Full wwPDB EM Validation Report ⓘ

Aug 15, 2023 – 08:03 pm BST

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

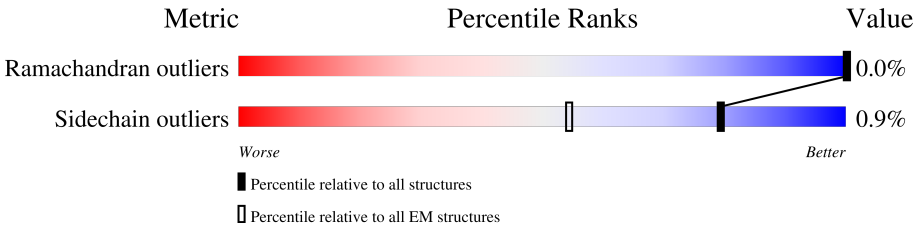
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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.



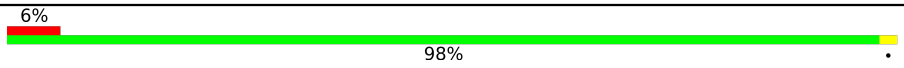
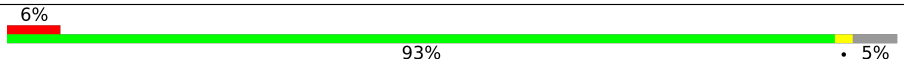
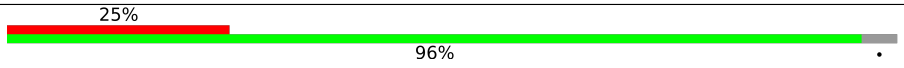
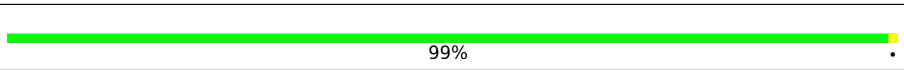
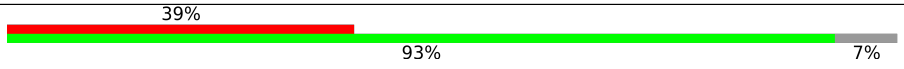
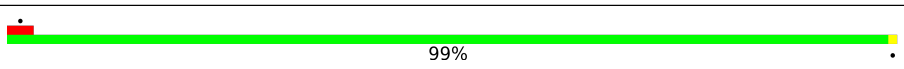
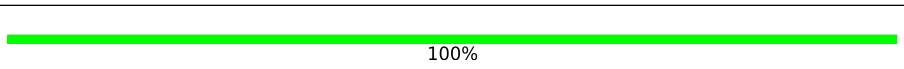
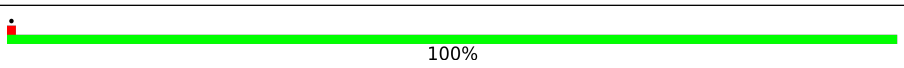
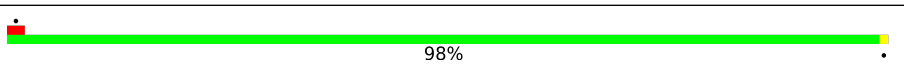
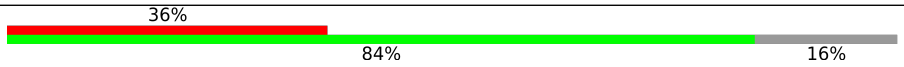
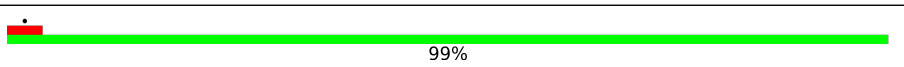
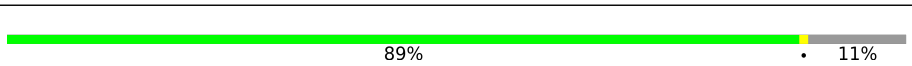
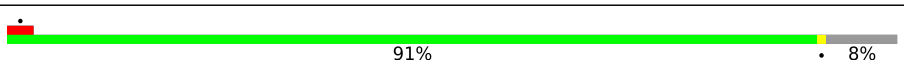
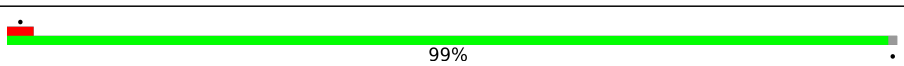
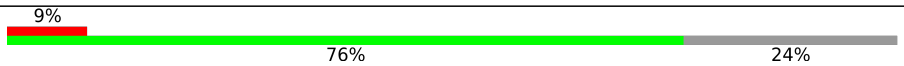
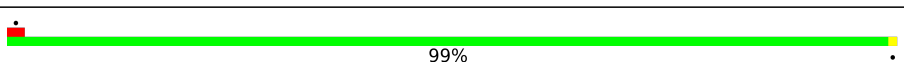
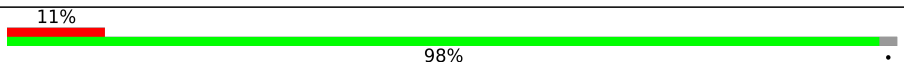
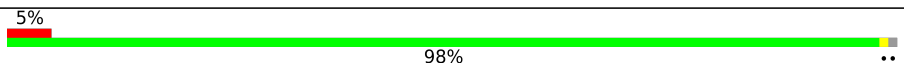
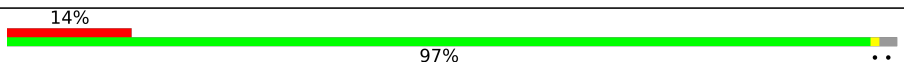
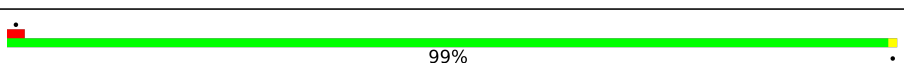
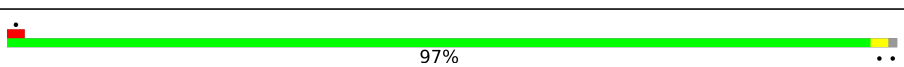
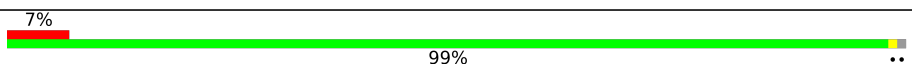
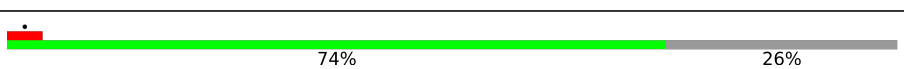
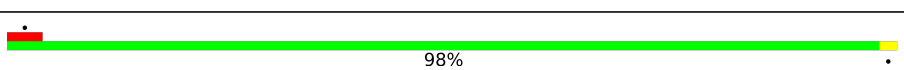
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%

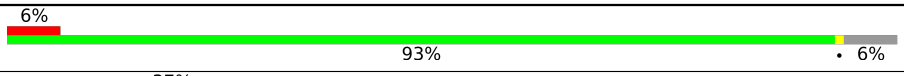
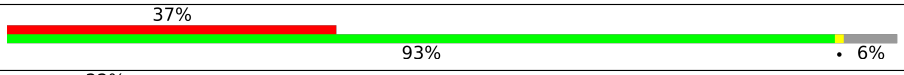
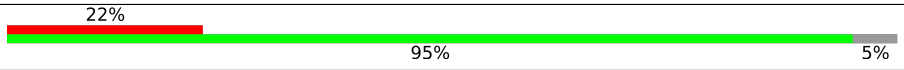
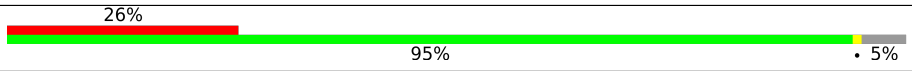
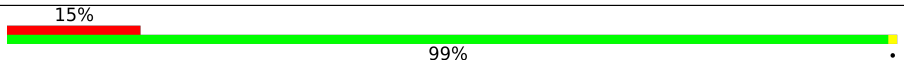
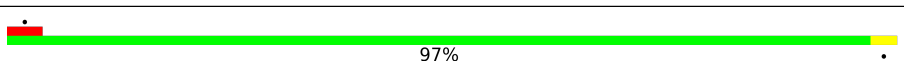
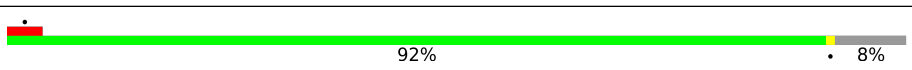
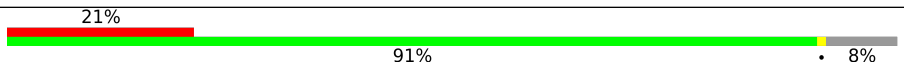
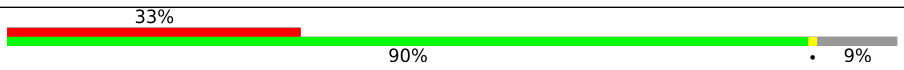
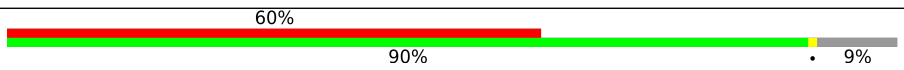
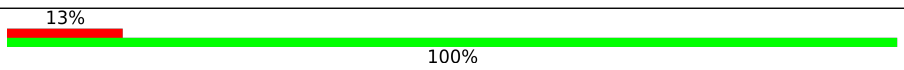
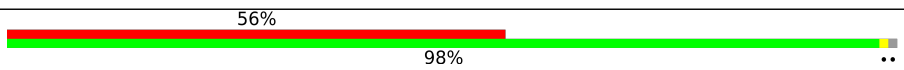
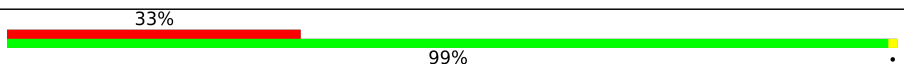
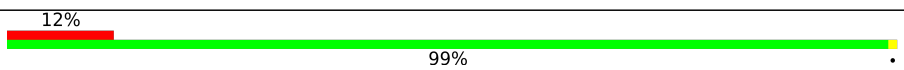
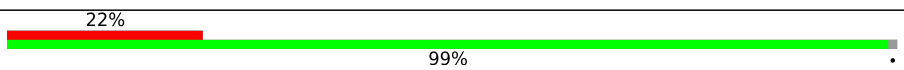
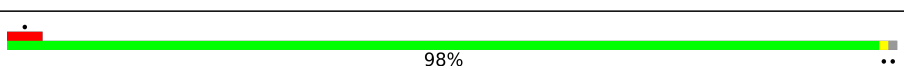
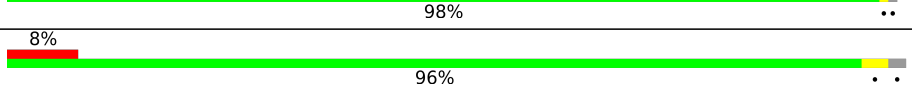
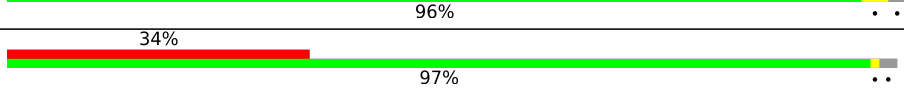
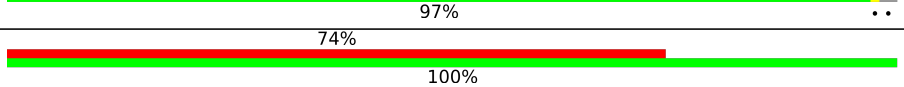
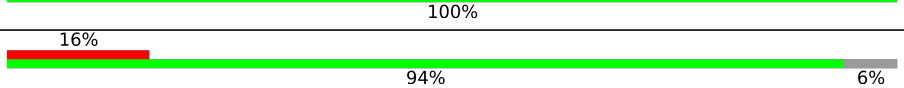
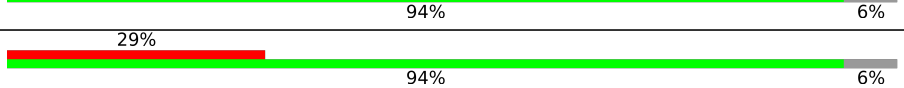
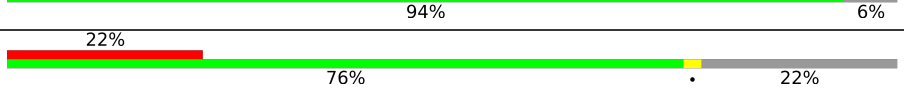
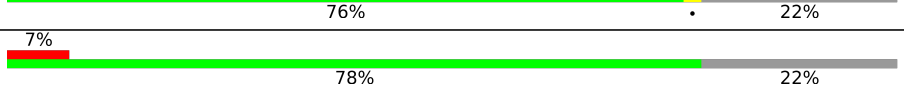
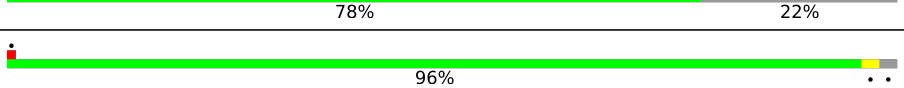
Continued on next page...

Continued from previous page...

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%

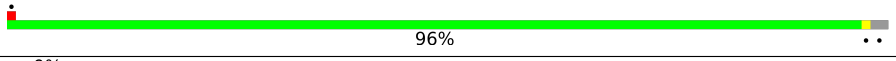
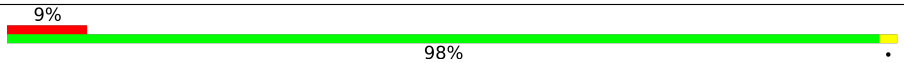
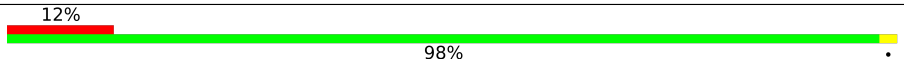
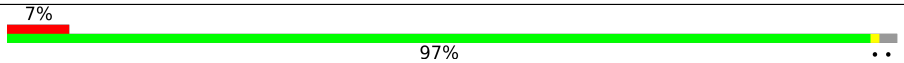
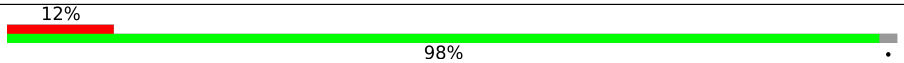
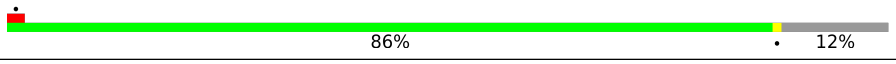
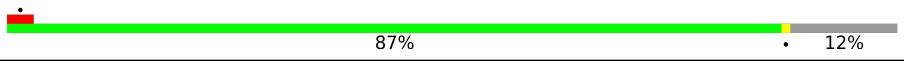
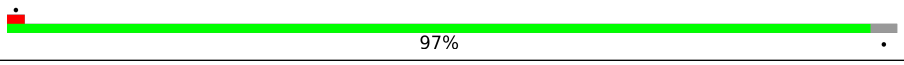
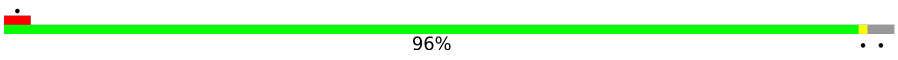
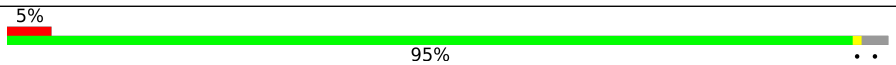
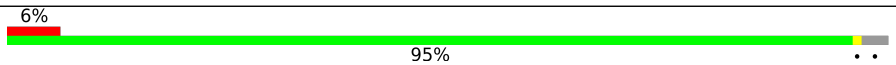
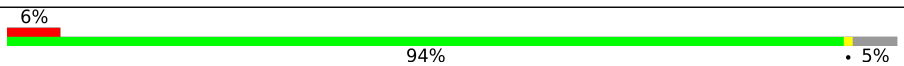
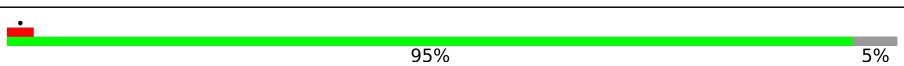
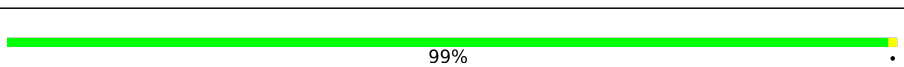
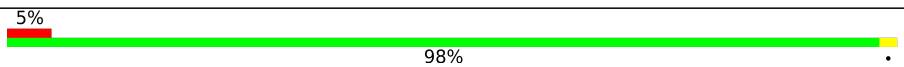
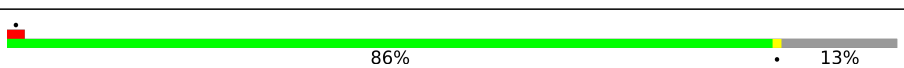
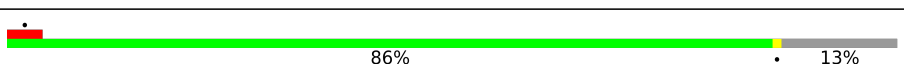
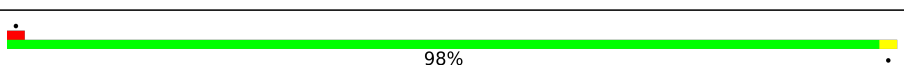
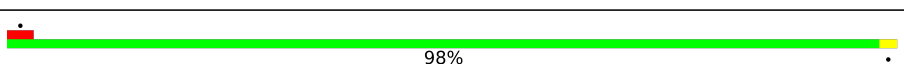
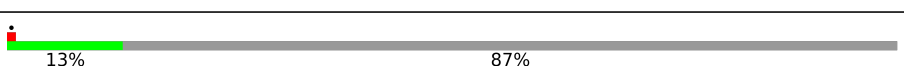
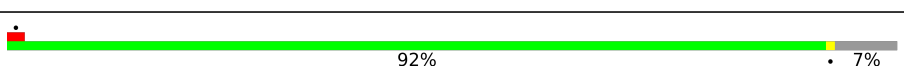
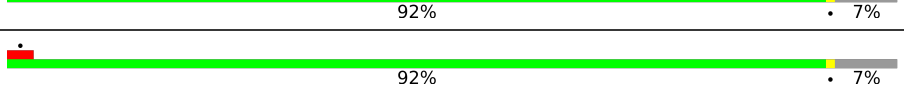
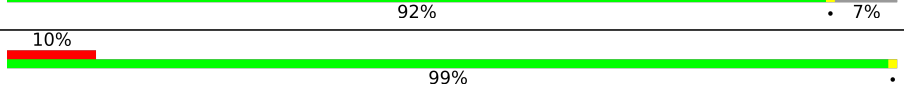
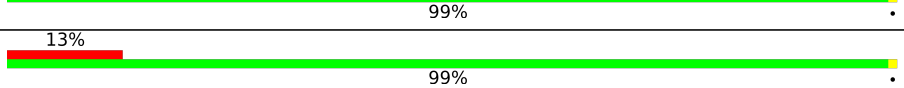
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
85	A	513	
85	a	513	
86	B	482	
86	b	482	
87	C	426	
87	c	426	
88	D	319	
88	d	319	
89	E	269	
89	e	269	
90	F	86	
90	f	86	
91	G	328	
91	g	328	
92	H	130	
92	h	130	
93	I	119	
93	i	119	
94	J	66	
94	j	66	
95	K	62	
95	k	62	
96	L	41	
96	l	41	
97	DA	688	

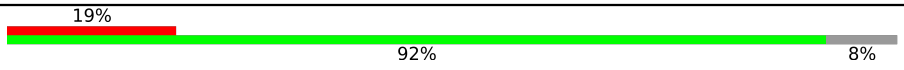
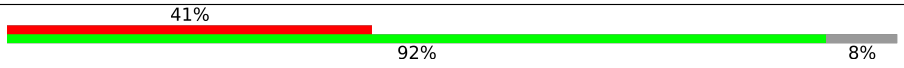
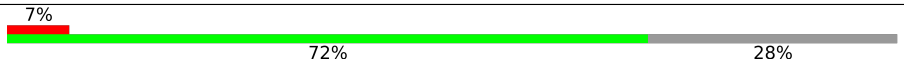
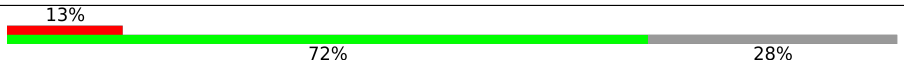
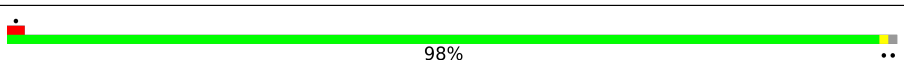
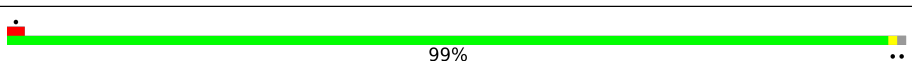
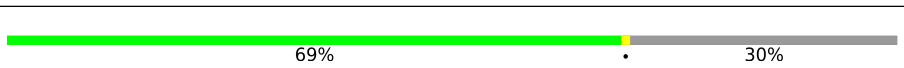
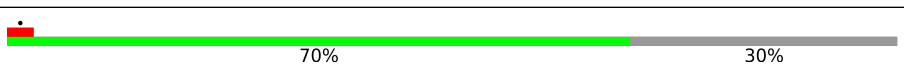
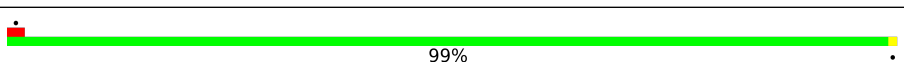
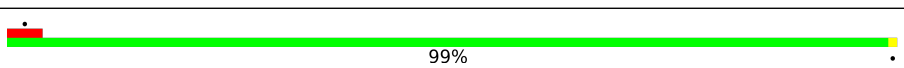
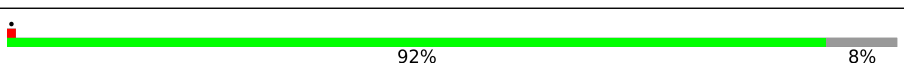
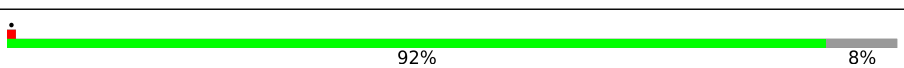
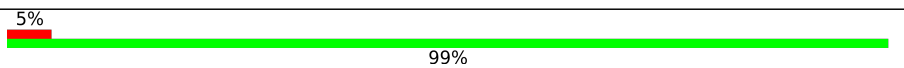
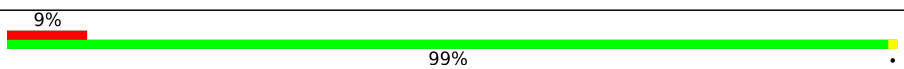
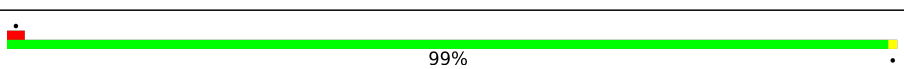
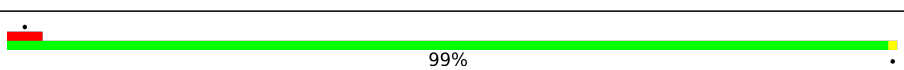
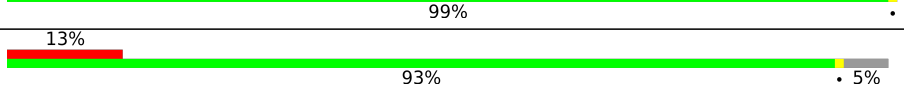
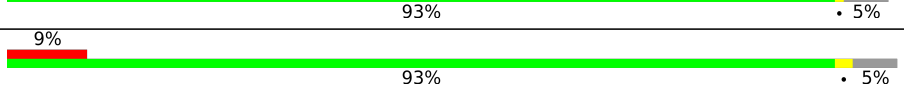
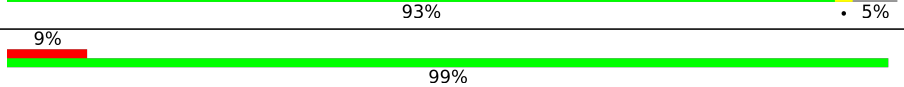
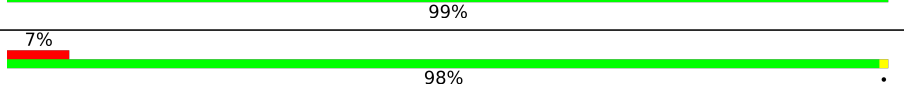
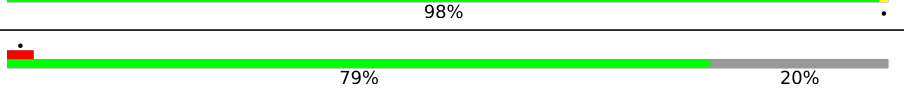
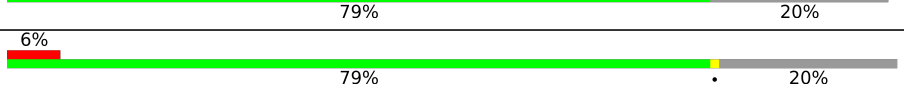
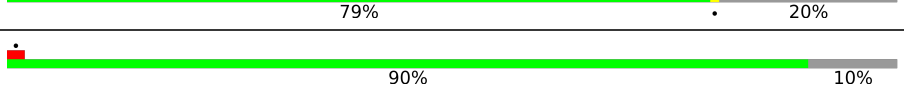
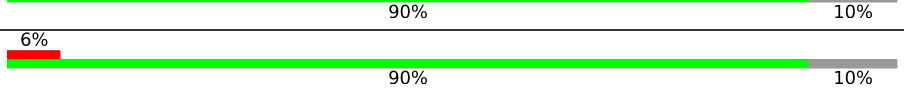
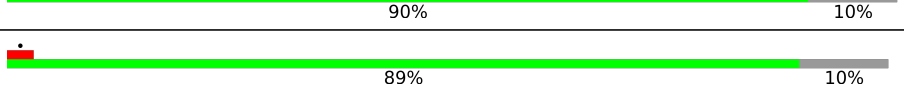
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
97	Da	688	
98	DB	604	
98	Db	604	
99	DC	594	
99	Dc	594	
100	DD	637	
100	Dd	637	
101	DE	130	
101	De	130	
102	DF	230	
102	Df	230	
103	DG	103	
103	Dg	103	
104	DH	133	
104	Dh	133	
105	DI	236	
105	Di	236	
106	DJ	220	
106	Dj	220	
107	DK	990	
107	Dk	990	
108	DM	490	
108	Dm	490	
109	DN	453	
109	Dn	453	

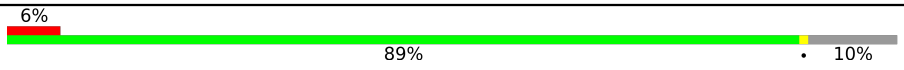
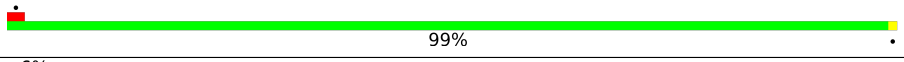
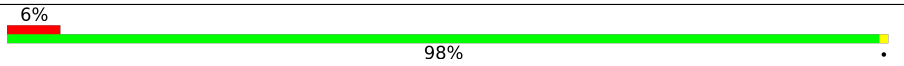
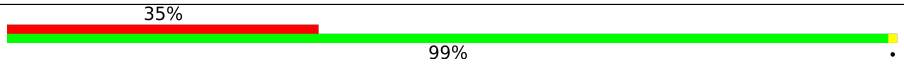
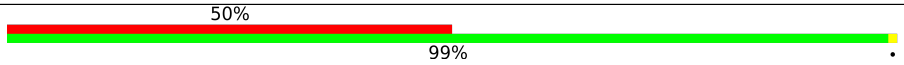
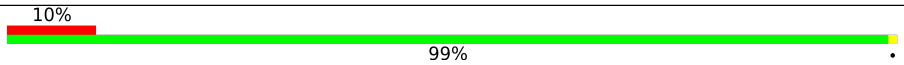
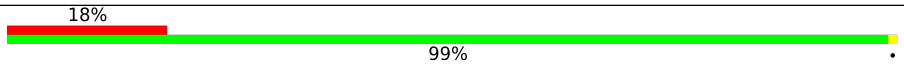
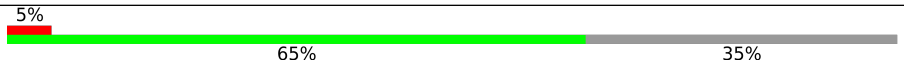
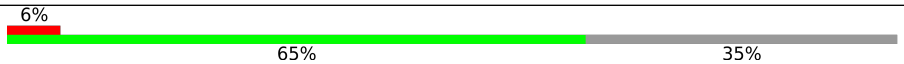
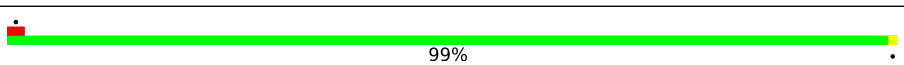
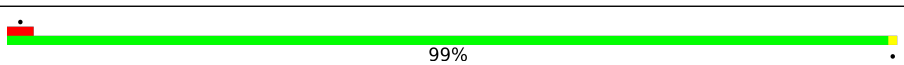
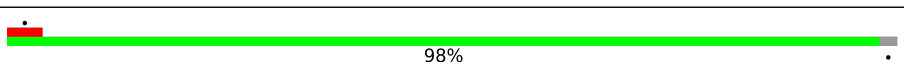
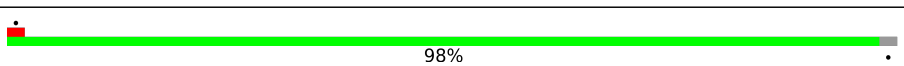
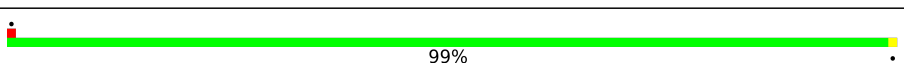
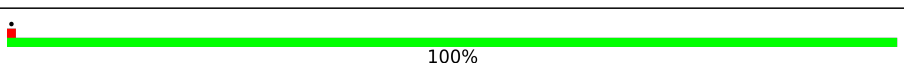
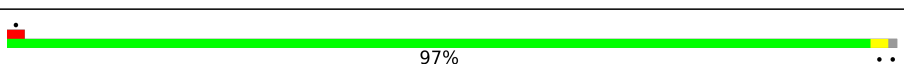
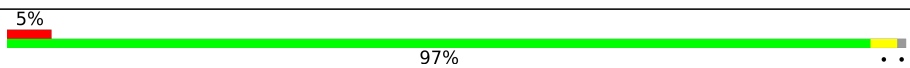
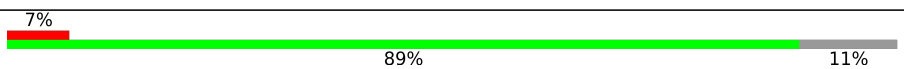
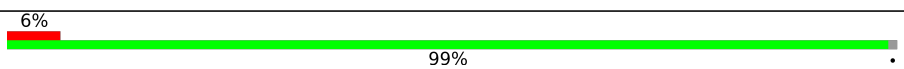
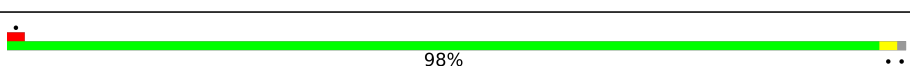
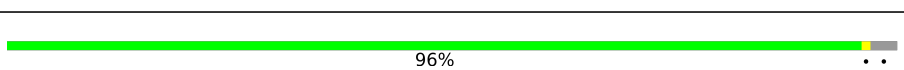
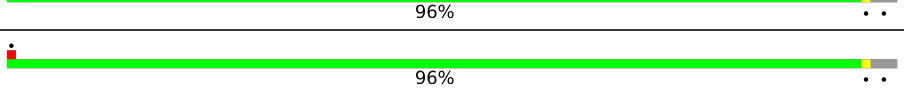
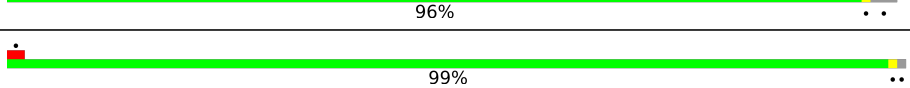
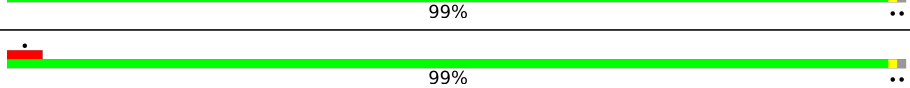
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
110	DO	473	
110	Do	473	
111	DP	402	
111	Dp	402	
112	DQ	385	
112	Dq	385	
113	DR	348	
113	Dr	348	
114	DS	346	
114	Ds	346	
115	DT	318	
115	Dt	318	
116	DU	330	
116	Du	330	
117	DV	318	
117	Dv	318	
118	DW	318	
118	Dw	318	
119	DX	252	
119	Dx	252	
120	DY	234	
120	Dy	234	
121	DZ	231	
121	Dz	231	
122	EA	215	

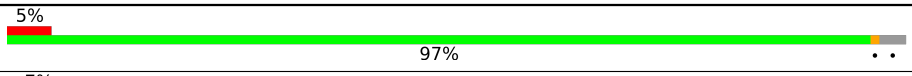
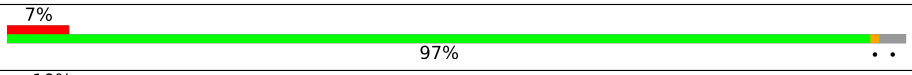
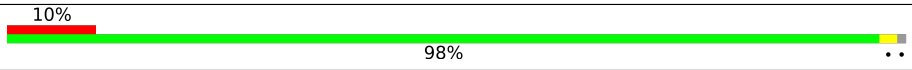
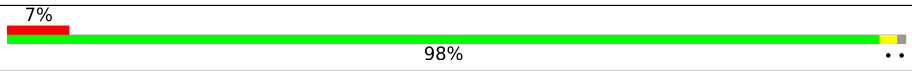
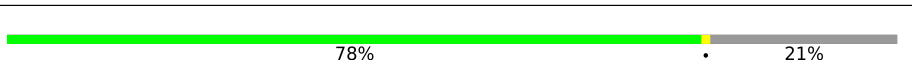
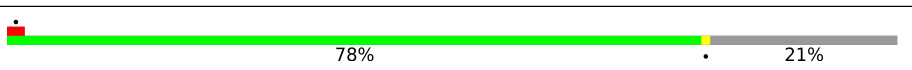
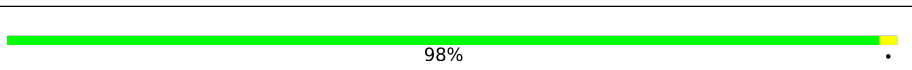
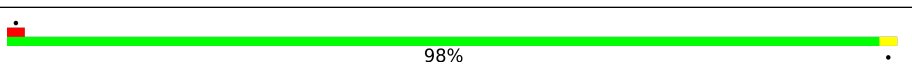
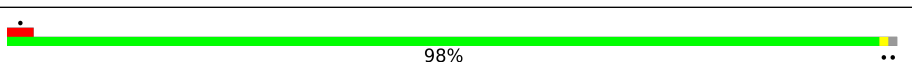
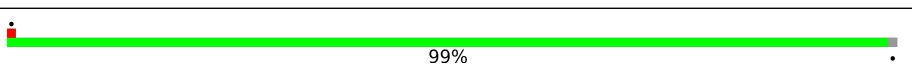
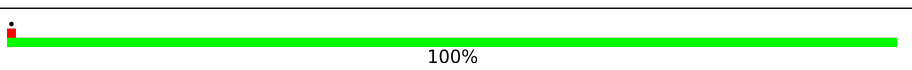
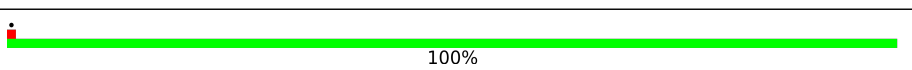
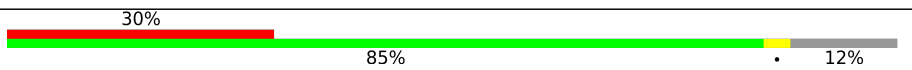
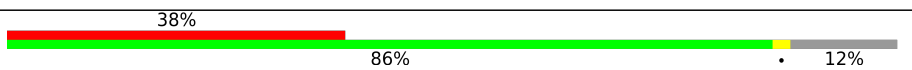
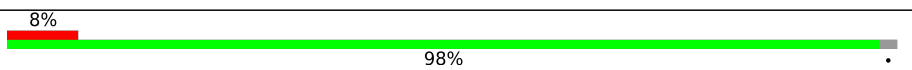
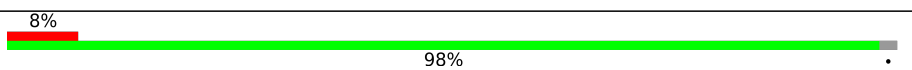
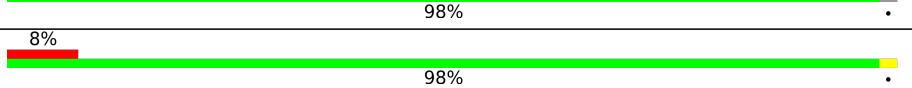
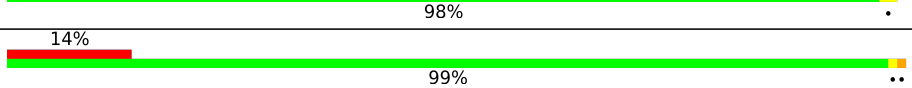
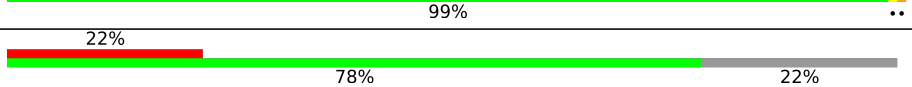
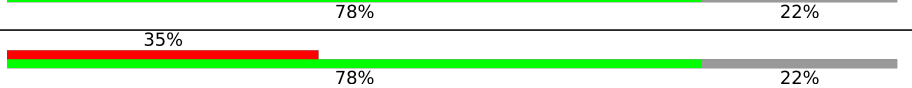
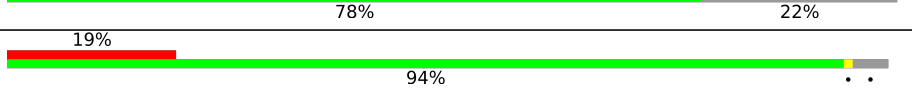
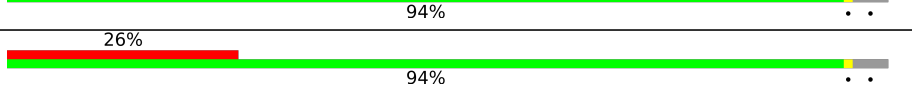
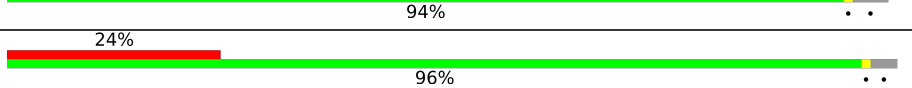
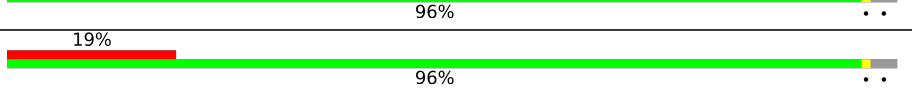
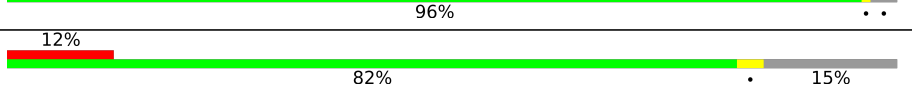
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
122	Ea	215	
123	EB	210	
123	Eb	210	
124	EC	212	
124	Ec	212	
125	ED	190	
125	Ed	190	
126	EE	193	
126	Ee	193	
127	EF	188	
127	Ef	188	
128	EG	100	
128	Eg	100	
129	EH	173	
129	Eh	173	
130	EI	173	
130	Ei	173	
131	EV	88	
131	Ev	88	
132	EK	170	
132	Ek	170	
133	EL	158	
133	El	158	
134	EM	154	
134	Em	154	

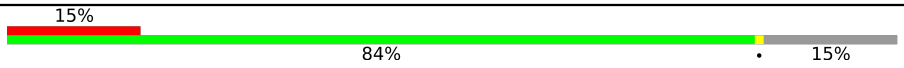
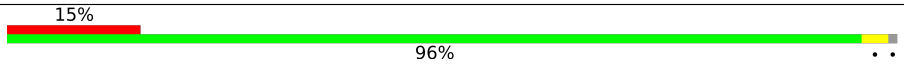
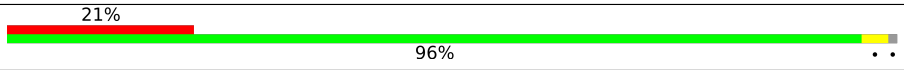
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
135	EN	149	
135	En	149	
136	EO	124	
136	Eo	124	
137	EP	127	
137	Ep	127	
138	EQ	122	
138	Eq	122	
139	ER	105	
139	Er	105	
140	ES	89	
140	Es	89	
141	ET	93	
141	Et	93	
142	EU	90	
142	Eu	90	
143	EJ	175	
143	Ej	175	
144	EW	81	
144	Ew	81	
145	EX	72	
145	Ex	72	
146	EY	72	
146	Ey	72	
147	EZ	68	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
147	Ez	68	
148	FA	72	
148	Fa	72	
149	DL	462	
149	Dl	462	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
169	HEA	DA	702	X	-	-	-
169	HEA	DA	703	X	-	-	-
169	HEA	Da	702	X	-	-	-
169	HEA	Da	703	X	-	-	-

2 Entry composition

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
7	A6	230	Total	C	H	N	O	S	0	0
			3770	1241	1862	322	340	5		

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

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

- Molecule 9 is a protein called ND5a.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called Ymf65.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 20 is a protein called Ymf62.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is a protein called Acyl carrier protein.

