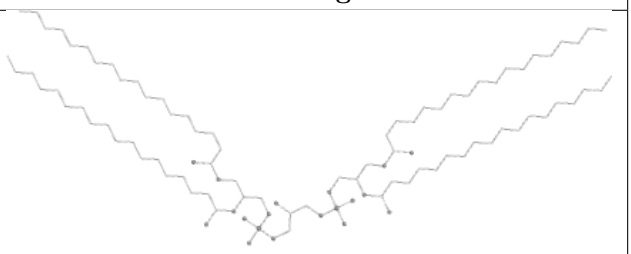


Bond angles

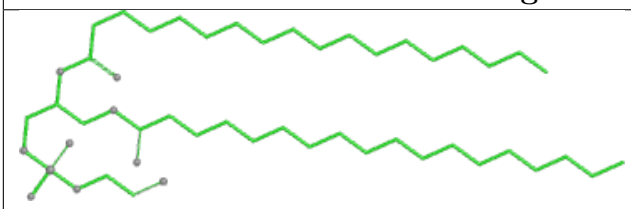


Torsions



Rings

Ligand 3PE Eo 202



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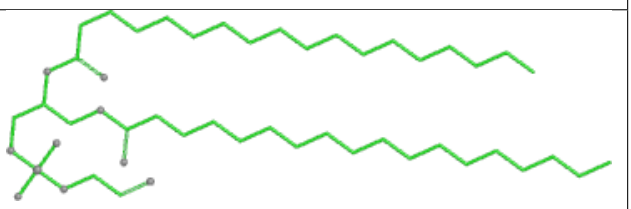
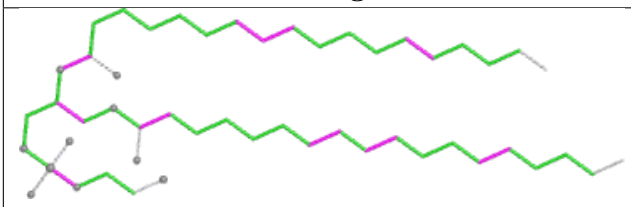


Bond angles



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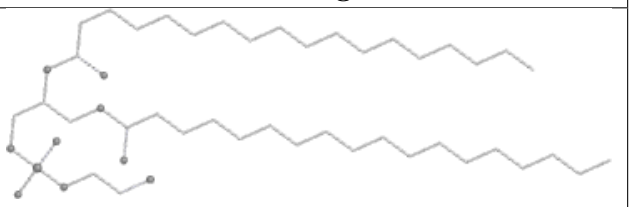
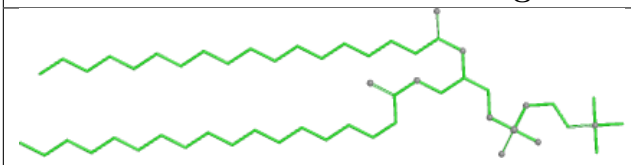


Rings

Ligand PC1 DC 603



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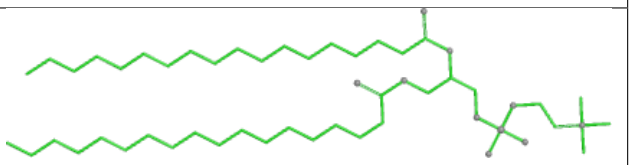
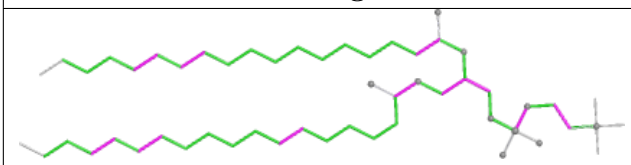


Bond angles



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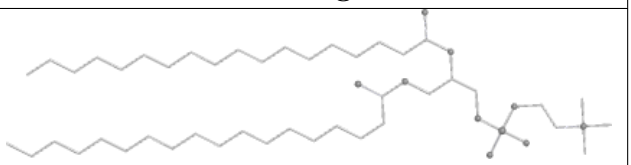
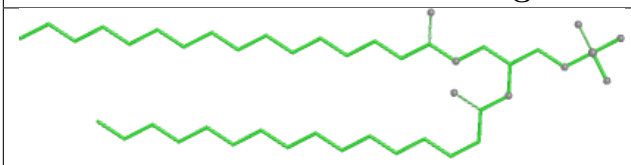
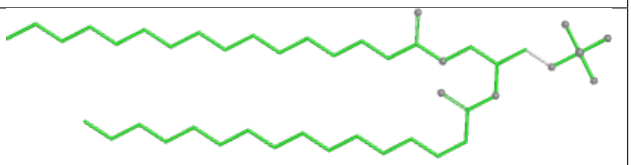


Rings

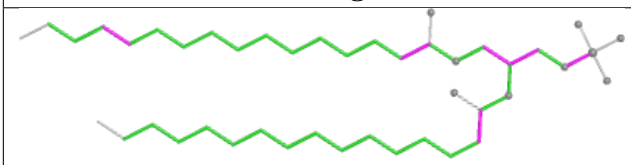
Ligand LPP AC 803



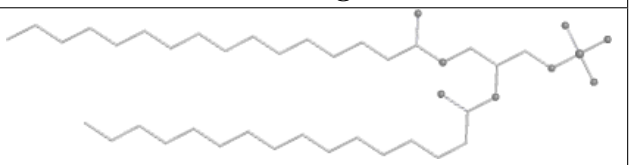
Bond lengths



Bond angles

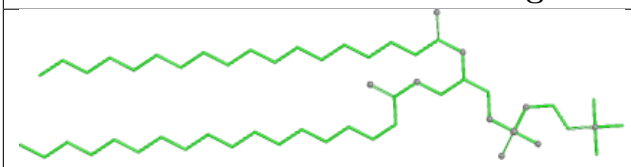


Torsions



Rings

Ligand PC1 K 501



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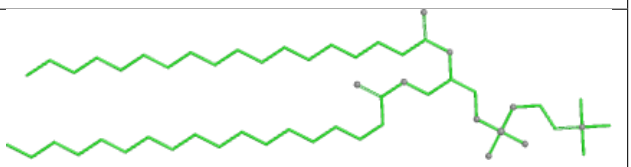
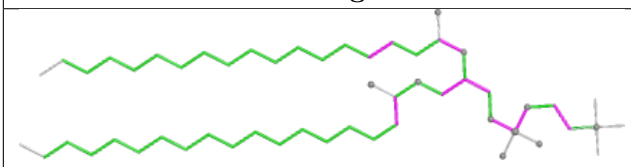
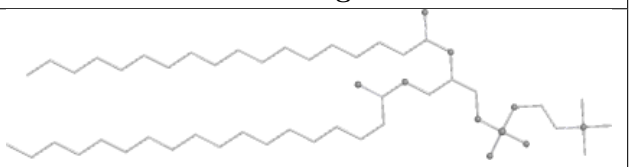


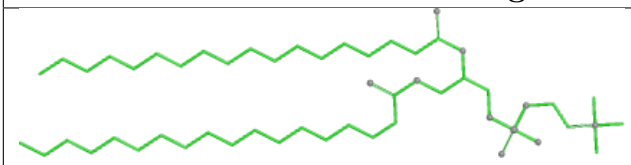
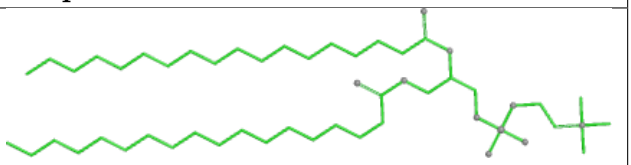
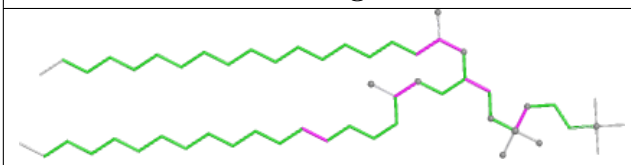
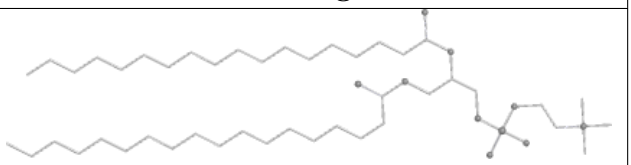
Bond angles

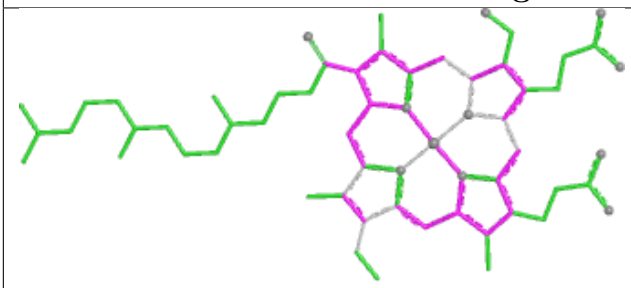
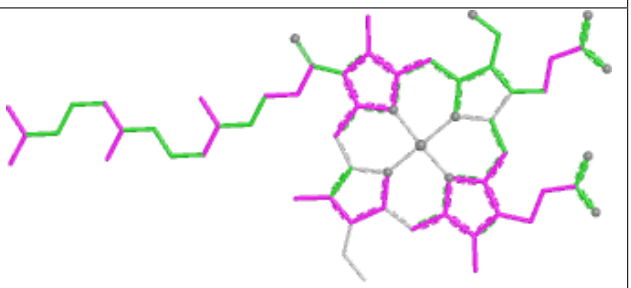
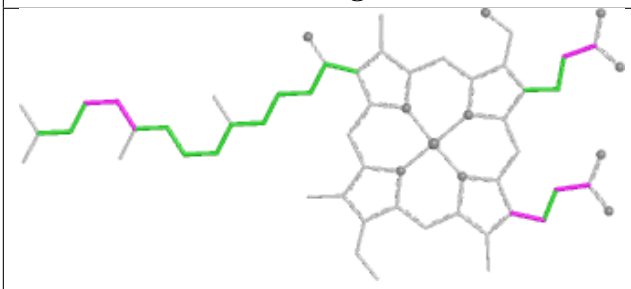
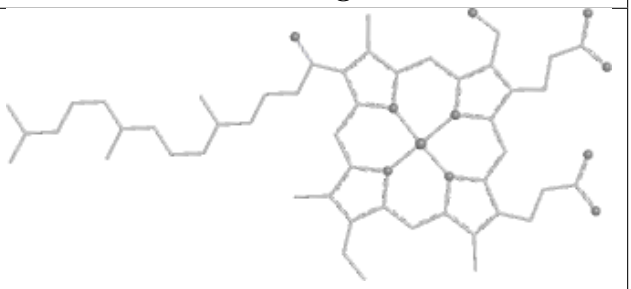


Torsions

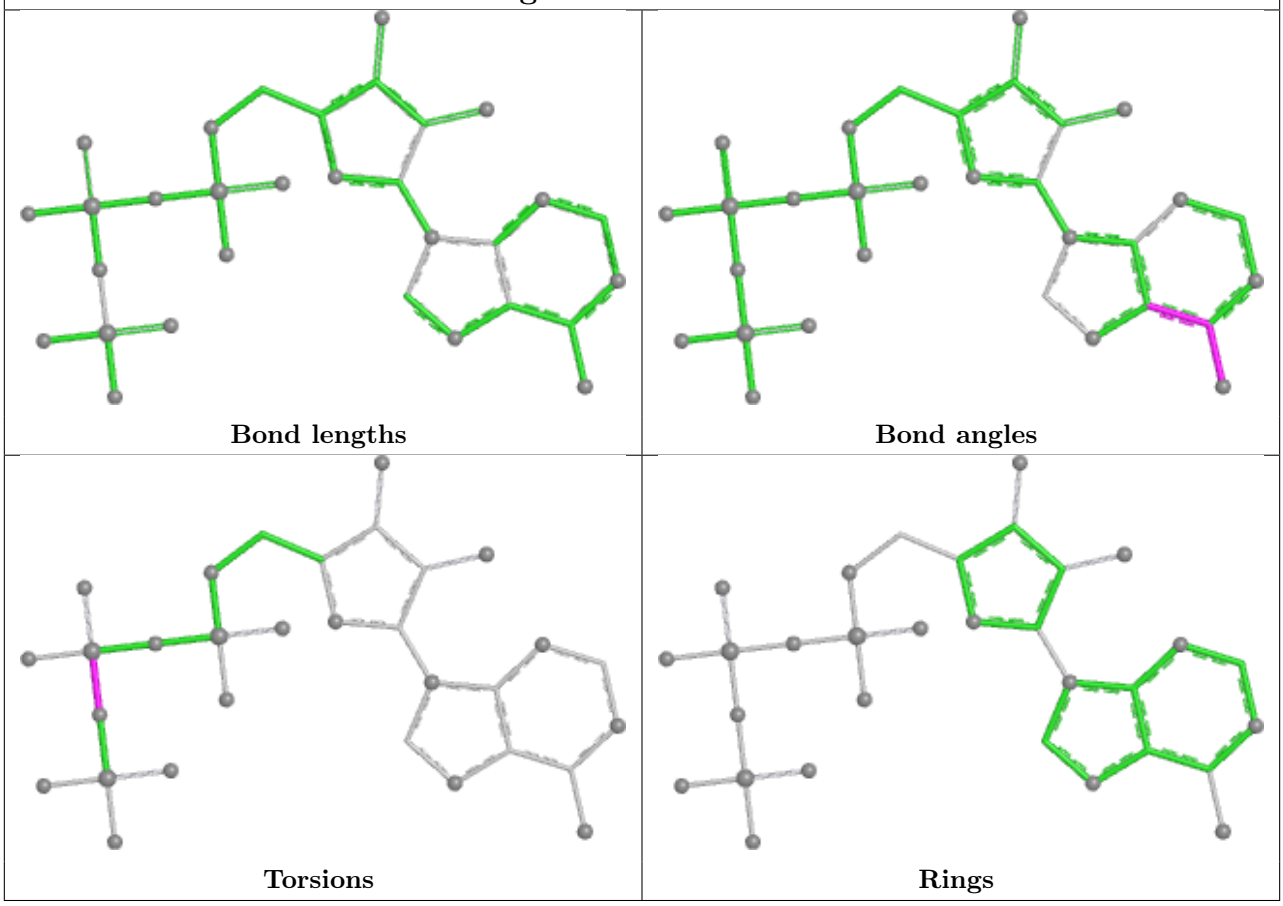


Rings

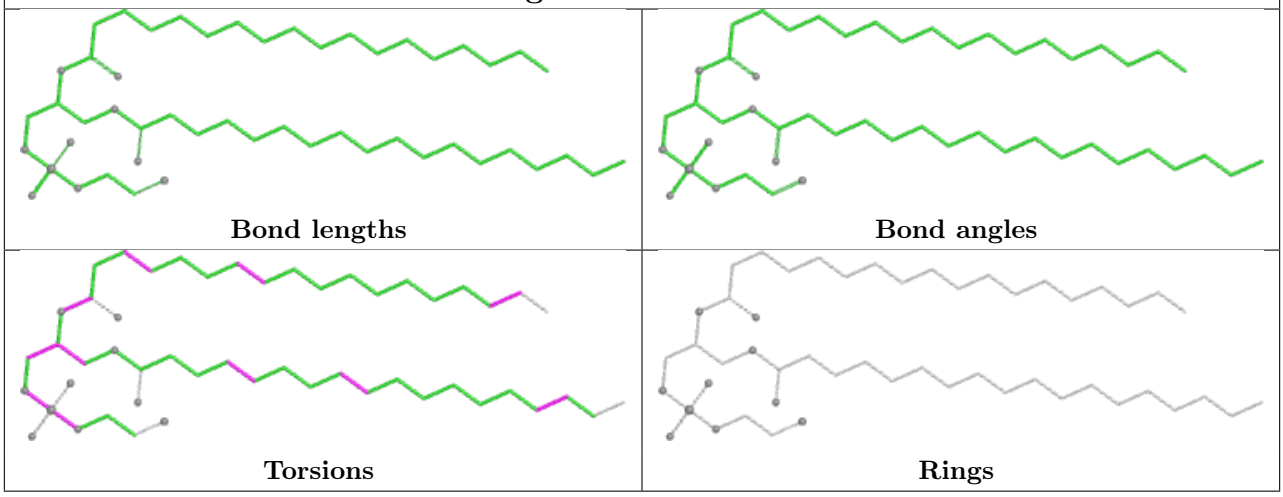
Ligand PC1 Dq 1404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA Da 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

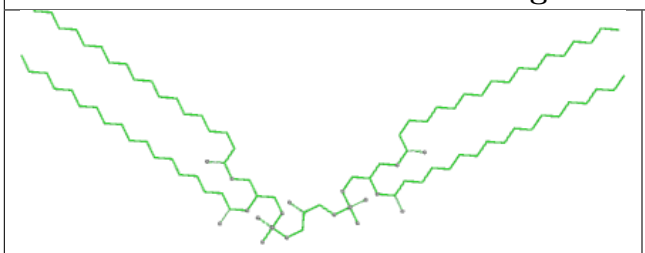
Ligand ATP Er 201



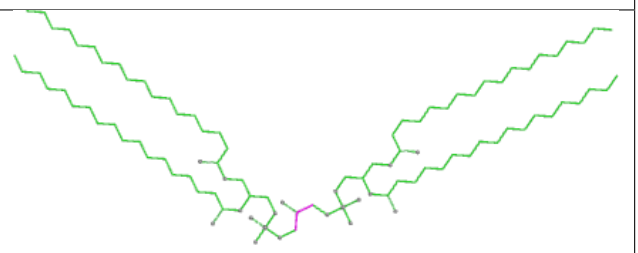
Ligand 3PE El 905



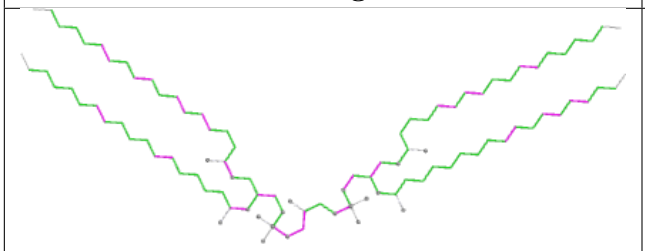
Ligand CDL c 502



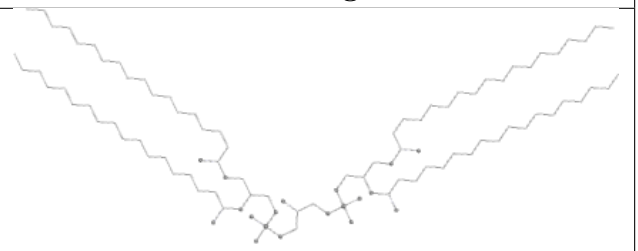
Bond lengths



Bond angles

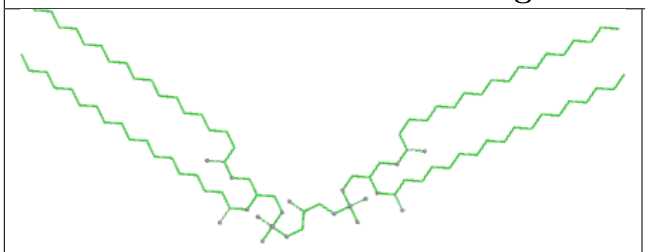


Torsions



Rings

Ligand CDL Dn 506



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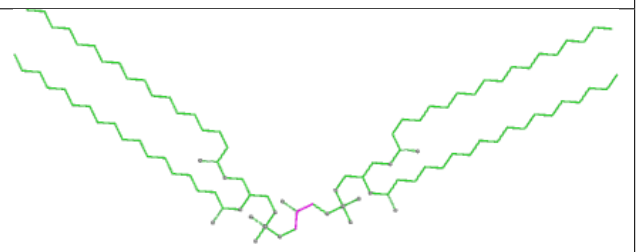
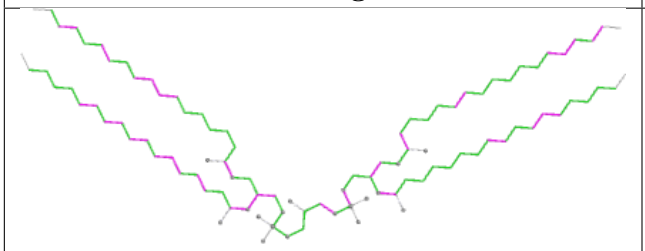


Bond angles



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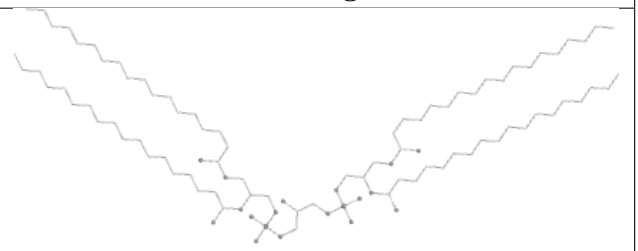
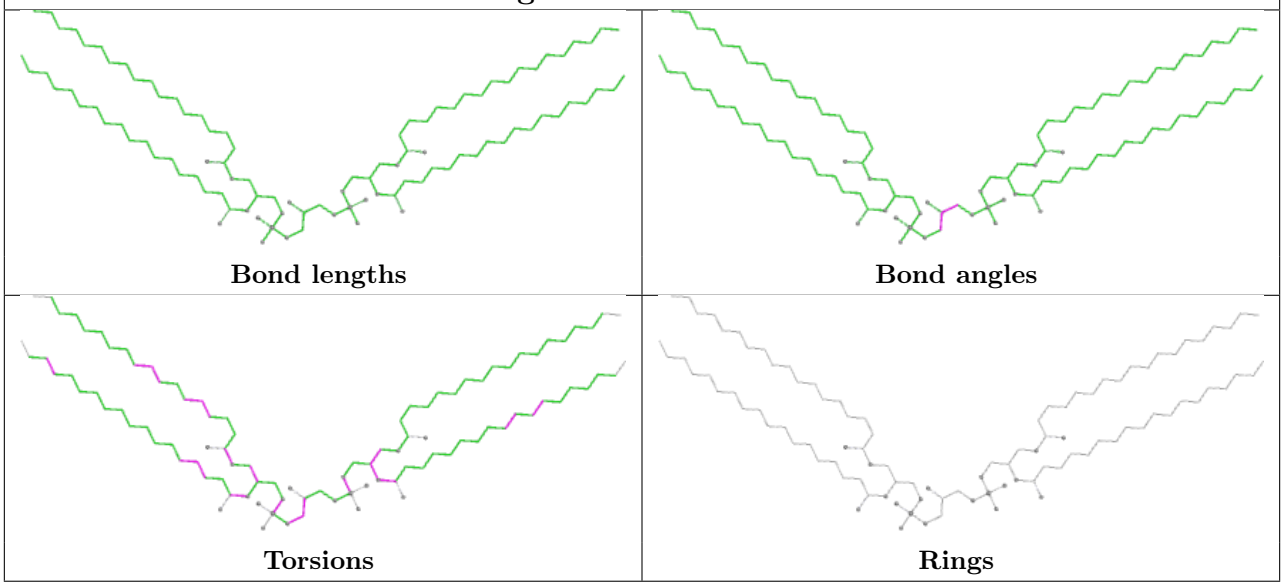
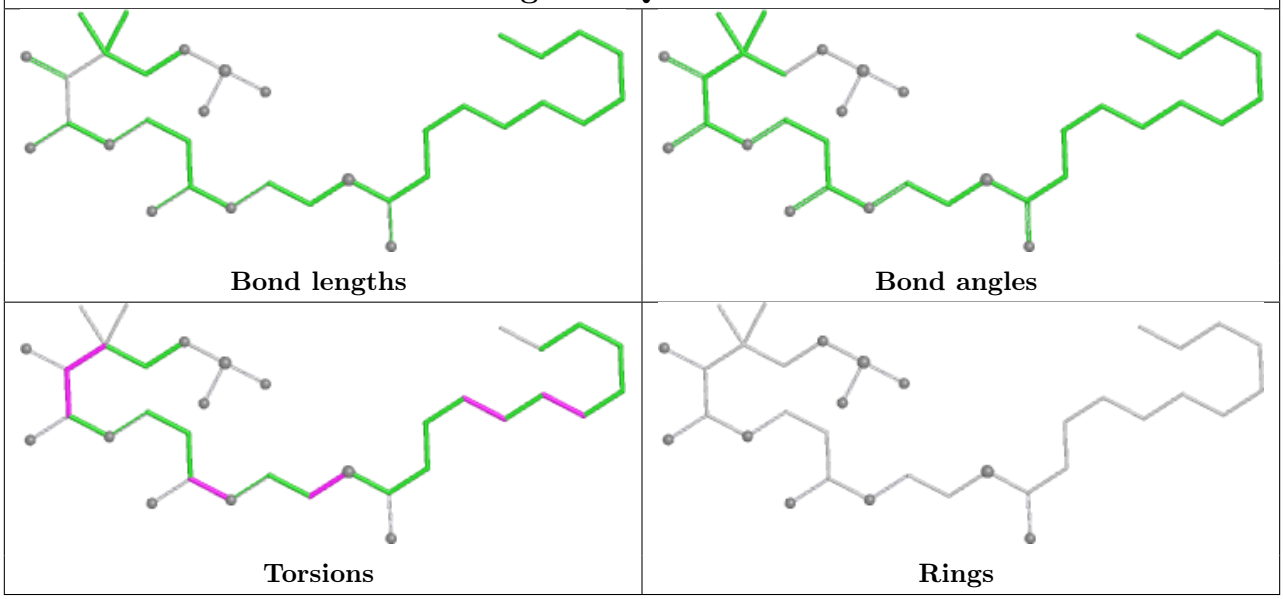


Rings

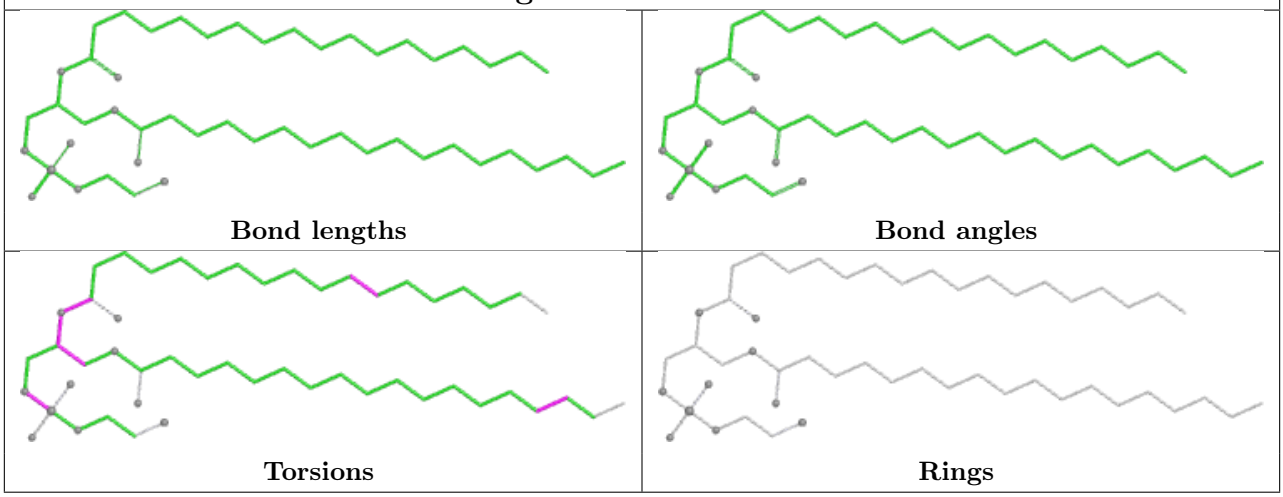
Ligand CDL Ds 401



Ligand 8Q1 AS 200



Ligand 3PE DC 606



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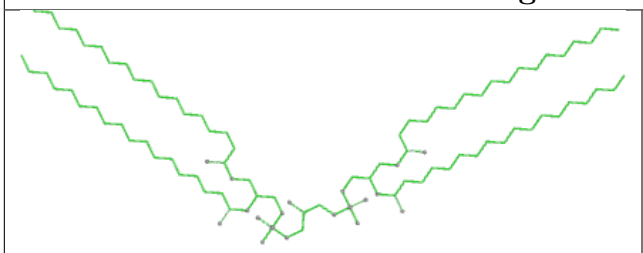
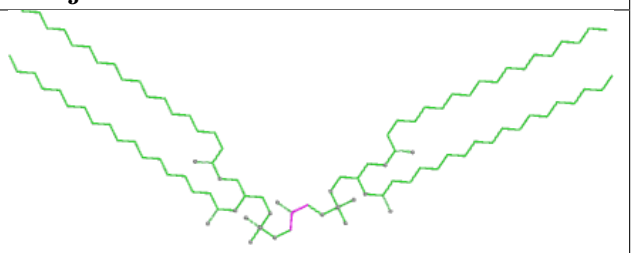
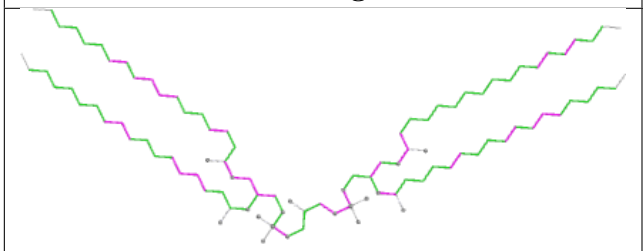
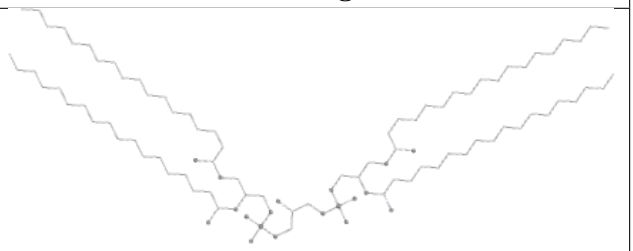
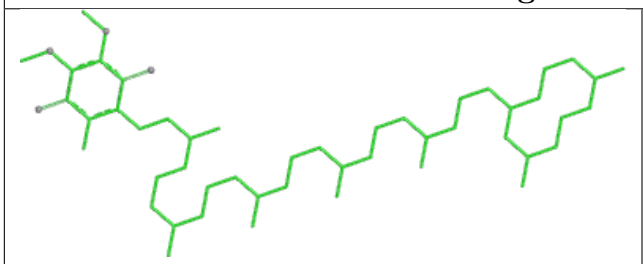
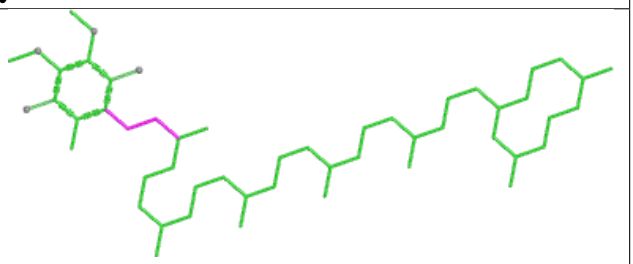
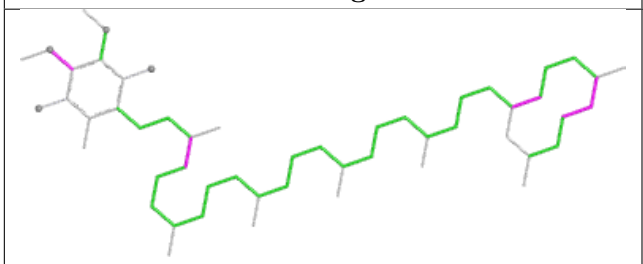
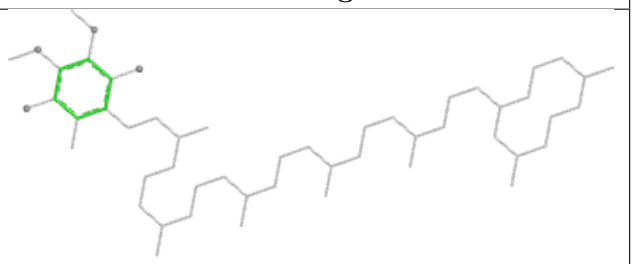
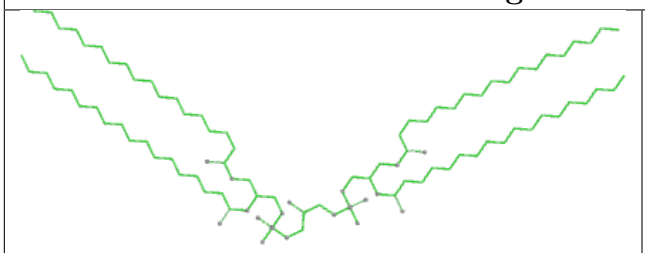
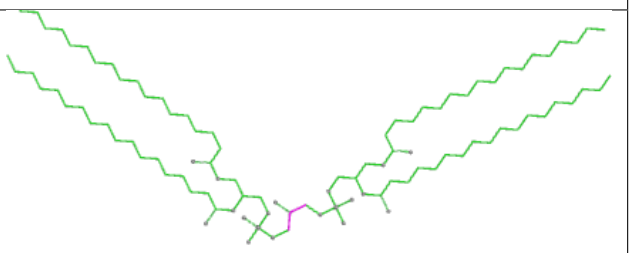
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ8 Ed 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

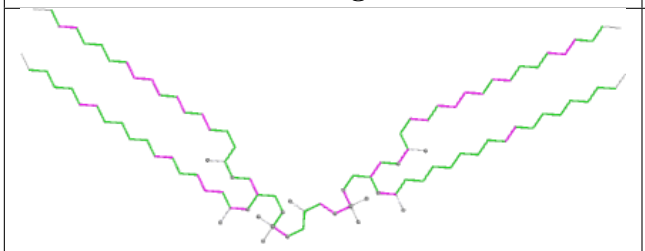
Ligand CDL Dx 1201



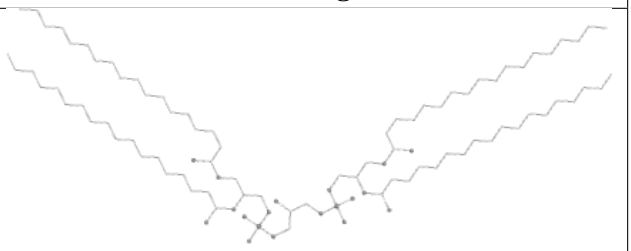
Bond lengths



Bond angles

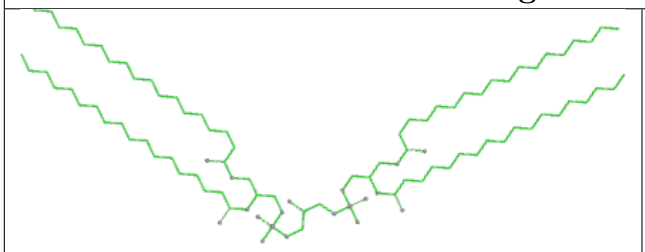


Torsions

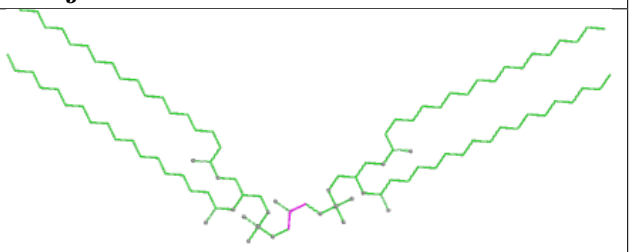


Rings

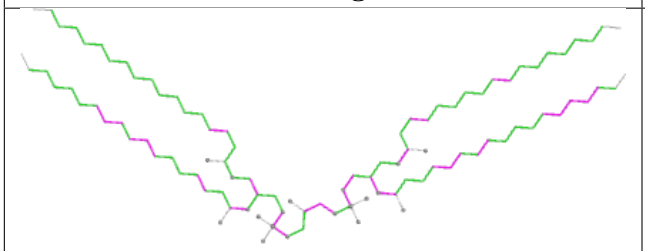
Ligand CDL Dj 404



Bond lengths



Bond angles



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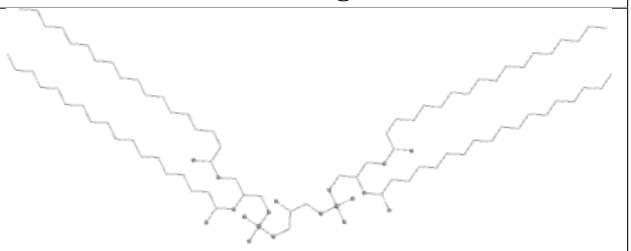
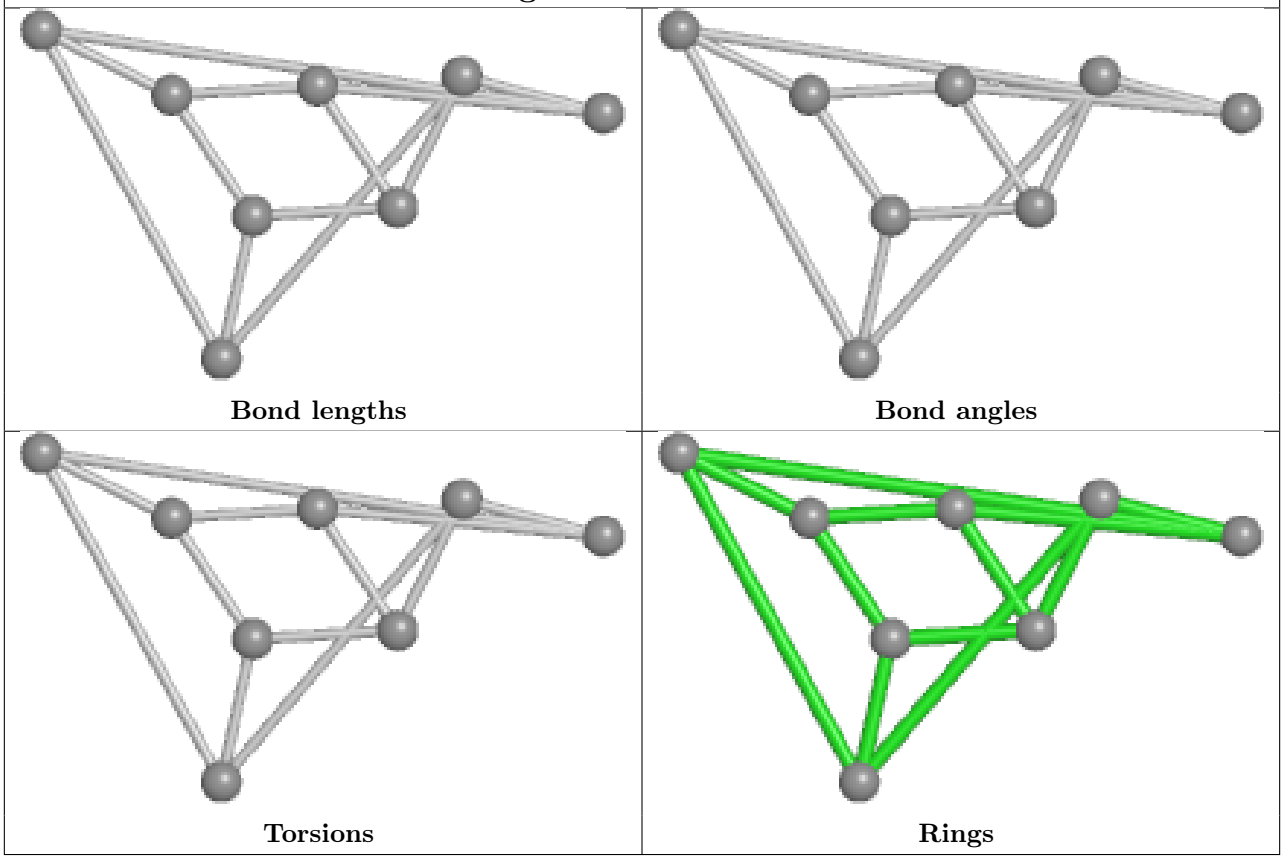
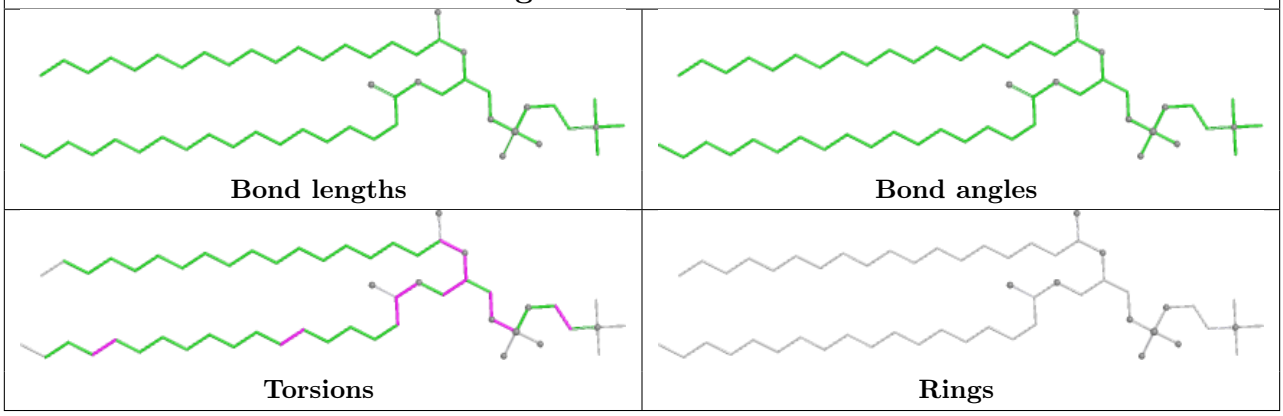


Rings

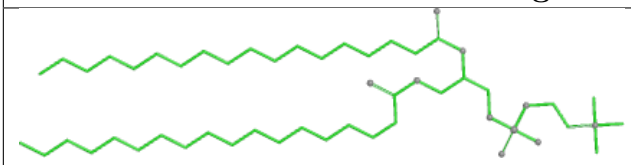
Ligand SF4 AB 802



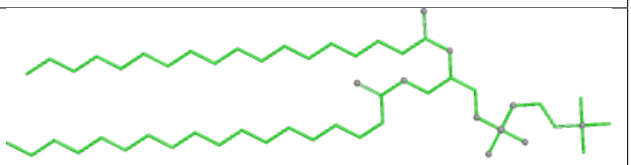
Ligand PC1 CC 302



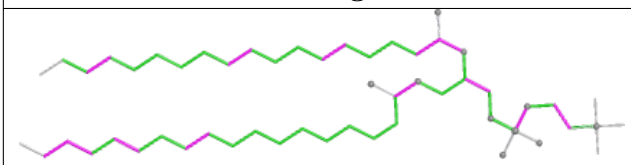
Ligand PC1 c 507



Bond lengths



Bond angles



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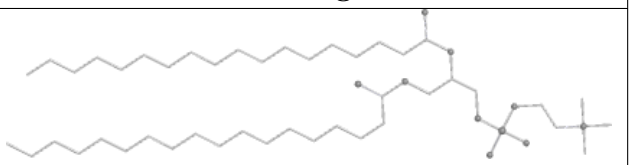
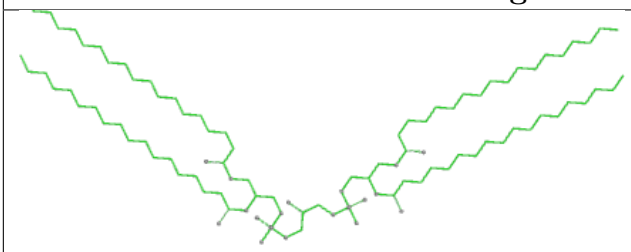


Rings

Ligand CDL DD 706



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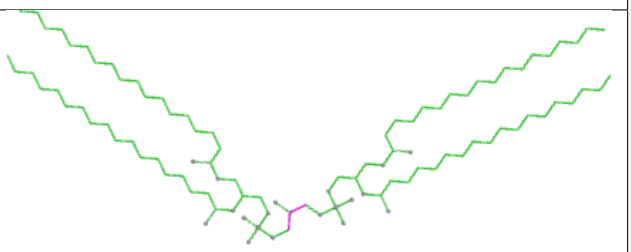
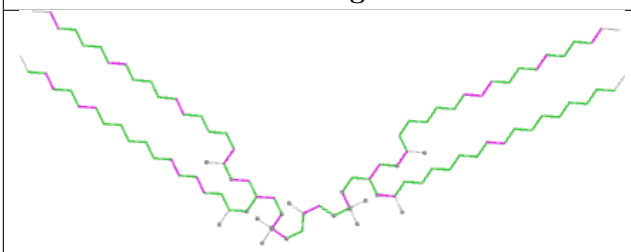


Bond angles



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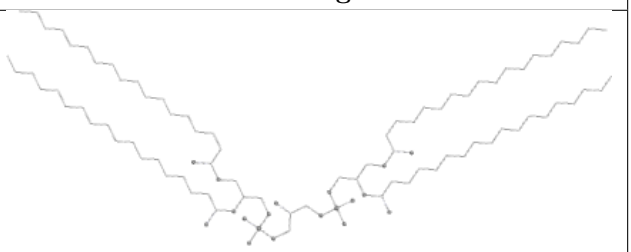
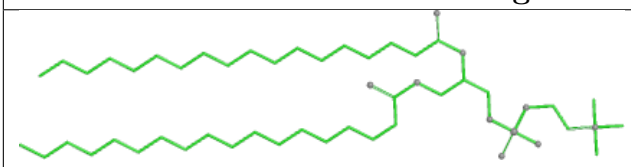
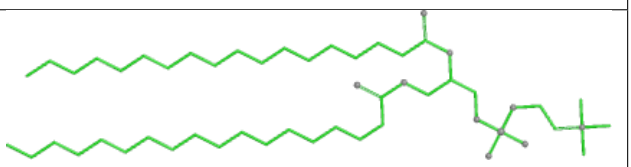


Rings

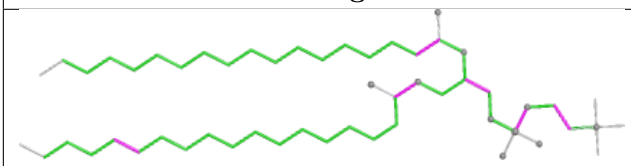
Ligand PC1 AH 301



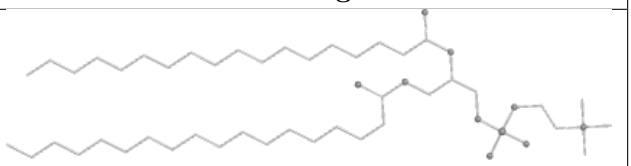
Bond lengths



Bond angles

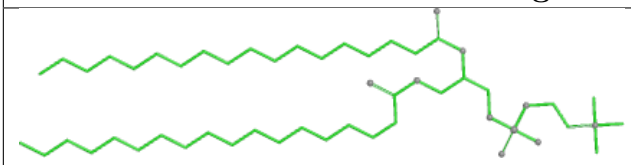


Torsions

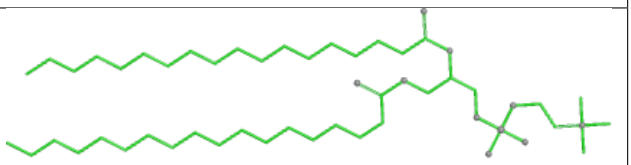


Rings

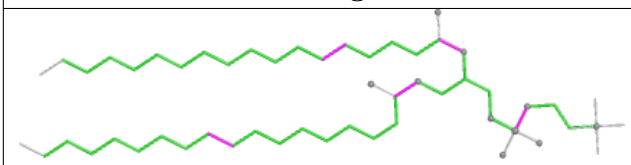
Ligand PC1 c 508



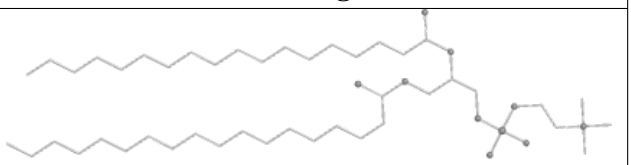
Bond lengths



Bond angles

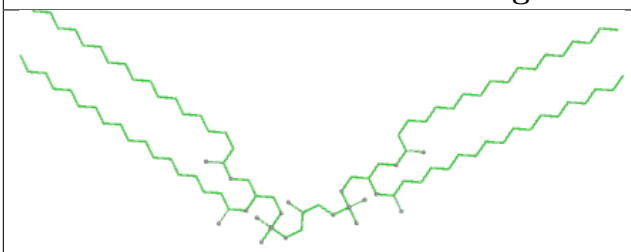


Torsions

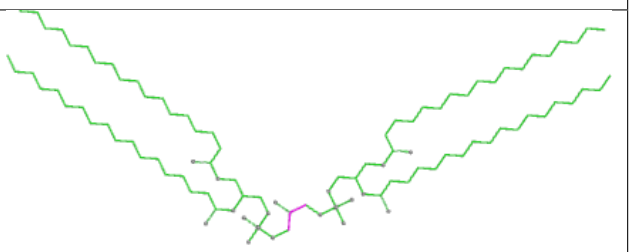


Rings

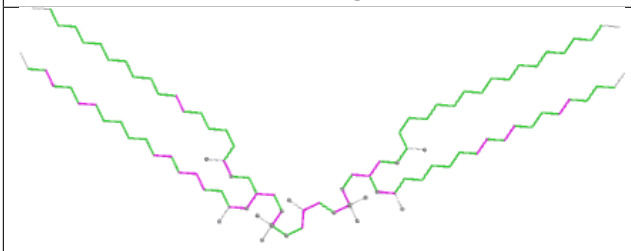
Ligand CDL EB 302



Bond lengths



Bond angles



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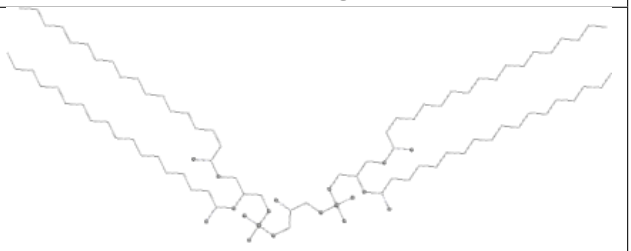
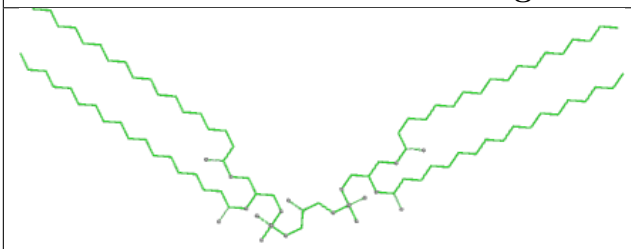
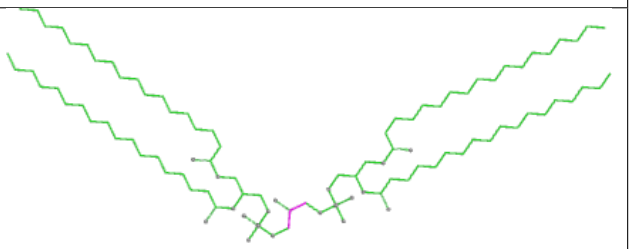


Rings

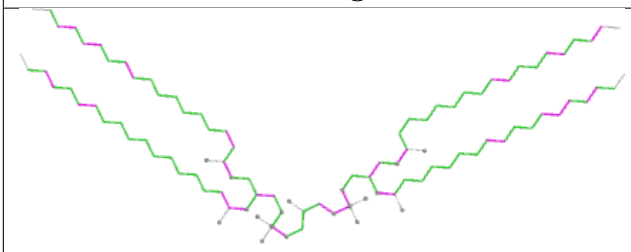
Ligand CDL EL 903



Bond lengths



Bond angles



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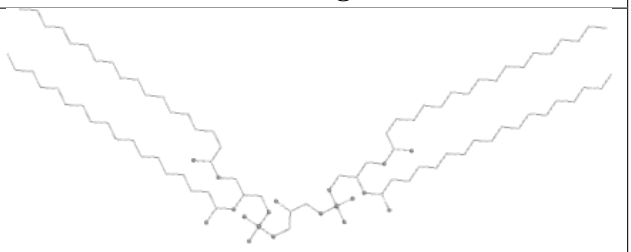
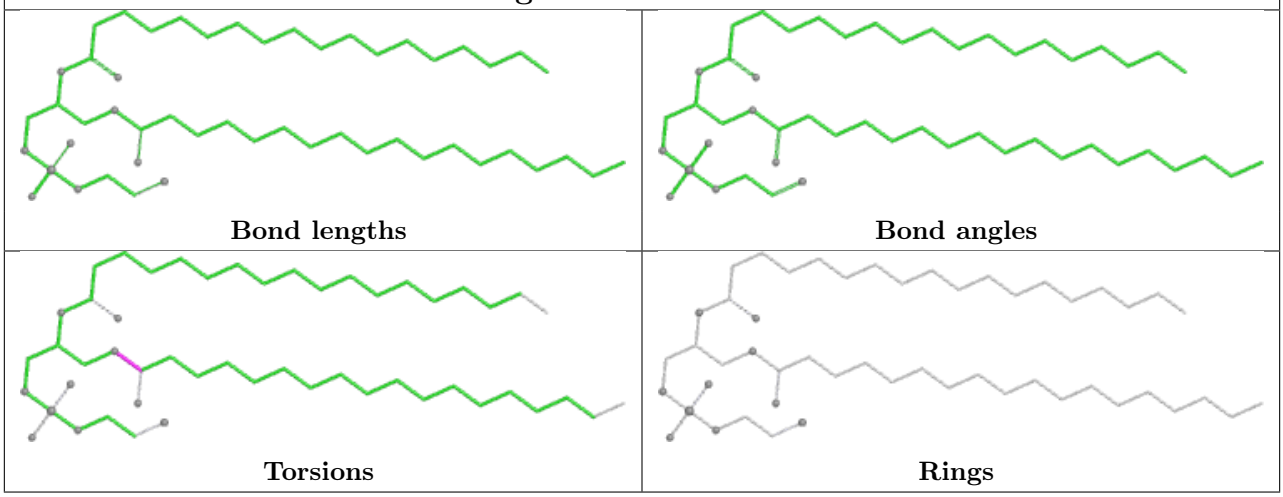
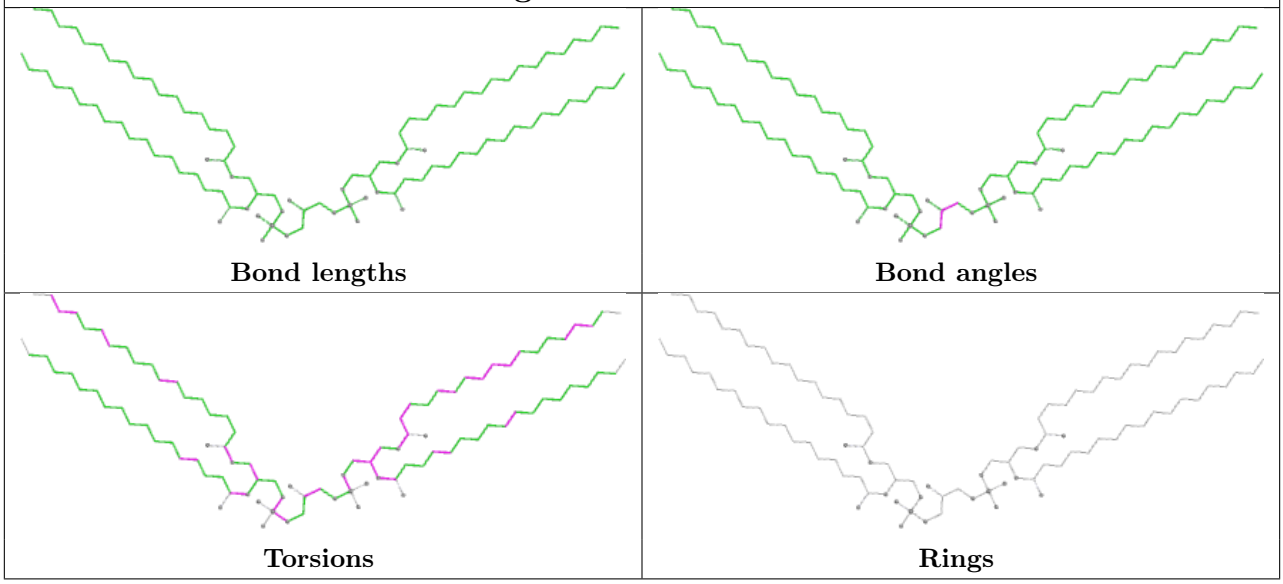


Rings

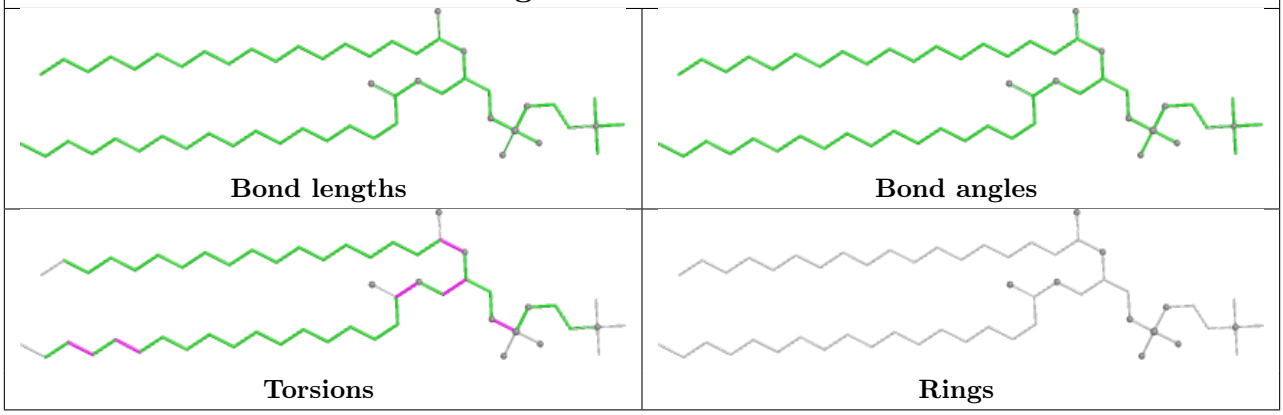
Ligand 3PE CK 101



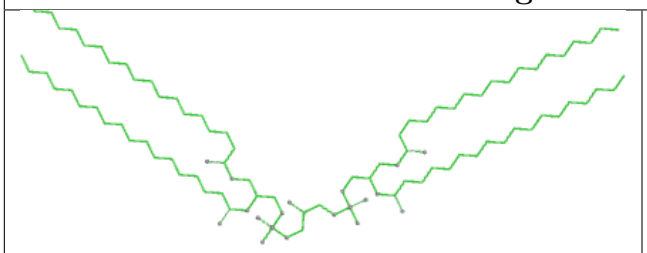
Ligand CDL Dn 501



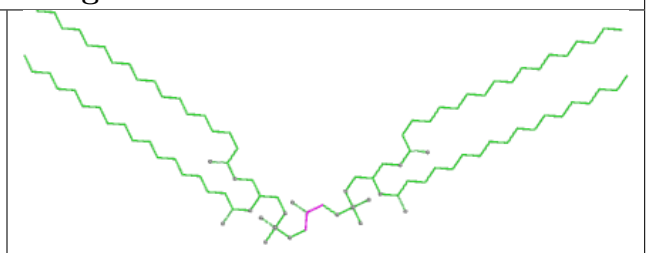
Ligand PC1 DA 708



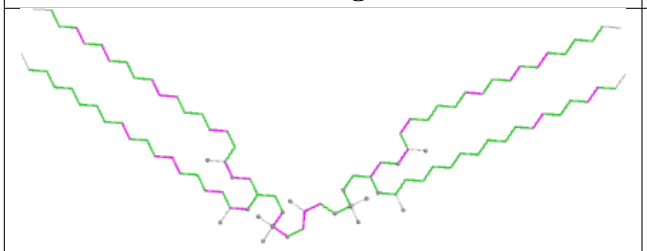
Ligand CDL Dg 202



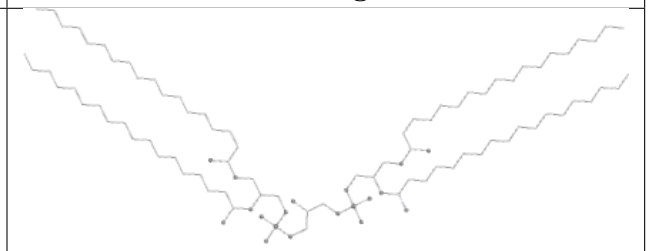
Bond lengths



Bond angles

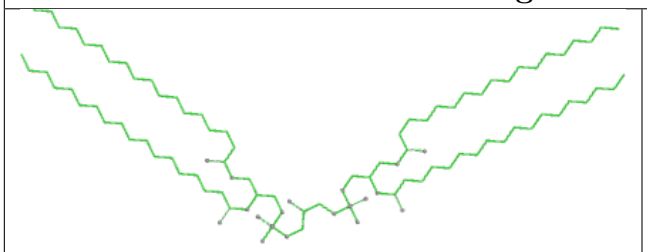


Torsions



Rings

Ligand CDL Da 709



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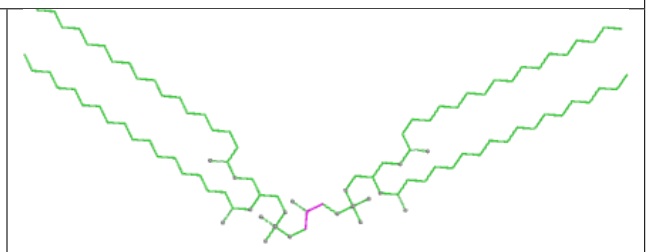
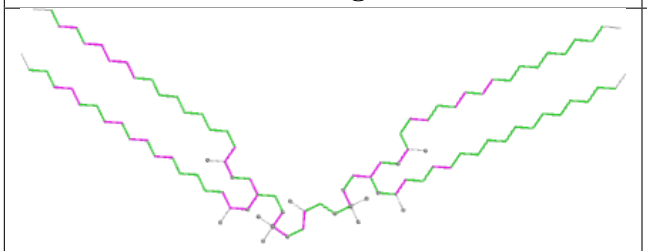


Bond angles



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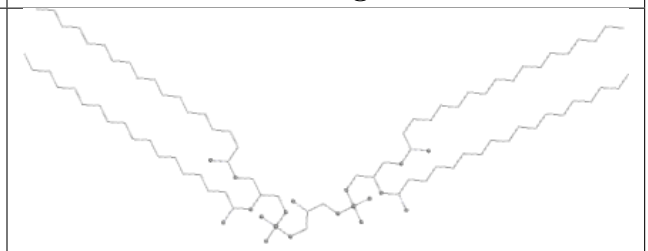
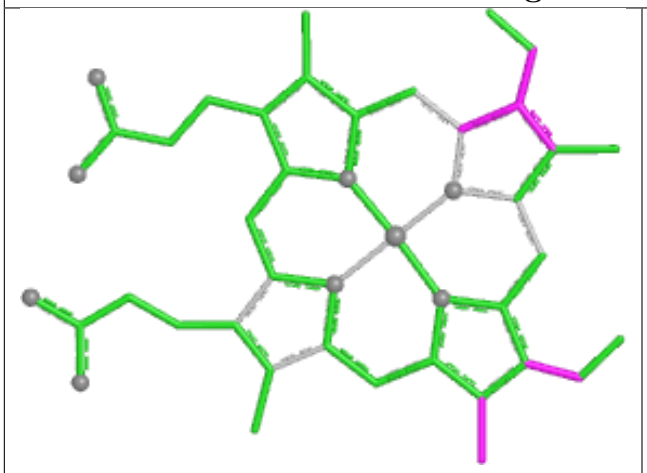


Rings

Ligand HEM c 504



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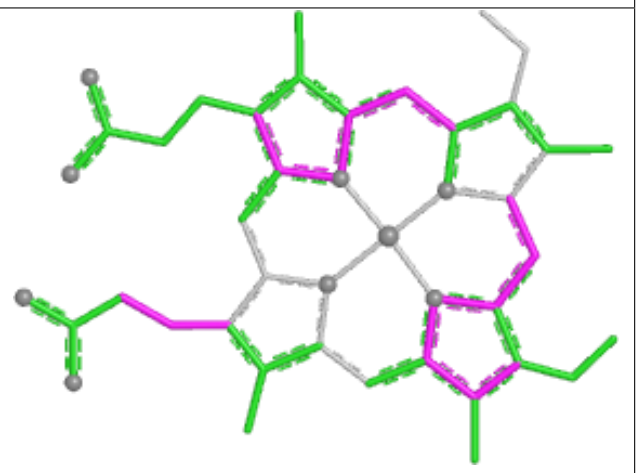
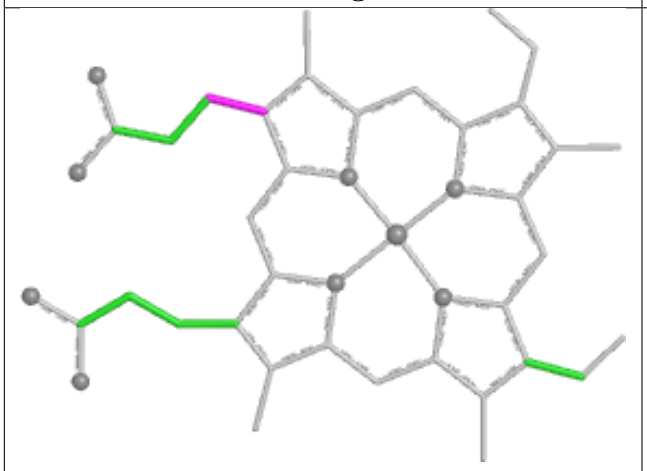


Bond angles



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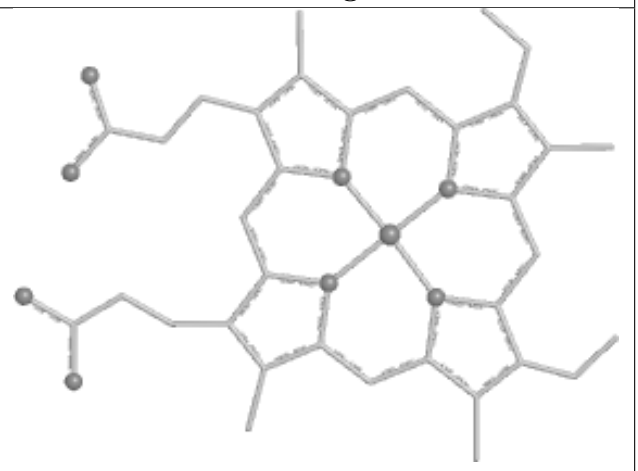
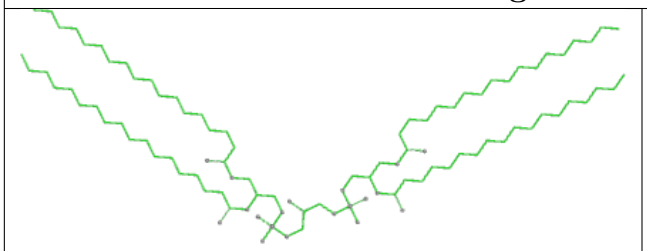


Rings

Ligand CDL Dm 502



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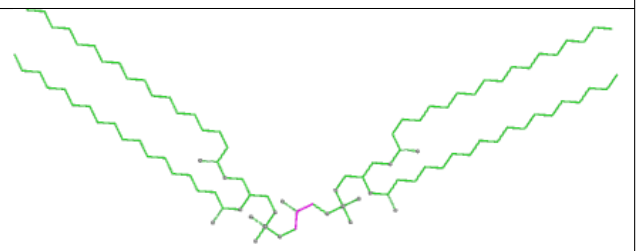
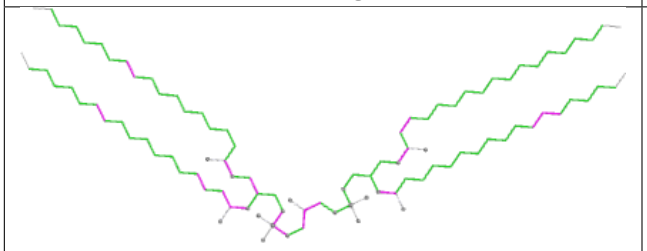


Bond angles



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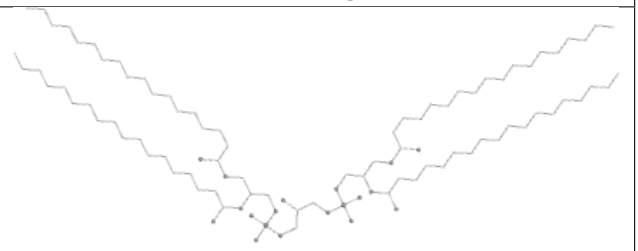

Rings

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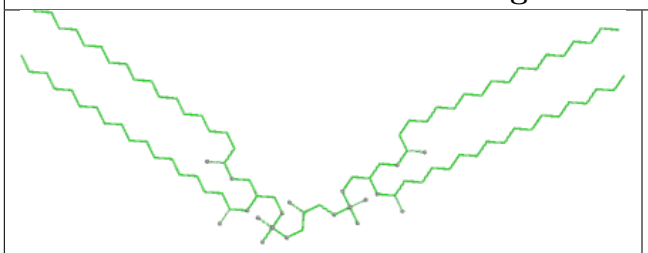

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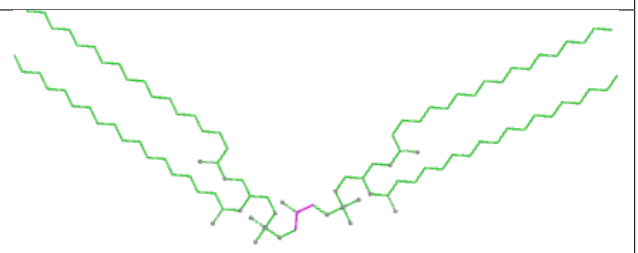
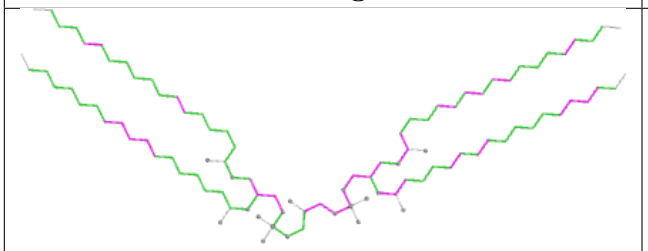
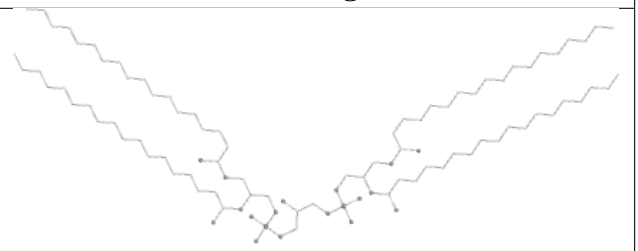