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

- Molecule 33 is a protein called Acyl carrier protein.

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

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

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

- Molecule 35 is a protein called Ymf58.

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

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

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

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

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

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

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

- Molecule 39 is a protein called GRAM domain protein.

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

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

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

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

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

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

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

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

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

- Molecule 44 is a protein called Transmembrane protein.

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

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

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

- Molecule 46 is a protein called NDUB8.

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

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

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

- Molecule 48 is a protein called NDUPH2.

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

- Molecule 49 is a protein called NDUB10.

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

- Molecule 50 is a protein called NDUA13.

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

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

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

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

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

- Molecule 53 is a protein called Thioredoxin.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 59 is a protein called NDUB6.

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

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

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

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

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

- Molecule 62 is a protein called NDUB4.

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

- Molecule 63 is a protein called NDUTT10.

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

- Molecule 64 is a protein called NDUTT11.

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

- Molecule 65 is a protein called NDUTT12.

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

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

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

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

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

- Molecule 68 is a protein called Ymf57.

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

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

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

- Molecule 70 is a protein called Diphthamide synthesis protein.

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

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

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

- Molecule 72 is a protein called Transposase.

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

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

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

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

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

- Molecule 75 is a protein called succinate dehydrogenase.

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

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

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

- Molecule 77 is a protein called Uncharacterized protein.

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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called Transmembrane protein.

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

- Molecule 83 is a protein called SDHTT11.

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

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

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

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

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

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

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

- Molecule 87 is a protein called Apocytochrome b.

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

- Molecule 88 is a protein called Cytochrome protein c1.

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

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

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

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

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

- Molecule 91 is a protein called UQCRTT1.

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

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

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

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

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

- Molecule 94 is a protein called UQCRTT3.

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 96 is a protein called UQCRTT2.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 98 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 99 is a protein called Ymf68.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	520	PSE	SER	modified residue	UNP Q23FF5
Dd	520	PSE	SER	modified residue	UNP Q23FF5

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

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

- Molecule 102 is a protein called Structural protein.

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

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

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

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

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

- Molecule 105 is a protein called Transmembrane protein.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	120	PSE	SER	modified residue	UNP W7X287
Di	120	PSE	SER	modified residue	UNP W7X287

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 109 is a protein called Ymf67.

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

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

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

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

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

- Molecule 112 is a protein called TraB family protein.

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

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

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

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

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

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

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

- Molecule 116 is a protein called Carrier protein.

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

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

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

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

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

- Molecule 119 is a protein called COXTT9.

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

- Molecule 120 is a protein called COXTT10.

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

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

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

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

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

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

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

- Molecule 124 is a protein called COXTT27.

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

Continued on next page...

Continued from previous page...

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

- Molecule 125 is a protein called Ymf75.

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

- Molecule 126 is a protein called Mobilization protein.

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

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

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

- Molecule 128 is a protein called COXTT28.

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

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

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

- Molecule 130 is a protein called Transmembrane protein.

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

- Molecule 131 is a protein called Decapping nuclease.

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

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

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

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

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

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

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

- Molecule 135 is a protein called COXTT22.

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

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

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

- Molecule 137 is a protein called Phage protein.

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

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

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

- Molecule 139 is a protein called Lysozyme.

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

- Molecule 140 is a protein called Ymf70.

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 142 is a protein called ABC transporter.

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

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

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

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

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

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

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

- Molecule 146 is a protein called Annexin.

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

- Molecule 147 is a protein called Transposase.

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

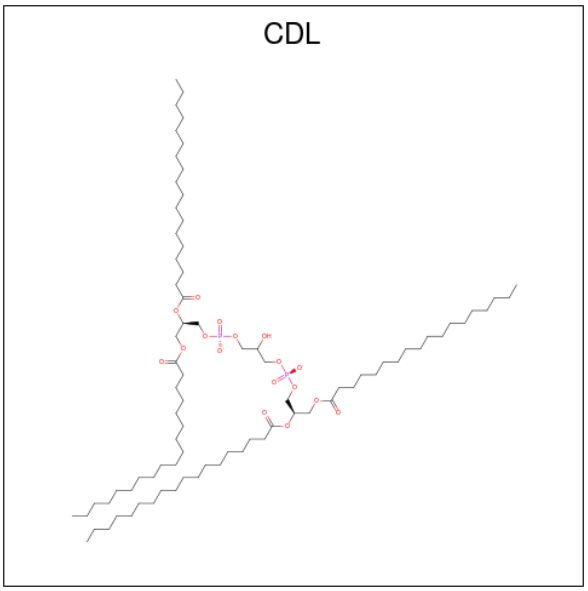
- Molecule 148 is a protein called Tim10/DDP family zinc finger protein.

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

- Molecule 149 is a protein called 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
149	Dl	380	Total	C	H	N	O	S	0	0
			5730	1856	2814	492	566	2		
149	DL	380	Total	C	H	N	O	S	0	0
			5730	1856	2814	492	566	2		

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

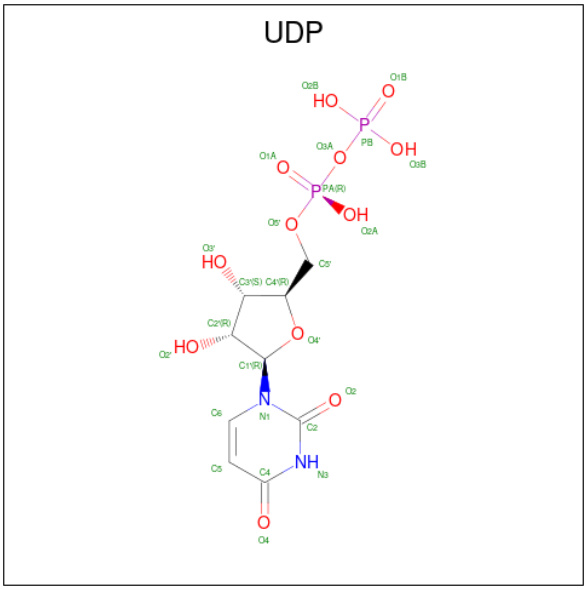
Mol	Chain	Residues	Atoms					AltConf
150	Du	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dv	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dv	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dv	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dx	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dx	1	Total	C	H	O	P	0
			256	81	156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

Continued on next page...

Continued from previous page...

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

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

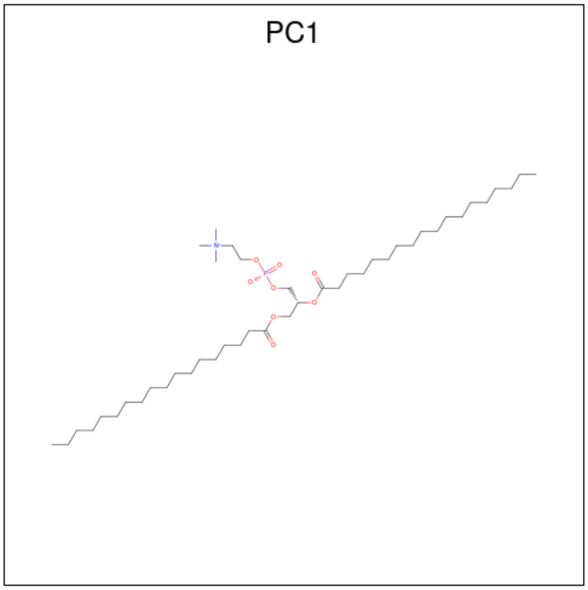


Mol	Chain	Residues	Atoms						AltConf
151	A0	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

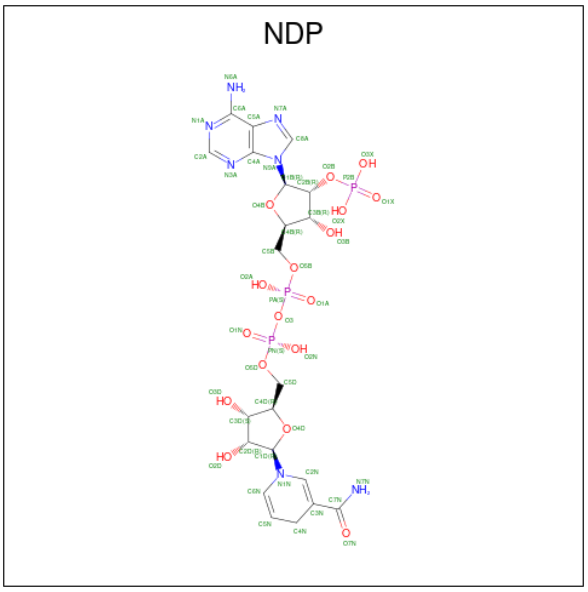
Mol	Chain	Residues	Atoms						AltConf
153	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
153	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
153	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
153	DX	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
153	DX	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
153	DY	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
153	EB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

Continued on next page...

Continued from previous page...

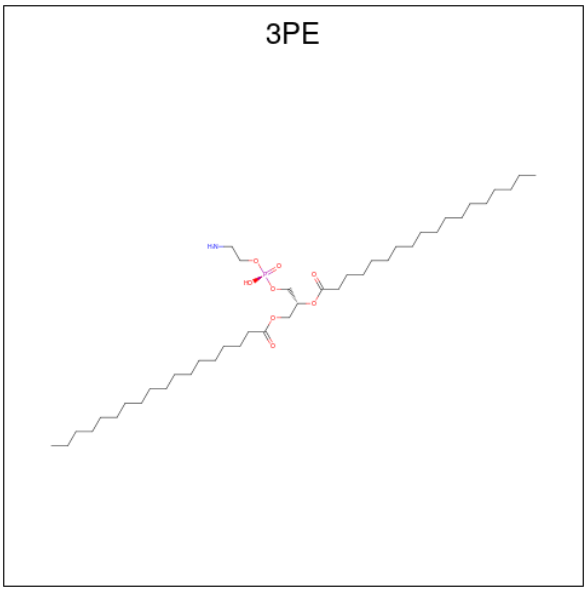
Mol	Chain	Residues	Atoms						AltConf
153	Dg	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Di	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Dj	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Dq	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Ds	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Dv	1	Total	C	H	N	O	P	0
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

- 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
154	A1	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

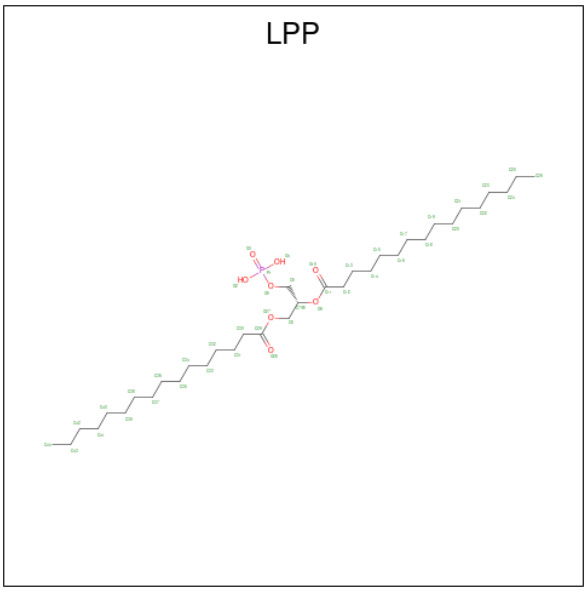
Mol	Chain	Residues	Atoms						AltConf
155	EL	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	EM	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	EN	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	EO	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	Da	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	Dc	1	Total	C	H	N	O	P	0
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

Continued on next page...

Continued from previous page...

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

- 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).



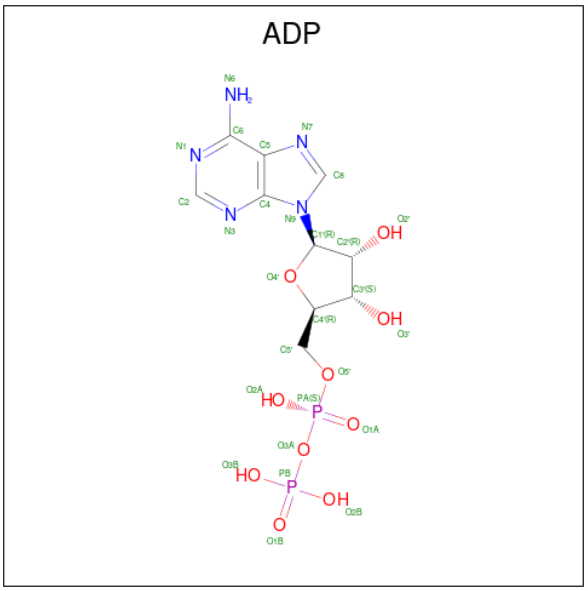
Mol	Chain	Residues	Atoms					AltConf
156	A6	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	AA	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	AC	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	AL	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	DA	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	DN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

Continued on next page...

Continued from previous page...

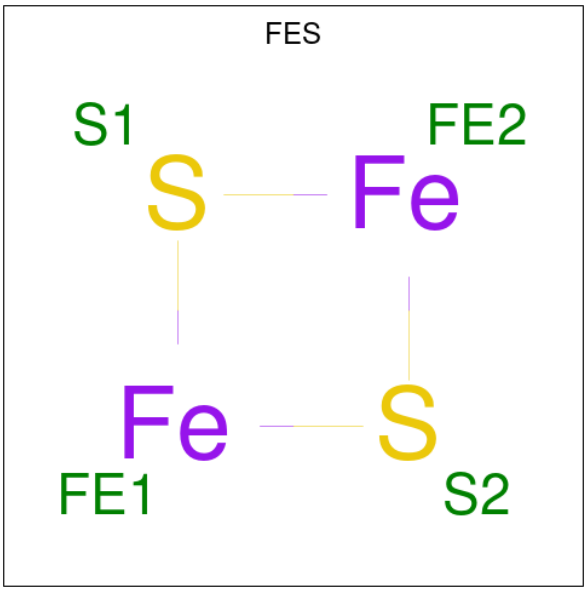
Mol	Chain	Residues	Atoms					AltConf
156	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	Ed	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	Dl	1	Total	C	H	O	P	0
			111	35	67	8	1	

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



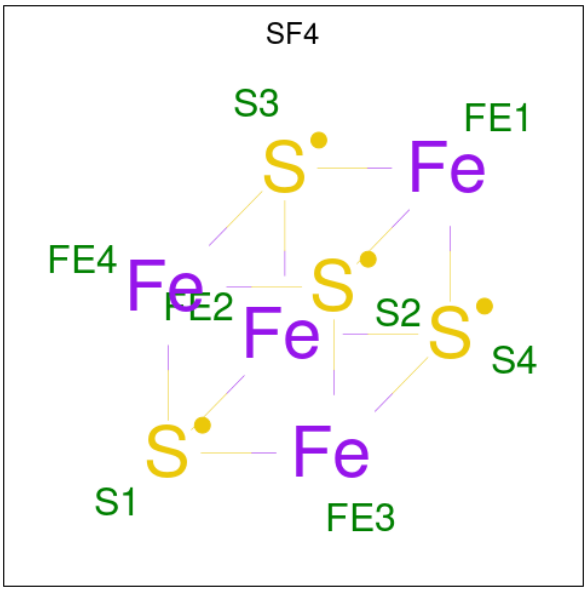
Mol	Chain	Residues	Atoms						AltConf
157	A8	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
157	AQ	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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



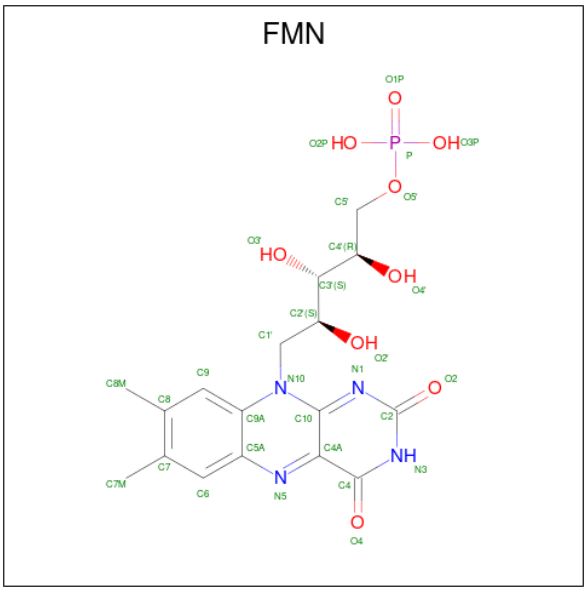
Mol	Chain	Residues	Atoms			AltConf
158	AB	1	Total	Fe	S	0
			4	2	2	
158	AI	1	Total	Fe	S	0
			4	2	2	
158	BI	1	Total	Fe	S	0
			4	2	2	
158	CB	1	Total	Fe	S	0
			4	2	2	
158	E	1	Total	Fe	S	0
			4	2	2	
158	e	1	Total	Fe	S	0
			4	2	2	
158	EF	1	Total	Fe	S	0
			4	2	2	
158	EF	1	Total	Fe	S	0
			4	2	2	
158	Ef	1	Total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

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



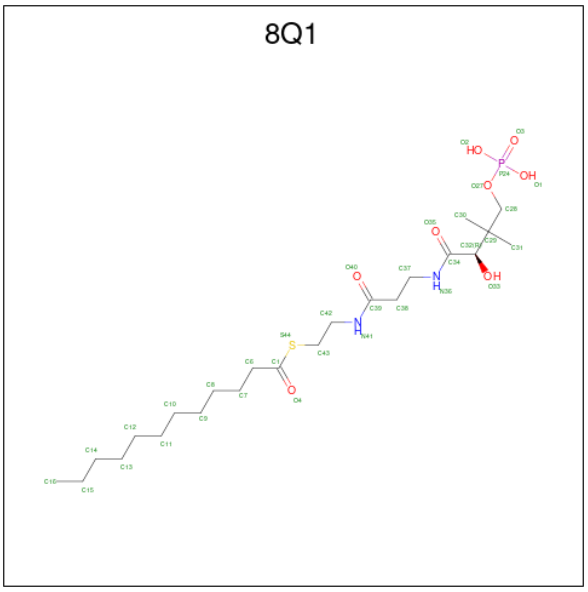
Mol	Chain	Residues	Atoms	AltConf
159	AB	1	Total Fe S 8 4 4	0
159	AB	1	Total Fe S 8 4 4	0
159	AD	1	Total Fe S 8 4 4	0
159	AL	1	Total Fe S 8 4 4	0
159	AL	1	Total Fe S 8 4 4	0
159	AT	1	Total Fe S 8 4 4	0
159	CB	1	Total Fe S 8 4 4	0

- 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
160	AD	1	Total	C	H	N	O	P	0
			49	17	18	4	9	1	

- 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
161	AS	1	Total	C	H	N	O	P	S	0
			77	23	43	2	7	1	1	

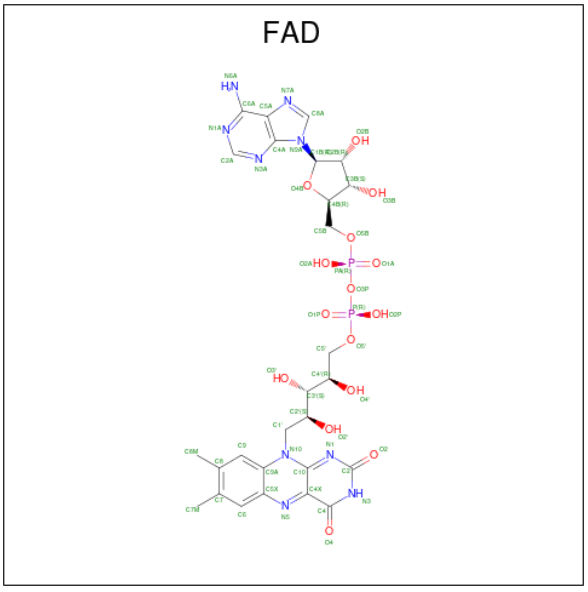
- Molecule 162 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

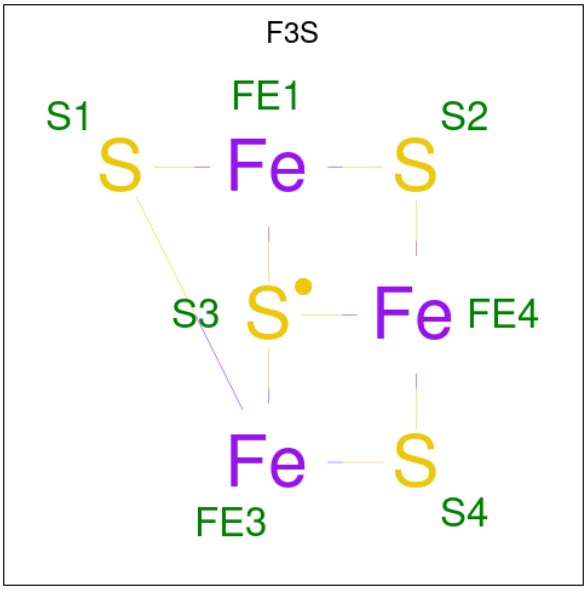
- Molecule 164 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

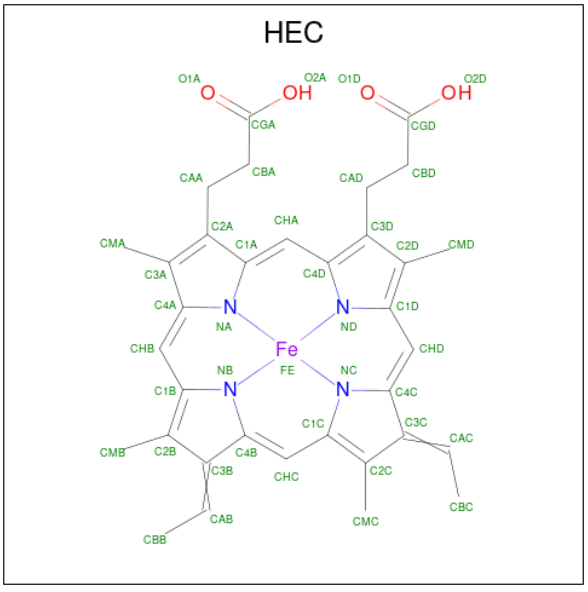
- Molecule 165 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4) (labeled as

"Ligand of Interest" by depositor).



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

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



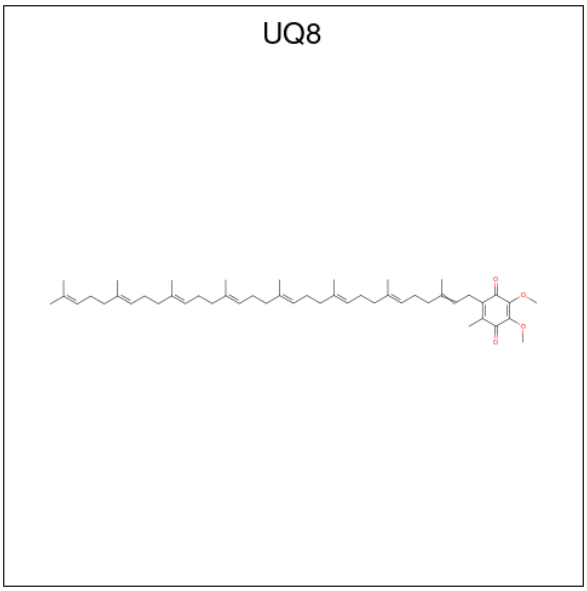
Mol	Chain	Residues	Atoms						AltConf
166	CE	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

Continued on next page...

Continued from previous page...

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

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



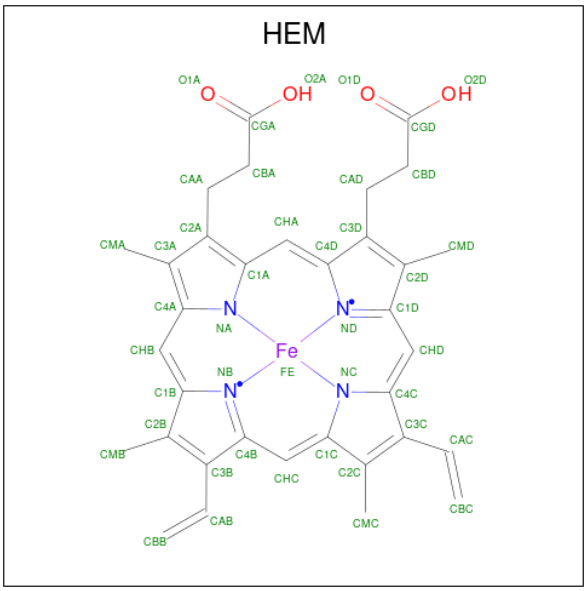
Mol	Chain	Residues	Atoms				AltConf
167	CC	1	Total	C	H	O	0
			127	49	74	4	
167	C	1	Total	C	O		0
			53	49	4		
167	C	1	Total	C	O		0
			53	49	4		
167	c	1	Total	C	O		0
			53	49	4		
167	DS	1	Total	C	H	O	0
			127	49	74	4	
167	ED	1	Total	C	H	O	0
			127	49	74	4	
167	EL	1	Total	C	H	O	0
			127	49	74	4	
167	EN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

Continued on next page...

Continued from previous page...

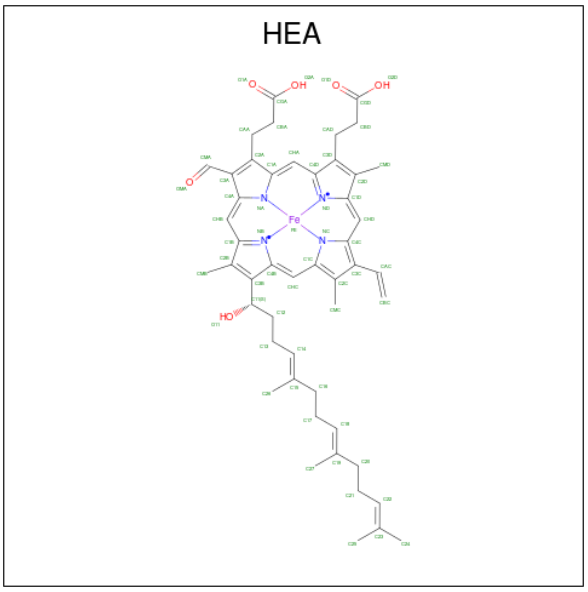
Mol	Chain	Residues	Atoms				AltConf
167	Ed	1	Total	C	H	O	0
			127	49	74	4	
167	El	1	Total	C	H	O	0
			127	49	74	4	
167	En	1	Total	C	H	O	0
			127	49	74	4	

- 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
168	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
168	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
168	c	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
168	c	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
168	ED	1	Total	C	Fe	H	N	O	0
			65	34	1	22	4	4	
168	Ed	1	Total	C	Fe	H	N	O	0
			67	34	1	24	4	4	

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

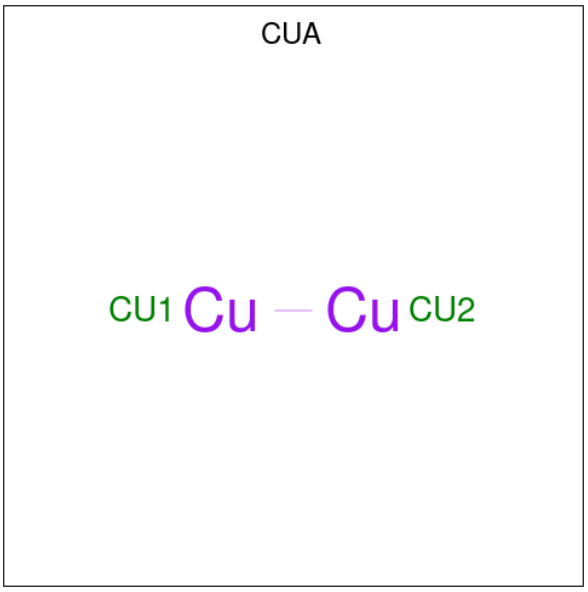


Mol	Chain	Residues	Atoms						AltConf
169	DA	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
169	DA	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
169	Da	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
169	Da	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

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

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

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

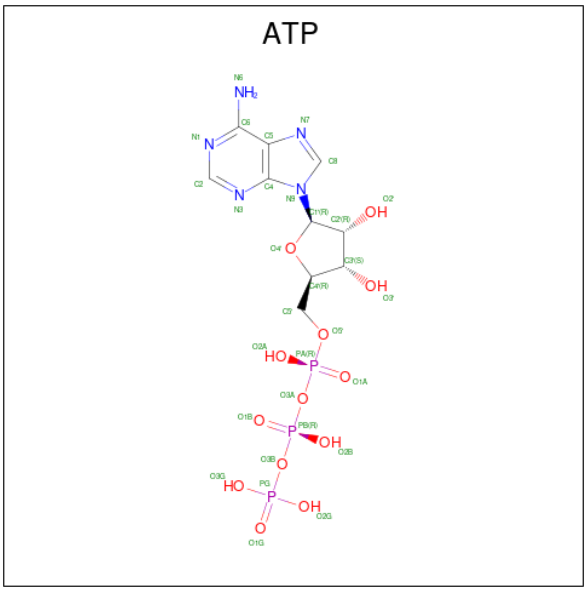


Mol	Chain	Residues	Atoms	AltConf
171	DB	1	Total Cu 2 2	0
171	Db	1	Total Cu 2 2	0

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

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

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



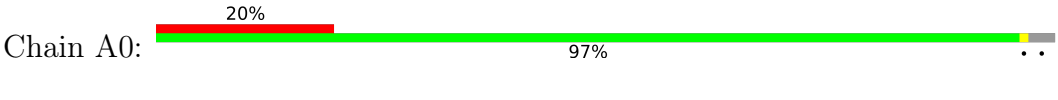
Mol	Chain	Residues	Atoms						AltConf
173	ER	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
173	Er	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

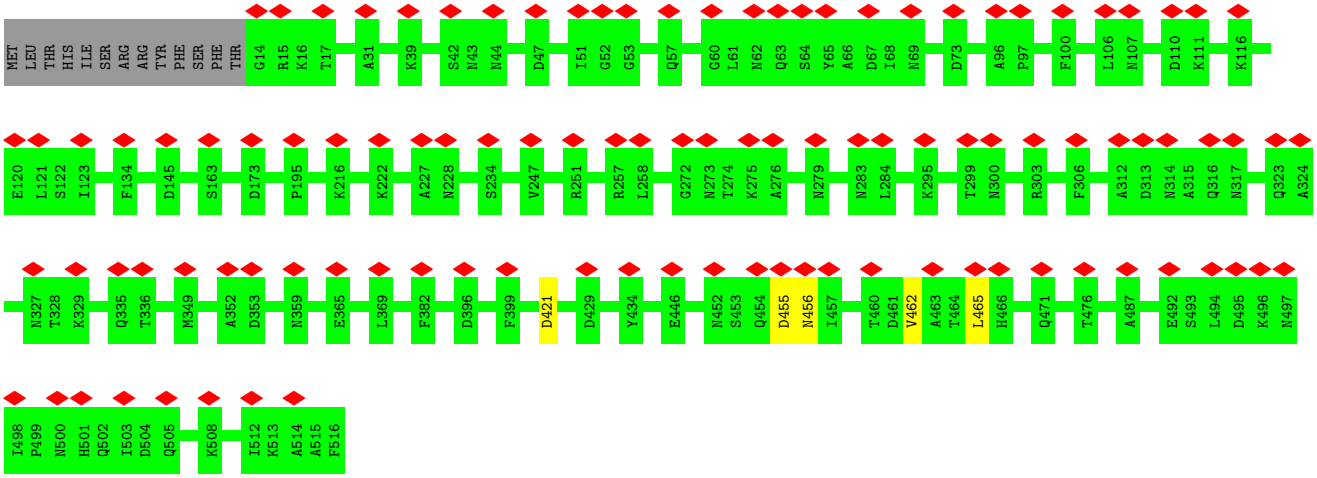
3 Residue-property plots (i)

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

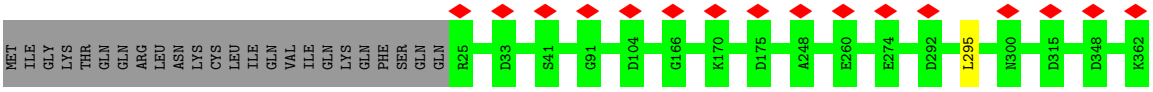
Chain A0:





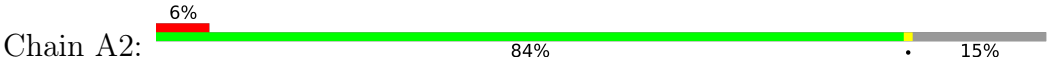
• Molecule 2: NAD-dependent epimerase/dehydratase family protein

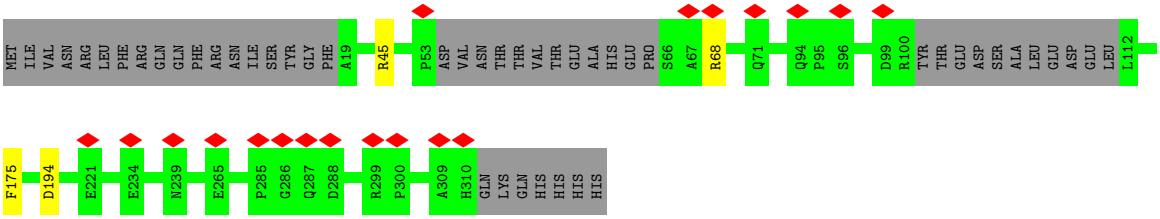
Chain A1:



• Molecule 3: DnaJ domain protein

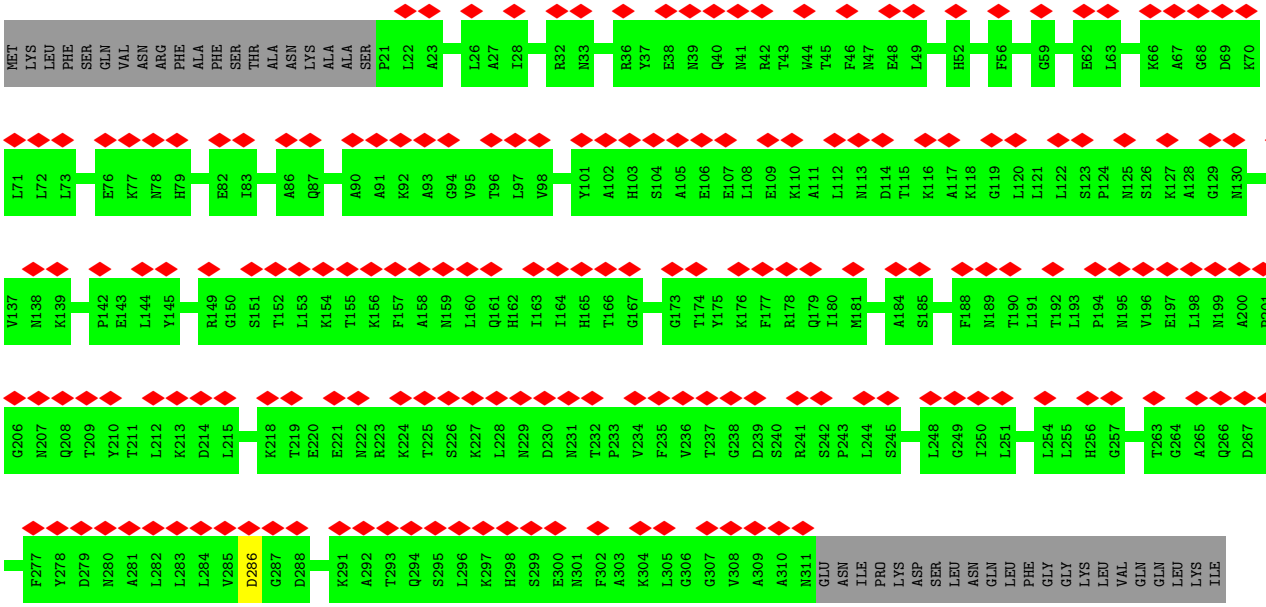
Chain A2:





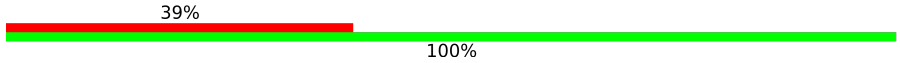
• Molecule 4: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

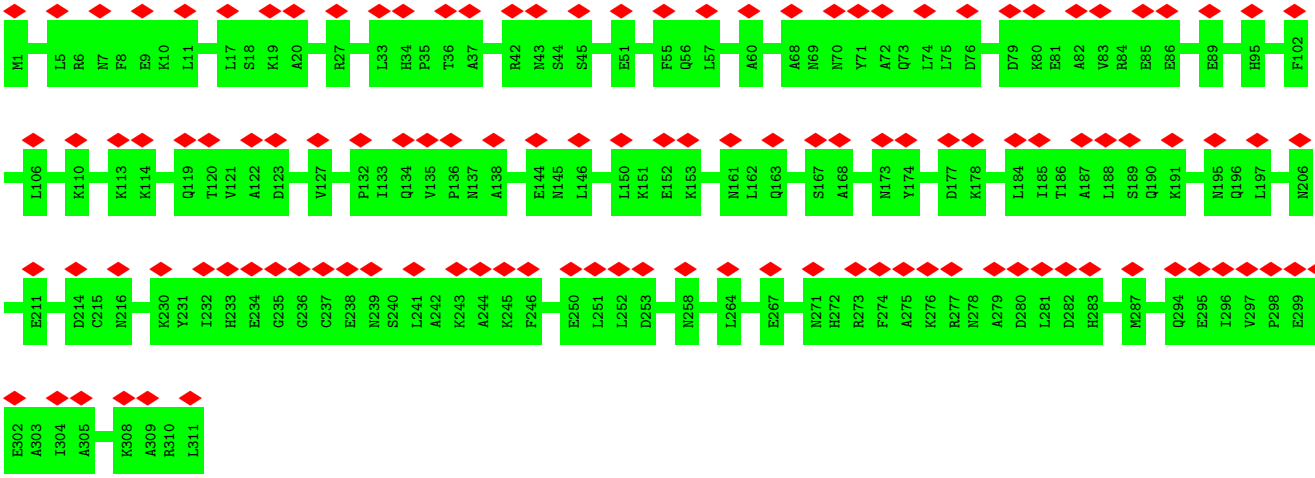
Chain A3:



• Molecule 5: RNase III domain-containing protein

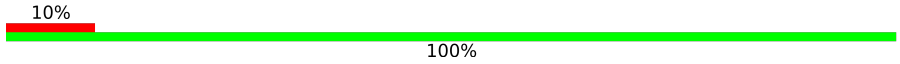
Chain A4:

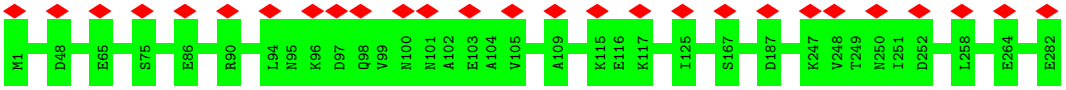




• Molecule 6: 37S ribosomal protein S25, mitochondrial

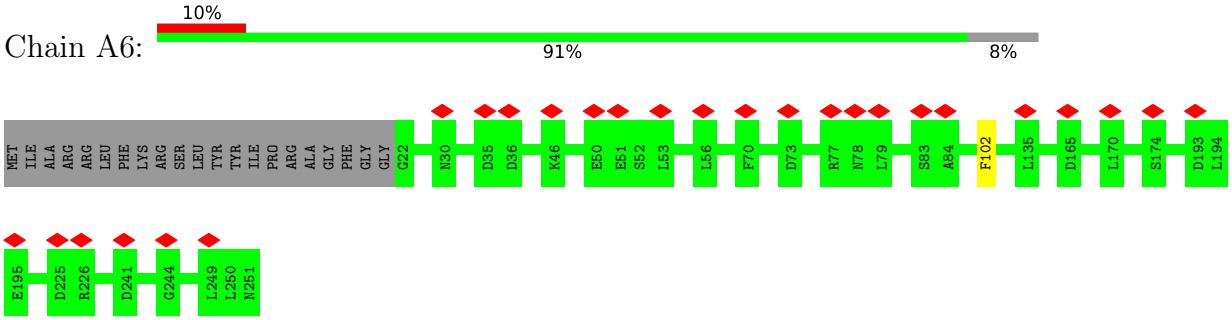
Chain A5:





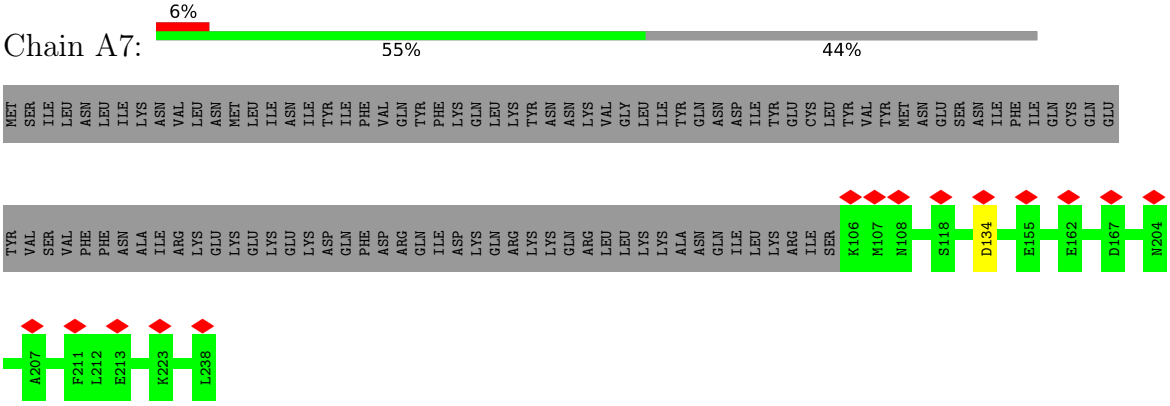
• Molecule 7: Transmembrane protein, putative

Chain A6:



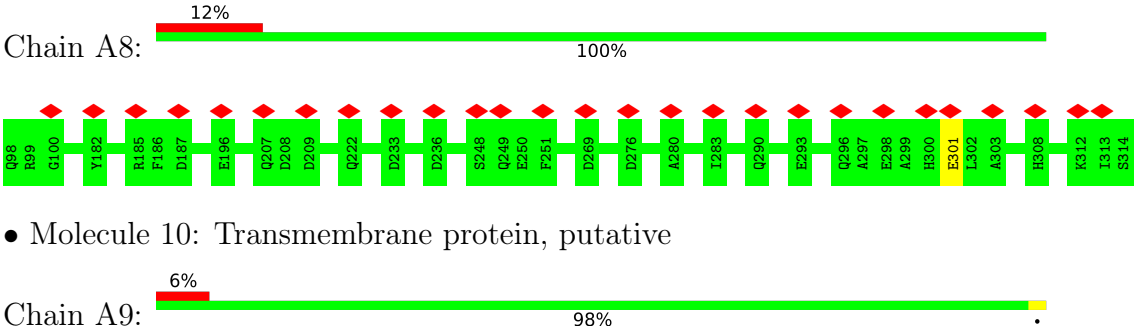
• Molecule 8: CX9C domain-containing protein

Chain A7:



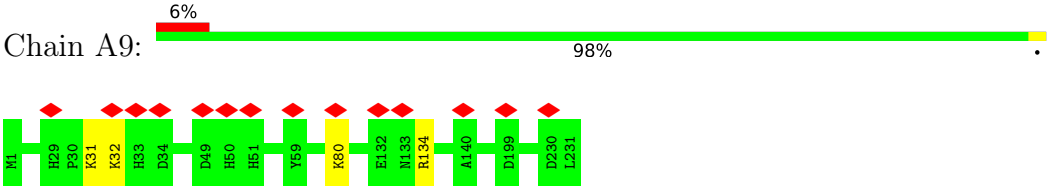
• Molecule 9: ND5a

Chain A8:



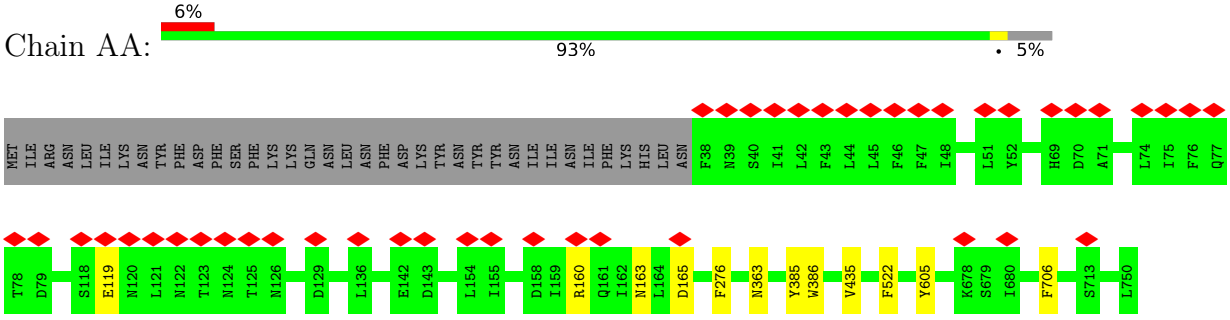
• Molecule 10: Transmembrane protein, putative

Chain A9:



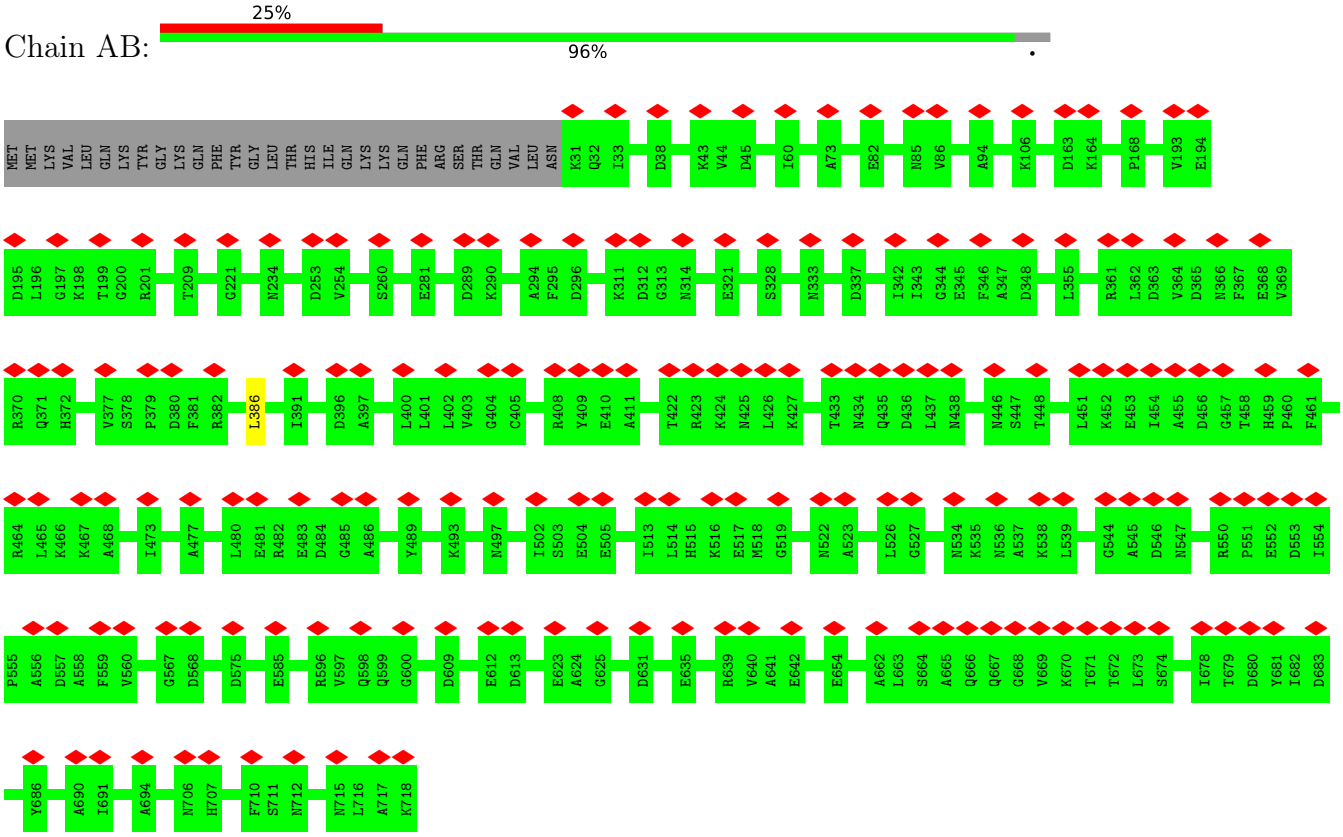
• Molecule 11: NADH dehydrogenase subunit 5

Chain AA:



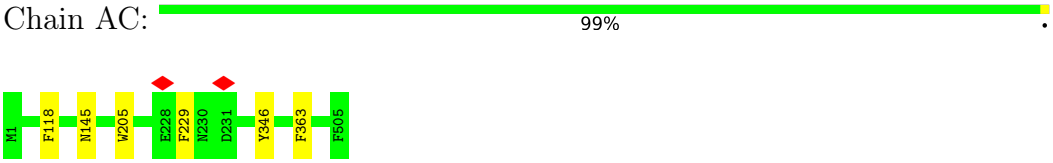
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain AB:



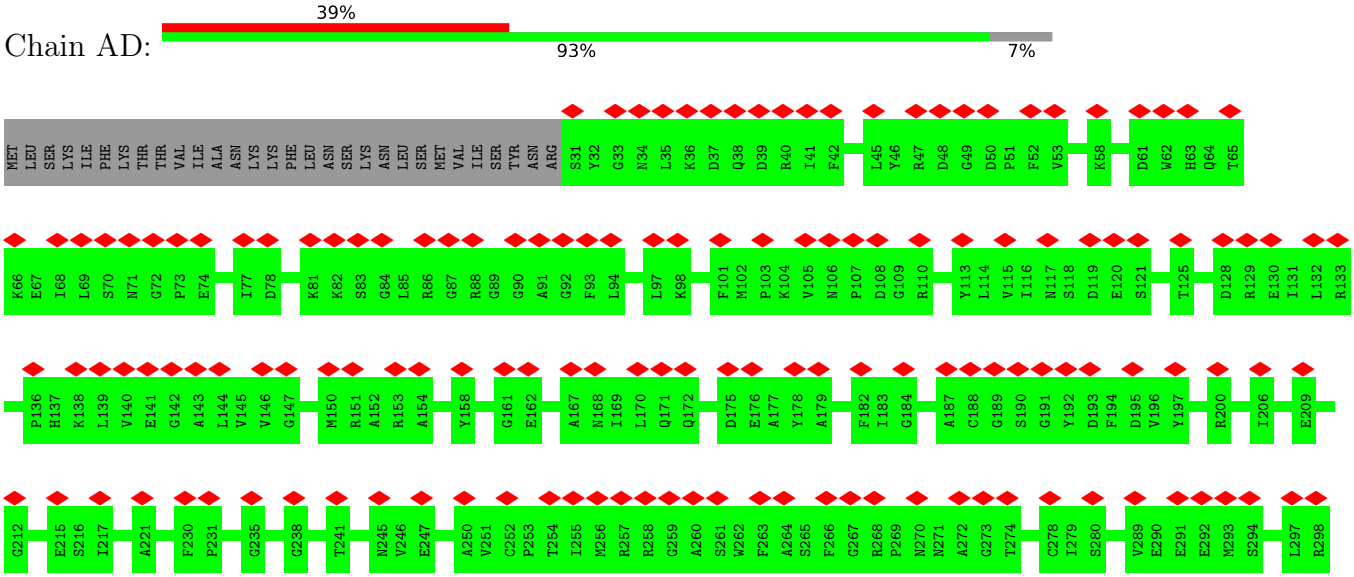
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

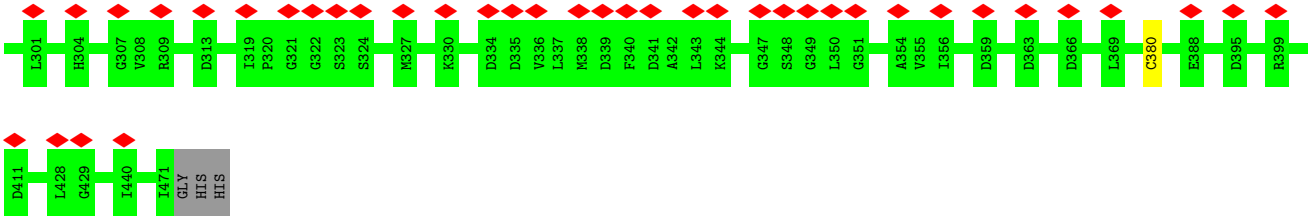
Chain AC:



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

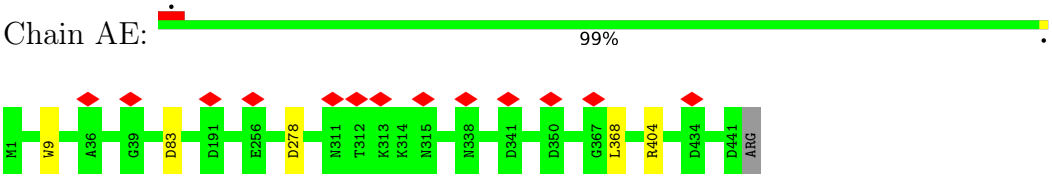
Chain AD:





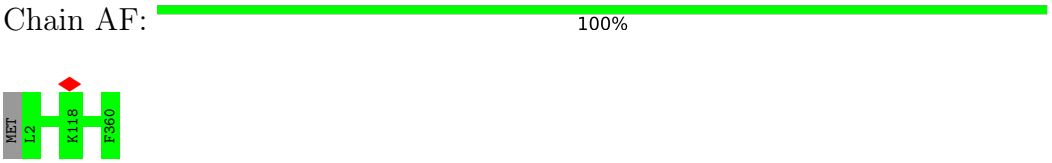
• Molecule 15: NADH dehydrogenase subunit 7

Chain AE:



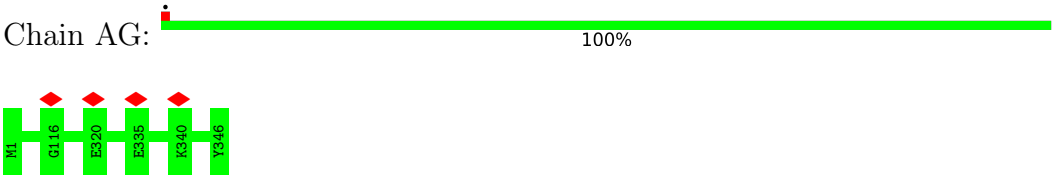
• Molecule 16: Ymf65

Chain AF:



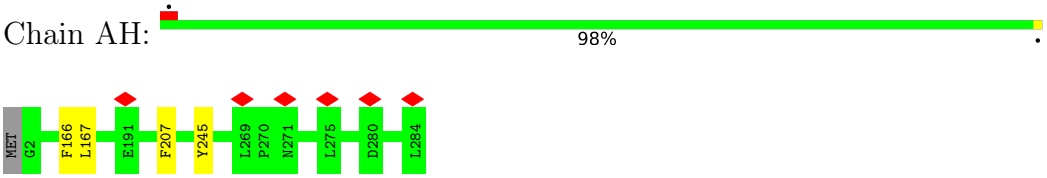
• Molecule 17: Transcription factor apfi protein, putative

Chain AG:



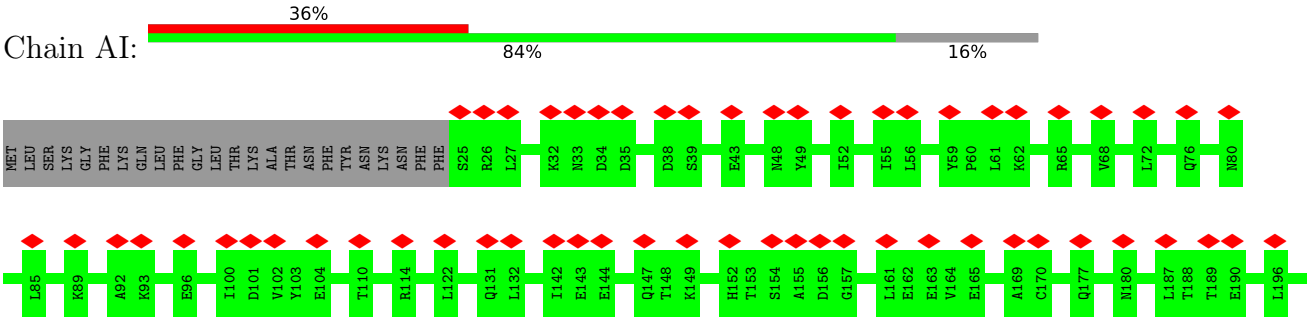
• Molecule 18: NADH-ubiquinone oxidoreductase chain 1

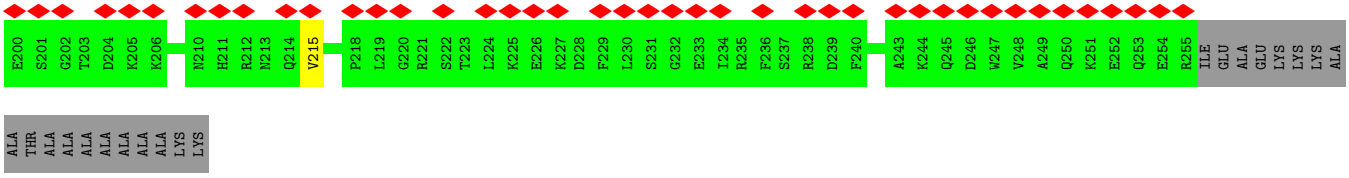
Chain AH:



• Molecule 19: NADH-ubiquinone oxidoreductase 24 kDa subunit

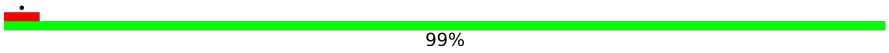
Chain AI:

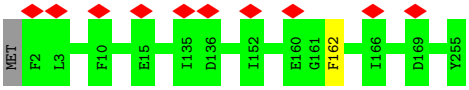




• Molecule 20: Ymf62

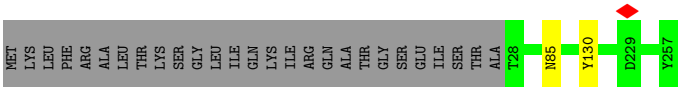
Chain AJ:





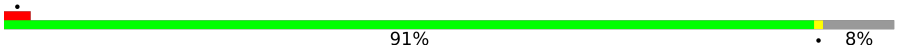
• Molecule 21: Gamma-carbonic anhydrase

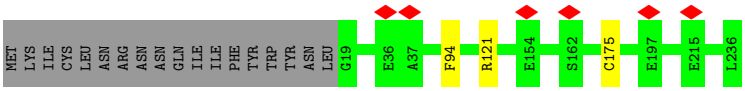
Chain AK:



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

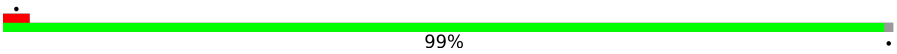
Chain AL:

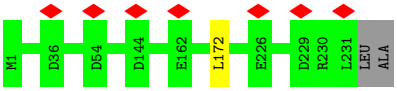




• Molecule 23: Gamma-carbonic anhydrase

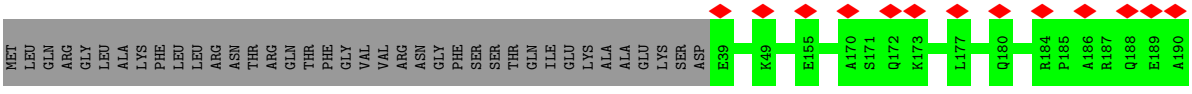
Chain AM:

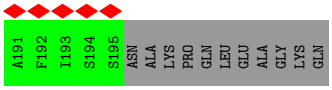




• Molecule 24: ETC complex I subunit motif protein

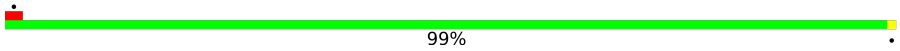
Chain AN:

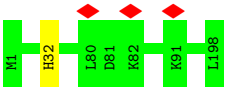




• Molecule 25: NADH dehydrogenase subunit 9

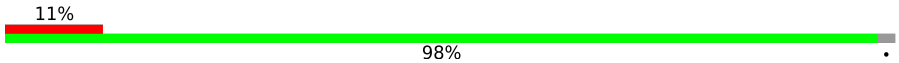
Chain AO:

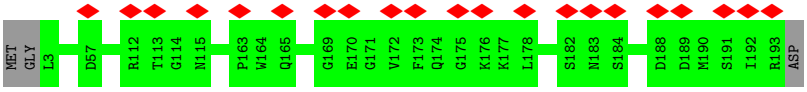




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

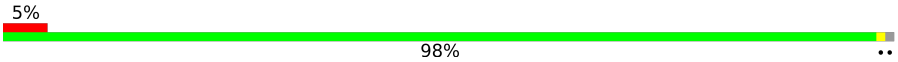
Chain AP:

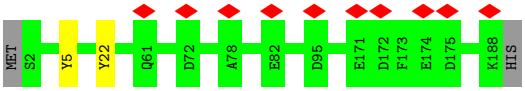




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

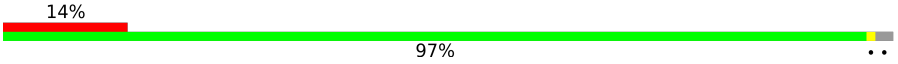
Chain AQ:

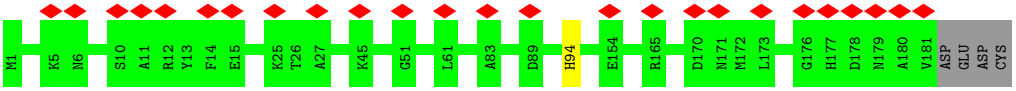




• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

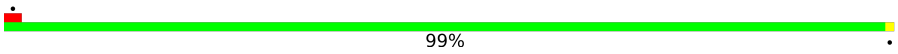
Chain AR:

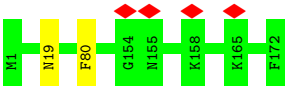




• Molecule 29: NADH dehydrogenase, putative

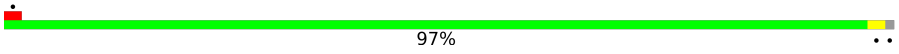
Chain AS:

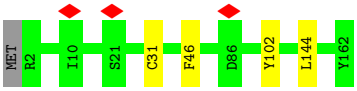




• Molecule 30: NADH dehydrogenase subunit 10

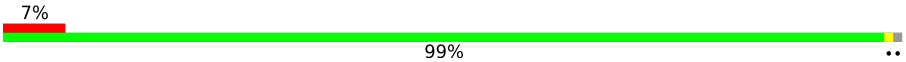
Chain AT:

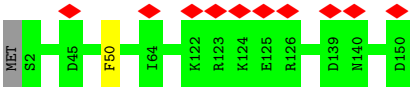




• Molecule 31: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

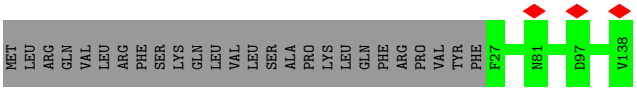
Chain AU:





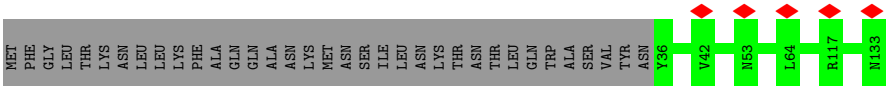
• Molecule 32: Acyl carrier protein

Chain AV:



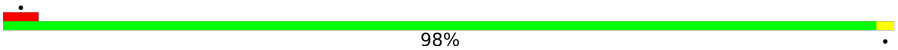
• Molecule 33: Acyl carrier protein

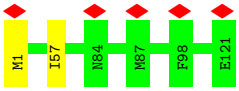
Chain AW:



• Molecule 34: NADH-ubiquinone oxidoreductase chain 3

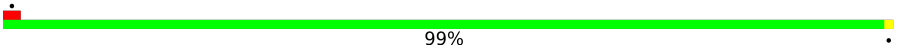
Chain AX:

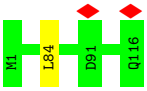




• Molecule 35: Ymf58

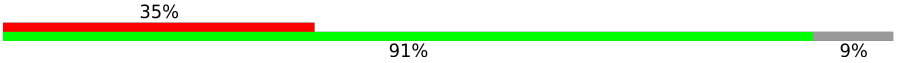
Chain AY:

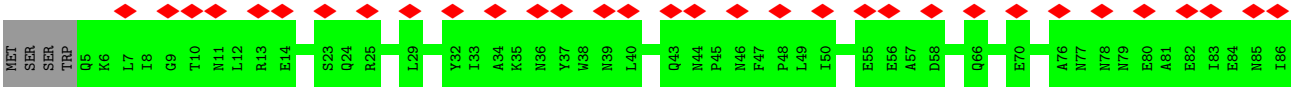


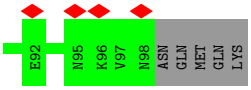


• Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein

Chain AZ:

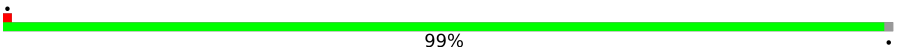


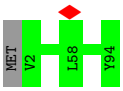




• Molecule 37: Transmembrane protein, putative

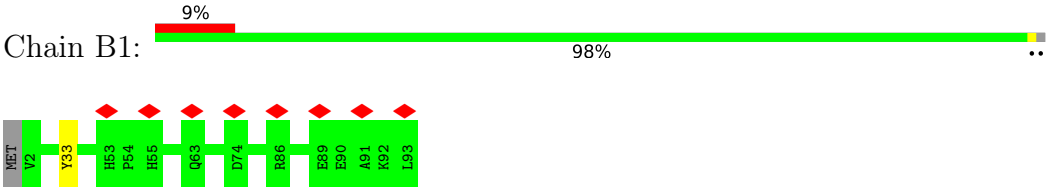
Chain B0:





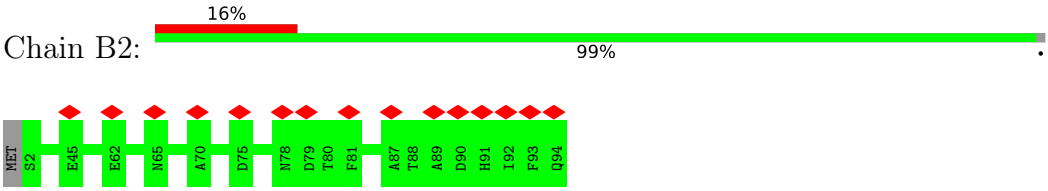
• Molecule 38: ATP synthase subunit e, mitochondrial

Chain B1:



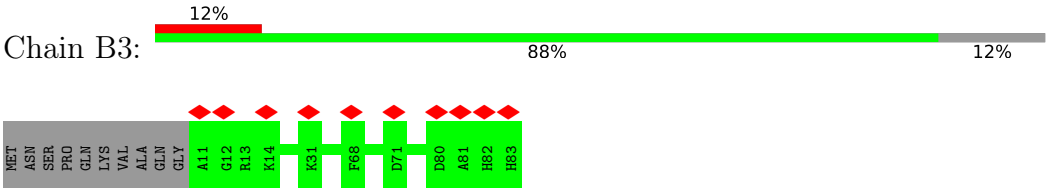
• Molecule 39: GRAM domain protein

Chain B2:



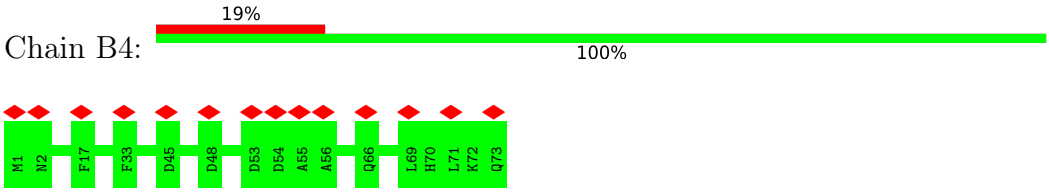
• Molecule 40: Transmembrane protein, putative

Chain B3:



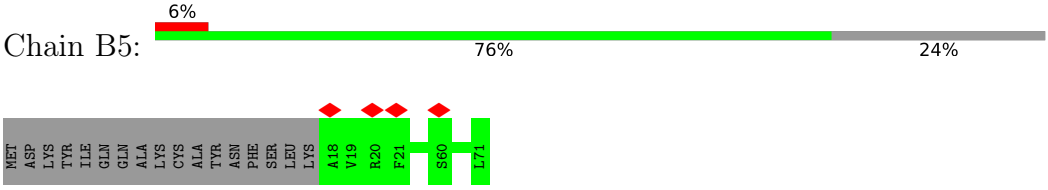
• Molecule 41: Transmembrane protein, putative

Chain B4:



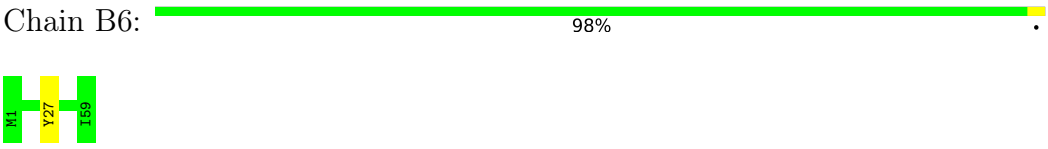
• Molecule 42: Transmembrane protein, putative

Chain B5:



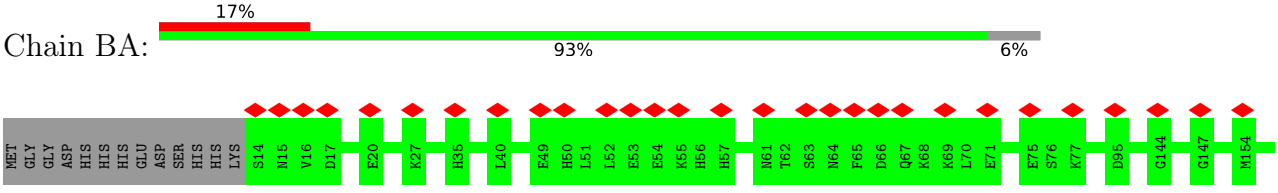
• Molecule 43: NADH dehydrogenase subunit 1

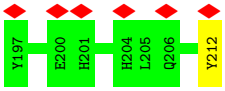
Chain B6:



• Molecule 44: Transmembrane protein

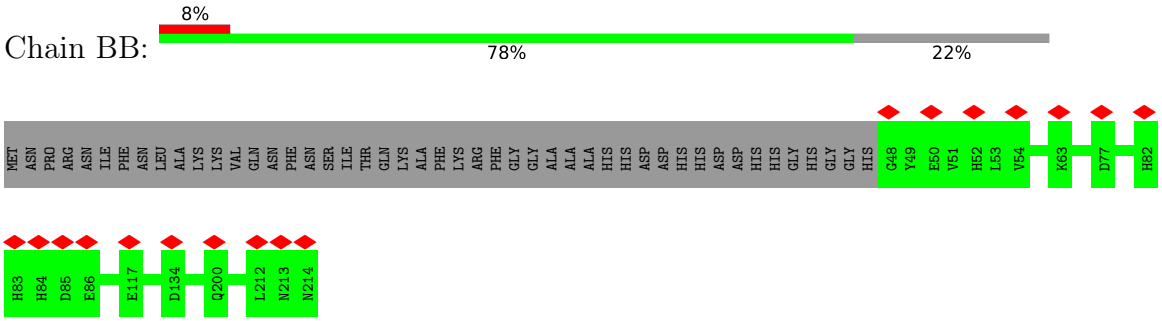
Chain BA:





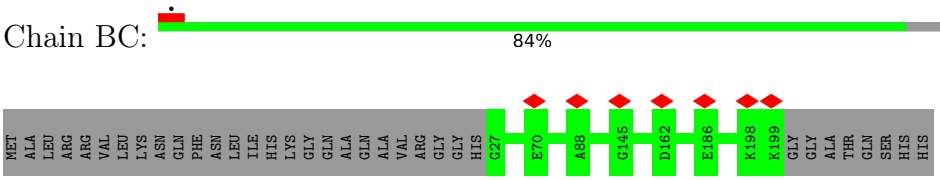
• Molecule 45: Transmembrane protein, putative

Chain BB:



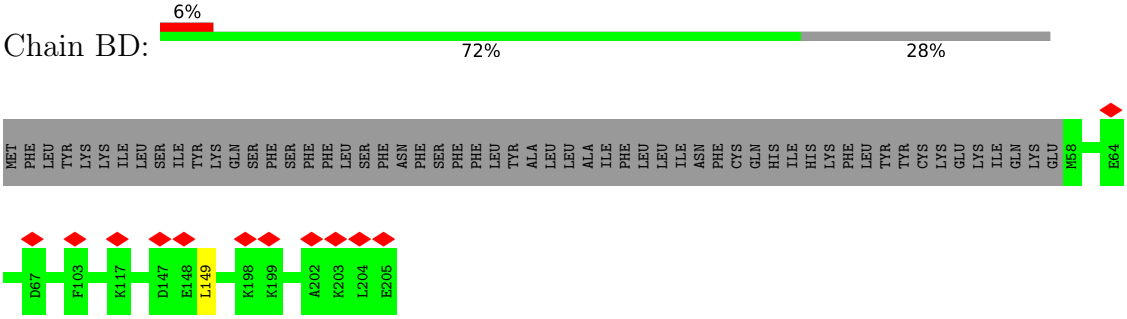
• Molecule 46: NDUB8

Chain BC:



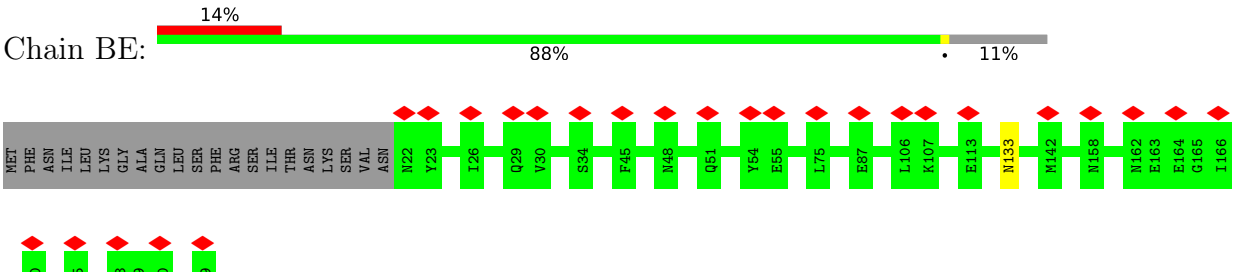
• Molecule 47: Transmembrane protein, putative

Chain BD:



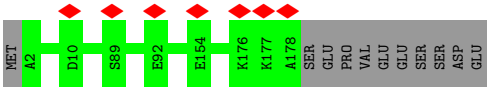
• Molecule 48: NDUPH2

Chain BE:



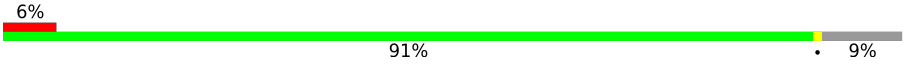
• Molecule 49: NDUB10

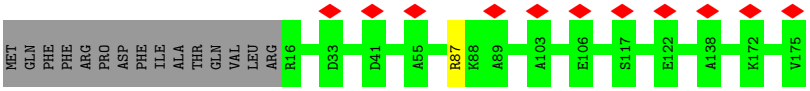
Chain BF:



• Molecule 50: NDUA13

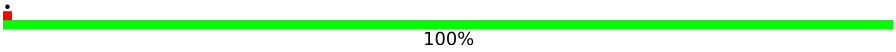
Chain BG:

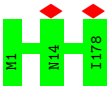




• Molecule 51: NADH dehydrogenase subunit 2

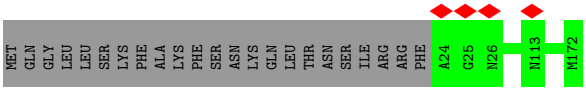
Chain BH:





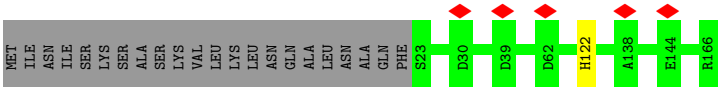
• Molecule 52: 2 iron, 2 sulfur cluster-binding protein

Chain BI:



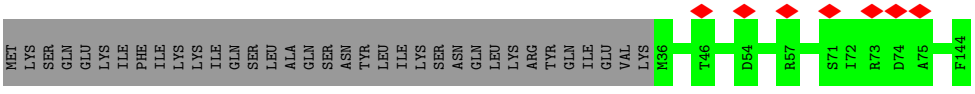
• Molecule 53: Thioredoxin

Chain BJ:



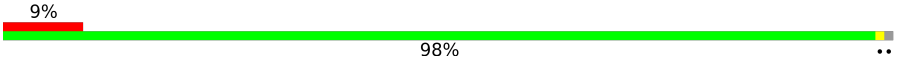
• Molecule 54: COX assembly mitochondrial protein

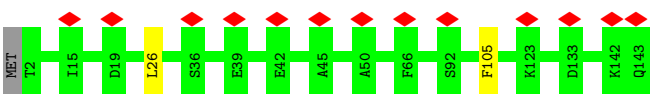
Chain BK:



• Molecule 55: Transmembrane protein, putative

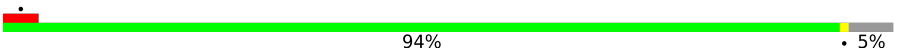
Chain BL:

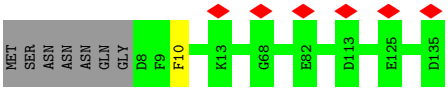




• Molecule 56: Transmembrane protein, putative

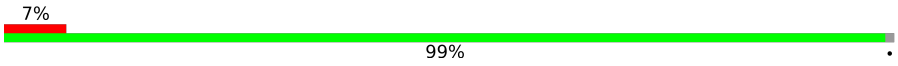
Chain BM:

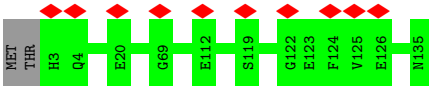




• Molecule 57: PH domain-containing protein

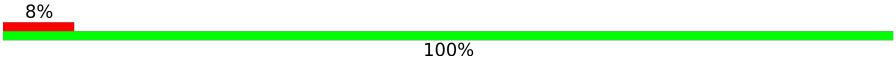
Chain BN:

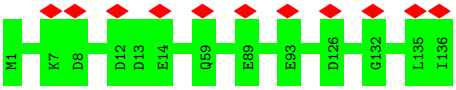




• Molecule 58: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

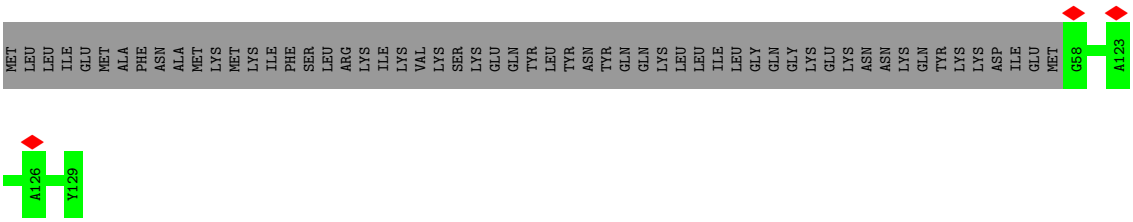
Chain BO:





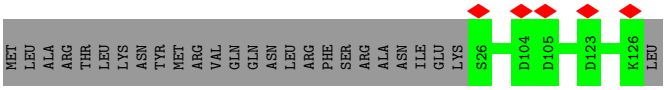
• Molecule 59: NDUB6

Chain BP:



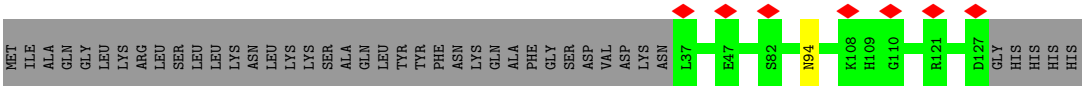
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain BQ:



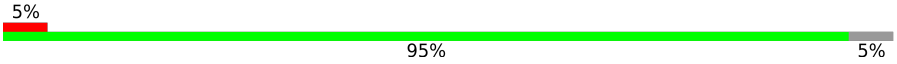
• Molecule 61: Zinc-finger protein

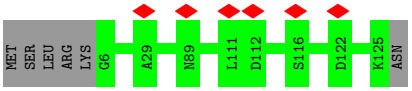
Chain BR:



• Molecule 62: NDUB4

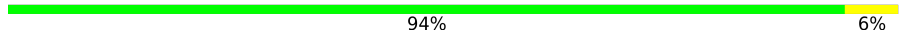
Chain BS:





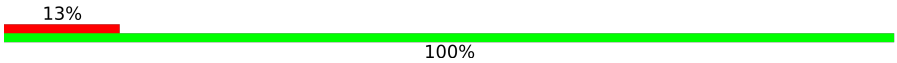
• Molecule 63: NDUTT10

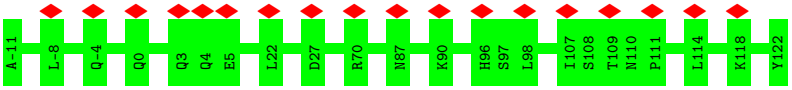
Chain BT:



• Molecule 64: NDUTT11

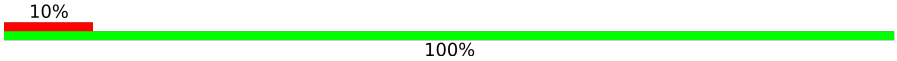
Chain BU:

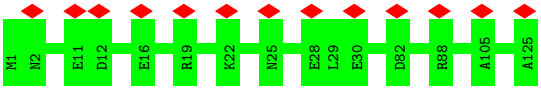




• Molecule 65: NDUTT12

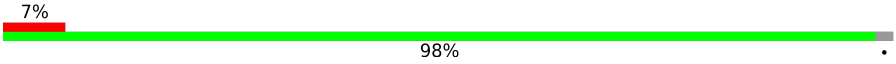
Chain BV:

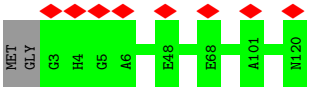




• Molecule 66: CHCH domain-containing protein

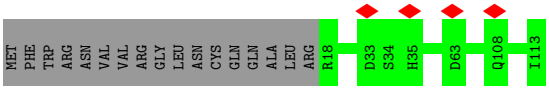
Chain BW:





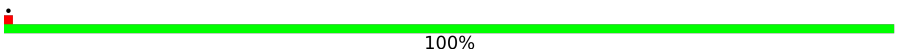
• Molecule 67: Transmembrane protein, putative

Chain BX:



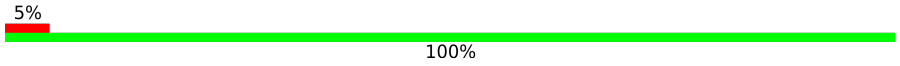
• Molecule 68: Ymf57

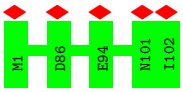
Chain BY:



• Molecule 69: Complex I-MNLL

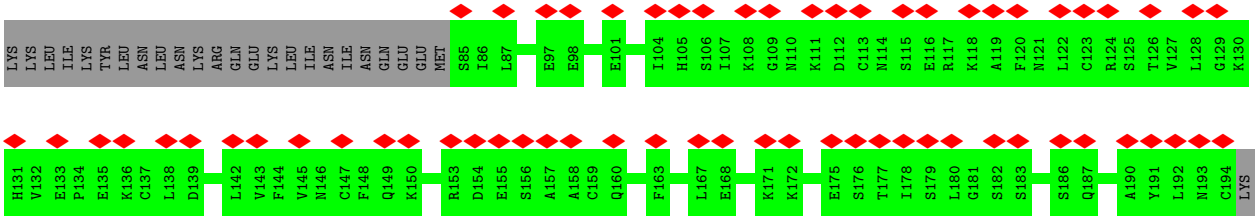
Chain BZ:





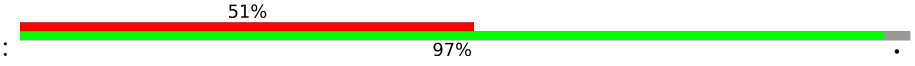
• Molecule 70: Diphthamide synthesis protein

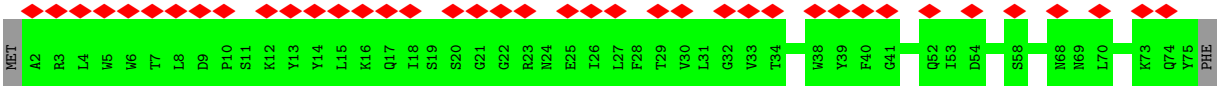
Chain CH:



• Molecule 71: Transmembrane protein, putative

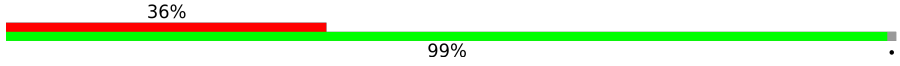
Chain CM:

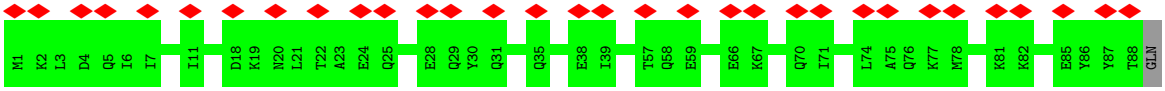




• Molecule 72: Transposase

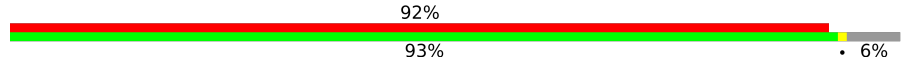
Chain CL:

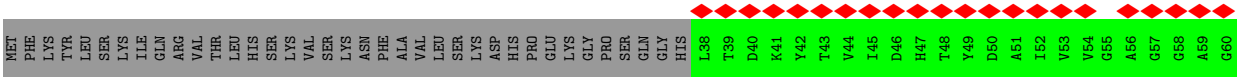


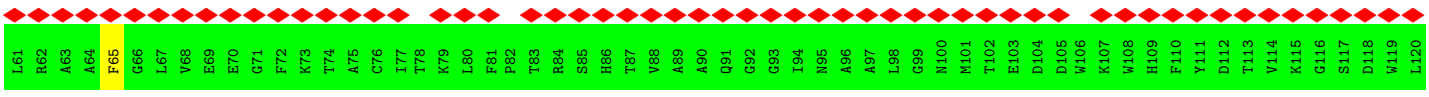


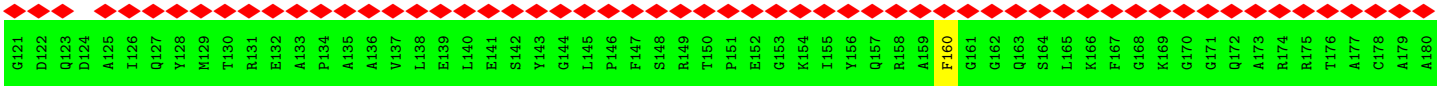
• Molecule 73: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

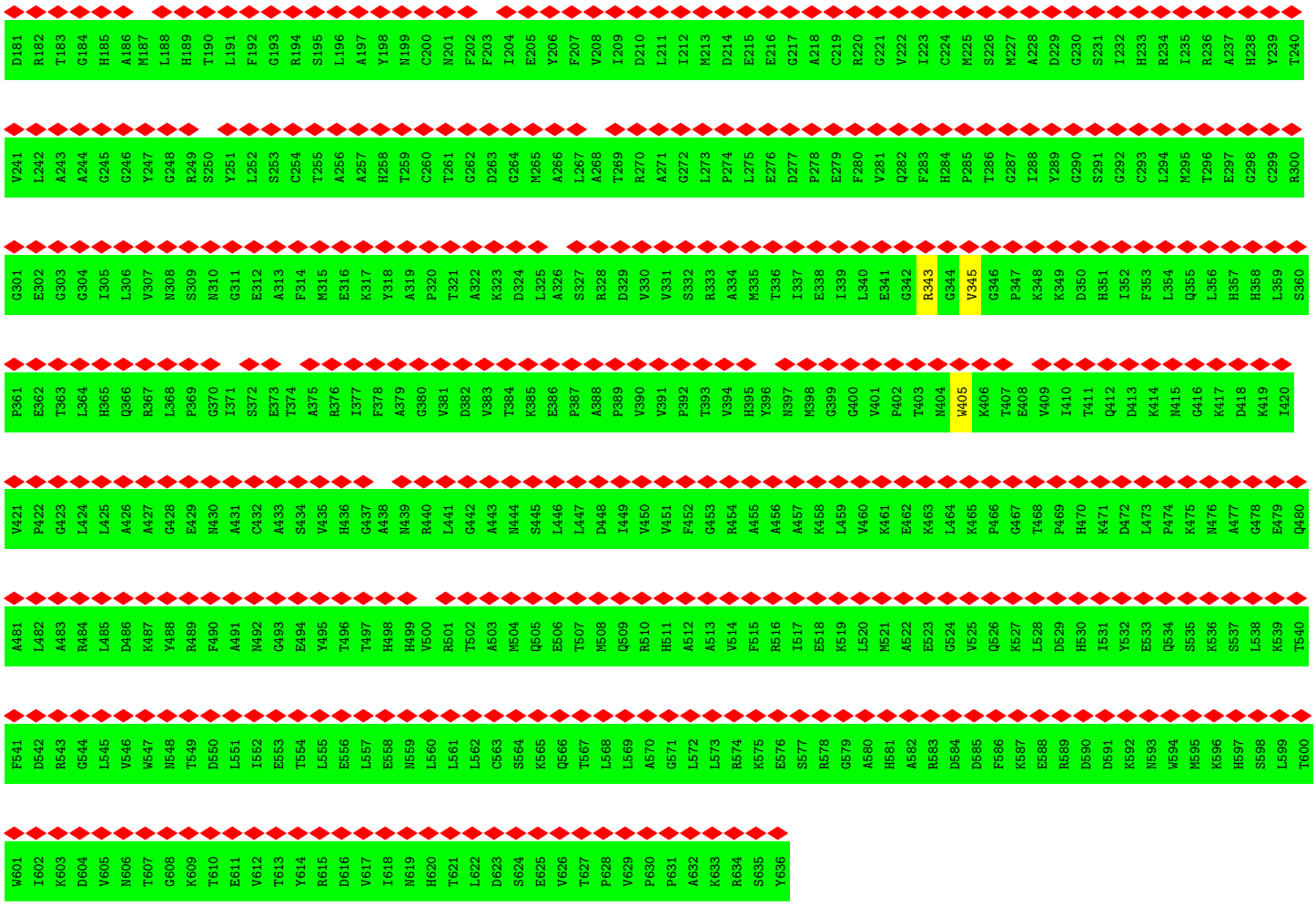
Chain CA:





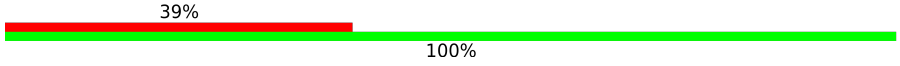


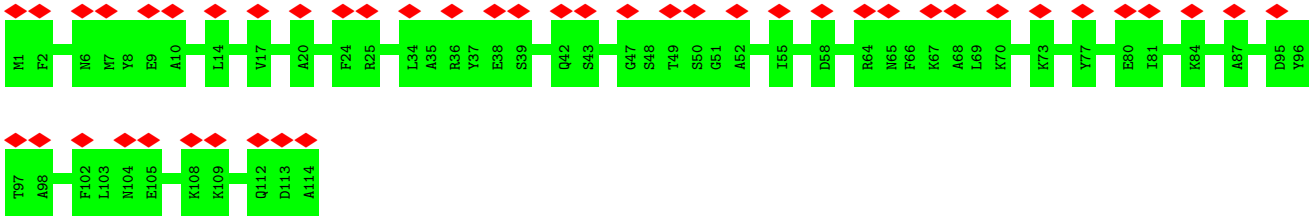




• Molecule 74: DUF4885 domain-containing protein

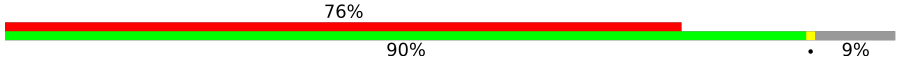
Chain CI:

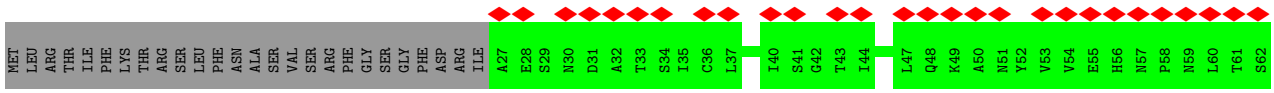


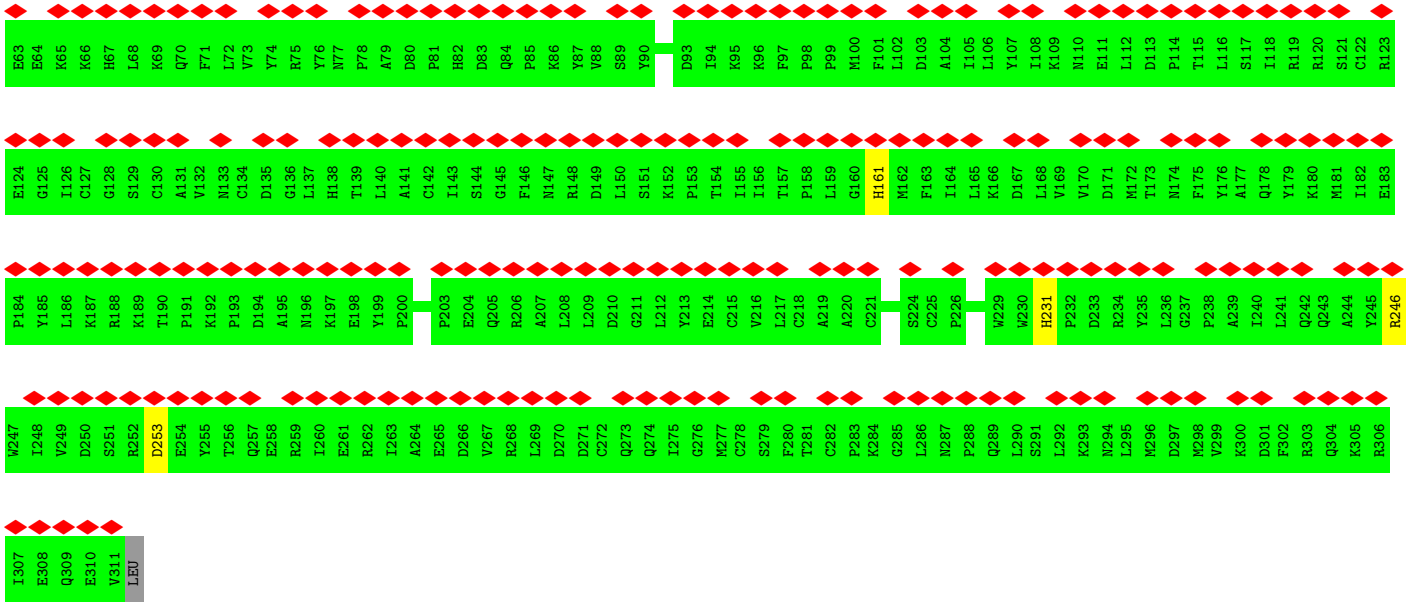


• Molecule 75: succinate dehydrogenase

Chain CB:

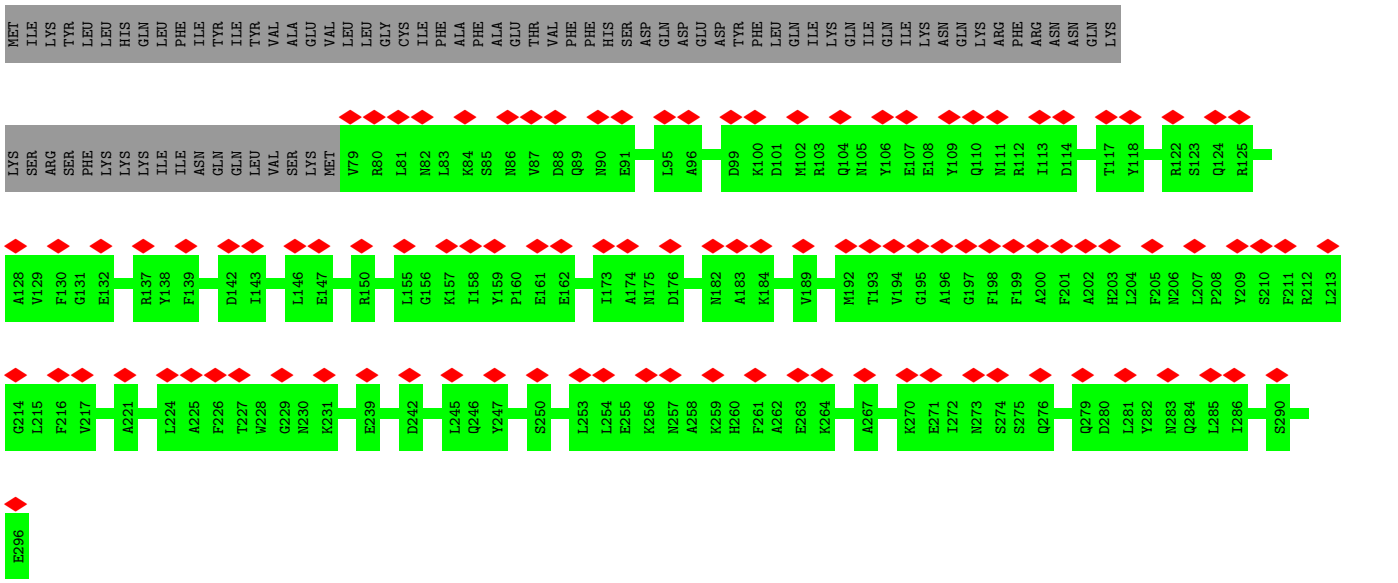






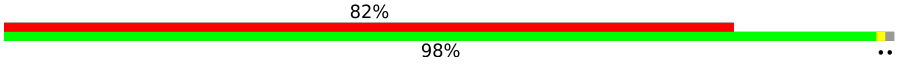
• Molecule 76: Transmembrane protein, putative

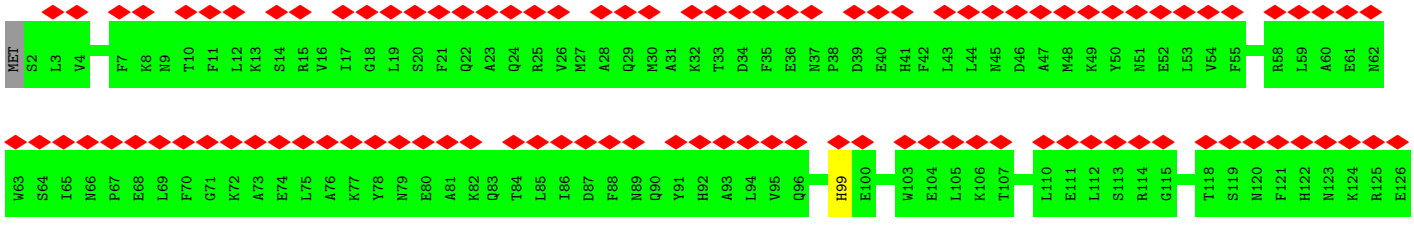
Chain CF:



• Molecule 77: Uncharacterized protein

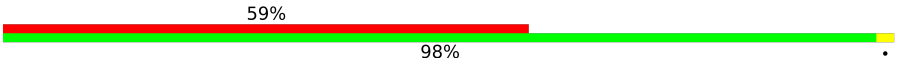
Chain CG:

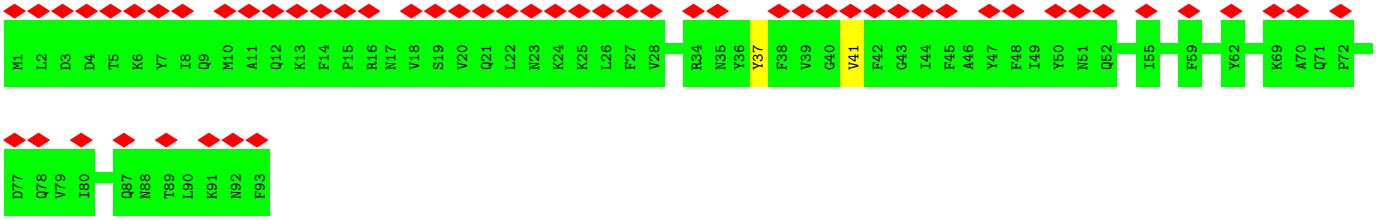




• Molecule 78: Transmembrane protein, putative

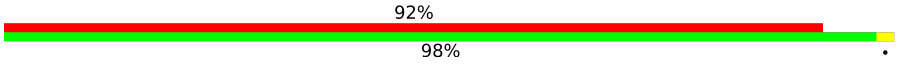
Chain CK:

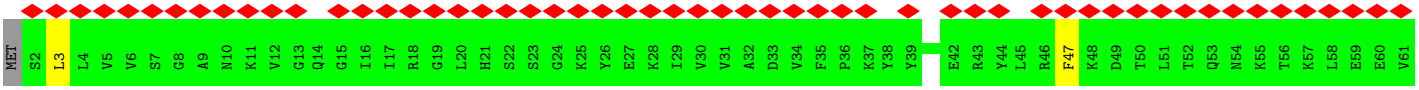


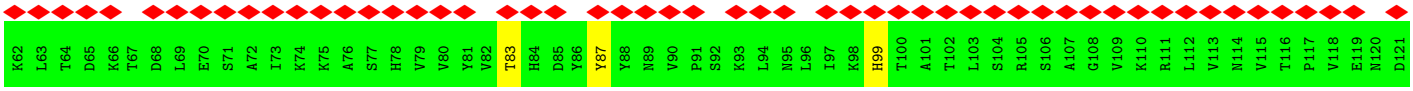


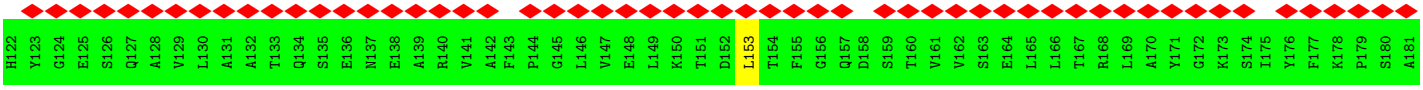
• Molecule 79: NmrA domain-containing protein

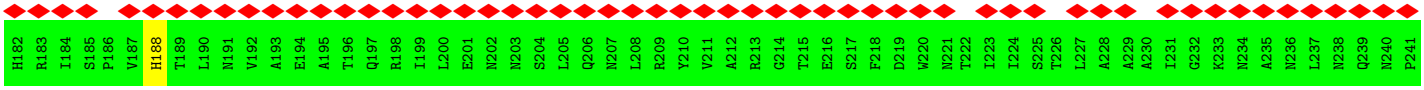
Chain CE:

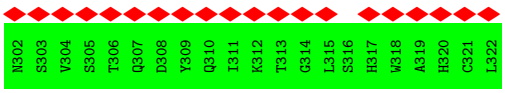






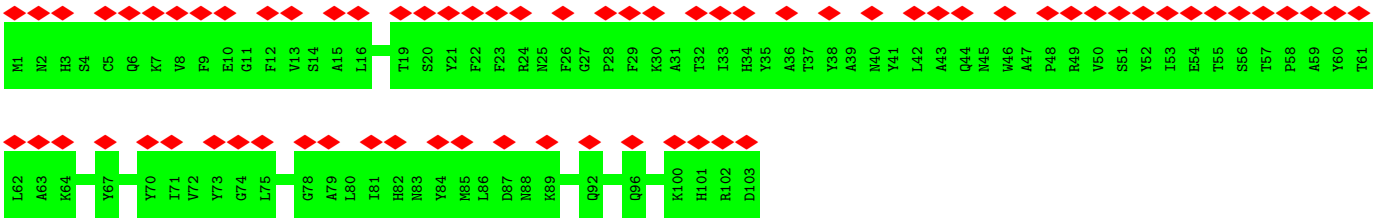




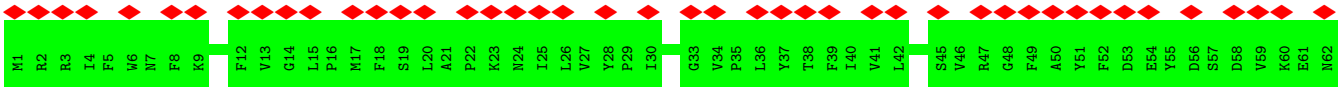


• Molecule 80: Transmembrane protein, putative

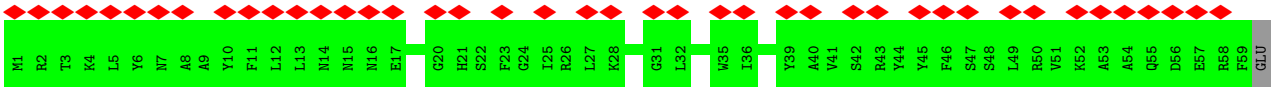
Chain CJ:



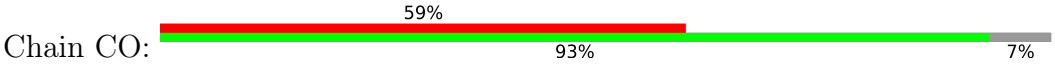
• Molecule 81: Transmembrane protein, putative

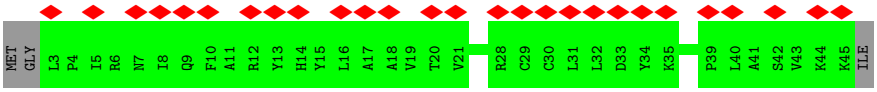


• Molecule 82: Transmembrane protein

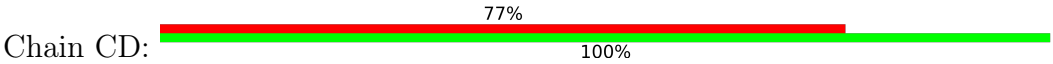


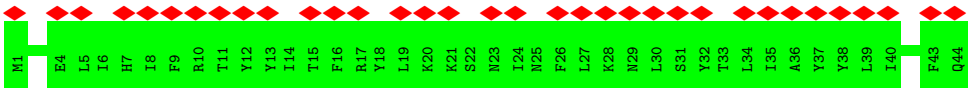
• Molecule 83: SDHTT11



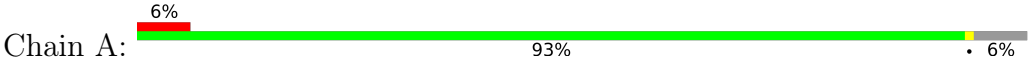


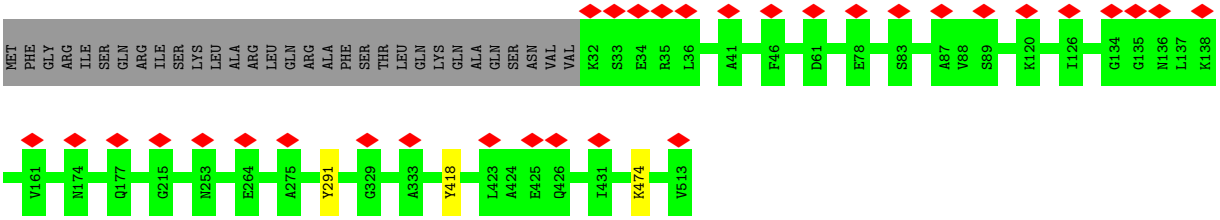
• Molecule 84: succinate dehydrogenase complex iron-sulfur subunit D





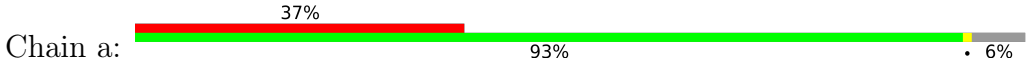
• Molecule 85: Peptidase M16 inactive domain protein

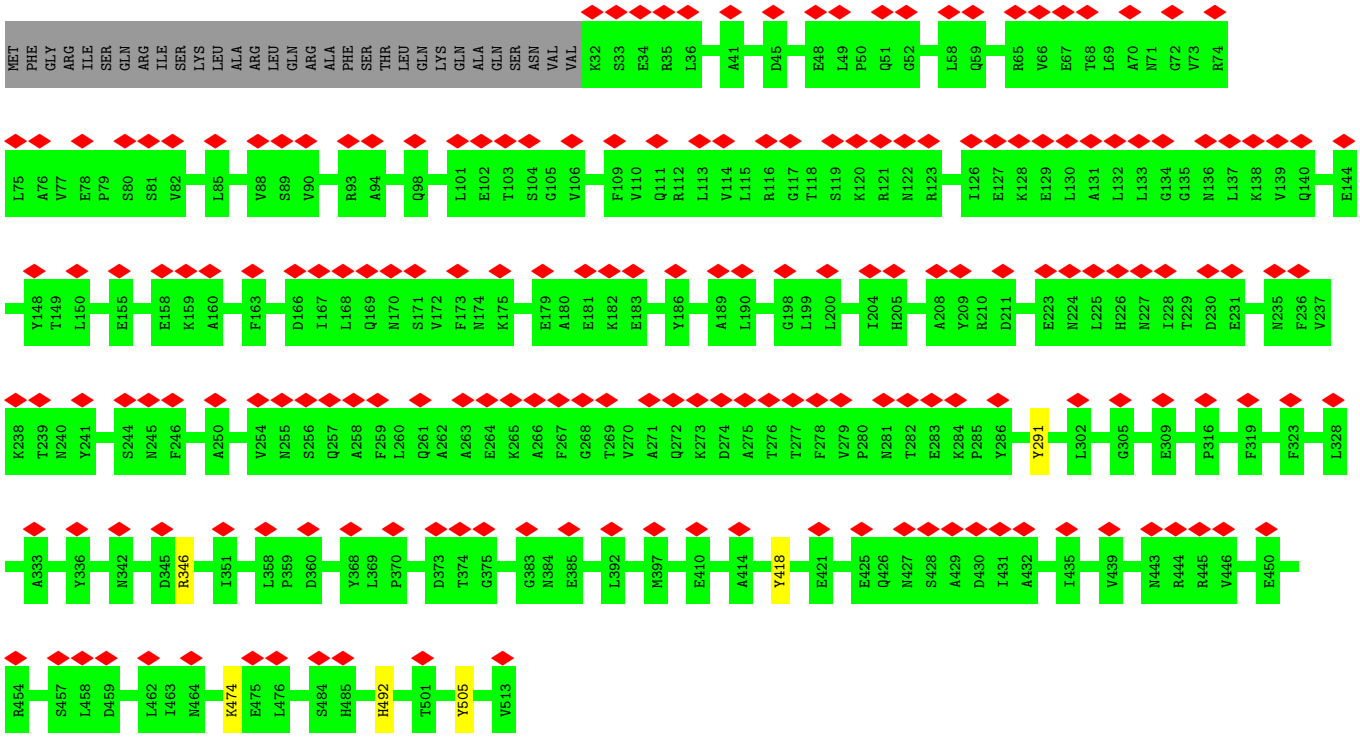




• Molecule 85: Peptidase M16 inactive domain protein

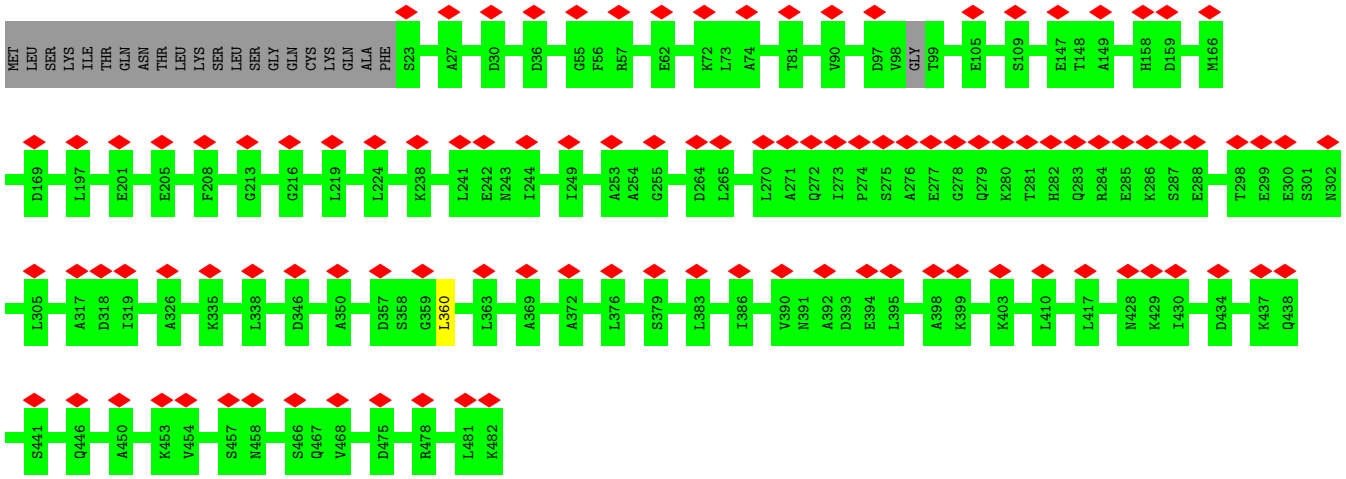
Chain a:





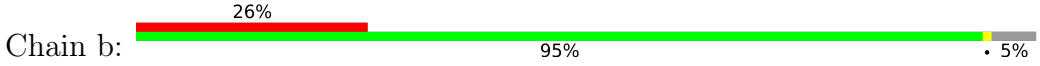
• Molecule 86: M16 family peptidase, putative

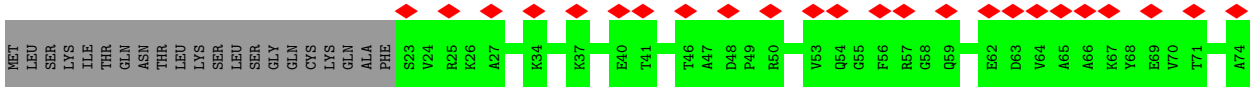
Chain B:

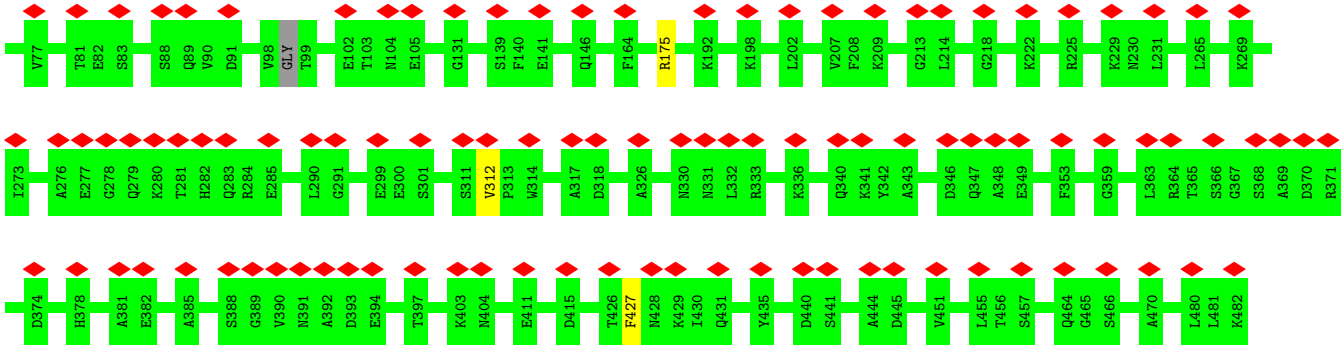


• Molecule 86: M16 family peptidase, putative

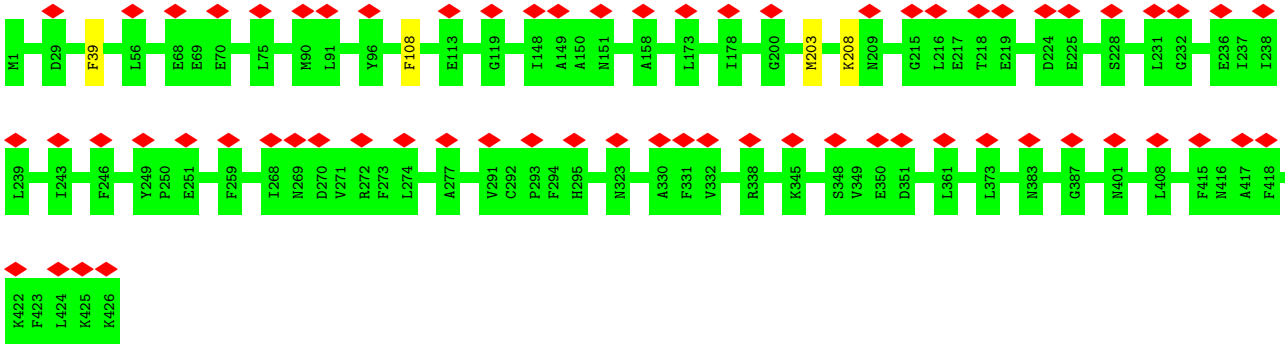
Chain b:



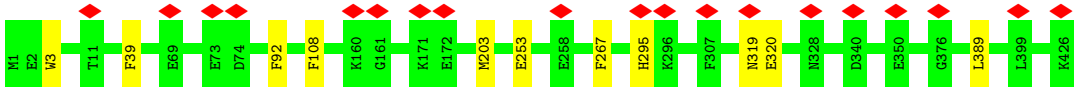




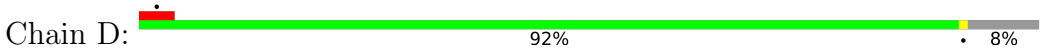
• Molecule 87: Apocytochrome b

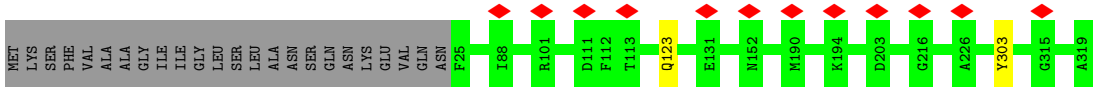


• Molecule 87: Apocytochrome b

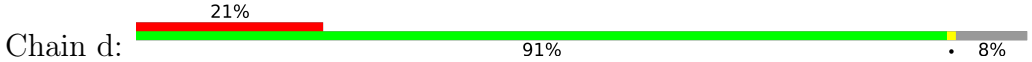


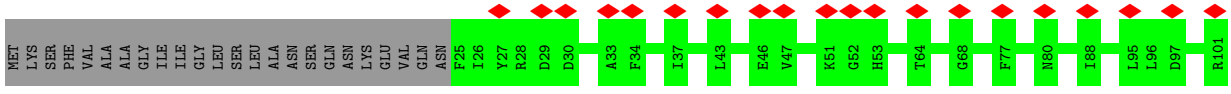
• Molecule 88: Cytochrome protein c1

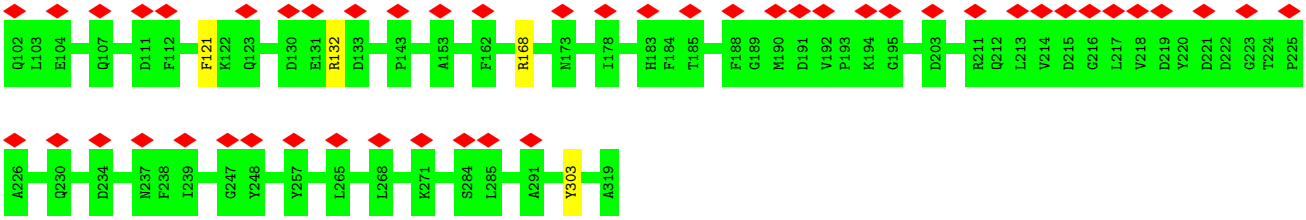




• Molecule 88: Cytochrome protein c1

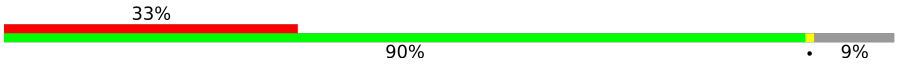


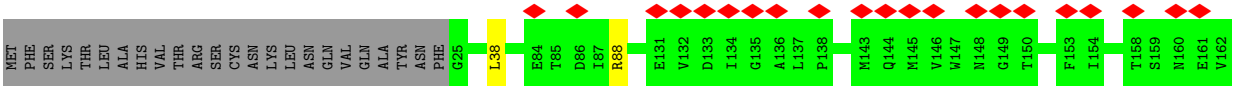


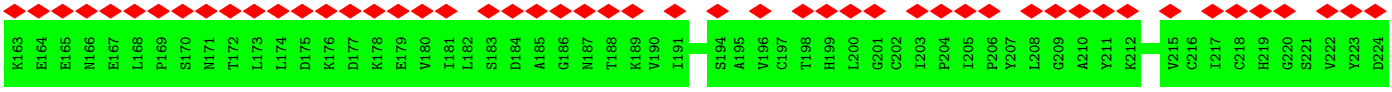


• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain E:

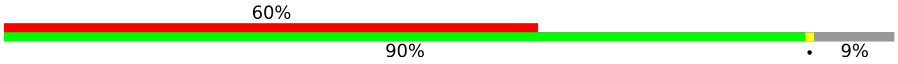


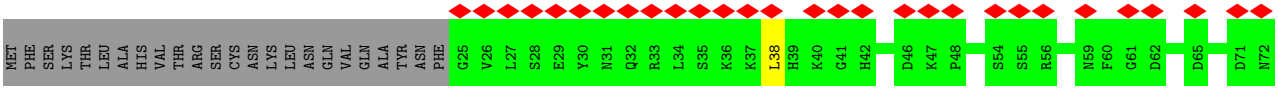


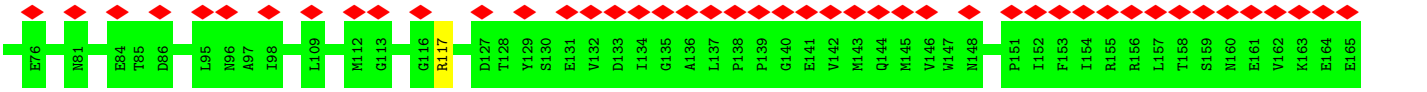


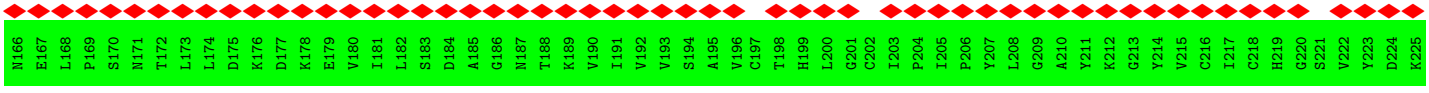
• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

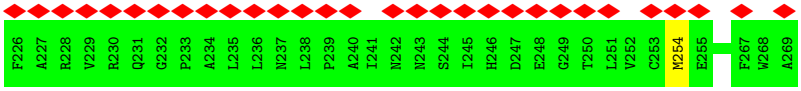
Chain e:





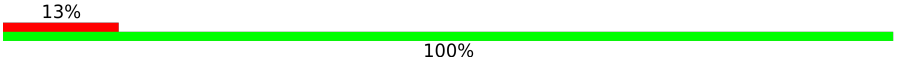


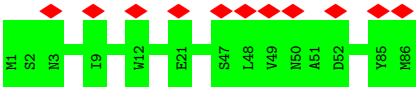




• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

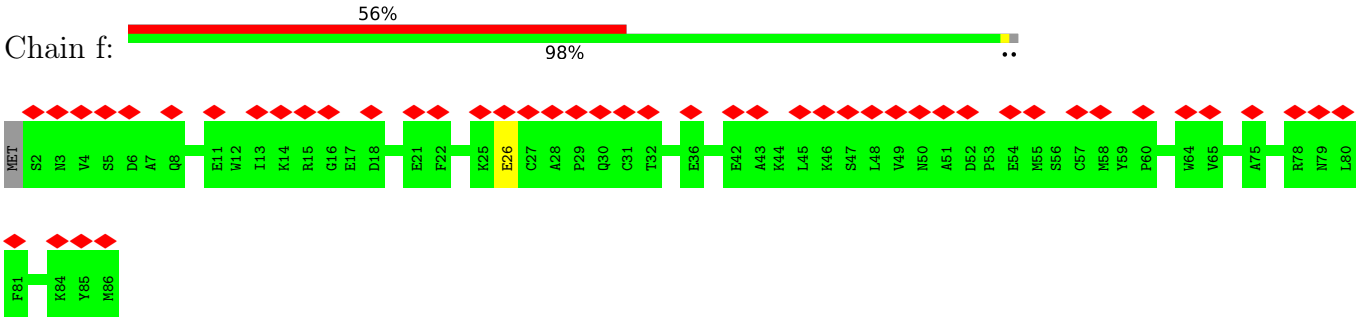
Chain F:





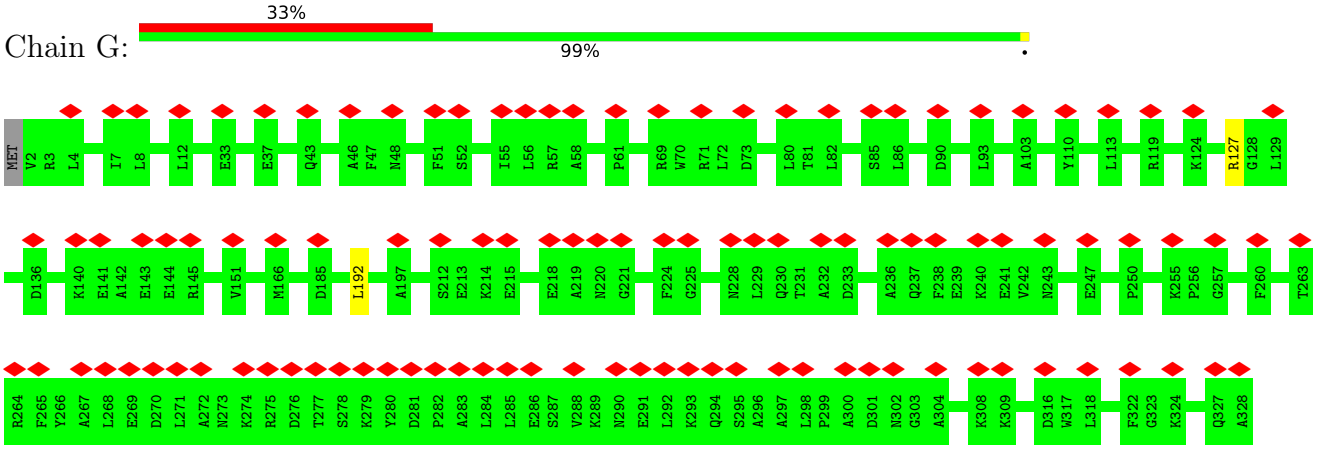
• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

Chain f:



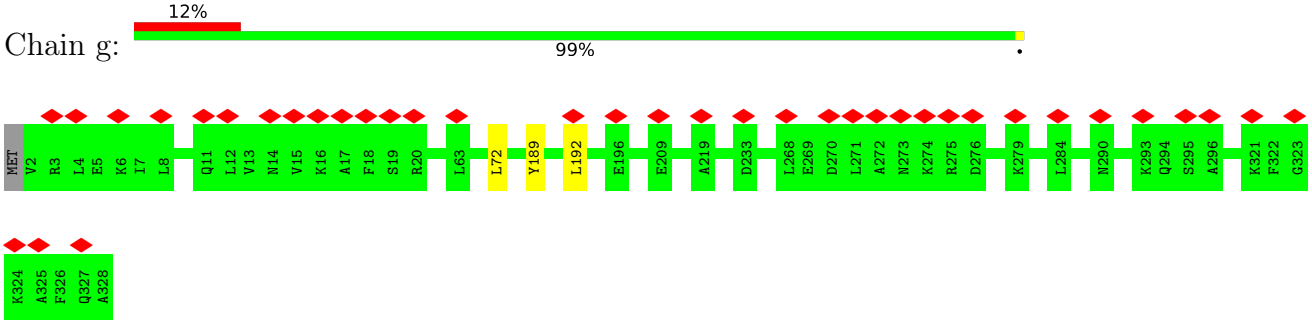
• Molecule 91: UQCRTT1

Chain G:



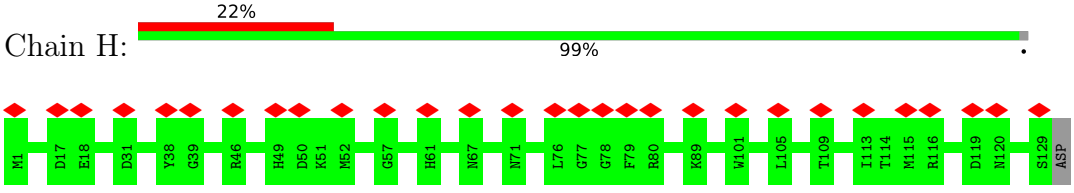
• Molecule 91: UQCRTT1

Chain g:



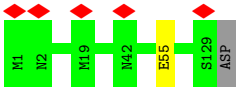
• Molecule 92: Transmembrane protein, putative

Chain H:



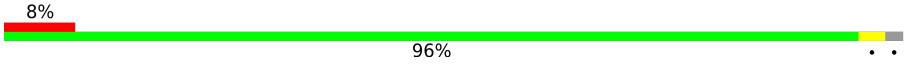
• Molecule 92: Transmembrane protein, putative

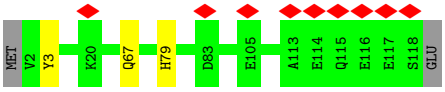
Chain h:



• Molecule 93: Transmembrane protein, putative

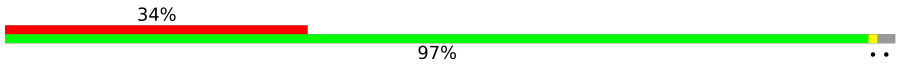
Chain I:

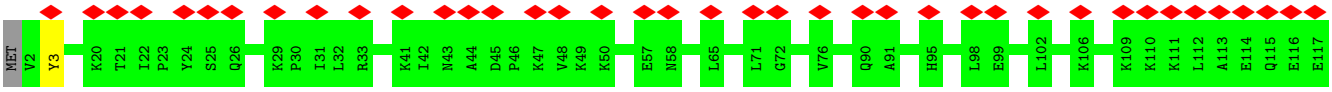




• Molecule 93: Transmembrane protein, putative

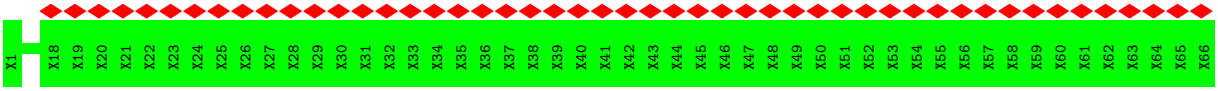
Chain i:





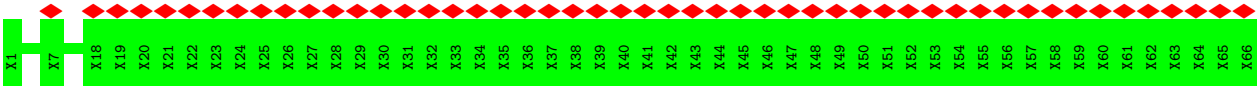
• Molecule 94: UQCRTT3

Chain J:



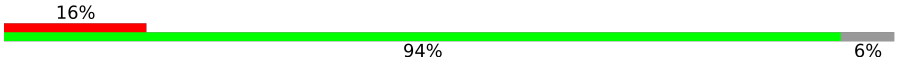
• Molecule 94: UQCRTT3

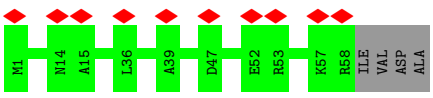
Chain j:



• Molecule 95: Transmembrane protein, putative

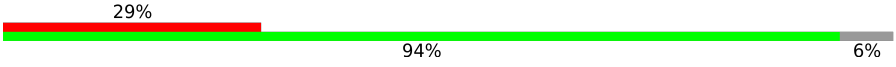
Chain K:

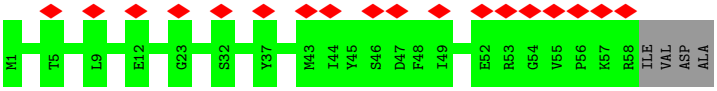




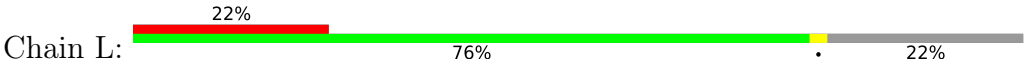
• Molecule 95: Transmembrane protein, putative

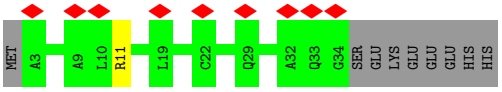
Chain k:



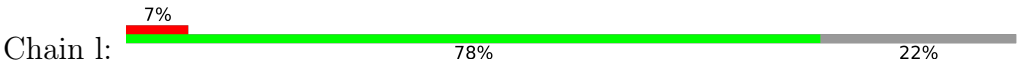


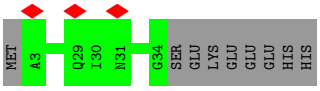
• Molecule 96: UQCRTT2



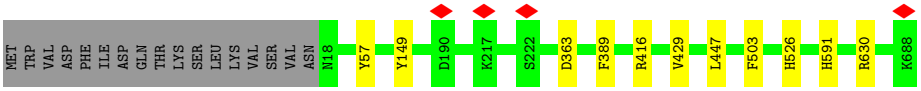


• Molecule 96: UQCRTT2

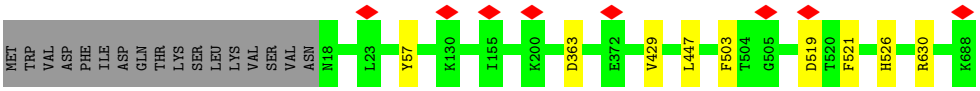




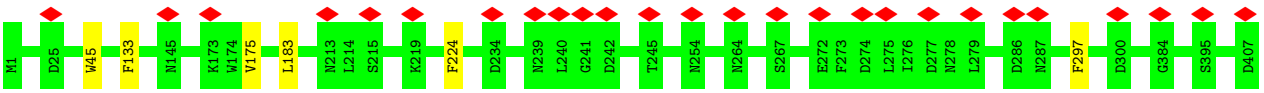
• Molecule 97: Cytochrome c oxidase subunit 1



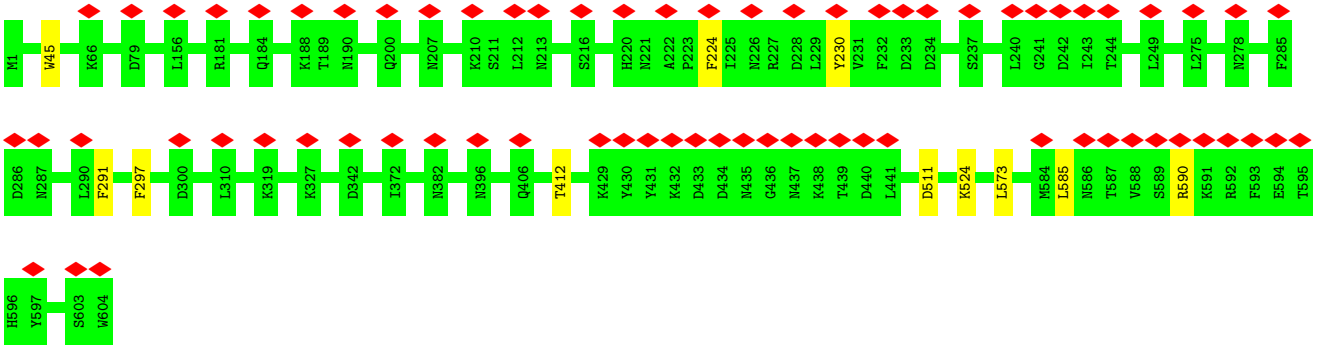
• Molecule 97: Cytochrome c oxidase subunit 1



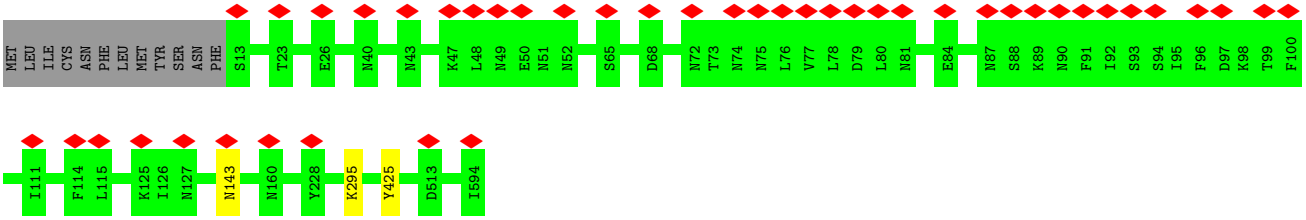
• Molecule 98: Cytochrome c oxidase subunit 2



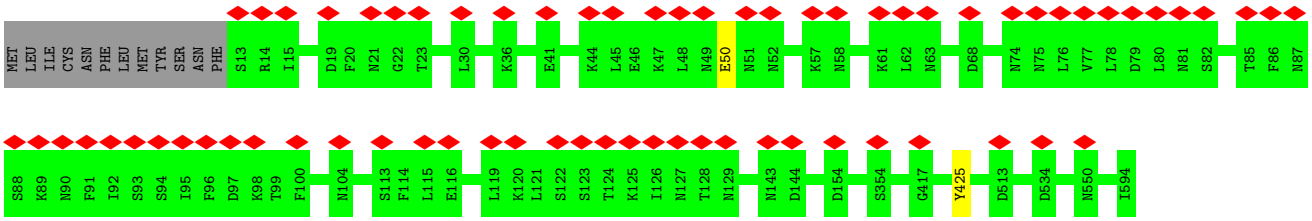
• Molecule 98: Cytochrome c oxidase subunit 2



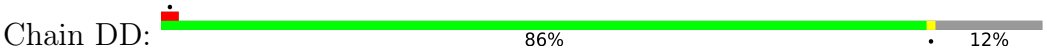
• Molecule 99: Ymf68

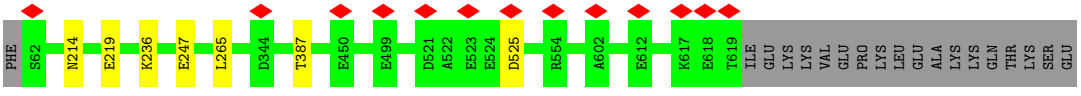


• Molecule 99: Ymf68

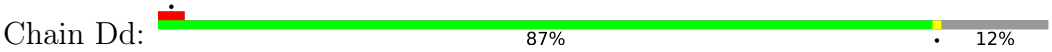


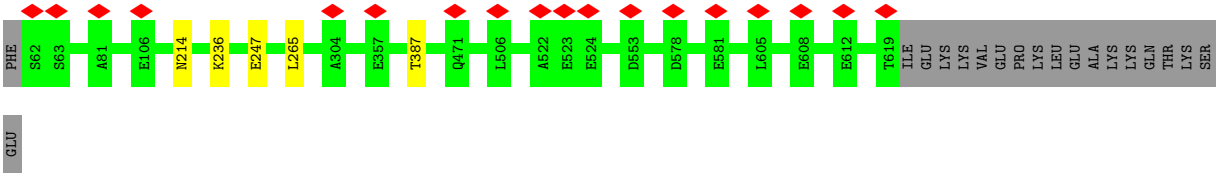
• Molecule 100: Cytochrome C oxidase subunit Vb protein





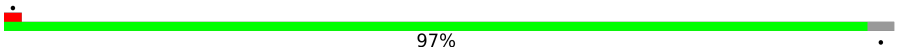
• Molecule 100: Cytochrome C oxidase subunit Vb protein

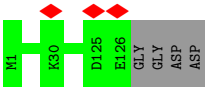




• Molecule 101: Transmembrane protein, putative

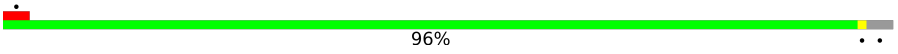
Chain DE:





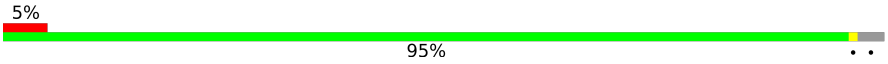
• Molecule 101: Transmembrane protein, putative

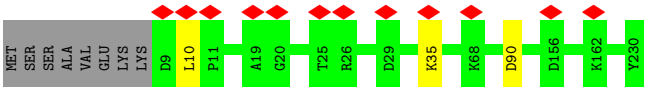
Chain De:



• Molecule 102: Structural protein

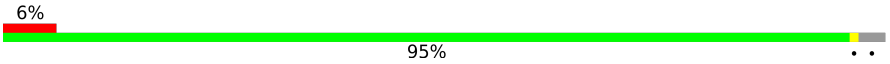
Chain DF:





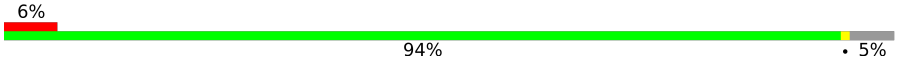
• Molecule 102: Structural protein

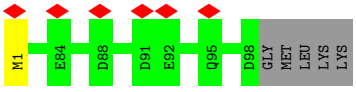
Chain Df:



• Molecule 103: Transmembrane protein, putative

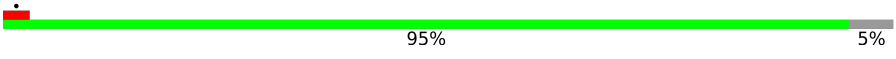
Chain DG:

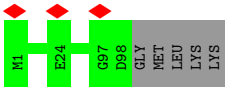




• Molecule 103: Transmembrane protein, putative

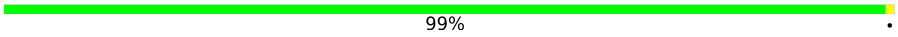
Chain Dg:





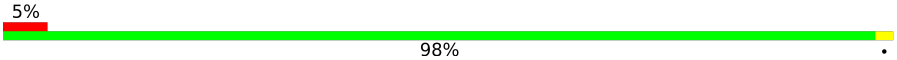
• Molecule 104: Transmembrane protein, putative

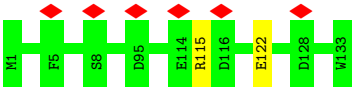
Chain DH:



• Molecule 104: Transmembrane protein, putative

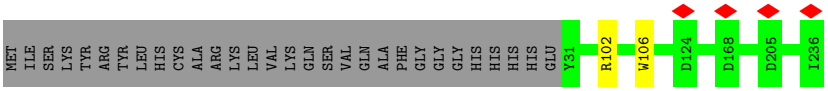
Chain Dh:





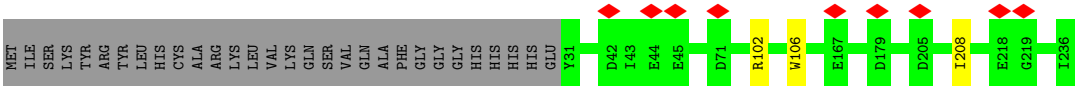
• Molecule 105: Transmembrane protein

Chain DI:



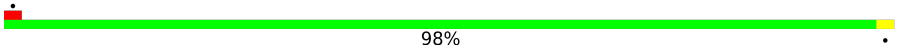
• Molecule 105: Transmembrane protein

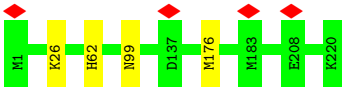
Chain Di:



• Molecule 106: Transmembrane protein, putative

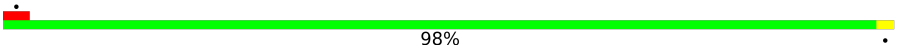
Chain DJ:

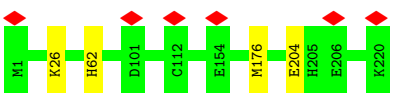




• Molecule 106: Transmembrane protein, putative

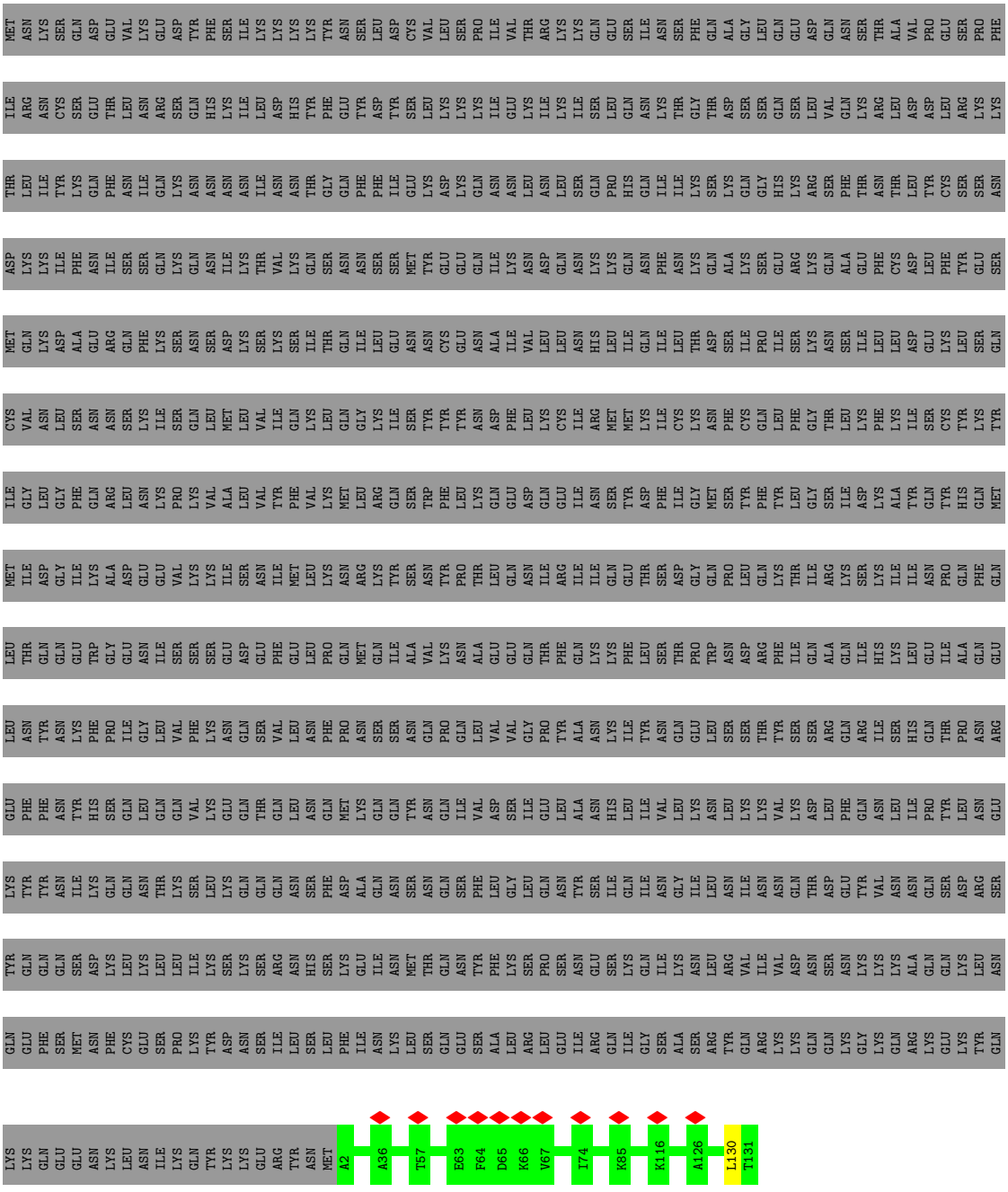
Chain Dj:





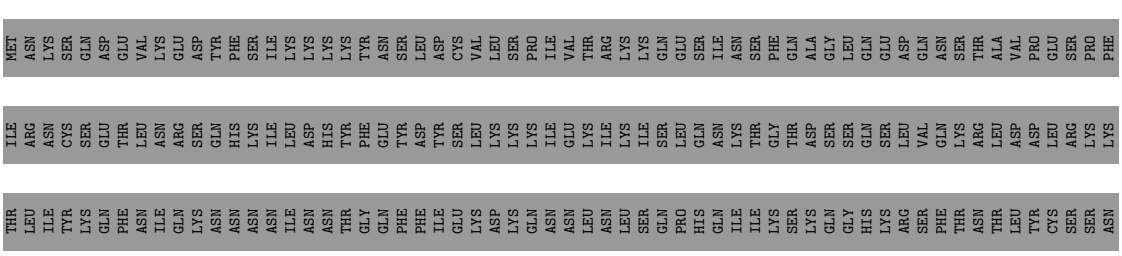
• Molecule 107: CTF/NF-I domain-containing protein

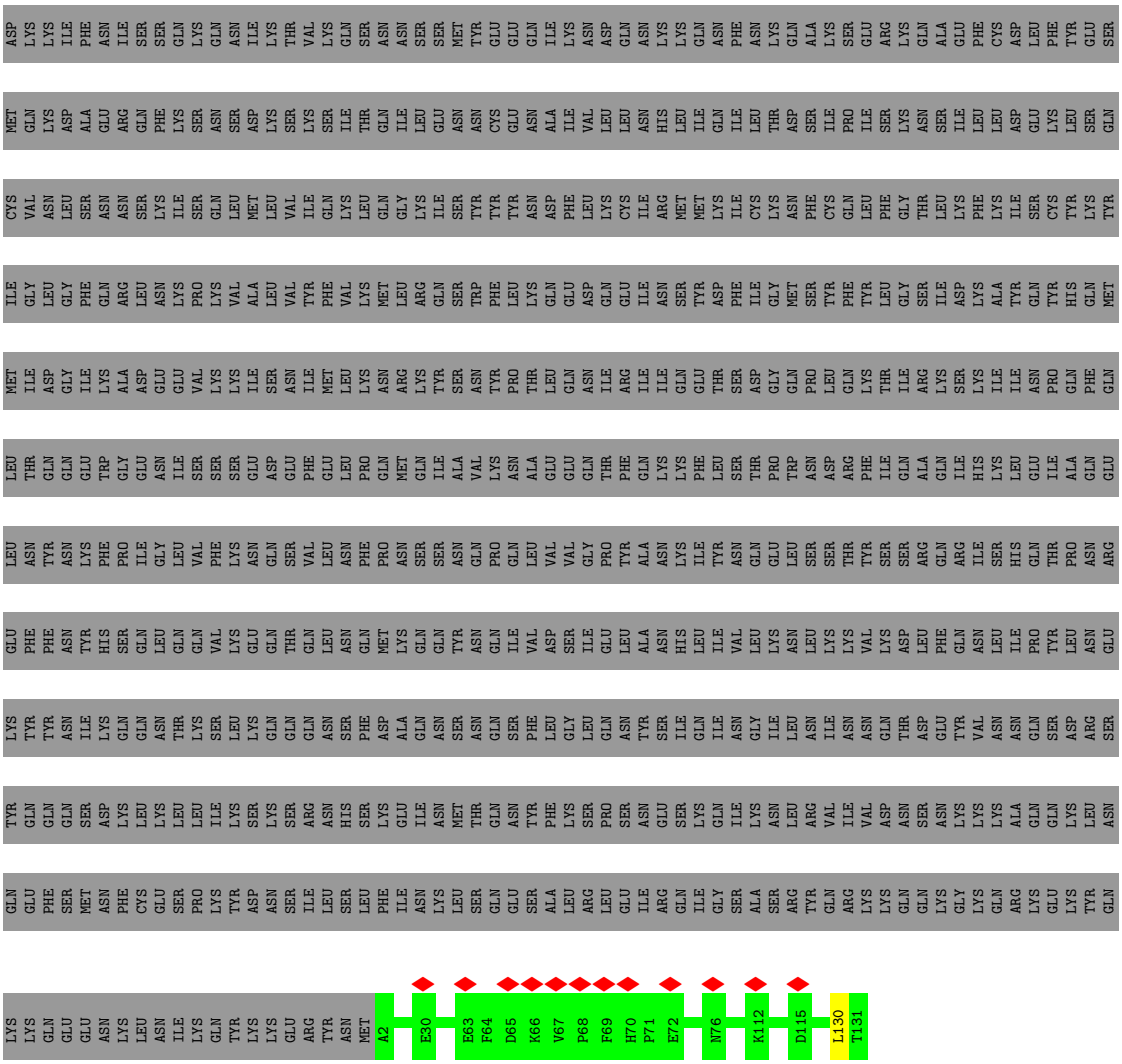
Chain DK:



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

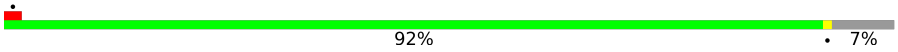
Chain Dk:

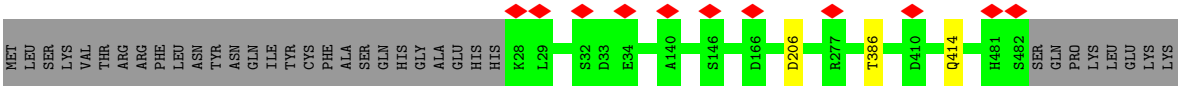




• Molecule 108: Transmembrane protein, putative

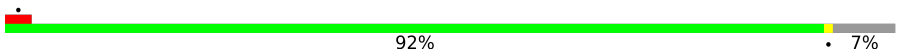
Chain DM:

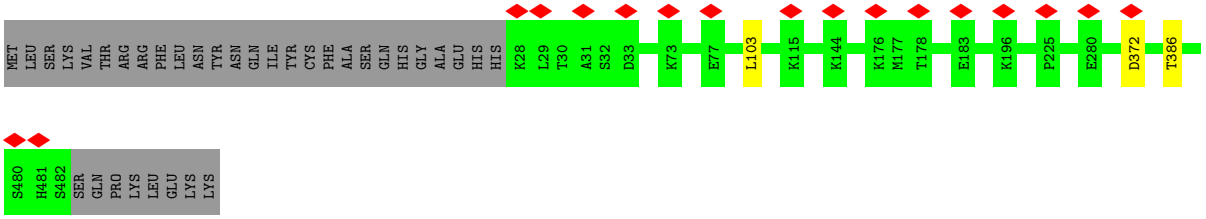




• Molecule 108: Transmembrane protein, putative

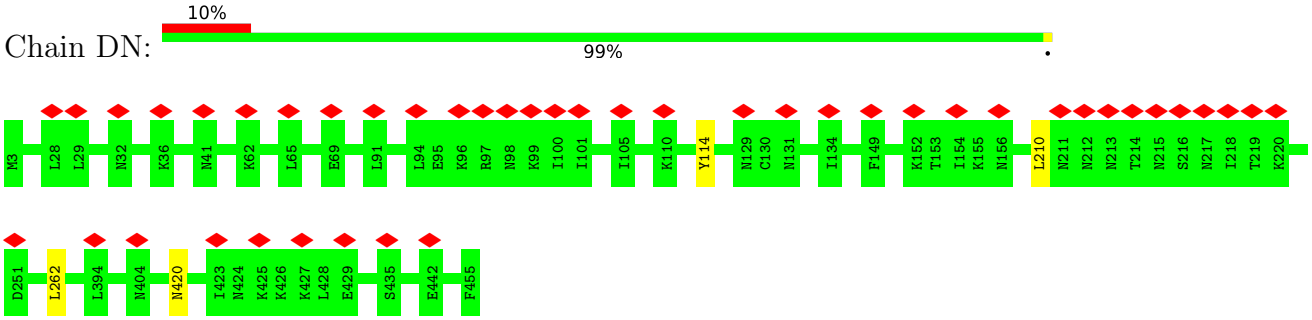
Chain Dm:





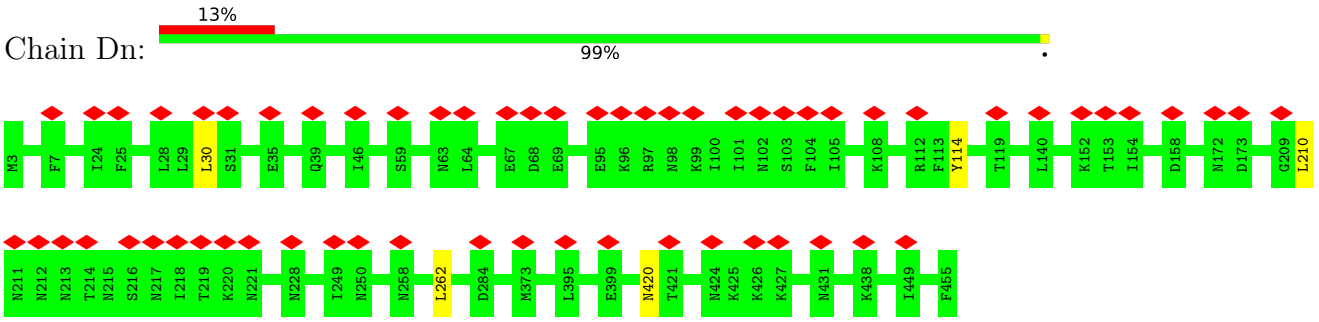
• Molecule 109: Ymf67

Chain DN:



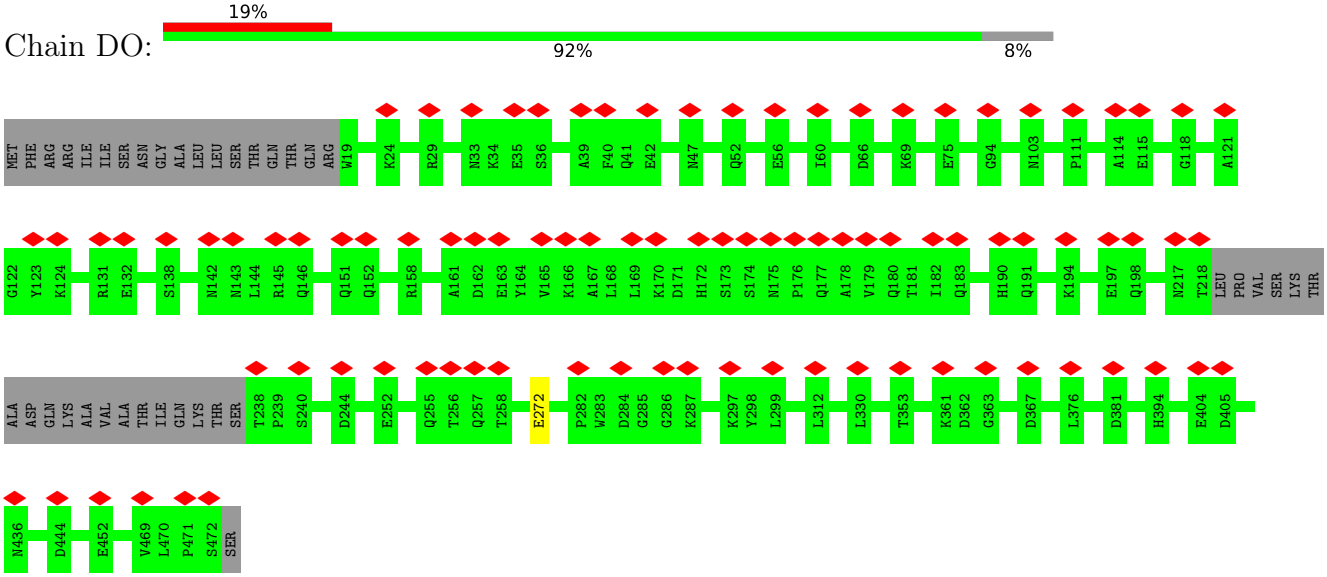
• Molecule 109: Ymf67

Chain Dn:



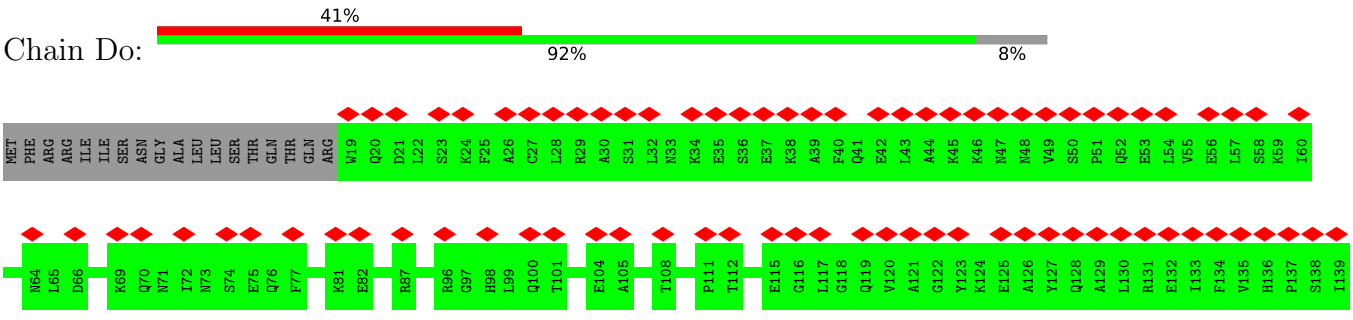
• Molecule 110: Protein phosphatase 2C, putative

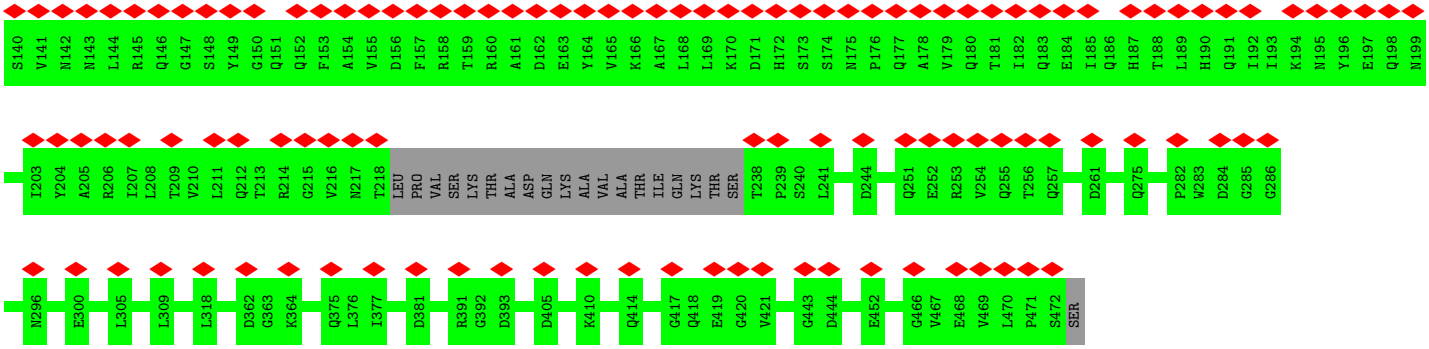
Chain DO:



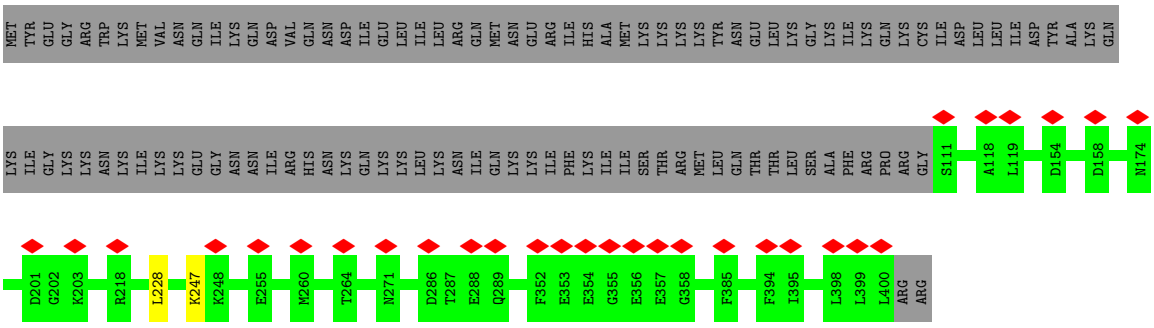
• Molecule 110: Protein phosphatase 2C, putative

Chain Do:

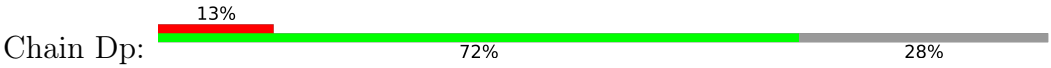


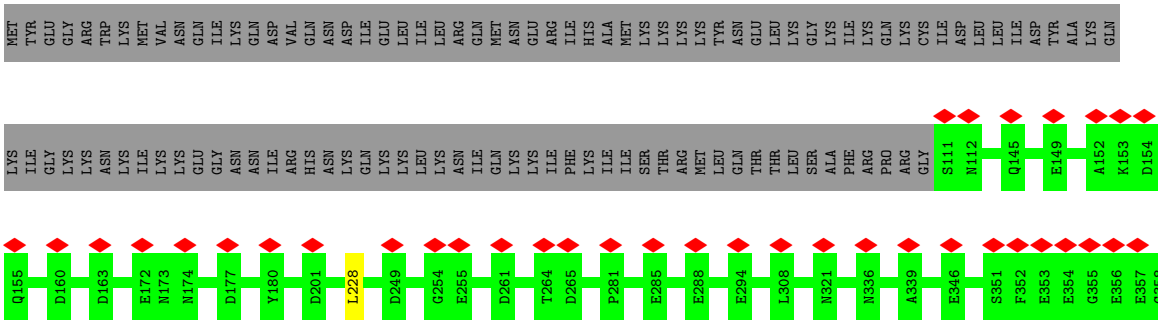


• Molecule 111: SURF1-like protein

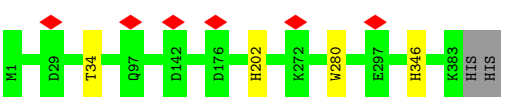


• Molecule 111: SURF1-like protein



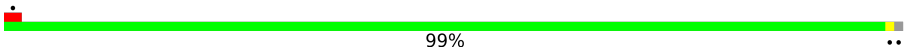


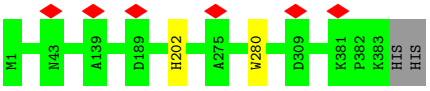
• Molecule 112: TraB family protein



• Molecule 112: TraB family protein

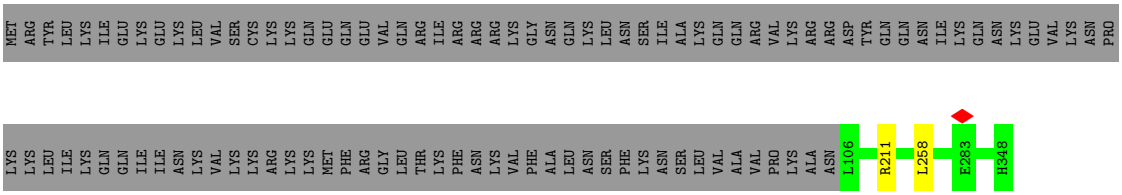
Chain Dq:





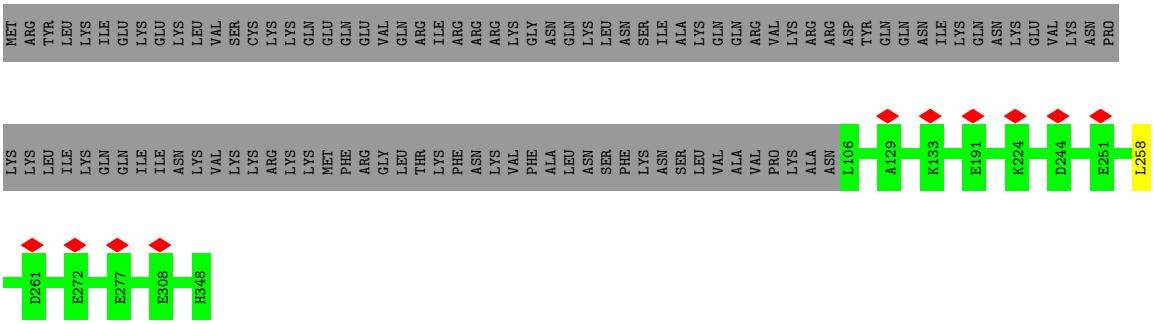
• Molecule 113: Transmembrane protein, putative

Chain DR:



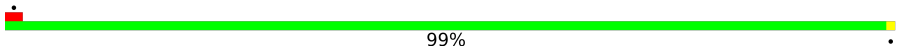
• Molecule 113: Transmembrane protein, putative

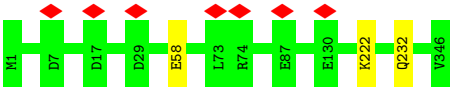
Chain Dr:



• Molecule 114: Oxoglutarate/malate translocator protein, putative

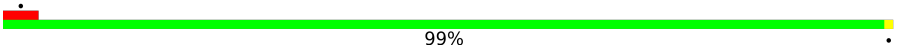
Chain DS:

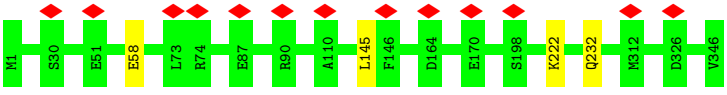




• Molecule 114: Oxoglutarate/malate translocator protein, putative

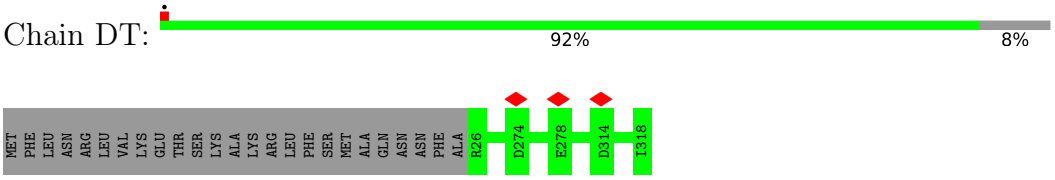
Chain Ds:





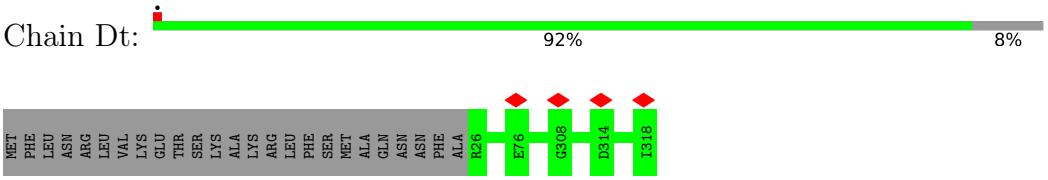
• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain DT:



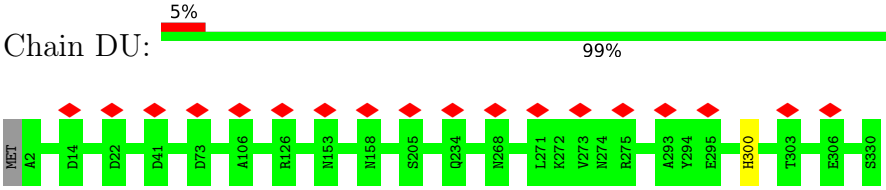
• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt:



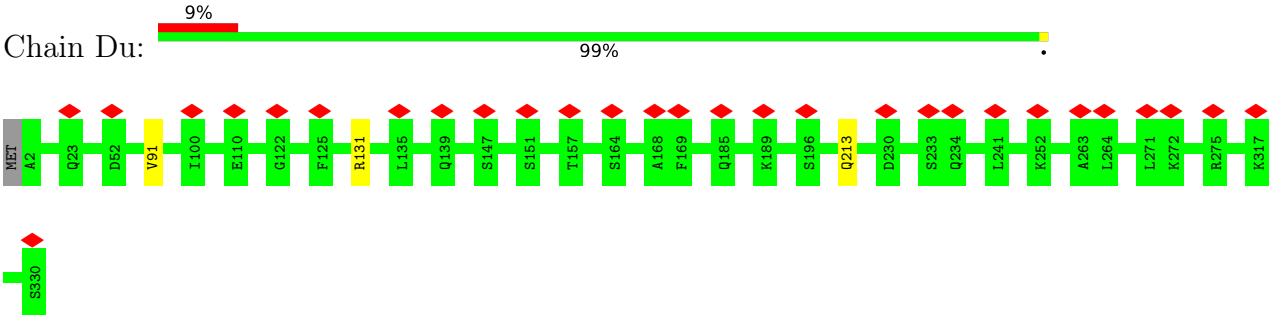
• Molecule 116: Carrier protein

Chain DU:



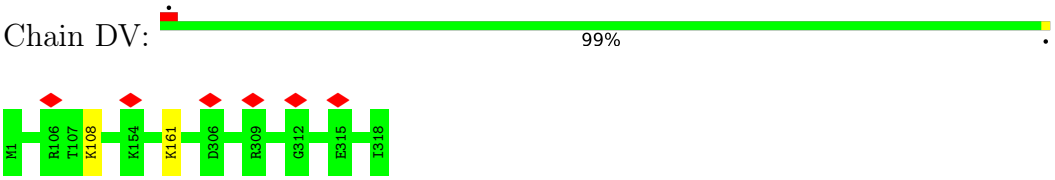
• Molecule 116: Carrier protein

Chain Du:



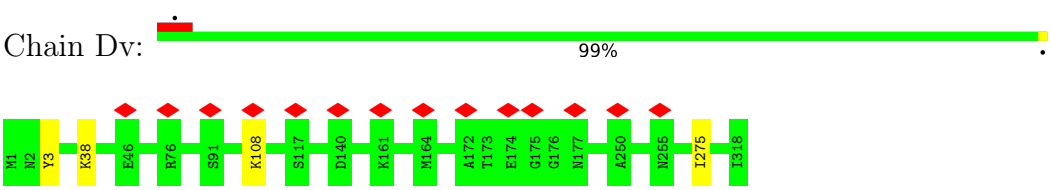
• Molecule 117: 2-oxoglutarate/malate carrier protein

Chain DV:



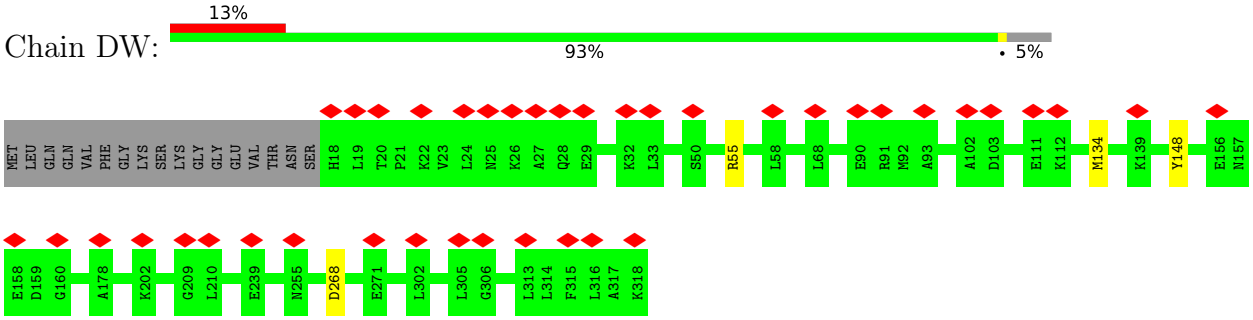
• Molecule 117: 2-oxoglutarate/malate carrier protein

Chain Dv:



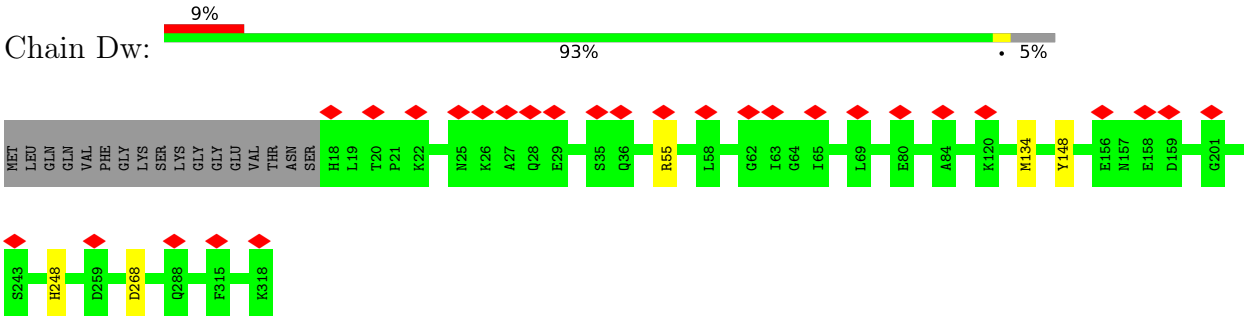
• Molecule 118: SURF1-like protein

Chain DW:



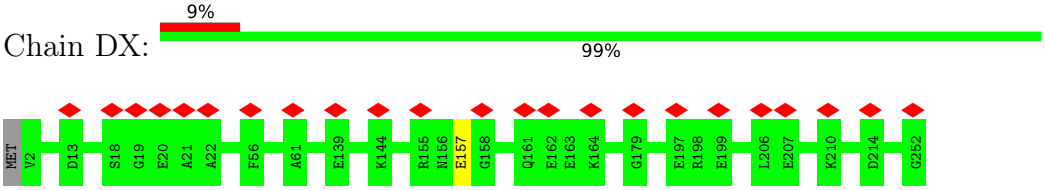
• Molecule 118: SURF1-like protein

Chain Dw:



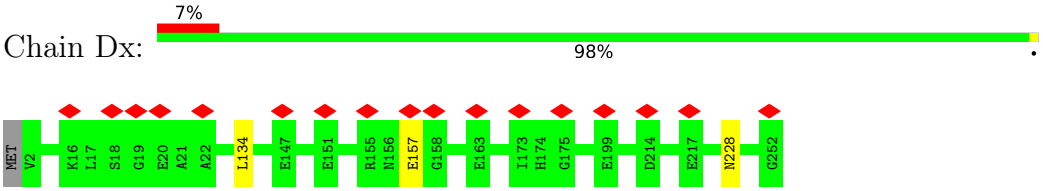
• Molecule 119: COXTT9

Chain DX:



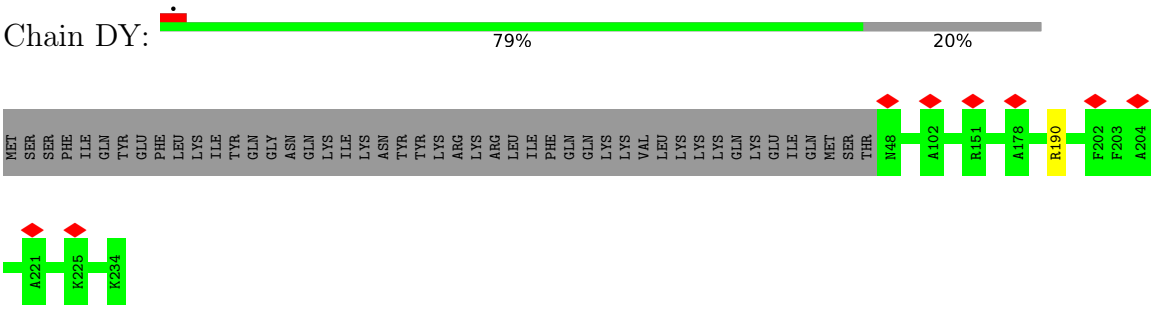
• Molecule 119: COXTT9

Chain Dx:



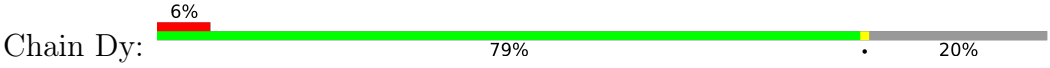
• Molecule 120: COXTT10

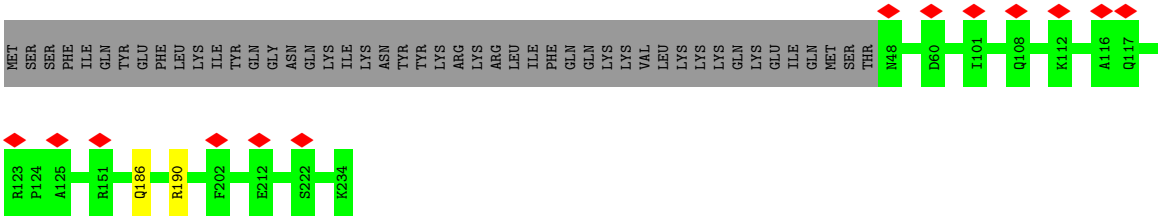
Chain DY:



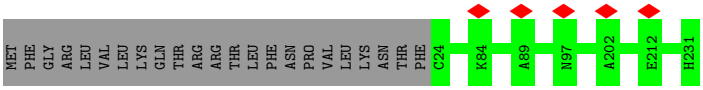
• Molecule 120: COXTT10

Chain Dy:

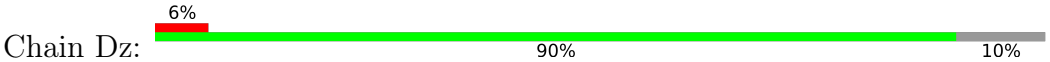


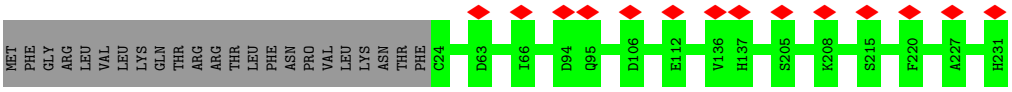


• Molecule 121: 39S ribosomal protein L9, mitochondrial

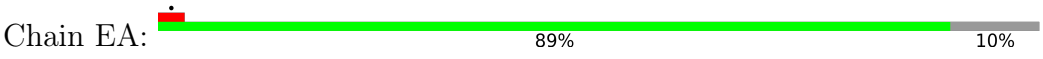


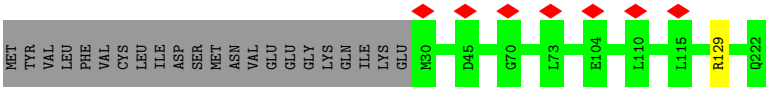
• Molecule 121: 39S ribosomal protein L9, mitochondrial



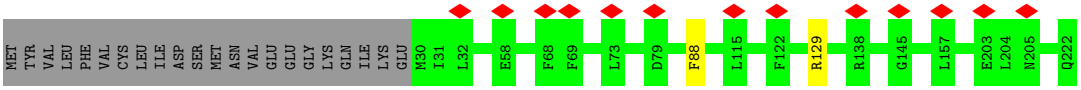


• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein

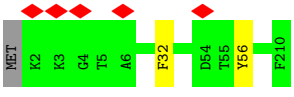




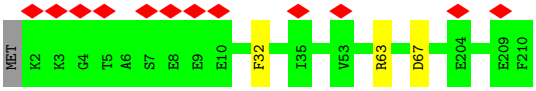
• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein



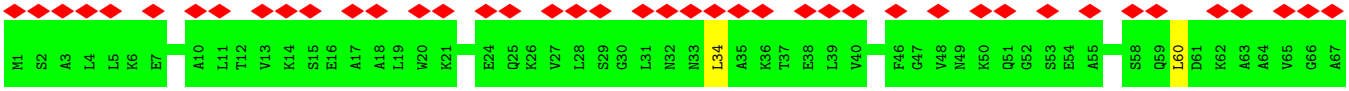
• Molecule 123: Transmembrane protein, putative

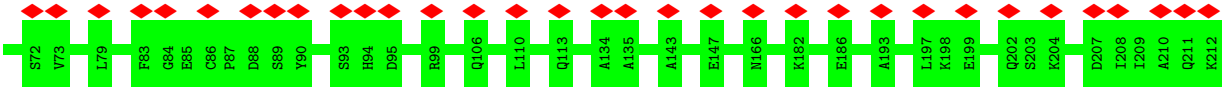


• Molecule 123: Transmembrane protein, putative

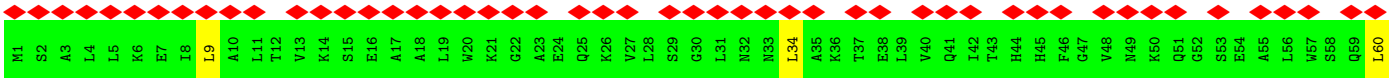


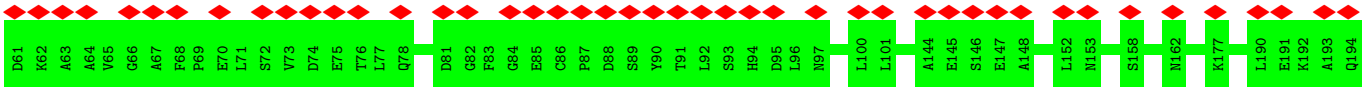
• Molecule 124: COXTT27

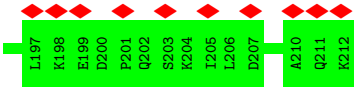




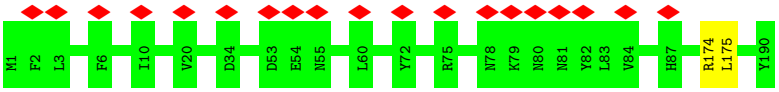
• Molecule 124: COXTT27



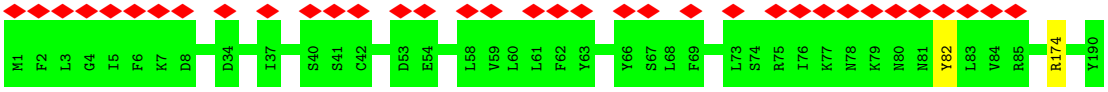




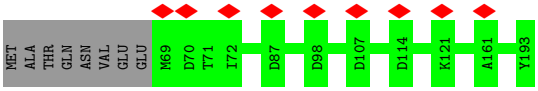
• Molecule 125: Ymf75



• Molecule 125: Ymf75

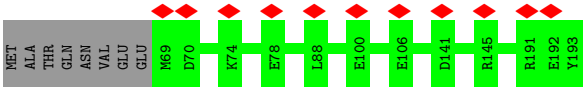


• Molecule 126: Mobilization protein



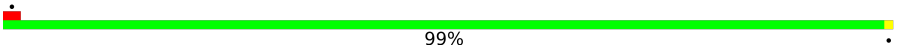
• Molecule 126: Mobilization protein

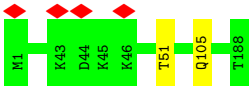
Chain Ee:



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

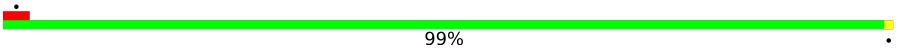
Chain EF:

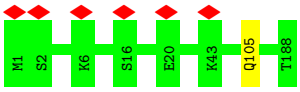




• Molecule 127: Iron-binding zinc finger CDGSH type protein

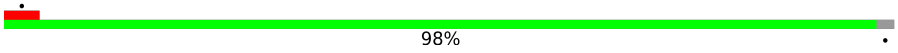
Chain Ef:

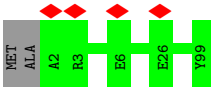




• Molecule 128: COXTT28

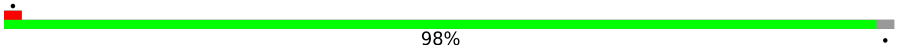
Chain EG:

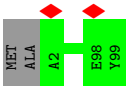




• Molecule 128: COXTT28

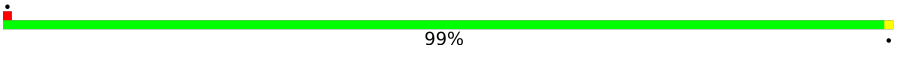
Chain Eg:

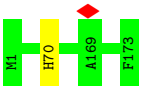




• Molecule 129: Transmembrane protein, putative

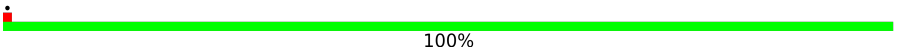
Chain EH:

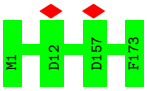




• Molecule 129: Transmembrane protein, putative

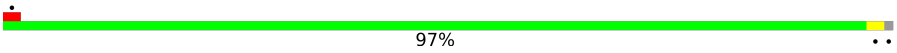
Chain Eh:

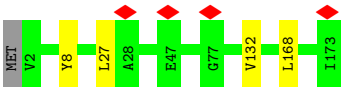




• Molecule 130: Transmembrane protein

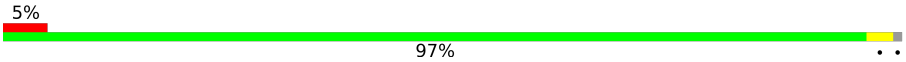
Chain EI:

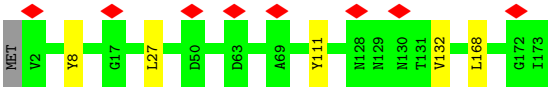




• Molecule 130: Transmembrane protein

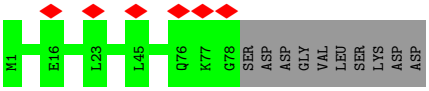
Chain Ei:





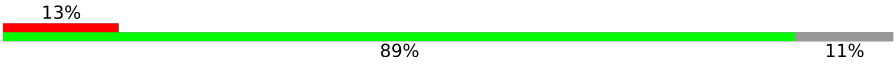
• Molecule 131: Decapping nuclease

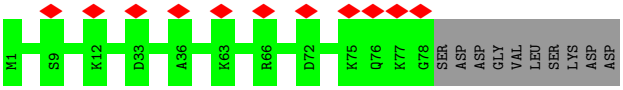
Chain EV:



• Molecule 131: Decapping nuclease

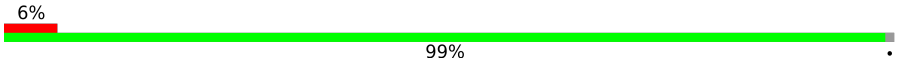
Chain Ev:

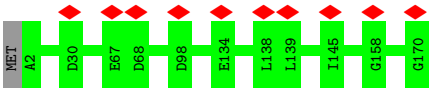




• Molecule 132: Complex III subunit VII

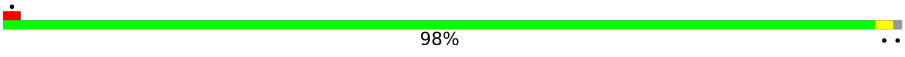
Chain EK:

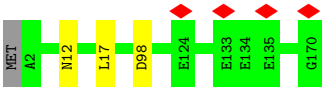




• Molecule 132: Complex III subunit VII

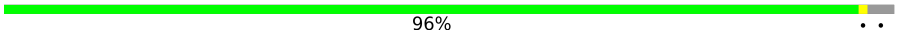
Chain Ek:

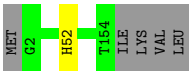




• Molecule 133: Transmembrane protein, putative

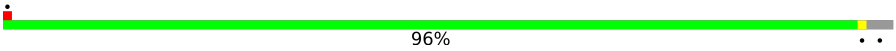
Chain EL:

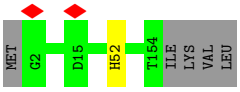




• Molecule 133: Transmembrane protein, putative

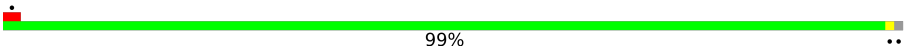
Chain El:

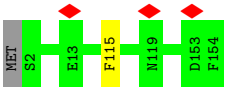




• Molecule 134: Transmembrane protein, putative

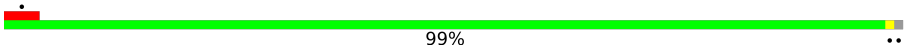
Chain EM:

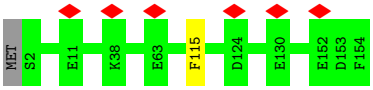




• Molecule 134: Transmembrane protein, putative

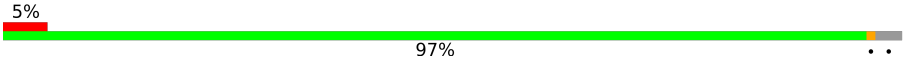
Chain Em:

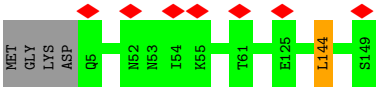




• Molecule 135: COXTT22

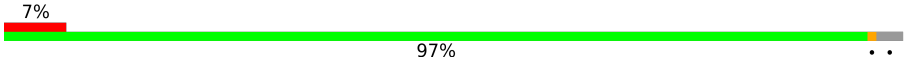
Chain EN:

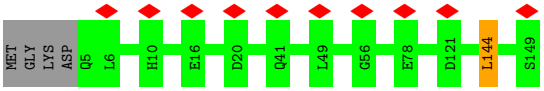




• Molecule 135: COXTT22

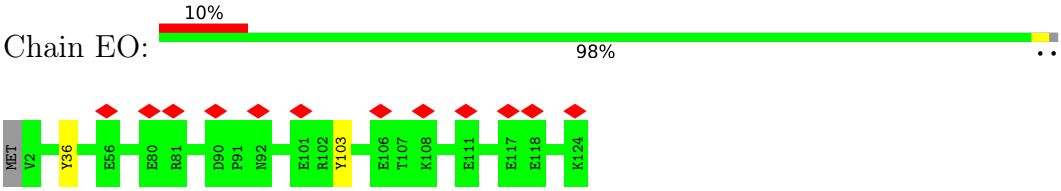
Chain En:





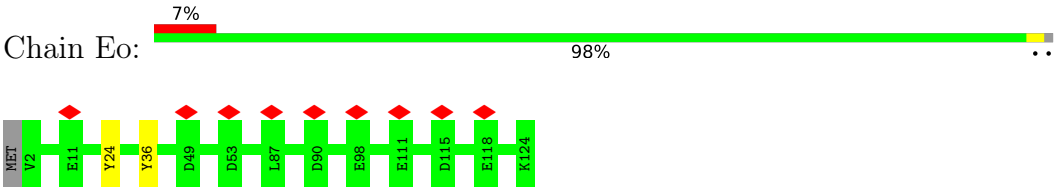
• Molecule 136: Transmembrane protein, putative

Chain EO:



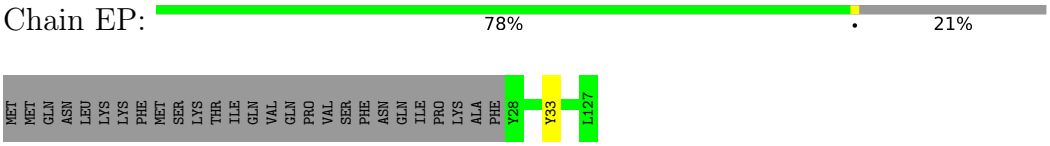
• Molecule 136: Transmembrane protein, putative

Chain Eo:



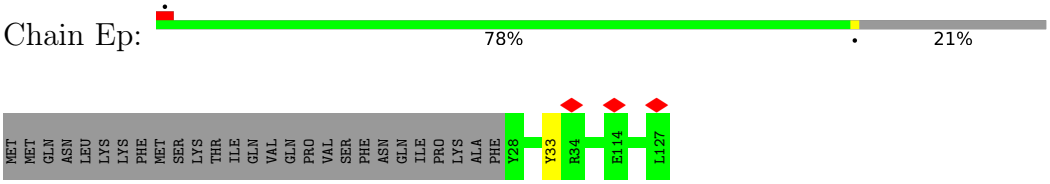
• Molecule 137: Phage protein

Chain EP:



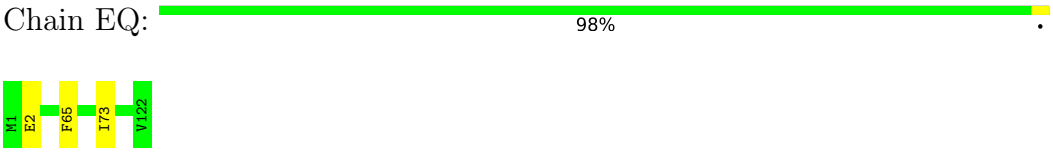
• Molecule 137: Phage protein

Chain Ep:



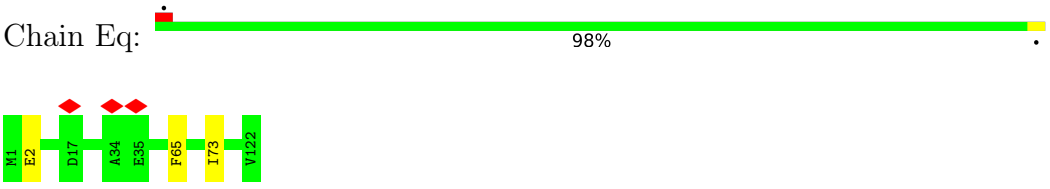
• Molecule 138: Transmembrane protein, putative

Chain EQ:



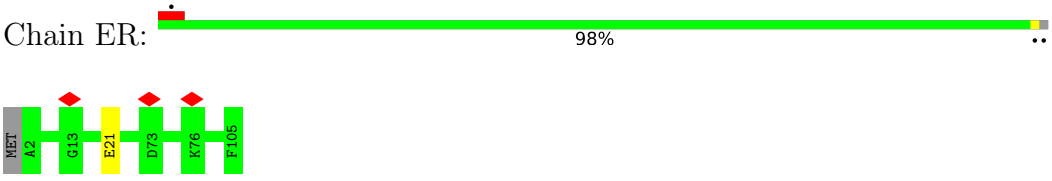
• Molecule 138: Transmembrane protein, putative

Chain Eq:



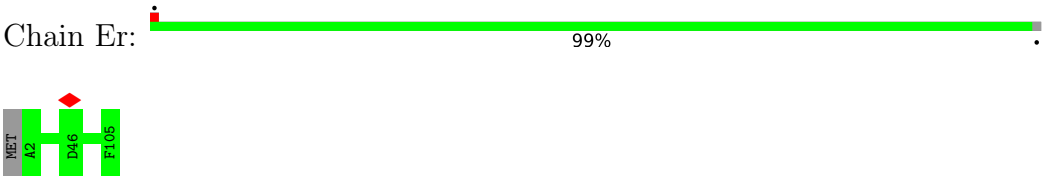
• Molecule 139: Lysozyme

Chain ER:



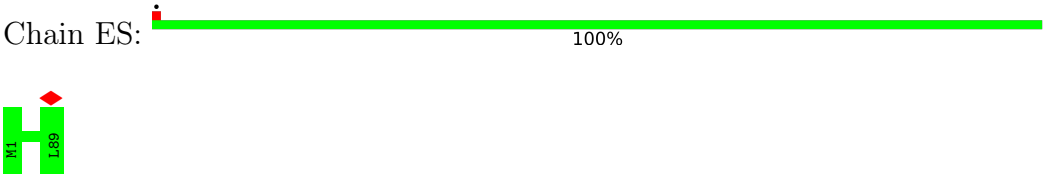
• Molecule 139: Lysozyme

Chain Er:



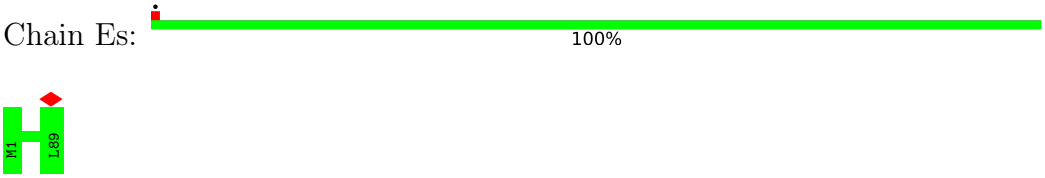
• Molecule 140: Ymf70

Chain ES:



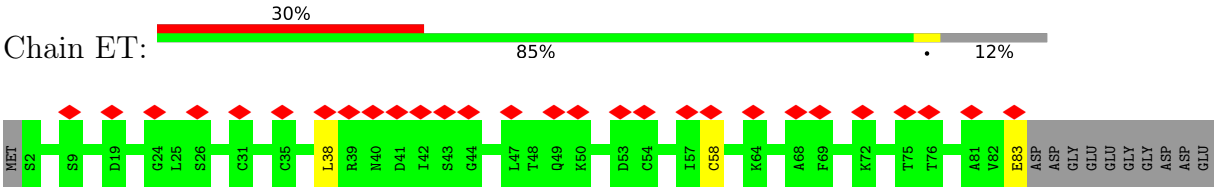
• Molecule 140: Ymf70

Chain Es:



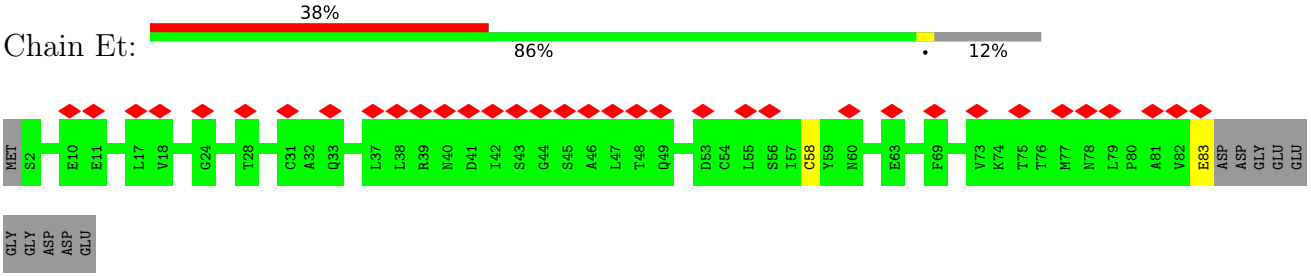
• Molecule 141: Zf-Tim10_DDP domain-containing protein

Chain ET:



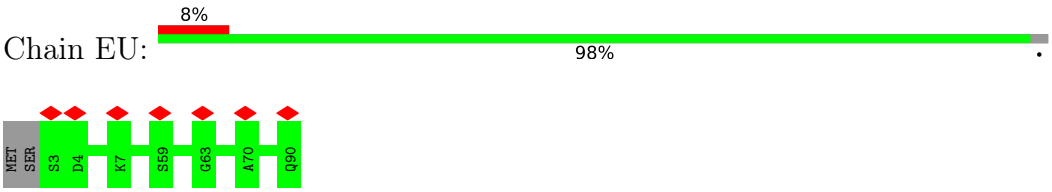
• Molecule 141: Zf-Tim10_DDP domain-containing protein

Chain Et:



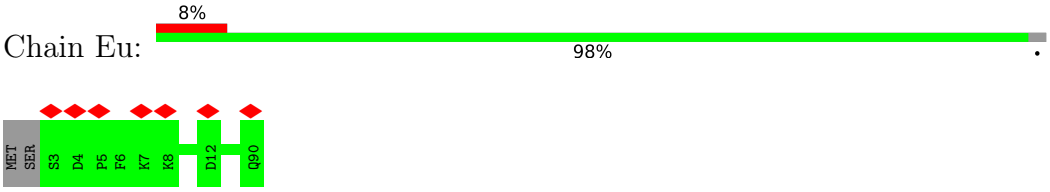
• Molecule 142: ABC transporter

Chain EU:



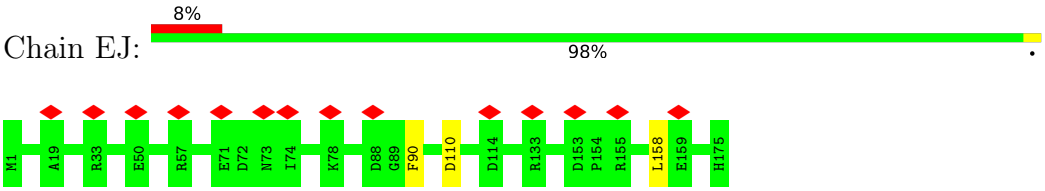
• Molecule 142: ABC transporter

Chain Eu:



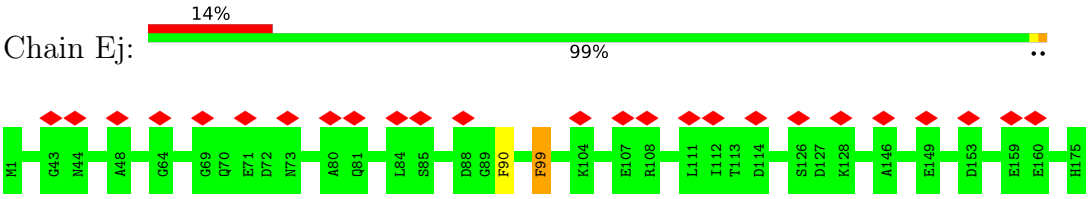
• Molecule 143: YflT domain-containing protein

Chain EJ:



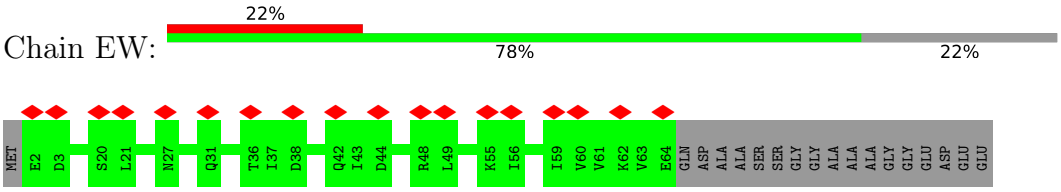
• Molecule 143: YflT domain-containing protein

Chain Ej:



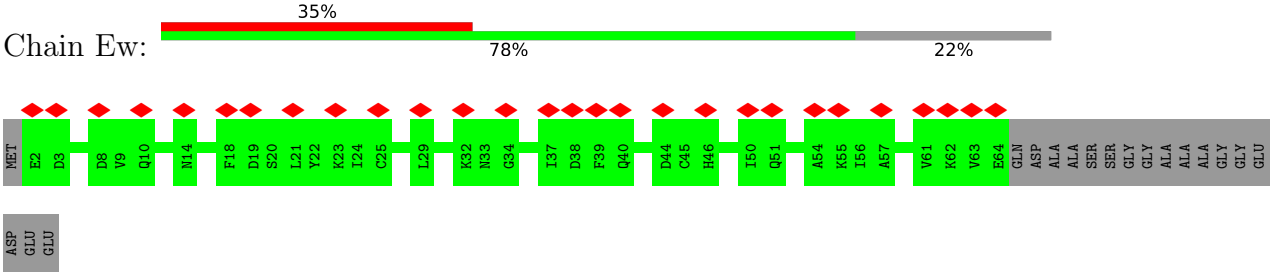
• Molecule 144: Cullin domain-containing protein

Chain EW:



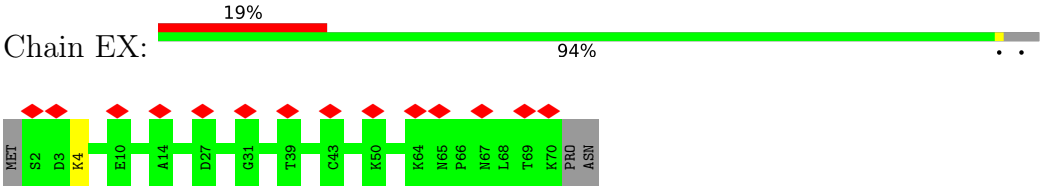
• Molecule 144: Cullin domain-containing protein

Chain Ew:



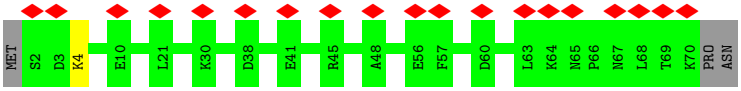
• Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain EX:



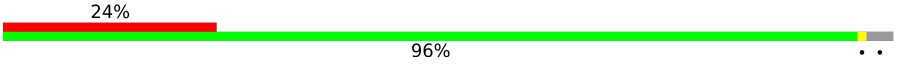
• Molecule 145: Zf-Tim10_DDP domain-containing protein

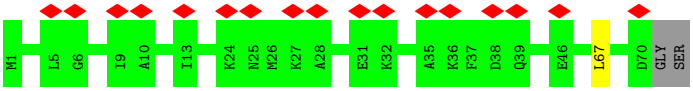
Chain Ex:



• Molecule 146: Annexin

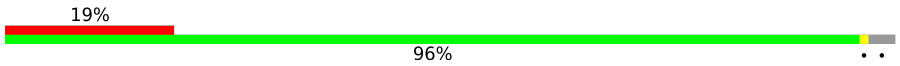
Chain EY:

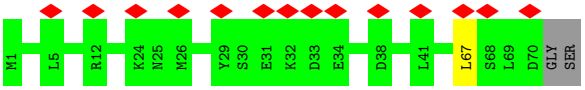




• Molecule 146: Annexin

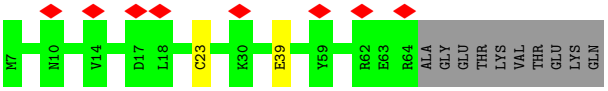
Chain Ey:





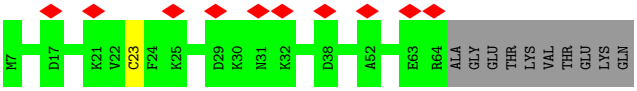
• Molecule 147: Transposase

Chain EZ:



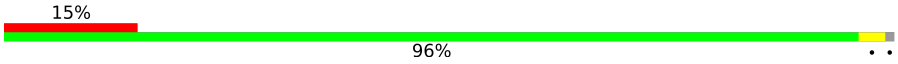
• Molecule 147: Transposase

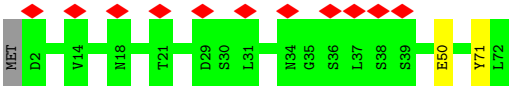
Chain Ez:



• Molecule 148: Tim10/DDP family zinc finger protein

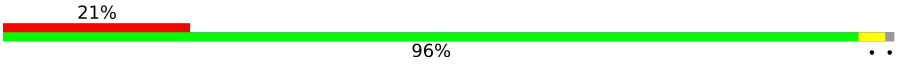
Chain FA:

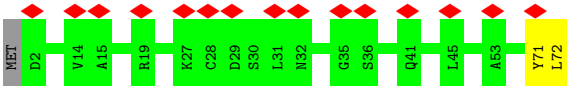




• Molecule 148: Tim10/DDP family zinc finger protein

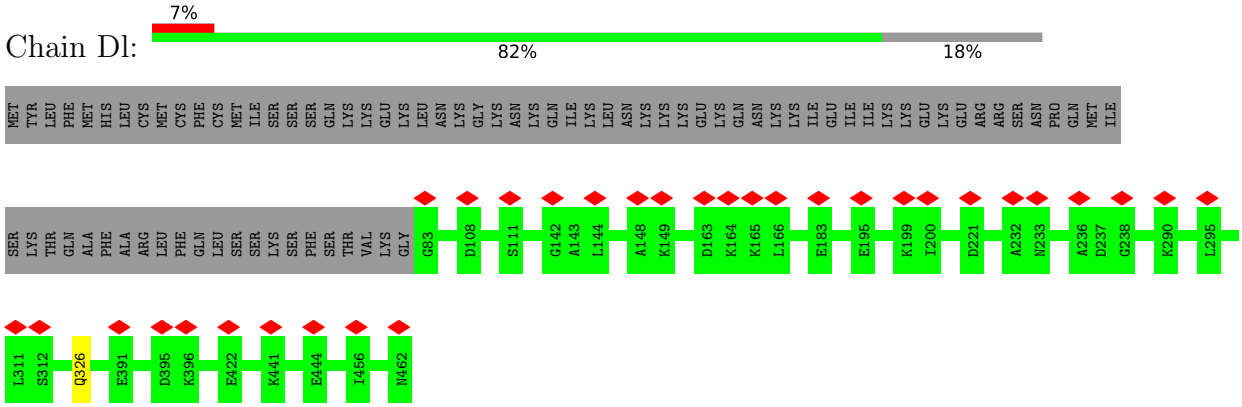
Chain Fa:





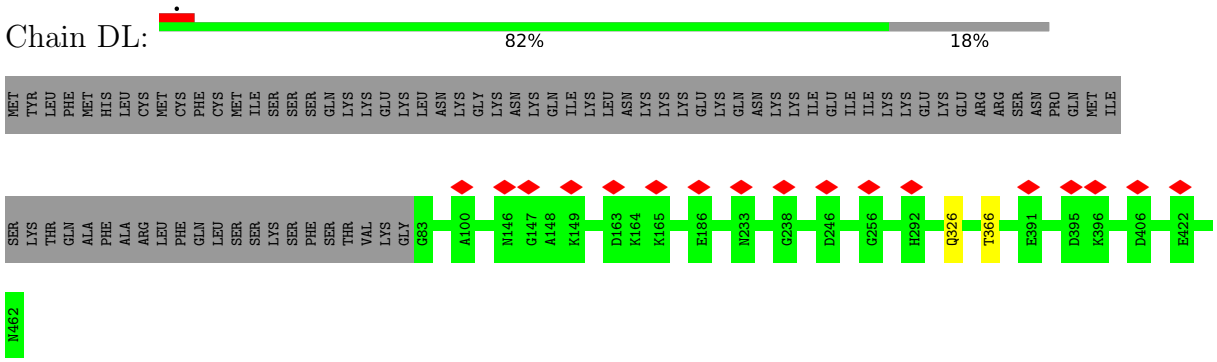
• Molecule 149: Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150

Chain Dl:



• Molecule 149: 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

5.1 Standard geometry

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

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	0/1199	0.46	0/1621
104	Dh	0.24	0/1199	0.46	0/1621
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	0/3247	0.44	0/4410
112	Dq	0.24	0/3247	0.45	0/4410
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	0/2950	0.44	0/4003
114	Ds	0.25	0/2950	0.44	0/4003
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	0/2622	0.44	0/3554
117	Dv	0.24	0/2622	0.45	0/3554
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	0/1471	0.43	0/1995
129	Eh	0.25	0/1471	0.44	0/1995
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	0.23	0/645	0.41	0/866
131	Ev	0.24	0/645	0.42	0/866
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	0.23	0/1035	0.42	0/1403
138	Eq	0.24	0/1035	0.43	0/1403
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	0/382811	0.44	44/518361 (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.

All (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
98	Db	573	LEU	CB-CG-CD2	5.98	121.16	111.00
100	Dd	265	LEU	CB-CG-CD1	5.98	121.16	111.00
100	DD	265	LEU	CB-CG-CD2	5.96	121.13	111.00
124	Ec	34	LEU	CB-CG-CD2	5.96	121.13	111.00
98	DB	573	LEU	CB-CG-CD2	5.93	121.09	111.00
124	EC	34	LEU	CB-CG-CD2	5.89	121.02	111.00
113	Dr	258	LEU	CB-CG-CD2	5.86	120.96	111.00
107	Dk	130	LEU	CB-CG-CD2	5.84	120.93	111.00
113	DR	258	LEU	CB-CG-CD2	5.79	120.85	111.00
100	DD	265	LEU	CB-CG-CD1	5.76	120.80	111.00
102	DF	10	LEU	CB-CG-CD1	5.74	120.76	111.00
107	DK	130	LEU	CB-CG-CD2	5.74	120.76	111.00
130	Ei	27	LEU	CB-CG-CD2	5.73	120.73	111.00
124	EC	60	LEU	CB-CG-CD2	5.72	120.73	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
130	EI	27	LEU	CB-CG-CD2	5.71	120.72	111.00
102	Df	10	LEU	CB-CG-CD1	5.70	120.69	111.00
124	Ec	60	LEU	CB-CG-CD2	5.68	120.66	111.00
135	EN	144	LEU	CB-CG-CD2	5.66	120.62	111.00
135	En	144	LEU	CB-CG-CD1	5.59	120.51	111.00
135	En	144	LEU	CB-CG-CD2	5.57	120.47	111.00
102	Df	10	LEU	CB-CG-CD2	5.56	120.45	111.00
135	EN	144	LEU	CB-CG-CD1	5.56	120.45	111.00
124	EC	34	LEU	CB-CG-CD1	5.55	120.43	111.00
124	Ec	60	LEU	CB-CG-CD1	5.54	120.42	111.00
124	EC	60	LEU	CB-CG-CD1	5.51	120.37	111.00
98	DB	573	LEU	CB-CG-CD1	5.50	120.35	111.00
146	Ey	67	LEU	CB-CG-CD1	5.48	120.32	111.00
124	Ec	34	LEU	CB-CG-CD1	5.48	120.31	111.00
98	Db	573	LEU	CB-CG-CD1	5.47	120.30	111.00
130	Ei	27	LEU	CB-CG-CD1	5.46	120.28	111.00
107	DK	130	LEU	CB-CG-CD1	5.45	120.27	111.00
113	DR	258	LEU	CB-CG-CD1	5.43	120.23	111.00
130	EI	27	LEU	CB-CG-CD1	5.43	120.23	111.00
107	Dk	130	LEU	CB-CG-CD1	5.41	120.20	111.00
102	DF	10	LEU	CB-CG-CD2	5.38	120.14	111.00
113	Dr	258	LEU	CB-CG-CD1	5.33	120.06	111.00
146	EY	67	LEU	CB-CG-CD1	5.32	120.04	111.00
130	EI	168	LEU	CB-CG-CD1	5.28	119.98	111.00
130	Ei	168	LEU	CB-CG-CD1	5.21	119.85	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%)	51	82
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	47	78
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%)	25	58
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

Continued on next page...

Continued from previous page...

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%)	47	78
99	Dc	580/594 (98%)	568 (98%)	12 (2%)	0	100	100
100	DD	552/637 (87%)	549 (100%)	3 (0%)	0	100	100
100	Dd	552/637 (87%)	548 (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

Continued on next page...

Continued from previous page...

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	131/133 (98%)	124 (95%)	7 (5%)	0	100	100
104	Dh	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
105	DI	201/236 (85%)	197 (98%)	4 (2%)	0	100	100
105	Di	201/236 (85%)	196 (98%)	5 (2%)	0	100	100
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	381/385 (99%)	375 (98%)	6 (2%)	0	100	100
112	Dq	381/385 (99%)	368 (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	344/346 (99%)	343 (100%)	1 (0%)	0	100	100
114	Ds	344/346 (99%)	342 (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	316/318 (99%)	314 (99%)	2 (1%)	0	100	100
117	Dv	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
118	DW	299/318 (94%)	297 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

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	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
129	Eh	171/173 (99%)	168 (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	76/88 (86%)	76 (100%)	0	0	100	100
131	Ev	76/88 (86%)	75 (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

Continued on next page...

Continued from previous page...

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	120/122 (98%)	120 (100%)	0	0	100	100
138	Eq	120/122 (98%)	119 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
149	Dl	378/462 (82%)	370 (98%)	8 (2%)	0	100	100
All	All	44774/50130 (89%)	43991 (98%)	778 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

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

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%)	73	92
2	A1	288/311 (93%)	287 (100%)	1 (0%)	92	98
3	A2	225/270 (83%)	221 (98%)	4 (2%)	59	85
4	A3	244/280 (87%)	243 (100%)	1 (0%)	91	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%)	88	96
8	A7	122/224 (54%)	121 (99%)	1 (1%)	81	94
9	A8	195/195 (100%)	194 (100%)	1 (0%)	88	96
10	A9	199/199 (100%)	195 (98%)	4 (2%)	55	82
11	AA	657/694 (95%)	646 (98%)	11 (2%)	60	86
12	AB	589/617 (96%)	588 (100%)	1 (0%)	93	98
13	AC	463/463 (100%)	457 (99%)	6 (1%)	69	90
14	AD	361/392 (92%)	360 (100%)	1 (0%)	92	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	AE	398/399 (100%)	393 (99%)	5 (1%)	69 90
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%)	62 86
19	AI	206/236 (87%)	205 (100%)	1 (0%)	88 96
20	AJ	243/244 (100%)	242 (100%)	1 (0%)	91 97
21	AK	196/218 (90%)	194 (99%)	2 (1%)	76 92
22	AL	197/215 (92%)	194 (98%)	3 (2%)	65 87
23	AM	196/197 (100%)	195 (100%)	1 (0%)	88 96
24	AN	146/186 (78%)	146 (100%)	0	100 100
25	AO	191/191 (100%)	190 (100%)	1 (0%)	88 96
26	AP	168/170 (99%)	168 (100%)	0	100 100
27	AQ	170/172 (99%)	168 (99%)	2 (1%)	71 91
28	AR	159/163 (98%)	158 (99%)	1 (1%)	86 96
29	AS	154/154 (100%)	152 (99%)	2 (1%)	69 90
30	AT	136/137 (99%)	132 (97%)	4 (3%)	42 76
31	AU	132/133 (99%)	131 (99%)	1 (1%)	81 94
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%)	59 85
35	AY	108/108 (100%)	107 (99%)	1 (1%)	78 93
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%)	71 91
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%)	59 85
44	BA	179/190 (94%)	178 (99%)	1 (1%)	86 96
45	BB	145/182 (80%)	145 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BC	155/180 (86%)	155 (100%)	0	100	100
47	BD	124/179 (69%)	123 (99%)	1 (1%)	81	94
48	BE	159/178 (89%)	158 (99%)	1 (1%)	86	96
49	BF	161/172 (94%)	161 (100%)	0	100	100
50	BG	142/156 (91%)	141 (99%)	1 (1%)	84	95
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%)	81	94
54	BK	97/131 (74%)	97 (100%)	0	100	100
55	BL	124/125 (99%)	122 (98%)	2 (2%)	62	86
56	BM	108/114 (95%)	107 (99%)	1 (1%)	78	93
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%)	71	91
62	BS	103/109 (94%)	103 (100%)	0	100	100
63	BT	110/110 (100%)	103 (94%)	7 (6%)	17	45
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%)	81	94
74	CI	97/97 (100%)	97 (100%)	0	100	100
75	CB	259/283 (92%)	255 (98%)	4 (2%)	65	87
76	CF	194/268 (72%)	194 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
77	CG	179/181 (99%)	177 (99%)	2 (1%)	73 92
78	CK	85/85 (100%)	83 (98%)	2 (2%)	49 79
79	CE	286/287 (100%)	281 (98%)	5 (2%)	60 86
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%)	84 95
85	a	411/440 (93%)	405 (98%)	6 (2%)	65 87
86	B	389/409 (95%)	388 (100%)	1 (0%)	92 98
86	b	389/409 (95%)	386 (99%)	3 (1%)	81 94
87	C	386/386 (100%)	382 (99%)	4 (1%)	76 92
87	c	386/386 (100%)	375 (97%)	11 (3%)	43 76
88	D	255/274 (93%)	253 (99%)	2 (1%)	81 94
88	d	255/274 (93%)	251 (98%)	4 (2%)	62 86
89	E	215/237 (91%)	213 (99%)	2 (1%)	78 93
89	e	215/237 (91%)	212 (99%)	3 (1%)	67 89
90	F	76/76 (100%)	76 (100%)	0	100 100
90	f	75/76 (99%)	74 (99%)	1 (1%)	69 90
91	G	288/289 (100%)	286 (99%)	2 (1%)	84 95
91	g	288/289 (100%)	285 (99%)	3 (1%)	76 92
92	H	117/118 (99%)	117 (100%)	0	100 100
92	h	117/118 (99%)	116 (99%)	1 (1%)	78 93
93	I	107/109 (98%)	104 (97%)	3 (3%)	43 76
93	i	107/109 (98%)	106 (99%)	1 (1%)	78 93
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%)	34 68
96	l	27/36 (75%)	27 (100%)	0	100 100
97	DA	596/613 (97%)	585 (98%)	11 (2%)	59 85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
97	Da	596/613 (97%)	587 (98%)	9 (2%)	65	87
98	DB	569/569 (100%)	560 (98%)	9 (2%)	62	86
98	Db	569/569 (100%)	559 (98%)	10 (2%)	59	85
99	DC	553/565 (98%)	551 (100%)	2 (0%)	91	97
99	Dc	553/565 (98%)	551 (100%)	2 (0%)	91	97
100	DD	506/579 (87%)	501 (99%)	5 (1%)	76	92
100	Dd	506/579 (87%)	503 (99%)	3 (1%)	86	96
101	DE	114/116 (98%)	114 (100%)	0	100	100
101	De	114/116 (98%)	113 (99%)	1 (1%)	78	93
102	DF	200/207 (97%)	198 (99%)	2 (1%)	76	92
102	Df	200/207 (97%)	198 (99%)	2 (1%)	76	92
103	DG	84/88 (96%)	83 (99%)	1 (1%)	71	91
103	Dg	84/88 (96%)	84 (100%)	0	100	100
104	DH	119/119 (100%)	118 (99%)	1 (1%)	81	94
104	Dh	119/119 (100%)	117 (98%)	2 (2%)	60	86
105	DI	193/218 (88%)	191 (99%)	2 (1%)	76	92
105	Di	193/218 (88%)	190 (98%)	3 (2%)	62	86
106	DJ	199/199 (100%)	195 (98%)	4 (2%)	55	82
106	Dj	199/199 (100%)	195 (98%)	4 (2%)	55	82
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%)	84	95
108	Dm	413/447 (92%)	410 (99%)	3 (1%)	84	95
109	DN	442/442 (100%)	438 (99%)	4 (1%)	78	93
109	Dn	442/442 (100%)	437 (99%)	5 (1%)	73	92
110	DO	380/413 (92%)	379 (100%)	1 (0%)	92	98
110	Do	380/413 (92%)	380 (100%)	0	100	100
111	DP	253/358 (71%)	251 (99%)	2 (1%)	81	94
111	Dp	253/358 (71%)	252 (100%)	1 (0%)	91	97
112	DQ	340/342 (99%)	336 (99%)	4 (1%)	71	91
112	Dq	340/342 (99%)	338 (99%)	2 (1%)	86	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
113	DR	219/318 (69%)	218 (100%)	1 (0%)	88 96
113	Dr	219/318 (69%)	219 (100%)	0	100 100
114	DS	293/293 (100%)	290 (99%)	3 (1%)	76 92
114	Ds	293/293 (100%)	289 (99%)	4 (1%)	67 89
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%)	91 97
116	Du	275/276 (100%)	272 (99%)	3 (1%)	73 92
117	DV	259/259 (100%)	257 (99%)	2 (1%)	81 94
117	Dv	259/259 (100%)	255 (98%)	4 (2%)	65 87
118	DW	258/272 (95%)	254 (98%)	4 (2%)	62 86
118	Dw	258/272 (95%)	253 (98%)	5 (2%)	57 84
119	DX	218/219 (100%)	217 (100%)	1 (0%)	88 96
119	Dx	218/219 (100%)	215 (99%)	3 (1%)	67 89
120	DY	169/216 (78%)	168 (99%)	1 (1%)	86 96
120	Dy	169/216 (78%)	167 (99%)	2 (1%)	71 91
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%)	86 96
122	Ea	180/201 (90%)	178 (99%)	2 (1%)	73 92
123	EB	180/181 (99%)	178 (99%)	2 (1%)	73 92
123	Eb	180/181 (99%)	177 (98%)	3 (2%)	60 86
124	EC	178/178 (100%)	178 (100%)	0	100 100
124	Ec	178/178 (100%)	177 (99%)	1 (1%)	86 96
125	ED	185/185 (100%)	183 (99%)	2 (1%)	73 92
125	Ed	185/185 (100%)	183 (99%)	2 (1%)	73 92
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%)	71 91
127	Ef	164/164 (100%)	163 (99%)	1 (1%)	86 96
128	EG	77/78 (99%)	77 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
128	Eg	77/78 (99%)	77 (100%)	0	100	100
129	EH	156/156 (100%)	155 (99%)	1 (1%)	86	96
129	Eh	156/156 (100%)	156 (100%)	0	100	100
130	EI	156/157 (99%)	154 (99%)	2 (1%)	69	90
130	Ei	156/157 (99%)	153 (98%)	3 (2%)	57	84
131	EV	71/80 (89%)	71 (100%)	0	100	100
131	Ev	71/80 (89%)	71 (100%)	0	100	100
132	EK	153/154 (99%)	153 (100%)	0	100	100
132	Ek	153/154 (99%)	150 (98%)	3 (2%)	55	82
133	EL	134/139 (96%)	133 (99%)	1 (1%)	84	95
133	El	134/139 (96%)	133 (99%)	1 (1%)	84	95
134	EM	137/138 (99%)	136 (99%)	1 (1%)	84	95
134	Em	137/138 (99%)	136 (99%)	1 (1%)	84	95
135	EN	132/135 (98%)	131 (99%)	1 (1%)	81	94
135	En	132/135 (98%)	131 (99%)	1 (1%)	81	94
136	EO	112/113 (99%)	110 (98%)	2 (2%)	59	85
136	Eo	112/113 (99%)	110 (98%)	2 (2%)	59	85
137	EP	87/113 (77%)	86 (99%)	1 (1%)	73	92
137	Ep	87/113 (77%)	86 (99%)	1 (1%)	73	92
138	EQ	104/104 (100%)	101 (97%)	3 (3%)	42	76
138	Eq	104/104 (100%)	101 (97%)	3 (3%)	42	76
139	ER	87/88 (99%)	86 (99%)	1 (1%)	73	92
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%)	31	65
141	Et	75/83 (90%)	73 (97%)	2 (3%)	44	77
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%)	57	84
143	Ej	157/157 (100%)	155 (99%)	2 (1%)	69	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
144	EW	57/66 (86%)	57 (100%)	0	100	100
144	Ew	57/66 (86%)	57 (100%)	0	100	100
145	EX	64/67 (96%)	63 (98%)	1 (2%)	62	86
145	Ex	64/67 (96%)	63 (98%)	1 (2%)	62	86
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%)	35	69
147	Ez	55/63 (87%)	54 (98%)	1 (2%)	59	85
148	FA	62/63 (98%)	60 (97%)	2 (3%)	39	73
148	Fa	62/63 (98%)	60 (97%)	2 (3%)	39	73
149	DL	308/386 (80%)	306 (99%)	2 (1%)	86	96
149	Dl	308/386 (80%)	307 (100%)	1 (0%)	92	98
All	All	40234/44788 (90%)	39882 (99%)	352 (1%)	79	93

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	421	ASP
1	A0	455	ASP
1	A0	456	ASN
1	A0	462	VAL
1	A0	465	LEU
2	A1	295	LEU
3	A2	45	ARG
3	A2	68	ARG
3	A2	175	PHE
3	A2	194	ASP
4	A3	286	ASP
7	A6	102	PHE
8	A7	134	ASP
9	A8	301	GLU
10	A9	31	LYS
10	A9	32	LYS
10	A9	80	LYS
10	A9	134	ARG
11	AA	160	ARG
11	AA	163	ASN
11	AA	165	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	AA	276	PHE
11	AA	363	ASN
11	AA	385	TYR
11	AA	386	TRP
11	AA	435	VAL
11	AA	522	PHE
11	AA	605	TYR
11	AA	706	PHE
12	AB	386	LEU
13	AC	118	PHE
13	AC	145	ASN
13	AC	205	TRP
13	AC	229	PHE
13	AC	346	TYR
13	AC	363	PHE
14	AD	380	CYS
15	AE	9	TRP
15	AE	83	ASP
15	AE	278	ASP
15	AE	368	LEU
15	AE	404	ARG
18	AH	166	PHE
18	AH	167	LEU
18	AH	207	PHE
18	AH	245	TYR
19	AI	215	VAL
20	AJ	162	PHE
21	AK	85	ASN
21	AK	130	TYR
22	AL	94	PHE
22	AL	121	ARG
22	AL	175	CYS
23	AM	172	LEU
25	AO	32	HIS
27	AQ	5	TYR
27	AQ	22	TYR
28	AR	94	HIS
29	AS	19	ASN
29	AS	80	PHE
30	AT	31	CYS
30	AT	46	PHE
30	AT	102	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	AT	144	LEU
31	AU	50	PHE
34	AX	1	MET
34	AX	57	ILE
35	AY	84	LEU
38	B1	33	TYR
43	B6	27	TYR
44	BA	212	TYR
47	BD	149	LEU
48	BE	133	ASN
50	BG	87	ARG
53	BJ	122	HIS
55	BL	26	LEU
55	BL	105	PHE
56	BM	10	PHE
61	BR	94	ASN
63	BT	40	GLN
63	BT	48	ASN
63	BT	52	VAL
63	BT	63	PHE
63	BT	122	LYS
63	BT	134	ASN
63	BT	141	GLN
73	CA	65	PHE
73	CA	160	PHE
73	CA	343	ARG
73	CA	345	VAL
75	CB	161	HIS
75	CB	231	HIS
75	CB	246	ARG
75	CB	253	ASP
77	CG	99	HIS
77	CG	169	HIS
78	CK	37	TYR
78	CK	41	VAL
79	CE	3	LEU
79	CE	47	PHE
79	CE	87	TYR
79	CE	99	HIS
79	CE	188	HIS
85	A	291	TYR
85	A	418	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	A	474	LYS
86	B	360	LEU
87	C	39	PHE
87	C	108	PHE
87	C	203	MET
87	C	208	LYS
88	D	123	GLN
88	D	303	TYR
89	E	38	LEU
89	E	88	ARG
91	G	127	ARG
91	G	192	LEU
93	I	3	TYR
93	I	67	GLN
93	I	79	HIS
96	L	11	ARG
85	a	291	TYR
85	a	346	ARG
85	a	418	TYR
85	a	474	LYS
85	a	492	HIS
85	a	505	TYR
86	b	175	ARG
86	b	312	VAL
86	b	427	PHE
87	c	3	TRP
87	c	39	PHE
87	c	92	PHE
87	c	108	PHE
87	c	203	MET
87	c	253	GLU
87	c	267	PHE
87	c	295	HIS
87	c	319	ASN
87	c	320	GLU
87	c	389	LEU
88	d	121	PHE
88	d	132	ARG
88	d	168	ARG
88	d	303	TYR
89	e	38	LEU
89	e	117	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
89	e	254	MET
90	f	26	GLU
91	g	72	LEU
91	g	189	TYR
91	g	192	LEU
92	h	55	GLU
93	i	3	TYR
97	DA	57	TYR
97	DA	149	TYR
97	DA	363	ASP
97	DA	389	PHE
97	DA	416	ARG
97	DA	429	VAL
97	DA	447	LEU
97	DA	503	PHE
97	DA	526	HIS
97	DA	591	HIS
97	DA	630	ARG
98	DB	45	TRP
98	DB	133	PHE
98	DB	175	VAL
98	DB	183	LEU
98	DB	224	PHE
98	DB	297	PHE
98	DB	524	LYS
98	DB	585	LEU
98	DB	590	ARG
99	DC	295	LYS
99	DC	425	TYR
100	DD	214	ASN
100	DD	219	GLU
100	DD	236	LYS
100	DD	247	GLU
100	DD	525	ASP
102	DF	35	LYS
102	DF	90	ASP
103	DG	1	MET
104	DH	115	ARG
105	DI	102	ARG
105	DI	106	TRP
106	DJ	26	LYS
106	DJ	62	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
106	DJ	99	ASN
106	DJ	176	MET
108	DM	206	ASP
108	DM	386	THR
108	DM	414	GLN
109	DN	114	TYR
109	DN	210	LEU
109	DN	262	LEU
109	DN	420	ASN
110	DO	272	GLU
111	DP	228	LEU
111	DP	247	LYS
112	DQ	34	THR
112	DQ	202	HIS
112	DQ	280	TRP
112	DQ	346	HIS
113	DR	211	ARG
114	DS	58	GLU
114	DS	222	LYS
114	DS	232	GLN
116	DU	300	HIS
117	DV	108	LYS
117	DV	161	LYS
118	DW	55	ARG
118	DW	134	MET
118	DW	148	TYR
118	DW	268	ASP
119	DX	157	GLU
120	DY	190	ARG
122	EA	129	ARG
123	EB	32	PHE
123	EB	56	TYR
125	ED	174	ARG
125	ED	175	LEU
127	EF	51	THR
127	EF	105	GLN
129	EH	70	HIS
130	EI	8	TYR
130	EI	132	VAL
133	EL	52	HIS
134	EM	115	PHE
135	EN	144	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
136	EO	36	TYR
136	EO	103	TYR
137	EP	33	TYR
138	EQ	2	GLU
138	EQ	65	PHE
138	EQ	73	ILE
139	ER	21	GLU
141	ET	38	LEU
141	ET	58	CYS
141	ET	83	GLU
143	EJ	90	PHE
143	EJ	110	ASP
143	EJ	158	LEU
145	EX	4	LYS
147	EZ	23	CYS
147	EZ	39	GLU
148	FA	50	GLU
148	FA	71	TYR
97	Da	57	TYR
97	Da	363	ASP
97	Da	429	VAL
97	Da	447	LEU
97	Da	503	PHE
97	Da	519	ASP
97	Da	521	PHE
97	Da	526	HIS
97	Da	630	ARG
98	Db	45	TRP
98	Db	224	PHE
98	Db	230	TYR
98	Db	291	PHE
98	Db	297	PHE
98	Db	412	THR
98	Db	511	ASP
98	Db	524	LYS
98	Db	585	LEU
98	Db	590	ARG
99	Dc	50	GLU
99	Dc	425	TYR
100	Dd	214	ASN
100	Dd	236	LYS
100	Dd	247	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
101	De	126	GLU
102	Df	35	LYS
102	Df	133	CYS
104	Dh	115	ARG
104	Dh	122	GLU
105	Di	102	ARG
105	Di	106	TRP
105	Di	208	ILE
106	Dj	26	LYS
106	Dj	62	HIS
106	Dj	176	MET
106	Dj	204	GLU
108	Dm	103	LEU
108	Dm	372	ASP
108	Dm	386	THR
109	Dn	30	LEU
109	Dn	114	TYR
109	Dn	210	LEU
109	Dn	262	LEU
109	Dn	420	ASN
111	Dp	228	LEU
112	Dq	202	HIS
112	Dq	280	TRP
114	Ds	58	GLU
114	Ds	145	LEU
114	Ds	222	LYS
114	Ds	232	GLN
116	Du	91	VAL
116	Du	131	ARG
116	Du	213	GLN
117	Dv	3	TYR
117	Dv	38	LYS
117	Dv	108	LYS
117	Dv	275	ILE
118	Dw	55	ARG
118	Dw	134	MET
118	Dw	148	TYR
118	Dw	248	HIS
118	Dw	268	ASP
119	Dx	134	LEU
119	Dx	157	GLU
119	Dx	228	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
120	Dy	186	GLN
120	Dy	190	ARG
122	Ea	88	PHE
122	Ea	129	ARG
123	Eb	32	PHE
123	Eb	63	ARG
123	Eb	67	ASP
124	Ec	9	LEU
125	Ed	82	TYR
125	Ed	174	ARG
127	Ef	105	GLN
130	Ei	8	TYR
130	Ei	111	TYR
130	Ei	132	VAL
132	Ek	12	ASN
132	Ek	17	LEU
132	Ek	98	ASP
133	El	52	HIS
134	Em	115	PHE
135	En	144	LEU
136	Eo	24	TYR
136	Eo	36	TYR
137	Ep	33	TYR
138	Eq	2	GLU
138	Eq	65	PHE
138	Eq	73	ILE
141	Et	58	CYS
141	Et	83	GLU
143	Ej	90	PHE
143	Ej	99	PHE
145	Ex	4	LYS
147	Ez	23	CYS
148	Fa	71	TYR
148	Fa	72	LEU
149	Dl	326	GLN
149	DL	326	GLN
149	DL	366	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
5	A4	283	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A9	133	ASN
10	A9	145	ASN
11	AA	68	HIS
11	AA	168	ASN
11	AA	290	ASN
12	AB	141	GLN
13	AC	101	ASN
13	AC	107	ASN
14	AD	134	ASN
14	AD	314	ASN
16	AF	133	ASN
20	AJ	114	HIS
20	AJ	118	ASN
27	AQ	63	ASN
28	AR	69	GLN
29	AS	17	GLN
34	AX	12	ASN
41	B4	64	GLN
46	BC	178	ASN
47	BD	68	GLN
47	BD	177	ASN
48	BE	150	ASN
61	BR	109	HIS
75	CB	70	GLN
75	CB	231	HIS
76	CF	153	GLN
79	CE	265	ASN
81	CN	24	ASN
81	CN	43	GLN
81	CN	44	ASN
84	CD	23	ASN
85	A	347	GLN
85	A	364	HIS
85	a	71	ASN
85	a	170	ASN
86	b	302	ASN
87	c	107	ASN
91	g	290	ASN
98	DB	198	GLN
98	DB	207	ASN
99	DC	224	ASN
101	DE	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
101	DE	73	GLN
106	DJ	106	GLN
108	DM	147	GLN
109	DN	32	ASN
109	DN	404	ASN
110	DO	198	GLN
110	DO	251	GLN
112	DQ	61	ASN
113	DR	262	GLN
115	DT	181	ASN
115	DT	220	ASN
117	DV	24	ASN
118	DW	214	ASN
119	DX	82	GLN
119	DX	228	ASN
119	DX	237	HIS
123	EB	121	GLN
129	EH	80	HIS
130	EI	64	ASN
135	EN	52	ASN
139	ER	91	ASN
143	EJ	105	GLN
98	Db	198	GLN
98	Db	207	ASN
98	Db	208	GLN
99	Dc	21	ASN
99	Dc	63	ASN
99	Dc	306	GLN
100	Dd	85	HIS
101	De	56	ASN
101	De	73	GLN
108	Dm	399	HIS
108	Dm	451	GLN
112	Dq	281	HIS
113	Dr	262	GLN
114	Ds	327	GLN
116	Du	17	ASN
116	Du	234	GLN
118	Dw	192	GLN
118	Dw	232	HIS
119	Dx	47	GLN
119	Dx	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
121	Dz	141	GLN
122	Ea	53	ASN
125	Ed	184	ASN
126	Ee	135	ASN
132	Ek	55	ASN
143	Ej	75	GLN
149	Dl	260	ASN
149	DL	90	GLN
149	DL	260	ASN
149	DL	336	ASN
149	DL	386	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