Bond angles

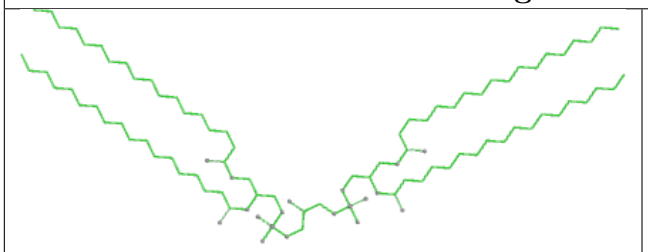


Torsions



Rings

Ligand CDL Dd 702



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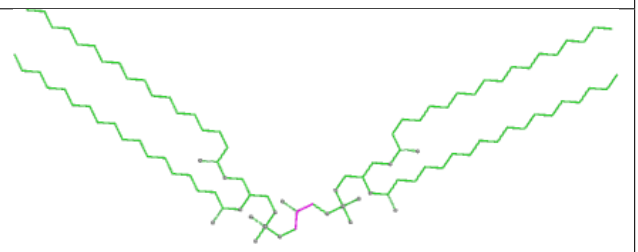
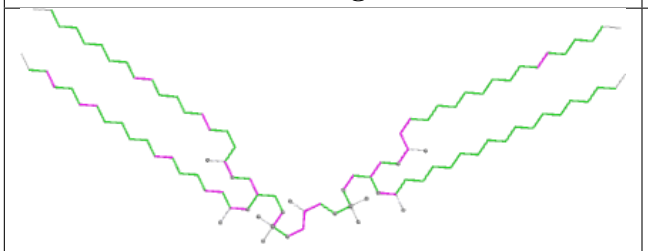


Bond angles



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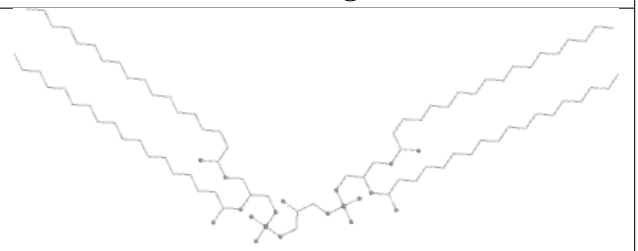
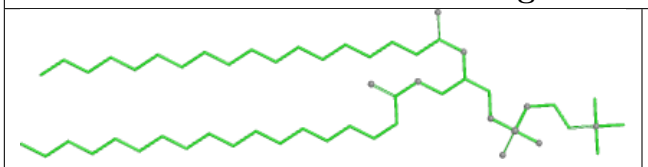


Rings

Ligand PC1 Db 702



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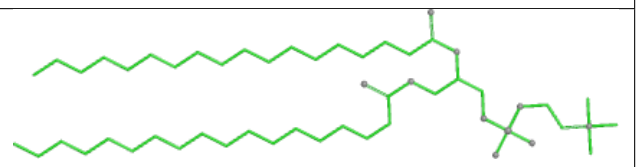
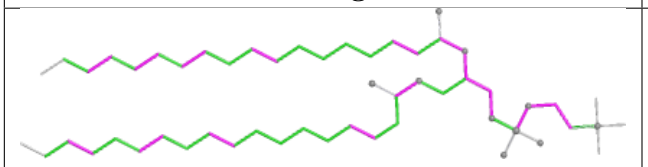


Bond angles



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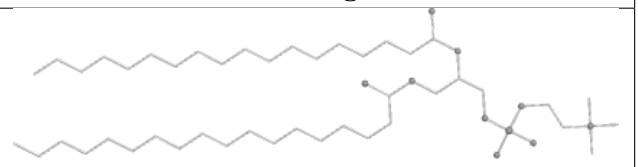
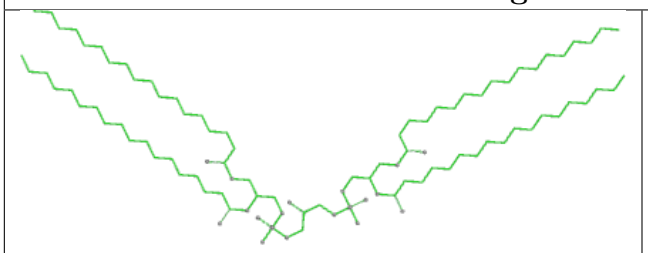


Rings

Ligand CDL DN 502



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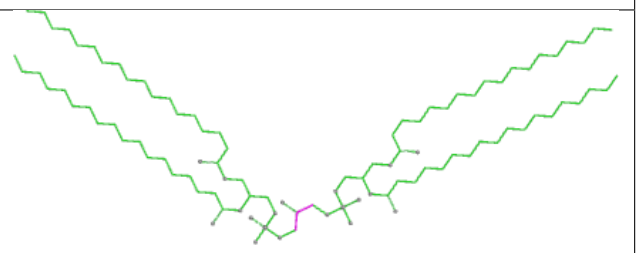
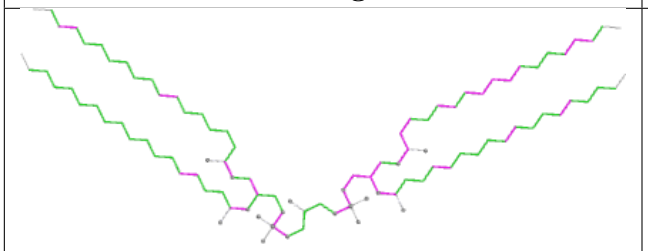


Bond angles



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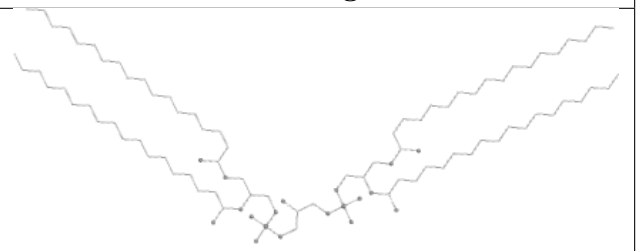
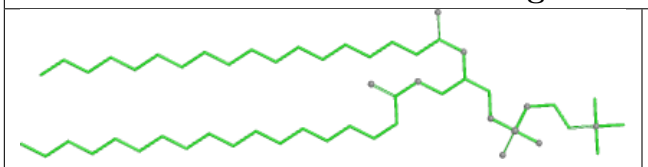
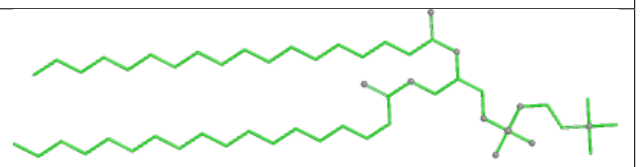


Rings

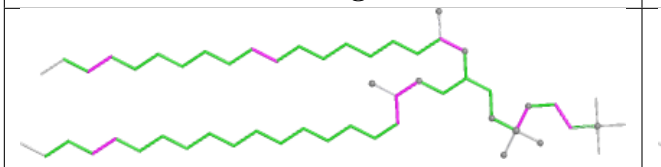
Ligand PC1 K 502



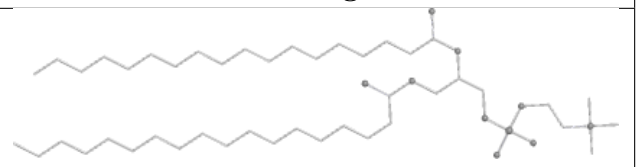
Bond lengths



Bond angles

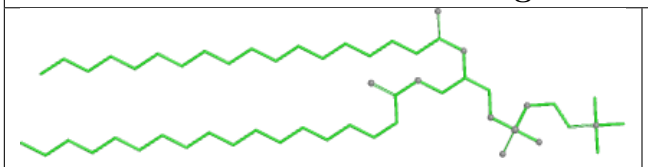


Torsions



Rings

Ligand PC1 AA 905



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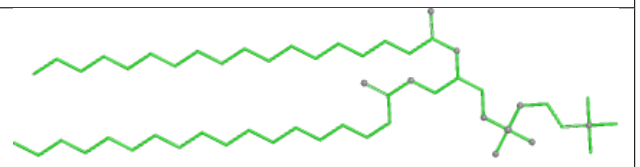
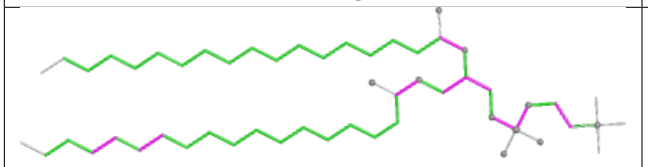


Bond angles



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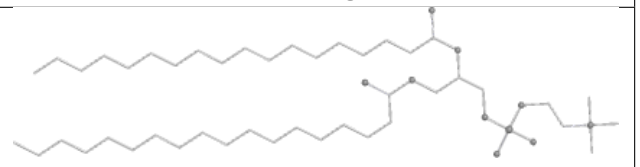
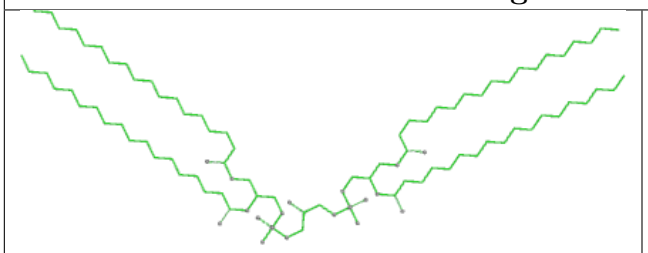
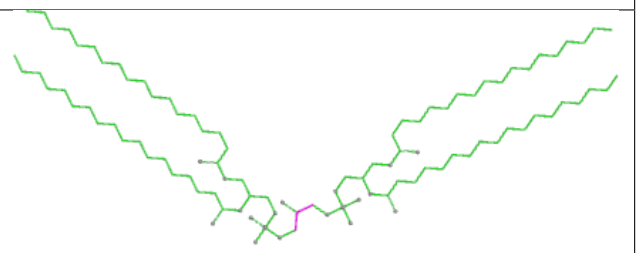


Rings

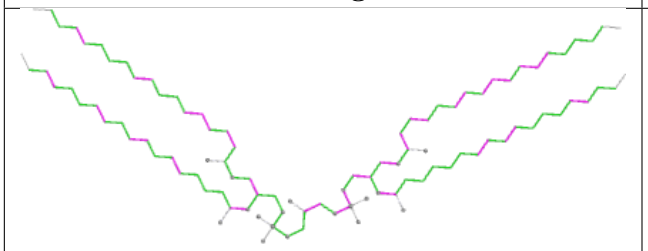
Ligand CDL Di 1103



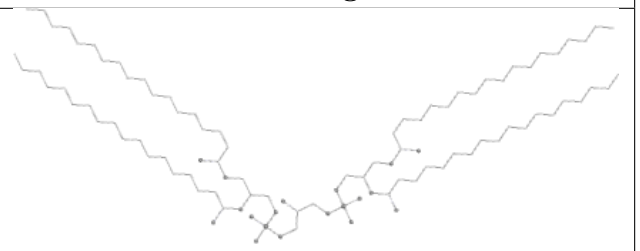
Bond lengths



Bond angles

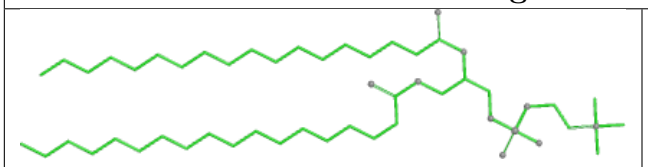


Torsions



Rings

Ligand PC1 BS 1302



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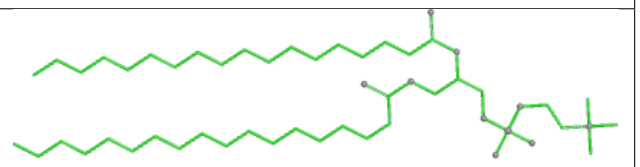

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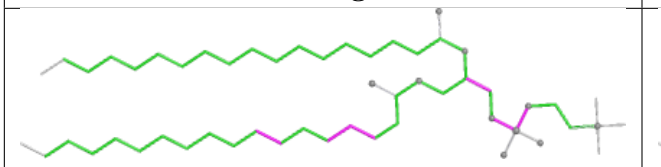

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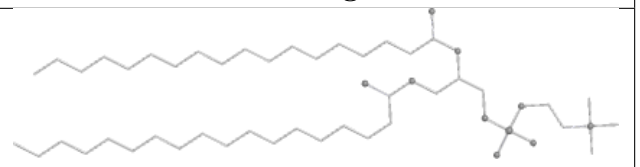
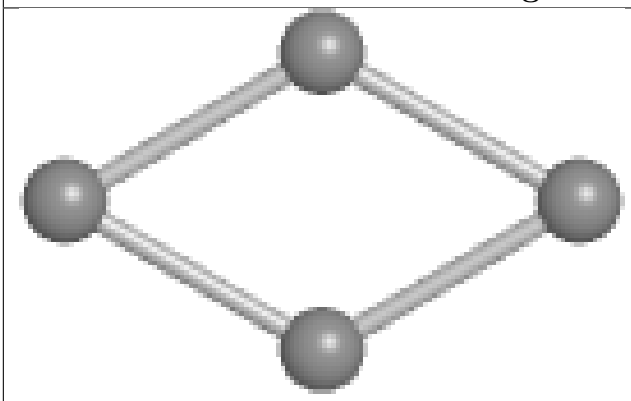


Rings

Ligand FES BI 201



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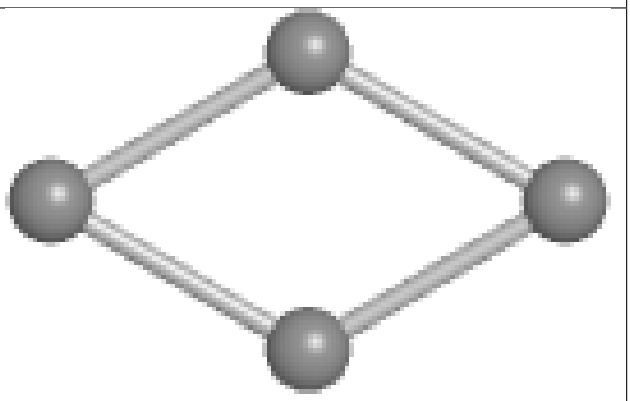
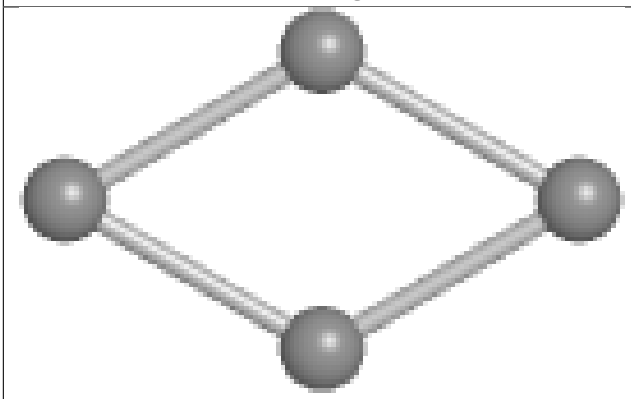


Bond angles



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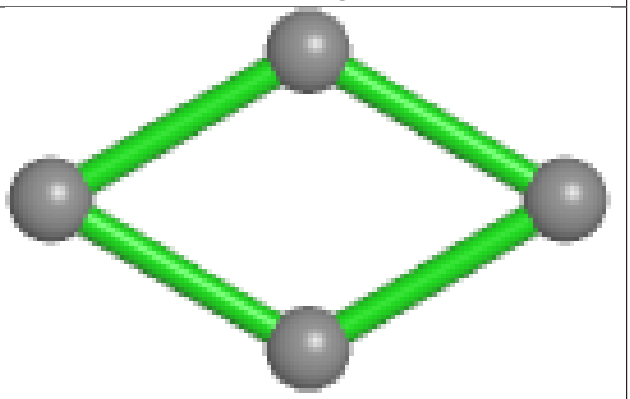
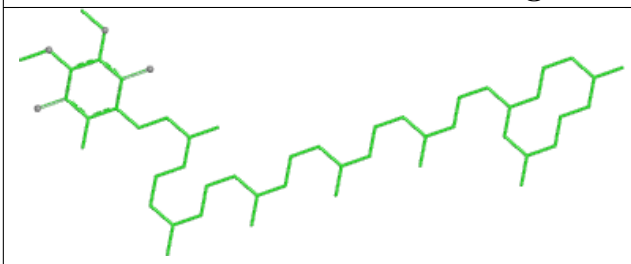


Rings

Ligand UQ8 C 512



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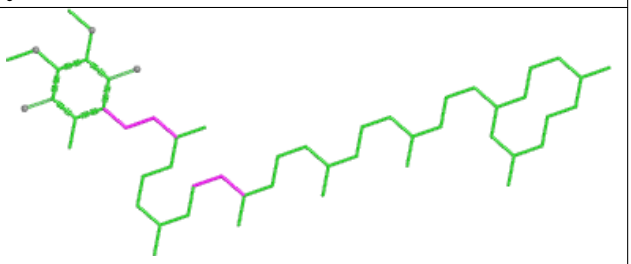
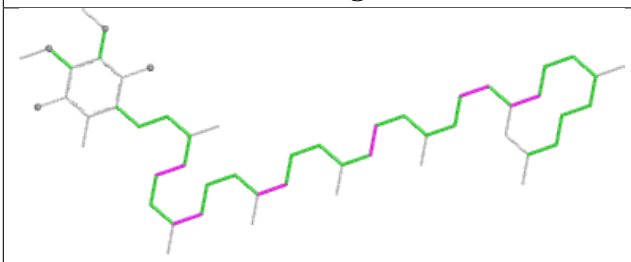


Bond angles



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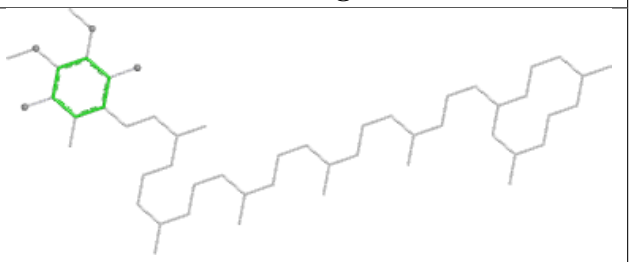
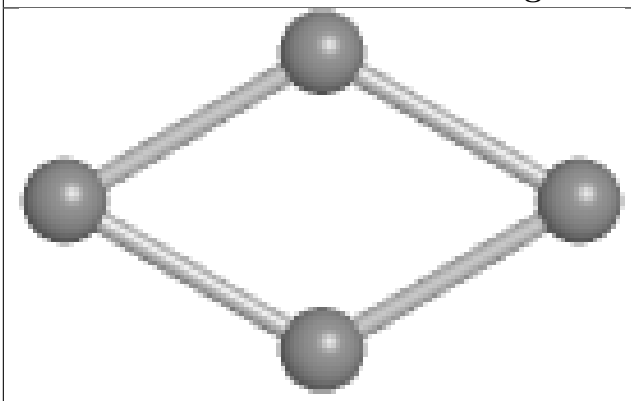


Rings

Ligand FES e 1102



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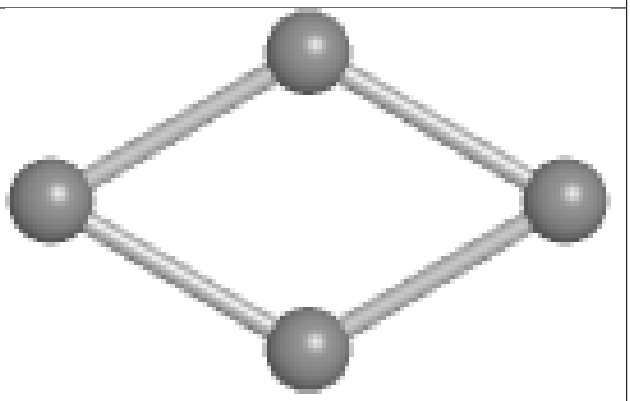

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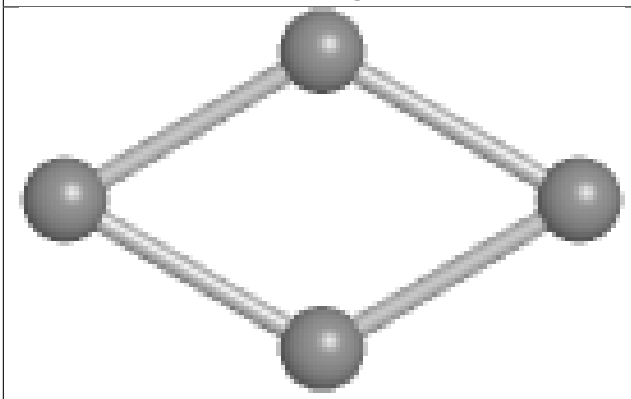

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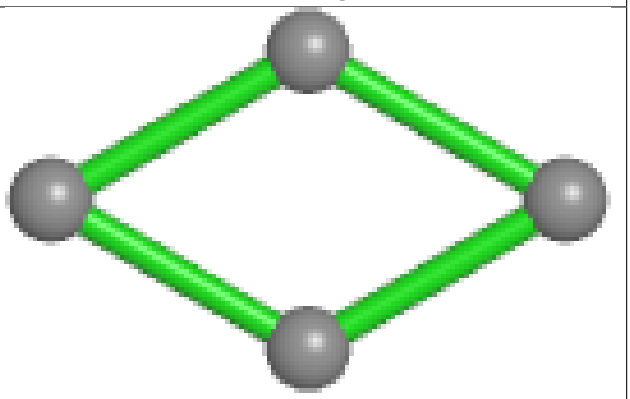
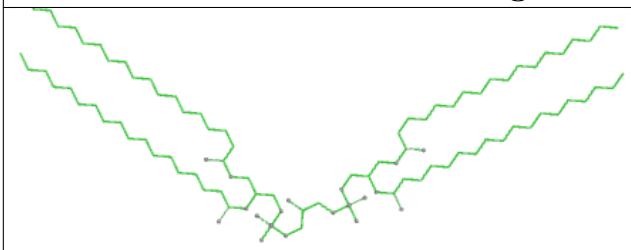


Rings

Ligand CDL DU 404



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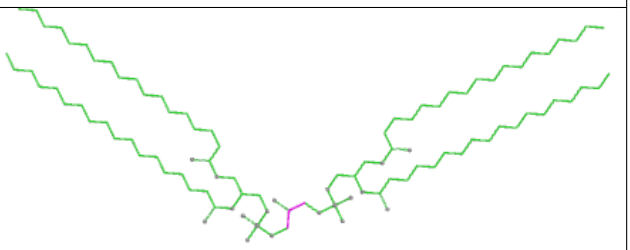

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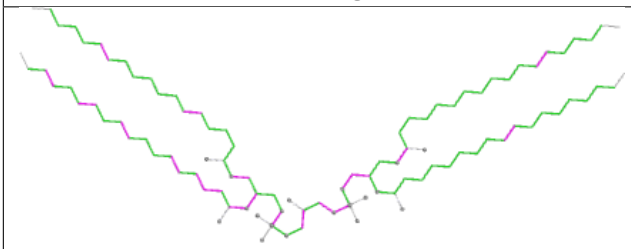

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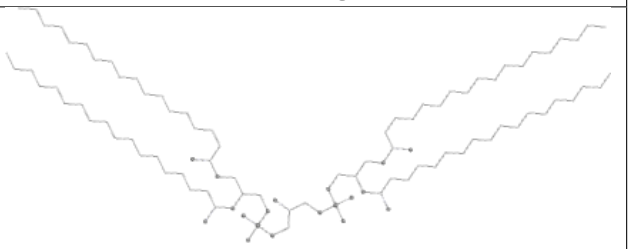
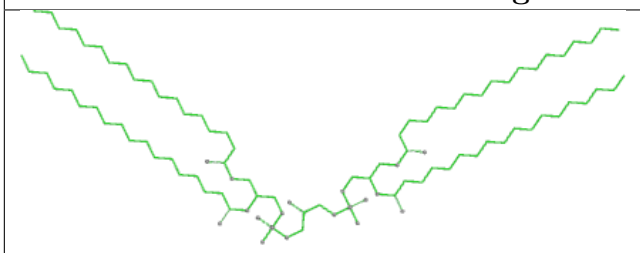


Rings

Ligand CDL ED 605



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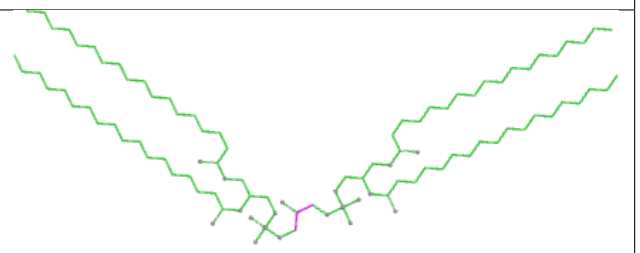
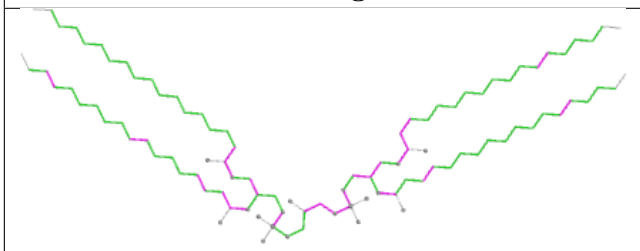


Bond angles



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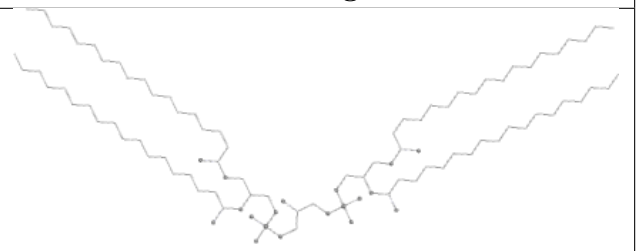
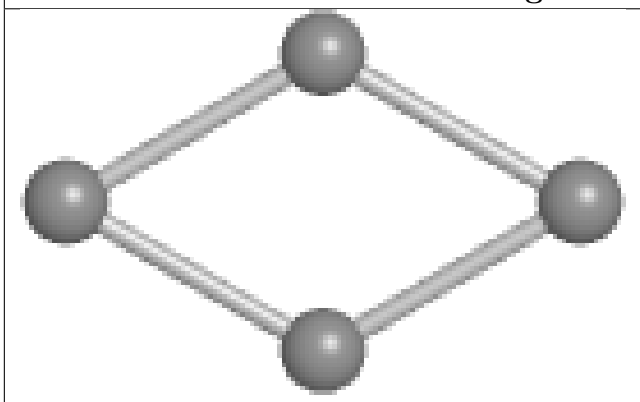


Rings

Ligand FES Ef 503



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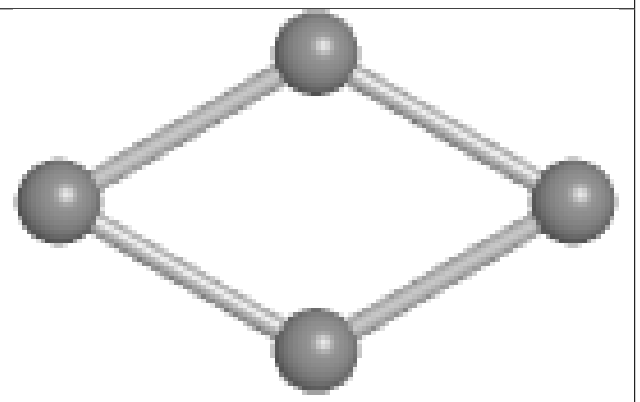

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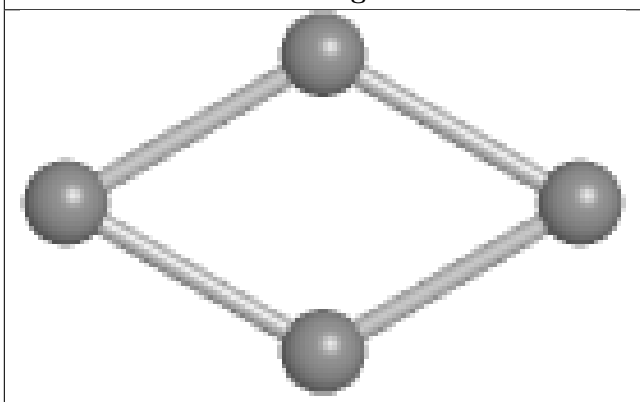

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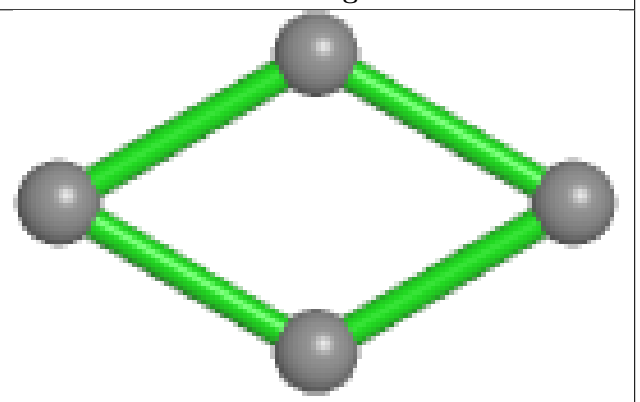
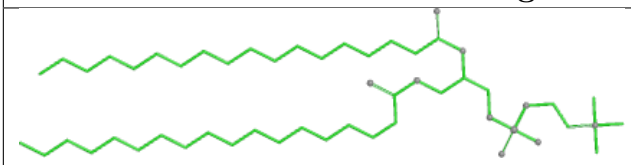


Rings

Ligand PC1 A1 403



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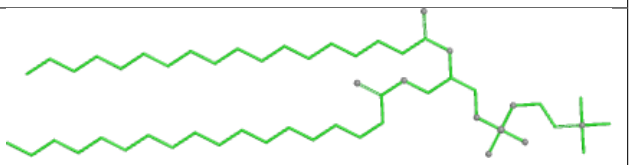
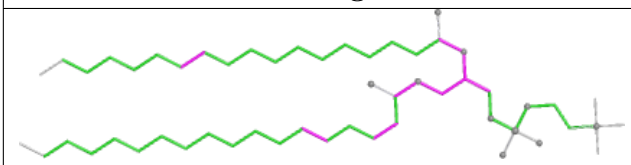


Bond angles



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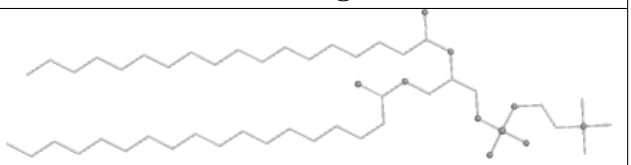
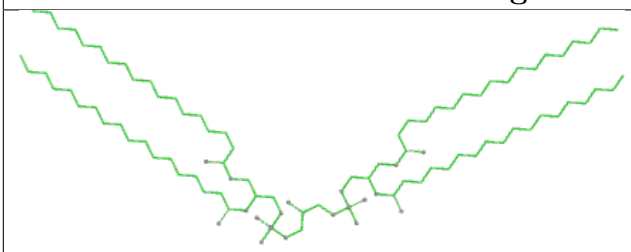


Rings

Ligand CDL AA 908



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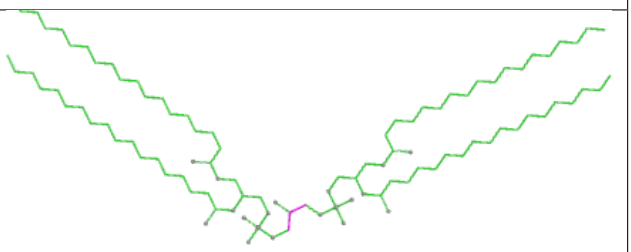
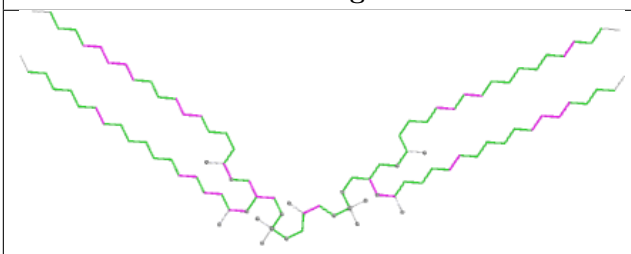


Bond angles



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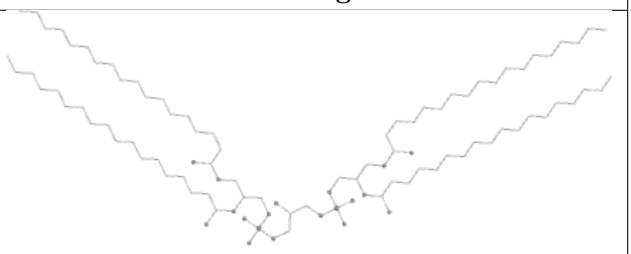
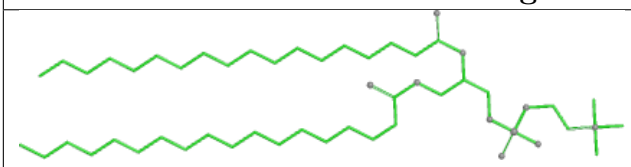


Rings

Ligand PC1 Eo 204



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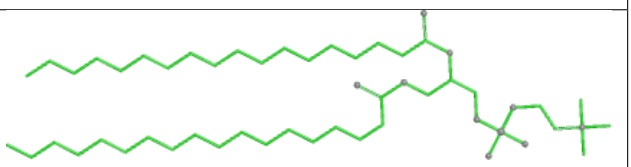
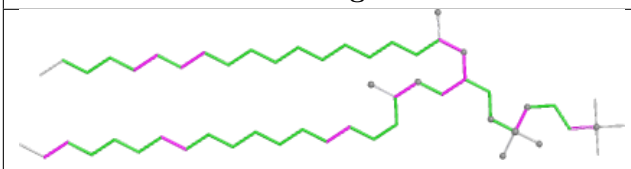


Bond angles



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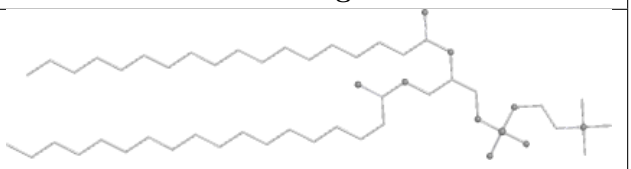
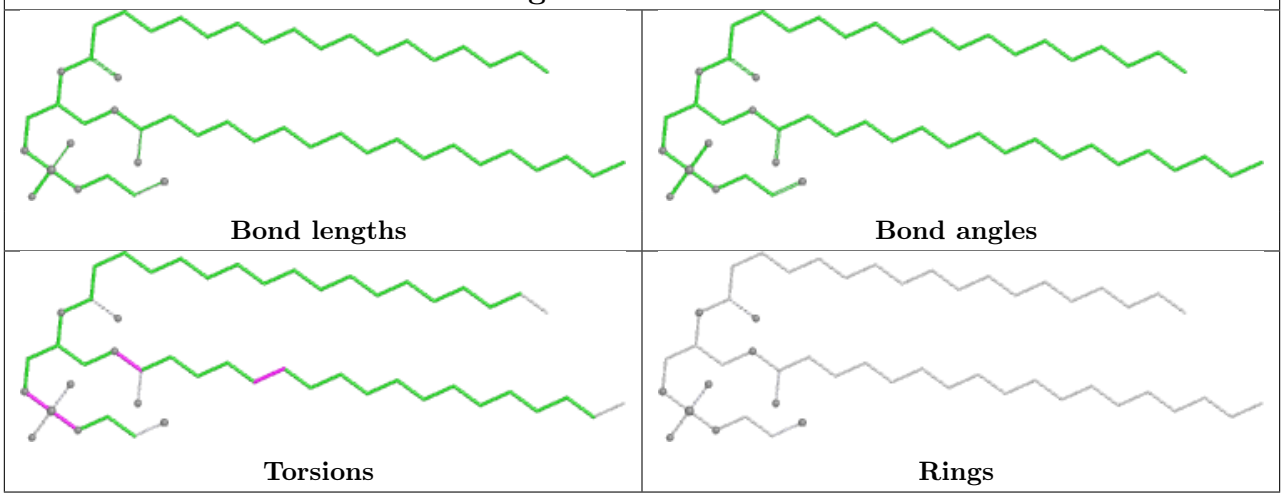
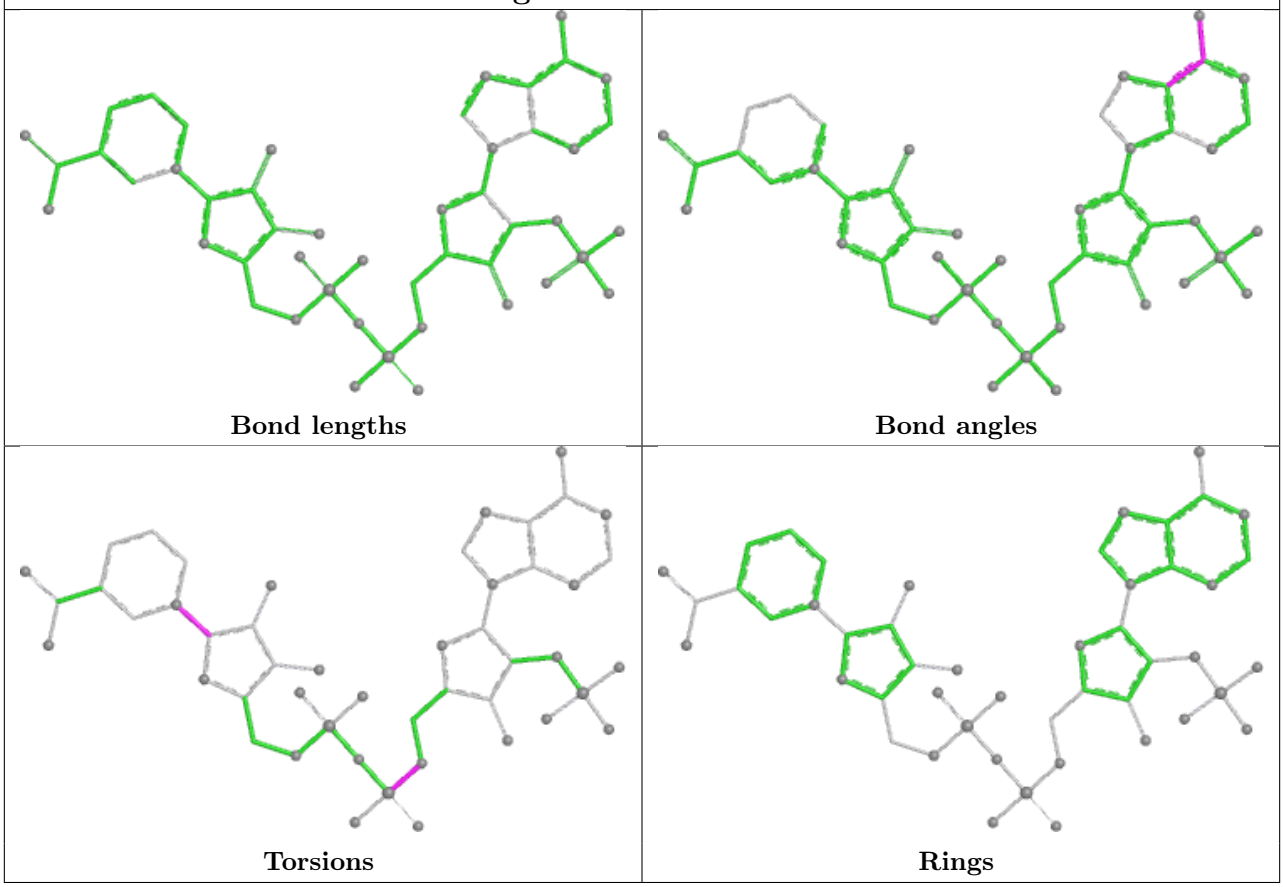


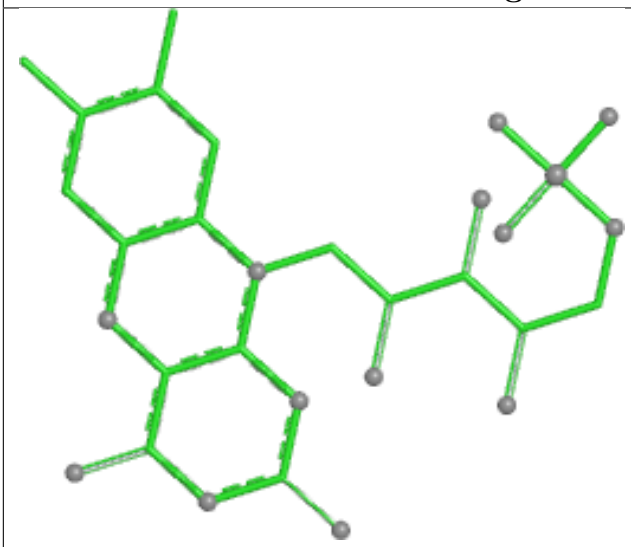
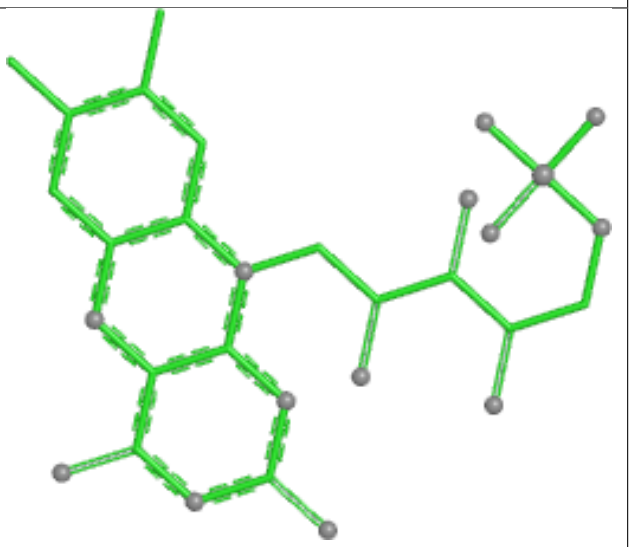
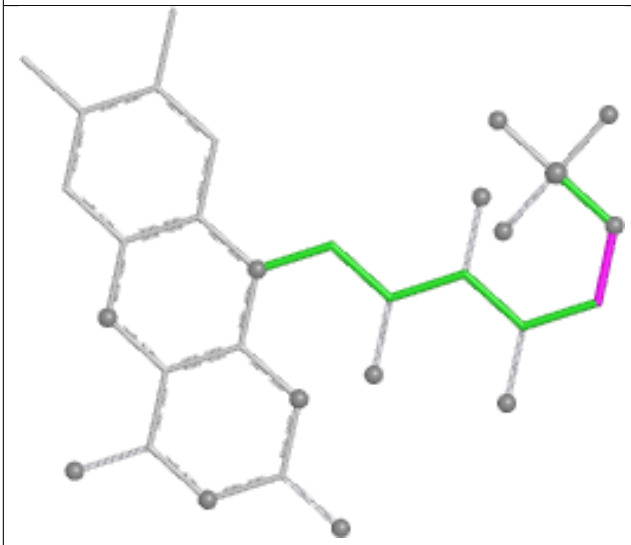
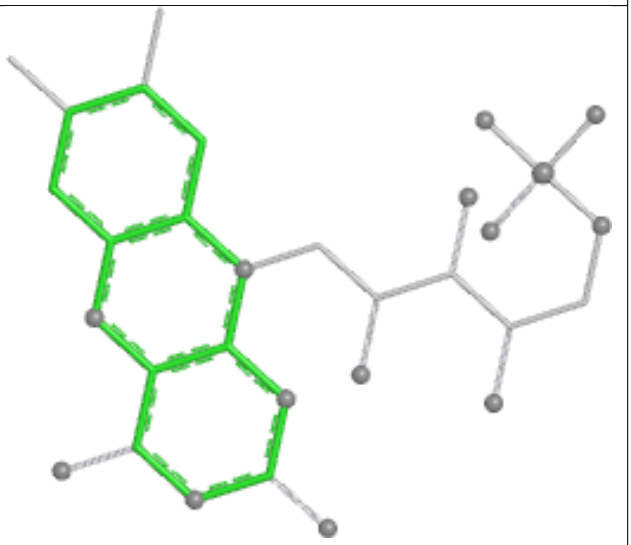
Rings

Ligand 3PE G 401

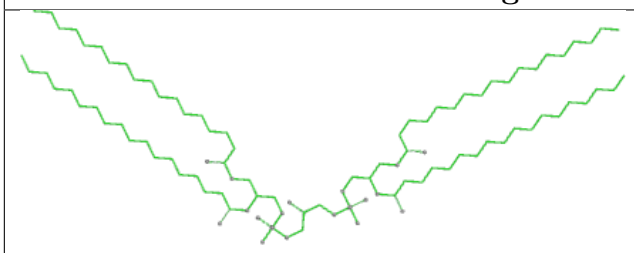


Ligand NDP A1 401

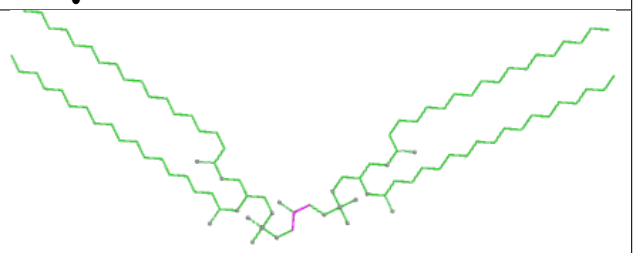


Ligand FMN AD 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

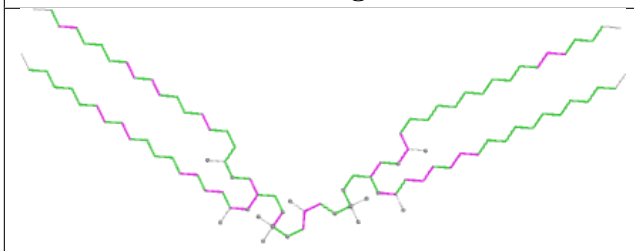
Ligand CDL DQ 1501



Bond lengths



Bond angles



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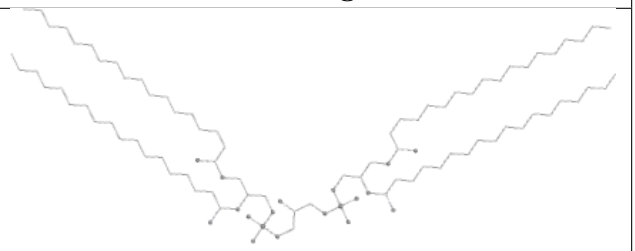
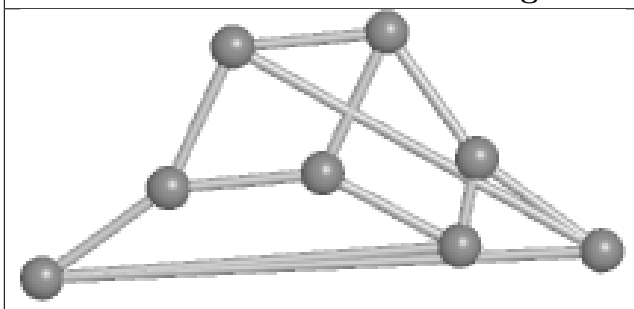
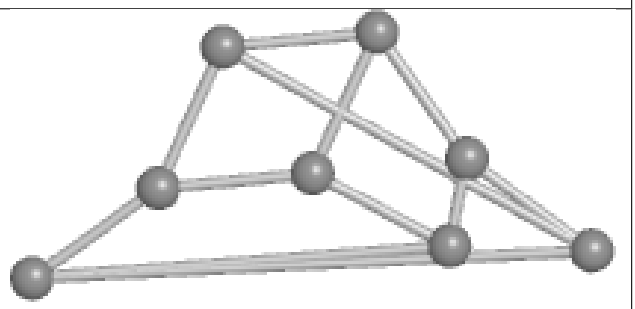


Rings

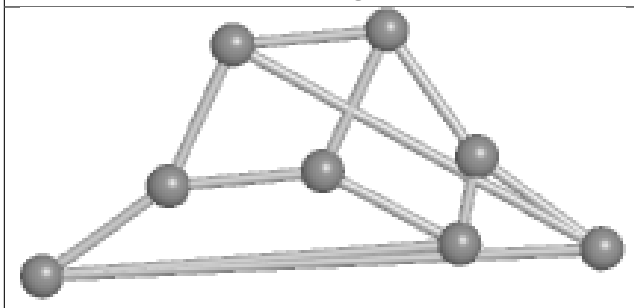
Ligand SF4 AT 201



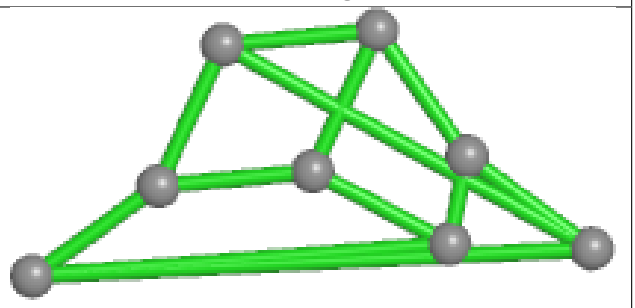
Bond lengths



Bond angles

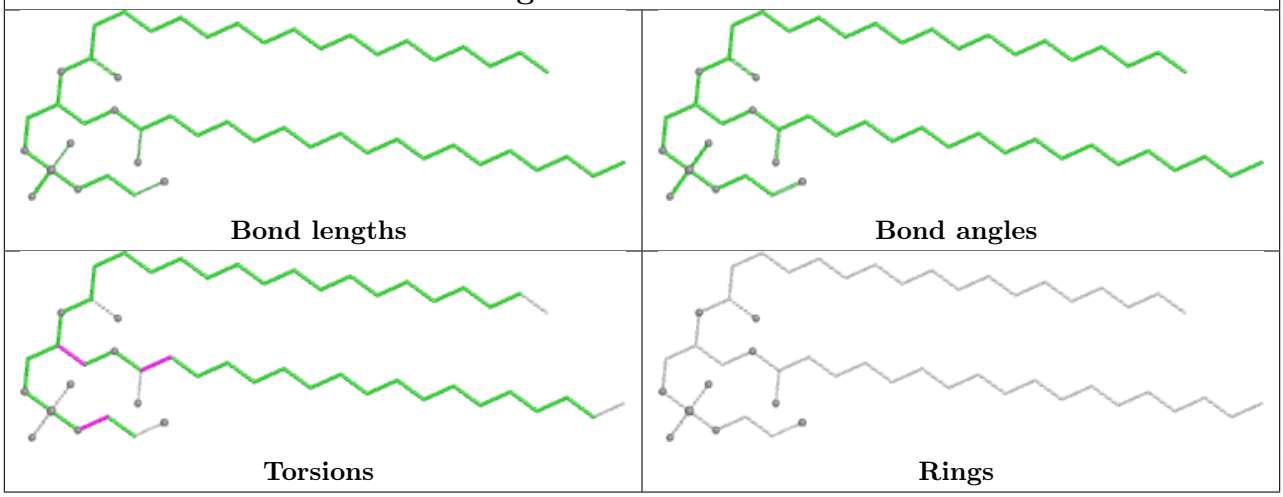


Torsions

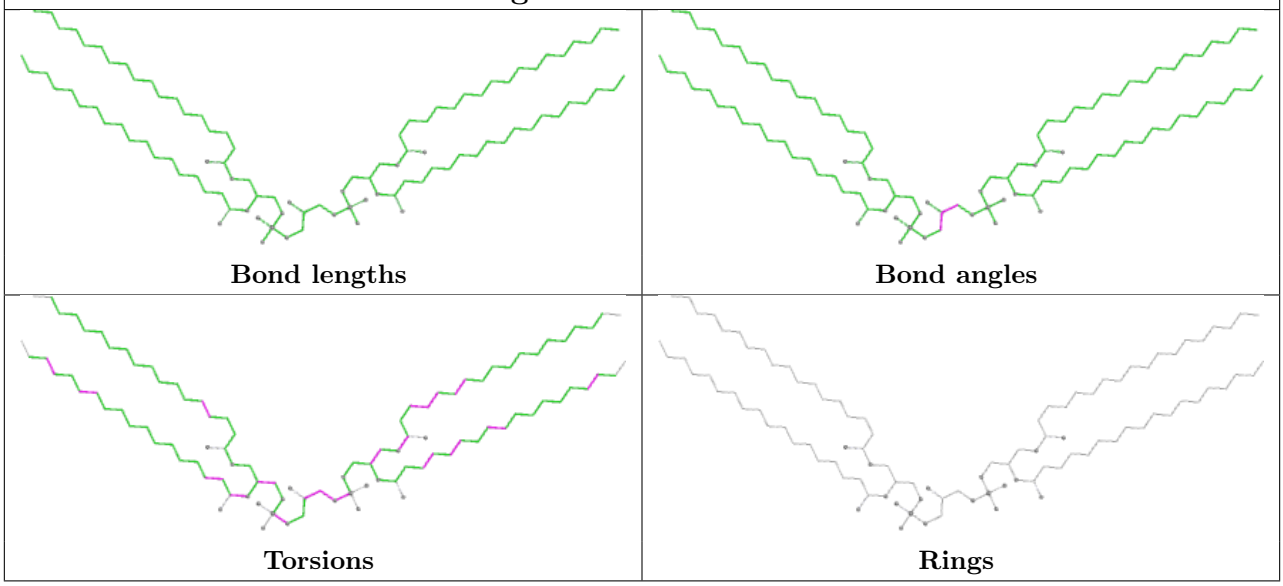


Rings

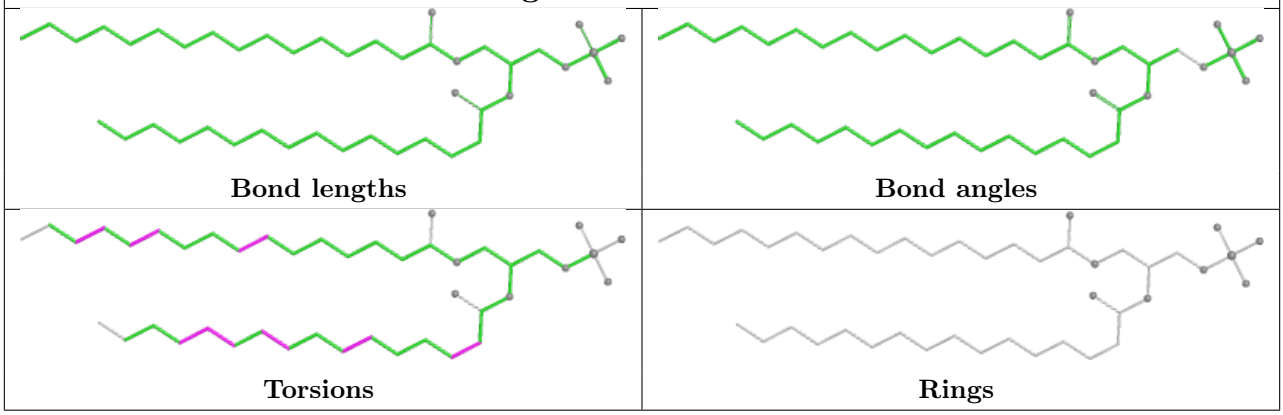
Ligand 3PE CC 301



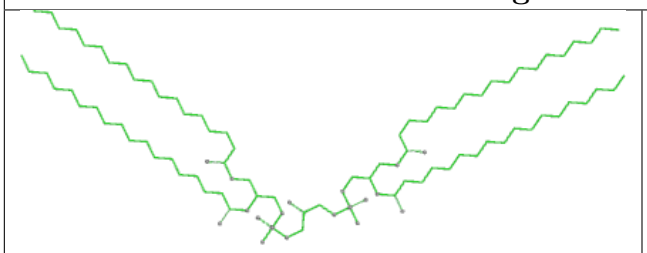
Ligand CDL CG 301



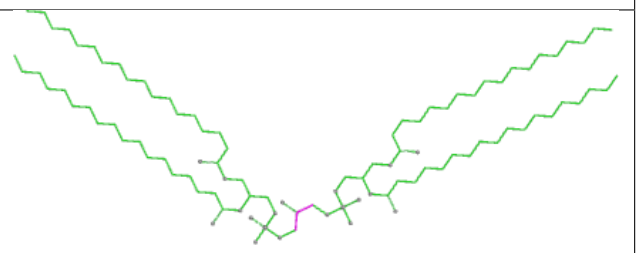
Ligand LPP EI 402



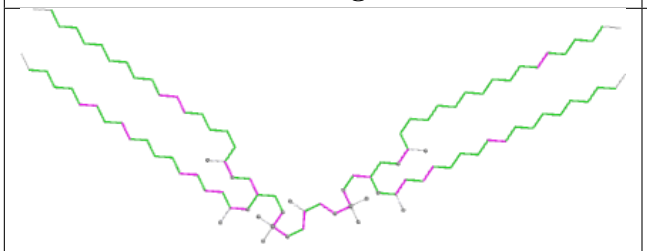
Ligand CDL ED 601



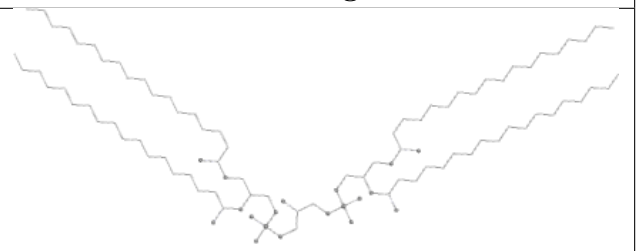
Bond lengths



Bond angles

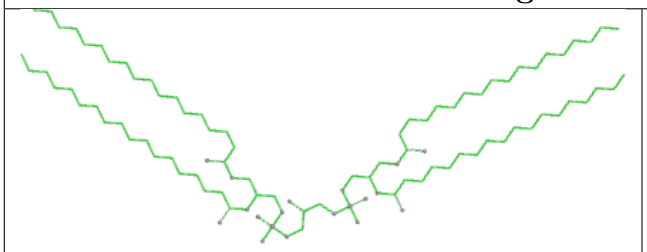


Torsions



Rings

Ligand CDL Eb 302



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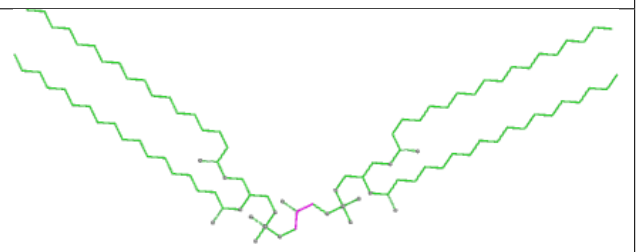
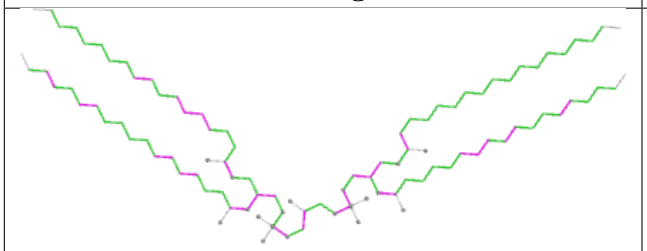


Bond angles



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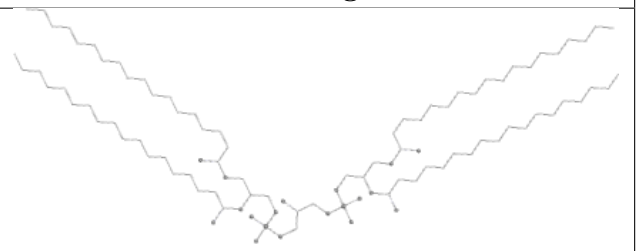
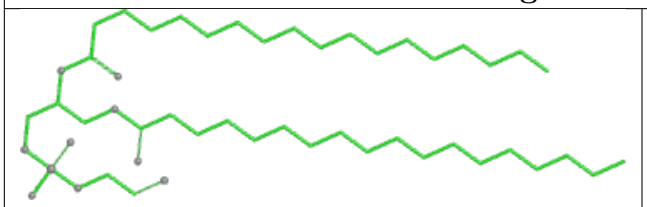


Rings

Ligand 3PE A9 602



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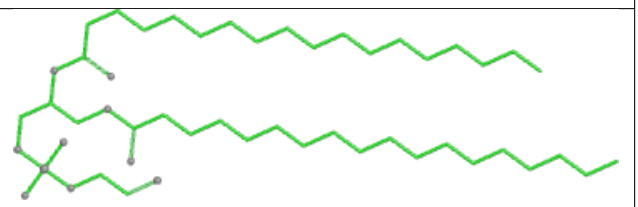
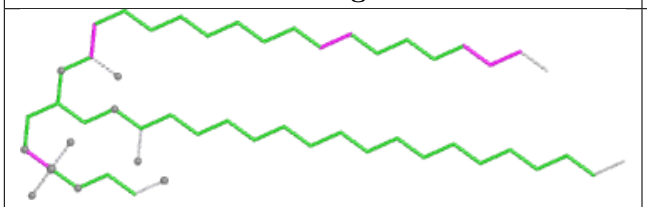


Bond angles



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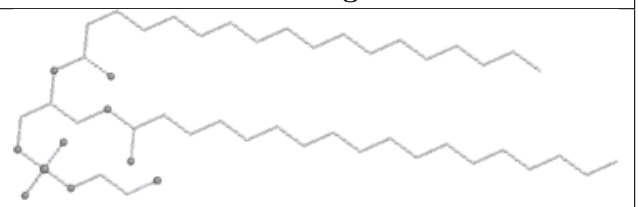
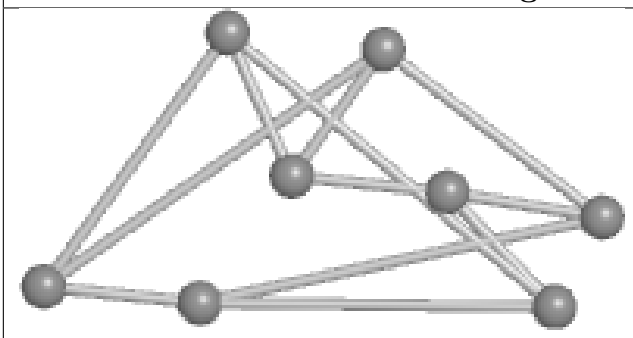


Rings

Ligand SF4 AL 302



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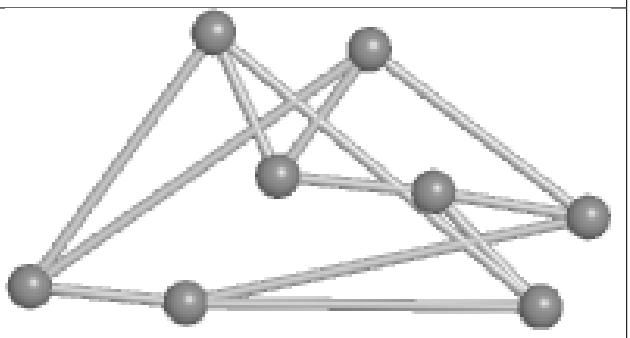
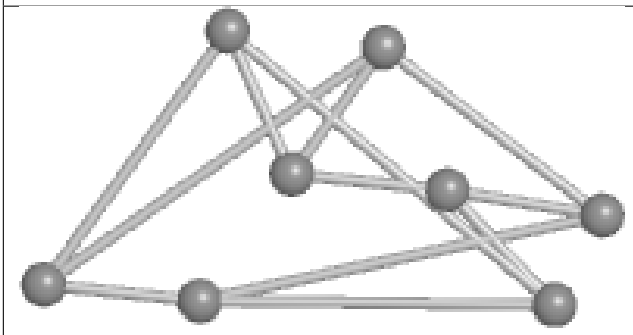
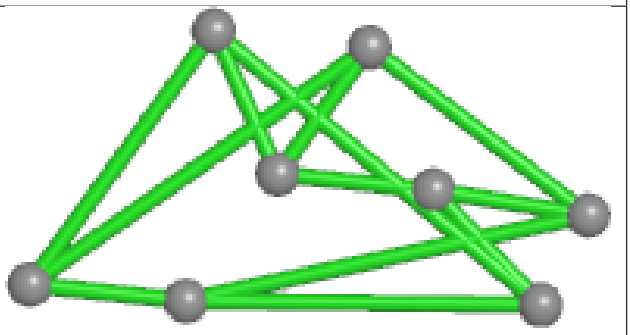


Bond angles

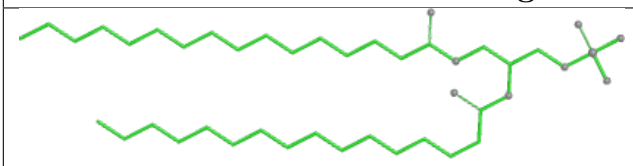


Torsions

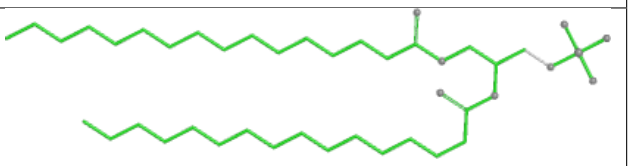


Rings

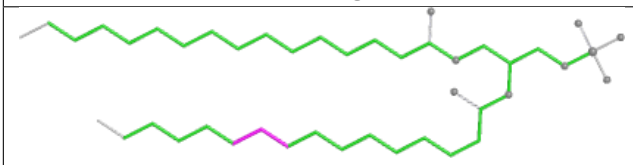
Ligand LPP Ed 203



Bond lengths



Bond angles



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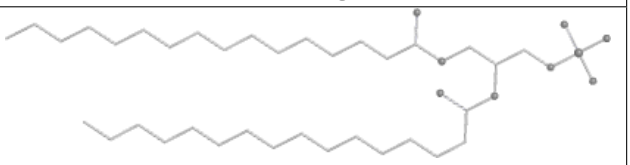
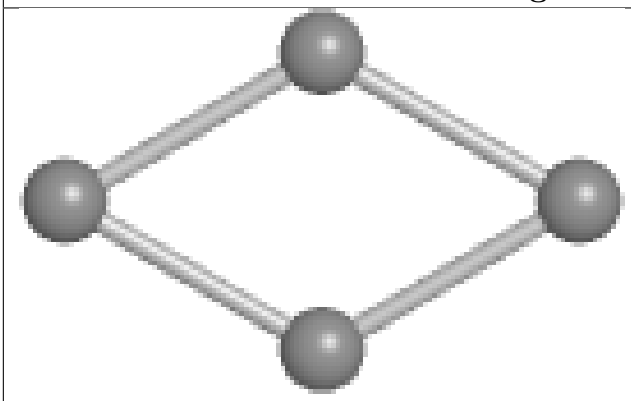


Rings

Ligand FES E 302



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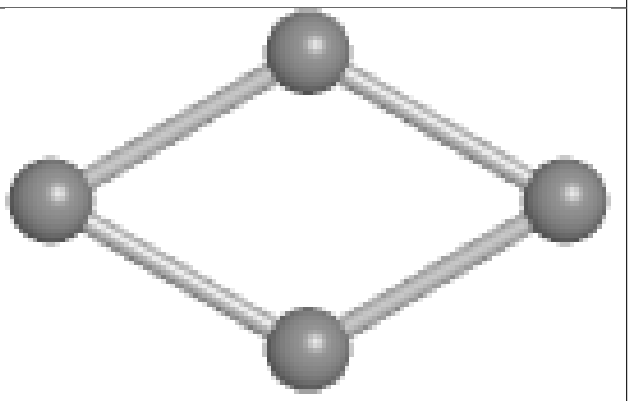

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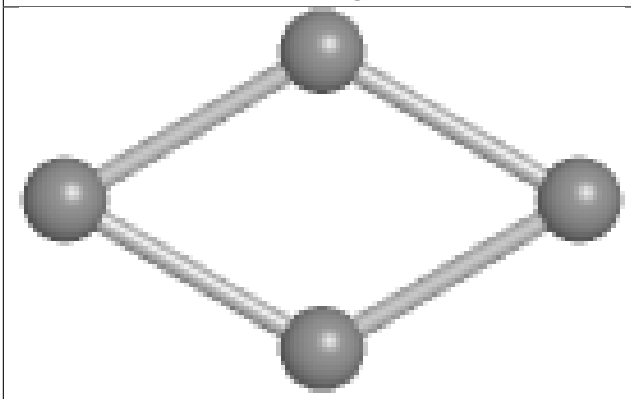

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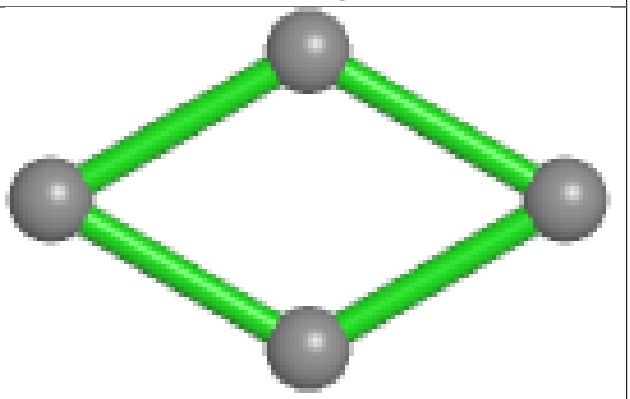
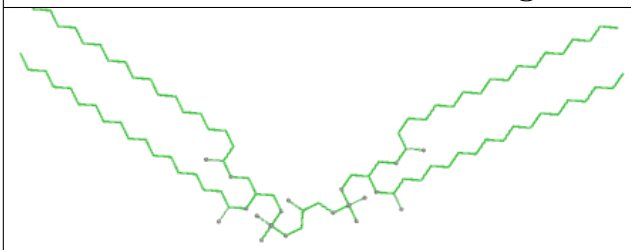


Rings

Ligand CDL Dj 407



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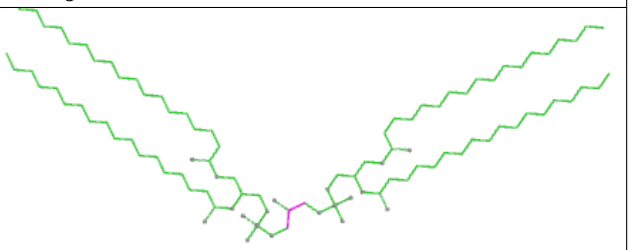
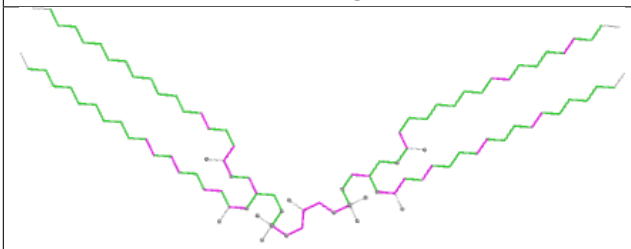
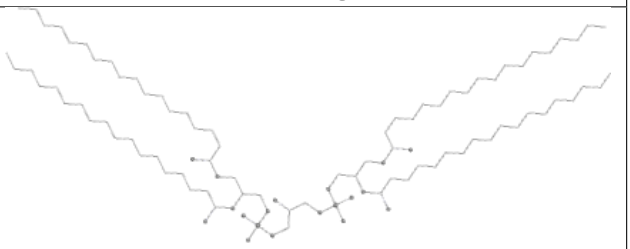


Bond angles

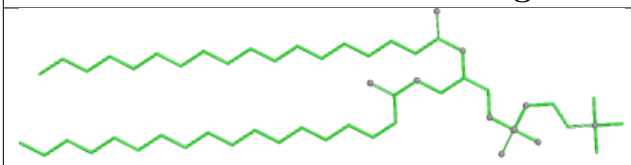


Torsions



Rings

Ligand PC1 DX 305



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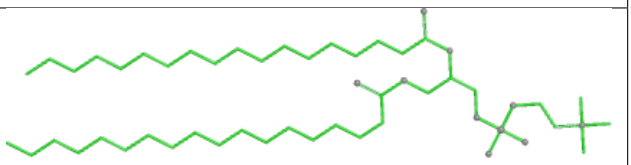
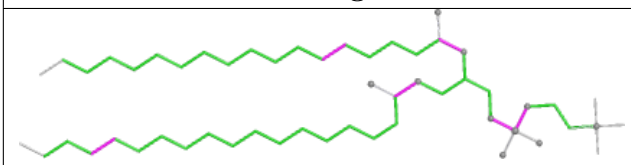


Bond angles



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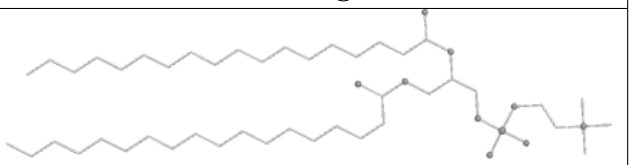
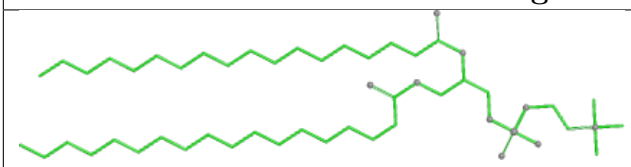


Rings

Ligand PC1 k 301



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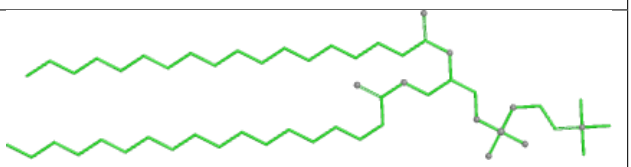
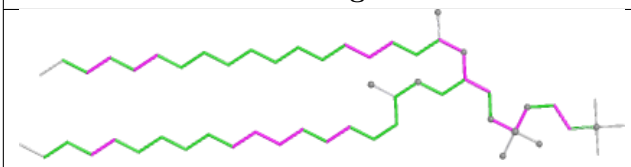
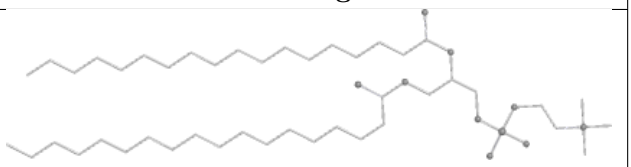


Bond angles

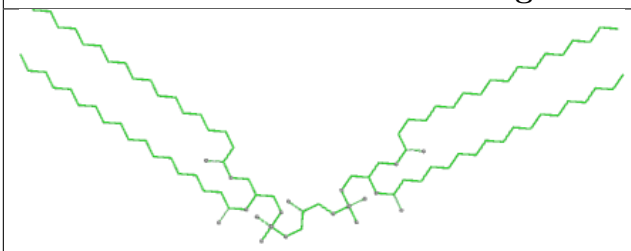


Torsions



Rings

Ligand CDL Dc 608



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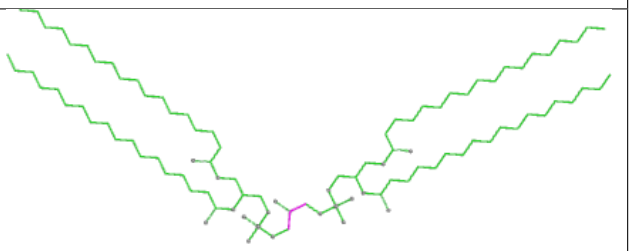
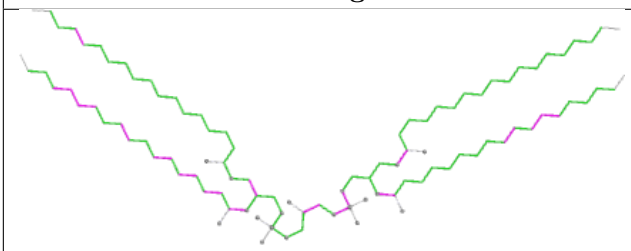


Bond angles



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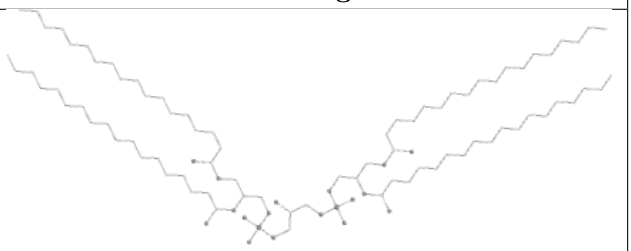
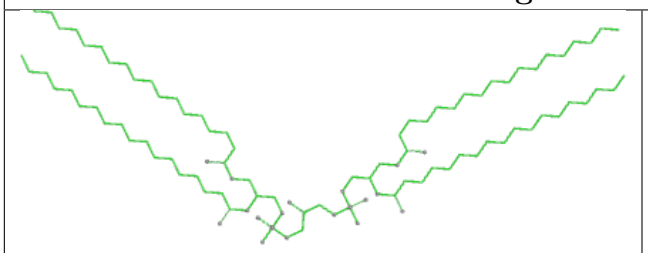
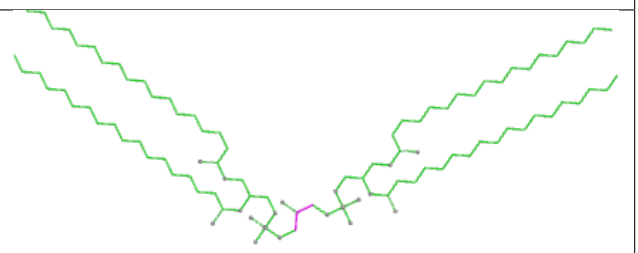


Rings

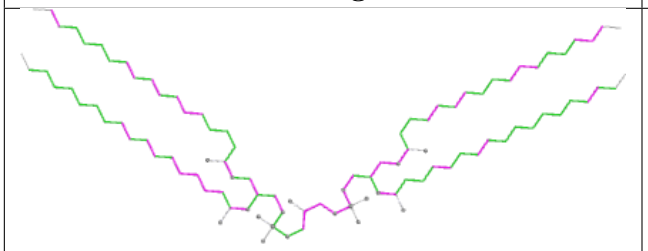
Ligand CDL EL 902



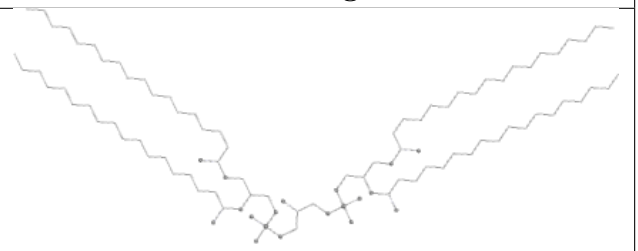
Bond lengths



Bond angles

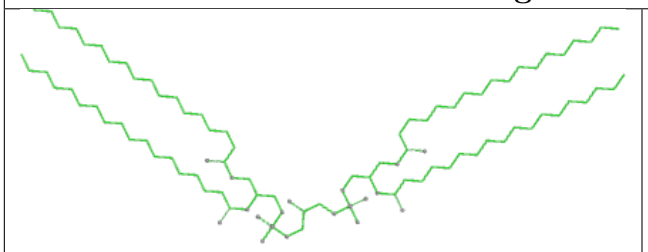


Torsions

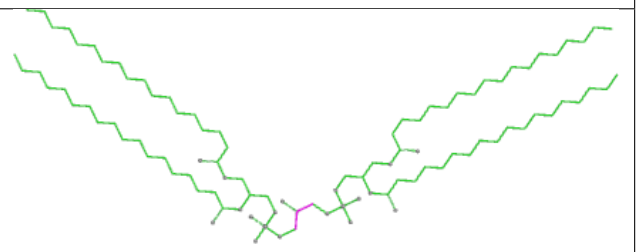


Rings

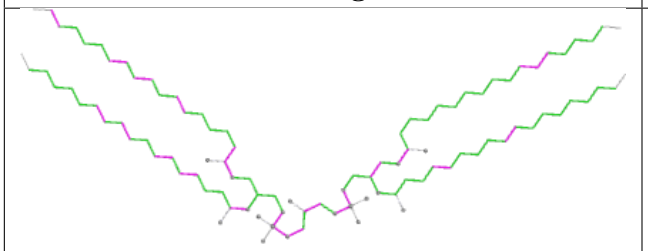
Ligand CDL Du 402



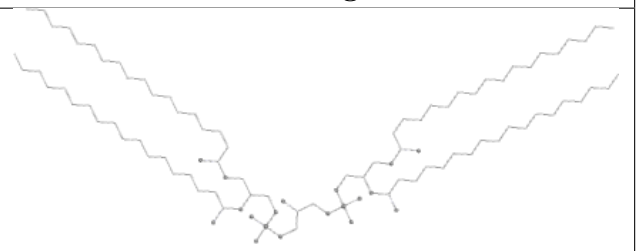
Bond lengths



Bond angles

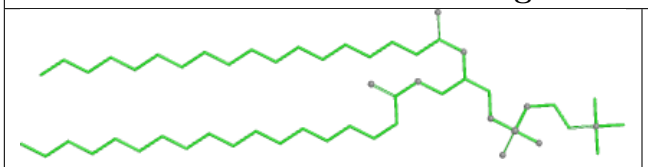


Torsions

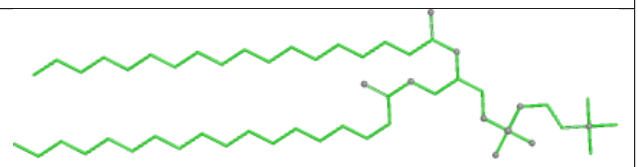


Rings

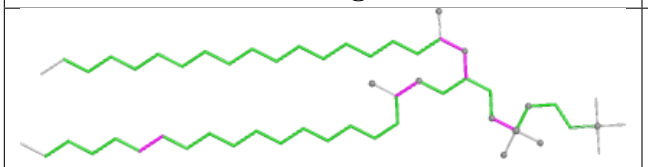
Ligand PC1 AX 401



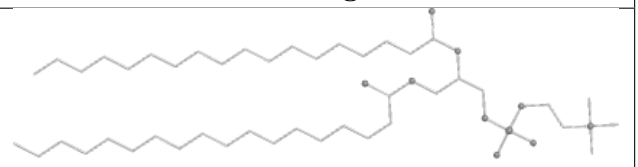
Bond lengths



Bond angles

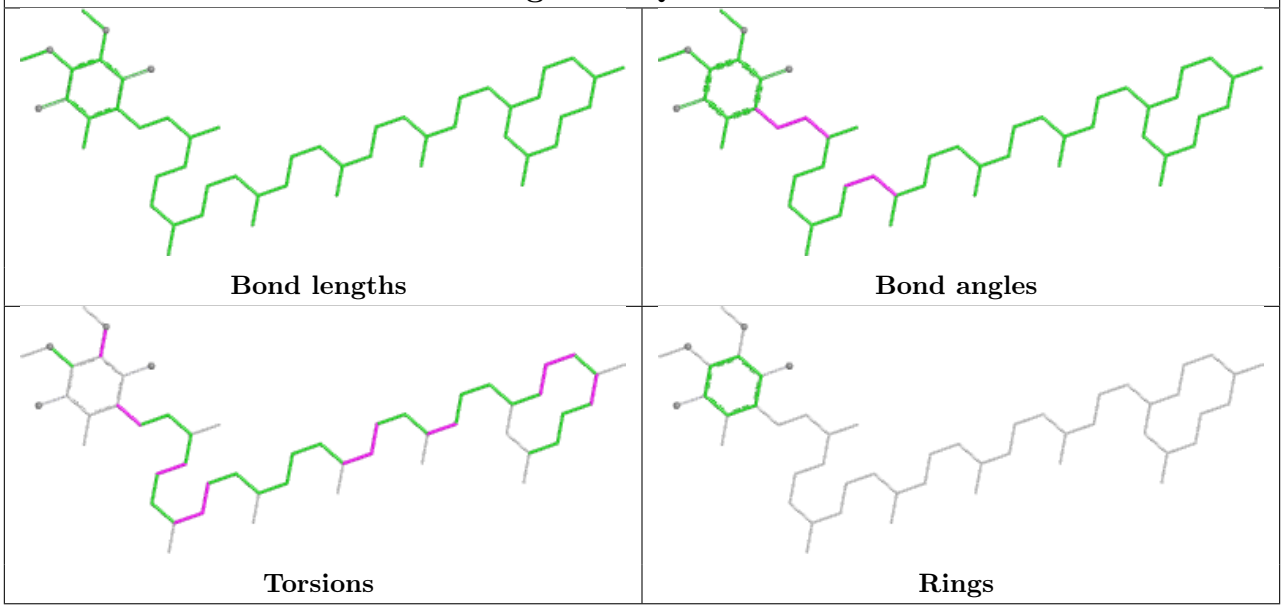


Torsions

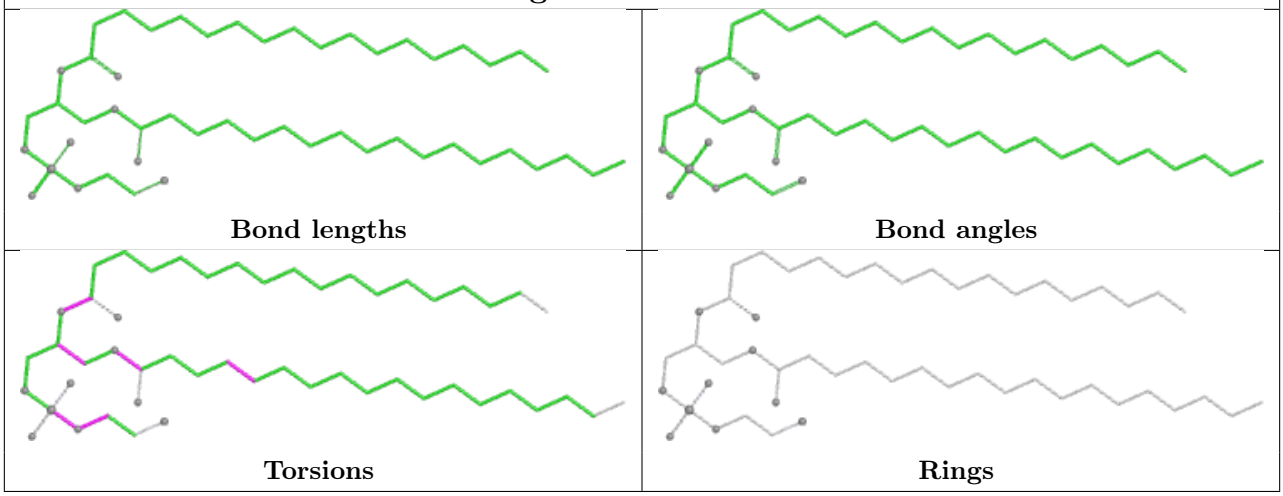


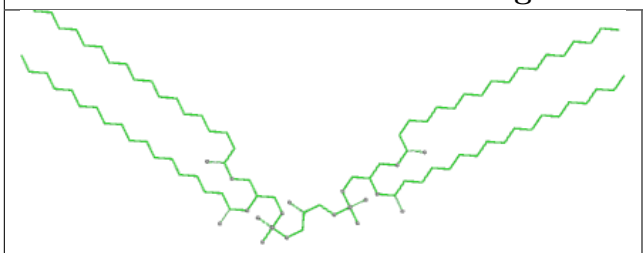
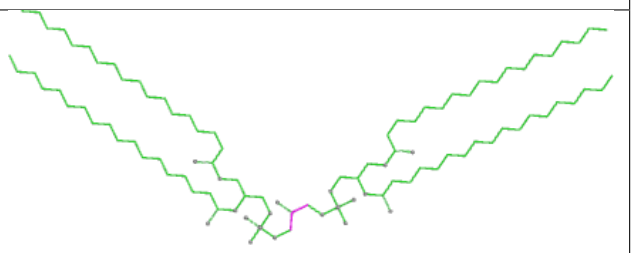
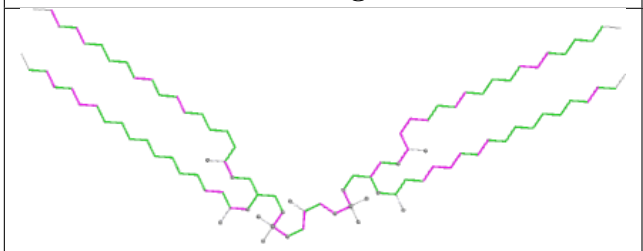
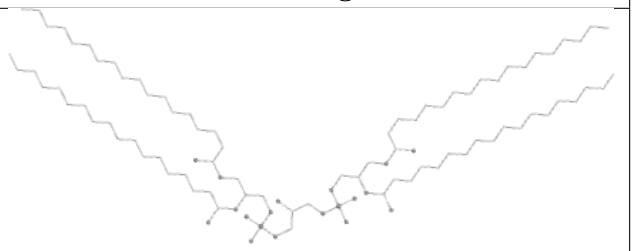
Rings

Ligand UQ8 C 511



Ligand 3PE C 513



Ligand CDL Dh 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

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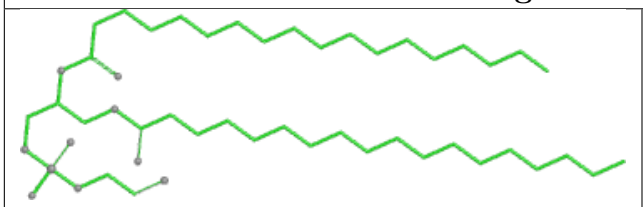
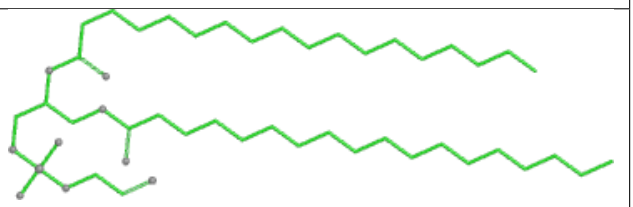
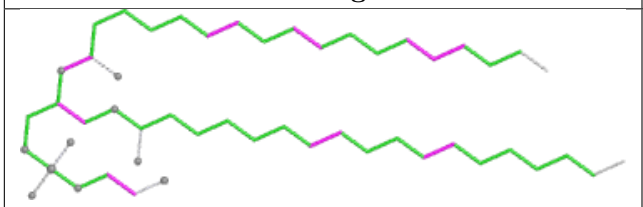
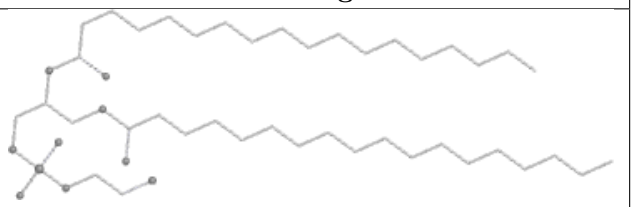
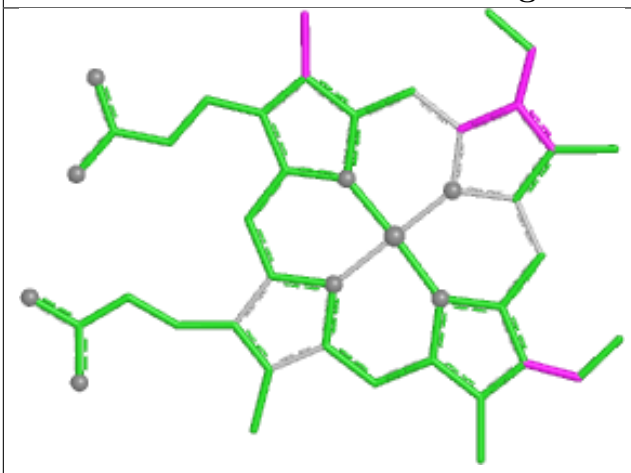
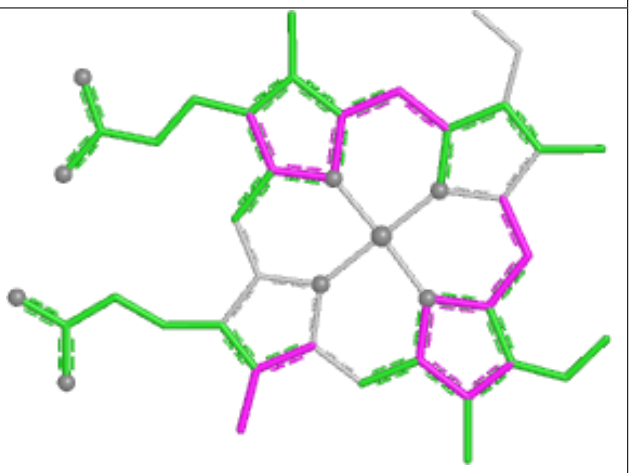
 Bond lengths	 Bond angles
 Torsions	 Rings

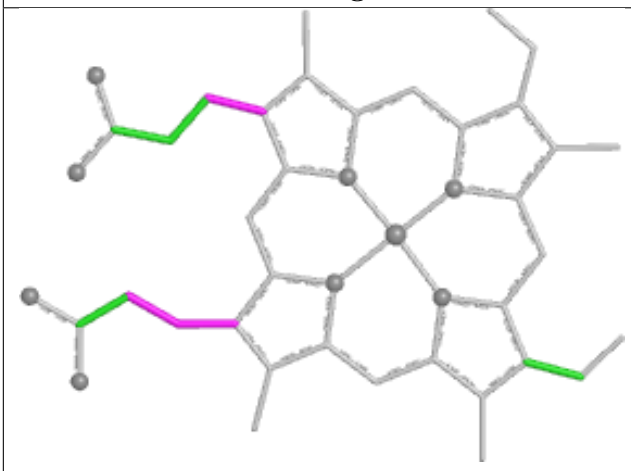
Ligand HEM C 501



Bond lengths



Bond angles



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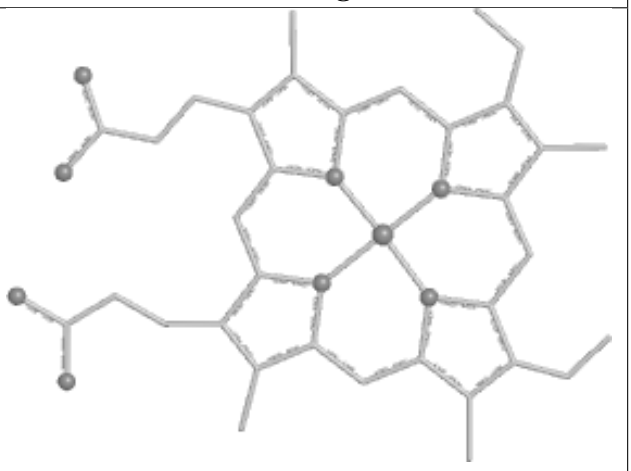
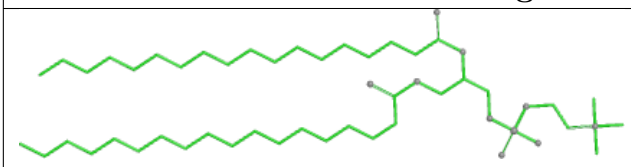


Rings

Ligand PC1 AL 303



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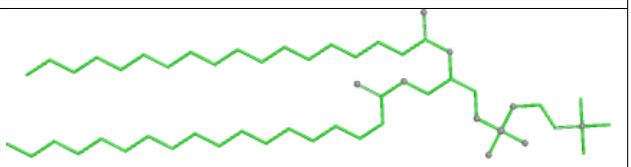
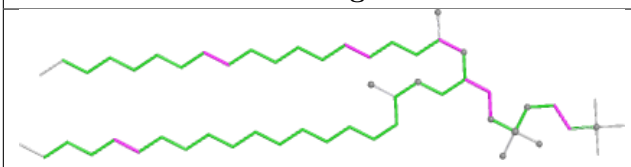


Bond angles



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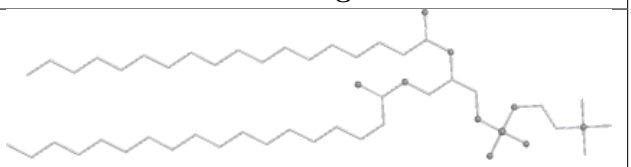
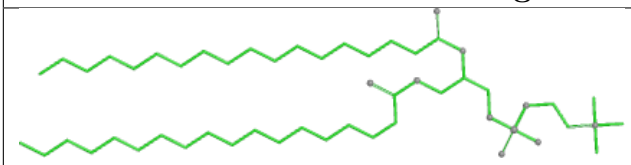


Rings

Ligand PC1 DA 707



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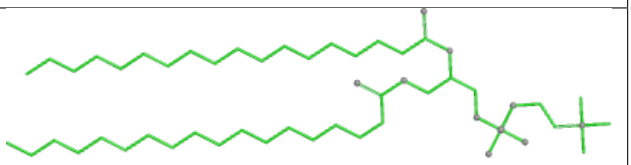
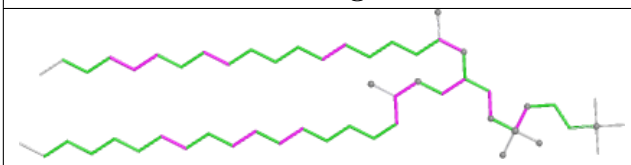


Bond angles



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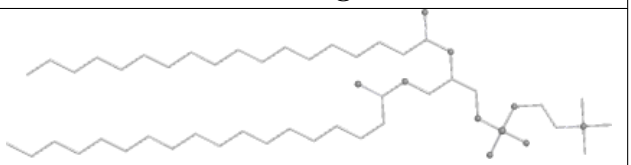
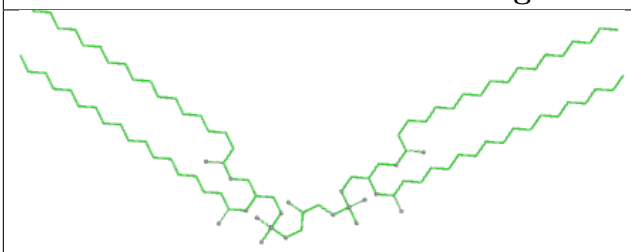


Rings

Ligand CDL Dy 301



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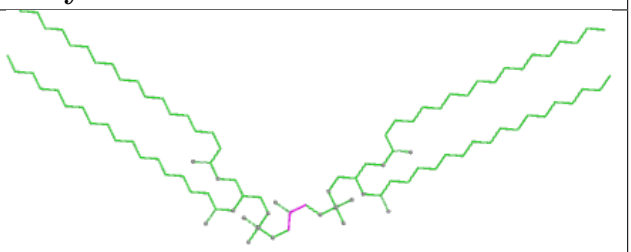
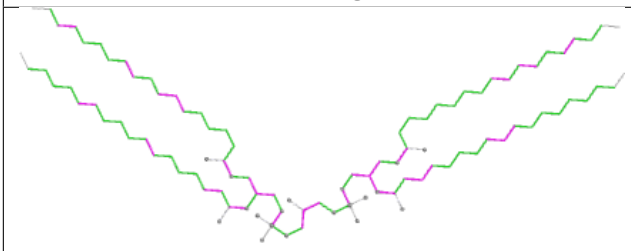


Bond angles



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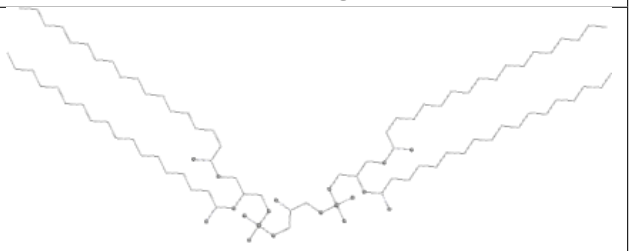

Rings

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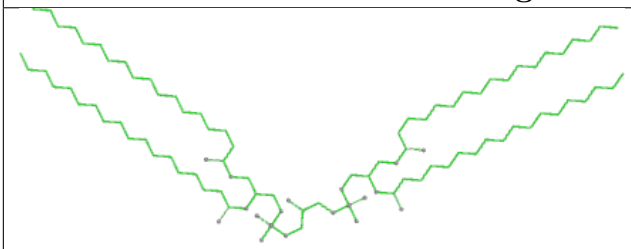

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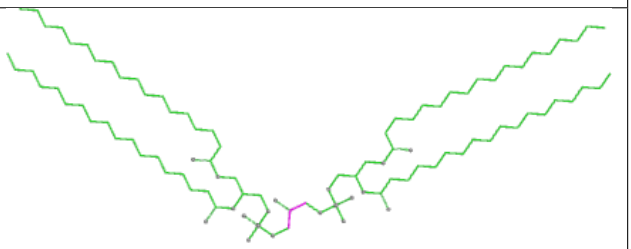
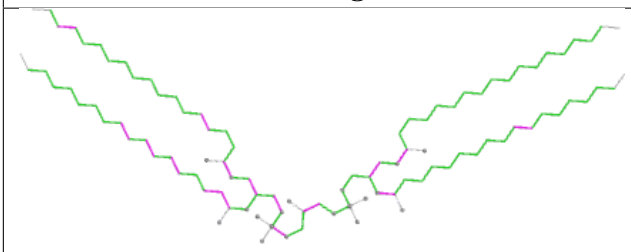
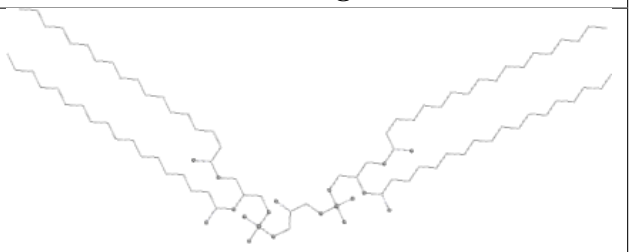


Bond angles

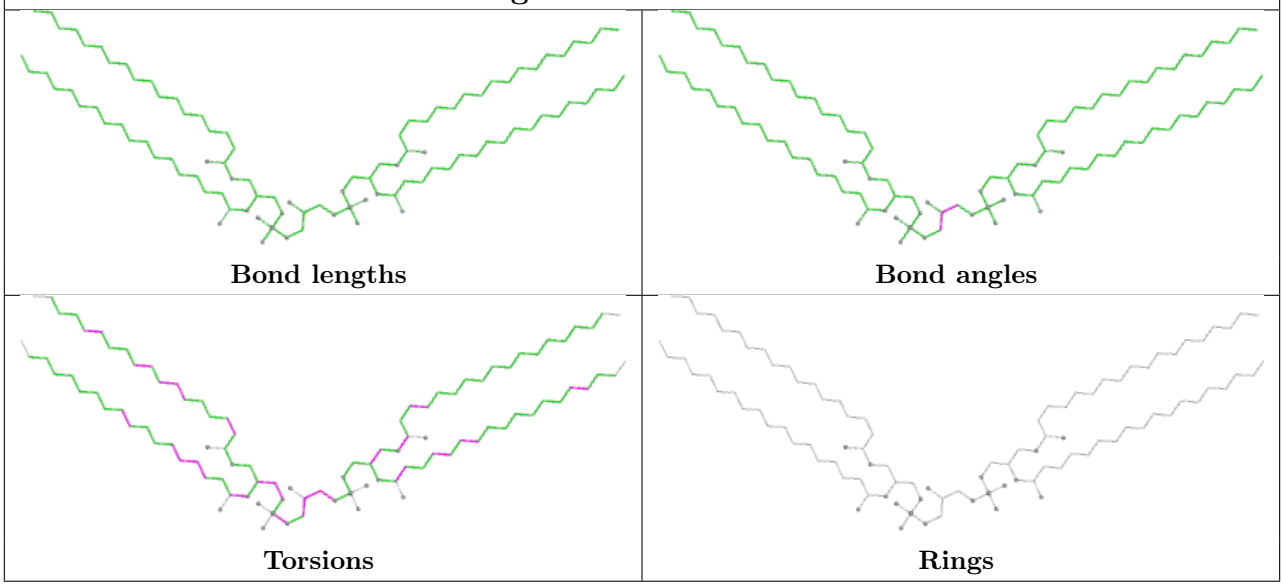


Torsions

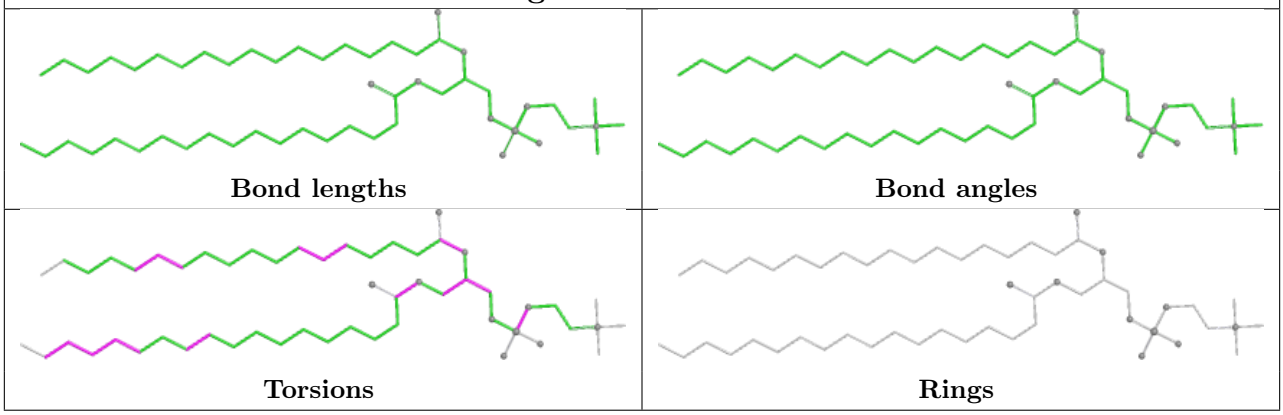


Rings

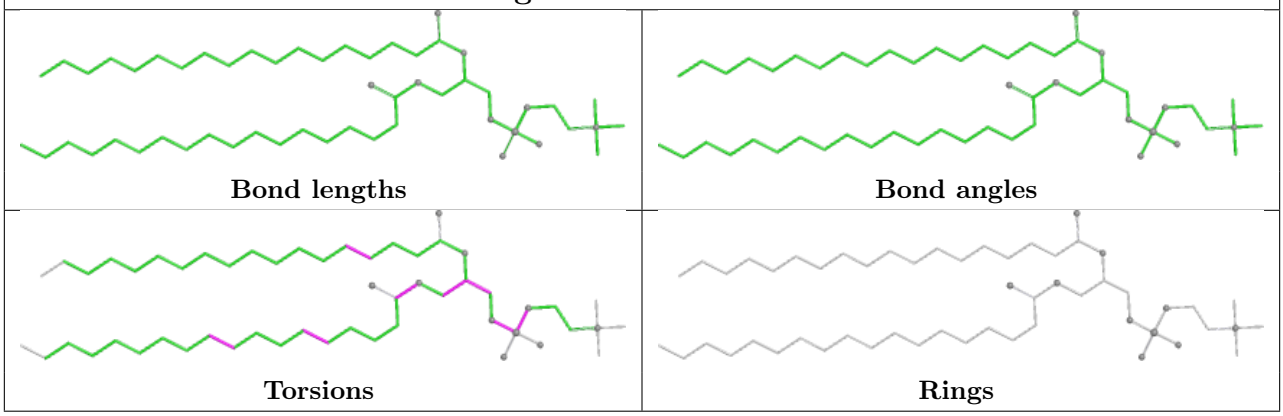
Ligand CDL DR 403



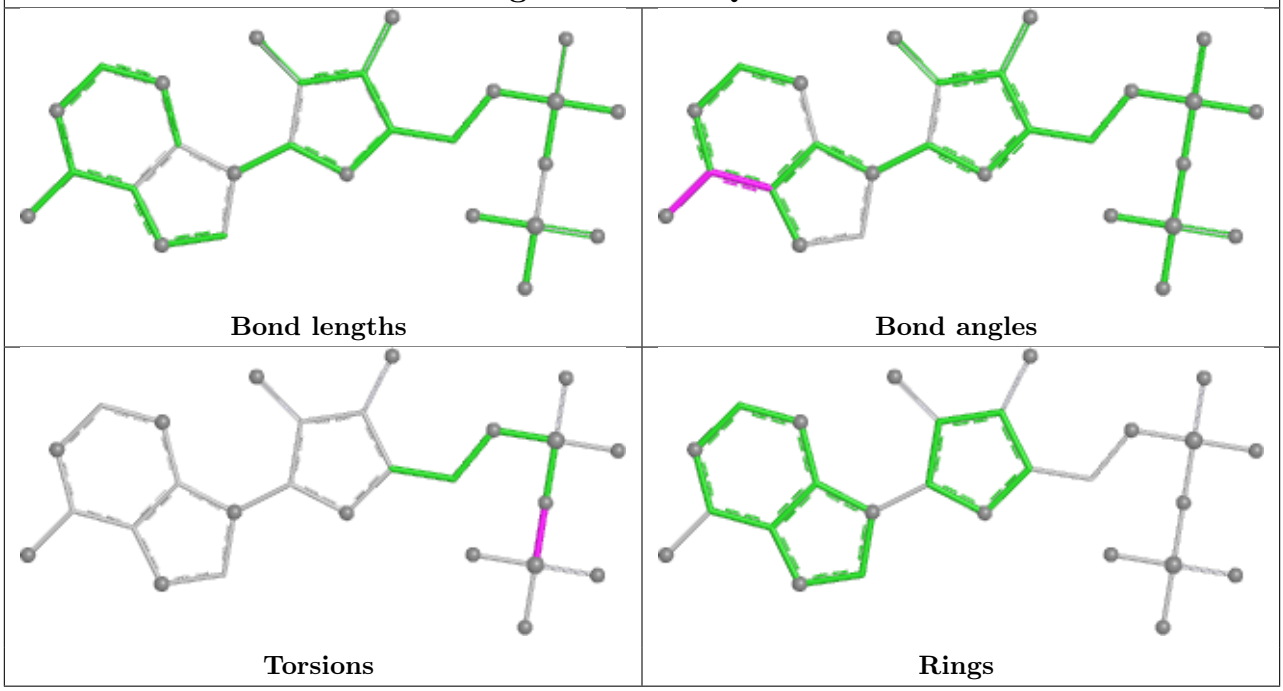
Ligand PC1 D 402



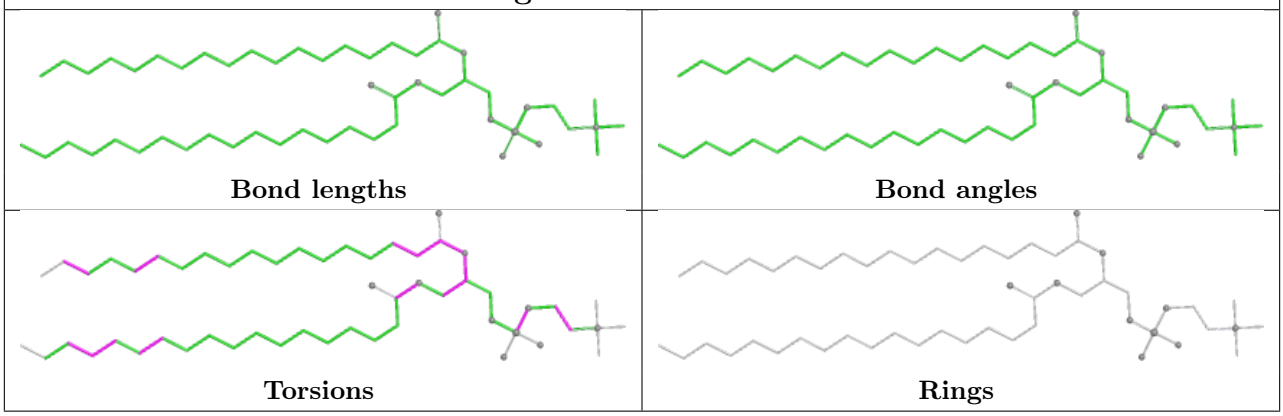
Ligand PC1 AA 903



Ligand ADP AQ 201



Ligand PC1 AA 906



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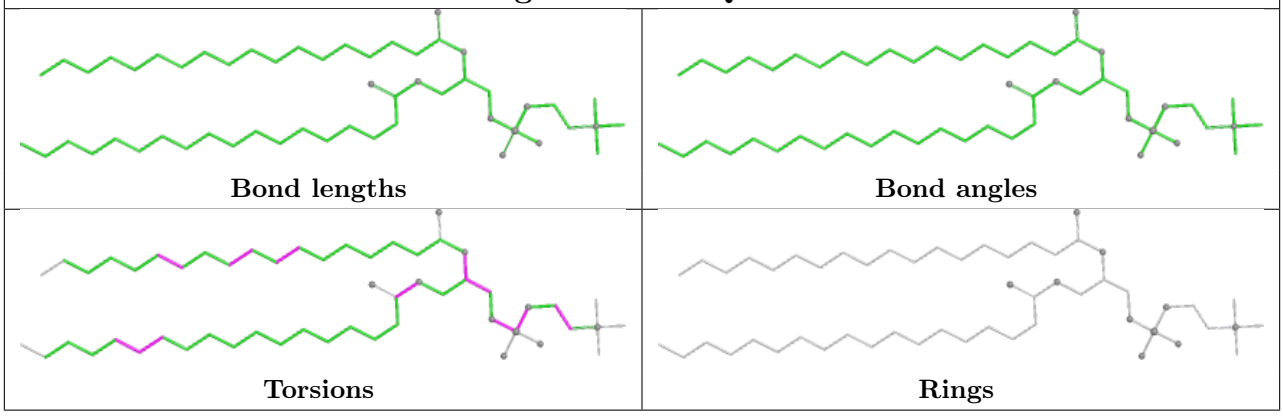

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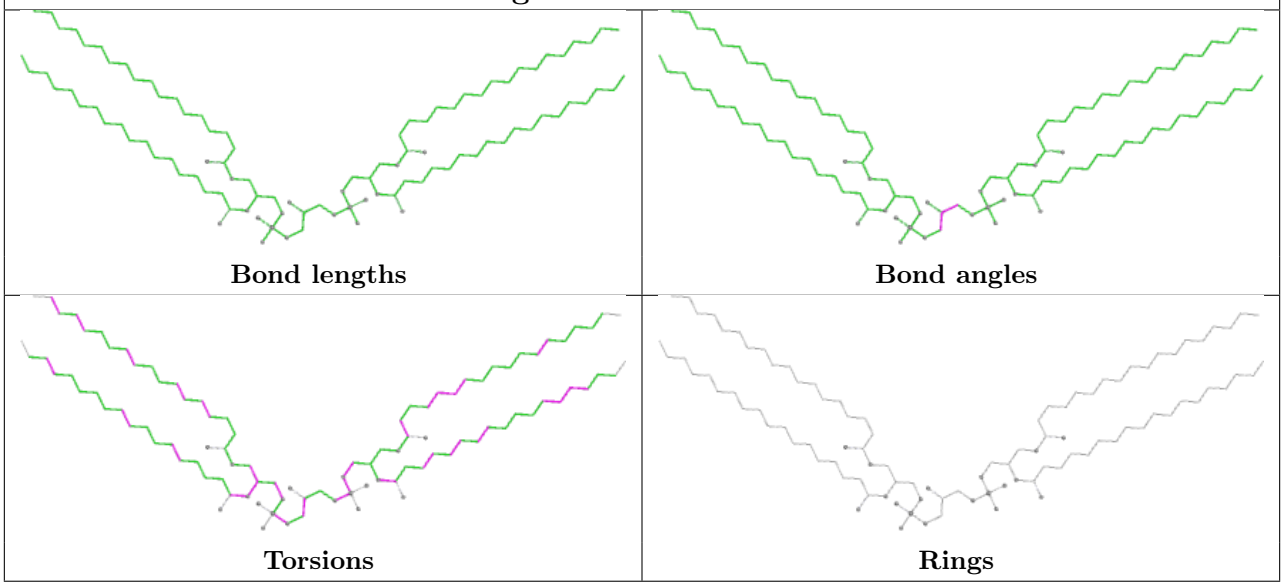

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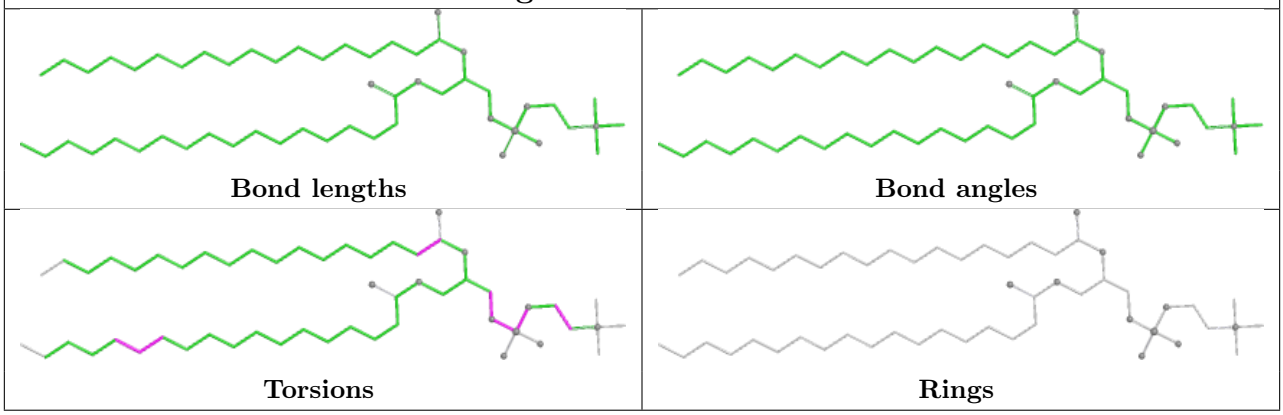

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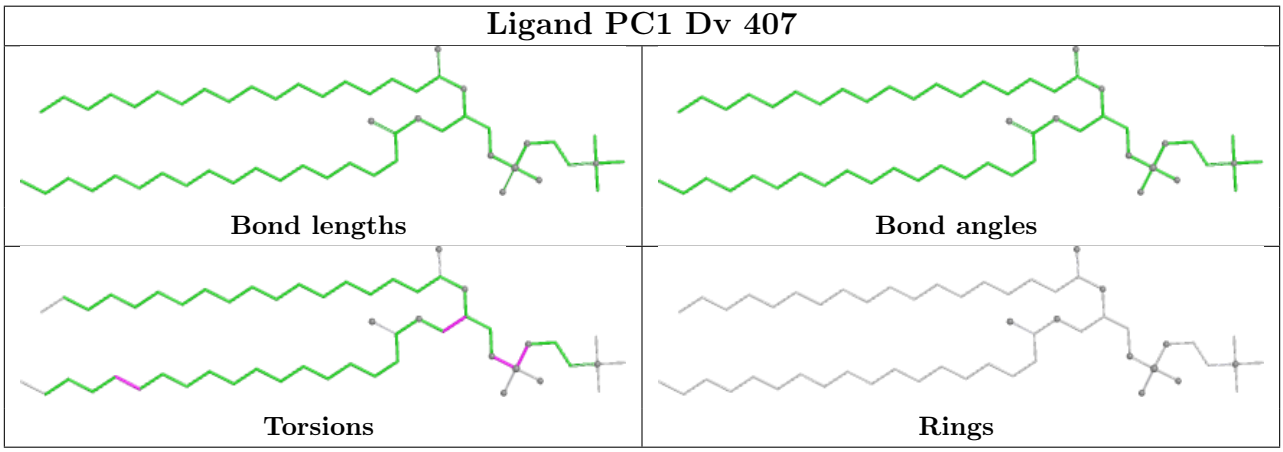
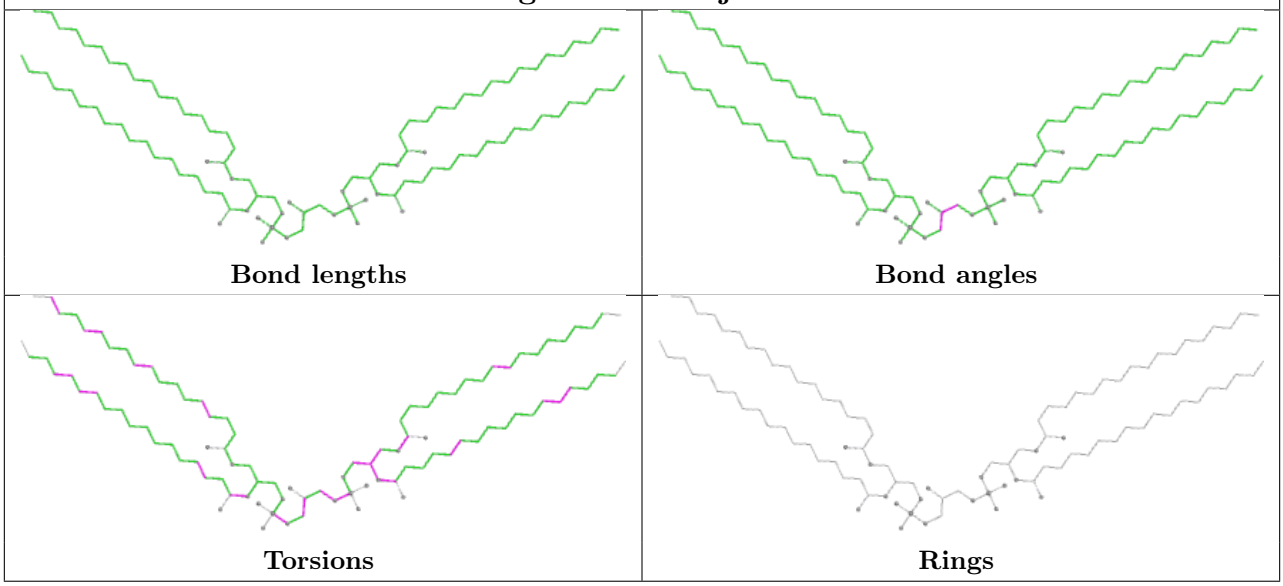


Ligand CDL Dj 405



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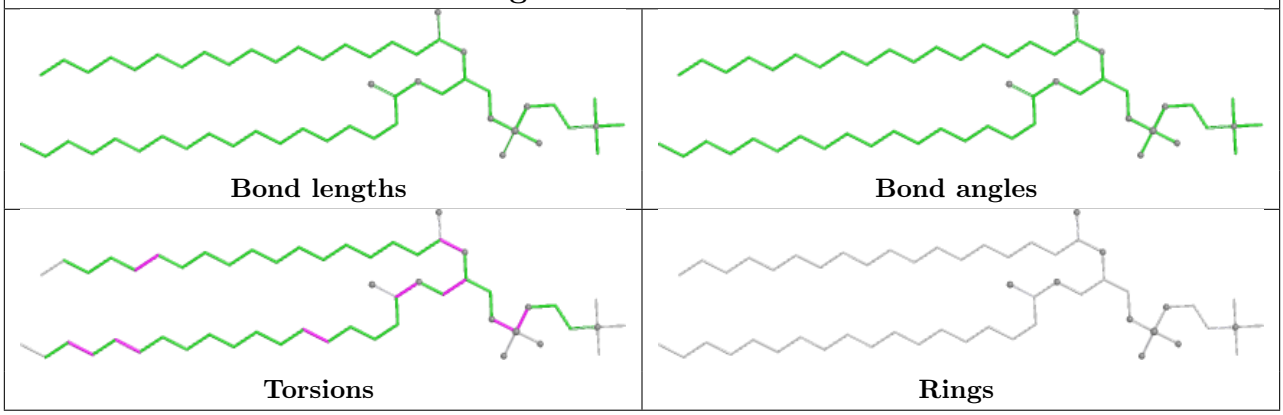
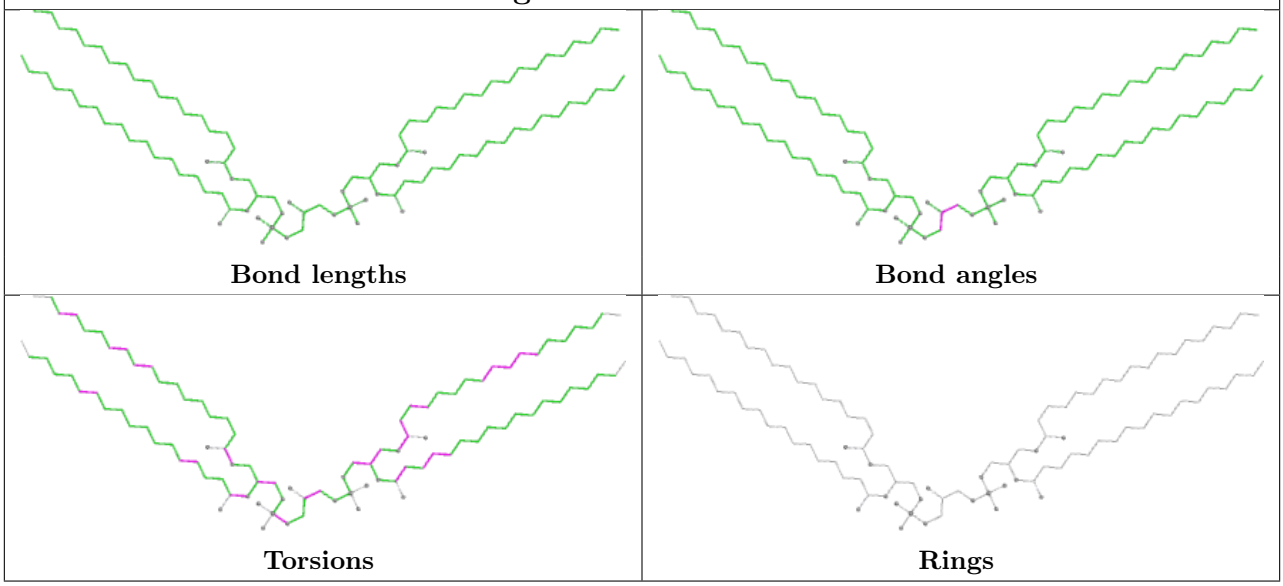


Ligand CDL AF 402



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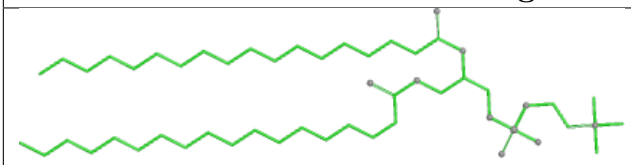
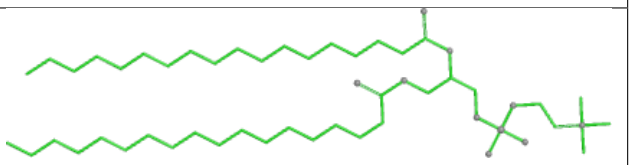
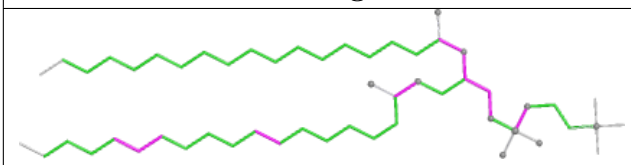
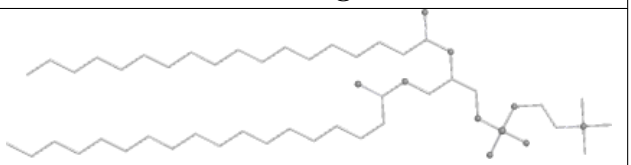
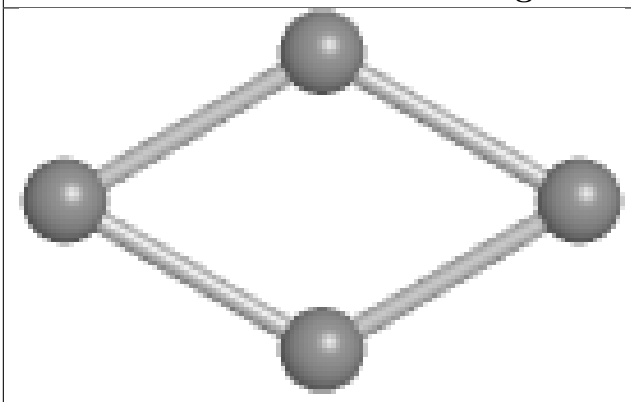
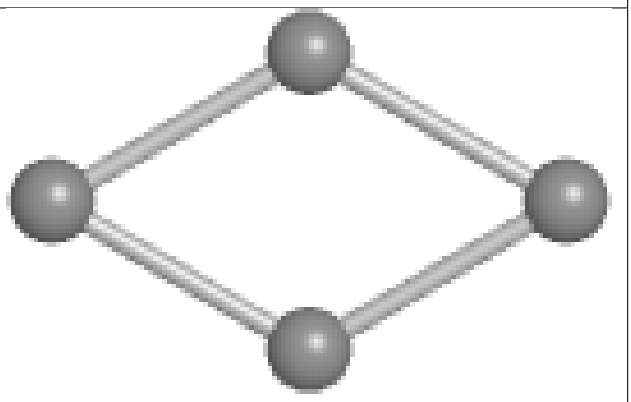
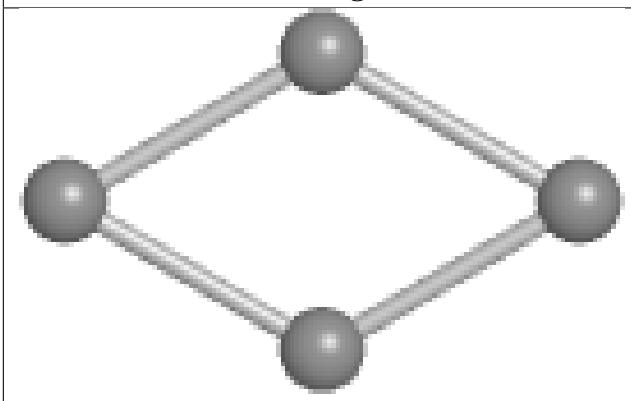
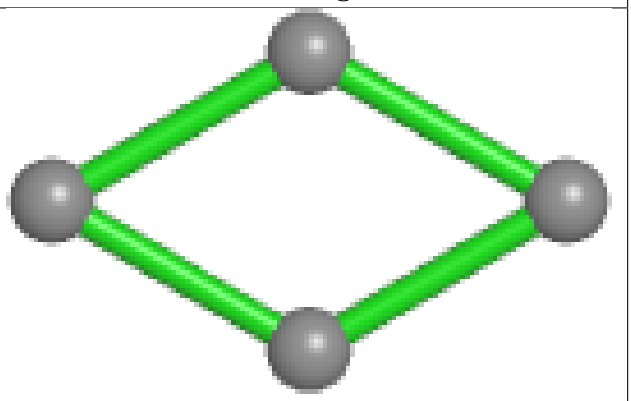
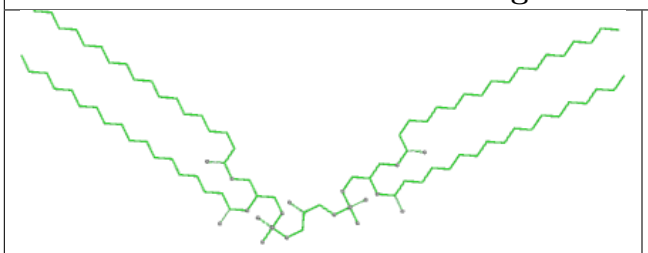
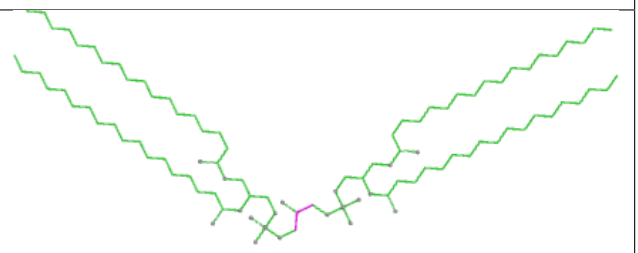
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES AB 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

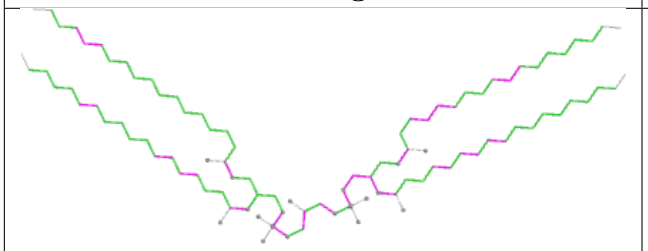
Ligand CDL CG 302



Bond lengths



Bond angles



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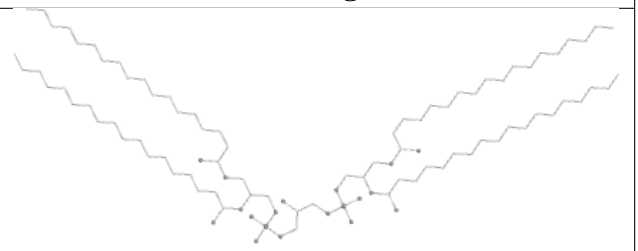
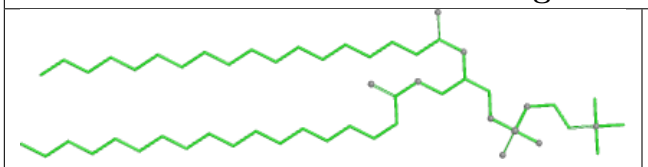


Rings

Ligand PC1 c 503



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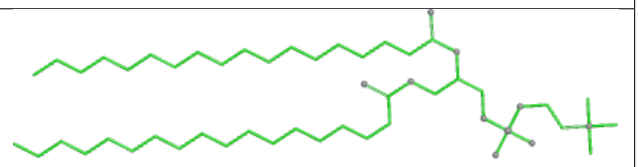

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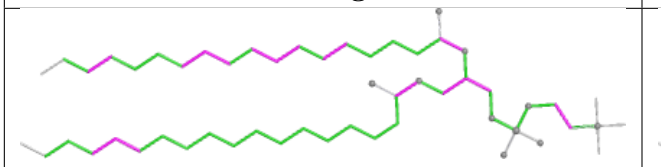

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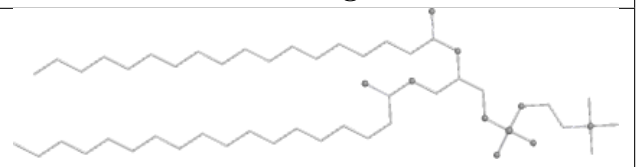
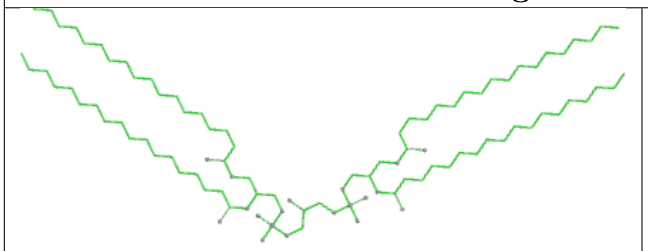


Rings

Ligand CDL AC 801



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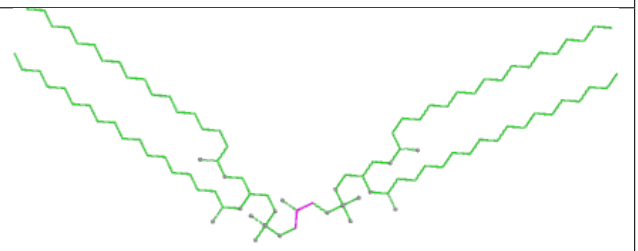

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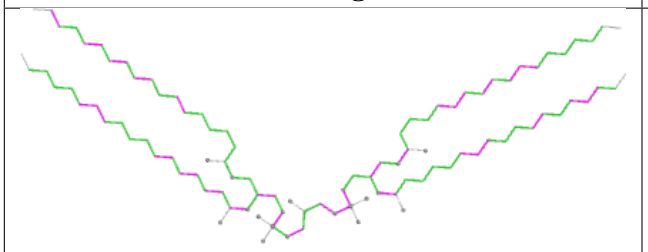

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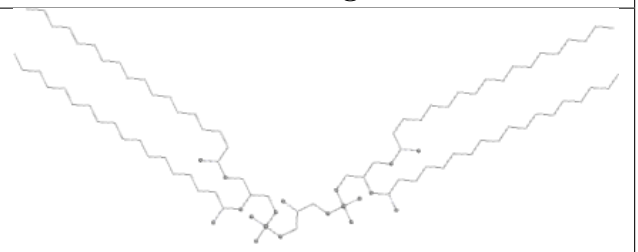
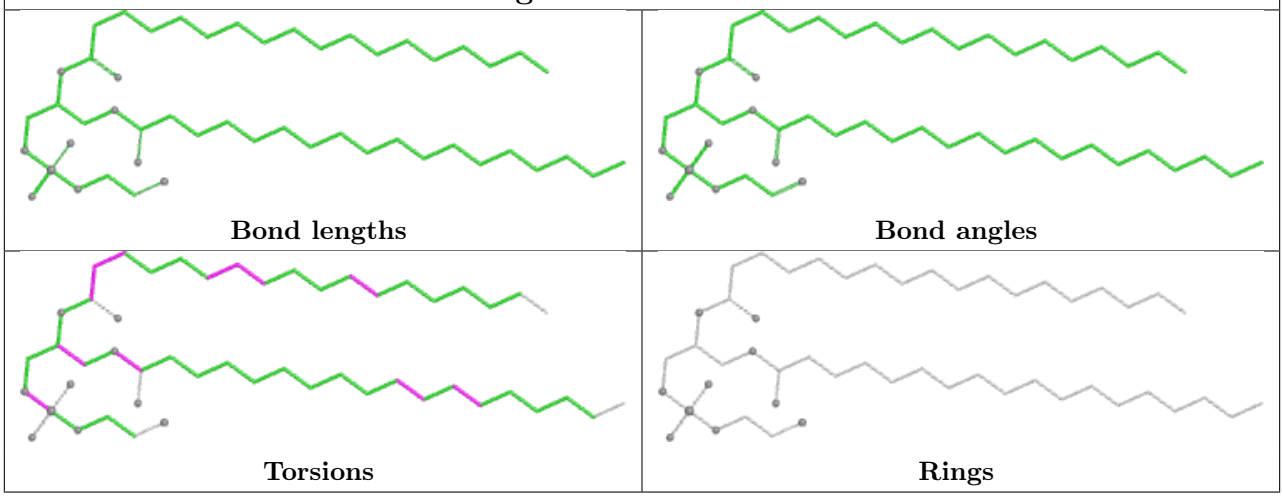
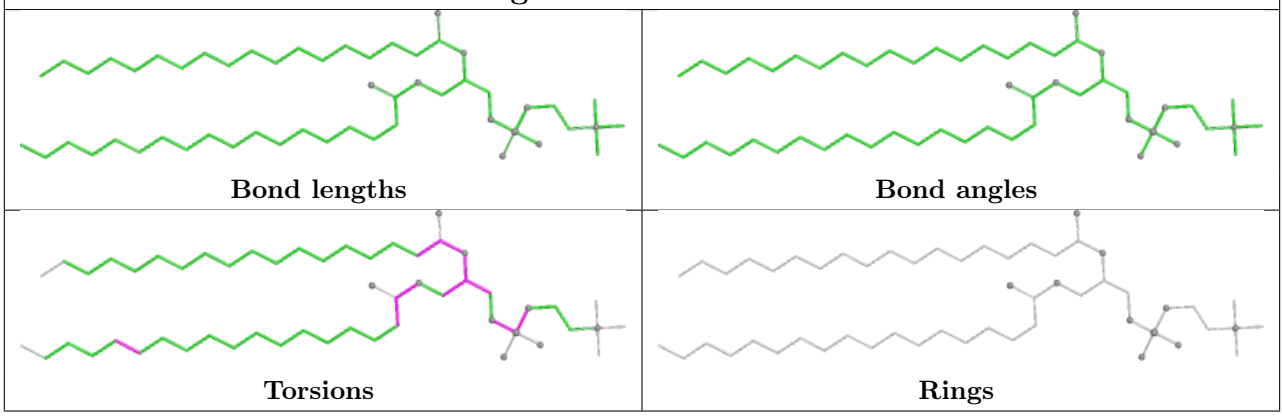


Rings

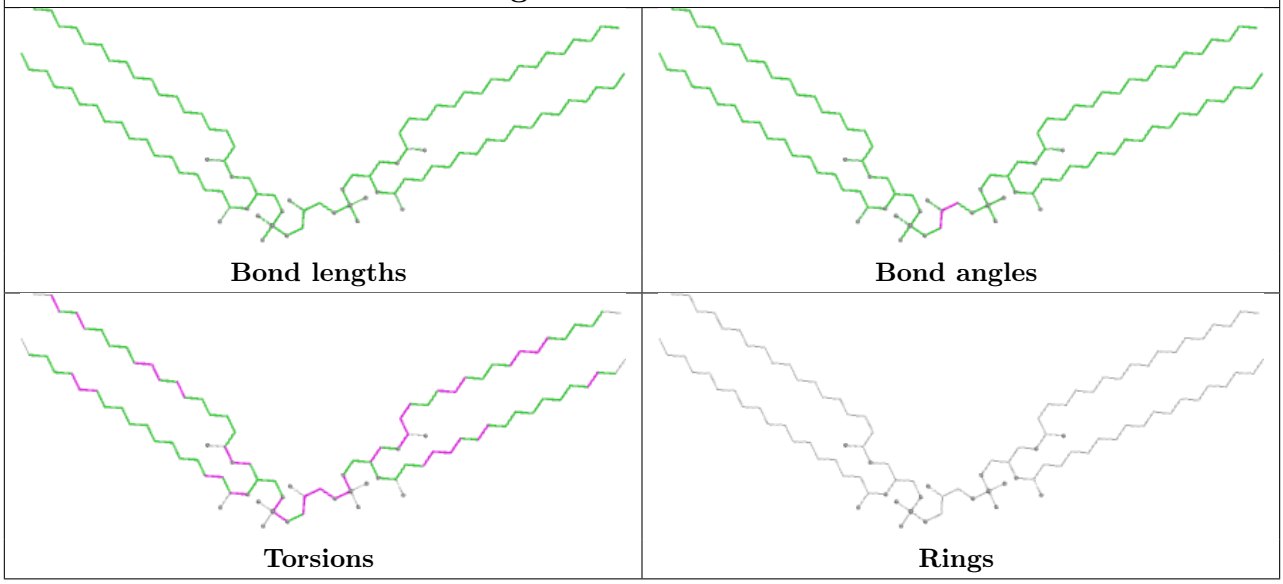
Ligand 3PE Em 901



Ligand PC1 AM 302



Ligand CDL DH 202



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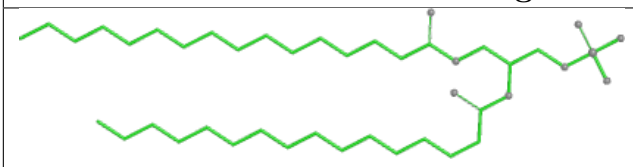

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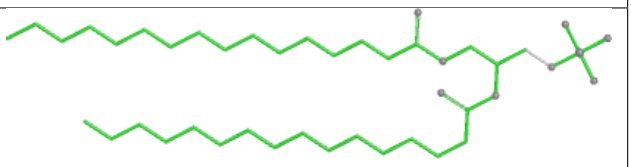
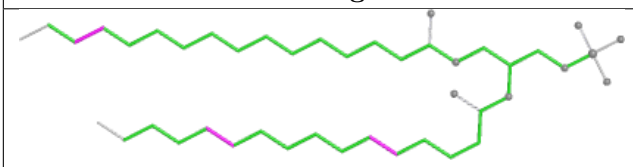
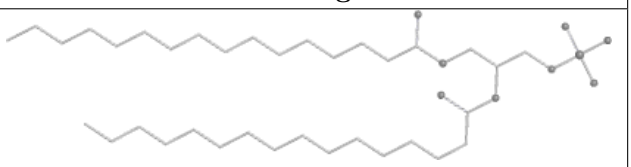


Bond angles



Torsions



Rings

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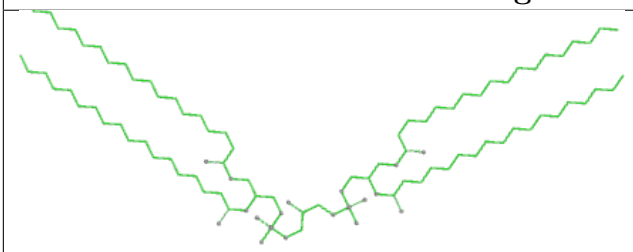

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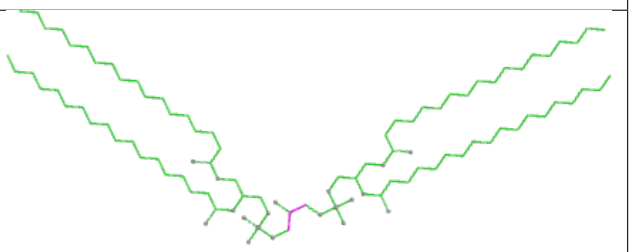

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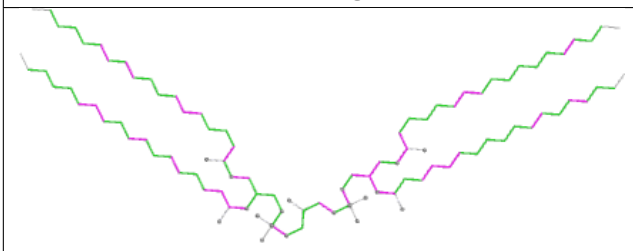

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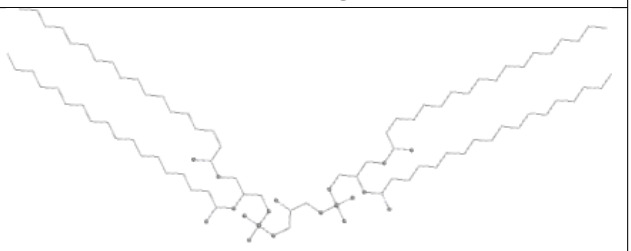

Rings

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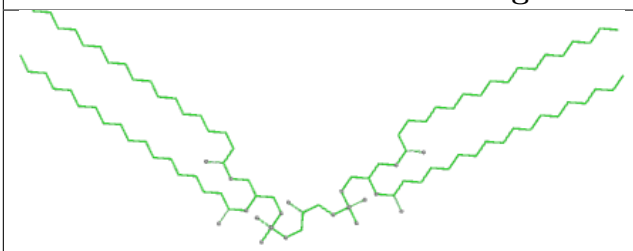

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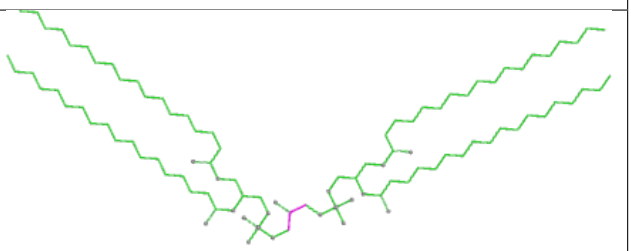

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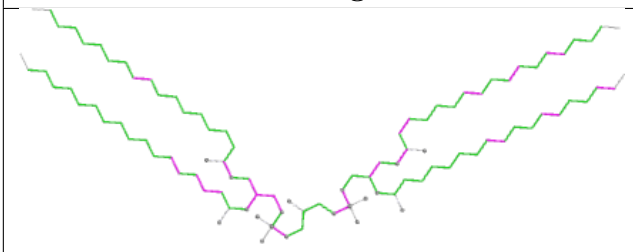

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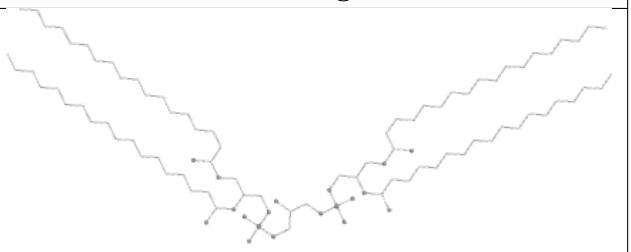

Rings

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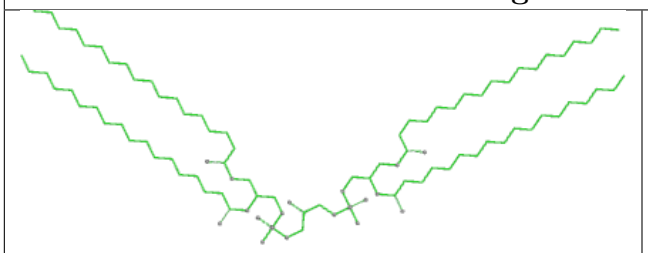

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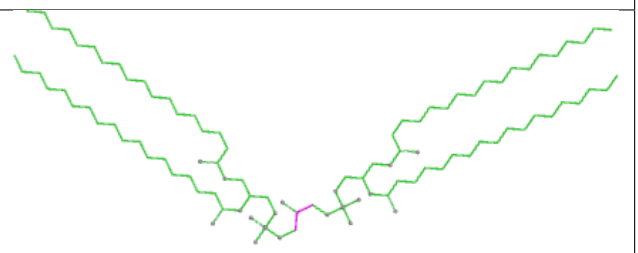

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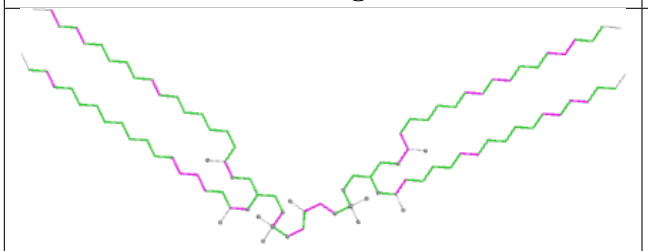

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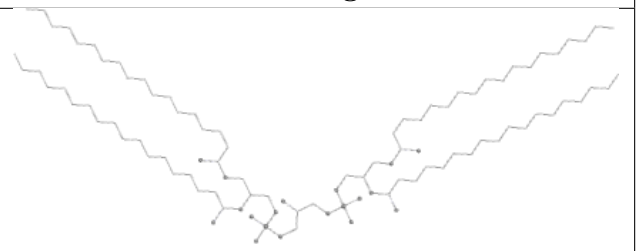
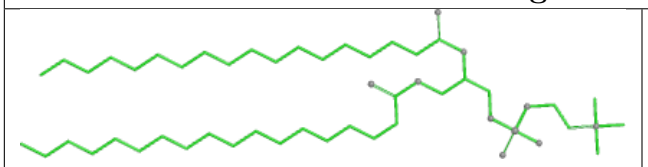


Rings

Ligand PC1 E 303



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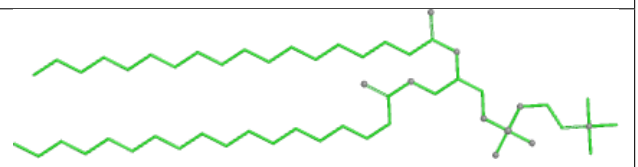

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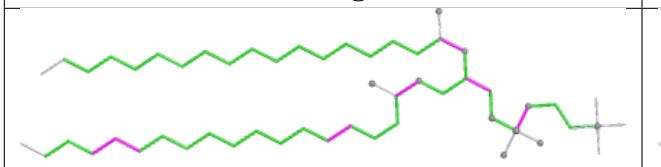

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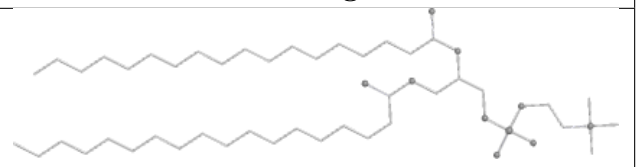
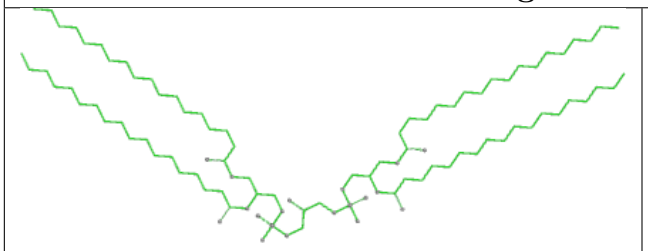


Rings

Ligand CDL Ds 402



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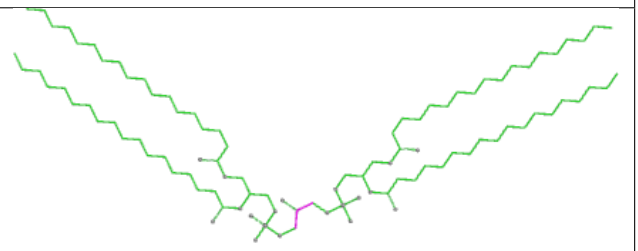
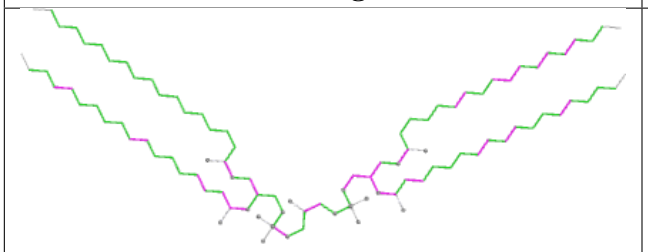


Bond angles



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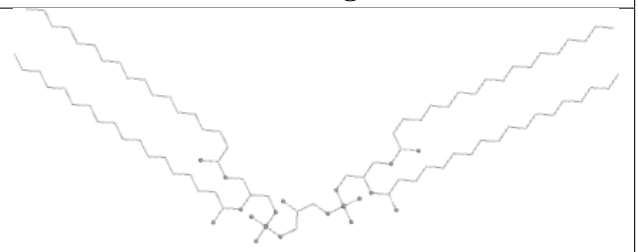
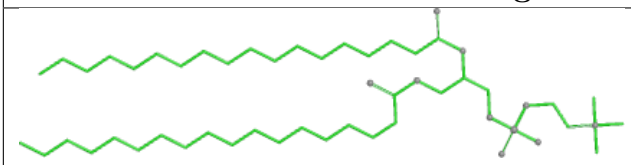


Rings

Ligand PC1 DB 702



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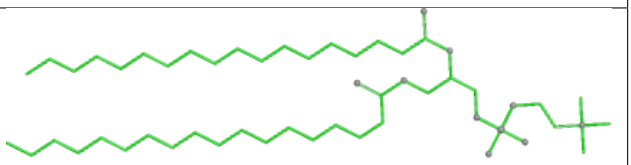
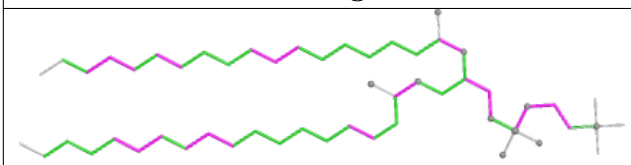


Bond angles



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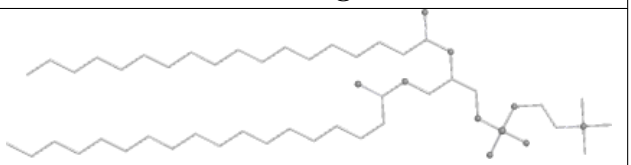
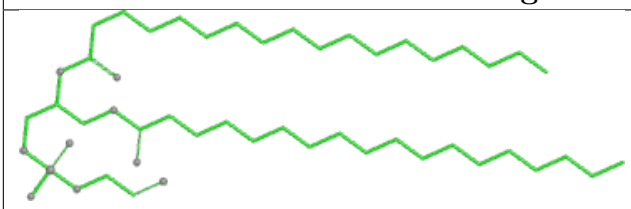


Rings

Ligand 3PE Ds 408



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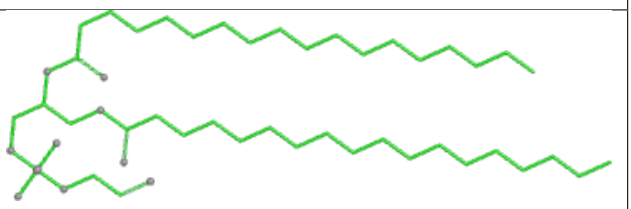

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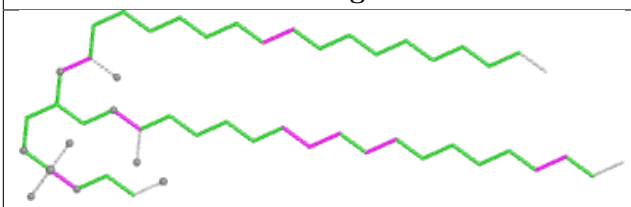

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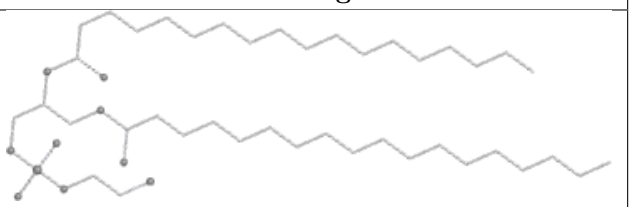
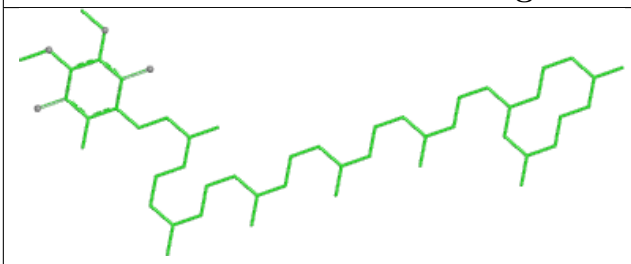


Rings

Ligand UQ8 EL 905



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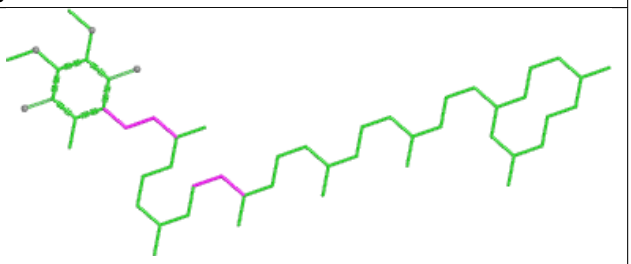
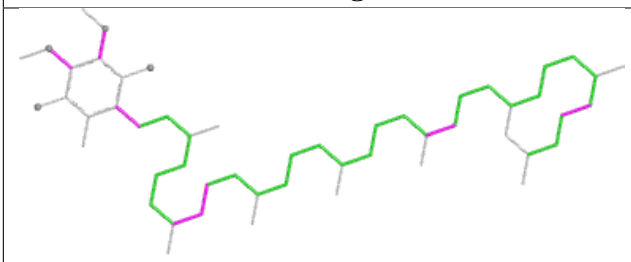


Bond angles



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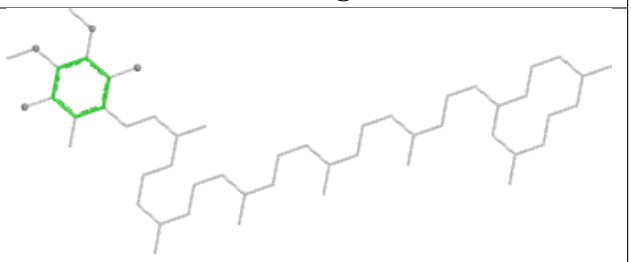
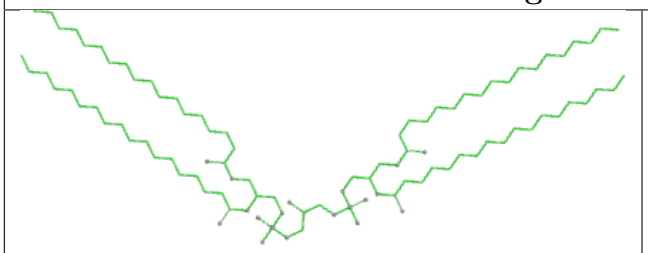


Rings

Ligand CDL C 507



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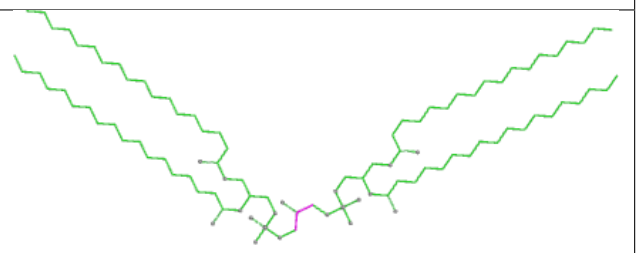
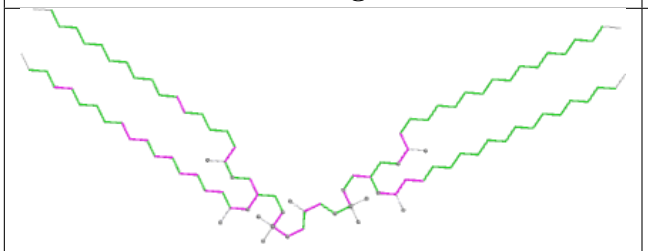
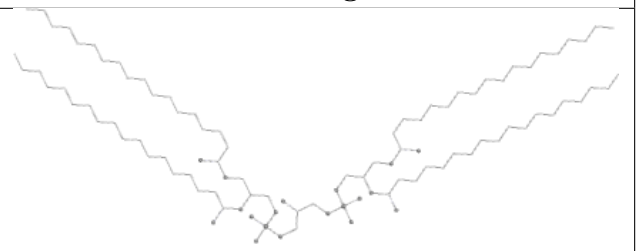


Bond angles

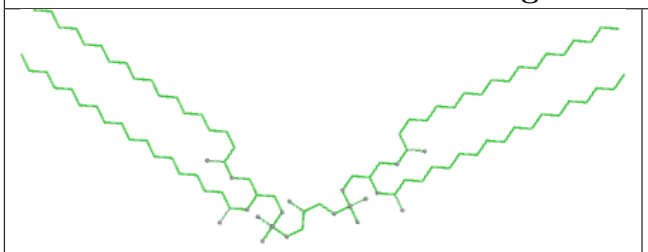


Torsions



Rings

Ligand CDL El 901



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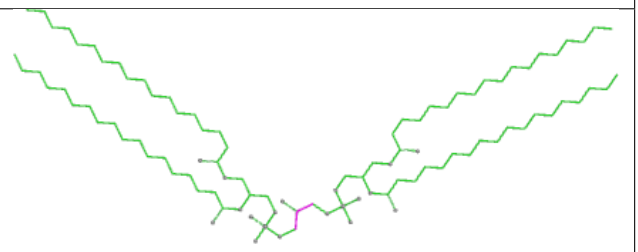

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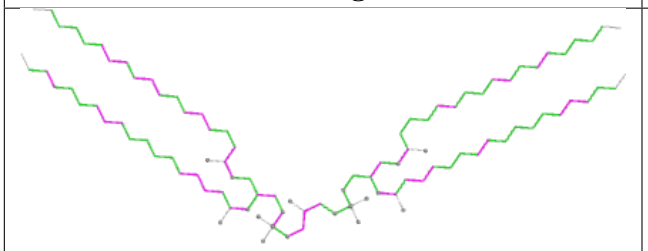

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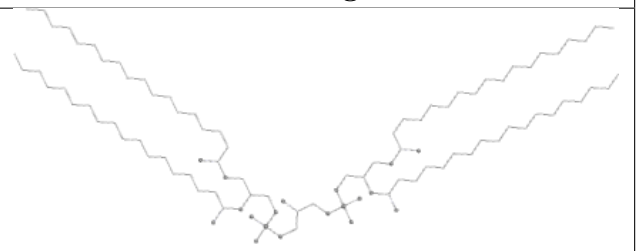
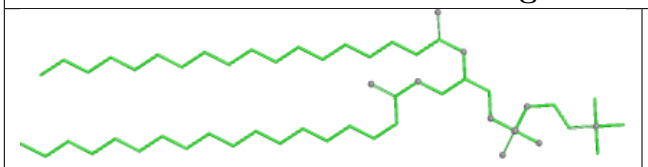


Rings

Ligand PC1 B1 401



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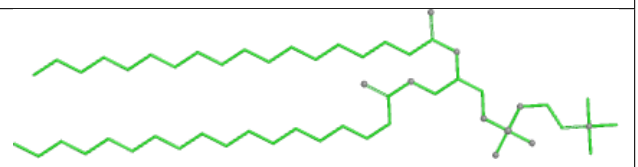
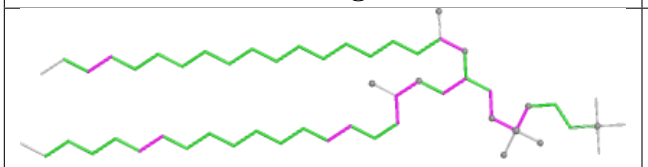


Bond angles



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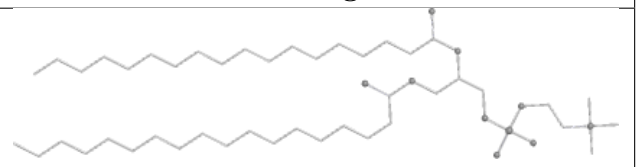
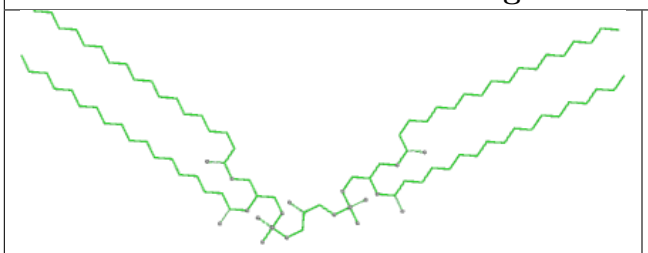


Rings

Ligand CDL EN 1202



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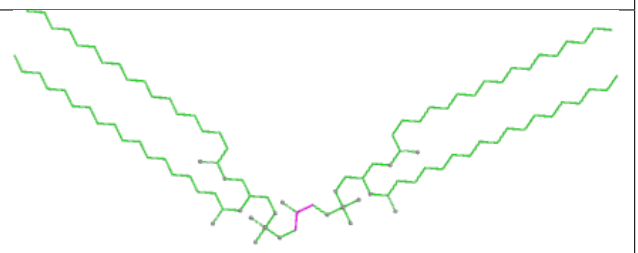
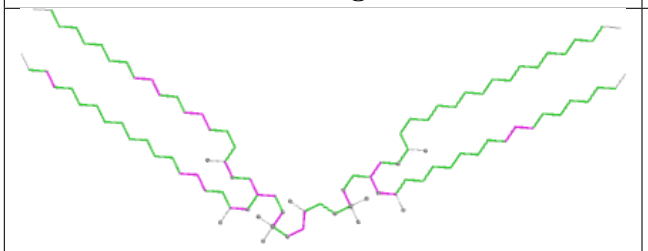


Bond angles



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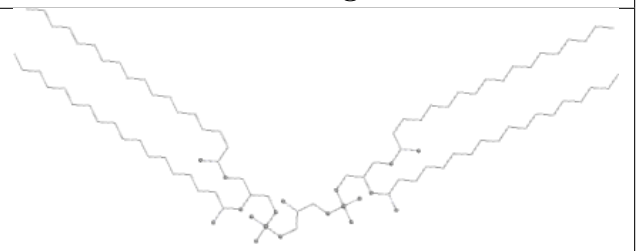
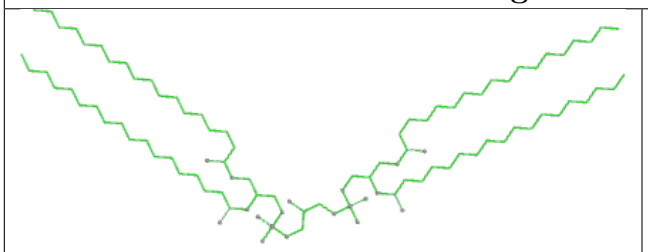


Rings

Ligand CDL DO 501



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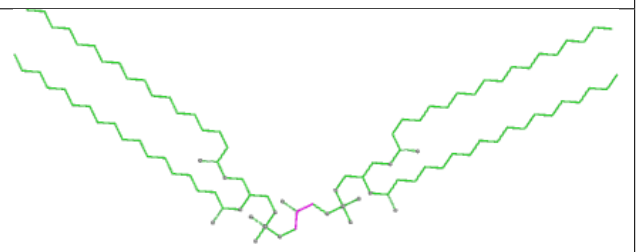

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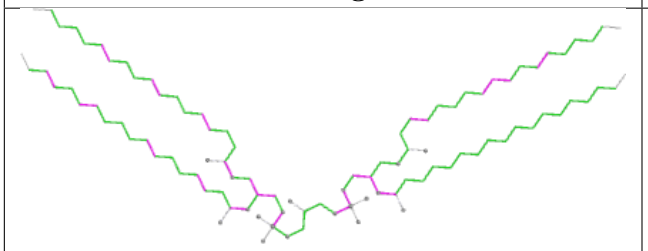

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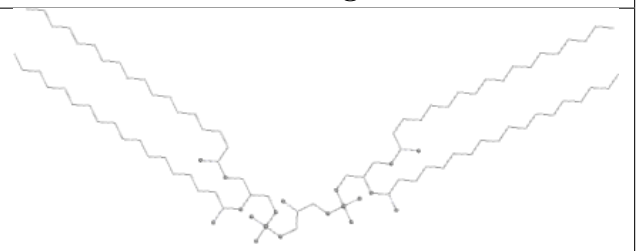
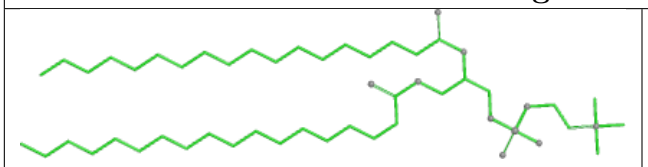


Rings

Ligand PC1 g 802



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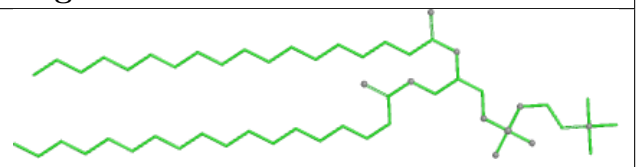
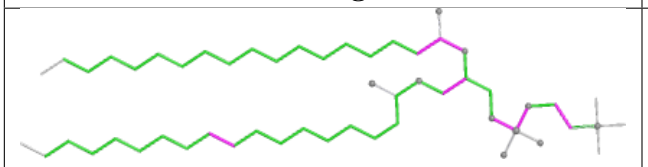


Bond angles



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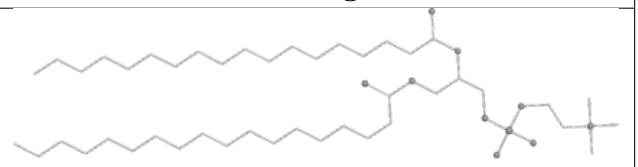
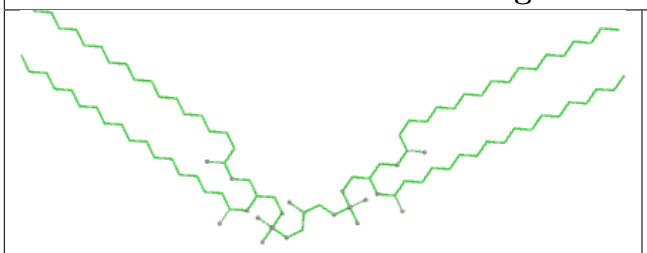


Rings

Ligand CDL Dd 705



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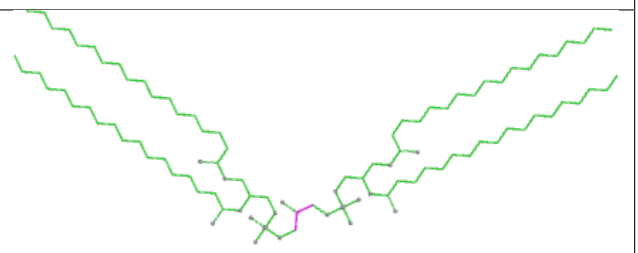

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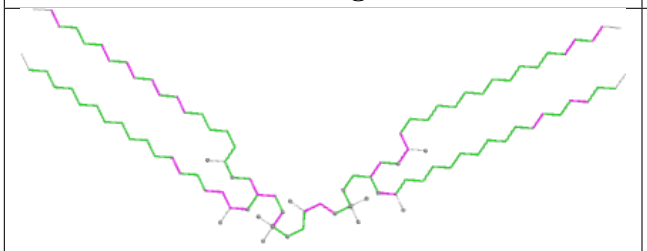

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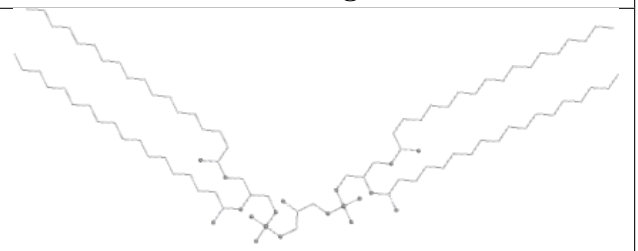
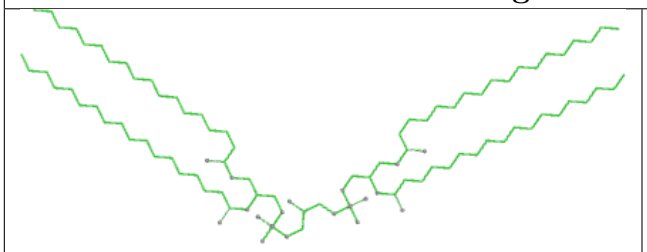


Rings

Ligand CDL AP 301



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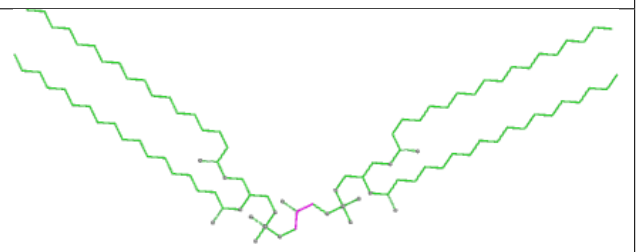

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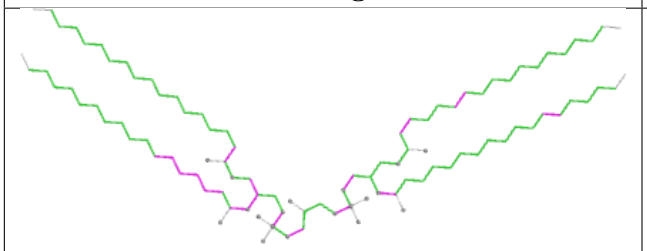

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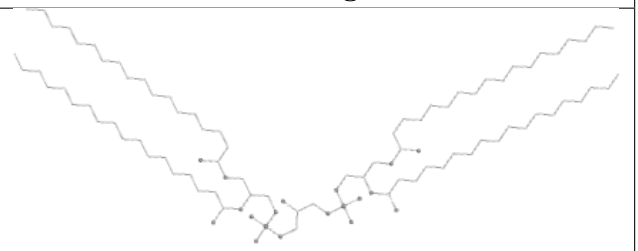
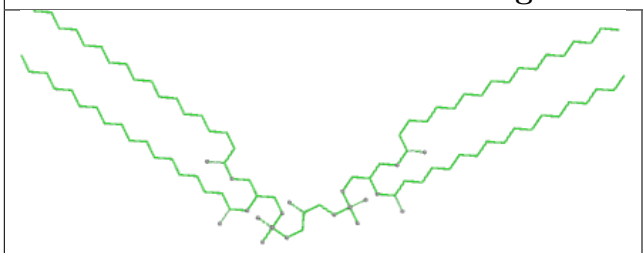


Rings

Ligand CDL A1 402



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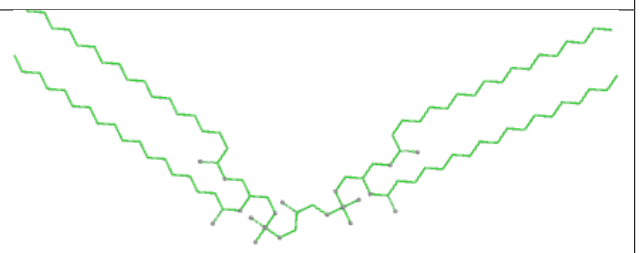
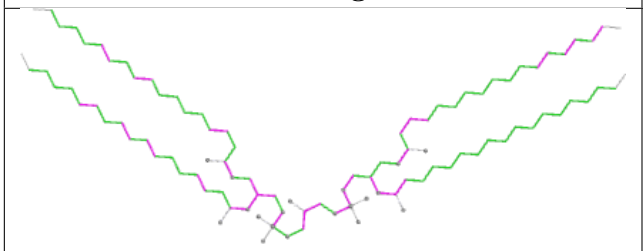


Bond angles



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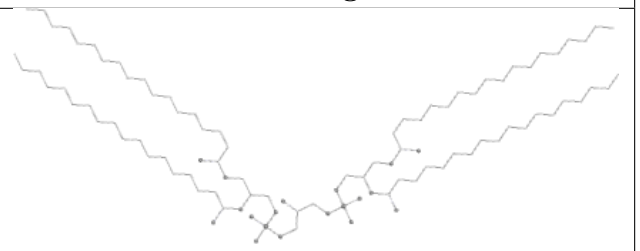

Rings

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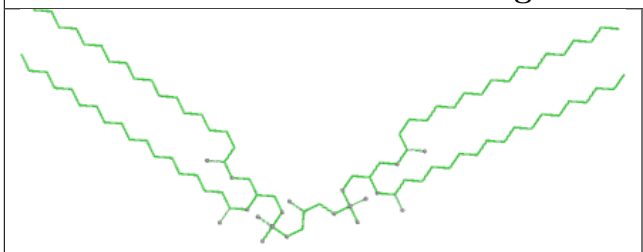

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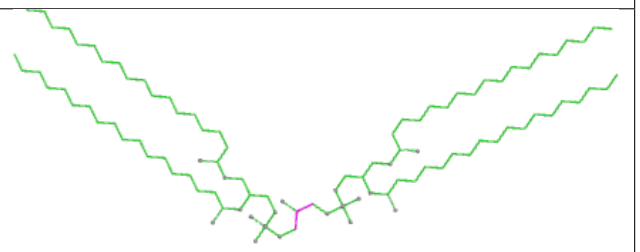

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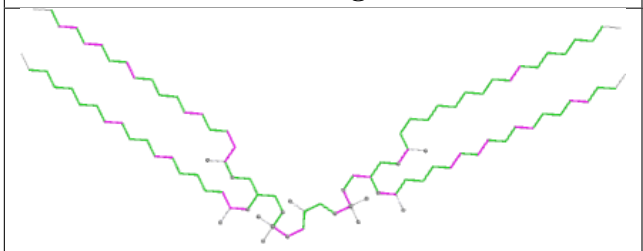

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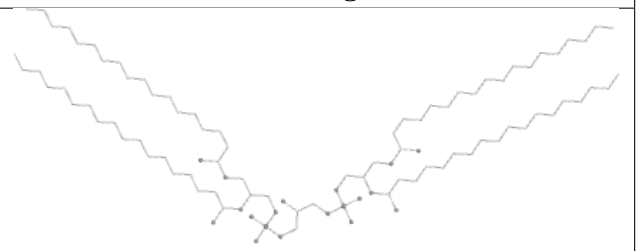
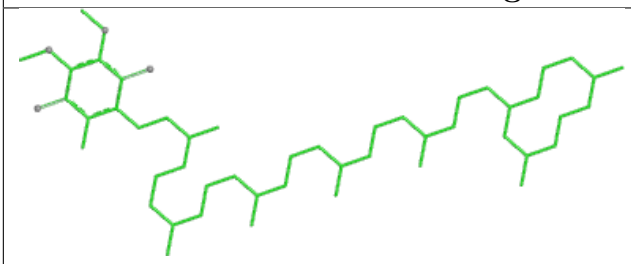


Rings

Ligand UQ8 EN 1205



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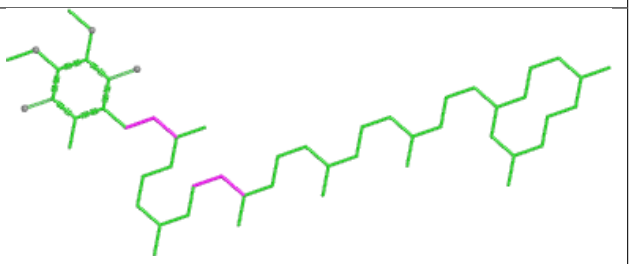

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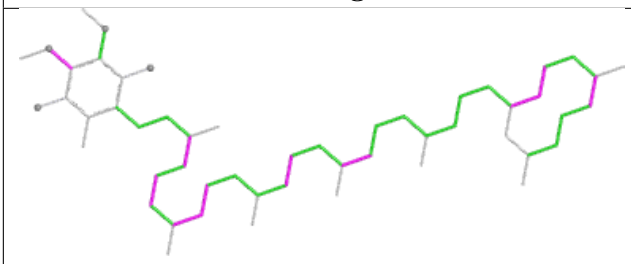

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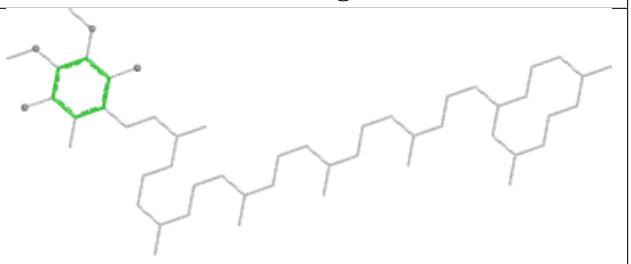
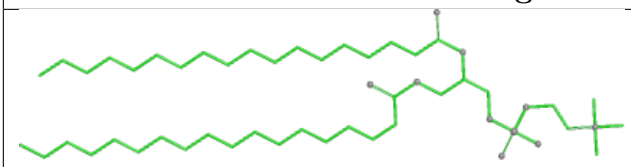


Rings

Ligand PC1 EO 201



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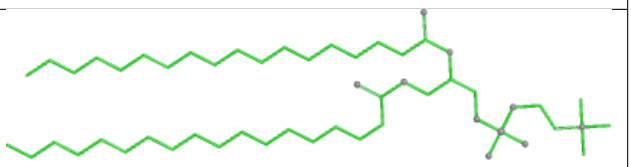

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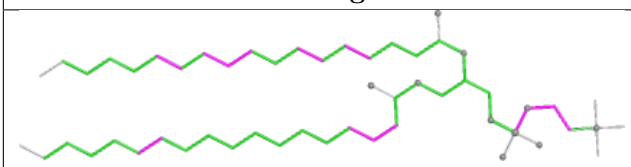

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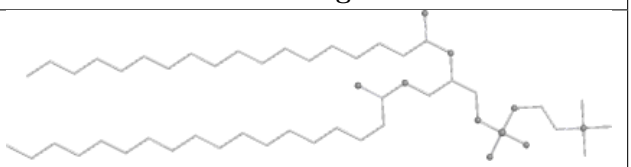
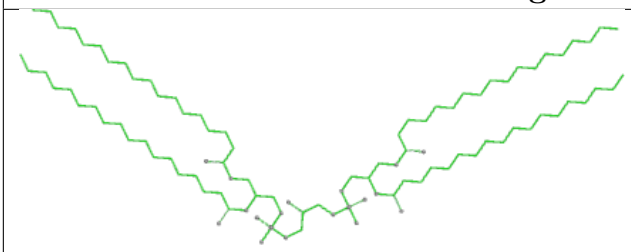


Rings

Ligand CDL c 509



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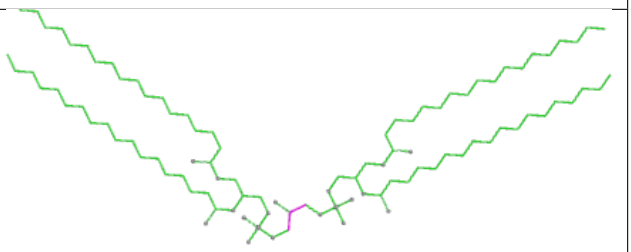
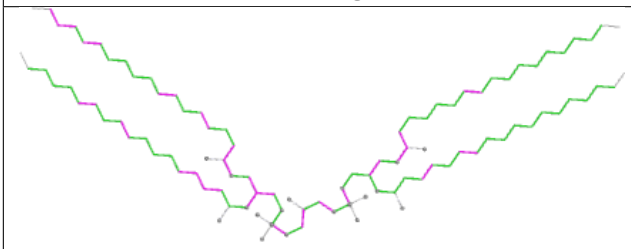


Bond angles



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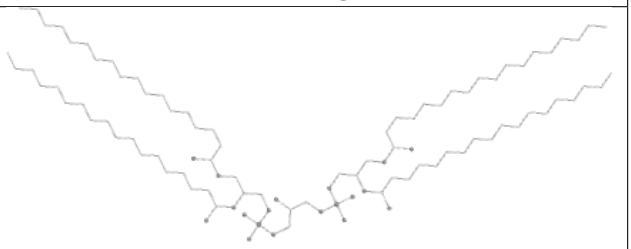

Rings

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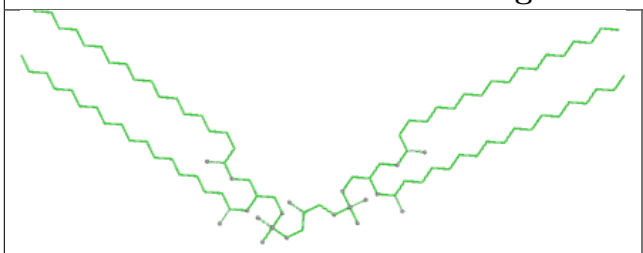
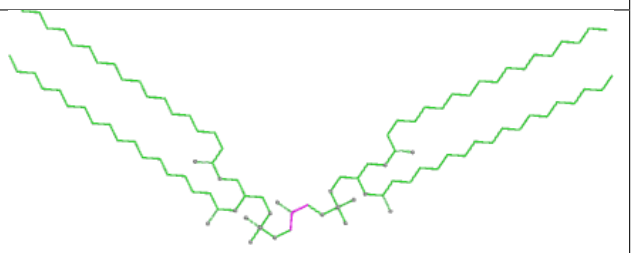
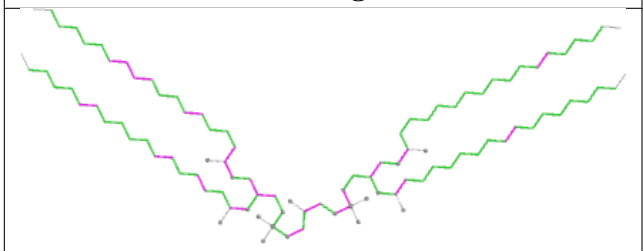
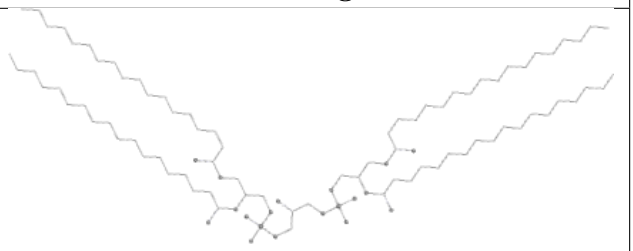
 Bond lengths	 Bond angles
 Torsions	 Rings

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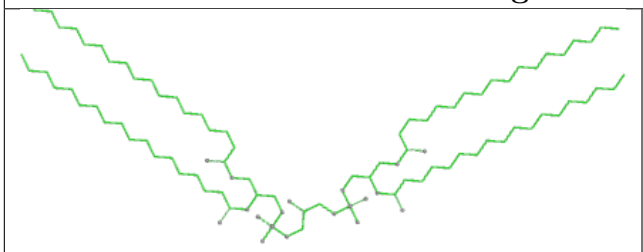
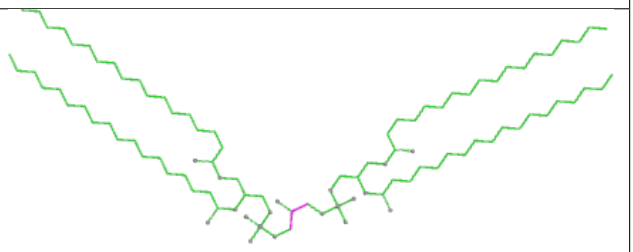
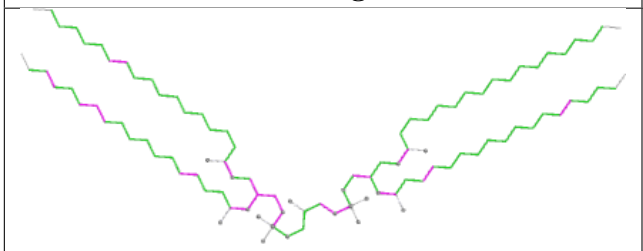
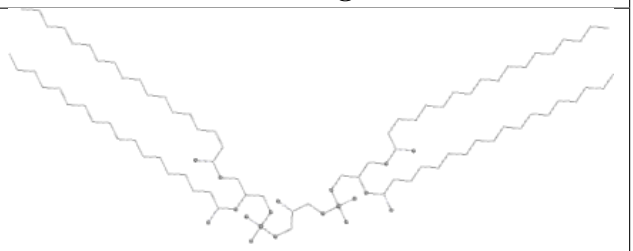
 Bond lengths	 Bond angles
 Torsions	 Rings

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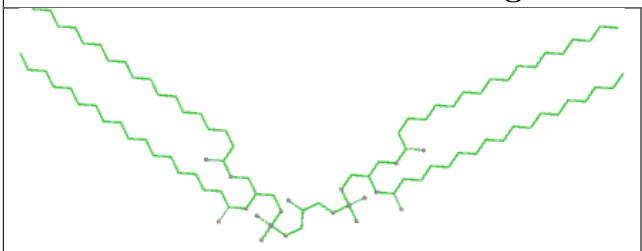
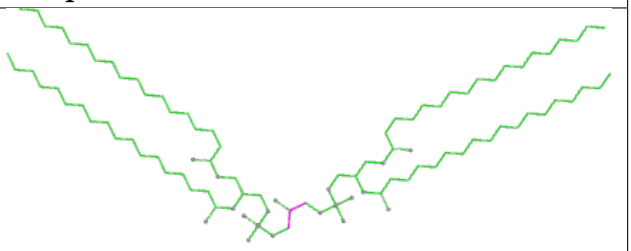
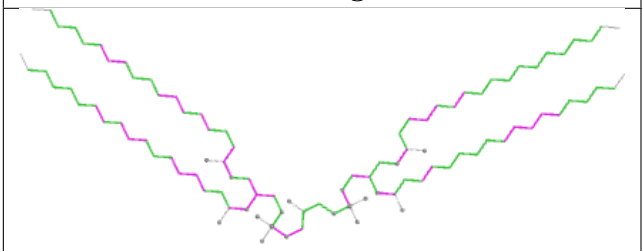
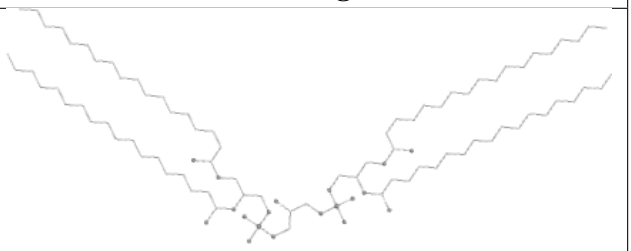
 Bond lengths	 Bond angles
 Torsions	 Rings

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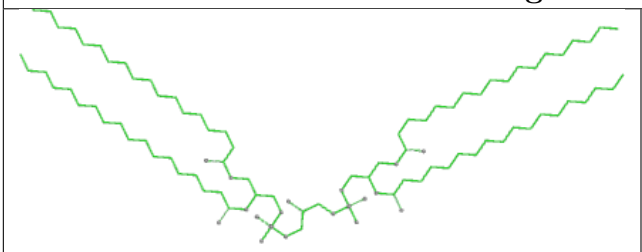
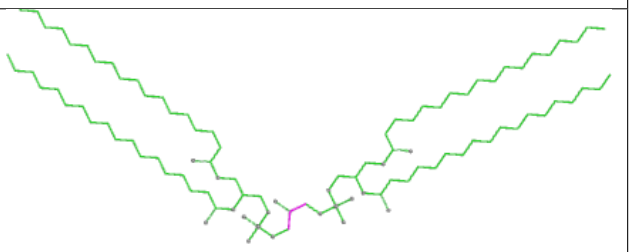
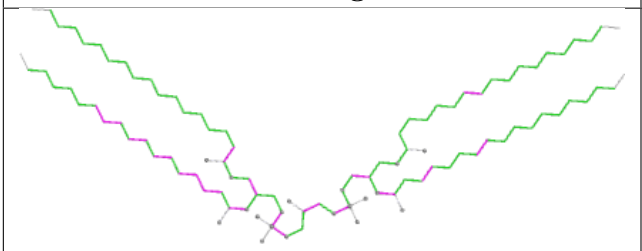
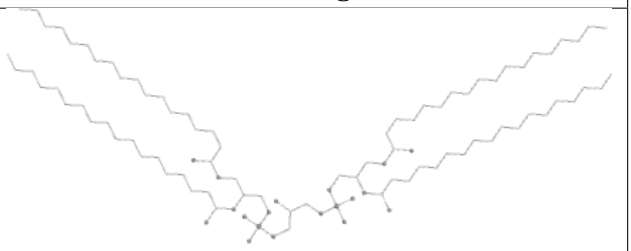
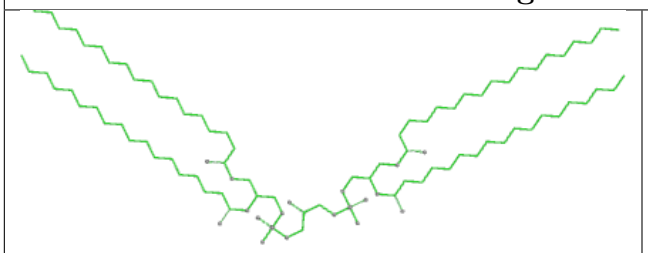
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Dr 402



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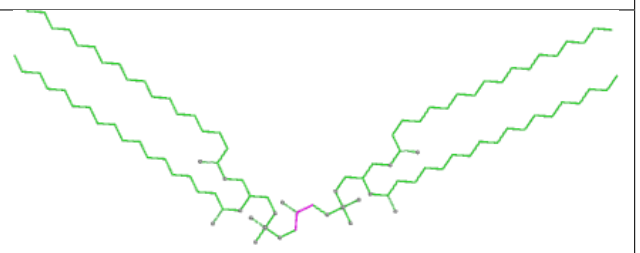

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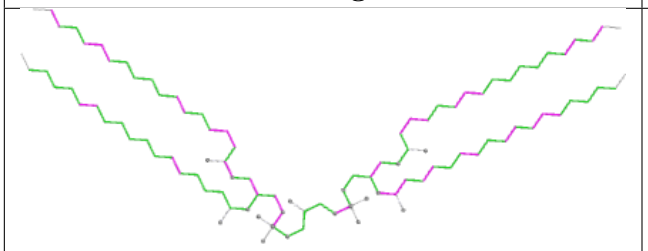

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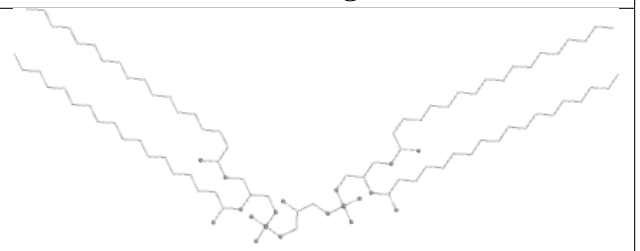
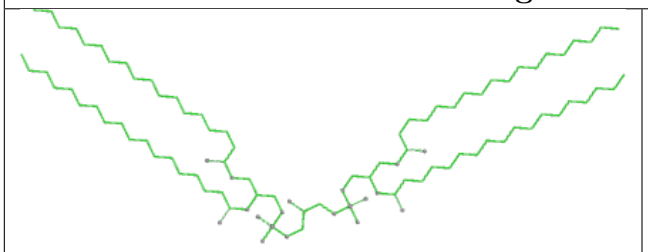


Rings

Ligand CDL A0 601



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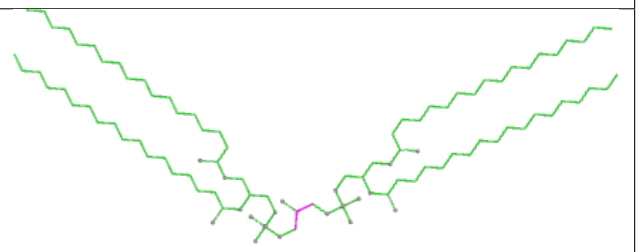

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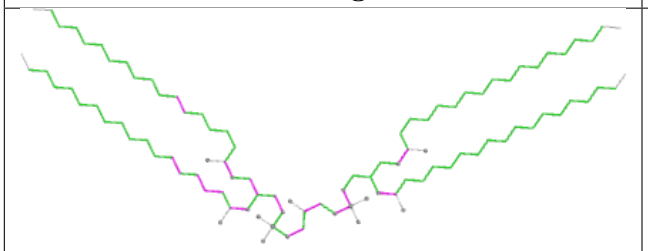

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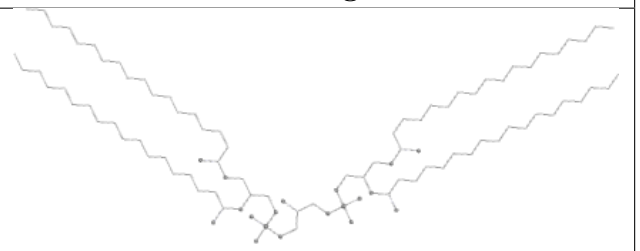
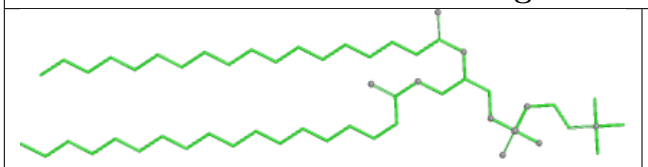


Rings

Ligand PC1 BG 202



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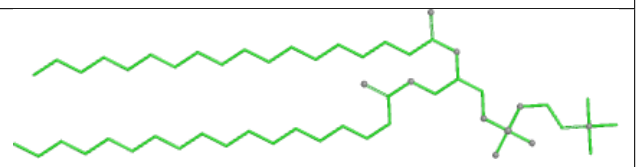
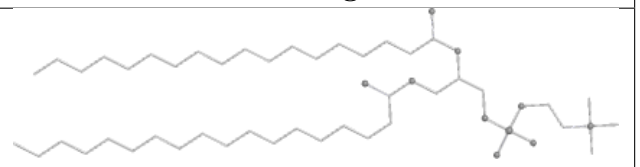
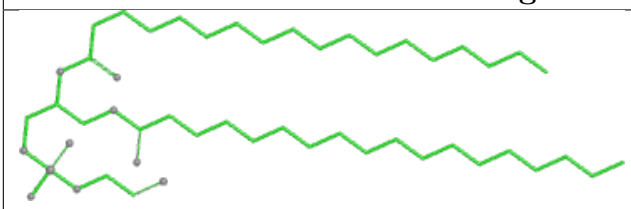
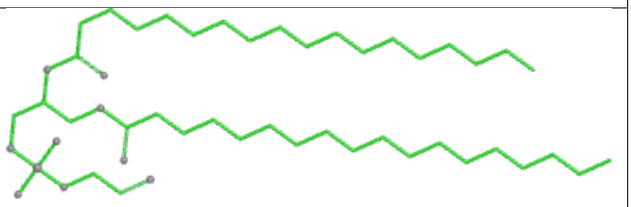
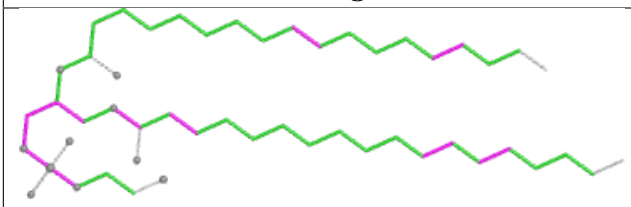
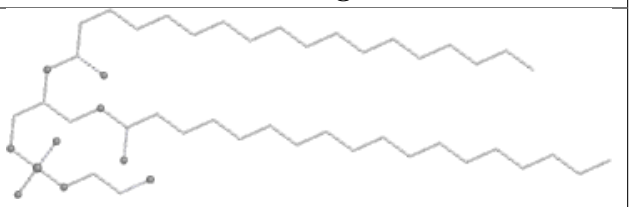


Bond angles

Torsions



Rings

Ligand 3PE Da 708	
 Bond lengths	 Bond angles
 Torsions	 Rings

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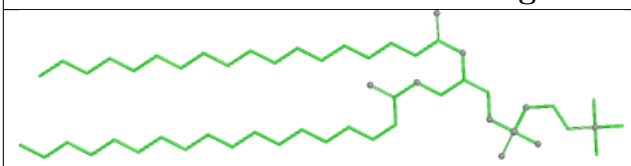
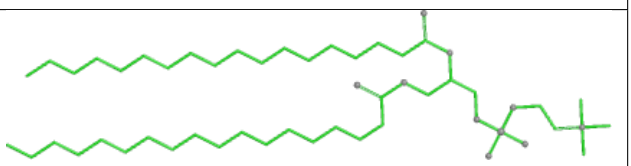
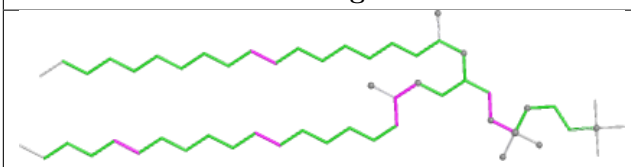
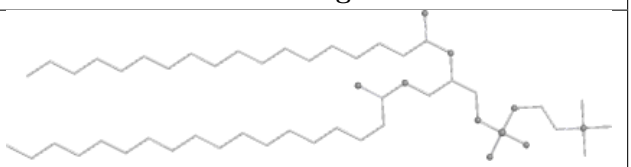
 Bond lengths	 Bond angles
 Torsions	 Rings

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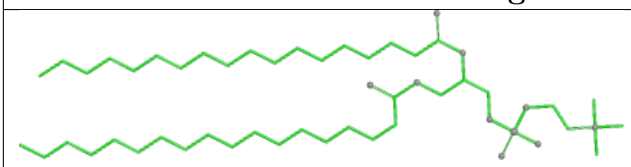
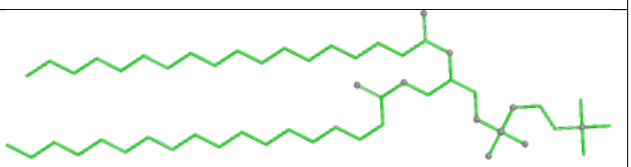
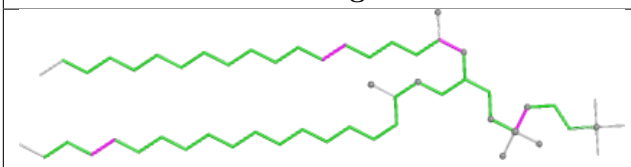
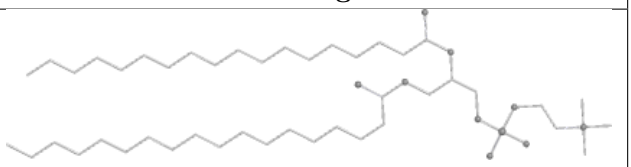
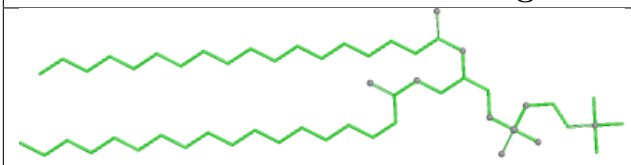
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 DS 406



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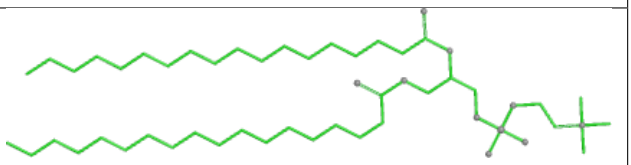
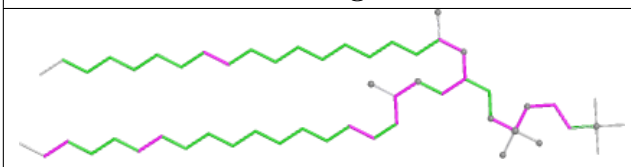


Bond angles



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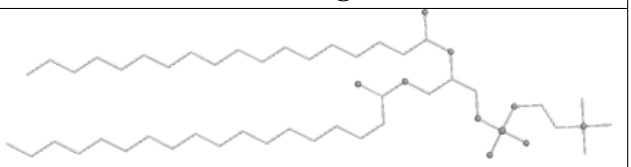
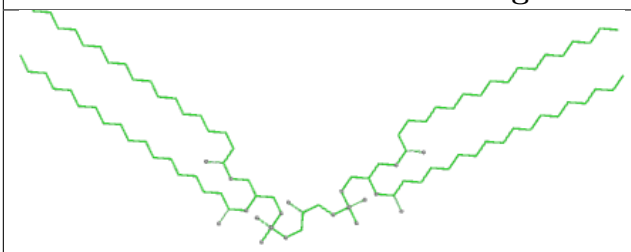


Rings

Ligand CDL EO 202



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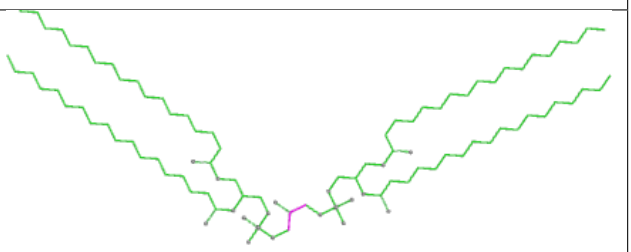

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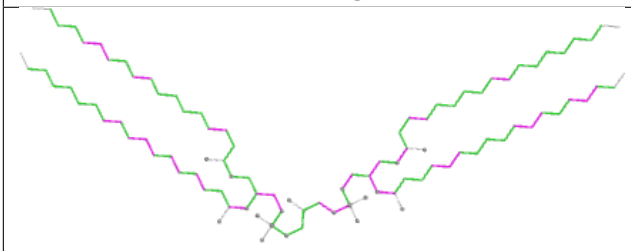

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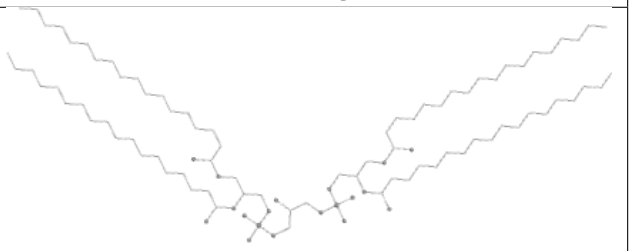

Rings

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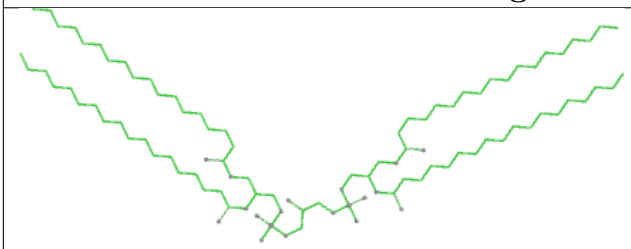

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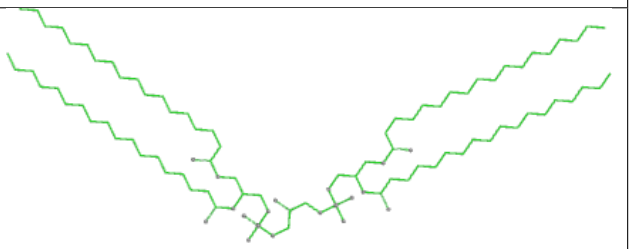
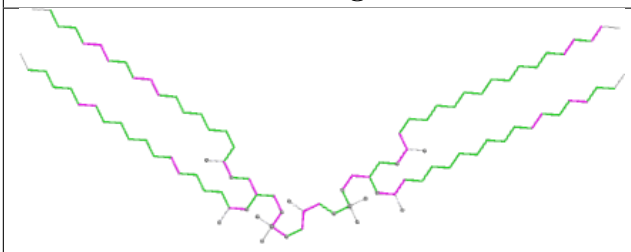


Bond angles



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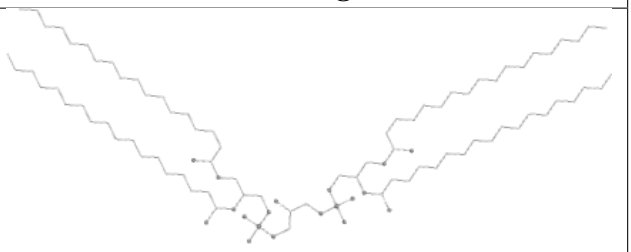
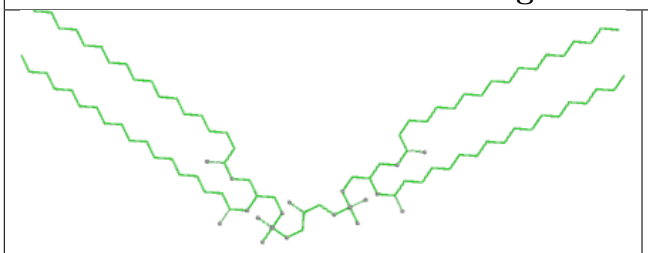


Rings

Ligand CDL B1 402



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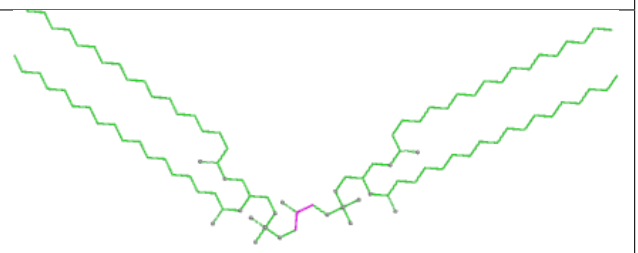

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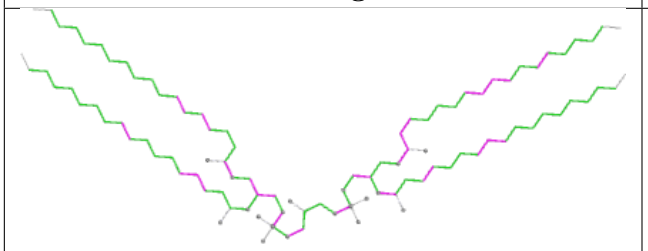

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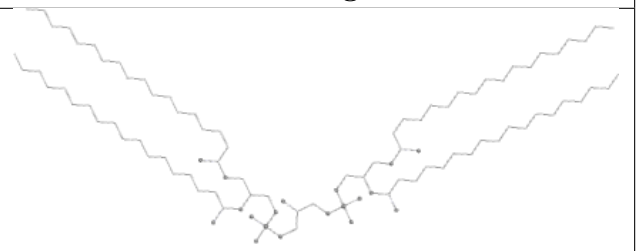
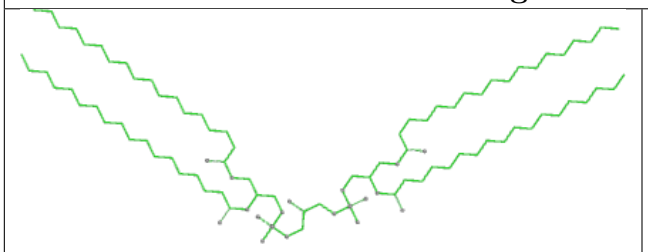
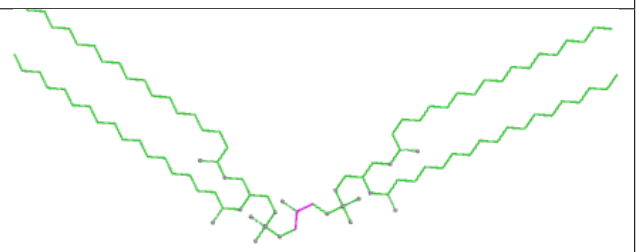


Rings

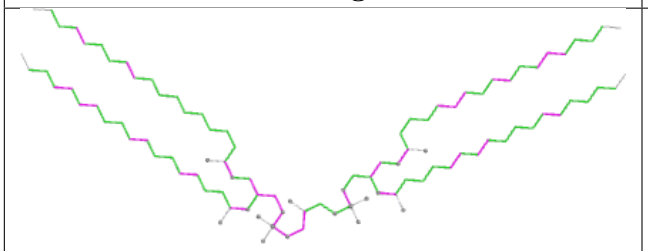
Ligand CDL DN 507



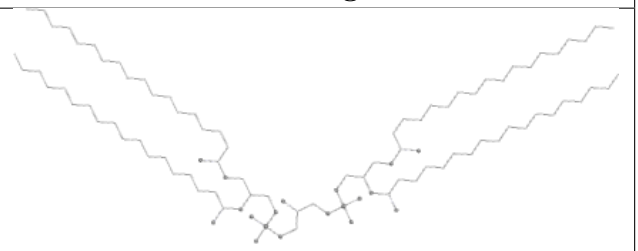
Bond lengths



Bond angles

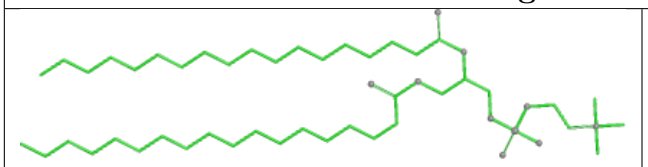


Torsions

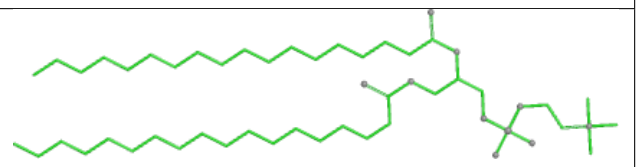


Rings

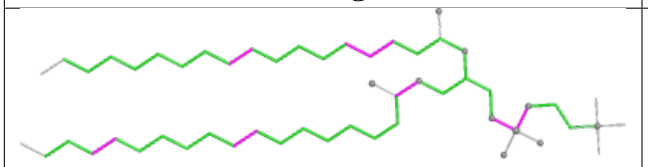
Ligand PC1 DJ 306



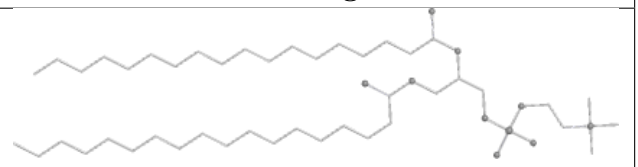
Bond lengths



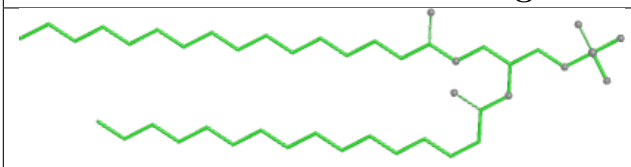
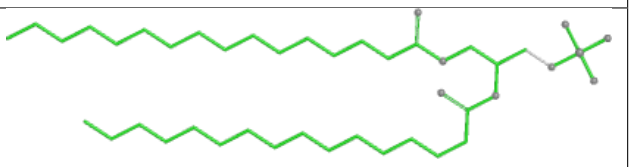
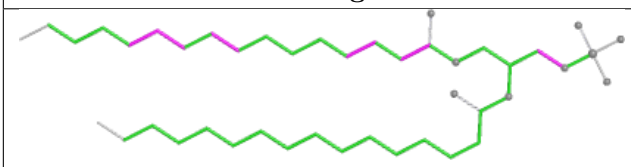
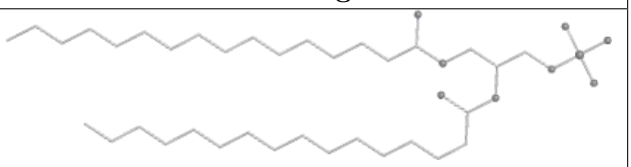
Bond angles

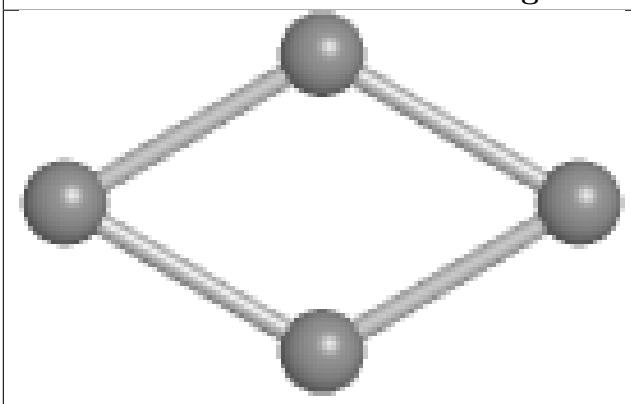
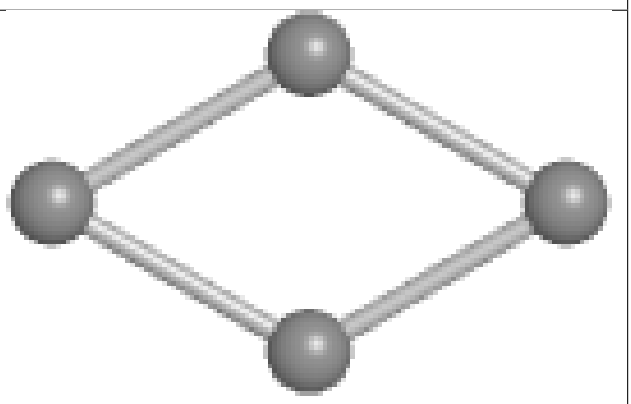
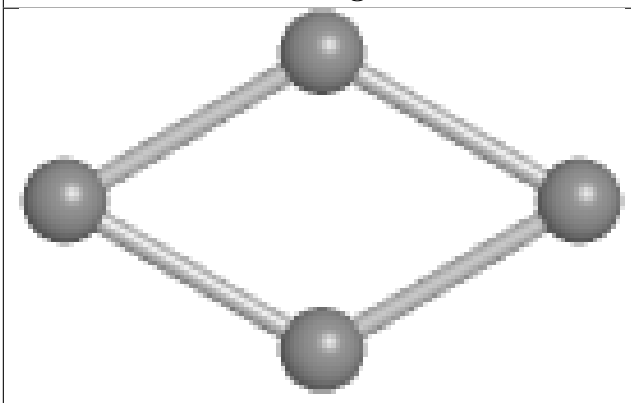
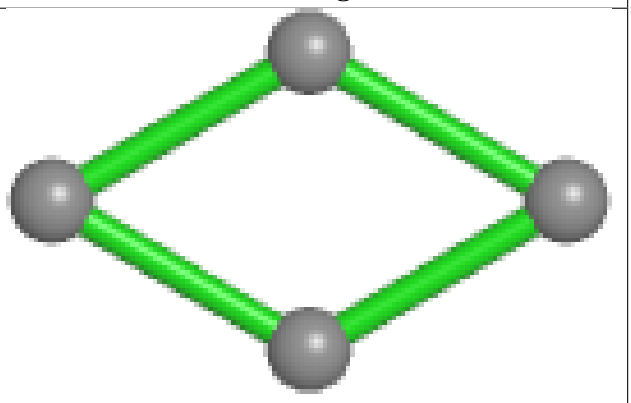


Torsions

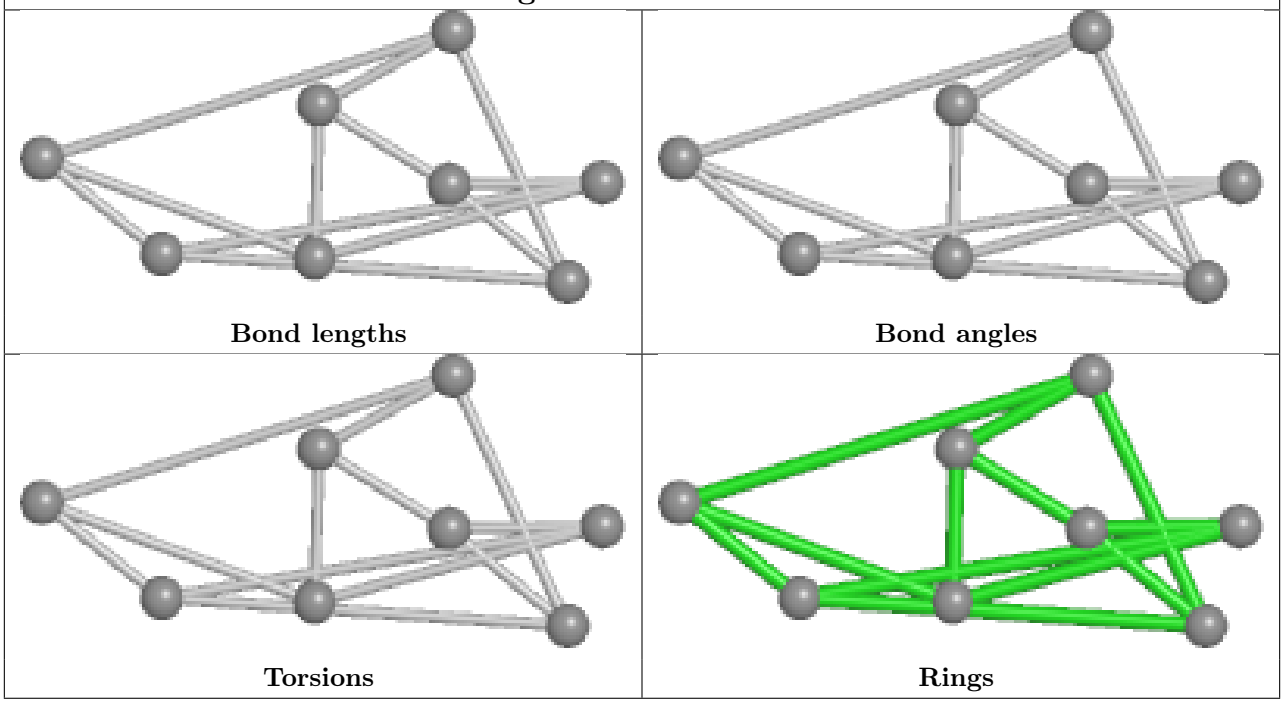


Rings

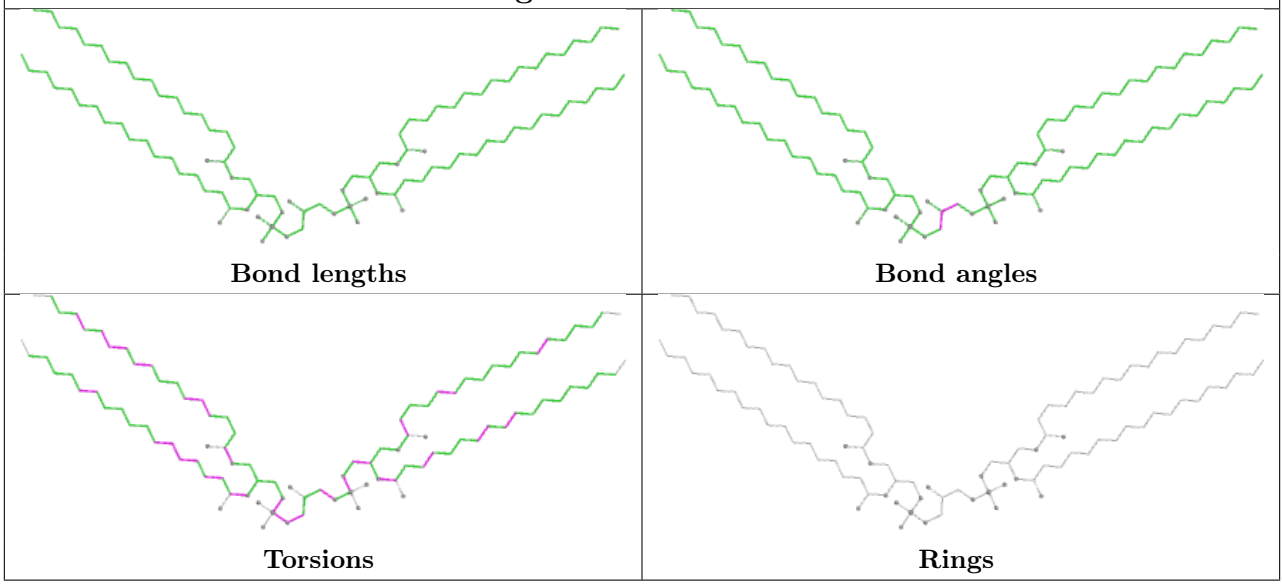
Ligand LPP Dn 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES AI 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

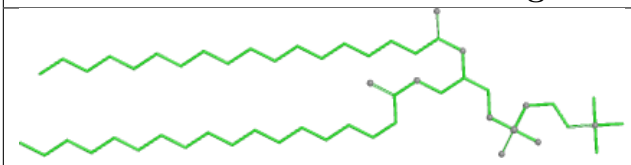
Ligand SF4 AD 501



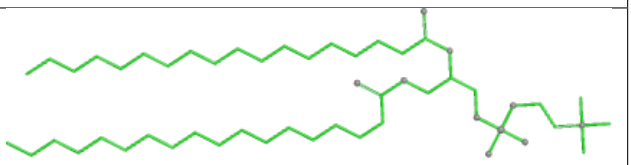
Ligand CDL A0 602



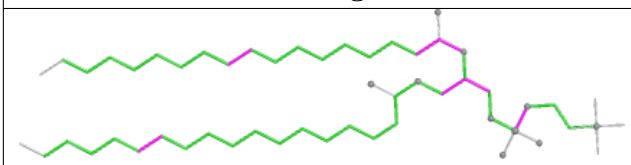
Ligand PC1 C 510



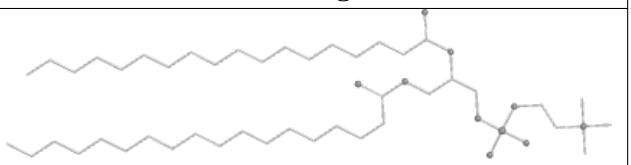
Bond lengths



Bond angles

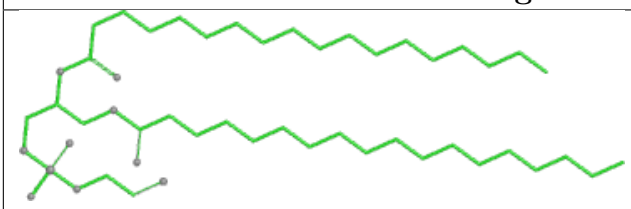


Torsions

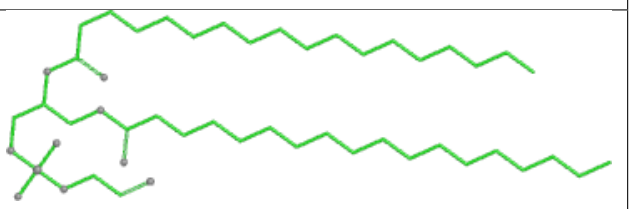


Rings

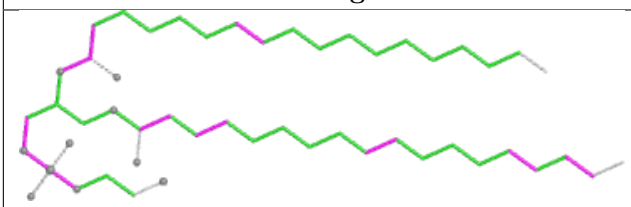
Ligand 3PE DX 303



Bond lengths



Bond angles



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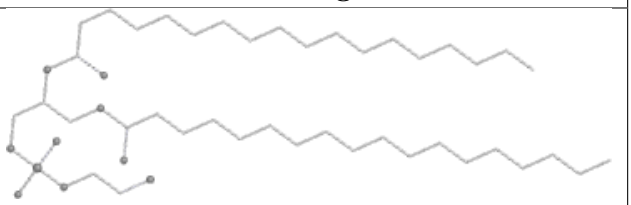
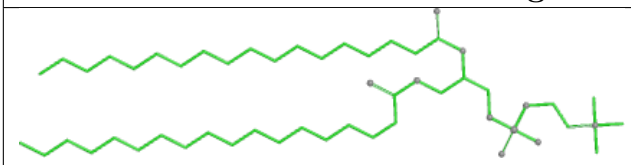


Rings

Ligand PC1 C 508



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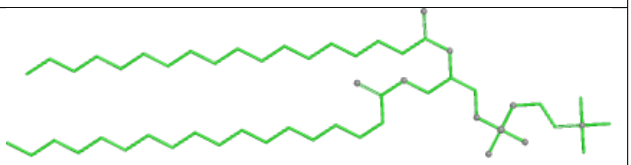
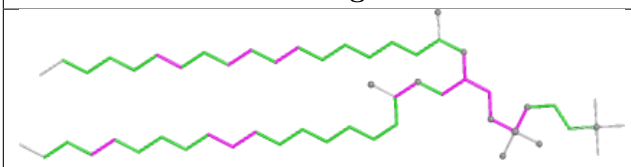
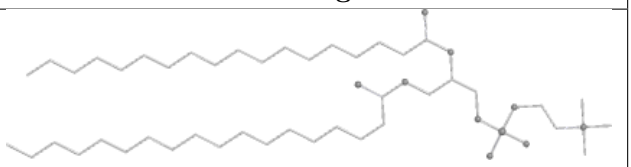


Bond angles

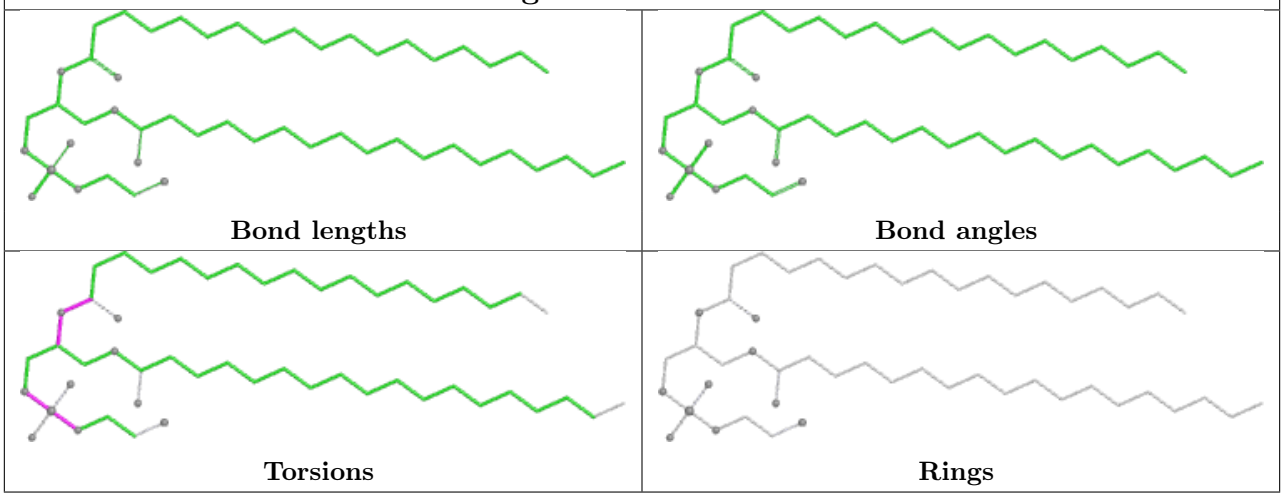


Torsions

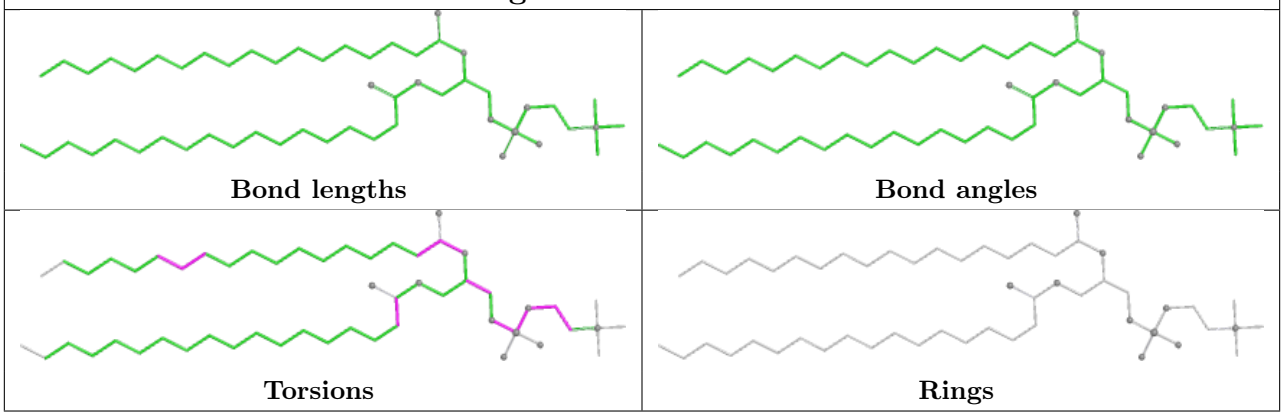


Rings

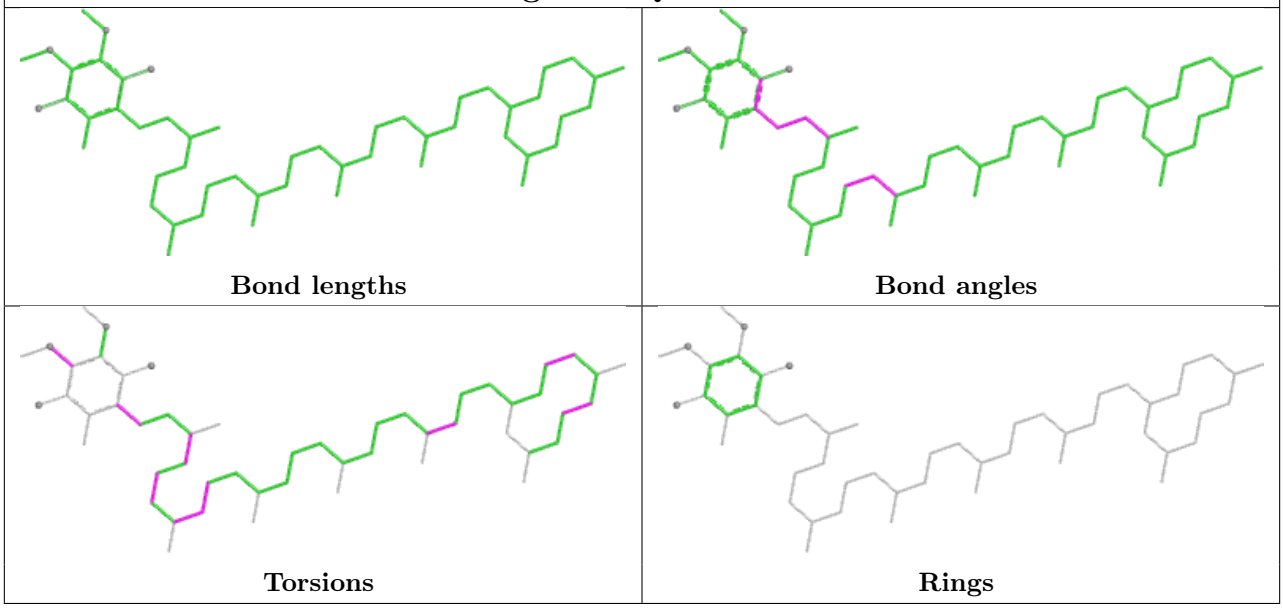
Ligand 3PE Eo 203



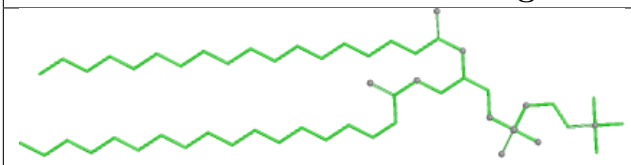
Ligand PC1 Dx 1203



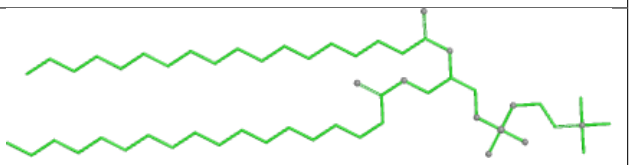
Ligand UQ8 El 906



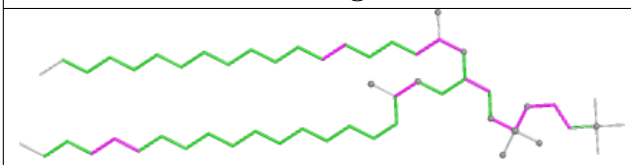
Ligand PC1 A9 603



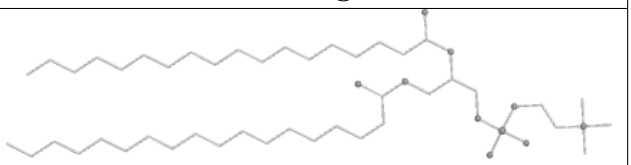
Bond lengths



Bond angles

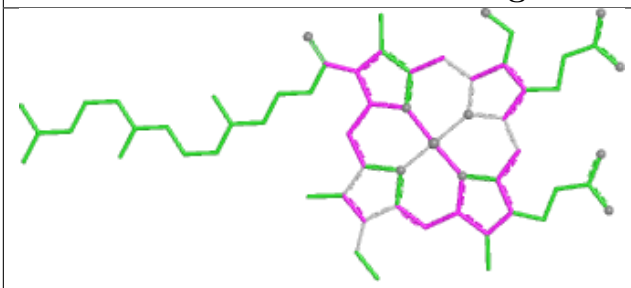


Torsions



Rings

Ligand HEA DA 703



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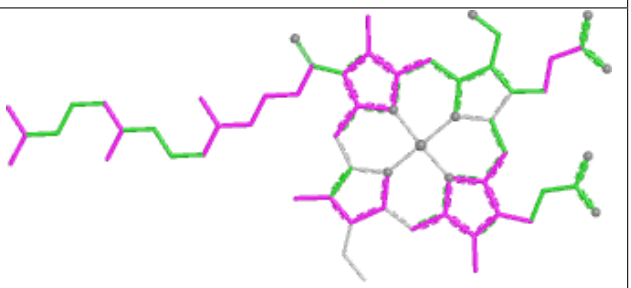
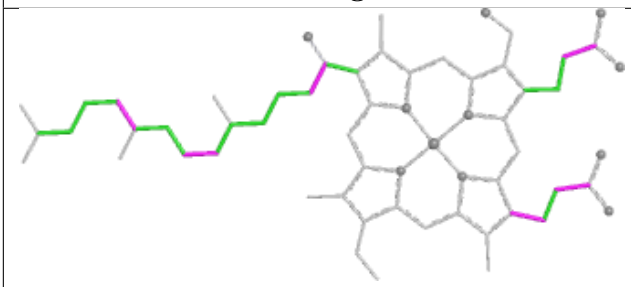
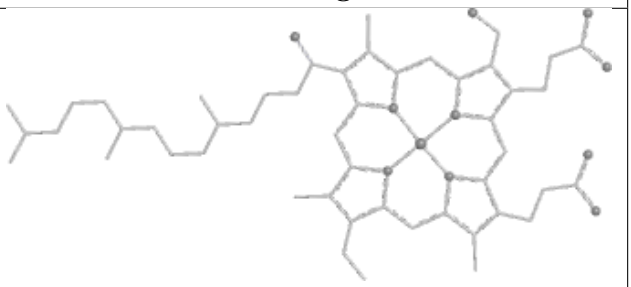


Bond angles

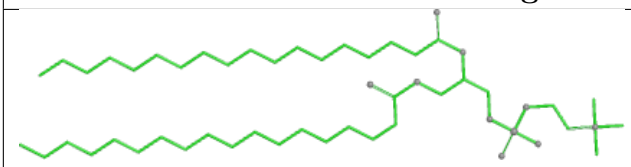


Torsions



Rings

Ligand PC1 Dj 406



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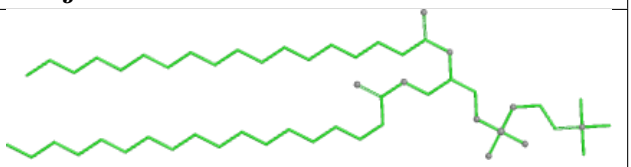
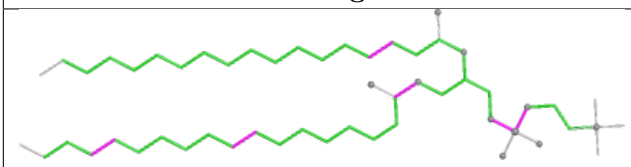
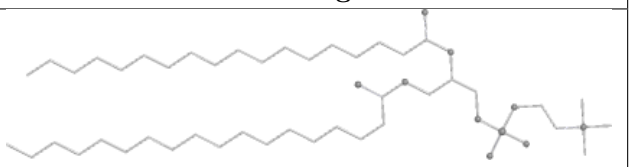


Bond angles

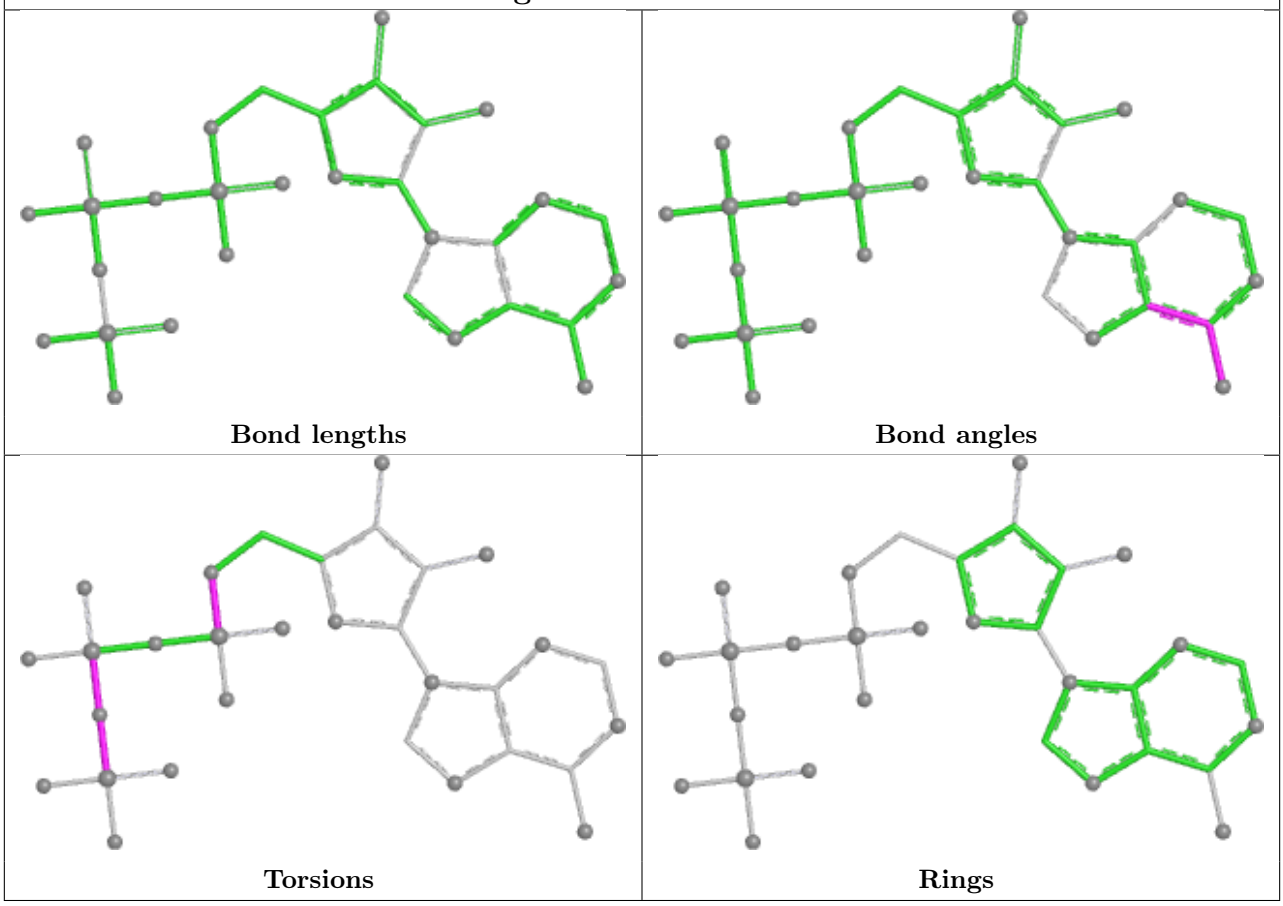


Torsions

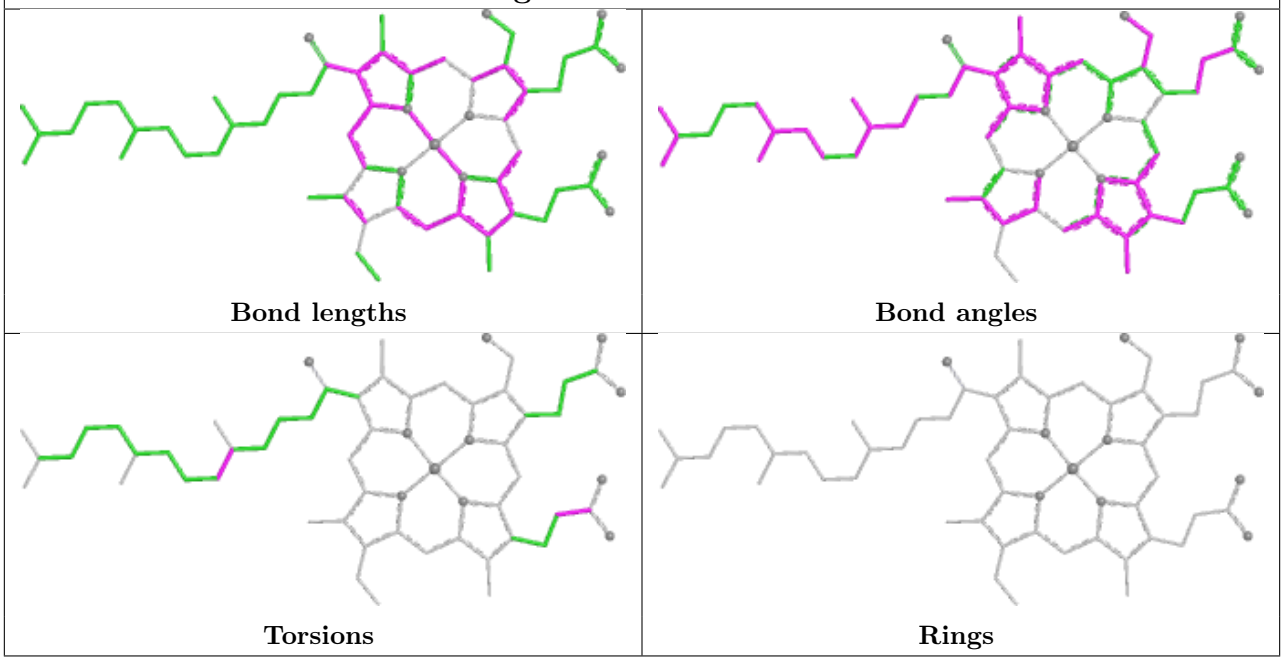


Rings

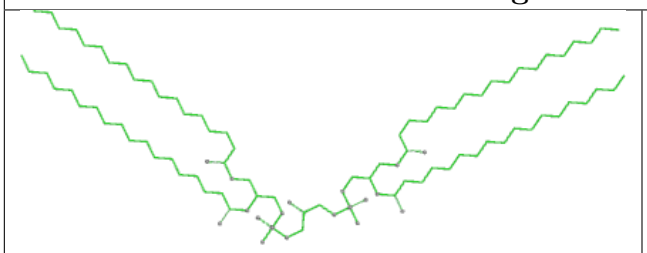
Ligand ATP ER 201



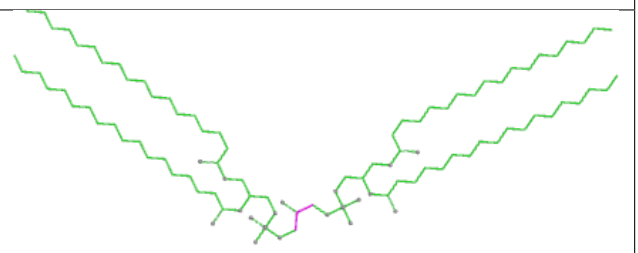
Ligand HEA Da 702



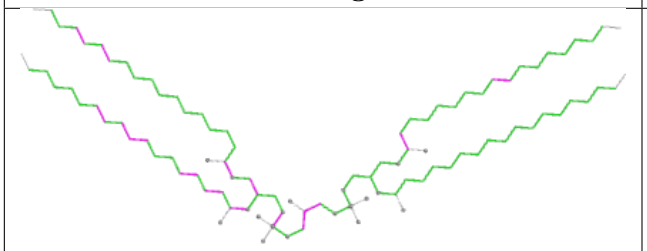
Ligand CDL DA 709



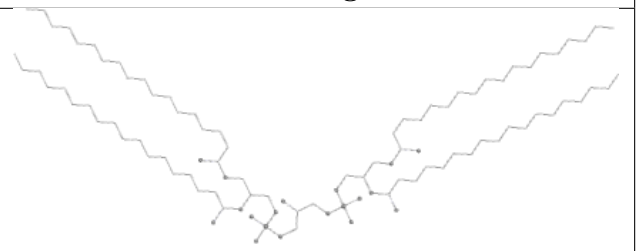
Bond lengths



Bond angles

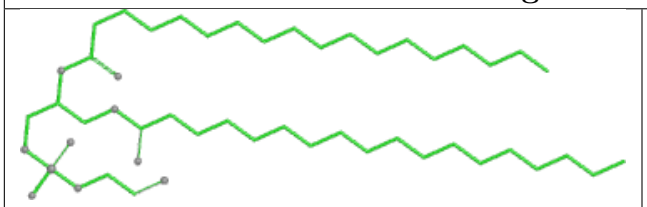


Torsions

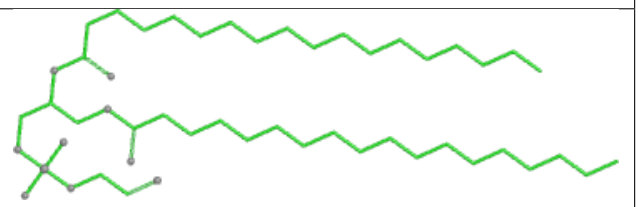


Rings

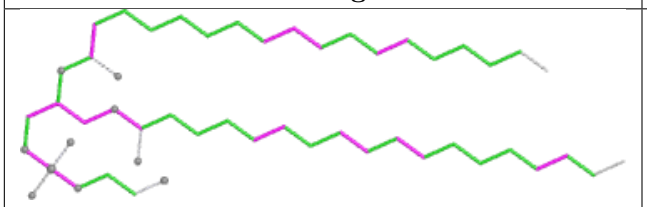
Ligand 3PE Ds 403



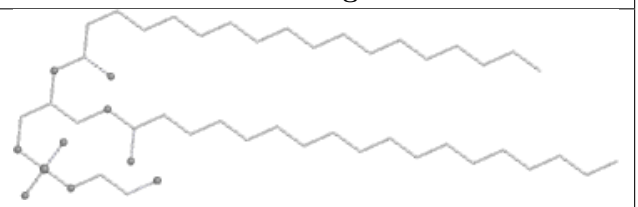
Bond lengths



Bond angles

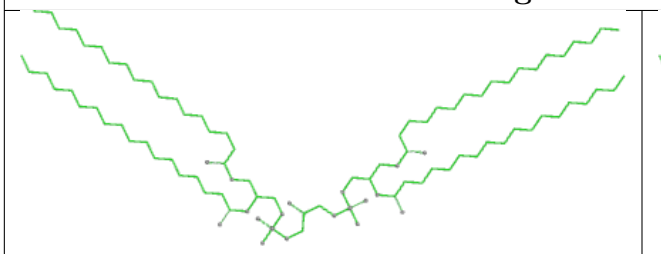


Torsions

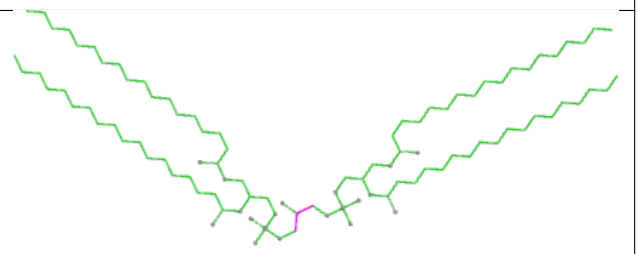


Rings

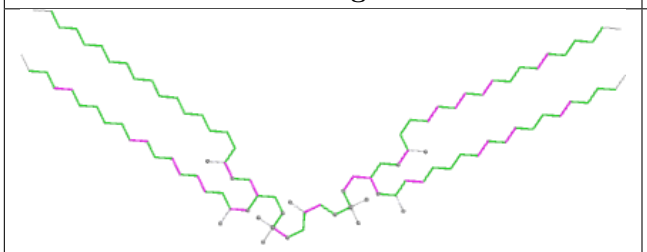
Ligand CDL DS 401



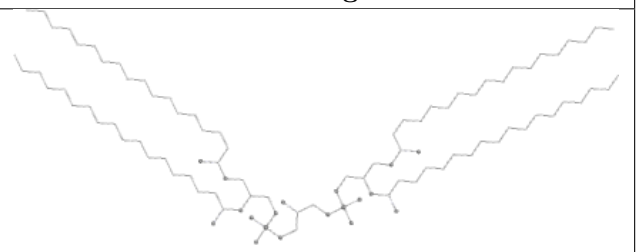
Bond lengths



Bond angles

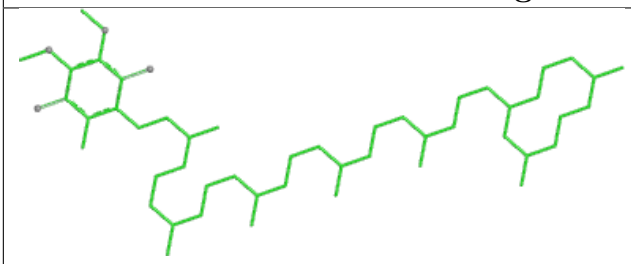


Torsions

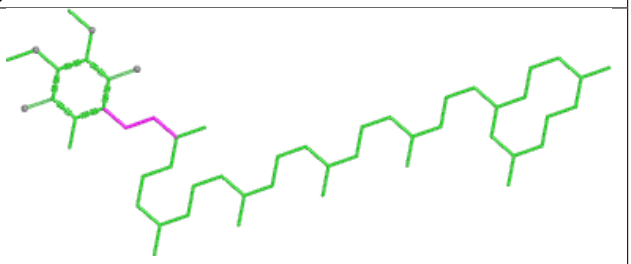


Rings

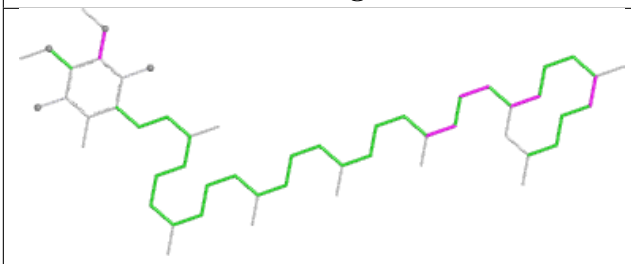
Ligand UQ8 DS 403



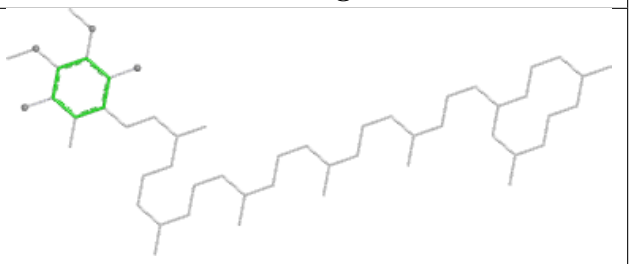
Bond lengths



Bond angles

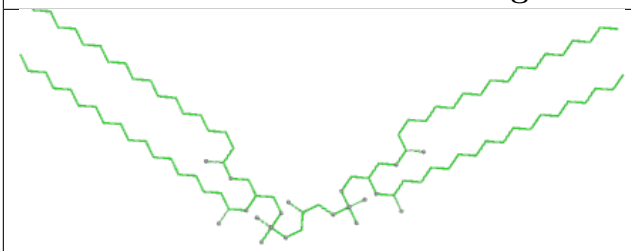


Torsions

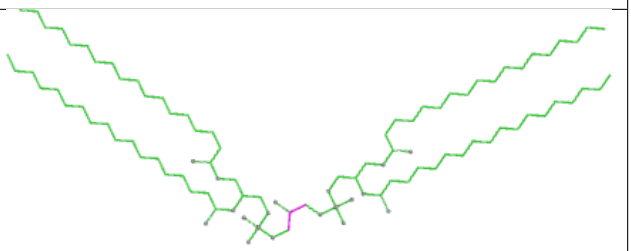


Rings

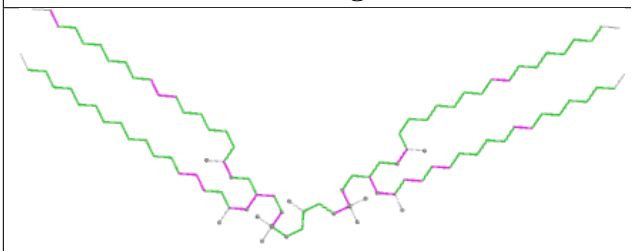
Ligand CDL CC 305



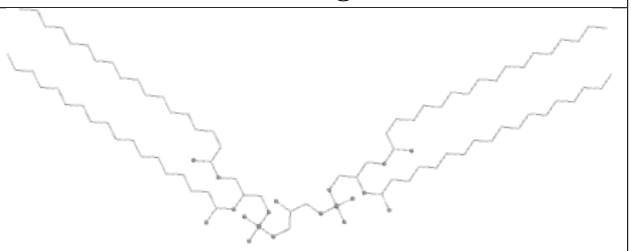
Bond lengths



Bond angles

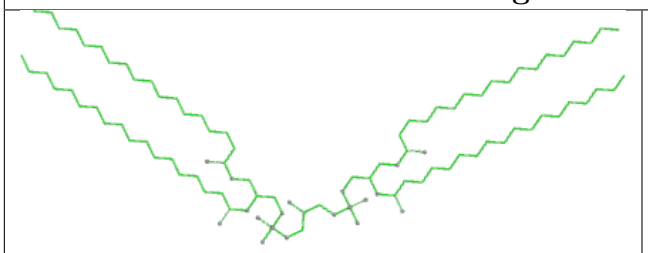


Torsions



Rings

Ligand CDL ED 604



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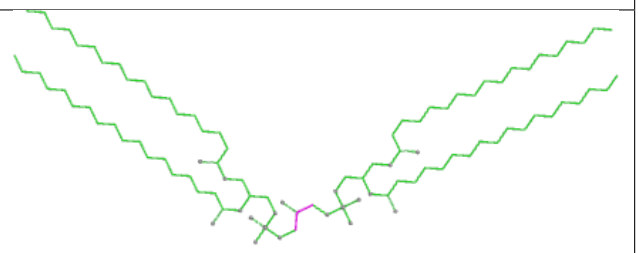
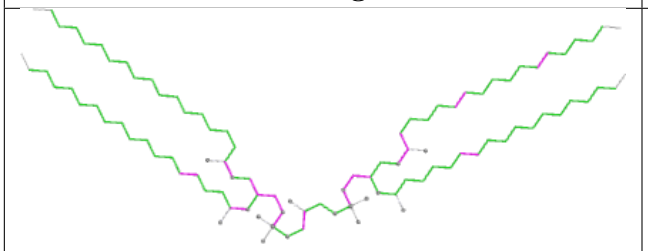


Bond angles



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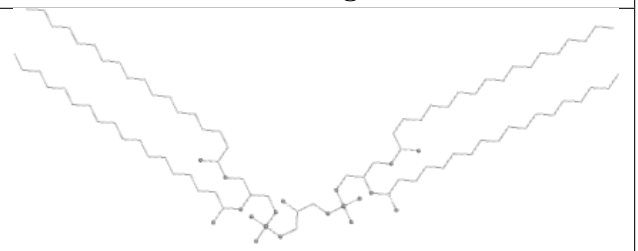
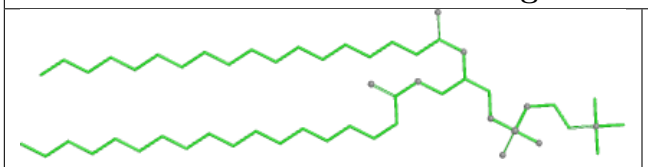


Rings

Ligand PC1 Eo 201



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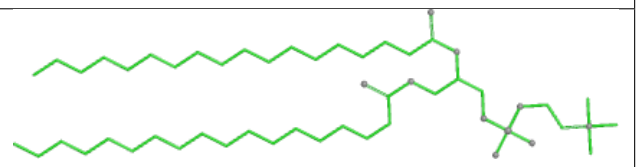
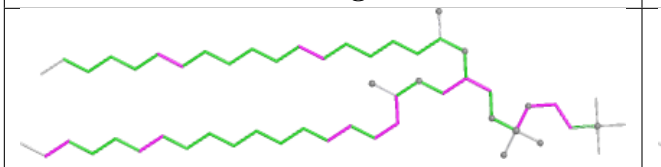


Bond angles



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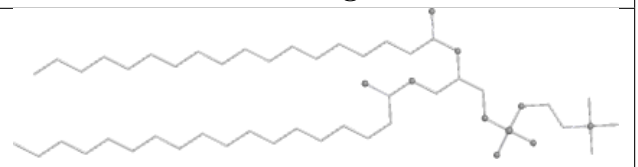
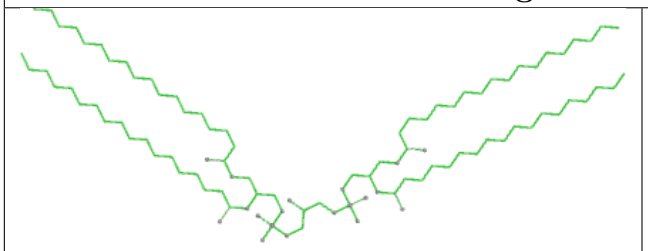
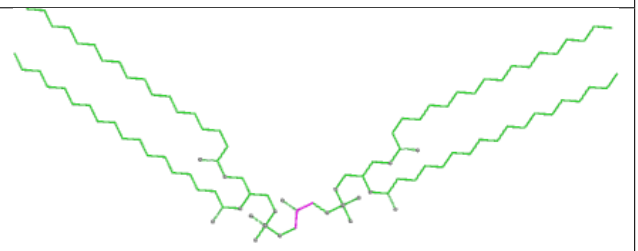


Rings

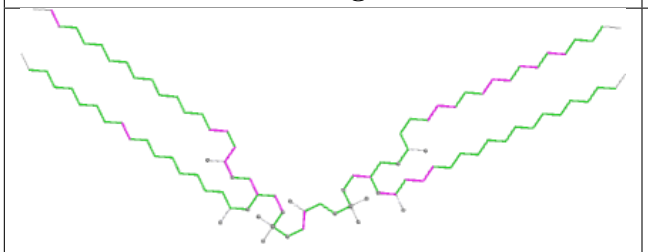
Ligand CDL CJ 201



Bond lengths



Bond angles



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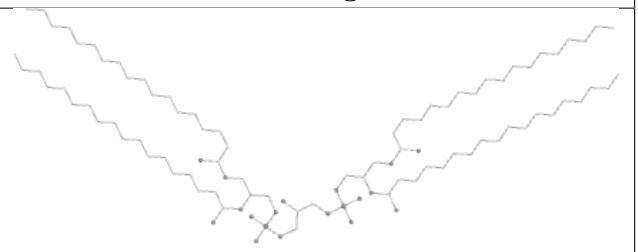
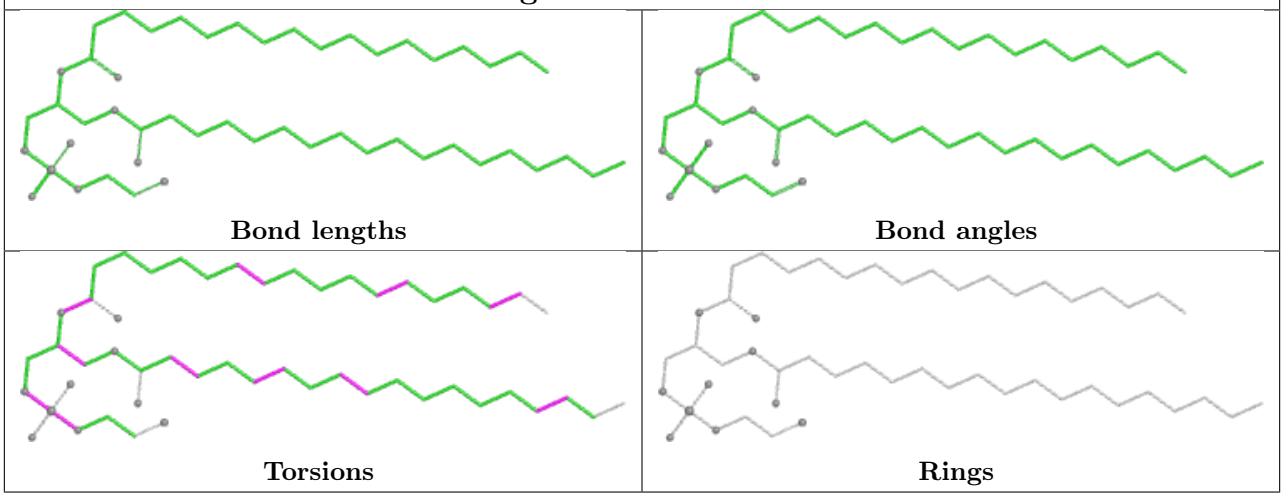
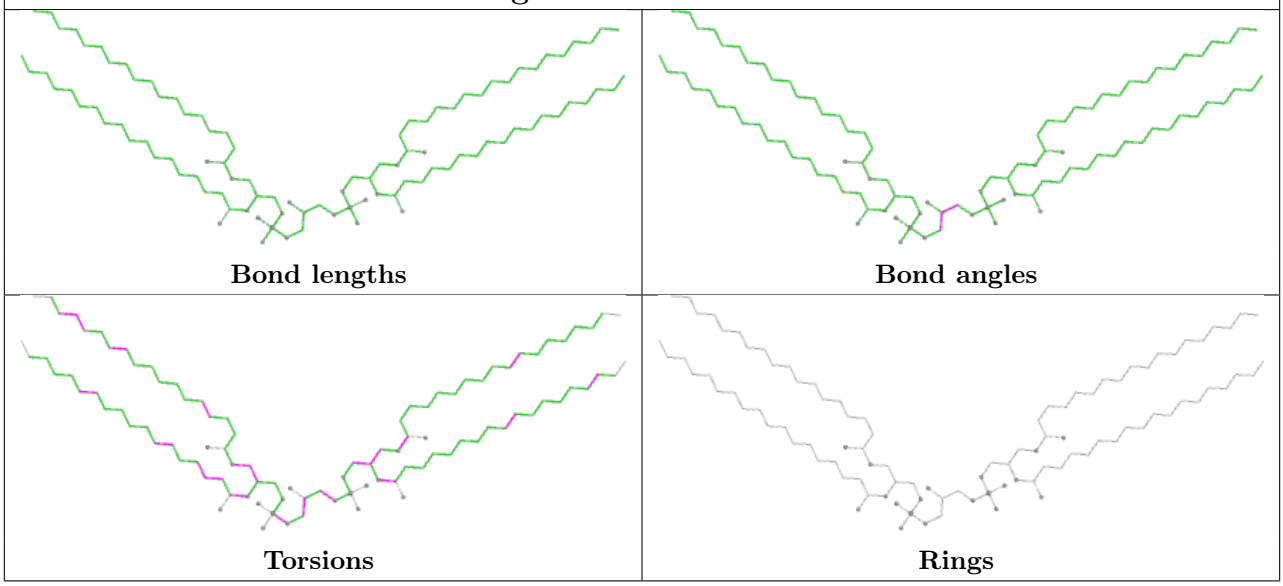


Rings

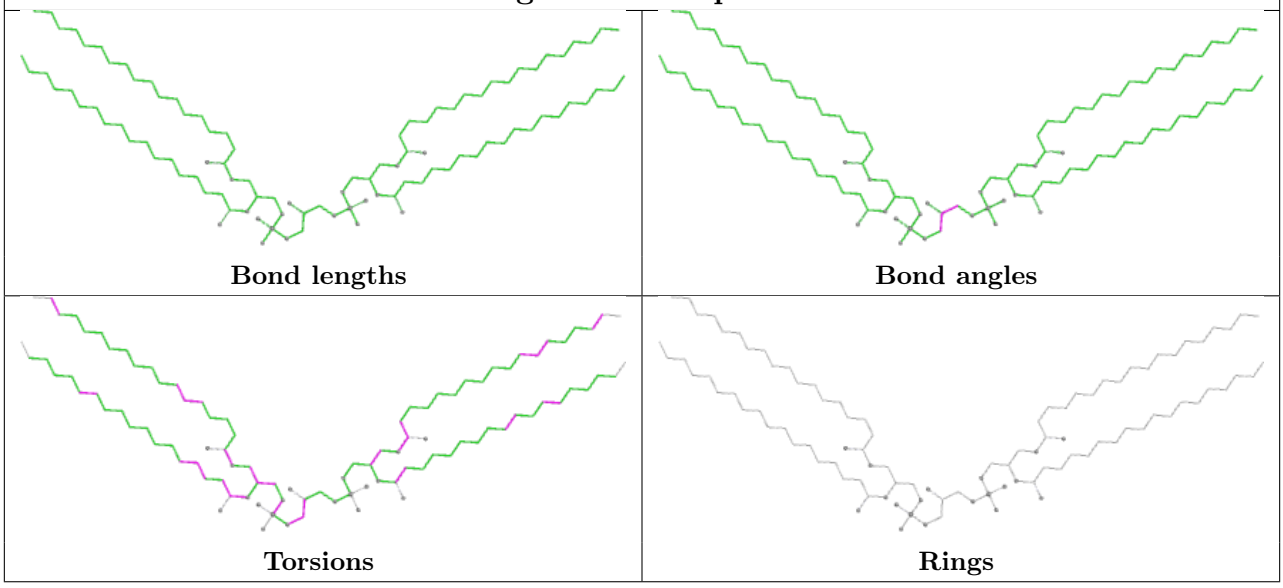
Ligand 3PE EL 904



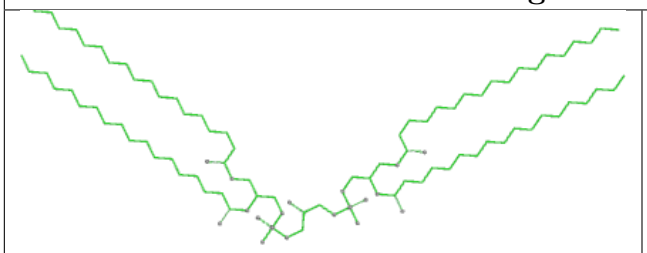
Ligand CDL DX 307



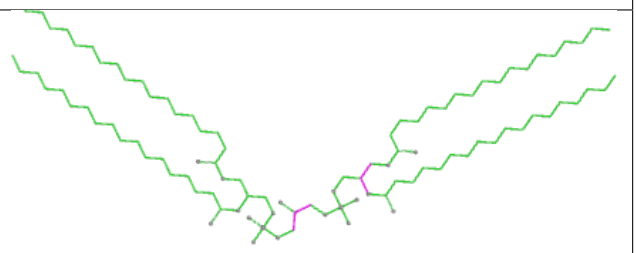
Ligand CDL Ep 701



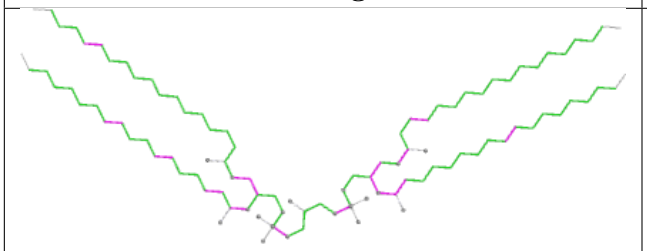
Ligand CDL h 501



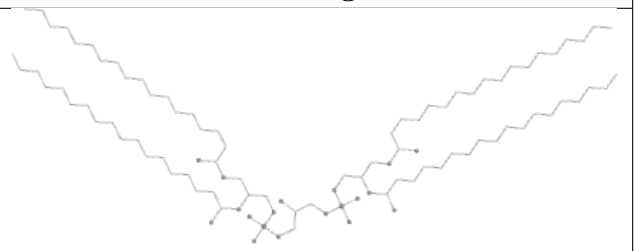
Bond lengths



Bond angles

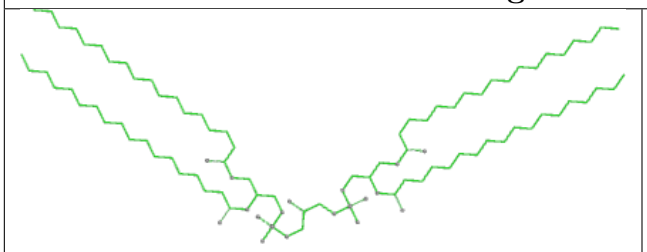


Torsions

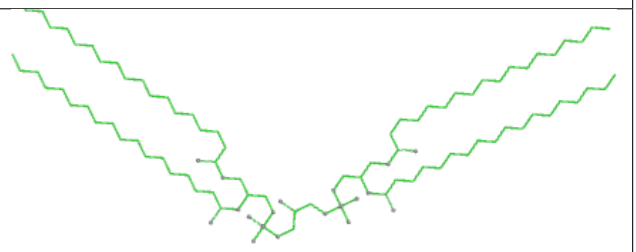


Rings

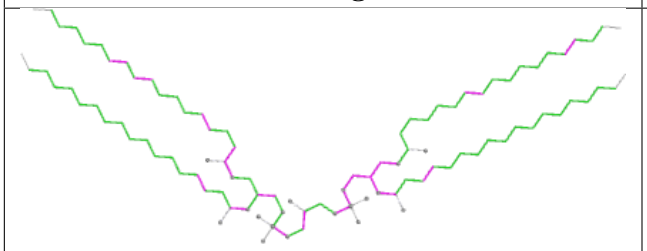
Ligand CDL AM 301



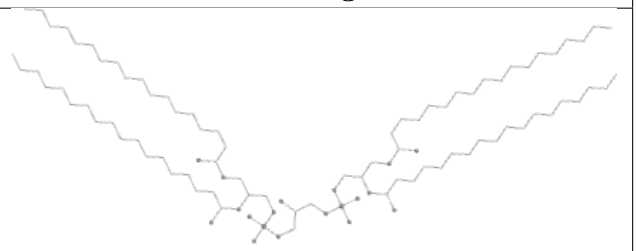
Bond lengths



Bond angles

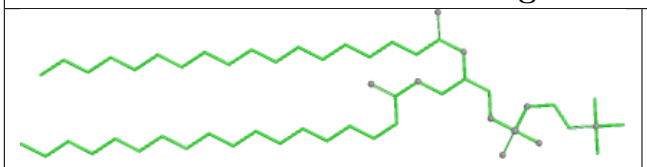


Torsions



Rings

Ligand PC1 A9 601



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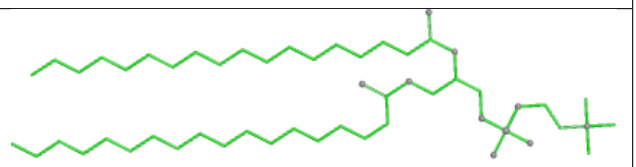
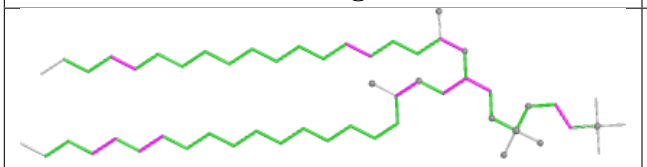
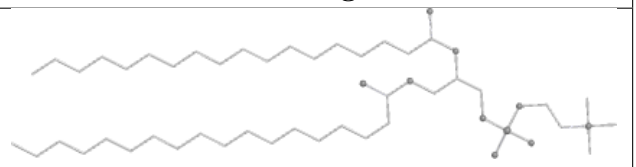


Bond angles

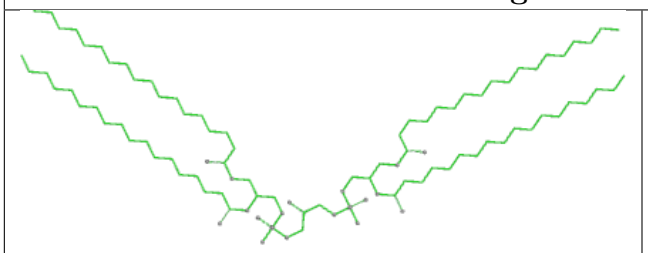


Torsions



Rings

Ligand CDL DU 401



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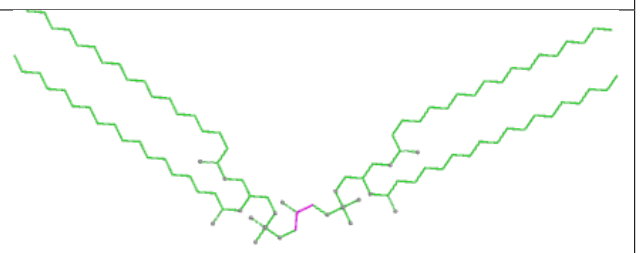
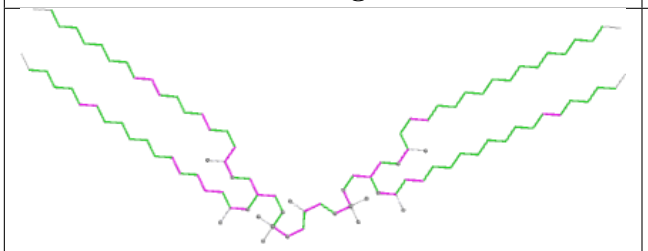


Bond angles



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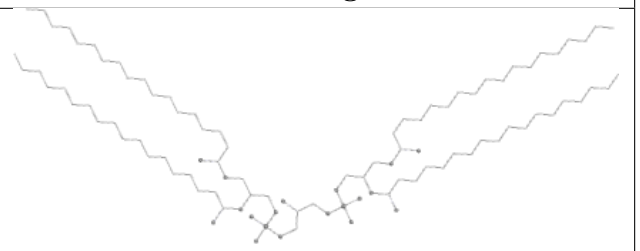
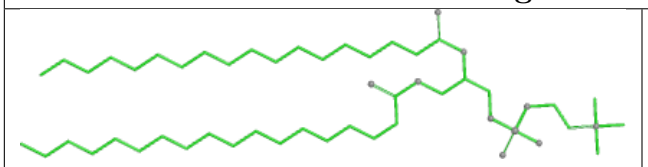
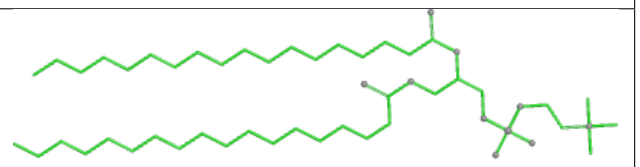


Rings

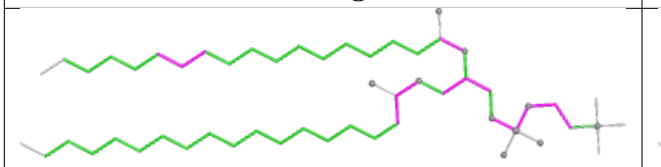
Ligand PC1 DX 308



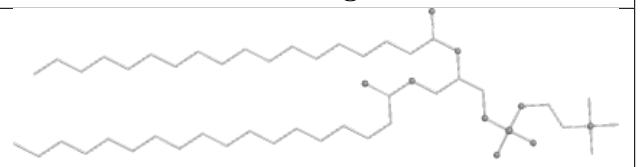
Bond lengths



Bond angles

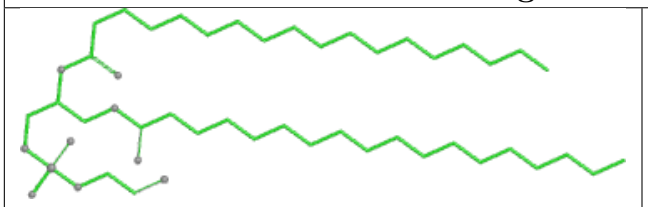


Torsions



Rings

Ligand 3PE EO 203



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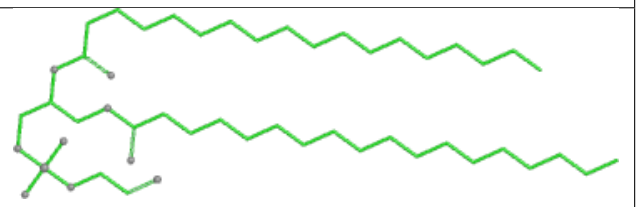
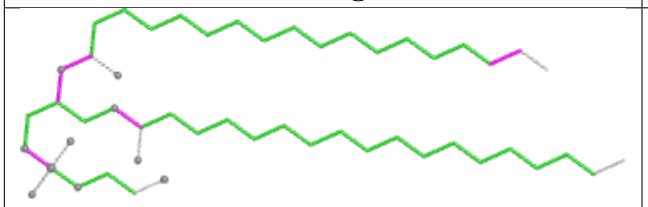
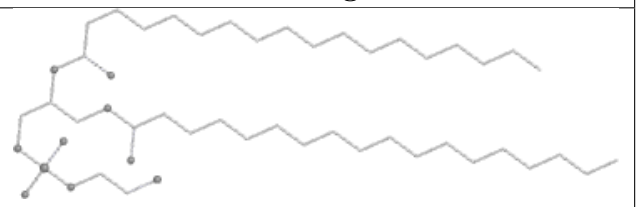


Bond angles

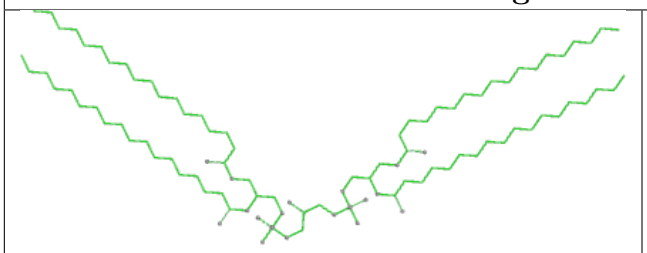


Torsions

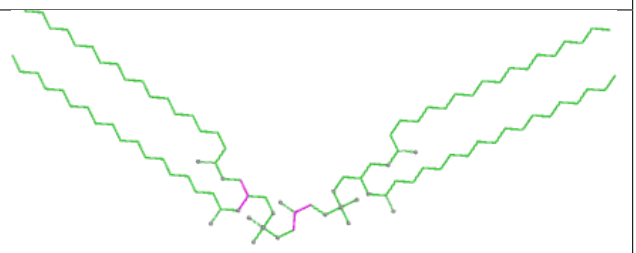


Rings

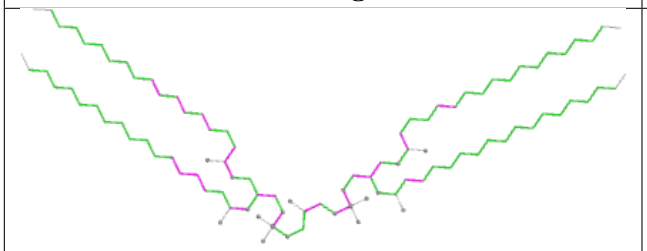
Ligand CDL BC 302



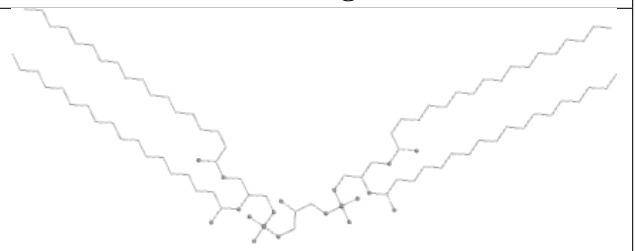
Bond lengths



Bond angles

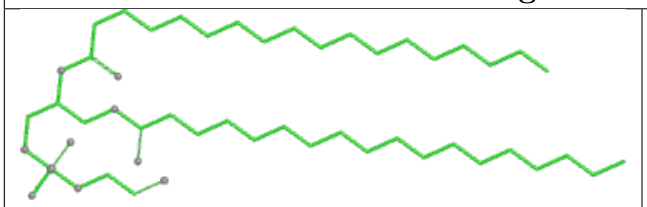


Torsions



Rings

Ligand 3PE Dd 703



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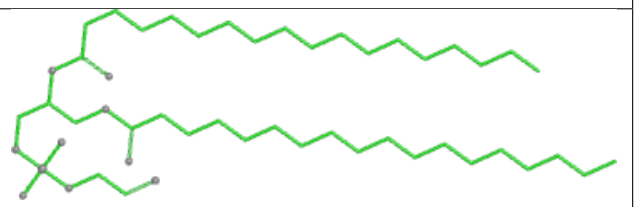
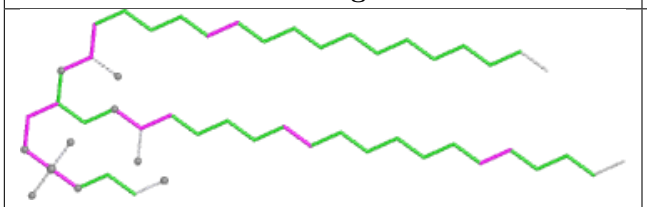


Bond angles



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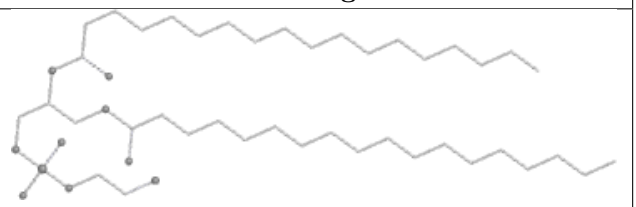
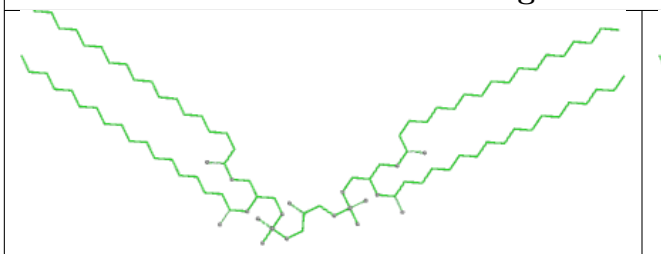


Rings

Ligand CDL Ea 501



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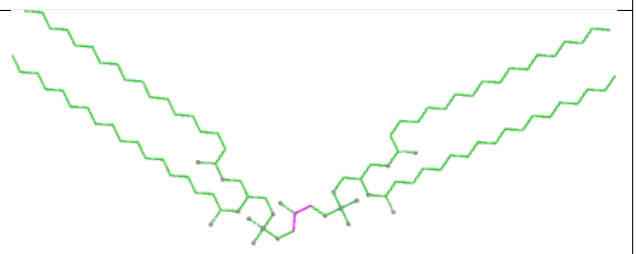

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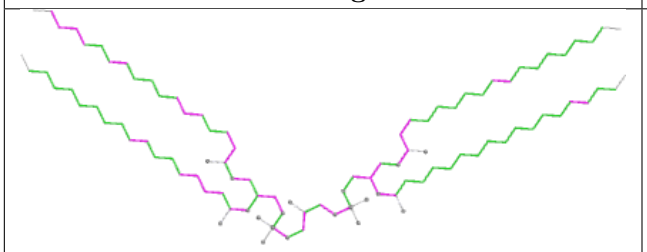

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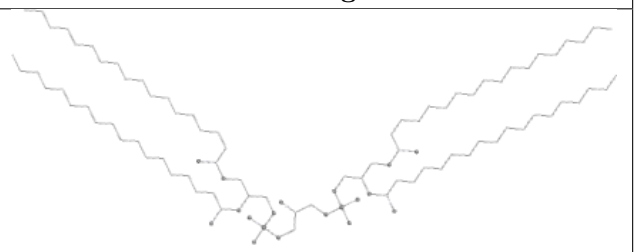
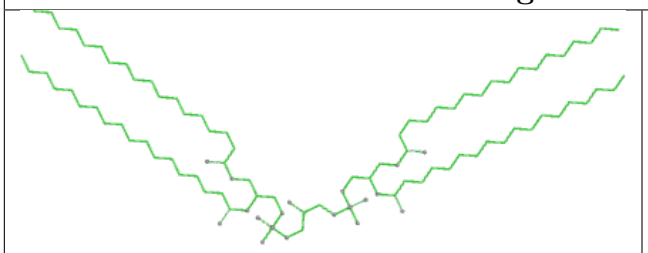


Rings

Ligand CDL Ek 201



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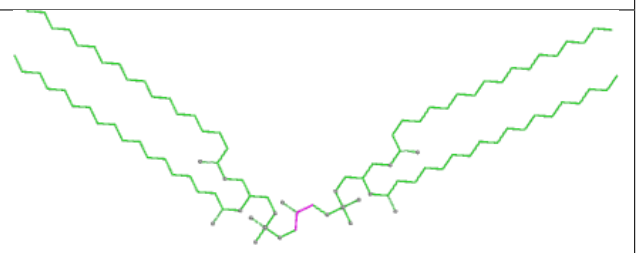

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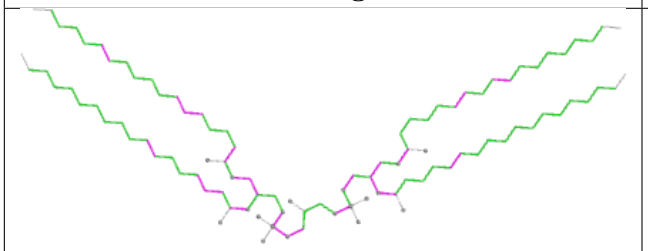

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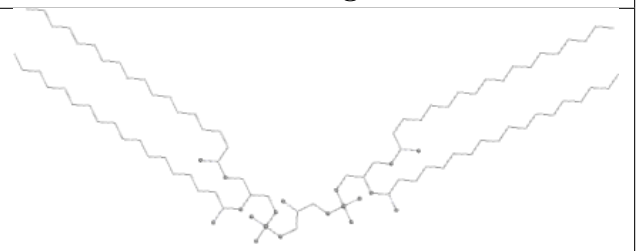
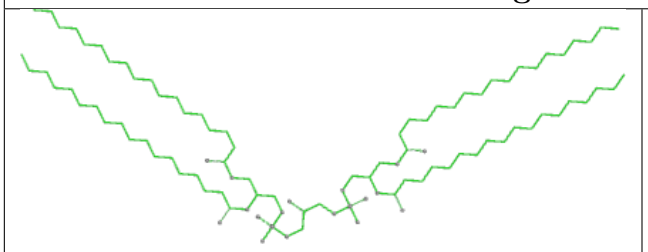


Rings

Ligand CDL BE 201



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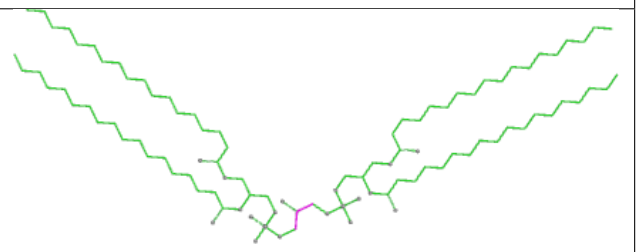
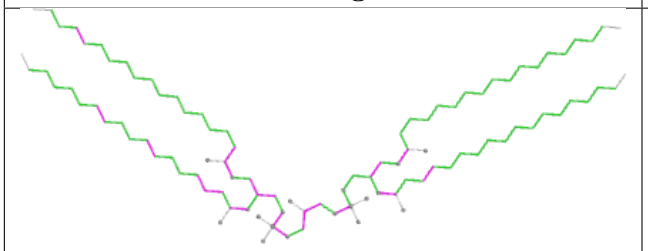


Bond angles



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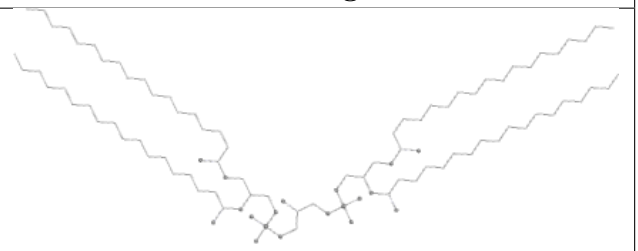
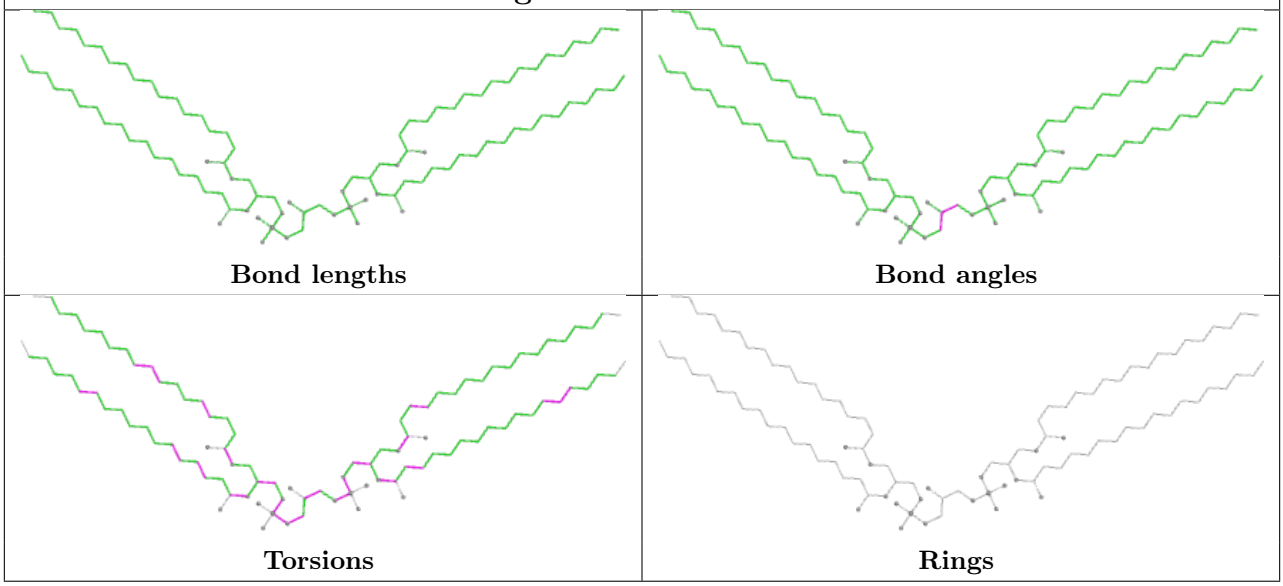
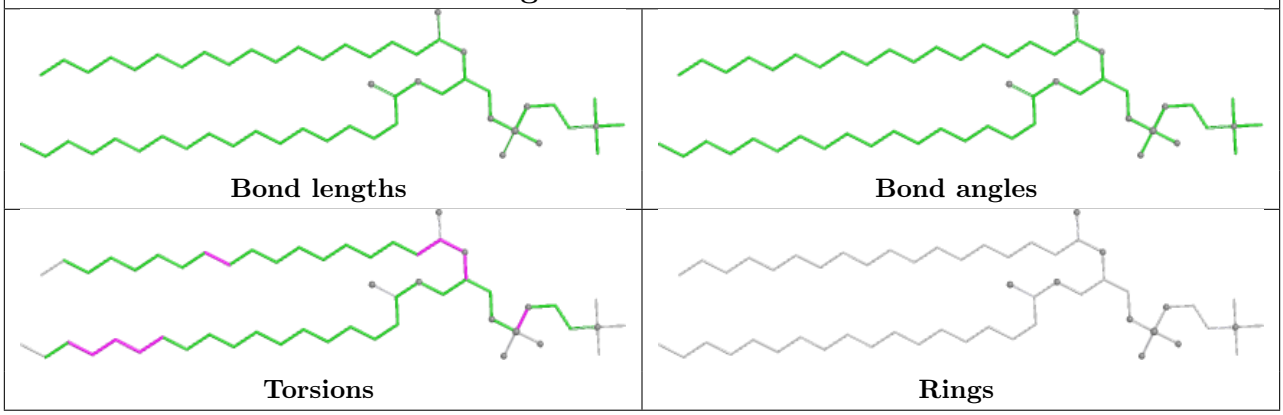


Rings

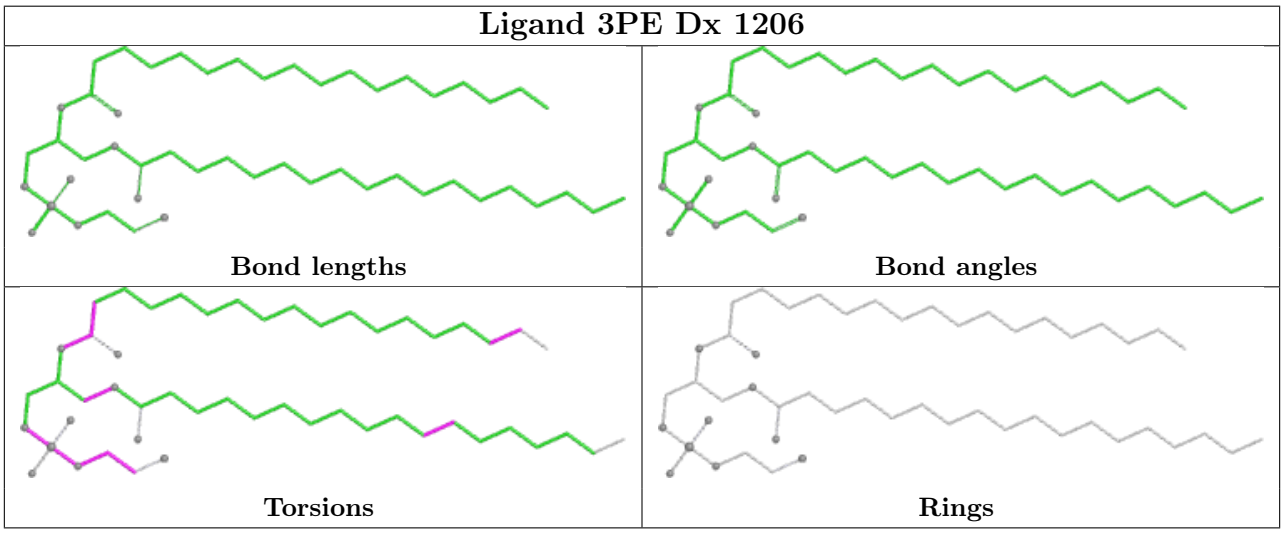
Ligand CDL Du 401



Ligand PC1 Eo 205



Ligand 3PE Dx 1206



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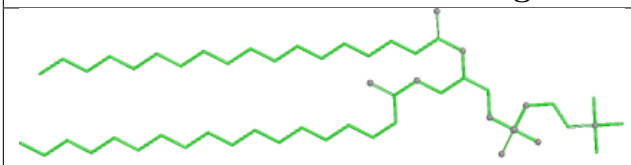
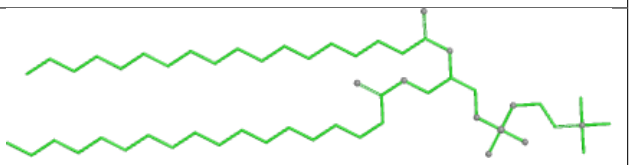
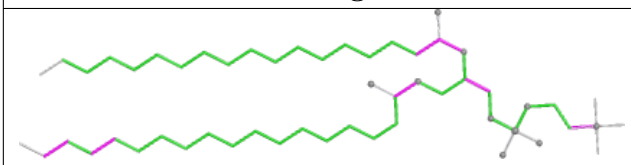


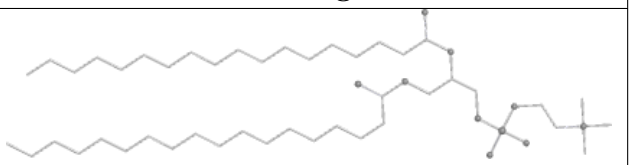
Bond lengths



Bond angles

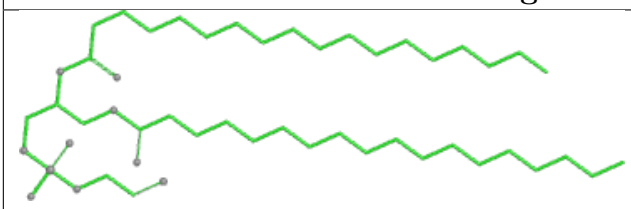


Torsions



Rings

Ligand 3PE Dr 404



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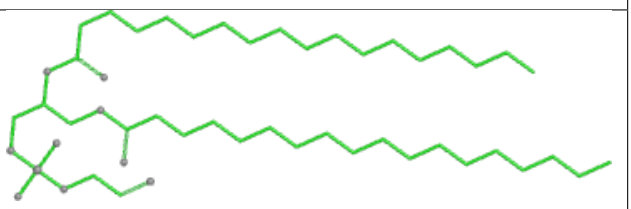
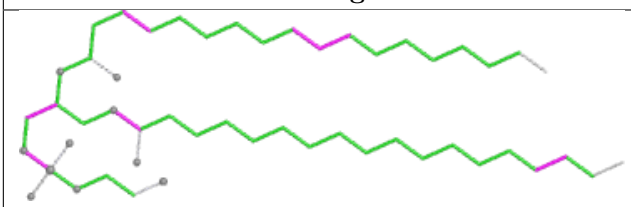


Bond angles



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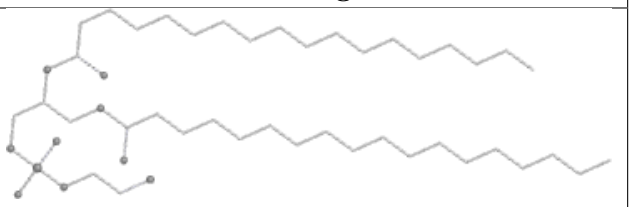
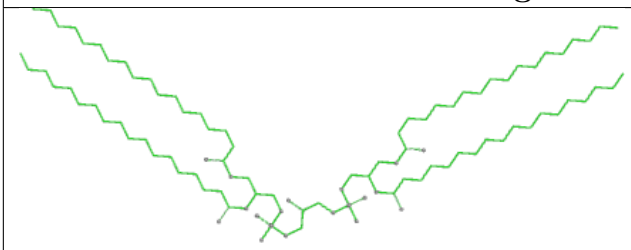


Rings

Ligand CDL DJ 303



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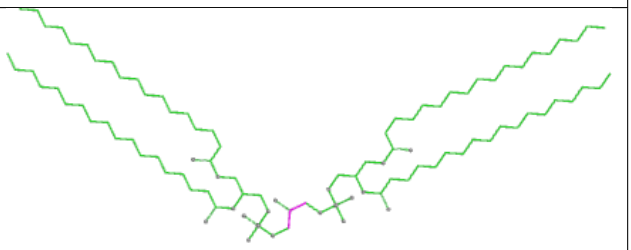
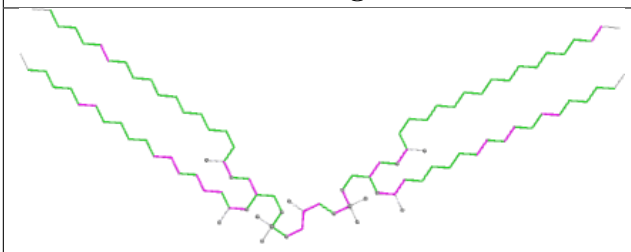
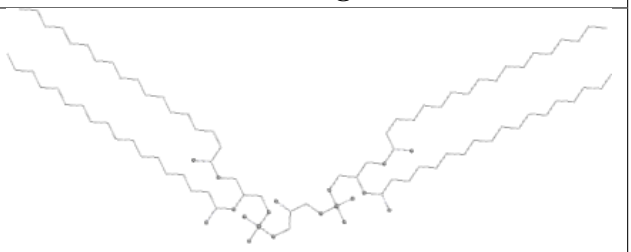


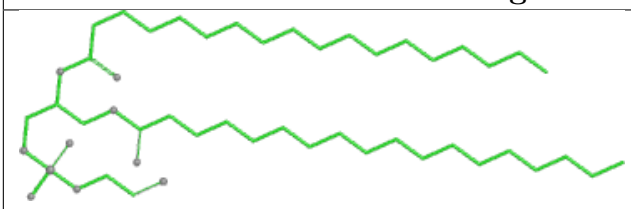
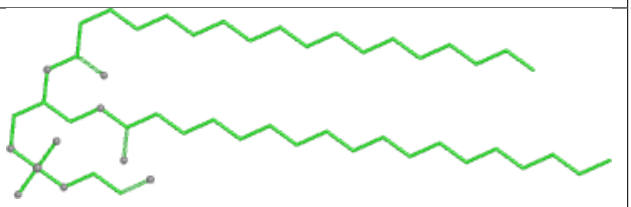
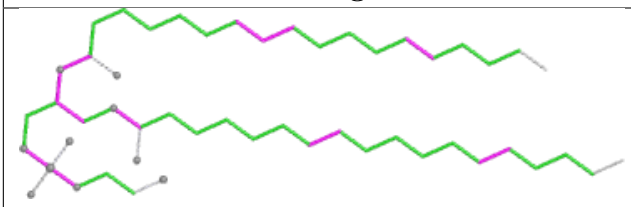
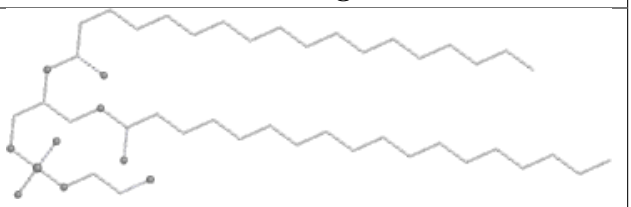
Bond angles

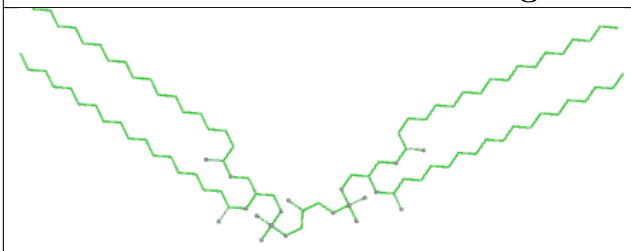
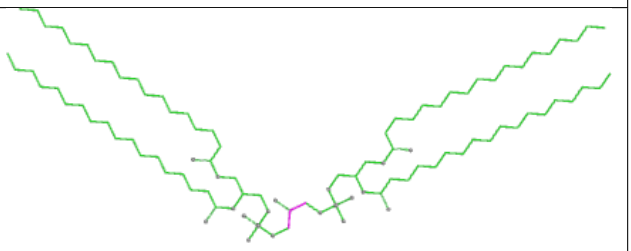
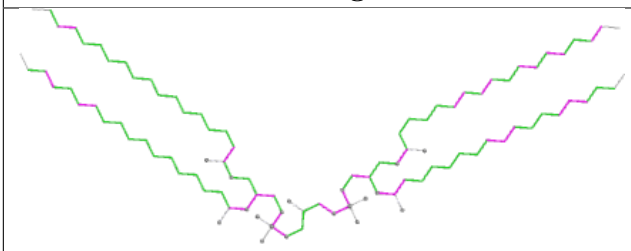
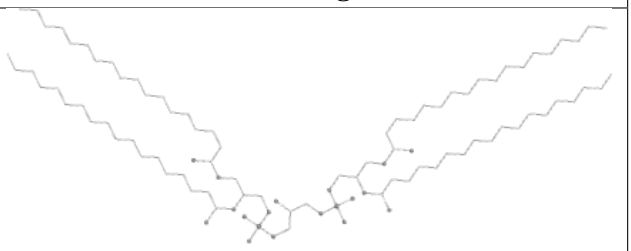


Torsions

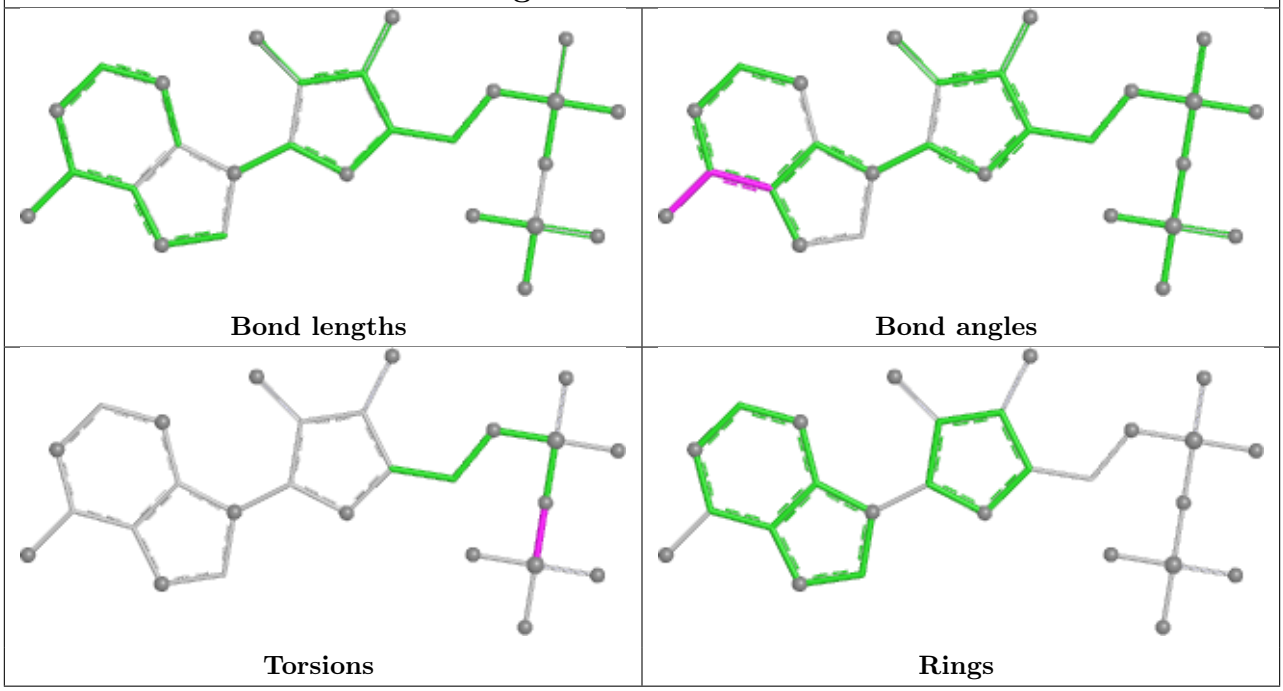


Rings

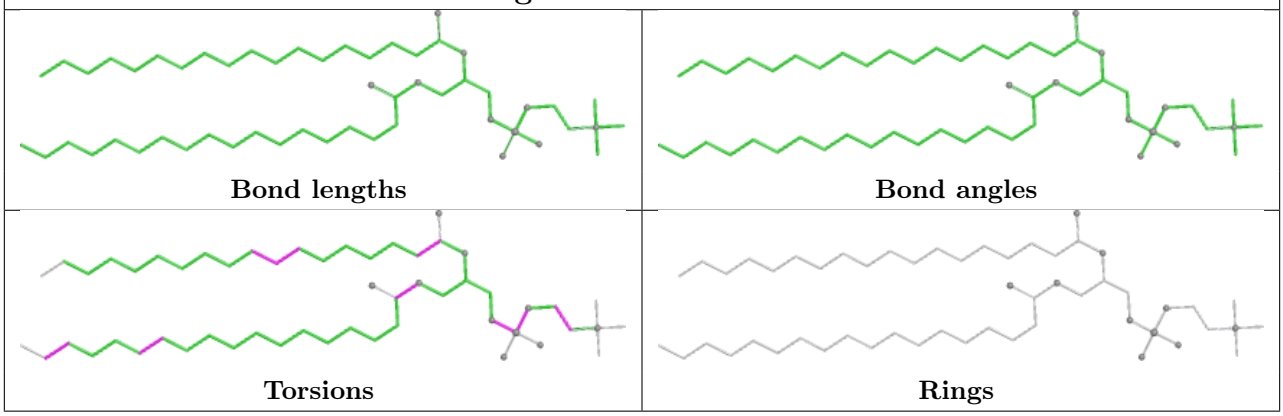
Ligand 3PE Dx 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL El 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

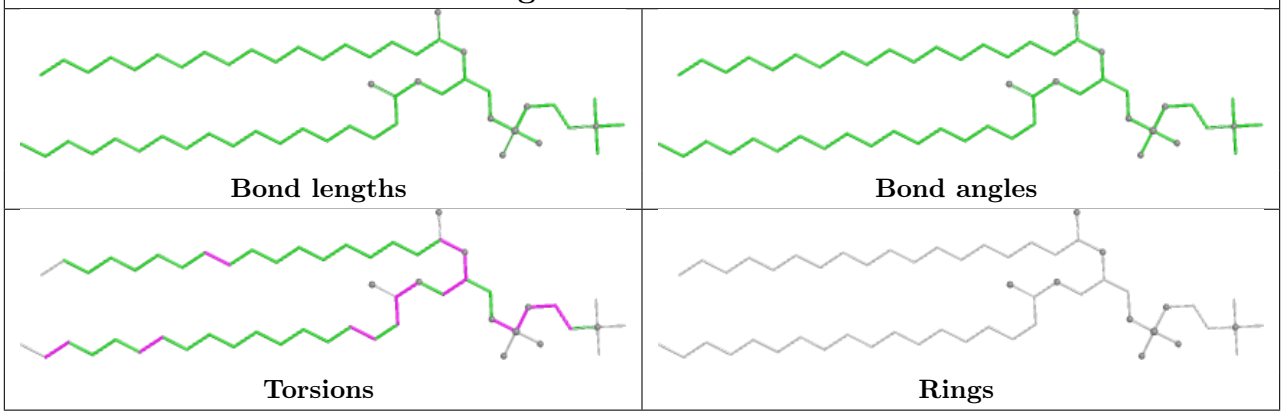
Ligand ADP A8 401



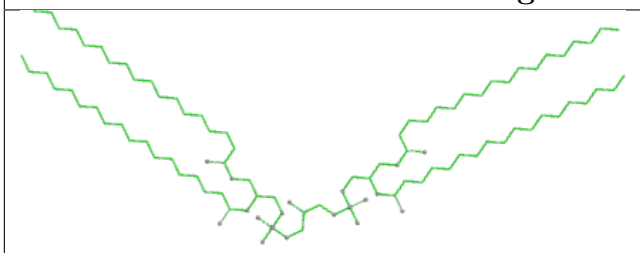
Ligand PC1 DC 604



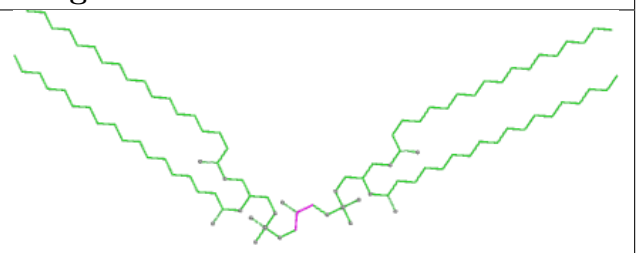
Ligand PC1 Dv 405



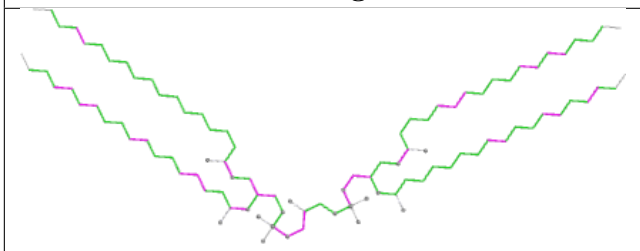
Ligand CDL Eg 101



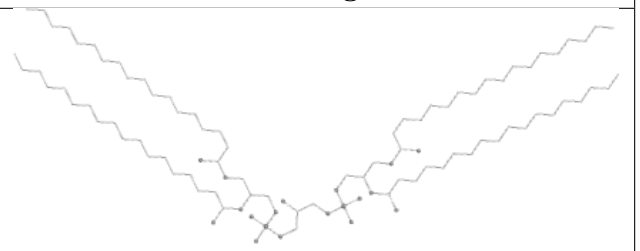
Bond lengths



Bond angles

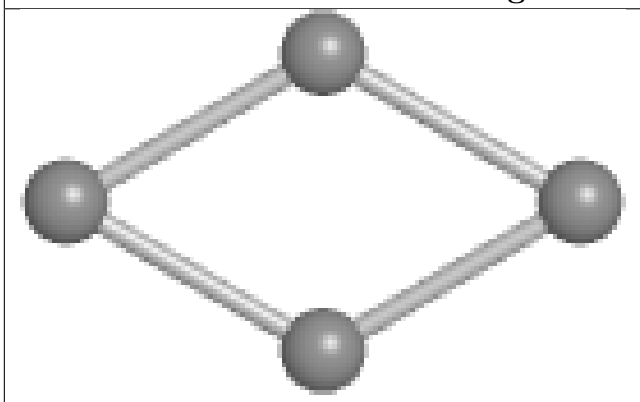


Torsions



Rings

Ligand FES CB 1000



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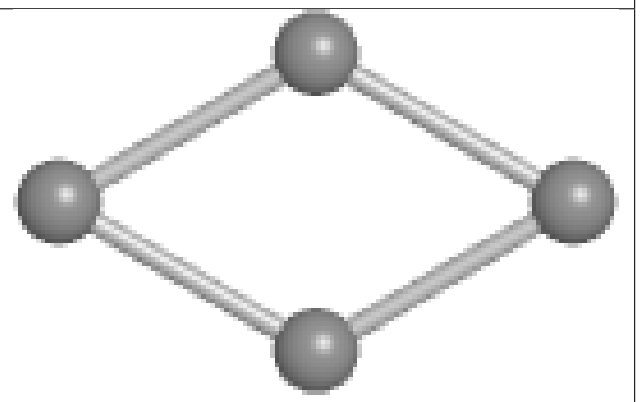
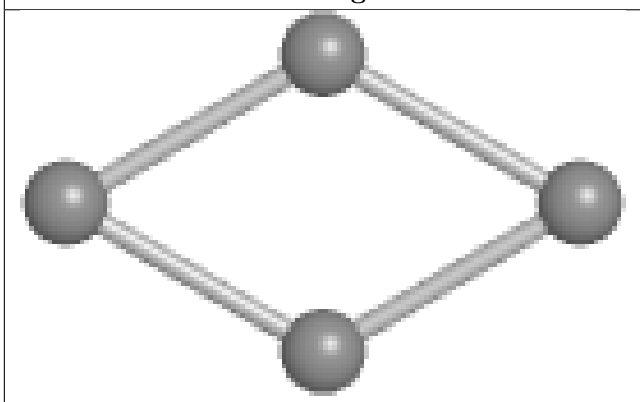


Bond angles



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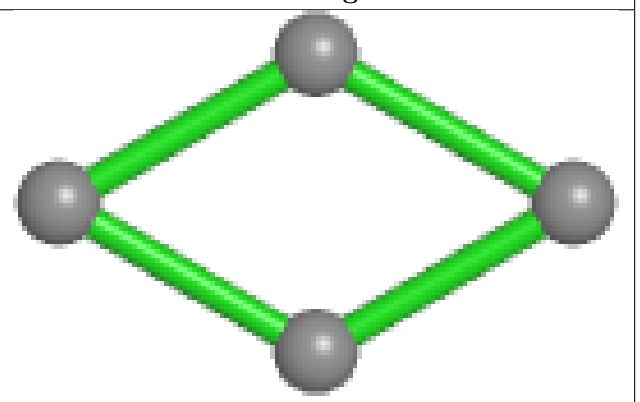
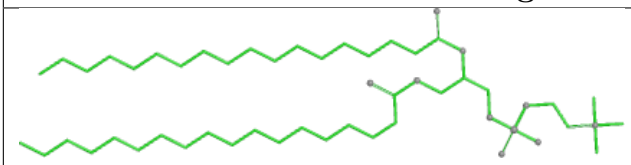


Rings

Ligand PC1 Dv 404



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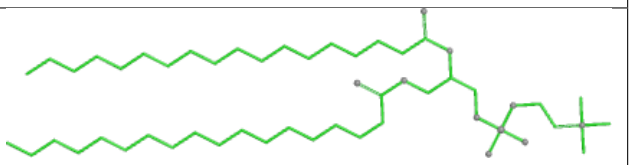
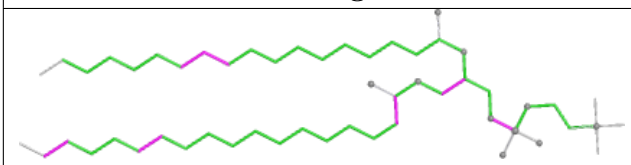
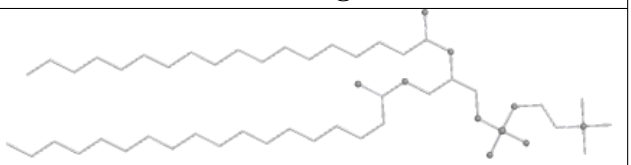


Bond angles

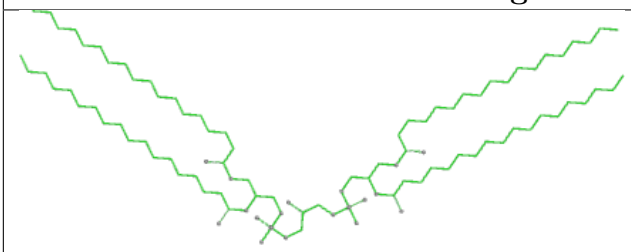


Torsions

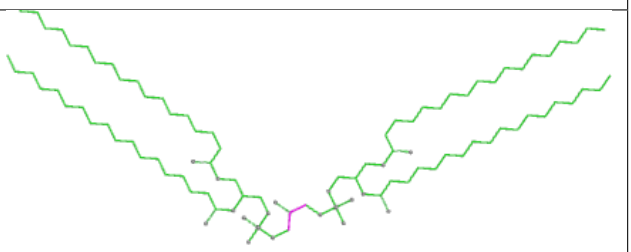


Rings

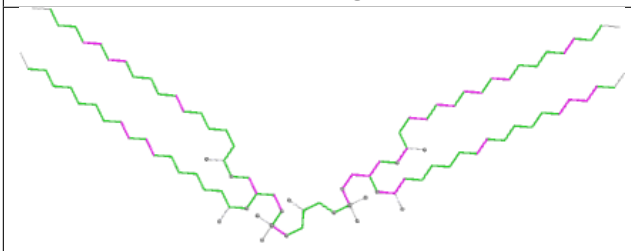
Ligand CDL DA 706



Bond lengths



Bond angles



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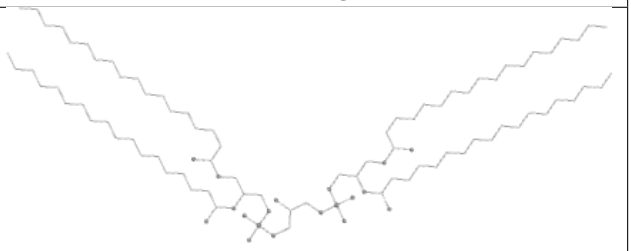
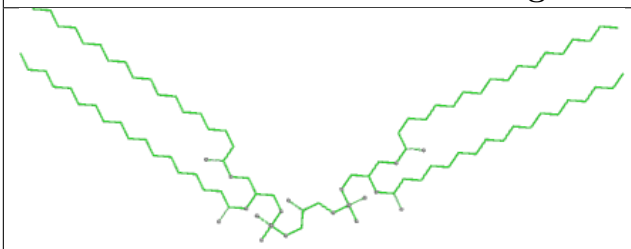


Rings

Ligand CDL g 801



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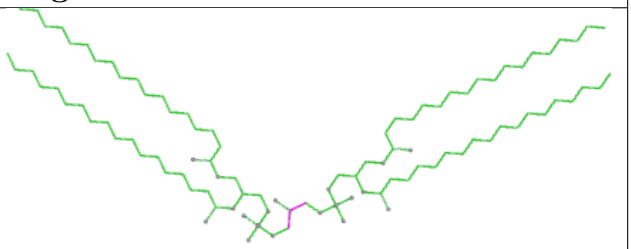
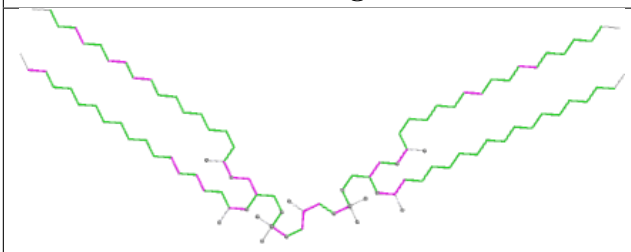


Bond angles



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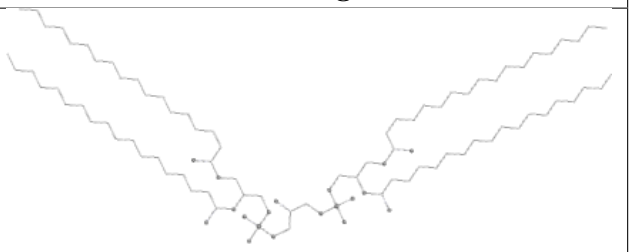
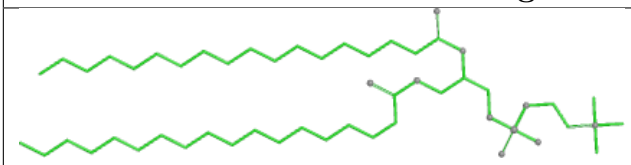


Rings

Ligand PC1 A0 605



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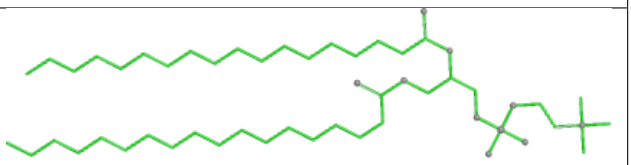
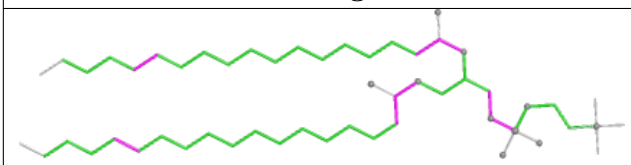


Bond angles



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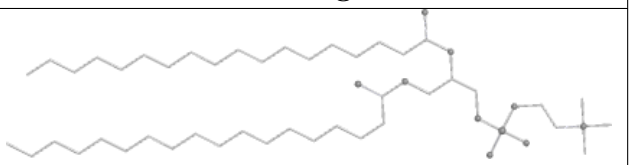
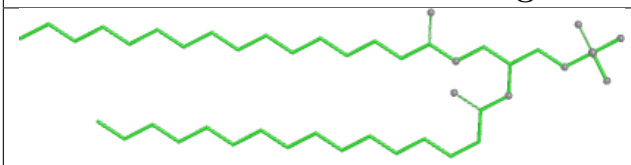


Rings

Ligand LPP A6 301



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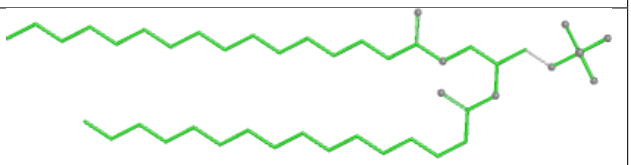
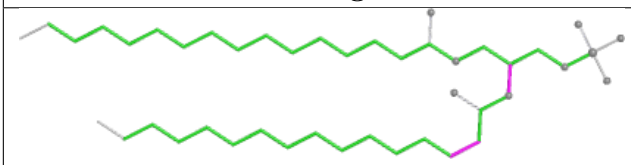


Bond angles



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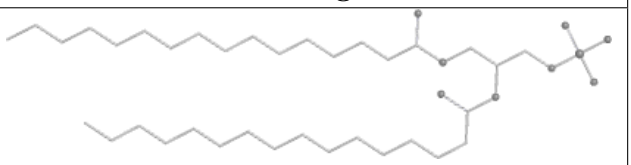
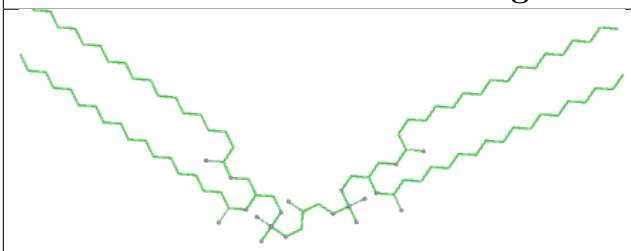


Rings

Ligand CDL EK 201



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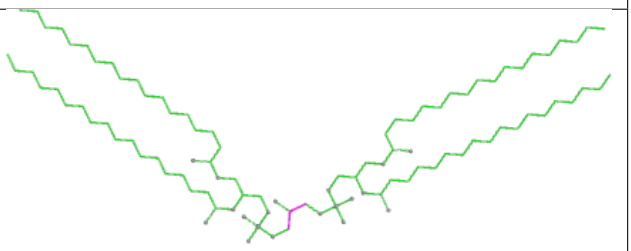
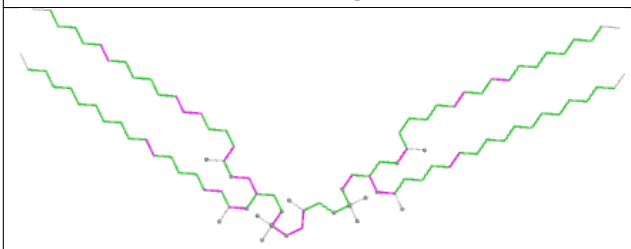


Bond angles



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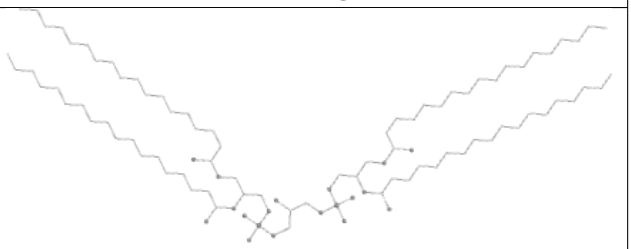
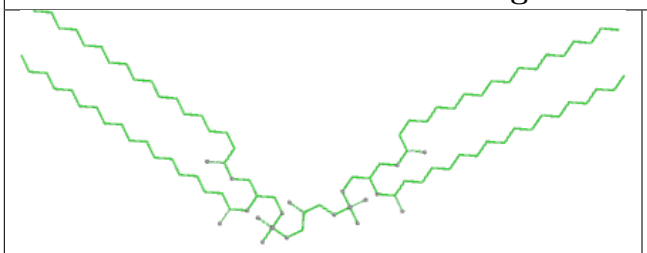


Rings

Ligand CDL DD 703



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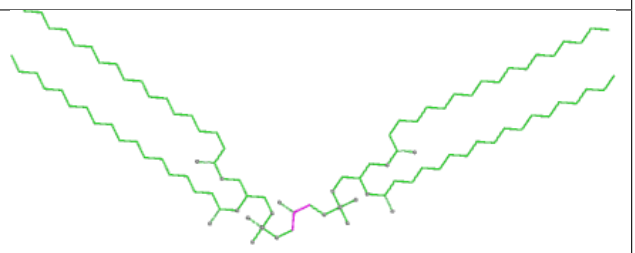
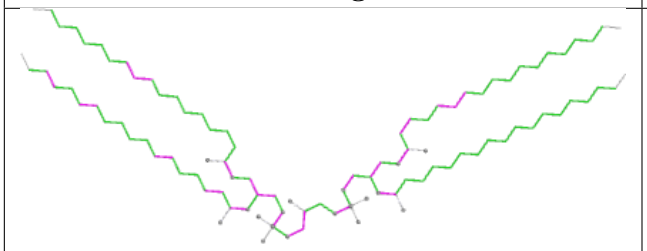


Bond angles



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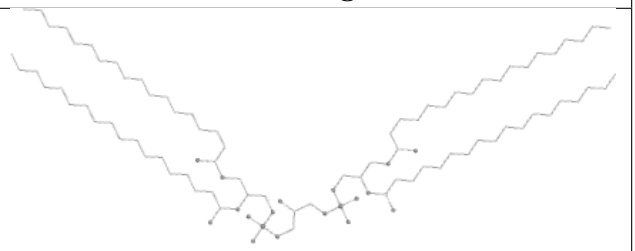
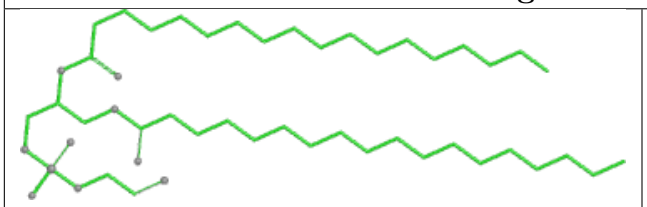


Rings

Ligand 3PE BP 201



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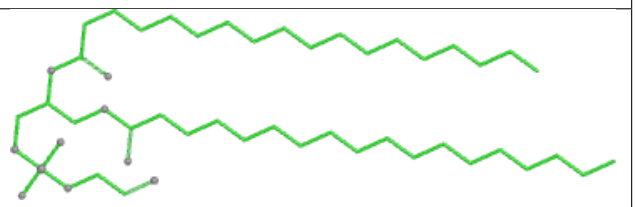

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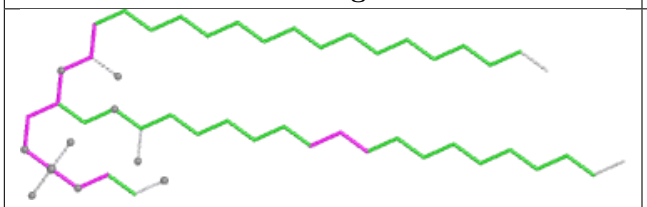

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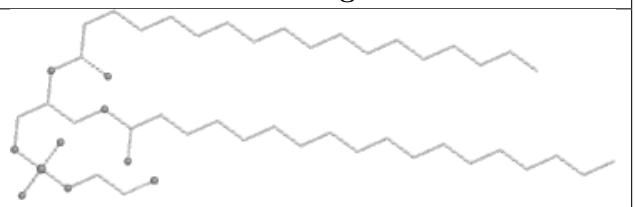
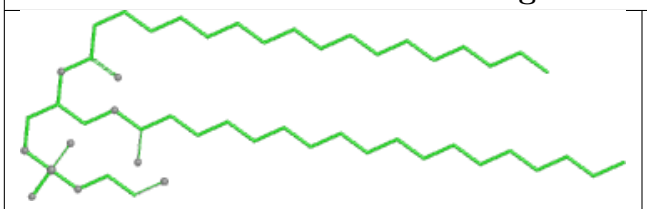


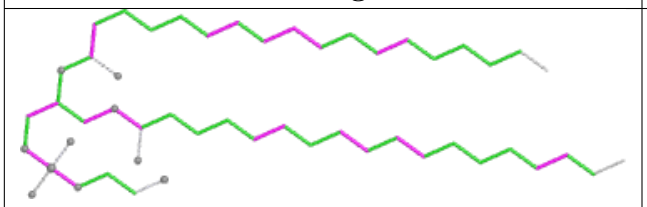
Rings

Ligand 3PE DS 402



Bond lengths

Bond angles



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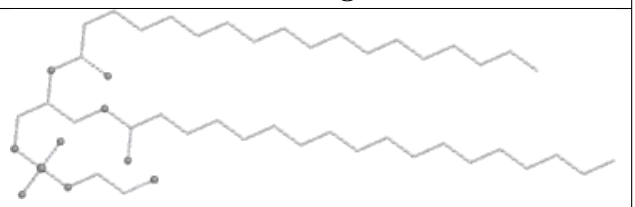
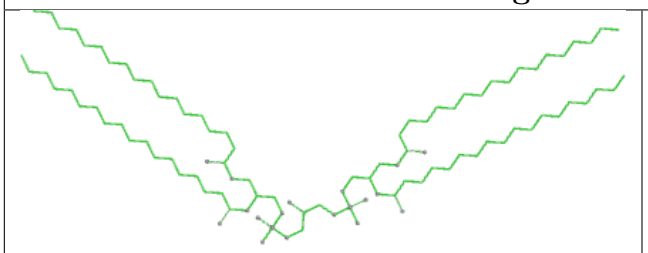


Rings

Ligand CDL BT 204



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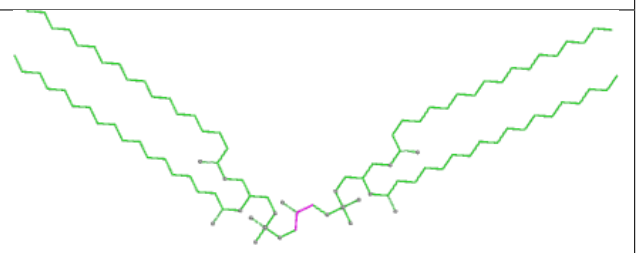
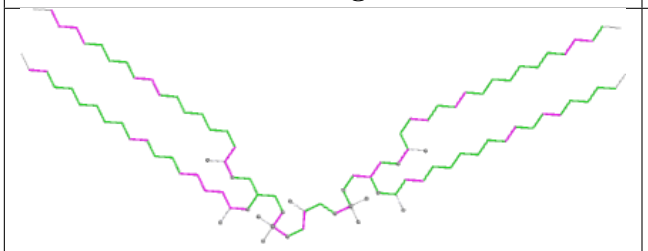


Bond angles



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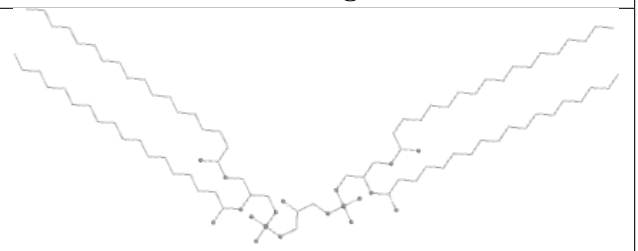
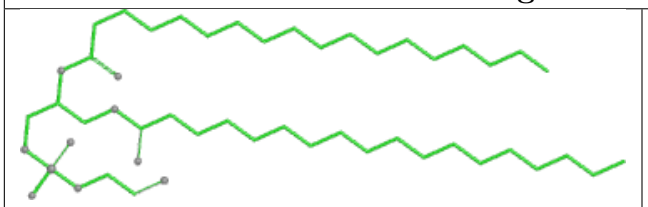


Rings

Ligand 3PE BT 201



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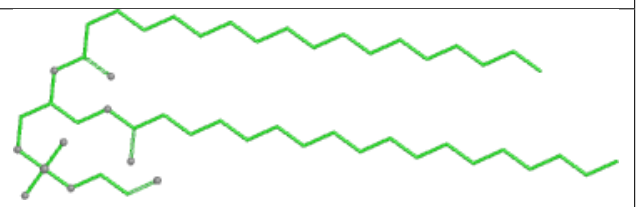
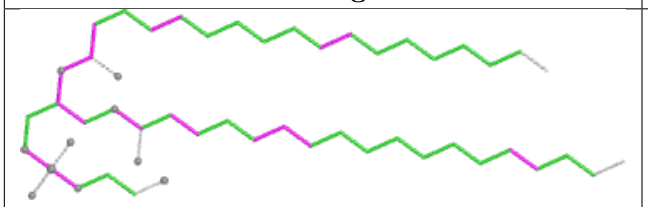


Bond angles



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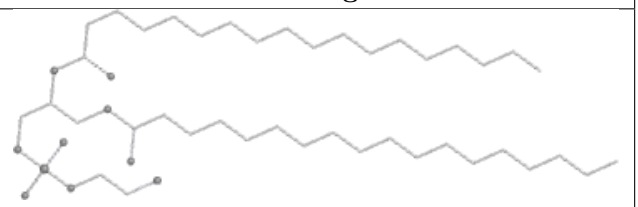
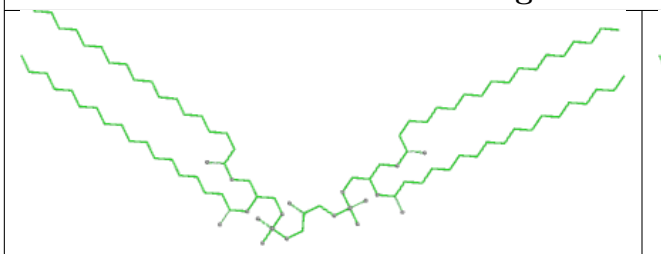


Rings

Ligand CDL Do 501



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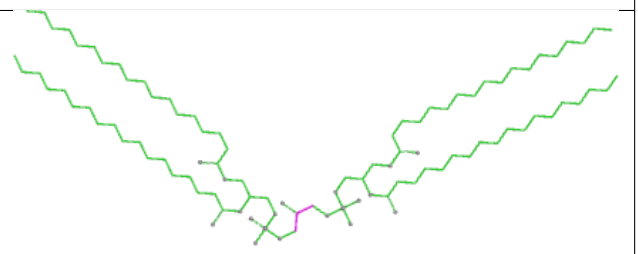
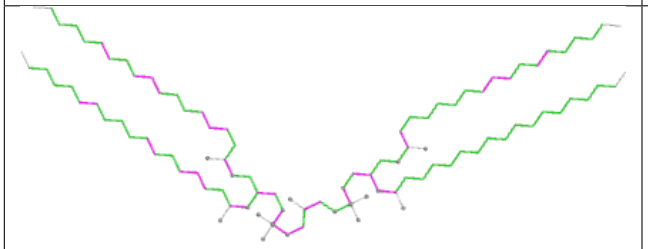


Bond angles



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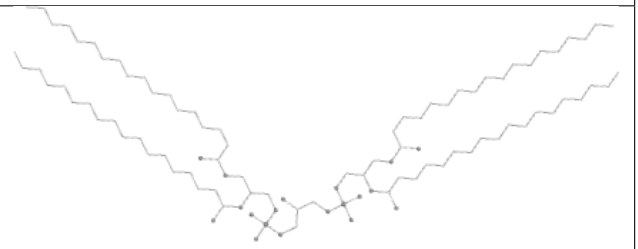
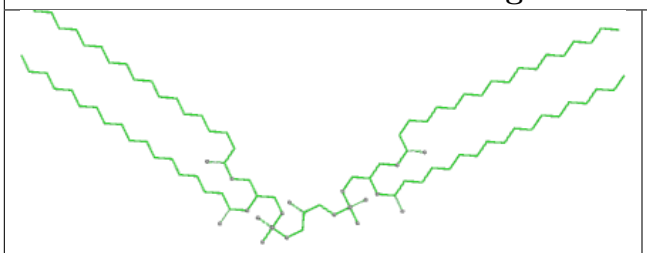


Rings

Ligand CDL Dq 1402



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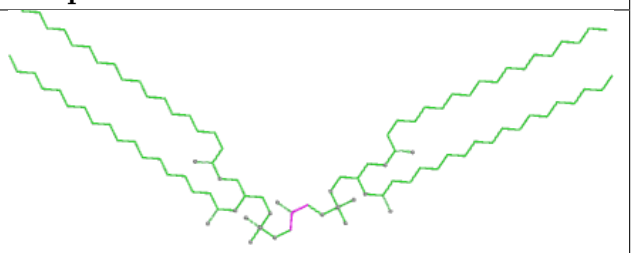
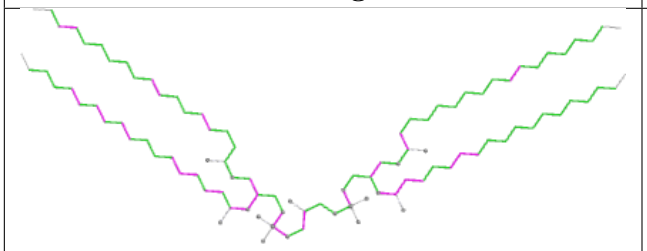
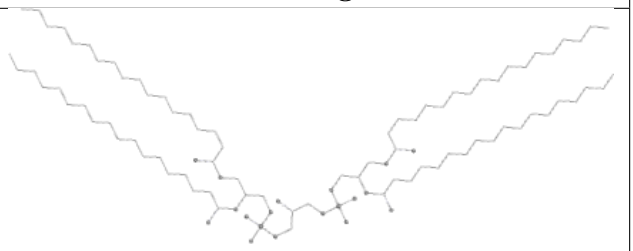


Bond angles

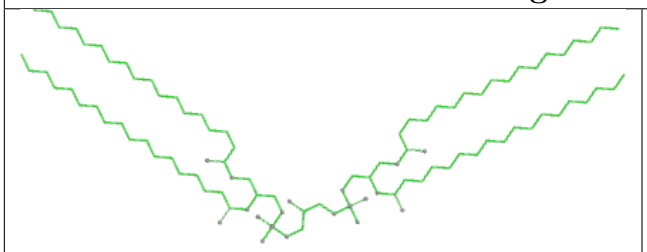


Torsions



Rings

Ligand CDL c 506



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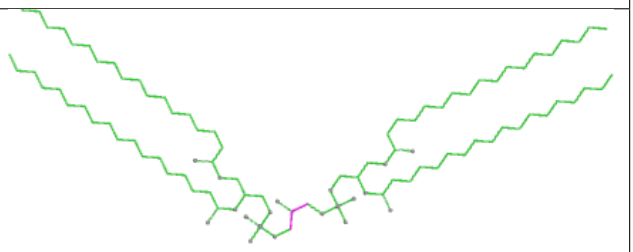
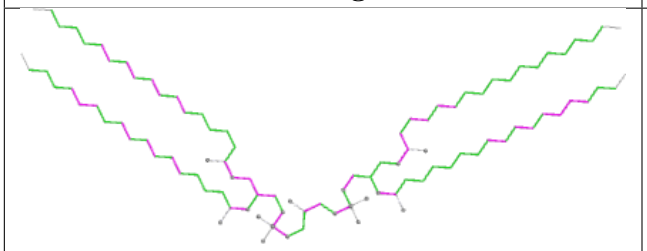
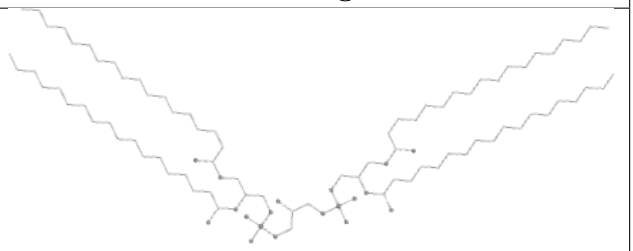


Bond angles

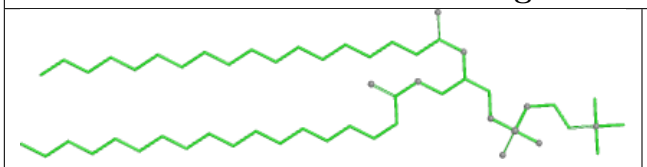


Torsions



Rings

Ligand PC1 AA 907



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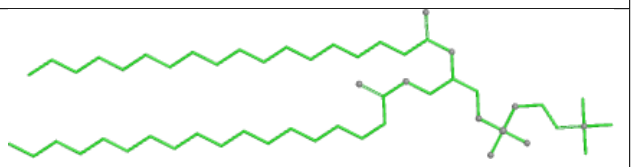
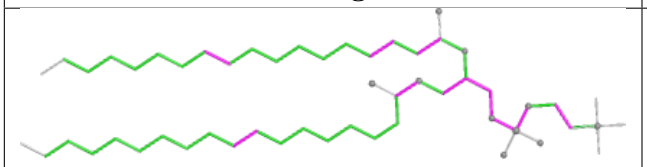
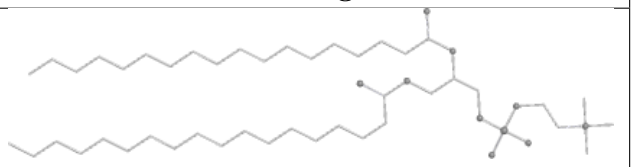


Bond angles

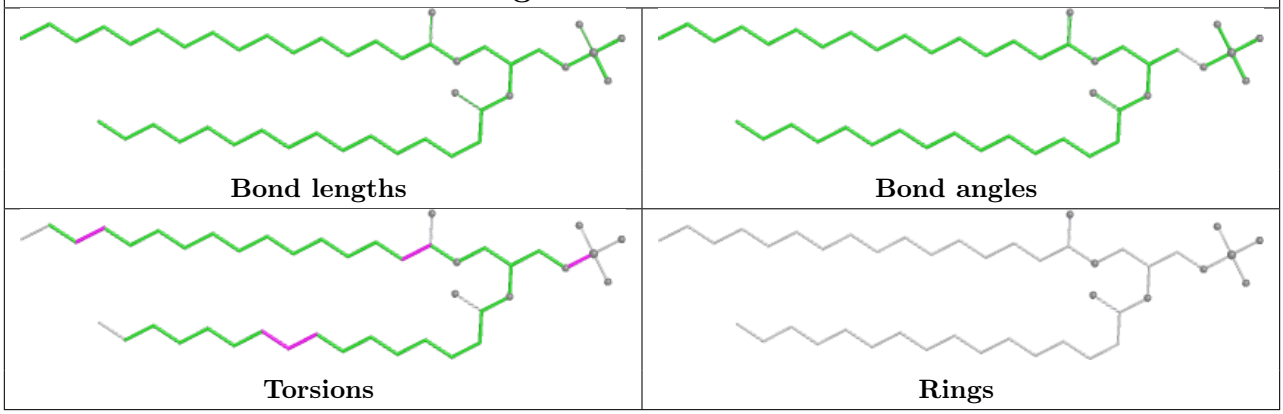


Torsions

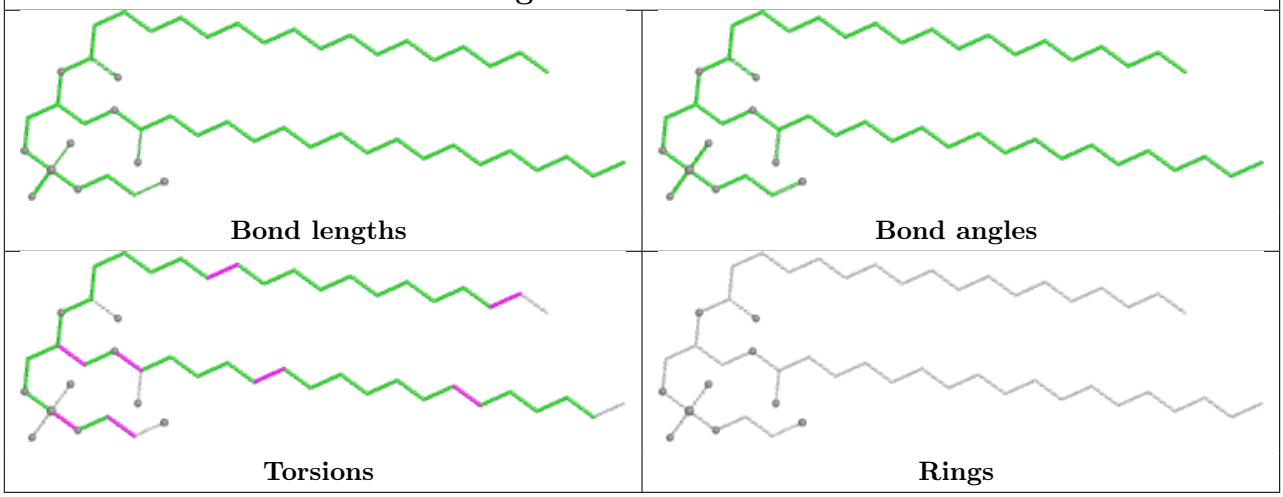


Rings

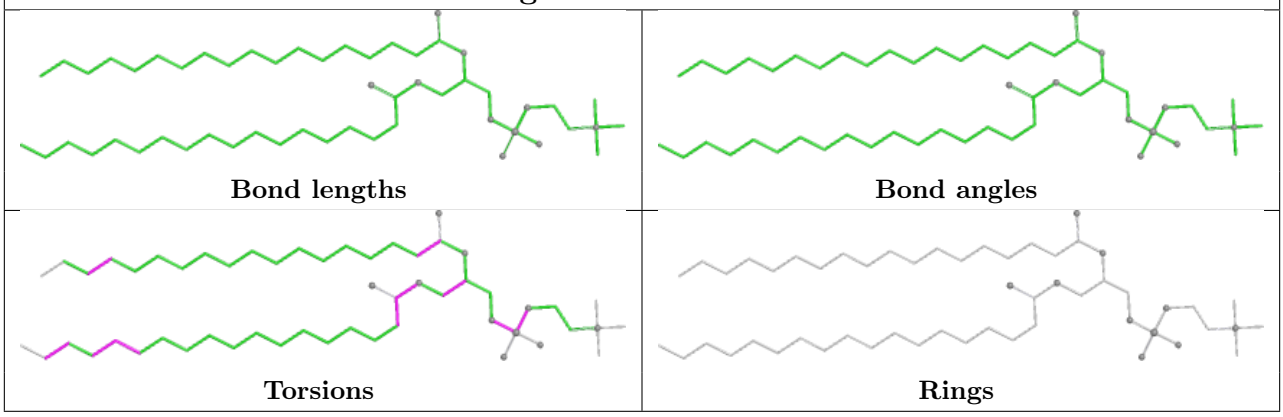
Ligand LPP DA 710



Ligand 3PE DC 607



Ligand PC1 Dc 602



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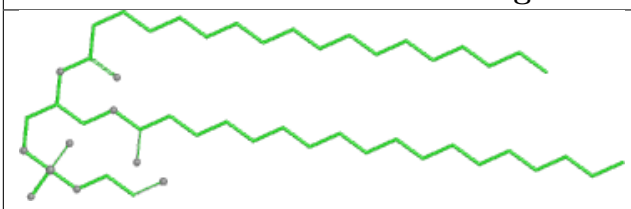
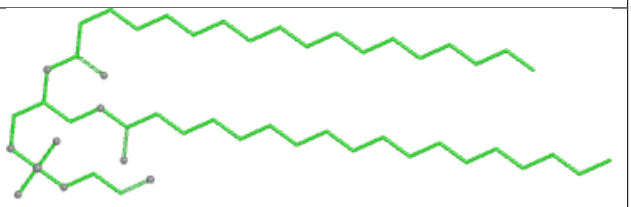
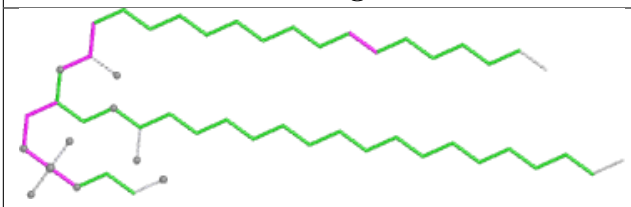
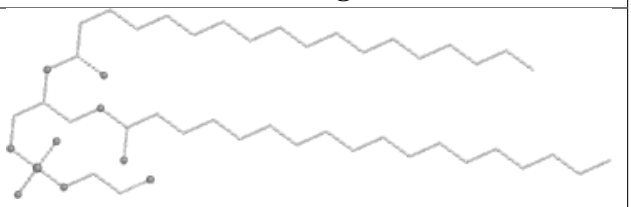
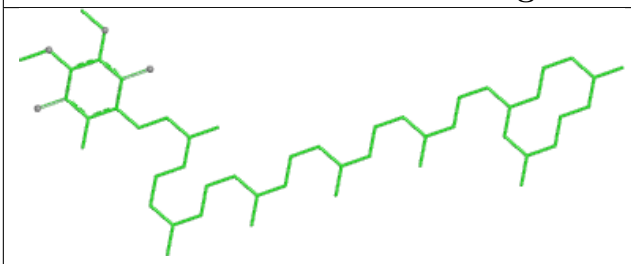
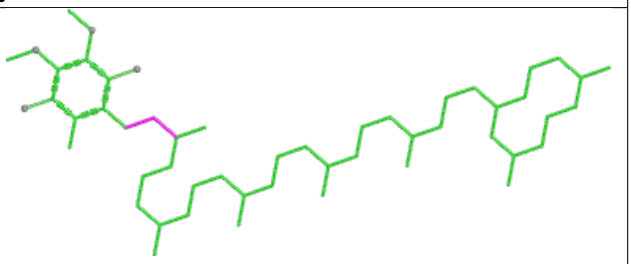
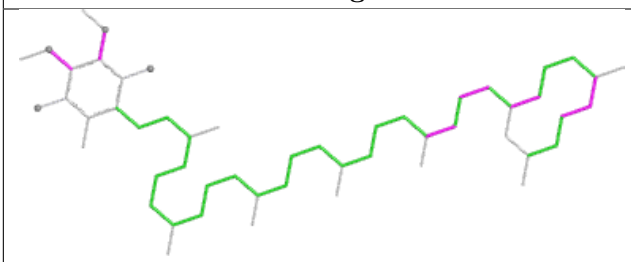
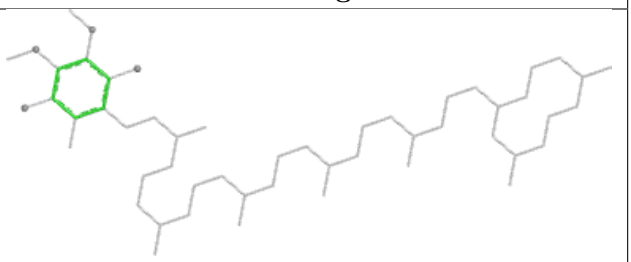
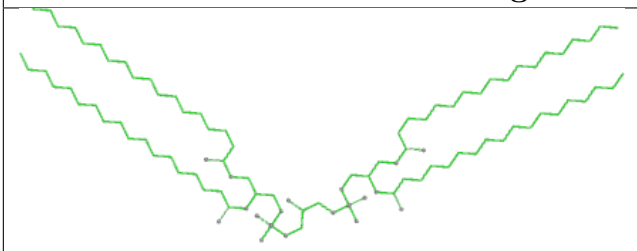
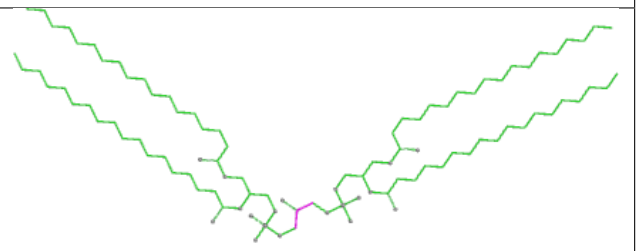
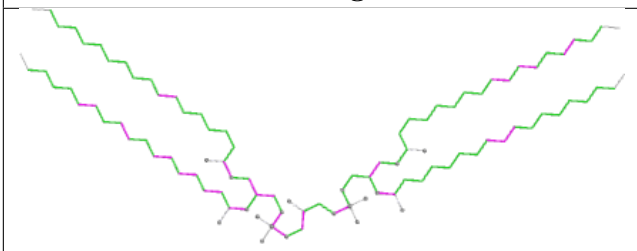
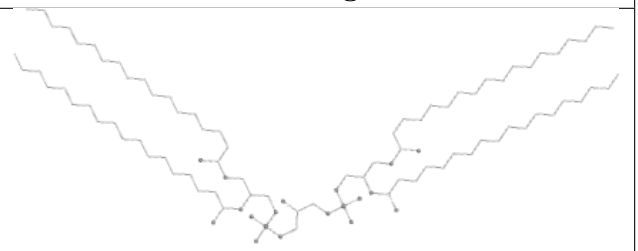
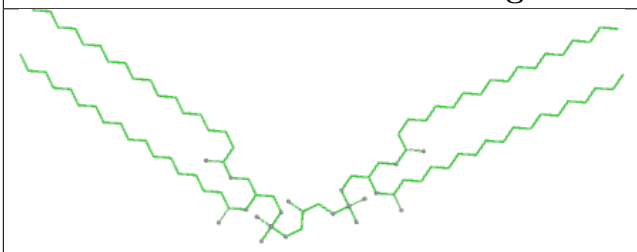
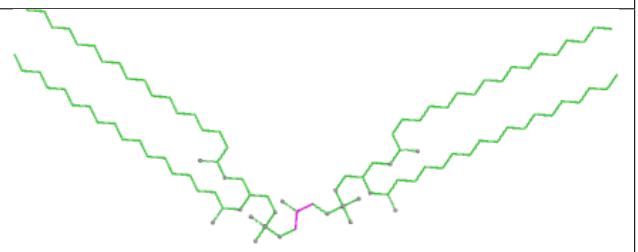
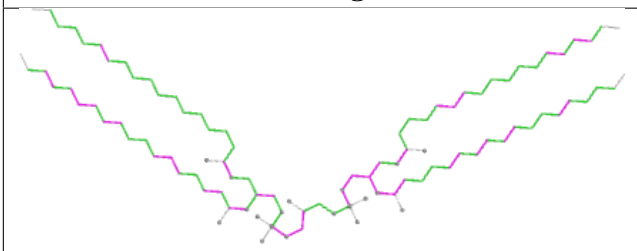
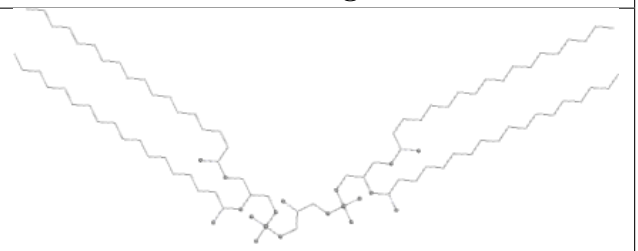
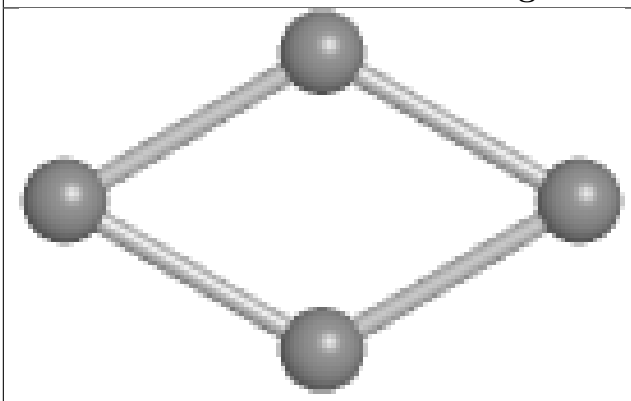
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ8 Ds 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

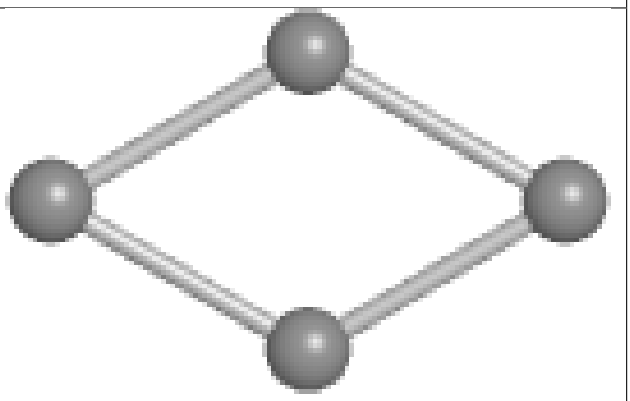
Ligand CDL DY 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Eh 1601	
 Bond lengths	 Bond angles
 Torsions	 Rings

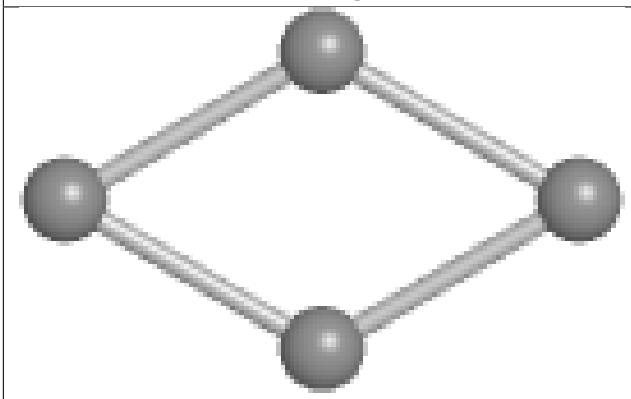
Ligand FES EF 201



Bond lengths



Bond angles



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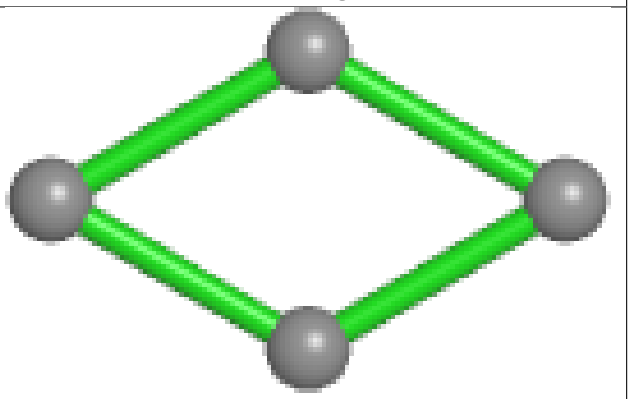
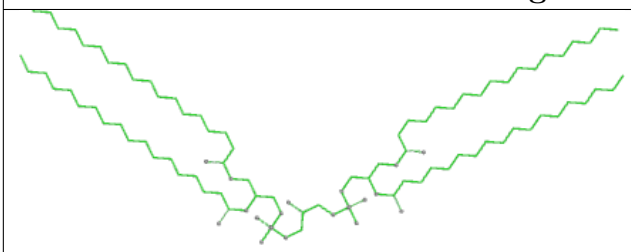


Rings

Ligand CDL c 501



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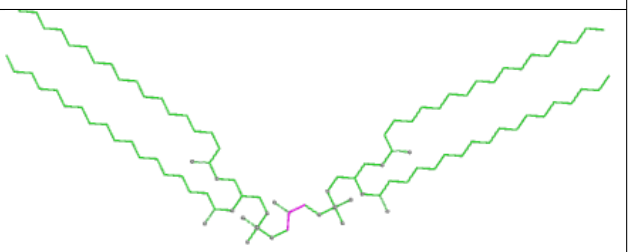

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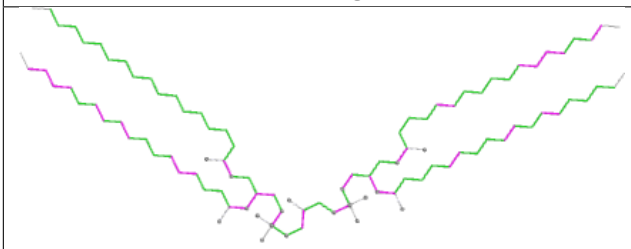

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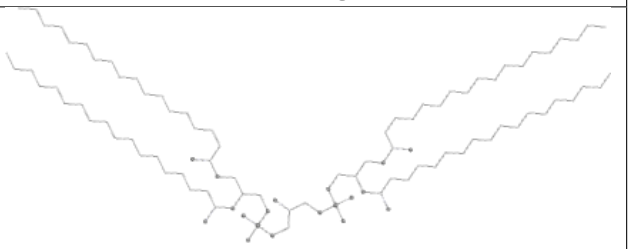
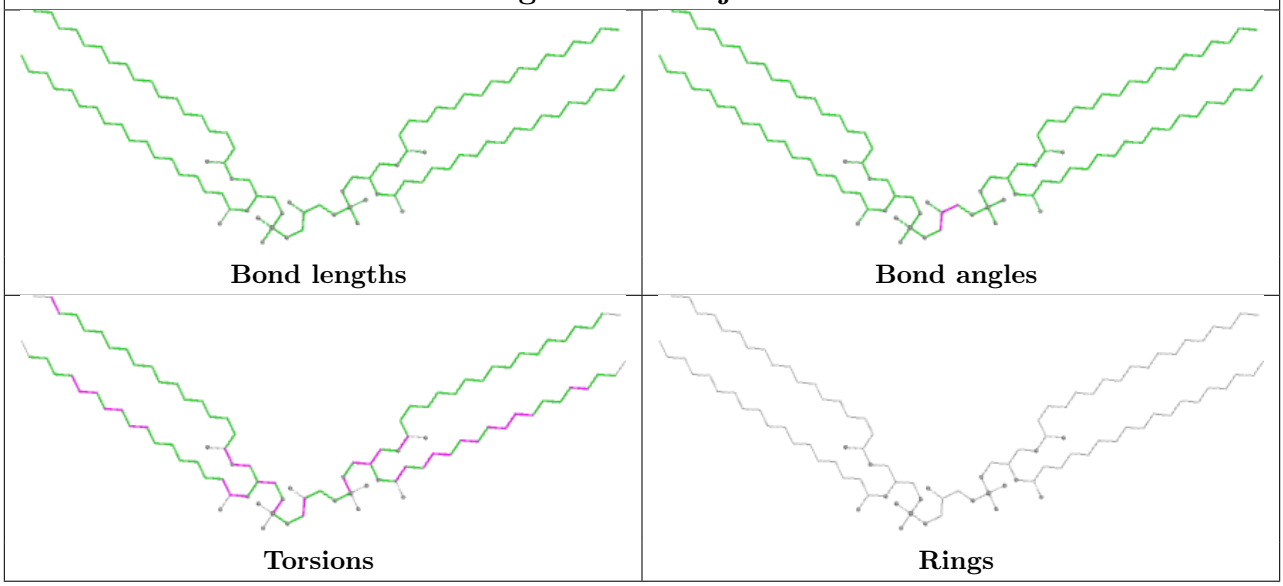
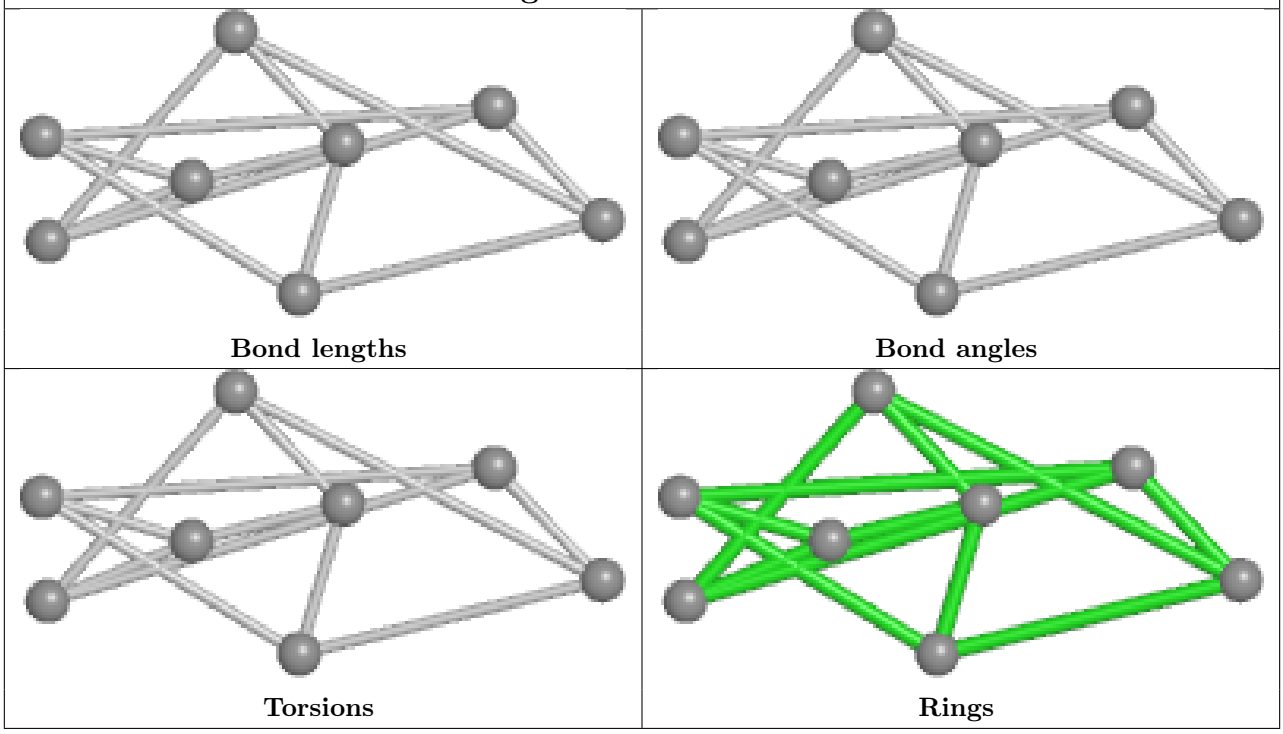


Rings

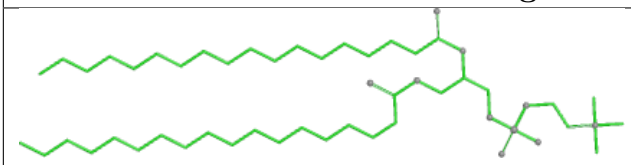
Ligand CDL Dj 402



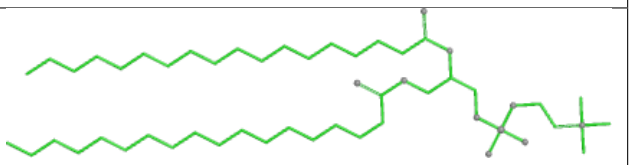
Ligand SF4 AL 301



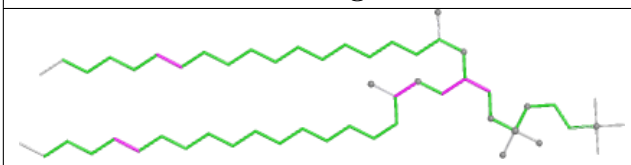
Ligand PC1 Ds 407



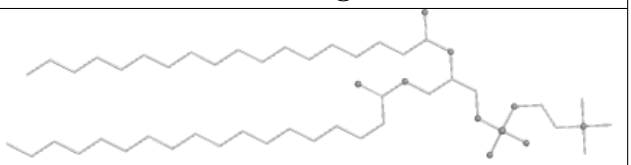
Bond lengths



Bond angles

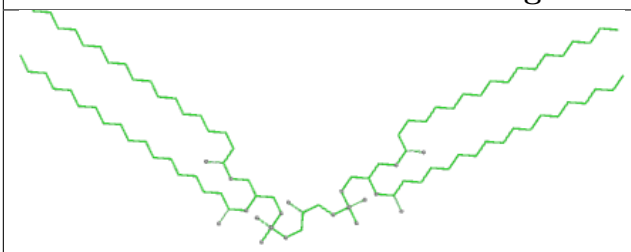


Torsions



Rings

Ligand CDL C 506



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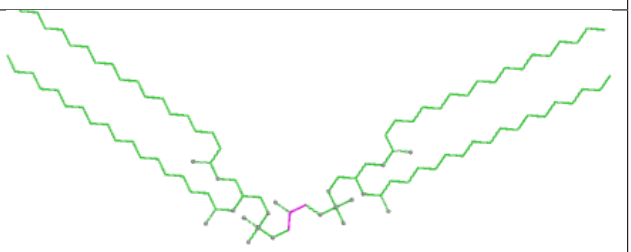

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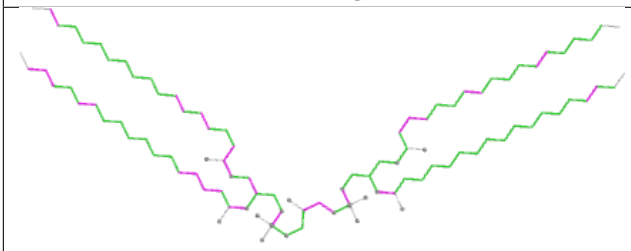

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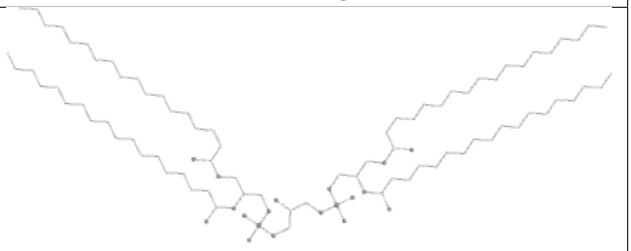
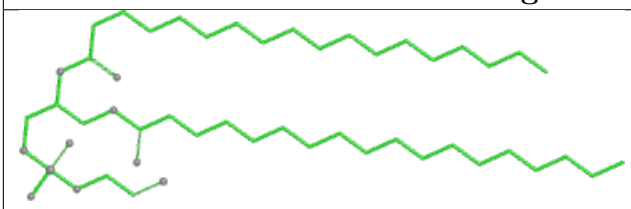


Rings

Ligand 3PE DI 301



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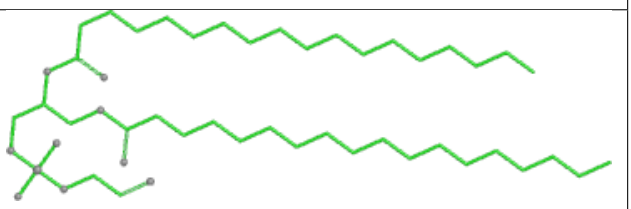
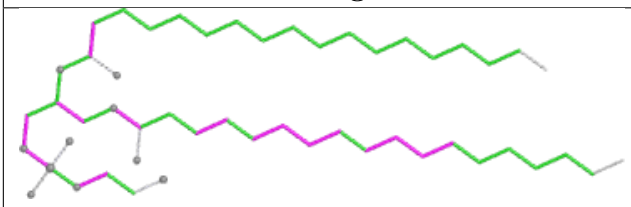


Bond angles



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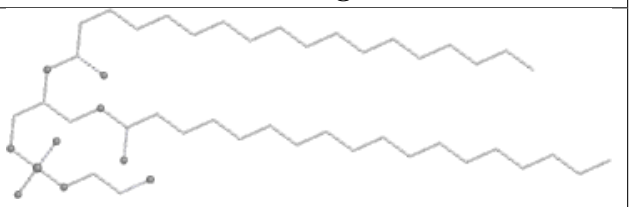
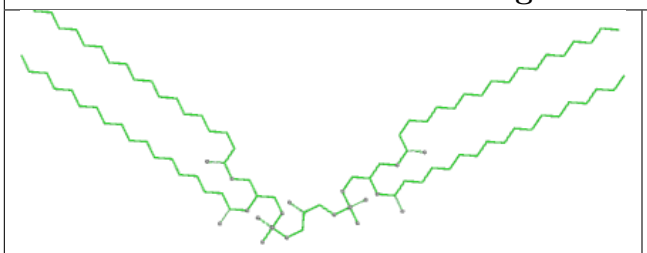


Rings

Ligand CDL EL 901



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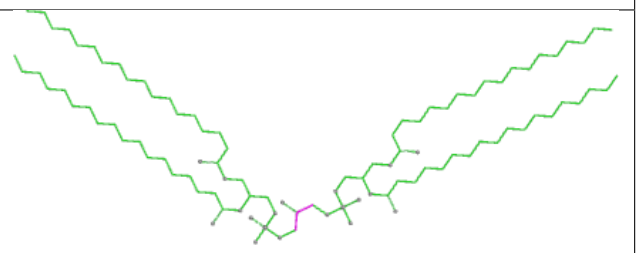
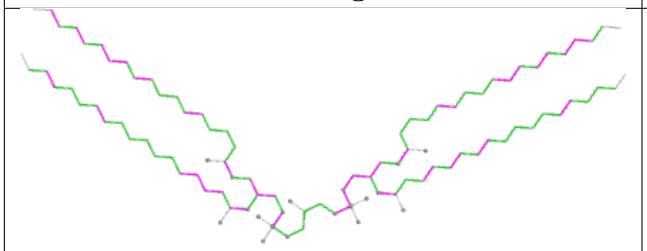


Bond angles



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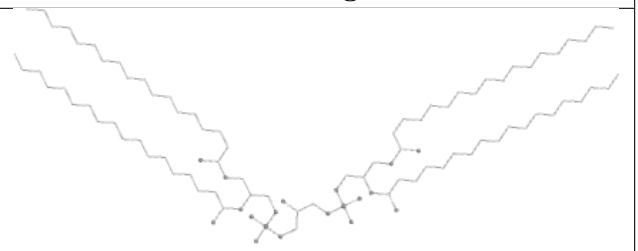
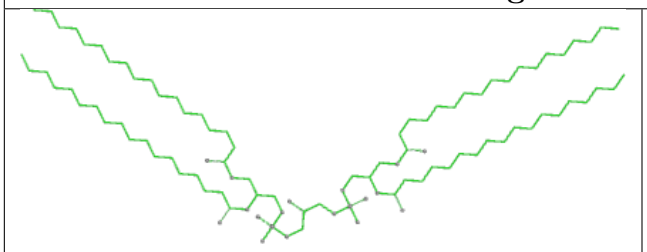


Rings

Ligand CDL DM 501



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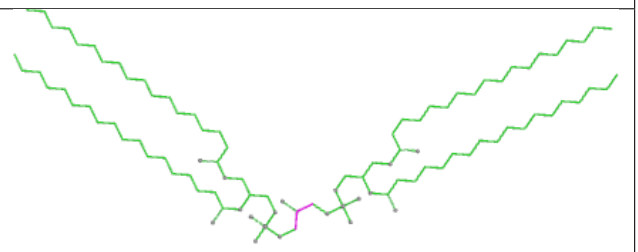
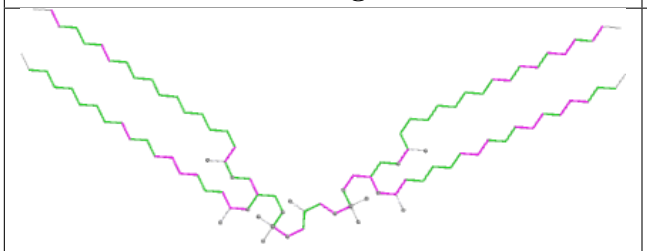


Bond angles



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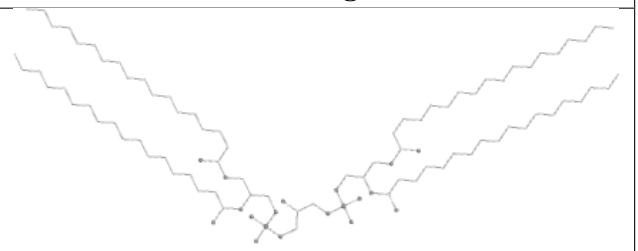
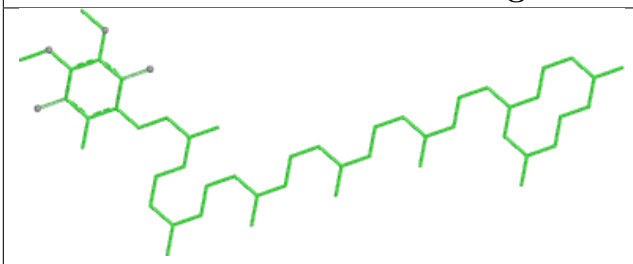


Rings

Ligand UQ8 En 1202



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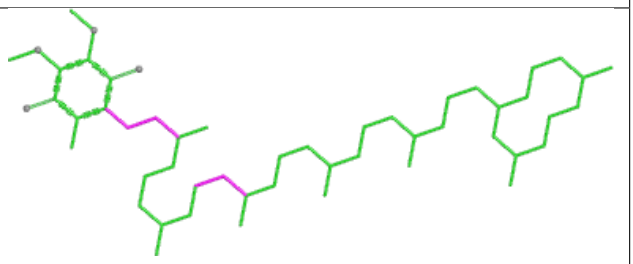
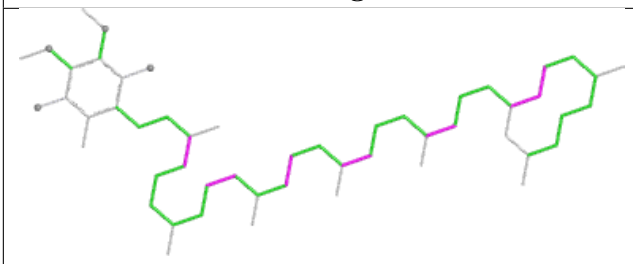
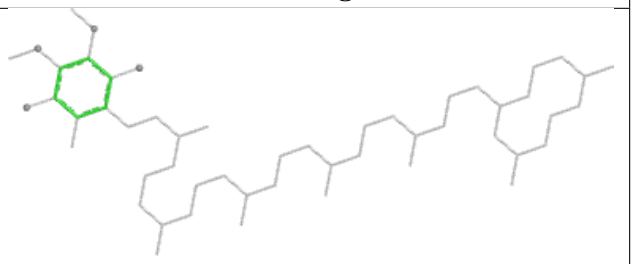


Bond angles

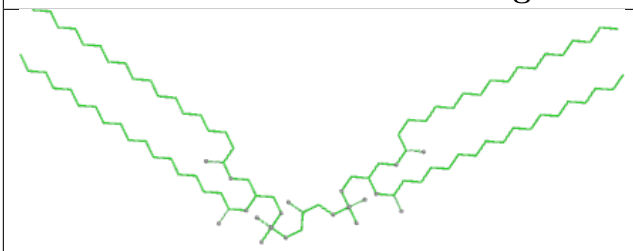


Torsions

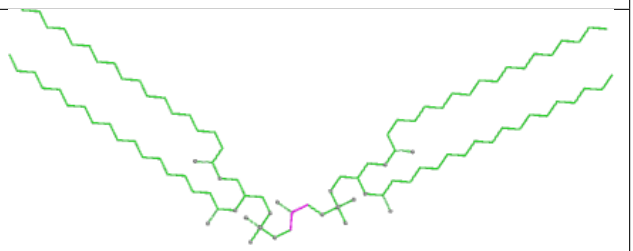


Rings

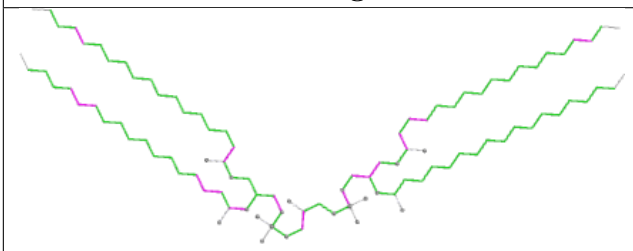
Ligand CDL BL 301



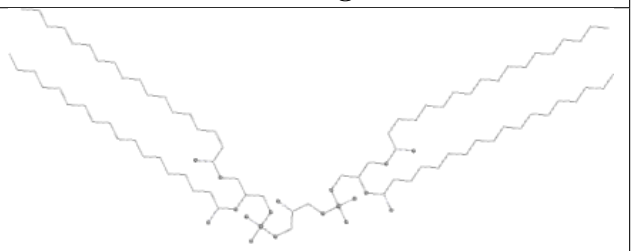
Bond lengths



Bond angles

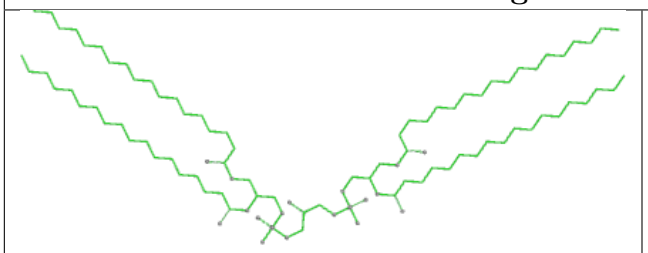


Torsions

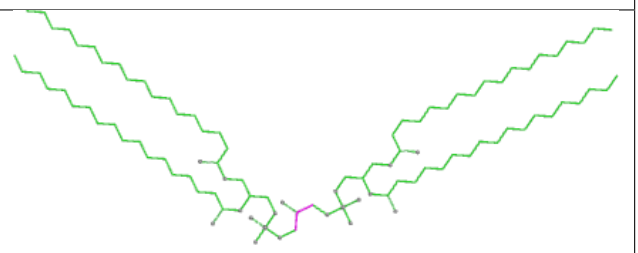


Rings

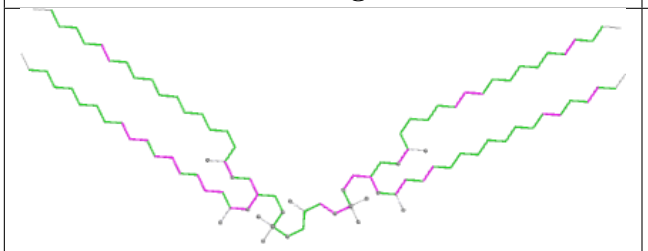
Ligand CDL DD 704



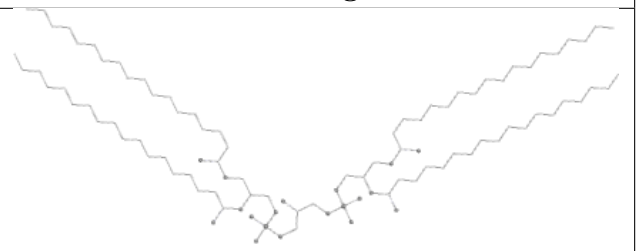
Bond lengths



Bond angles

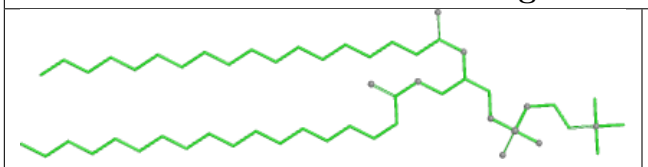


Torsions



Rings

Ligand PC1 AJ 501



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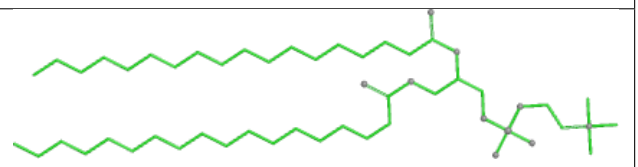
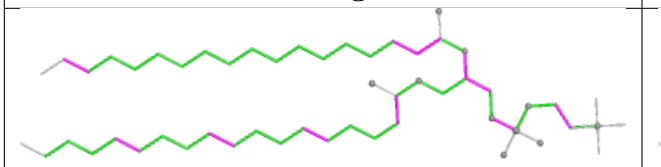
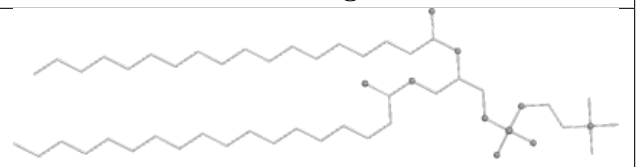


Bond angles

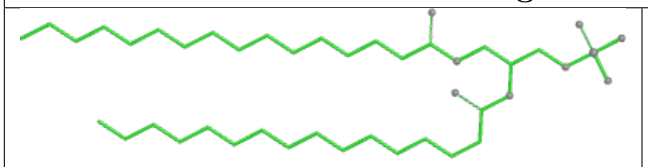


Torsions



Rings

Ligand LPP Dn 504



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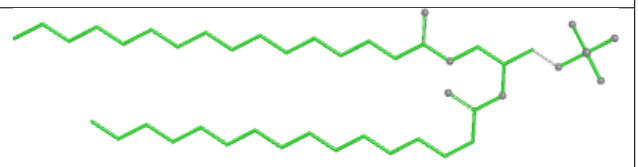
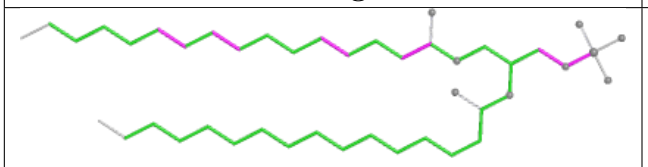
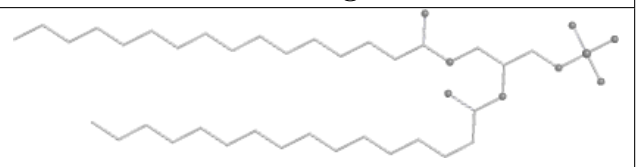


Bond angles

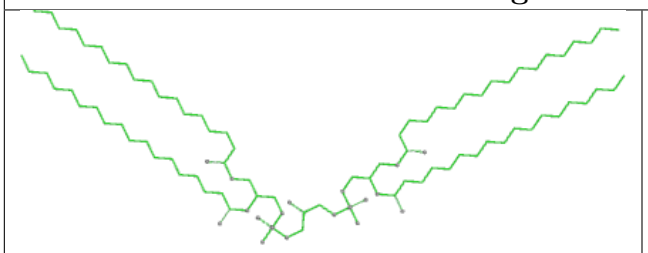


Torsions



Rings

Ligand CDL DR 402



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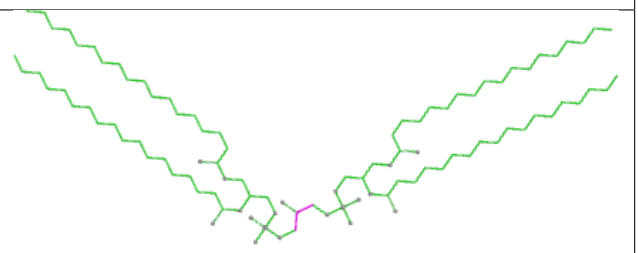
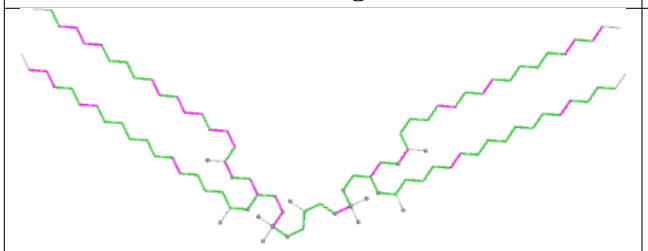
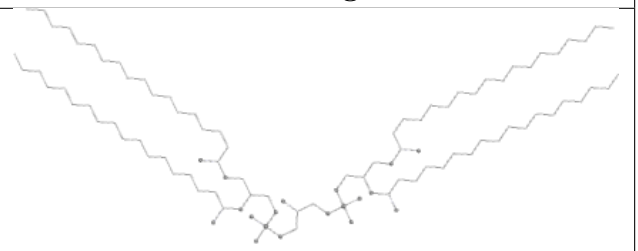


Bond angles

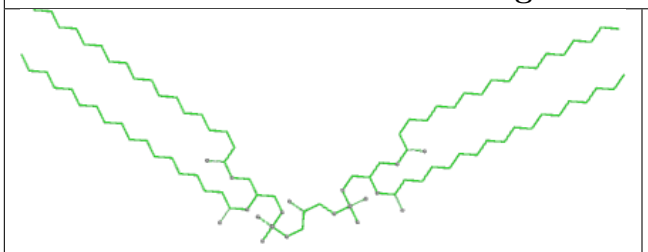


Torsions

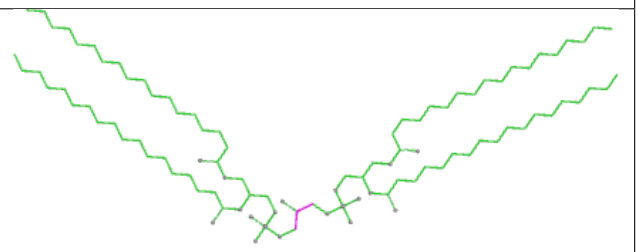


Rings

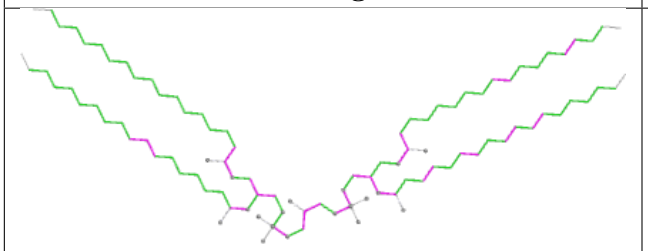
Ligand CDL DJ 307



Bond lengths



Bond angles



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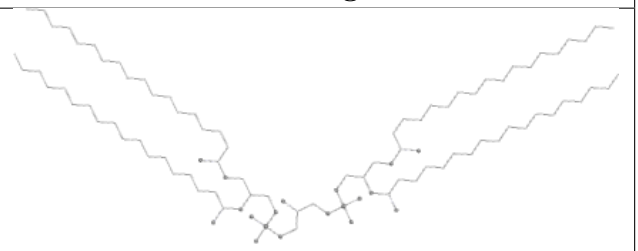
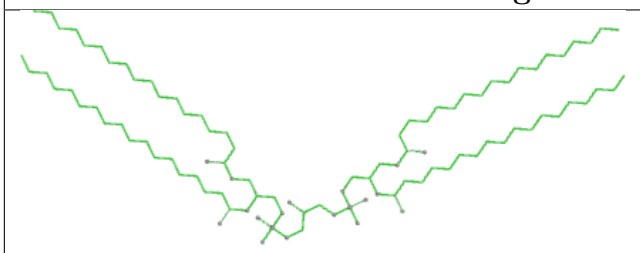


Rings

Ligand CDL DZ 501



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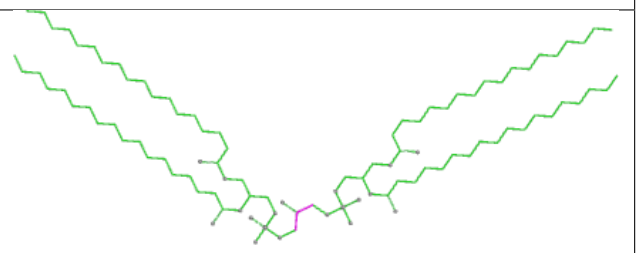
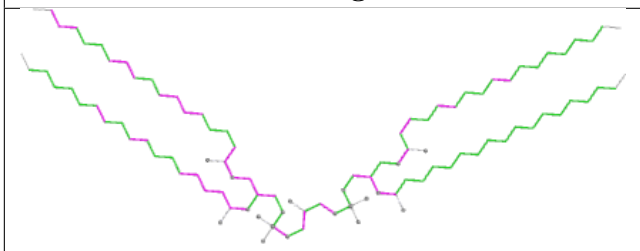


Bond angles



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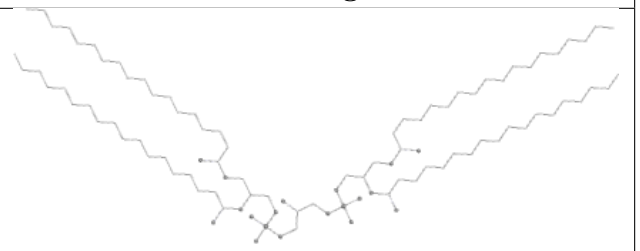
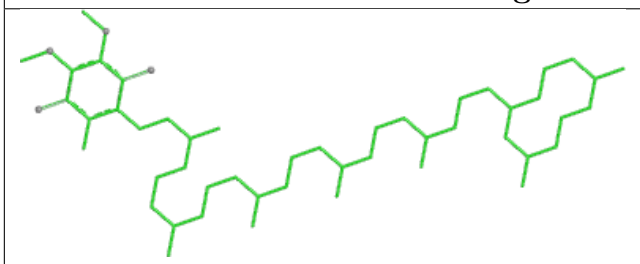


Rings

Ligand UQ8 CC 303



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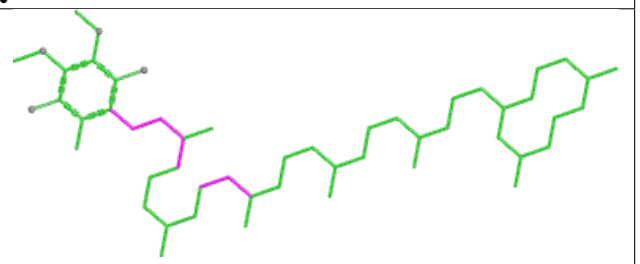
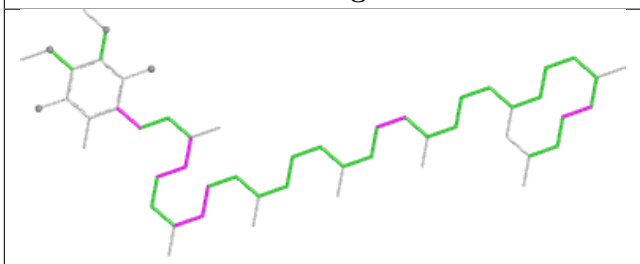
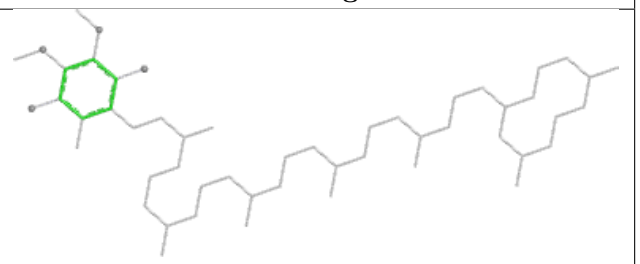


Bond angles

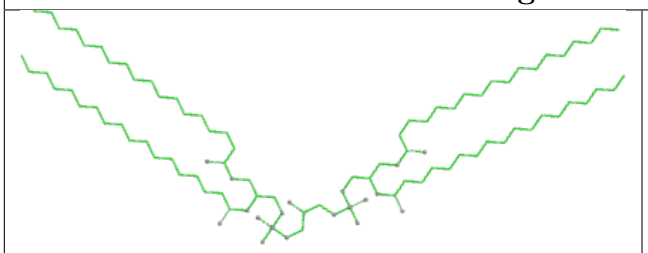


Torsions



Rings

Ligand CDL DI 302



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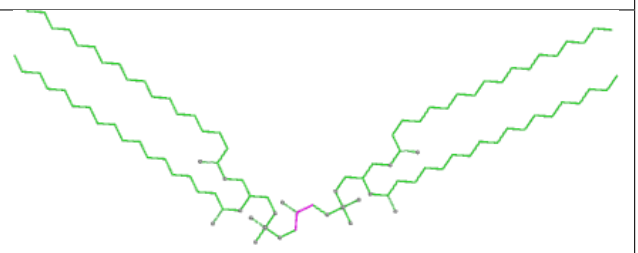
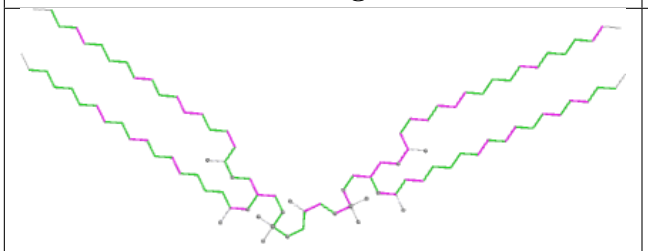


Bond angles



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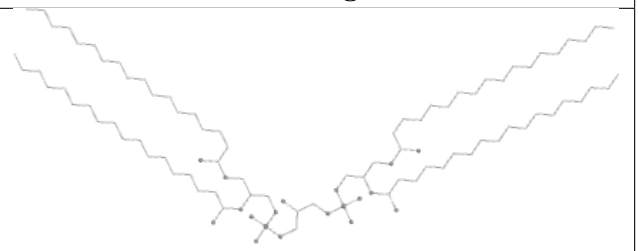
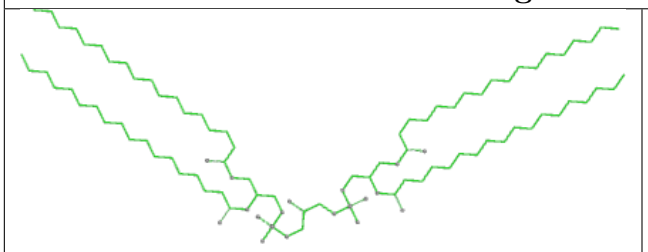


Rings

Ligand CDL Dv 401



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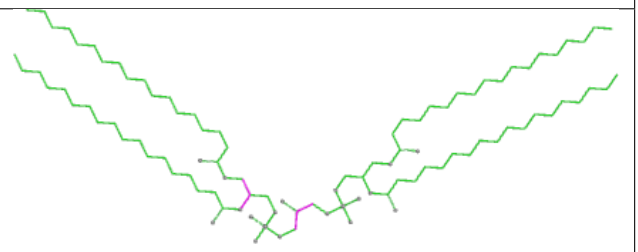
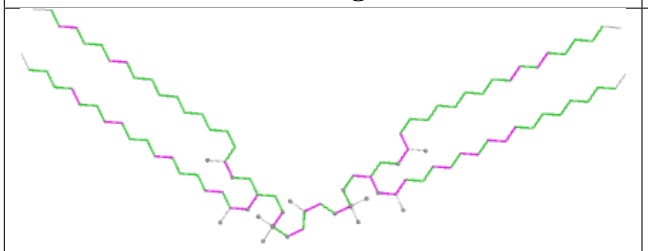


Bond angles



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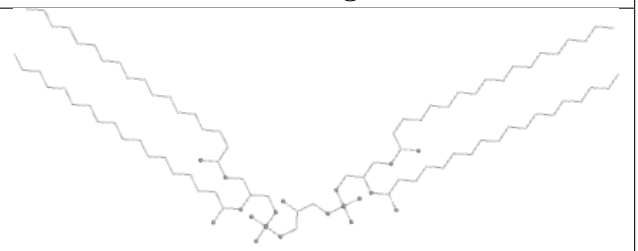
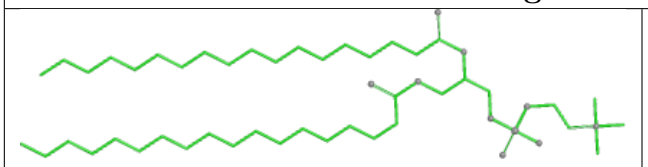


Rings

Ligand PC1 Ef 501



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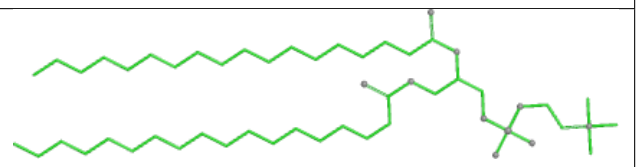
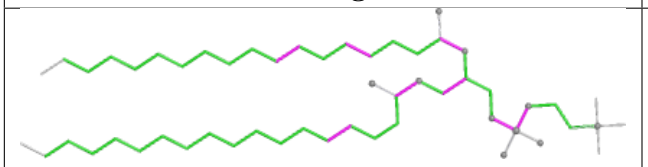


Bond angles



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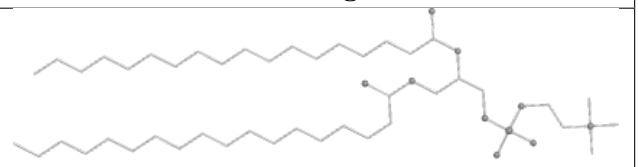
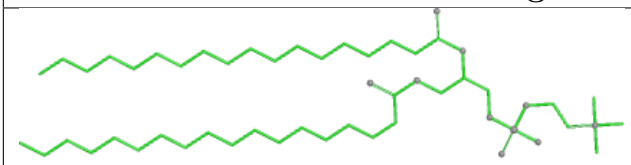


Rings

Ligand PC1 C 509



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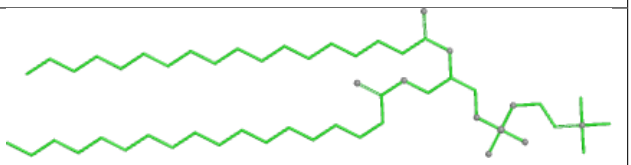
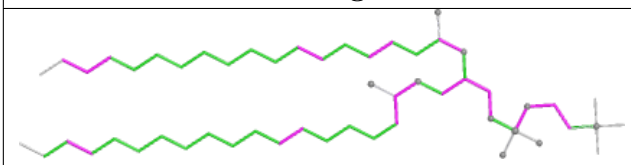
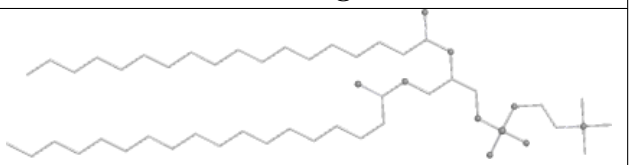


Bond angles

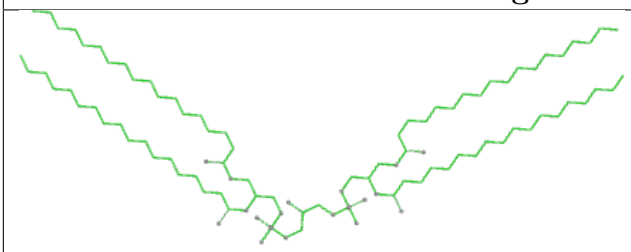


Torsions

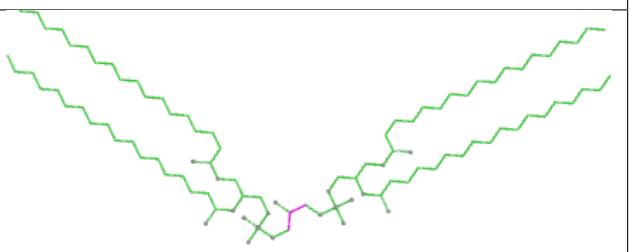


Rings

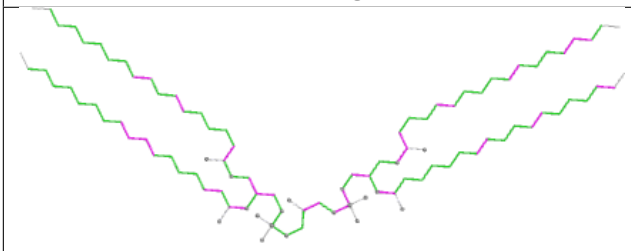
Ligand CDL BT 202



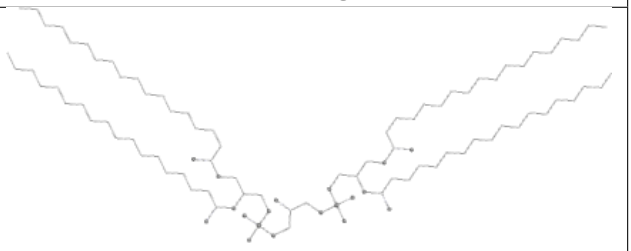
Bond lengths



Bond angles

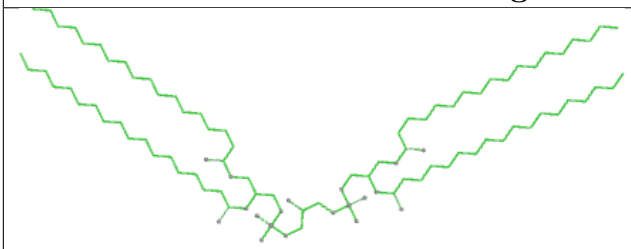


Torsions

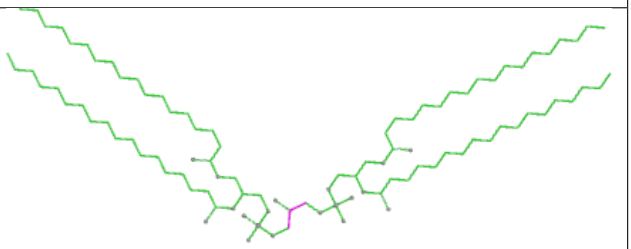


Rings

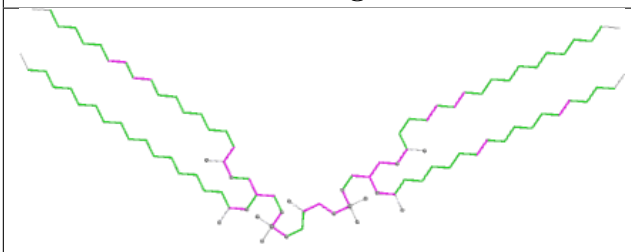
Ligand CDL CD 301



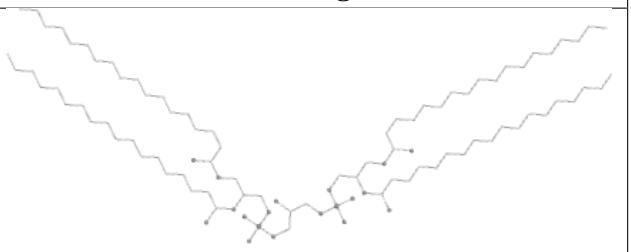
Bond lengths



Bond angles

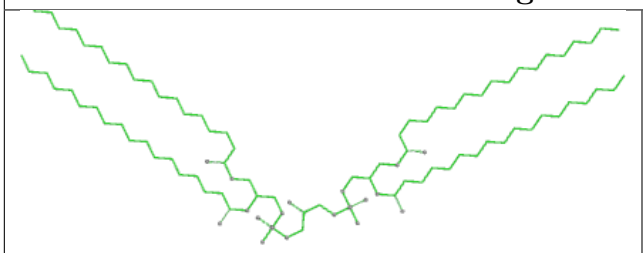


Torsions

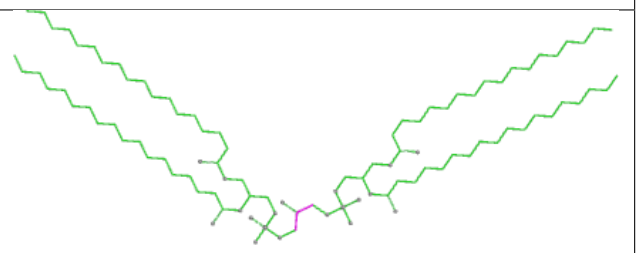


Rings

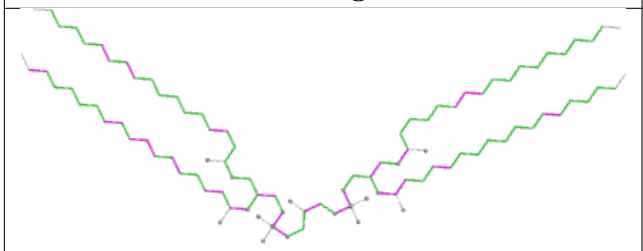
Ligand CDL B0 101



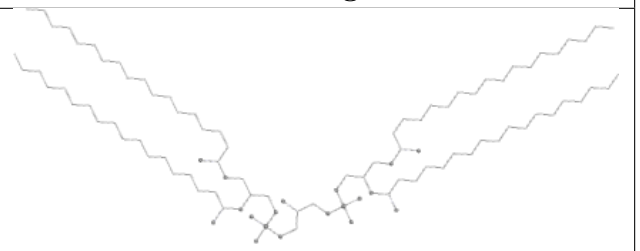
Bond lengths



Bond angles

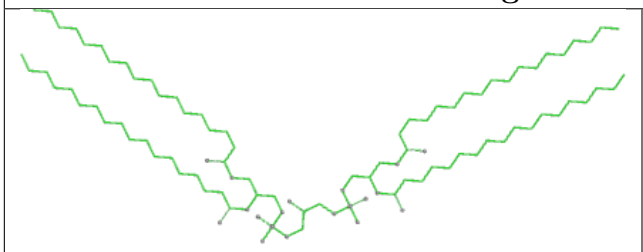


Torsions

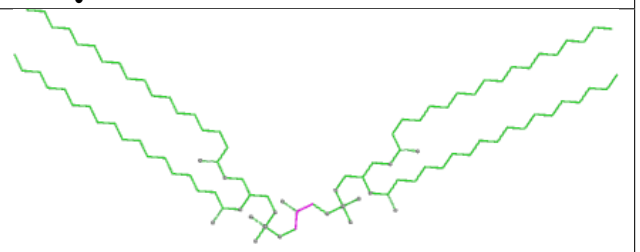


Rings

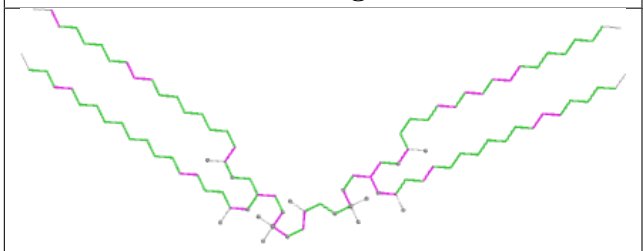
Ligand CDL DQ 1502



Bond lengths



Bond angles



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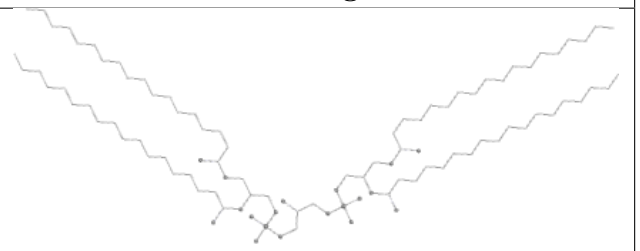
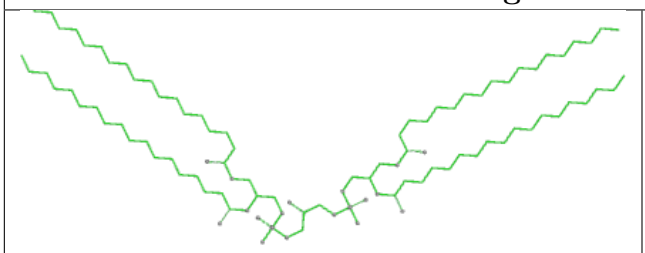
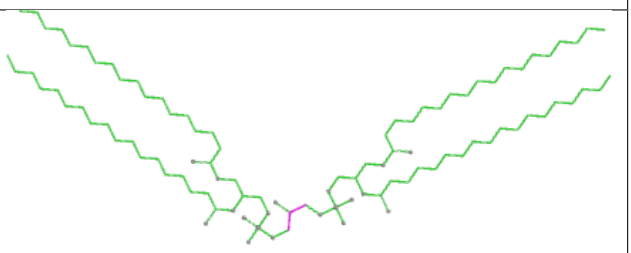


Rings

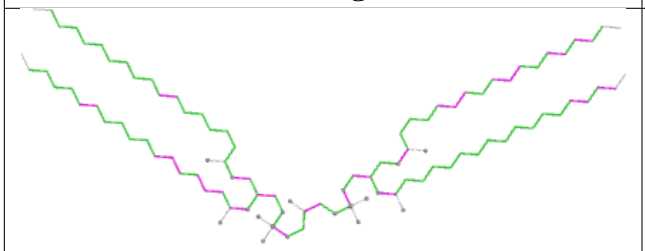
Ligand CDL EH 1601



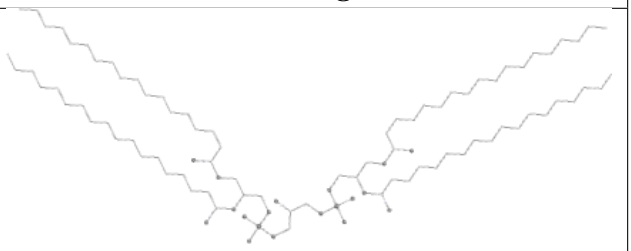
Bond lengths



Bond angles

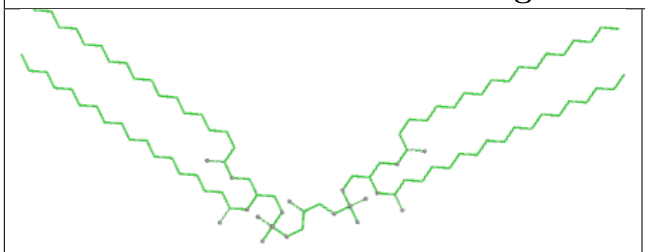


Torsions

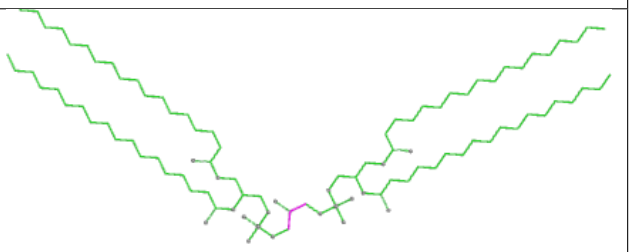


Rings

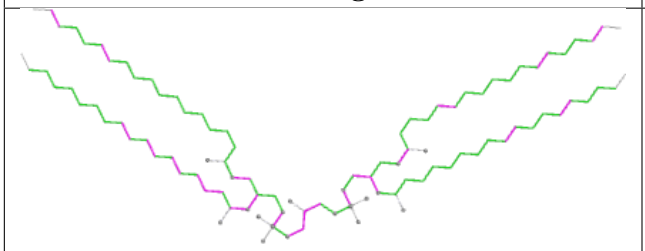
Ligand CDL Du 403



Bond lengths



Bond angles



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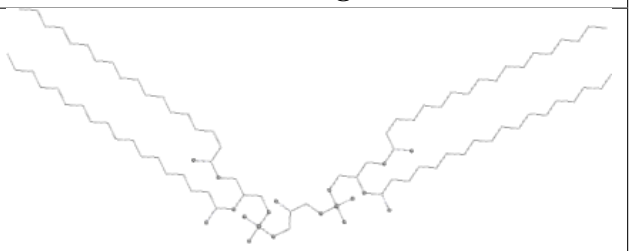
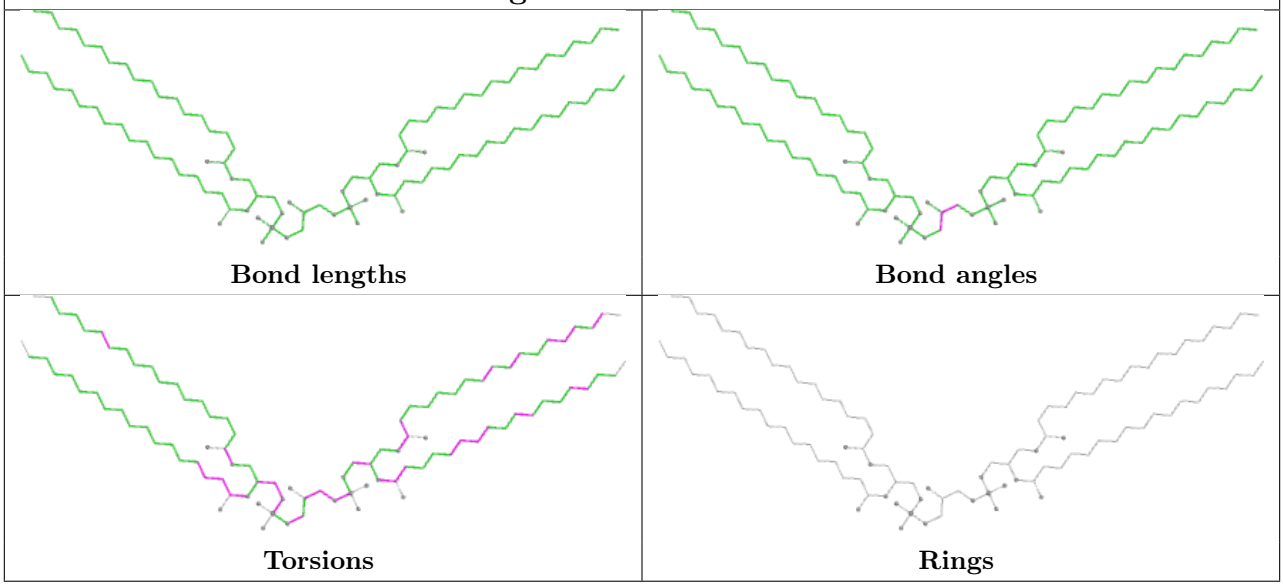
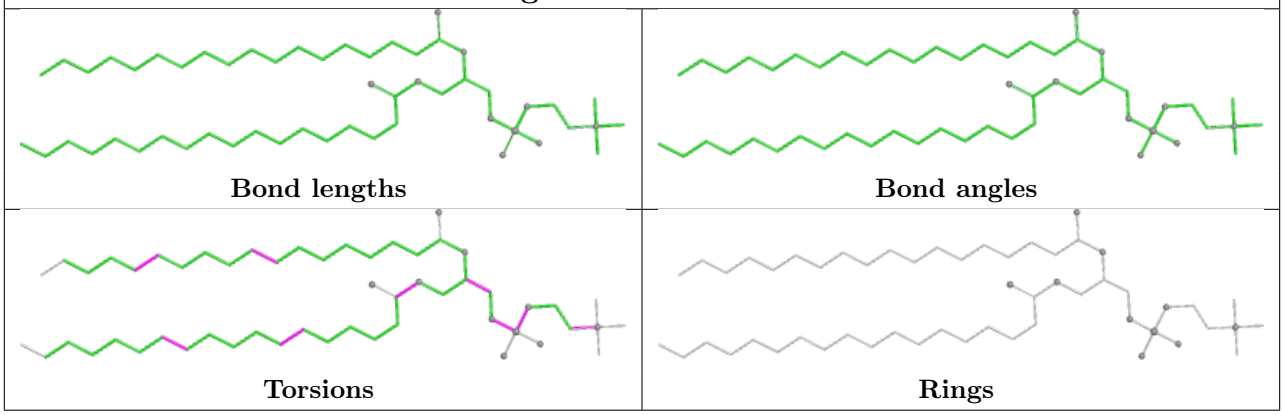


Rings

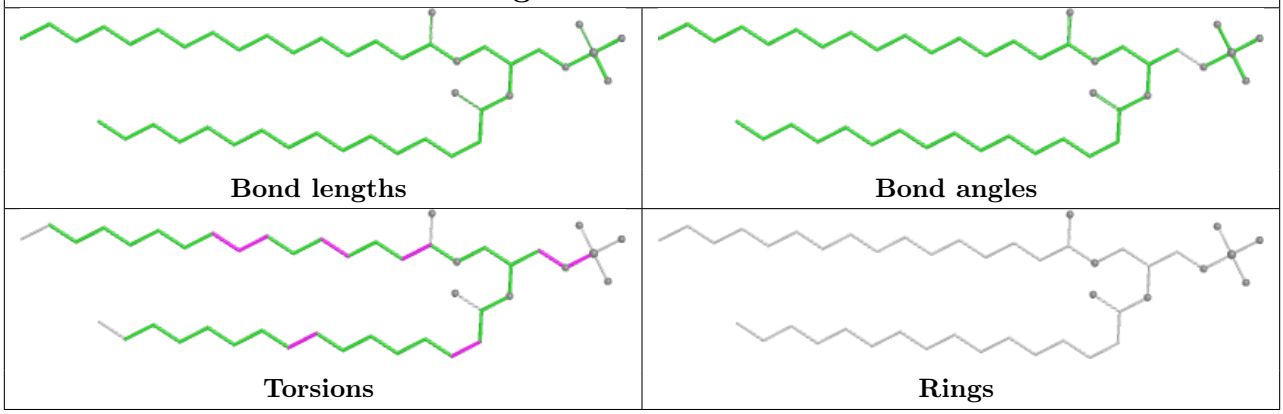
Ligand CDL Dm 501



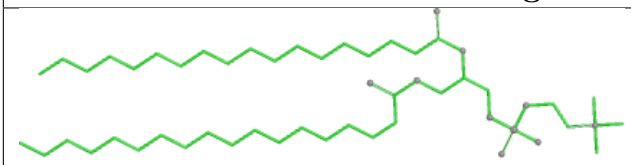
Ligand PC1 DI 303



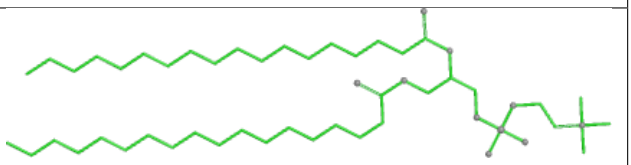
Ligand LPP AA 902



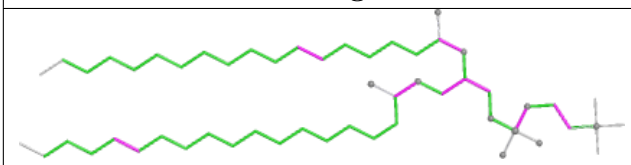
Ligand PC1 e 1101



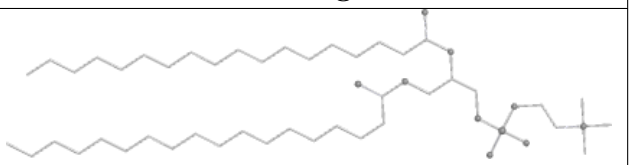
Bond lengths



Bond angles

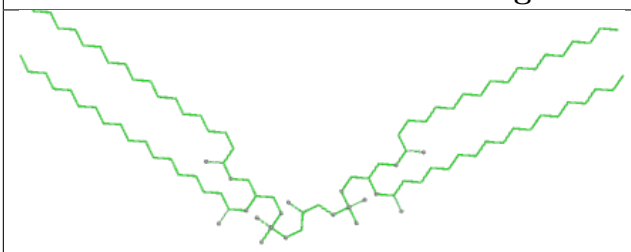


Torsions

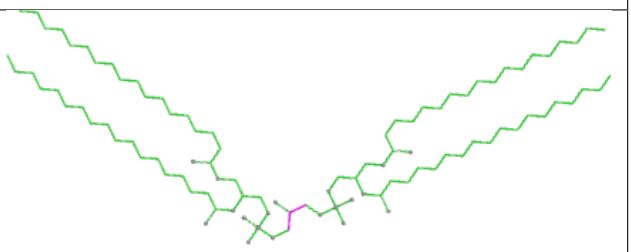


Rings

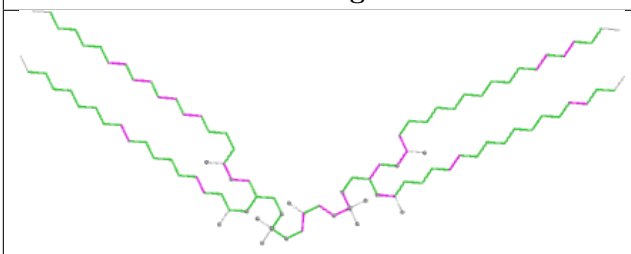
Ligand CDL DJ 302



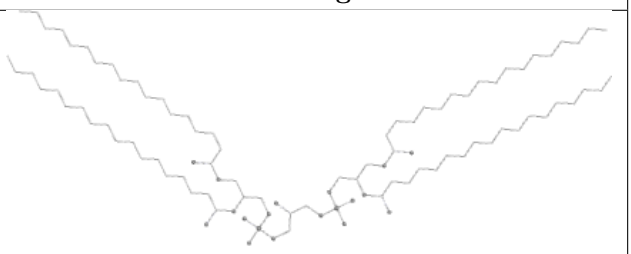
Bond lengths



Bond angles

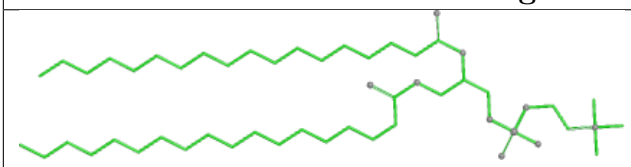


Torsions

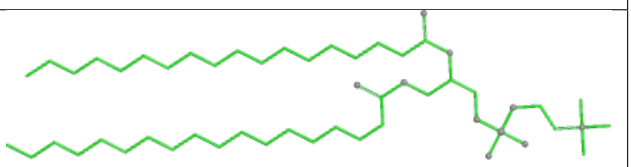


Rings

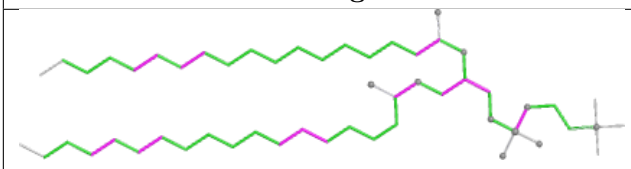
Ligand PC1 Dc 603



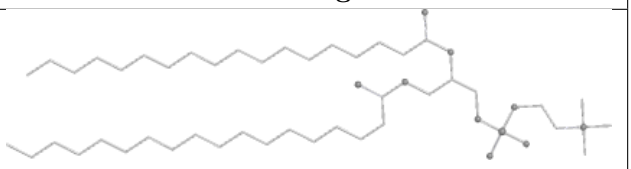
Bond lengths



Bond angles

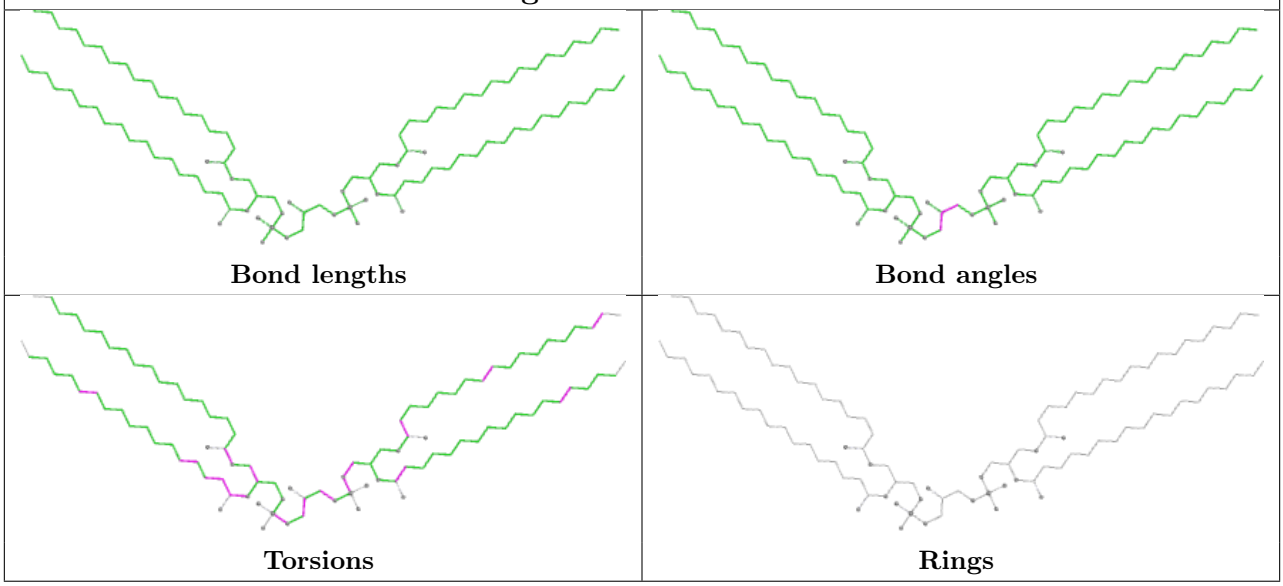


Torsions

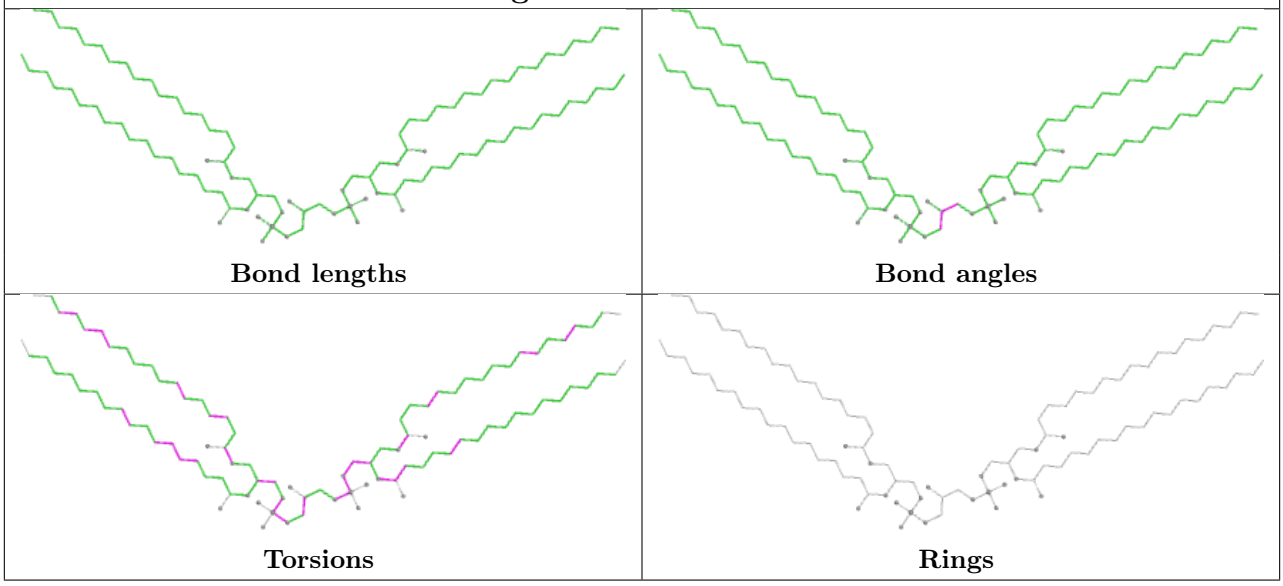


Rings

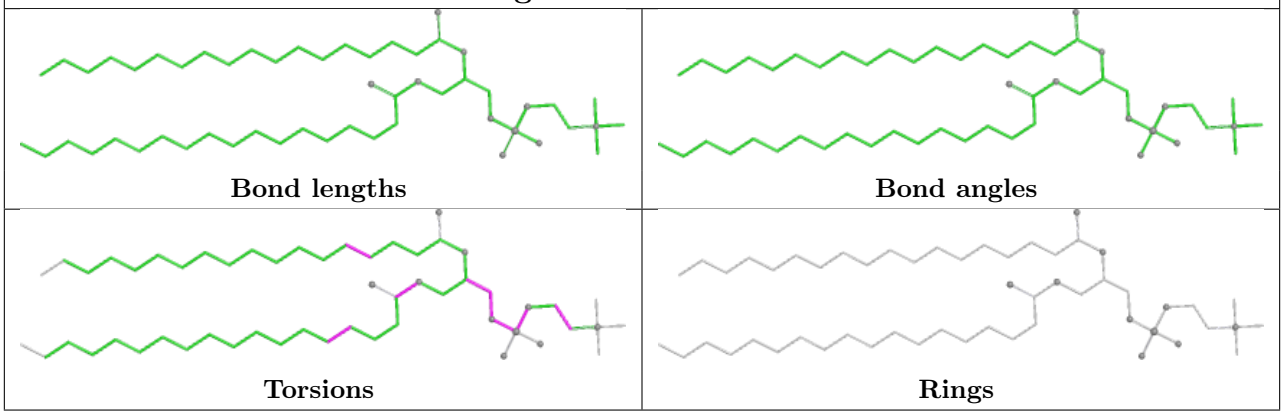
Ligand CDL Ei 401



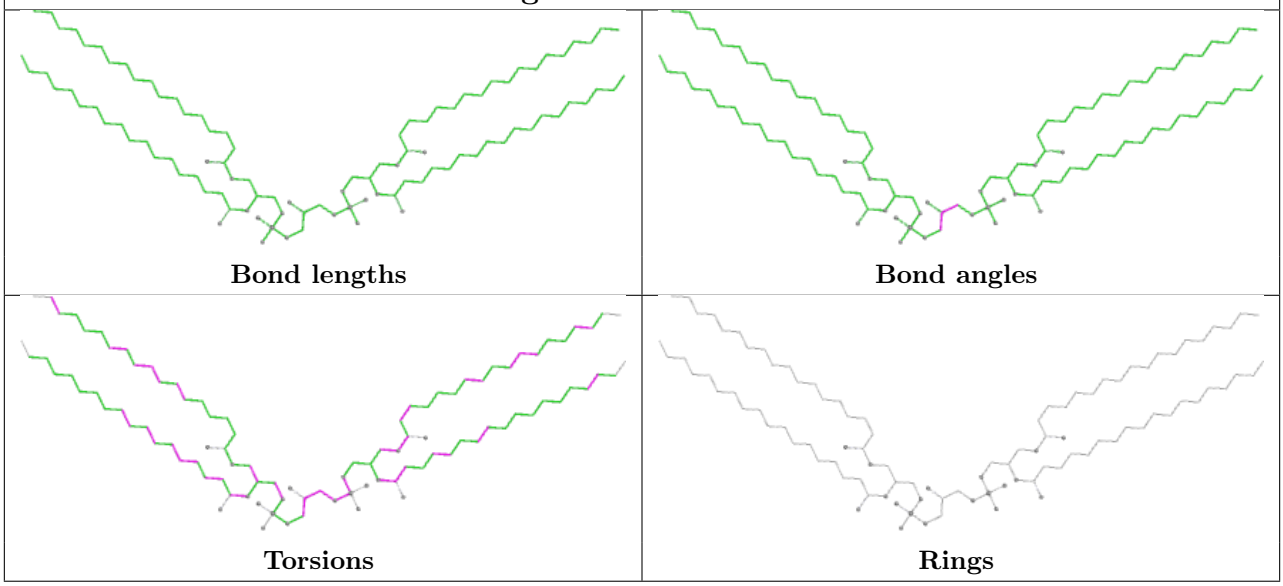
Ligand CDL DV 403



Ligand PC1 AU 201



Ligand CDL El 902



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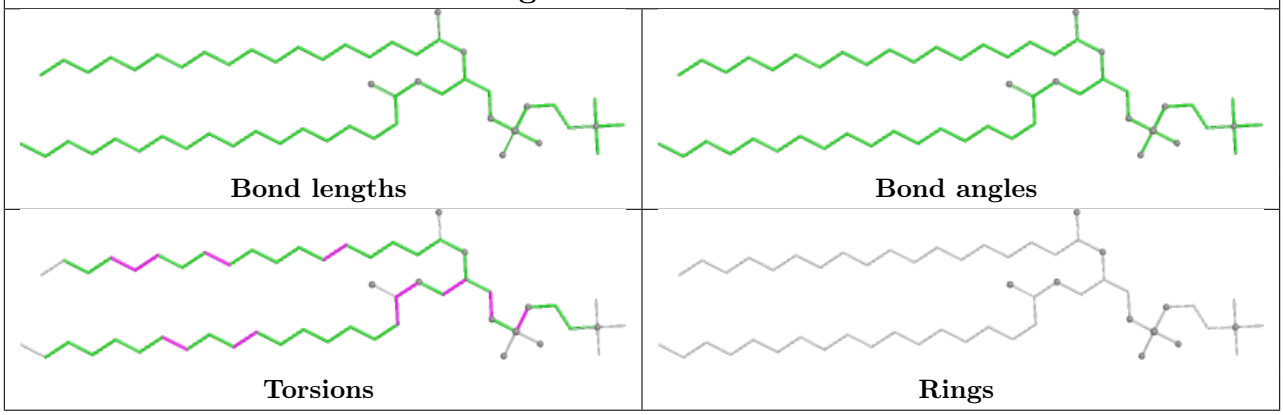
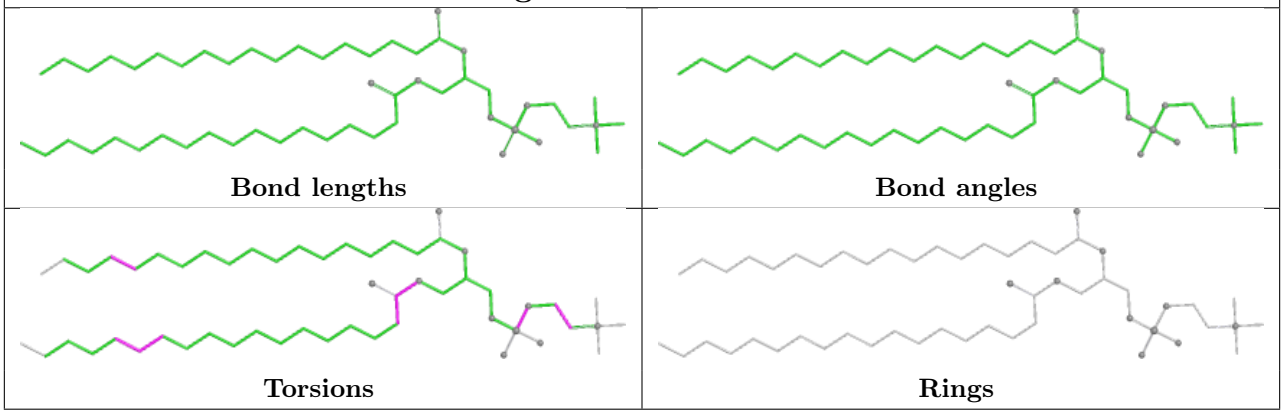
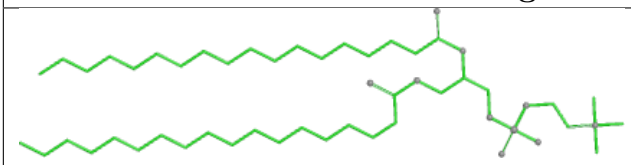


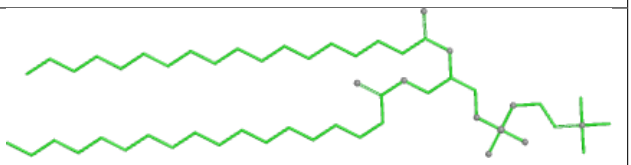
Ligand PC1 DV 405



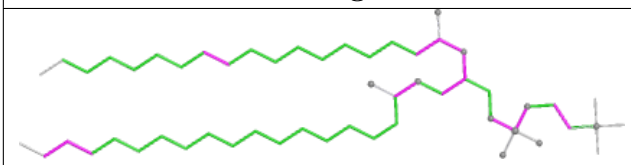
Ligand PC1 Dc 605



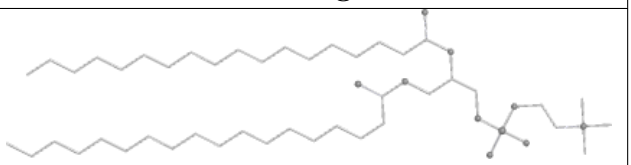
Bond lengths



Bond angles

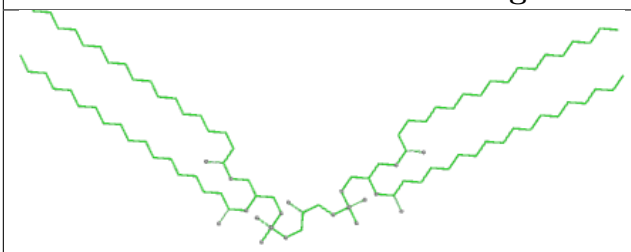


Torsions

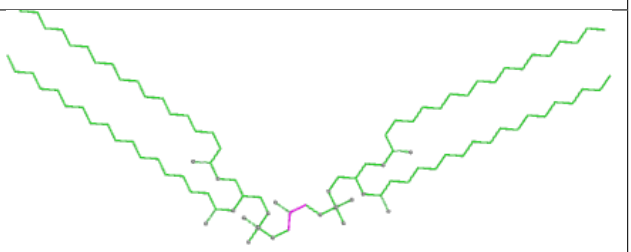


Rings

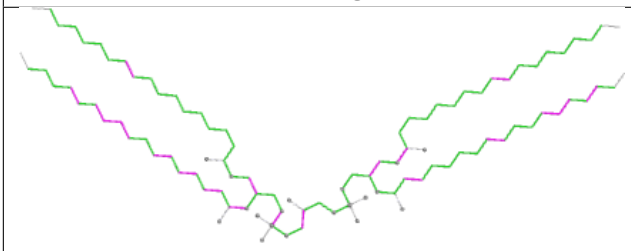
Ligand CDL DH 201



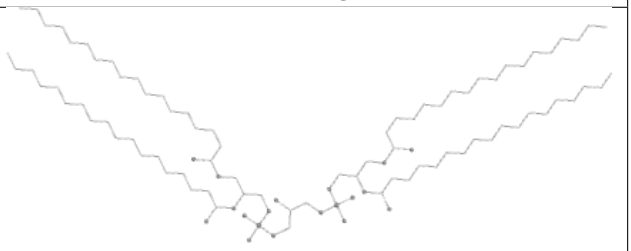
Bond lengths



Bond angles

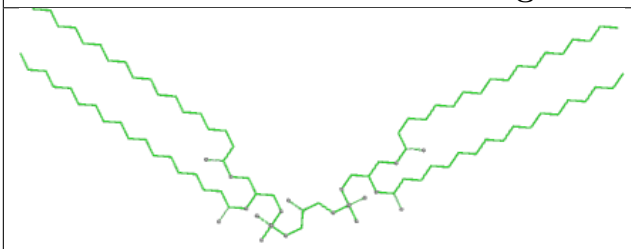


Torsions

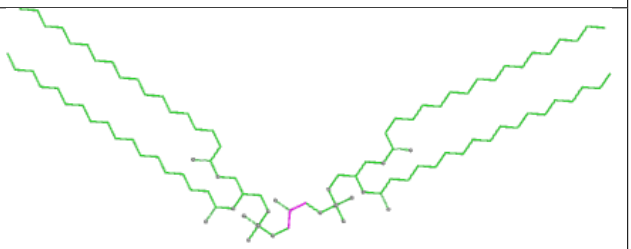


Rings

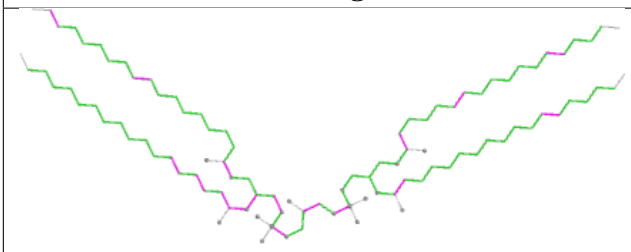
Ligand CDL Ea 502



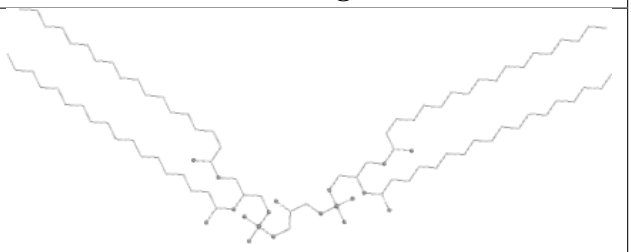
Bond lengths



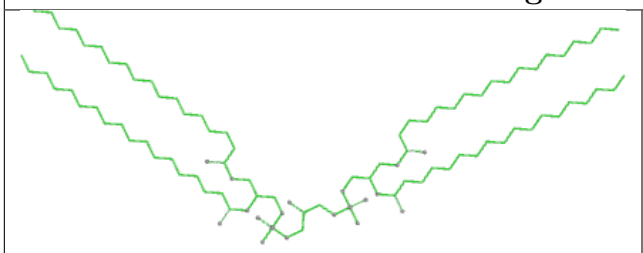
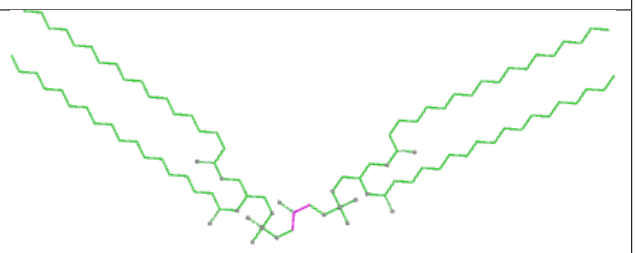
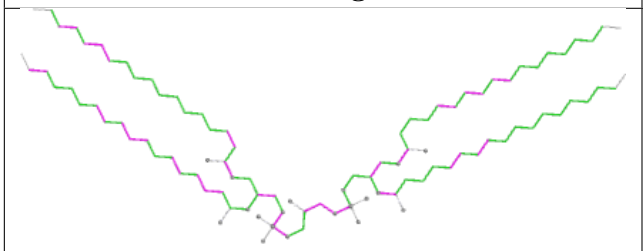
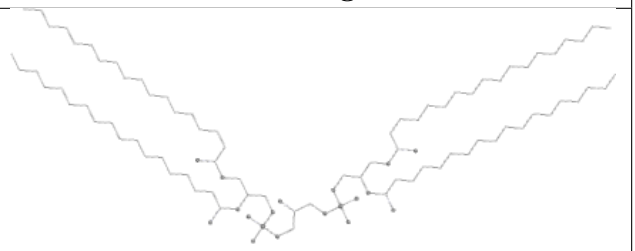
Bond angles

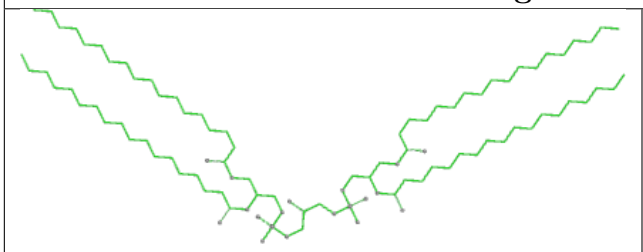
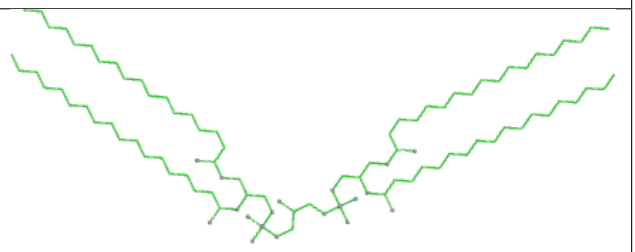
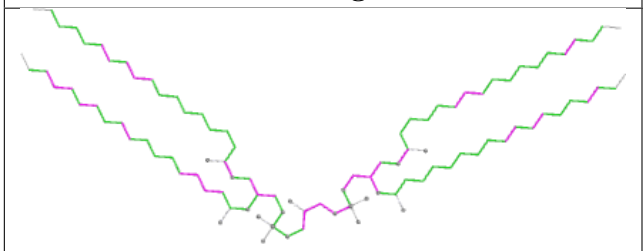
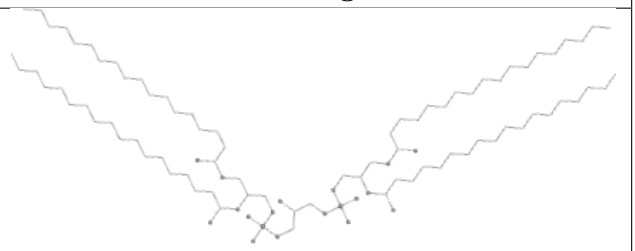


Torsions



Rings

Ligand CDL C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Dd 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

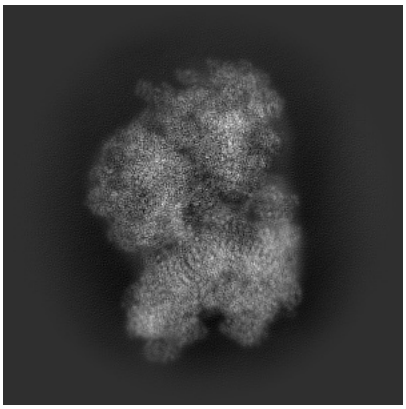
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16184. These allow visual inspection of the internal detail of the map and identification of artifacts.

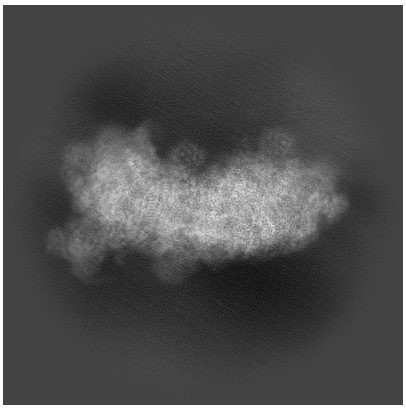
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

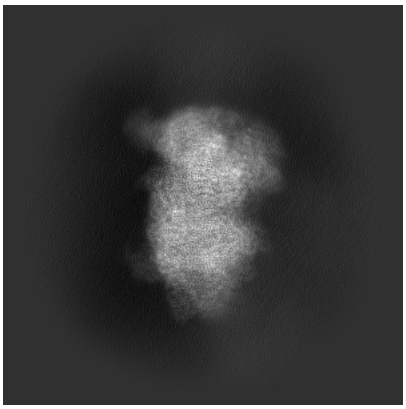
6.1.1 Primary map



X

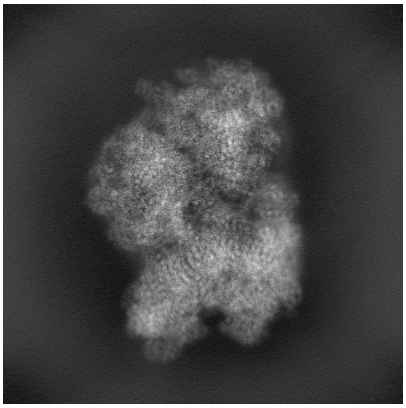


Y

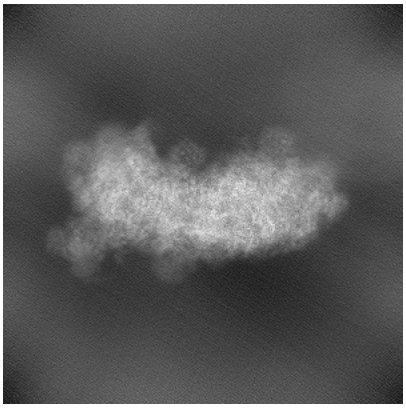


Z

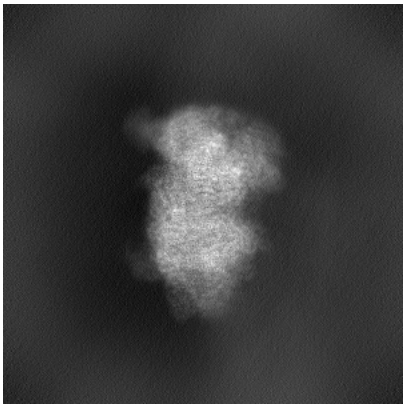
6.1.2 Raw map



X



Y

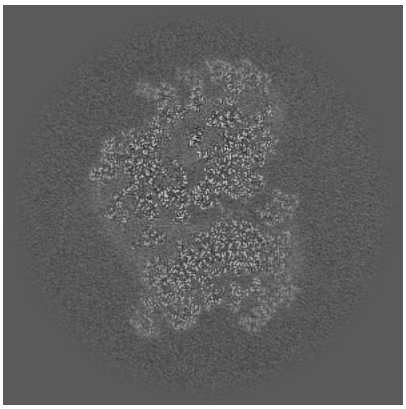


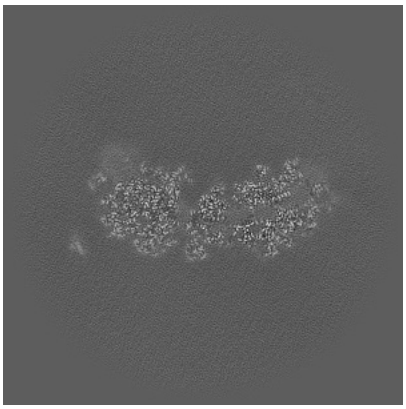
Z

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

6.2 Central slices (i)

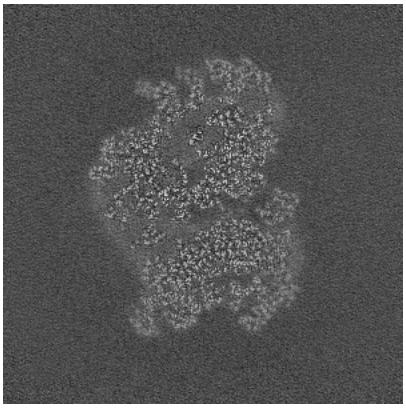
6.2.1 Primary map

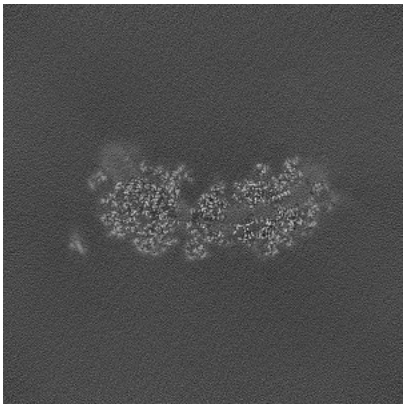

X Index: 240

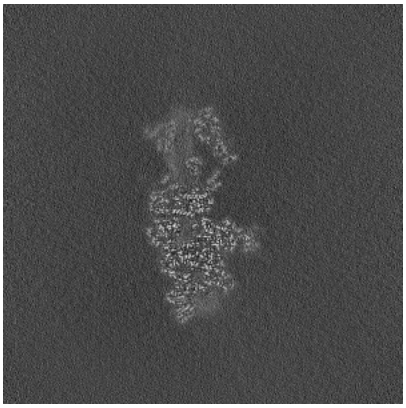

Y Index: 240

Z Index: 240

6.2.2 Raw map


X Index: 240

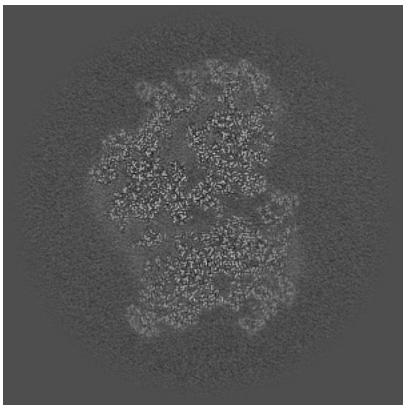

Y Index: 240

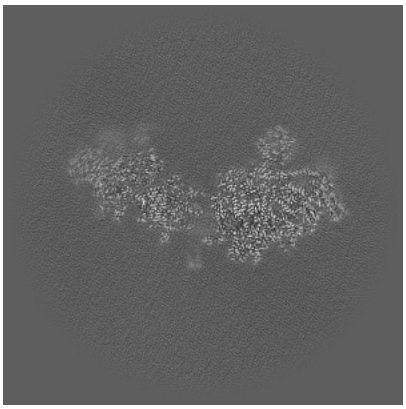

Z Index: 240

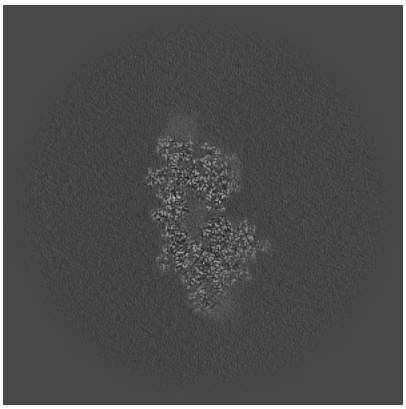
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

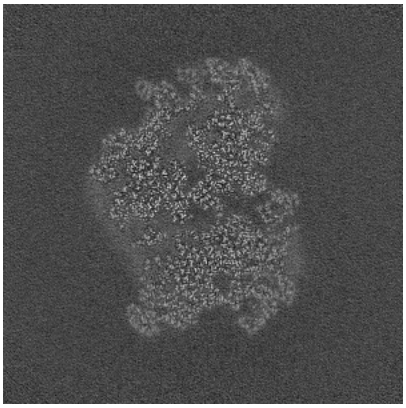
6.3.1 Primary map

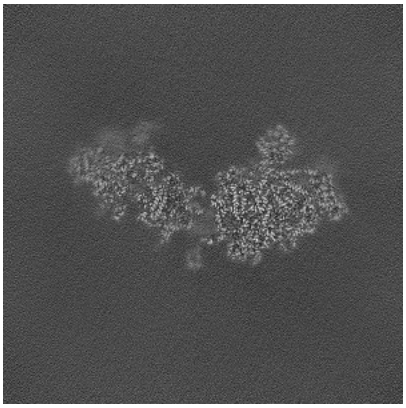

X Index: 243

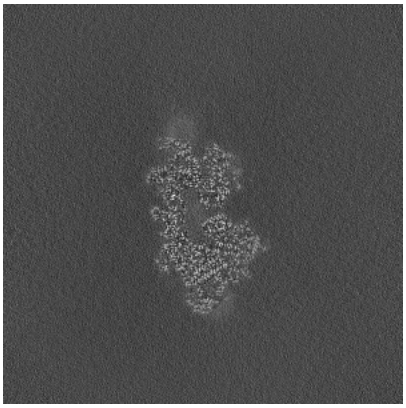

Y Index: 272


Z Index: 287

6.3.2 Raw map


X Index: 243

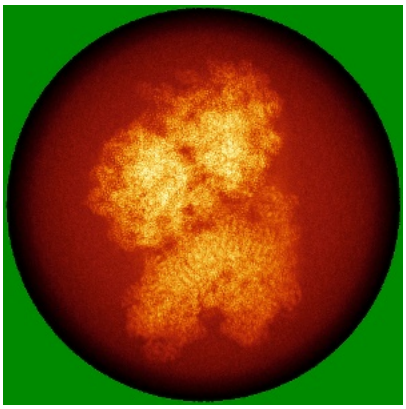

Y Index: 271

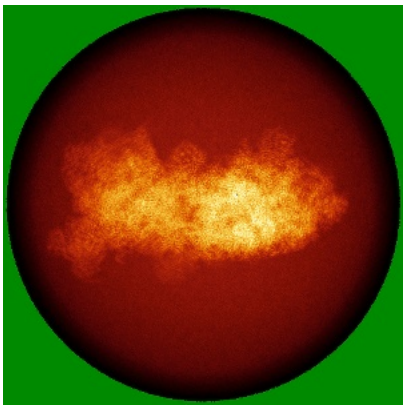

Z Index: 284

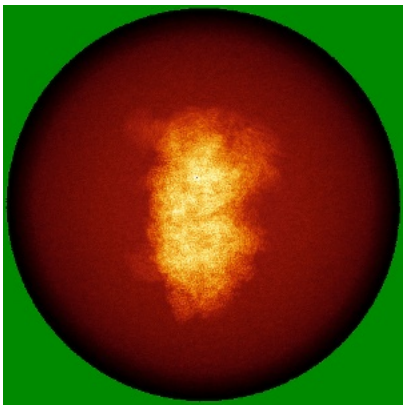
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

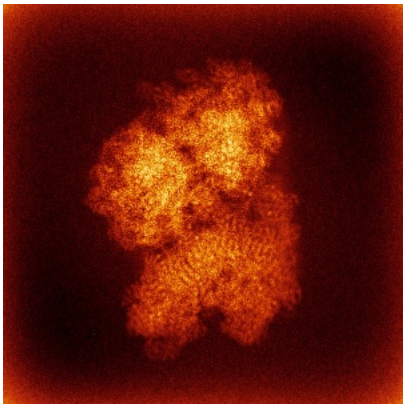
6.4.1 Primary map

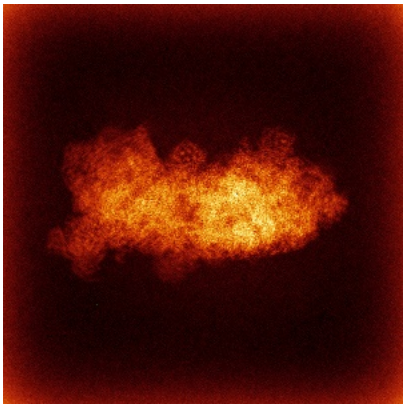

X

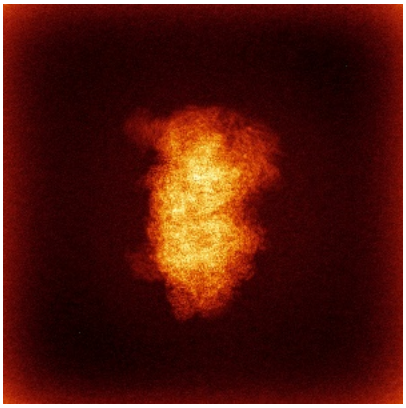

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

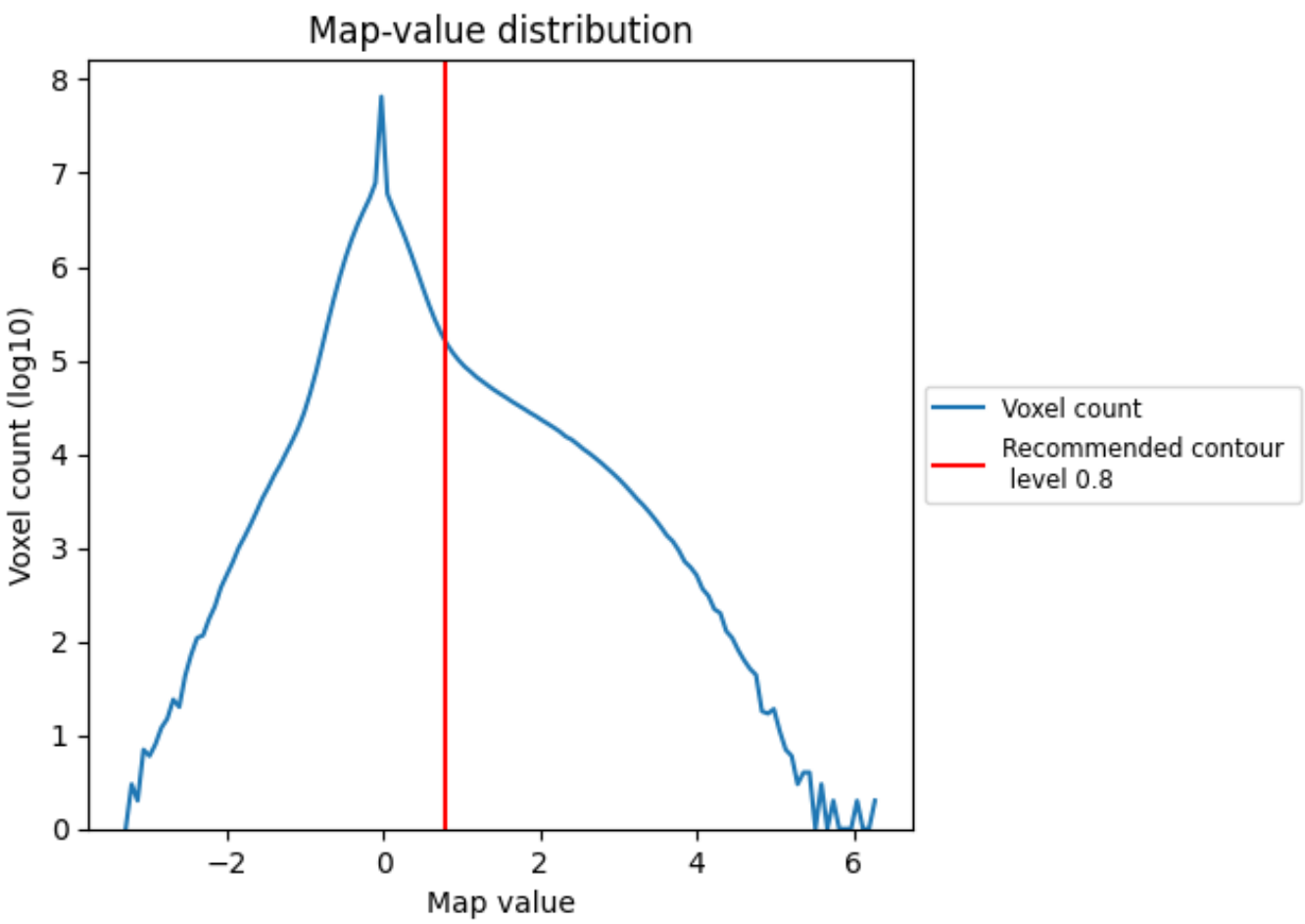
6.6 Mask visualisation (i)

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

7 Map analysis (i)

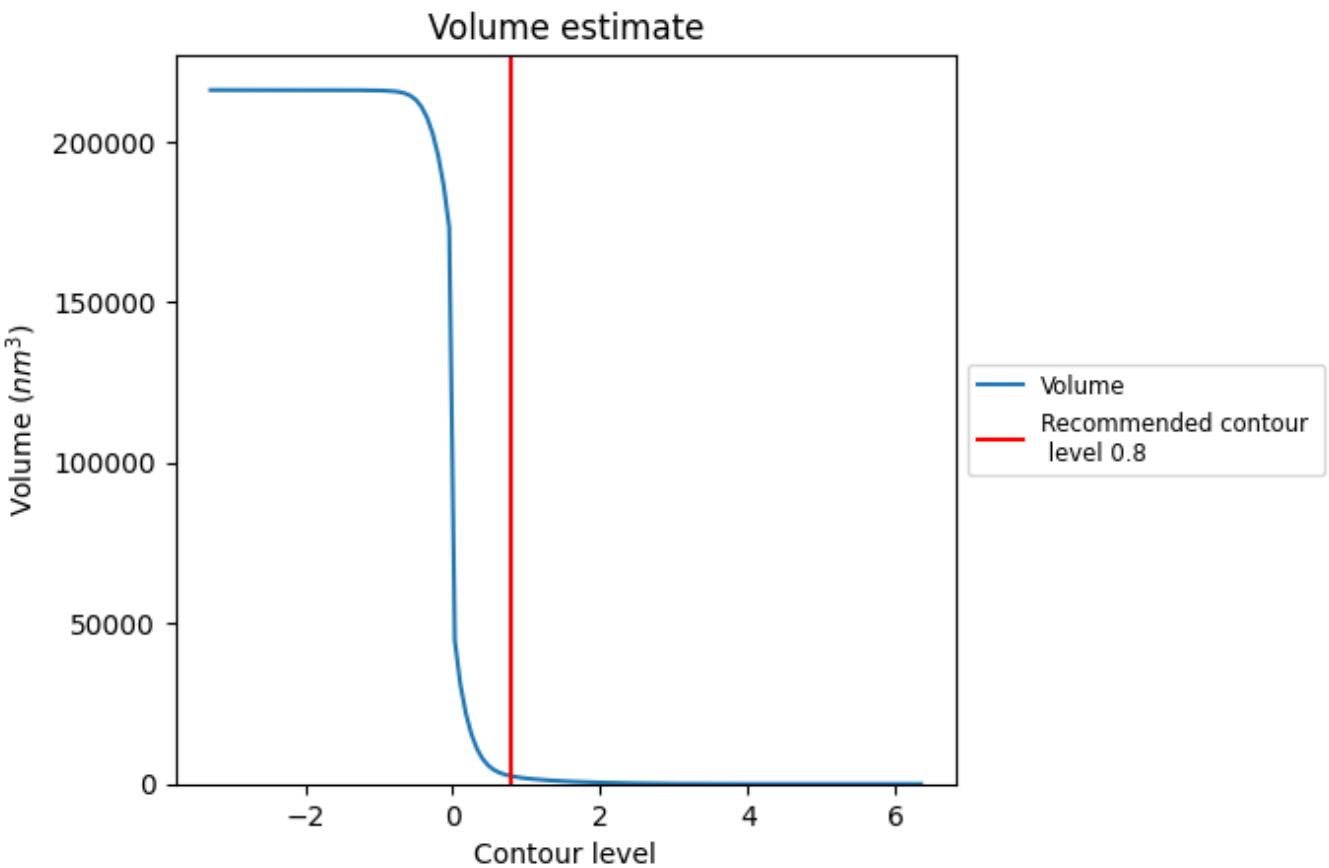
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

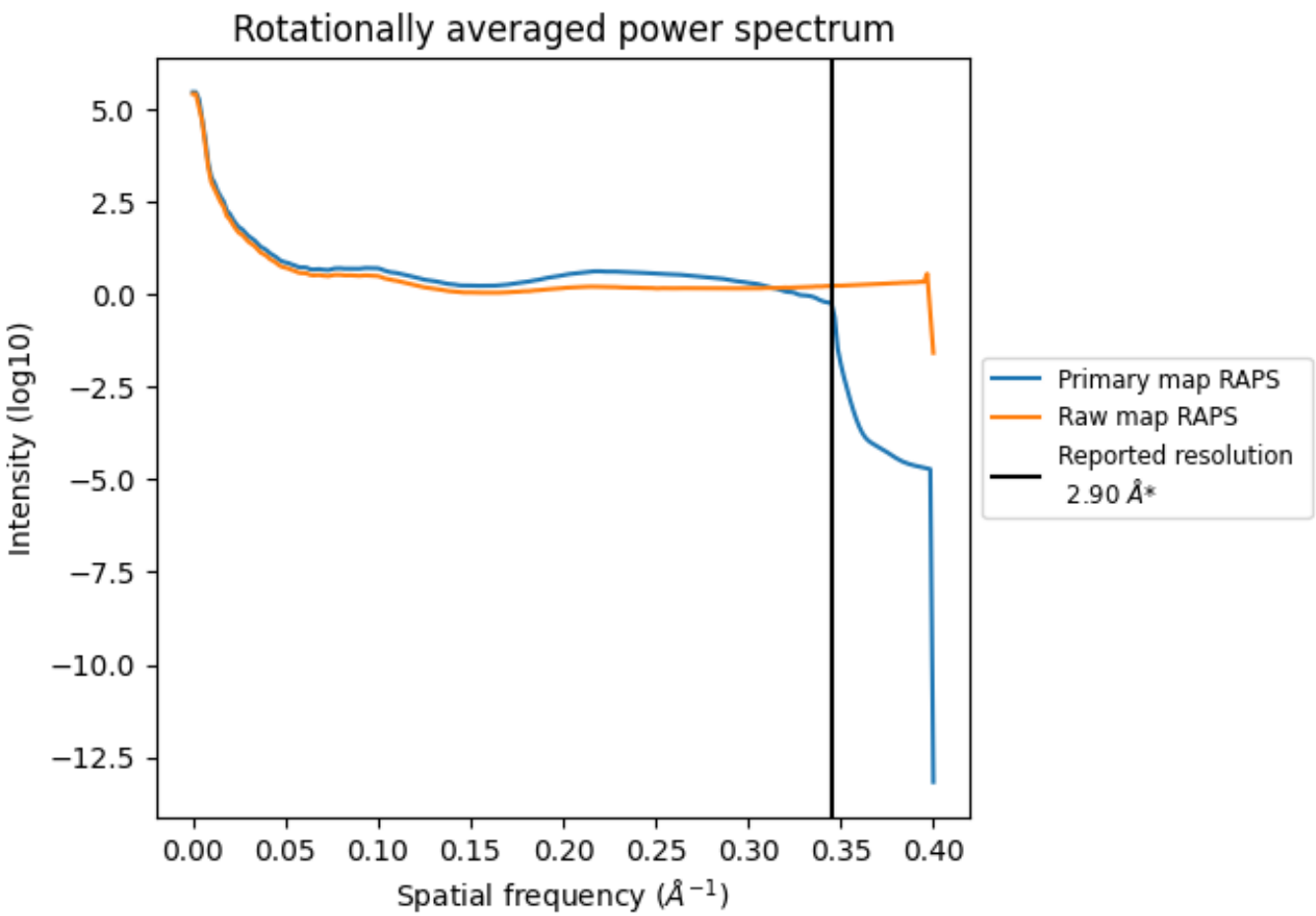
7.2 Volume estimate (i)



The volume at the recommended contour level is 2424 nm^3; this corresponds to an approximate mass of 2189 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 (i)

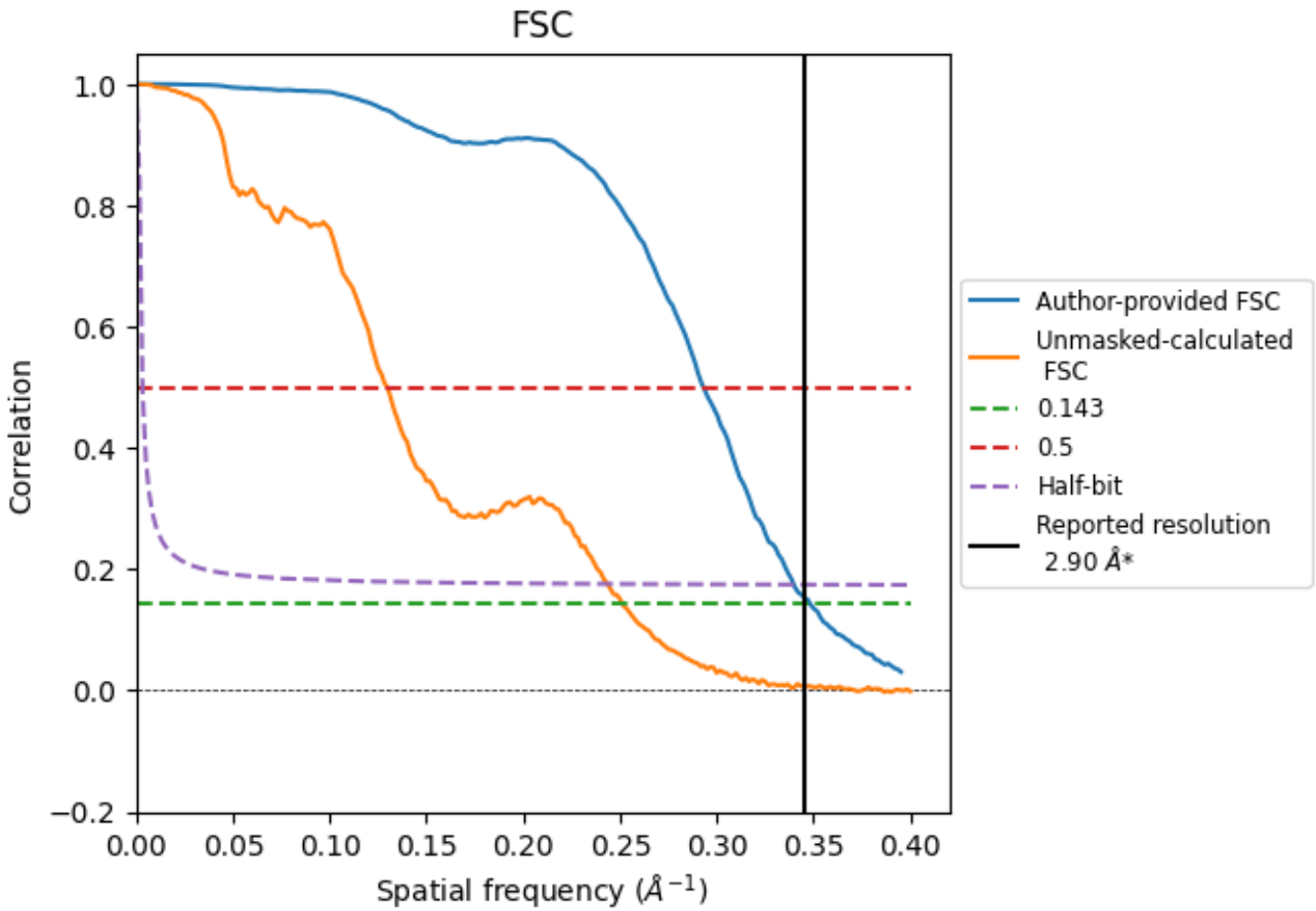


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

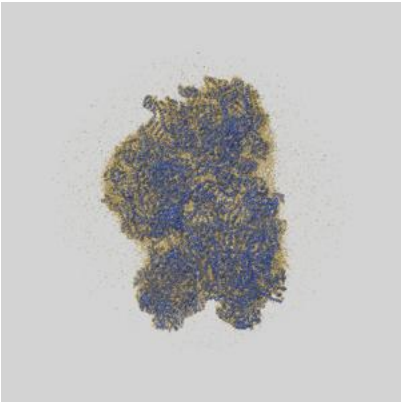
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.41	2.94
Unmasked-calculated*	3.98	7.70	4.11

*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 3.98 differs from the reported value 2.9 by more than 10 %

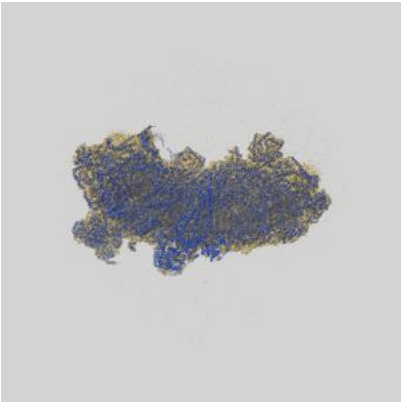
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16184 and PDB model 8BQS. Per-residue inclusion information can be found in section 3 on page 67.

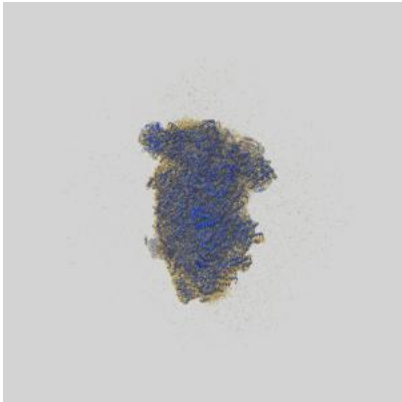
9.1 Map-model overlay (i)



X



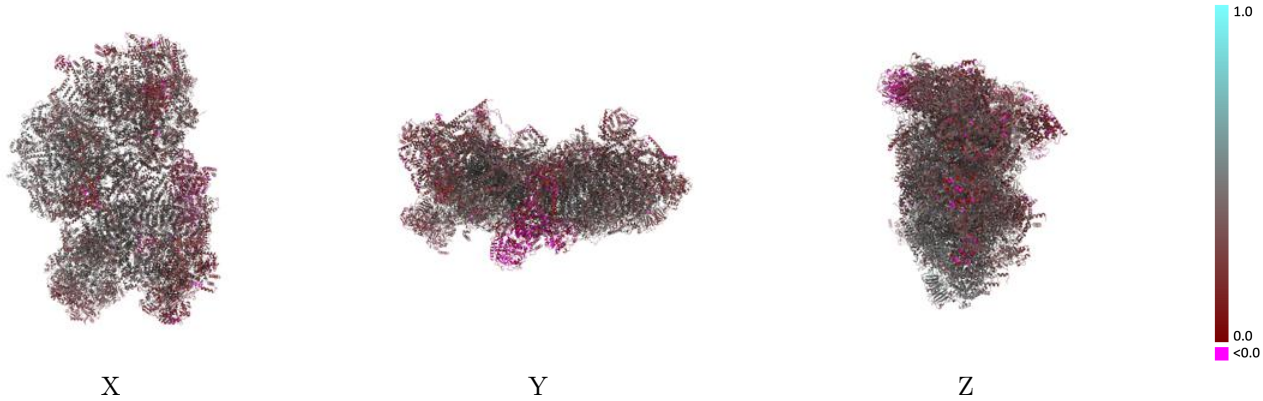
Y



Z

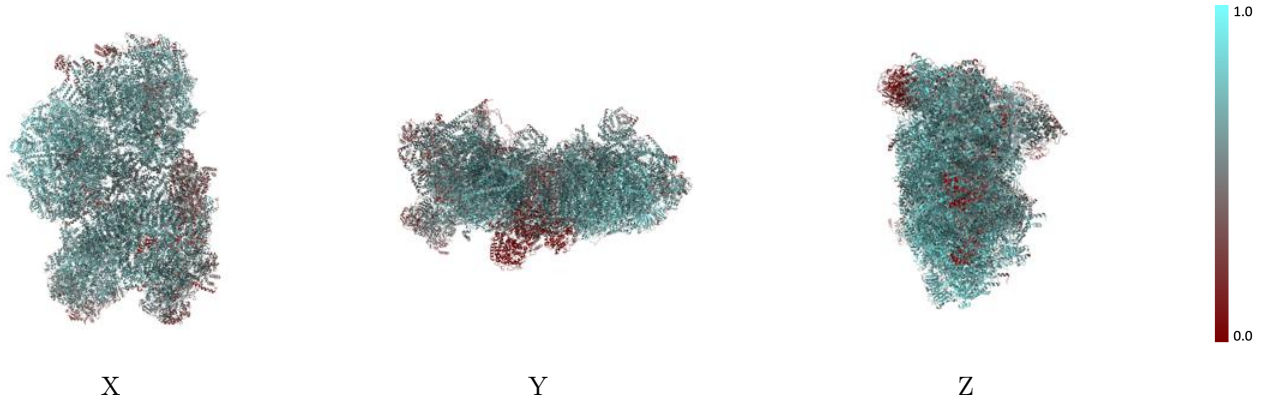
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



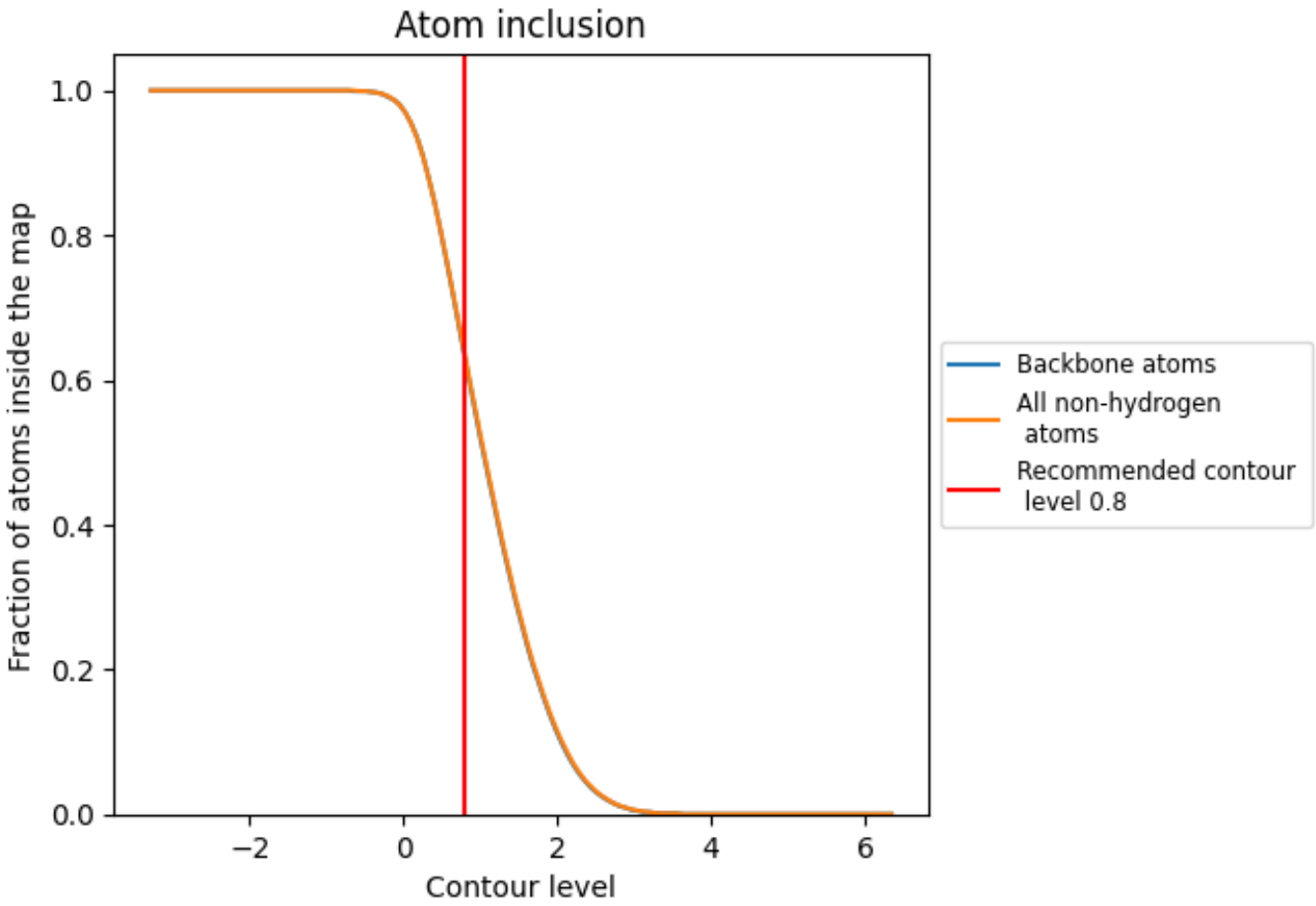
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.3560
A	0.6900	0.3680
A0	0.5580	0.3130
A1	0.7020	0.3880
A2	0.6870	0.3940
A3	0.3210	0.2170
A4	0.4820	0.2530
A5	0.6710	0.3790
A6	0.6190	0.3420
A7	0.6260	0.3520
A8	0.6270	0.3590
A9	0.6910	0.4030
AA	0.6900	0.4060
AB	0.5450	0.3140
AC	0.7630	0.4460
AD	0.4530	0.2660
AE	0.7470	0.4290
AF	0.7650	0.4510
AG	0.7390	0.4310
AH	0.7210	0.4310
AI	0.4290	0.2420
AJ	0.7330	0.4260
AK	0.7970	0.4740
AL	0.7440	0.4280
AM	0.7170	0.4340
AN	0.6640	0.4060
AO	0.7280	0.4250
AP	0.6560	0.3770
AQ	0.7170	0.4030
AR	0.6200	0.3650
AS	0.7760	0.4190
AT	0.7660	0.4360
AU	0.6920	0.4320
AV	0.7320	0.4140
AW	0.7000	0.3880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AX	0.7350	0.4400
AY	0.7720	0.4600
AZ	0.4770	0.2770
B	0.5680	0.2810
B0	0.6460	0.3860
B1	0.6240	0.3660
B2	0.6540	0.3950
B3	0.6780	0.3670
B4	0.5530	0.3230
B5	0.6580	0.3610
B6	0.8040	0.4730
BA	0.5800	0.3170
BB	0.6660	0.3950
BC	0.6700	0.3910
BD	0.6770	0.3970
BE	0.5990	0.3310
BF	0.7270	0.4090
BG	0.6600	0.3950
BH	0.7940	0.4630
BI	0.7970	0.4560
BJ	0.7320	0.3940
BK	0.6760	0.3950
BL	0.6280	0.3700
BM	0.7640	0.4460
BN	0.7100	0.4250
BO	0.6560	0.3790
BP	0.7250	0.4360
BQ	0.6750	0.4090
BR	0.6530	0.3620
BS	0.6550	0.3740
BT	0.6870	0.4100
BU	0.6240	0.3820
BV	0.6690	0.4090
BW	0.6940	0.3750
BX	0.7270	0.4310
BY	0.7240	0.4230
BZ	0.7560	0.4420
C	0.5340	0.3100
CA	0.0900	0.0450
CB	0.2010	0.0700
CC	0.2300	0.1240
CD	0.2130	0.0990

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Chain	Atom inclusion	Q-score
CE	0.1450	0.0770
CF	0.4250	0.1950
CG	0.2040	0.0900
CH	0.3990	0.1510
CI	0.4700	0.2050
CJ	0.2820	0.1180
CK	0.3240	0.1560
CL	0.4740	0.2290
CM	0.4110	0.1910
CN	0.2580	0.0950
CO	0.3660	0.1480
D	0.7510	0.4300
DA	0.7960	0.4530
DB	0.7030	0.3700
DC	0.7190	0.4010
DD	0.7360	0.4190
DE	0.7810	0.4510
DF	0.7410	0.3800
DG	0.6970	0.4000
DH	0.7460	0.4420
DI	0.7430	0.4290
DJ	0.6900	0.4050
DK	0.6650	0.3370
DL	0.7430	0.4470
DM	0.7690	0.4470
DN	0.6450	0.3720
DO	0.5870	0.3200
DP	0.6520	0.3330
DQ	0.7510	0.4280
DR	0.7590	0.4340
DS	0.7370	0.4220
DT	0.8250	0.4740
DU	0.6570	0.3630
DV	0.7340	0.4220
DW	0.6420	0.3390
DX	0.6340	0.3670
DY	0.7110	0.3960
DZ	0.7190	0.4110
Da	0.7620	0.4040
Db	0.6650	0.3340
Dc	0.6630	0.3450
Dd	0.7010	0.3790

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Chain	Atom inclusion	Q-score
De	0.7560	0.3930
Df	0.7050	0.3580
Dg	0.6730	0.3780
Dh	0.7200	0.3970
Di	0.6850	0.3690
Dj	0.6590	0.3870
Dk	0.6730	0.3480
Dl	0.6650	0.3490
Dm	0.7170	0.3750
Dn	0.5970	0.3270
Do	0.4320	0.2450
Dp	0.5860	0.2780
Dq	0.7400	0.4180
Dr	0.6920	0.3840
Ds	0.6680	0.3580
Dt	0.7780	0.4270
Du	0.6080	0.3040
Dv	0.6530	0.3460
Dw	0.6450	0.3190
Dx	0.6430	0.3670
Dy	0.6540	0.3360
Dz	0.6690	0.3440
E	0.5140	0.3080
EA	0.6640	0.3560
EB	0.7100	0.4000
EC	0.4860	0.2670
ED	0.6160	0.3610
EE	0.7020	0.3540
EF	0.8180	0.4530
EG	0.7370	0.3980
EH	0.7540	0.4230
EI	0.6930	0.3780
EJ	0.6870	0.3770
EK	0.6680	0.3640
EL	0.6940	0.4140
EM	0.7180	0.3840
EN	0.7070	0.4260
EO	0.6360	0.3690
EP	0.8090	0.4600
EQ	0.7660	0.4150
ER	0.7790	0.4080
ES	0.7710	0.4480

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Chain	Atom inclusion	Q-score
ET	0.5080	0.2210
EU	0.6900	0.3830
EV	0.6310	0.3140
EW	0.5360	0.2420
EX	0.5960	0.2900
EY	0.5790	0.2580
EZ	0.6110	0.2880
Ea	0.6200	0.3120
Eb	0.6740	0.3430
Ec	0.4020	0.2370
Ed	0.5810	0.3500
Ee	0.6410	0.2900
Ef	0.7580	0.4130
Eg	0.6830	0.3710
Eh	0.7250	0.3840
Ei	0.6840	0.3720
Ej	0.6250	0.3040
Ek	0.6970	0.3910
El	0.6710	0.3830
Em	0.7140	0.3660
En	0.6810	0.3720
Eo	0.6640	0.3570
Ep	0.7390	0.4240
Eq	0.7470	0.3750
Er	0.7920	0.3860
Es	0.8220	0.4520
Et	0.4450	0.1610
Eu	0.6080	0.3500
Ev	0.6280	0.2880
Ew	0.4570	0.1760
Ex	0.5400	0.2120
Ey	0.5610	0.2420
Ez	0.5880	0.2520
F	0.6180	0.3650
FA	0.6260	0.2810
Fa	0.6000	0.2590
G	0.5030	0.2540
H	0.5110	0.2820
I	0.7290	0.4120
J	0.2640	0.2030
K	0.6340	0.3540
L	0.5490	0.2780

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Chain	Atom inclusion	Q-score
a	0.4730	0.2720
b	0.5200	0.2780
c	0.6660	0.3990
d	0.5600	0.3130
e	0.3240	0.2050
f	0.3590	0.2060
g	0.6290	0.3850
h	0.7170	0.4140
i	0.4860	0.2600
j	0.2180	0.1610
k	0.5070	0.3230
l	0.6160	0.4010