16 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	TPO	DD	387	100	8,10,11	1.57	1 (12%)	10,14,16	1.90	1 (10%)
104	AME	Dh	1	104	9,10,11	0.22	0	9,11,13	0.49	0
129	AME	EH	1	129	9,10,11	0.20	0	9,11,13	0.48	0
114	AME	Ds	1	114	9,10,11	0.22	0	9,11,13	0.56	0
114	AME	DS	1	114	9,10,11	0.22	0	9,11,13	0.50	0
117	AME	Dv	1	117	9,10,11	0.22	0	9,11,13	0.57	0
138	AME	Eq	1	138	9,10,11	0.23	0	9,11,13	0.49	0
129	AME	Eh	1	129	9,10,11	0.23	0	9,11,13	0.50	0
131	AME	Ev	1	131	9,10,11	0.23	0	9,11,13	0.51	0
112	AME	Dq	1	112	9,10,11	0.23	0	9,11,13	0.47	0
117	AME	DV	1	117	9,10,11	0.23	0	9,11,13	0.57	0
138	AME	EQ	1	138	9,10,11	0.24	0	9,11,13	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
131	AME	EV	1	131	9,10,11	0.24	0	9,11,13	0.51	0
112	AME	DQ	1	112	9,10,11	0.23	0	9,11,13	0.47	0
104	AME	DH	1	104	9,10,11	0.22	0	9,11,13	0.49	0
100	TPO	Dd	387	100	8,10,11	1.57	1 (12%)	10,14,16	1.83	1 (10%)

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	TPO	DD	387	100	-	2/9/11/13	-
104	AME	Dh	1	104	-	0/9/10/12	-
129	AME	EH	1	129	-	1/9/10/12	-
114	AME	Ds	1	114	-	1/9/10/12	-
114	AME	DS	1	114	-	0/9/10/12	-
117	AME	Dv	1	117	-	0/9/10/12	-
138	AME	Eq	1	138	-	1/9/10/12	-
129	AME	Eh	1	129	-	2/9/10/12	-
131	AME	Ev	1	131	-	0/9/10/12	-
112	AME	Dq	1	112	-	0/9/10/12	-
117	AME	DV	1	117	-	0/9/10/12	-
138	AME	EQ	1	138	-	0/9/10/12	-
131	AME	EV	1	131	-	1/9/10/12	-
112	AME	DQ	1	112	-	0/9/10/12	-
104	AME	DH	1	104	-	0/9/10/12	-
100	TPO	Dd	387	100	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
100	DD	387	TPO	P-O1P	3.34	1.61	1.50
100	Dd	387	TPO	P-O1P	3.32	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
100	DD	387	TPO	P-OG1-CB	-5.46	106.71	123.21
100	Dd	387	TPO	P-OG1-CB	-5.27	107.29	123.21

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
129	EH	1	AME	O-C-CA-CB
131	EV	1	AME	C-CA-N-CT1
100	Dd	387	TPO	C-CA-CB-CG2
129	Eh	1	AME	O-C-CA-CB
138	Eq	1	AME	O-C-CA-CB
100	DD	387	TPO	C-CA-CB-CG2
129	Eh	1	AME	N-CA-CB-CG
114	Ds	1	AME	C-CA-CB-CG
100	DD	387	TPO	O-C-CA-CB
100	Dd	387	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
150	CDL	Dm	502	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	BT	204	-	99,99,99	0.33	0	105,111,111	0.59	1 (0%)
153	PC1	AU	201	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	DA	708	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	DO	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	h	501	-	99,99,99	0.30	0	105,111,111	0.54	2 (1%)
155	3PE	DI	301	-	50,50,50	0.26	0	53,55,55	0.23	0
150	CDL	AM	301	-	99,99,99	0.30	0	105,111,111	0.51	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	0.54	1 (0%)
158	FES	e	1102	89	0,4,4	-	-	-		
153	PC1	Eo	204	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	C	509	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	DN	501	-	50,50,50	0.26	0	53,55,55	0.20	0
156	LPP	DA	710	-	43,43,43	0.23	0	47,48,48	0.28	0
155	3PE	CK	101	-	50,50,50	0.26	0	53,55,55	0.21	0
161	8Q1	AS	200	-	27,33,34	0.12	0	32,40,43	0.33	0
150	CDL	Dq	1403	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
168	HEM	C	502	87	41,50,50	1.45	4 (9%)	45,82,82	1.28	3 (6%)
150	CDL	DS	405	-	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	0.56	1 (0%)
150	CDL	Dj	407	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
167	UQ8	En	1202	-	53,53,53	0.51	0	64,67,67	0.63	2 (3%)
150	CDL	Dr	403	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	H	1301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	E	303	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	Dq	1401	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
158	FES	EF	202	127	0,4,4	-	-	-		
150	CDL	Dg	202	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DS	406	-	53,53,53	0.29	0	59,61,61	0.25	0
150	CDL	EH	1601	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
173	ATP	Er	201	-	26,33,33	0.62	0	31,52,52	1.05	2 (6%)
150	CDL	Dj	401	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
153	PC1	Dc	604	-	53,53,53	0.28	0	59,61,61	0.28	0
153	PC1	DX	308	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	k	301	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	Eh	1601	-	99,99,99	0.31	0	105,111,111	0.51	1 (0%)
156	LPP	EI	402	-	43,43,43	0.23	0	47,48,48	0.27	0
150	CDL	DX	306	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
167	UQ8	El	906	-	53,53,53	0.53	0	64,67,67	0.84	3 (4%)
160	FMN	AD	502	-	33,33,33	0.19	0	48,50,50	0.32	0
150	CDL	Dv	403	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
156	LPP	A6	301	-	43,43,43	0.30	0	47,48,48	0.44	1 (2%)
167	UQ8	DS	403	-	53,53,53	0.50	0	64,67,67	0.66	1 (1%)
150	CDL	DJ	304	-	99,99,99	0.30	0	105,111,111	0.49	1 (0%)
155	3PE	Dx	1208	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	BS	1302	-	53,53,53	0.28	0	59,61,61	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	Dx	1205	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	A0	602	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
150	CDL	DM	501	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Eo	201	-	53,53,53	0.29	0	59,61,61	0.28	0
153	PC1	A1	403	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DR	402	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
156	LPP	Dn	505	-	43,43,43	0.22	0	47,48,48	0.28	0
150	CDL	c	509	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
153	PC1	AQ	202	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	AH	301	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	C	508	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	CC	302	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	DV	404	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	DN	503	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
150	CDL	DX	307	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
150	CDL	Dx	1204	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
153	PC1	c	503	-	53,53,53	0.28	0	59,61,61	0.30	0
153	PC1	Dc	609	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	H	1302	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	Dx	1206	-	50,50,50	0.27	0	53,55,55	0.21	0
153	PC1	A9	603	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DV	401	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	AU	202	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	Dn	504	-	43,43,43	0.23	0	47,48,48	0.33	0
169	HEA	Da	702	97	57,67,67	2.19	19 (33%)	61,103,103	2.28	26 (42%)
150	CDL	DN	506	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DA	707	-	53,53,53	0.28	0	59,61,61	0.27	0
169	HEA	Da	703	97	57,67,67	2.18	19 (33%)	61,103,103	2.35	26 (42%)
155	3PE	Dg	204	-	50,50,50	0.26	0	53,55,55	0.22	0
150	CDL	g	801	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Dv	401	-	99,99,99	0.30	0	105,111,111	0.52	2 (1%)
150	CDL	DD	705	-	99,99,99	0.31	0	105,111,111	0.53	0
155	3PE	Da	708	-	50,50,50	0.25	0	53,55,55	0.21	0
153	PC1	Dg	203	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	Dn	506	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	EO	205	-	53,53,53	0.30	0	59,61,61	0.27	0
150	CDL	DQ	1504	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
153	PC1	DG	203	-	53,53,53	0.29	0	59,61,61	0.28	0
167	UQ8	Ds	404	-	53,53,53	0.51	0	64,67,67	0.66	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	EO	204	-	53,53,53	0.28	0	59,61,61	0.28	0
155	3PE	DS	402	-	50,50,50	0.27	0	53,55,55	0.19	0
153	PC1	d	801	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	DA	706	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
166	HEC	d	802	88	32,50,50	2.39	12 (37%)	24,82,82	2.23	5 (20%)
150	CDL	DH	201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	DN	502	-	99,99,99	0.31	0	105,111,111	0.51	1 (0%)
153	PC1	DI	303	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Ea	501	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	ES	1101	-	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	0.55	1 (0%)
150	CDL	B1	402	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	CD	302	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
155	3PE	Dx	1207	-	50,50,50	0.26	0	53,55,55	0.20	0
155	3PE	Eo	202	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	DH	202	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dj	404	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
168	HEM	C	501	87	41,50,50	1.45	4 (9%)	45,82,82	1.36	7 (15%)
150	CDL	DD	703	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	AF	401	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	Dv	407	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	DU	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
167	UQ8	EL	905	-	53,53,53	0.51	0	64,67,67	0.80	3 (4%)
150	CDL	Eb	302	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
150	CDL	BC	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	c	508	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	EK	201	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	Ed	204	-	99,99,99	0.30	0	105,111,111	0.47	1 (0%)
159	SF4	AB	803	12	0,12,12	-	-	-		
159	SF4	CB	1001	75	0,12,12	-	-	-		
150	CDL	DA	709	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
150	CDL	CC	304	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
150	CDL	DS	404	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	CG	302	-	99,99,99	0.29	0	105,111,111	0.50	1 (0%)
167	UQ8	C	512	-	53,53,53	0.50	0	64,67,67	0.68	3 (4%)
153	PC1	B1	401	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DD	704	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	DV	406	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	A0	601	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	ED	605	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	Ds	405	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	AA	907	-	53,53,53	0.29	0	59,61,61	0.27	0
155	3PE	Eo	203	-	50,50,50	0.27	0	53,55,55	0.20	0
156	LPP	Ed	203	-	43,43,43	0.22	0	47,48,48	0.27	0
150	CDL	Ds	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	E	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	AJ	501	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	DJ	303	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DV	405	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	g	802	-	53,53,53	0.29	0	59,61,61	0.25	0
153	PC1	DJ	306	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	BT	203	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	Dq	1404	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	EN	1201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	c	502	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DI	302	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
153	PC1	DC	608	-	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	0.52	1 (0%)
155	3PE	BP	201	-	50,50,50	0.27	0	53,55,55	0.22	0
150	CDL	BT	202	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	DQ	1502	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	El	902	-	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	0.47	0
150	CDL	Dd	706	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	A6	303	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	Da	707	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	DC	601	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	CC	301	-	50,50,50	0.26	0	53,55,55	0.22	0
164	FAD	CA	702	-	53,58,58	0.62	0	68,89,89	0.70	2 (2%)
150	CDL	Dy	301	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
166	HEC	CE	401	79	32,50,50	2.90	10 (31%)	24,82,82	2.02	5 (20%)
150	CDL	EL	903	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	B1	403	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	DY	302	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	C	510	-	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	$\#\|Z\|>2$
150	CDL	Dn	503	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	DR	401	-	50,50,50	0.27	0	53,55,55	0.22	0
150	CDL	ED	604	-	99,99,99	0.30	0	105,111,111	0.47	1 (0%)
155	3PE	DC	606	-	50,50,50	0.27	0	53,55,55	0.22	0
150	CDL	AA	908	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
156	LPP	Dl	1101	-	43,43,43	0.23	0	47,48,48	0.26	0
150	CDL	Du	403	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
173	ATP	ER	201	-	26,33,33	0.62	0	31,52,52	1.05	2 (6%)
150	CDL	Ds	402	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
150	CDL	DS	401	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	Dx	1209	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	Ef	501	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	AA	904	-	53,53,53	0.28	0	59,61,61	0.30	0
156	LPP	AL	304	-	43,43,43	0.22	0	47,48,48	0.28	0
150	CDL	A1	402	-	99,99,99	0.30	0	105,111,111	0.50	0
150	CDL	BG	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
158	FES	Ef	502	127	0,4,4	-	-	-		
150	CDL	CD	301	-	99,99,99	0.29	0	105,111,111	0.51	1 (0%)
171	CUA	DB	701	98	0,1,1	-	-	-		
153	PC1	A9	601	-	53,53,53	0.29	0	59,61,61	0.26	0
168	HEM	ED	602	125	41,50,50	1.46	3 (7%)	45,82,82	1.45	8 (17%)
167	UQ8	CC	303	-	53,53,53	0.50	0	64,67,67	0.71	4 (6%)
165	F3S	CB	1002	75	0,9,9	-	-	-		
150	CDL	Dd	702	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
167	UQ8	c	510	-	53,53,53	0.50	0	64,67,67	0.70	2 (3%)
156	LPP	DN	504	-	43,43,43	0.23	0	47,48,48	0.35	0
150	CDL	B0	102	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Du	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	AA	905	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	A2	401	-	50,50,50	0.27	0	53,55,55	0.21	0
155	3PE	EN	1204	-	50,50,50	0.27	0	53,55,55	0.20	0
169	HEA	DA	702	97	57,67,67	2.19	19 (33%)	61,103,103	2.27	25 (40%)
150	CDL	EI	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	AJ	502	-	50,50,50	0.26	0	53,55,55	0.23	0
156	LPP	AA	902	-	43,43,43	0.22	0	47,48,48	0.29	0
155	3PE	EO	203	-	50,50,50	0.27	0	53,55,55	0.21	0
150	CDL	Ep	701	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	EB	303	-	53,53,53	0.29	0	59,61,61	0.27	0
155	3PE	EL	904	-	50,50,50	0.28	0	53,55,55	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	Eb	303	-	53,53,53	0.29	0	59,61,61	0.27	0
155	3PE	DG	205	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	Dc	603	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	Ds	407	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	Dy	302	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	El	905	-	50,50,50	0.28	0	53,55,55	0.21	0
167	UQ8	ED	603	-	53,53,53	0.51	0	64,67,67	0.70	3 (4%)
150	CDL	Eg	101	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	DG	204	-	50,50,50	0.26	0	53,55,55	0.20	0
155	3PE	Dx	1202	-	50,50,50	0.27	0	53,55,55	0.21	0
168	HEM	Ed	201	125	41,50,50	1.47	3 (7%)	45,82,82	1.50	8 (17%)
150	CDL	Dr	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dn	502	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	DD	706	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	CJ	201	-	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	0.56	1 (0%)
150	CDL	DJ	305	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Dj	403	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
155	3PE	A9	602	-	50,50,50	0.28	0	53,55,55	0.22	0
150	CDL	Di	1103	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
153	PC1	e	1101	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	c	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	BA	301	-	50,50,50	0.27	0	53,55,55	0.21	0
153	PC1	DB	702	-	53,53,53	0.29	0	59,61,61	0.25	0
150	CDL	Dm	501	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	EO	201	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	Dv	402	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Dh	202	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	EN	1202	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	AX	401	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	BC	302	-	99,99,99	0.30	0	105,111,111	0.57	2 (1%)
150	CDL	AA	901	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DG	201	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
153	PC1	Dv	405	-	53,53,53	0.29	0	59,61,61	0.25	0
153	PC1	Db	702	-	53,53,53	0.29	0	59,61,61	0.25	0
155	3PE	CD	303	-	50,50,50	0.27	0	53,55,55	0.22	0
153	PC1	Eo	205	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	EB	302	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
150	CDL	DV	402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	C	503	-	99,99,99	0.30	0	105,111,111	0.52	0
159	SF4	AB	802	12	0,12,12	-	-	-		
150	CDL	C	506	-	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%)
155	3PE	DX	304	-	50,50,50	0.27	0	53,55,55	0.20	0
155	3PE	Di	1102	-	50,50,50	0.26	0	53,55,55	0.24	0
150	CDL	Dd	705	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Dj	405	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
155	3PE	Ds	403	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	AA	903	-	53,53,53	0.29	0	59,61,61	0.26	0
158	FES	AI	301	19	0,4,4	-	-	-		
150	CDL	Ds	406	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	AA	906	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	AC	803	-	43,43,43	0.23	0	47,48,48	0.28	0
155	3PE	Dc	607	-	50,50,50	0.28	0	53,55,55	0.20	0
150	CDL	C	507	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DY	301	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	DC	605	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Ek	201	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
153	PC1	A2	402	-	53,53,53	0.28	0	59,61,61	0.26	0
157	ADP	A8	401	152	24,29,29	0.61	0	29,45,45	0.61	1 (3%)
153	PC1	AM	302	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	DU	403	-	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	0.56	1 (0%)
153	PC1	Dx	1203	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	BY	201	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	Do	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	BT	201	-	50,50,50	0.28	0	53,55,55	0.20	0
150	CDL	DU	404	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
155	3PE	Dr	404	-	50,50,50	0.26	0	53,55,55	0.20	0
159	SF4	AT	201	30	0,12,12	-	-	-		
150	CDL	Dq	1402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	B0	101	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
155	3PE	C	513	-	50,50,50	0.26	0	53,55,55	0.21	0
155	3PE	DX	302	-	50,50,50	0.26	0	53,55,55	0.19	0
150	CDL	En	1201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	AF	402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	DC	604	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Dx	1201	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
153	PC1	BG	202	-	53,53,53	0.28	0	59,61,61	0.25	0
159	SF4	AL	301	22	0,12,12	-	-	-		
166	HEC	D	401	88	32,50,50	2.43	12 (37%)	24,82,82	2.24	5 (20%)
150	CDL	BV	201	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	Dc	606	-	50,50,50	0.28	0	53,55,55	0.20	0
153	PC1	A6	302	-	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	0.26	0
171	CUA	Db	701	98	0,1,1	-	-	-		
159	SF4	AL	302	22	0,12,12	-	-	-		
167	UQ8	C	511	-	53,53,53	0.51	0	64,67,67	0.75	3 (4%)
153	PC1	K	501	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	BS	1301	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	Ds	408	-	50,50,50	0.27	0	53,55,55	0.20	0
154	NDP	A1	401	-	45,52,52	0.50	0	53,80,80	0.54	1 (1%)
150	CDL	DZ	501	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	CG	301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Da	709	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Dh	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Dj	406	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	CC	305	-	99,99,99	0.29	0	105,111,111	0.53	1 (0%)
150	CDL	DV	403	-	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	0.55	1 (0%)
150	CDL	EA	301	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	EO	206	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	AP	301	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	DX	301	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
153	PC1	EB	301	-	53,53,53	0.29	0	59,61,61	0.25	0
150	CDL	Dn	501	-	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	0.53	1 (0%)
150	CDL	DJ	307	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
167	UQ8	Ed	202	-	53,53,53	0.52	0	64,67,67	0.72	3 (4%)
153	PC1	Di	1104	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	EL	901	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
155	3PE	G	401	-	50,50,50	0.26	0	53,55,55	0.22	0
153	PC1	DC	603	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	AC	801	-	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	EL	902	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	c	506	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	C	504	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Ed	205	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	Du	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
168	HEM	c	505	87	41,50,50	1.46	3 (7%)	45,82,82	1.36	4 (8%)
151	UDP	A0	603	152	24,26,26	0.38	0	37,40,40	0.76	2 (5%)
150	CDL	Dc	608	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	c	507	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Dj	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	Dc	602	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	BL	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	D	402	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	Dc	601	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	DM	502	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	Em	901	-	50,50,50	0.27	0	53,55,55	0.19	0
159	SF4	AD	501	14	0,12,12	-	-	-		
158	FES	BI	201	52	0,4,4	-	-	-		
150	CDL	Di	1101	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	BE	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	Dd	703	-	50,50,50	0.28	0	53,55,55	0.20	0
150	CDL	Dg	201	-	99,99,99	0.31	0	105,111,111	0.51	1 (0%)
153	PC1	AL	303	-	53,53,53	0.28	0	59,61,61	0.28	0
155	3PE	DC	607	-	50,50,50	0.27	0	53,55,55	0.20	0
155	3PE	DX	303	-	50,50,50	0.26	0	53,55,55	0.21	0
158	FES	Ef	503	127	0,4,4	-	-	-		
150	CDL	AC	802	-	99,99,99	0.29	0	105,111,111	0.53	1 (0%)
158	FES	E	302	89	0,4,4	-	-	-		
153	PC1	Dv	406	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	A0	605	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	Eb	301	-	53,53,53	0.28	0	59,61,61	0.25	0
150	CDL	El	901	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
169	HEA	DA	703	97	57,67,67	2.17	19 (33%)	61,103,103	2.37	26 (42%)
158	FES	EF	201	127	0,4,4	-	-	-		
150	CDL	DQ	1501	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	El	904	-	53,53,53	0.27	0	59,61,61	0.28	0
167	UQ8	EN	1205	-	53,53,53	0.51	0	64,67,67	0.67	2 (3%)
150	CDL	ED	601	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	Dv	404	-	53,53,53	0.29	0	59,61,61	0.27	0
155	3PE	Dr	401	-	50,50,50	0.26	0	53,55,55	0.22	0
155	3PE	EM	901	-	50,50,50	0.27	0	53,55,55	0.20	0
155	3PE	DJ	301	-	50,50,50	0.27	0	53,55,55	0.21	0
153	PC1	A	1201	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	DQ	1503	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Ei	401	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
153	PC1	EN	1203	-	53,53,53	0.29	0	59,61,61	0.25	0
153	PC1	K	502	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	DN	505	-	43,43,43	0.22	0	47,48,48	0.28	0
153	PC1	DC	602	-	53,53,53	0.28	0	59,61,61	0.27	0
168	HEM	c	504	87	41,50,50	1.46	3 (7%)	45,82,82	1.35	6 (13%)
150	CDL	DJ	302	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
157	ADP	AQ	201	-	24,29,29	0.61	0	29,45,45	0.63	1 (3%)
158	FES	CB	1000	75	0,4,4	-	-	-		
153	PC1	AC	804	-	53,53,53	0.30	0	59,61,61	0.27	0
158	FES	AB	801	12	0,4,4	-	-	-		
153	PC1	Da	706	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	DX	305	-	53,53,53	0.29	0	59,61,61	0.26	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
150	CDL	Dm	502	-	-	27/110/110/110	-
150	CDL	BT	204	-	-	39/110/110/110	-
153	PC1	AU	201	-	-	12/57/57/57	-
153	PC1	DA	708	-	-	10/57/57/57	-
150	CDL	DO	501	-	-	29/110/110/110	-
150	CDL	h	501	-	-	26/110/110/110	-
155	3PE	DI	301	-	-	18/54/54/54	-
150	CDL	AM	301	-	-	31/110/110/110	-
150	CDL	DR	403	-	-	29/110/110/110	-
158	FES	e	1102	89	-	-	0/1/1/1
153	PC1	Eo	204	-	-	20/57/57/57	-
153	PC1	C	509	-	-	24/57/57/57	-
155	3PE	DN	501	-	-	12/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
156	LPP	DA	710	-	-	7/45/45/45	-
155	3PE	CK	101	-	-	3/54/54/54	-
161	8Q1	AS	200	-	-	12/38/40/41	-
150	CDL	Dq	1403	-	-	34/110/110/110	-
168	HEM	C	502	87	-	5/12/54/54	-
150	CDL	DS	405	-	-	32/110/110/110	-
150	CDL	DN	507	-	-	38/110/110/110	-
150	CDL	Dj	407	-	-	32/110/110/110	-
167	UQ8	En	1202	-	-	11/51/75/75	0/1/1/1
150	CDL	Dr	403	-	-	30/110/110/110	-
150	CDL	H	1301	-	-	29/110/110/110	-
153	PC1	E	303	-	-	12/57/57/57	-
150	CDL	Dq	1401	-	-	40/110/110/110	-
158	FES	EF	202	127	-	-	0/1/1/1
150	CDL	Dg	202	-	-	32/110/110/110	-
153	PC1	DS	406	-	-	19/57/57/57	-
150	CDL	EH	1601	-	-	32/110/110/110	-
173	ATP	Er	201	-	-	2/18/38/38	0/3/3/3
150	CDL	Dj	401	-	-	38/110/110/110	-
153	PC1	Dc	604	-	-	11/57/57/57	-
153	PC1	DX	308	-	-	18/57/57/57	-
153	PC1	k	301	-	-	17/57/57/57	-
150	CDL	Eh	1601	-	-	40/110/110/110	-
156	LPP	EI	402	-	-	7/45/45/45	-
150	CDL	DX	306	-	-	34/110/110/110	-
167	UQ8	El	906	-	-	13/51/75/75	0/1/1/1
160	FMN	AD	502	-	-	1/18/18/18	0/3/3/3
150	CDL	Dv	403	-	-	40/110/110/110	-
156	LPP	A6	301	-	-	3/45/45/45	-
167	UQ8	DS	403	-	-	8/51/75/75	0/1/1/1
150	CDL	DJ	304	-	-	40/110/110/110	-
155	3PE	Dx	1208	-	-	13/54/54/54	-
153	PC1	BS	1302	-	-	10/57/57/57	-
153	PC1	Dx	1205	-	-	14/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	A0	602	-	-	36/110/110/110	-
150	CDL	DM	501	-	-	41/110/110/110	-
153	PC1	Eo	201	-	-	15/57/57/57	-
153	PC1	A1	403	-	-	14/57/57/57	-
150	CDL	DR	402	-	-	33/110/110/110	-
156	LPP	Dn	505	-	-	6/45/45/45	-
150	CDL	c	509	-	-	33/110/110/110	-
153	PC1	AQ	202	-	-	15/57/57/57	-
153	PC1	AH	301	-	-	9/57/57/57	-
153	PC1	C	508	-	-	20/57/57/57	-
153	PC1	CC	302	-	-	15/57/57/57	-
153	PC1	DV	404	-	-	14/57/57/57	-
150	CDL	DN	503	-	-	26/110/110/110	-
150	CDL	DX	307	-	-	29/110/110/110	-
150	CDL	Dx	1204	-	-	46/110/110/110	-
153	PC1	c	503	-	-	16/57/57/57	-
153	PC1	Dc	609	-	-	17/57/57/57	-
150	CDL	H	1302	-	-	29/110/110/110	-
155	3PE	Dx	1206	-	-	15/54/54/54	-
153	PC1	A9	603	-	-	21/57/57/57	-
150	CDL	DV	401	-	-	32/110/110/110	-
153	PC1	AU	202	-	-	14/57/57/57	-
156	LPP	Dn	504	-	-	9/45/45/45	-
169	HEA	Da	702	97	3/3/16/16	5/32/76/76	-
150	CDL	DN	506	-	-	37/110/110/110	-
169	HEA	Da	703	97	3/3/16/16	9/32/76/76	-
153	PC1	DA	707	-	-	18/57/57/57	-
155	3PE	Dg	204	-	-	13/54/54/54	-
150	CDL	g	801	-	-	31/110/110/110	-
150	CDL	Dv	401	-	-	37/110/110/110	-
150	CDL	DD	705	-	-	34/110/110/110	-
155	3PE	Da	708	-	-	17/54/54/54	-
153	PC1	Dg	203	-	-	13/57/57/57	-
150	CDL	Dn	506	-	-	35/110/110/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	PC1	EO	205	-	-	25/57/57/57	-
150	CDL	DQ	1504	-	-	36/110/110/110	-
153	PC1	DG	203	-	-	9/57/57/57	-
167	UQ8	Ds	404	-	-	12/51/75/75	0/1/1/1
153	PC1	EO	204	-	-	10/57/57/57	-
155	3PE	DS	402	-	-	20/54/54/54	-
153	PC1	d	801	-	-	18/57/57/57	-
150	CDL	DA	706	-	-	33/110/110/110	-
166	HEC	d	802	88	-	2/10/54/54	-
150	CDL	DH	201	-	-	27/110/110/110	-
150	CDL	DN	502	-	-	40/110/110/110	-
153	PC1	DI	303	-	-	18/57/57/57	-
150	CDL	Ea	501	-	-	37/110/110/110	-
150	CDL	ES	1101	-	-	39/110/110/110	-
150	CDL	Eu	101	-	-	32/110/110/110	-
150	CDL	B1	402	-	-	33/110/110/110	-
150	CDL	CD	302	-	-	28/110/110/110	-
155	3PE	Dx	1207	-	-	19/54/54/54	-
155	3PE	Eo	202	-	-	14/54/54/54	-
150	CDL	DH	202	-	-	39/110/110/110	-
150	CDL	Dj	404	-	-	35/110/110/110	-
168	HEM	C	501	87	-	4/12/54/54	-
150	CDL	DD	703	-	-	31/110/110/110	-
150	CDL	AF	401	-	-	22/110/110/110	-
153	PC1	Dv	407	-	-	9/57/57/57	-
150	CDL	DU	401	-	-	37/110/110/110	-
167	UQ8	EL	905	-	-	11/51/75/75	0/1/1/1
150	CDL	Eb	302	-	-	37/110/110/110	-
150	CDL	BC	301	-	-	22/110/110/110	-
153	PC1	c	508	-	-	8/57/57/57	-
150	CDL	EK	201	-	-	31/110/110/110	-
150	CDL	Ed	204	-	-	27/110/110/110	-
159	SF4	AB	803	12	-	-	0/6/5/5
159	SF4	CB	1001	75	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	DA	709	-	-	23/110/110/110	-
150	CDL	CC	304	-	-	22/110/110/110	-
150	CDL	DS	404	-	-	36/110/110/110	-
150	CDL	CG	302	-	-	36/110/110/110	-
167	UQ8	C	512	-	-	10/51/75/75	0/1/1/1
153	PC1	B1	401	-	-	18/57/57/57	-
150	CDL	DD	704	-	-	32/110/110/110	-
153	PC1	DV	406	-	-	9/57/57/57	-
150	CDL	A0	601	-	-	23/110/110/110	-
150	CDL	ED	605	-	-	36/110/110/110	-
150	CDL	Ds	405	-	-	40/110/110/110	-
153	PC1	AA	907	-	-	21/57/57/57	-
155	3PE	Eo	203	-	-	8/54/54/54	-
156	LPP	Ed	203	-	-	2/45/45/45	-
150	CDL	Ds	401	-	-	28/110/110/110	-
150	CDL	E	301	-	-	28/110/110/110	-
153	PC1	AJ	501	-	-	15/57/57/57	-
150	CDL	DJ	303	-	-	31/110/110/110	-
153	PC1	DV	405	-	-	9/57/57/57	-
153	PC1	g	802	-	-	13/57/57/57	-
153	PC1	DJ	306	-	-	12/57/57/57	-
153	PC1	BT	203	-	-	16/57/57/57	-
153	PC1	Dq	1404	-	-	10/57/57/57	-
150	CDL	EN	1201	-	-	28/110/110/110	-
150	CDL	c	502	-	-	29/110/110/110	-
150	CDL	DI	302	-	-	41/110/110/110	-
153	PC1	DC	608	-	-	16/57/57/57	-
150	CDL	EO	202	-	-	33/110/110/110	-
155	3PE	BP	201	-	-	15/54/54/54	-
150	CDL	BT	202	-	-	36/110/110/110	-
150	CDL	DQ	1502	-	-	33/110/110/110	-
150	CDL	El	902	-	-	39/110/110/110	-
150	CDL	Dd	704	-	-	34/110/110/110	-
150	CDL	Dd	706	-	-	29/110/110/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	PC1	A6	303	-	-	11/57/57/57	-
153	PC1	Da	707	-	-	12/57/57/57	-
150	CDL	DC	601	-	-	39/110/110/110	-
155	3PE	CC	301	-	-	5/54/54/54	-
164	FAD	CA	702	-	-	15/30/50/50	0/6/6/6
150	CDL	Dy	301	-	-	40/110/110/110	-
166	HEC	CE	401	79	-	5/10/54/54	-
150	CDL	EL	903	-	-	37/110/110/110	-
153	PC1	B1	403	-	-	16/57/57/57	-
153	PC1	DY	302	-	-	9/57/57/57	-
153	PC1	C	510	-	-	12/57/57/57	-
150	CDL	Dn	503	-	-	30/110/110/110	-
155	3PE	DR	401	-	-	9/54/54/54	-
150	CDL	ED	604	-	-	26/110/110/110	-
155	3PE	DC	606	-	-	10/54/54/54	-
150	CDL	AA	908	-	-	29/110/110/110	-
156	LPP	Dl	1101	-	-	8/45/45/45	-
150	CDL	Du	403	-	-	30/110/110/110	-
173	ATP	ER	201	-	-	6/18/38/38	0/3/3/3
150	CDL	Ds	402	-	-	33/110/110/110	-
150	CDL	DS	401	-	-	29/110/110/110	-
153	PC1	Dx	1209	-	-	5/57/57/57	-
153	PC1	Ef	501	-	-	14/57/57/57	-
153	PC1	AA	904	-	-	14/57/57/57	-
156	LPP	AL	304	-	-	3/45/45/45	-
150	CDL	A1	402	-	-	40/110/110/110	-
150	CDL	BG	201	-	-	34/110/110/110	-
158	FES	Ef	502	127	-	-	0/1/1/1
150	CDL	CD	301	-	-	38/110/110/110	-
153	PC1	A9	601	-	-	13/57/57/57	-
168	HEM	ED	602	125	-	0/12/54/54	-
167	UQ8	CC	303	-	-	10/51/75/75	0/1/1/1
165	F3S	CB	1002	75	-	-	2/3/3/3
150	CDL	Dd	702	-	-	30/110/110/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
167	UQ8	c	510	-	-	12/51/75/75	0/1/1/1
156	LPP	DN	504	-	-	9/45/45/45	-
150	CDL	B0	102	-	-	25/110/110/110	-
150	CDL	Du	401	-	-	38/110/110/110	-
153	PC1	AA	905	-	-	15/57/57/57	-
155	3PE	A2	401	-	-	9/54/54/54	-
169	HEA	DA	702	97	3/3/16/16	4/32/76/76	-
155	3PE	EN	1204	-	-	14/54/54/54	-
150	CDL	EI	401	-	-	23/110/110/110	-
155	3PE	AJ	502	-	-	14/54/54/54	-
156	LPP	AA	902	-	-	11/45/45/45	-
155	3PE	EO	203	-	-	9/54/54/54	-
150	CDL	Ep	701	-	-	33/110/110/110	-
153	PC1	EB	303	-	-	6/57/57/57	-
155	3PE	EL	904	-	-	17/54/54/54	-
153	PC1	Eb	303	-	-	6/57/57/57	-
155	3PE	DG	205	-	-	15/54/54/54	-
153	PC1	Dc	603	-	-	14/57/57/57	-
153	PC1	Ds	407	-	-	9/57/57/57	-
153	PC1	Dy	302	-	-	12/57/57/57	-
155	3PE	El	905	-	-	17/54/54/54	-
167	UQ8	ED	603	-	-	9/51/75/75	0/1/1/1
150	CDL	Eg	101	-	-	32/110/110/110	-
155	3PE	DG	204	-	-	16/54/54/54	-
155	3PE	Dx	1202	-	-	18/54/54/54	-
168	HEM	Ed	201	125	-	0/12/54/54	-
150	CDL	Dr	402	-	-	35/110/110/110	-
150	CDL	Dn	502	-	-	41/110/110/110	-
150	CDL	DD	706	-	-	31/110/110/110	-
150	CDL	CJ	201	-	-	24/110/110/110	-
150	CDL	DG	202	-	-	27/110/110/110	-
150	CDL	DJ	305	-	-	25/110/110/110	-
150	CDL	Dj	403	-	-	35/110/110/110	-
155	3PE	A9	602	-	-	8/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Di	1103	-	-	35/110/110/110	-
153	PC1	e	1101	-	-	12/57/57/57	-
150	CDL	c	501	-	-	34/110/110/110	-
155	3PE	BA	301	-	-	17/54/54/54	-
153	PC1	DB	702	-	-	21/57/57/57	-
150	CDL	Dm	501	-	-	39/110/110/110	-
153	PC1	EO	201	-	-	12/57/57/57	-
150	CDL	Dv	402	-	-	39/110/110/110	-
150	CDL	Dh	202	-	-	39/110/110/110	-
150	CDL	EN	1202	-	-	29/110/110/110	-
153	PC1	AX	401	-	-	8/57/57/57	-
150	CDL	BC	302	-	-	32/110/110/110	-
150	CDL	AA	901	-	-	32/110/110/110	-
150	CDL	DG	201	-	-	37/110/110/110	-
153	PC1	Dv	405	-	-	19/57/57/57	-
153	PC1	Db	702	-	-	22/57/57/57	-
155	3PE	CD	303	-	-	12/54/54/54	-
153	PC1	Eo	205	-	-	14/57/57/57	-
150	CDL	EB	302	-	-	33/110/110/110	-
150	CDL	DV	402	-	-	32/110/110/110	-
150	CDL	C	503	-	-	35/110/110/110	-
159	SF4	AB	802	12	-	-	0/6/5/5
150	CDL	C	506	-	-	31/110/110/110	-
150	CDL	Ea	502	-	-	26/110/110/110	-
155	3PE	DX	304	-	-	13/54/54/54	-
155	3PE	Di	1102	-	-	17/54/54/54	-
150	CDL	Dd	705	-	-	31/110/110/110	-
150	CDL	Dj	405	-	-	29/110/110/110	-
155	3PE	Ds	403	-	-	20/54/54/54	-
153	PC1	AA	903	-	-	13/57/57/57	-
158	FES	AI	301	19	-	-	0/1/1/1
150	CDL	Ds	406	-	-	35/110/110/110	-
153	PC1	AA	906	-	-	20/57/57/57	-
156	LPP	AC	803	-	-	11/45/45/45	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
155	3PE	Dc	607	-	-	18/54/54/54	-
150	CDL	C	507	-	-	34/110/110/110	-
150	CDL	DY	301	-	-	35/110/110/110	-
153	PC1	DC	605	-	-	12/57/57/57	-
150	CDL	Ek	201	-	-	30/110/110/110	-
153	PC1	A2	402	-	-	9/57/57/57	-
157	ADP	A8	401	152	-	2/12/32/32	0/3/3/3
153	PC1	AM	302	-	-	19/57/57/57	-
150	CDL	DU	403	-	-	30/110/110/110	-
150	CDL	DU	402	-	-	29/110/110/110	-
153	PC1	Dx	1203	-	-	18/57/57/57	-
150	CDL	BY	201	-	-	28/110/110/110	-
150	CDL	Do	501	-	-	36/110/110/110	-
155	3PE	BT	201	-	-	21/54/54/54	-
150	CDL	DU	404	-	-	26/110/110/110	-
155	3PE	Dr	404	-	-	10/54/54/54	-
159	SF4	AT	201	30	-	-	0/6/5/5
150	CDL	Dq	1402	-	-	31/110/110/110	-
150	CDL	B0	101	-	-	34/110/110/110	-
155	3PE	C	513	-	-	11/54/54/54	-
155	3PE	DX	302	-	-	14/54/54/54	-
150	CDL	En	1201	-	-	32/110/110/110	-
150	CDL	AF	402	-	-	29/110/110/110	-
153	PC1	DC	604	-	-	15/57/57/57	-
150	CDL	Dx	1201	-	-	37/110/110/110	-
153	PC1	BG	202	-	-	22/57/57/57	-
159	SF4	AL	301	22	-	-	0/6/5/5
166	HEC	D	401	88	-	1/10/54/54	-
150	CDL	BV	201	-	-	24/110/110/110	-
155	3PE	Dc	606	-	-	5/54/54/54	-
153	PC1	A6	302	-	-	11/57/57/57	-
153	PC1	Dc	605	-	-	18/57/57/57	-
159	SF4	AL	302	22	-	-	0/6/5/5
167	UQ8	C	511	-	-	16/51/75/75	0/1/1/1
153	PC1	K	501	-	-	15/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	PC1	BS	1301	-	-	16/57/57/57	-
155	3PE	Ds	408	-	-	12/54/54/54	-
154	NDP	A1	401	-	-	6/30/77/77	0/5/5/5
150	CDL	DZ	501	-	-	37/110/110/110	-
150	CDL	CG	301	-	-	27/110/110/110	-
150	CDL	Da	709	-	-	41/110/110/110	-
150	CDL	Dh	201	-	-	34/110/110/110	-
153	PC1	Dj	406	-	-	10/57/57/57	-
150	CDL	CC	305	-	-	29/110/110/110	-
150	CDL	DV	403	-	-	37/110/110/110	-
150	CDL	C	505	-	-	36/110/110/110	-
150	CDL	EA	301	-	-	28/110/110/110	-
153	PC1	EO	206	-	-	17/57/57/57	-
150	CDL	AP	301	-	-	25/110/110/110	-
150	CDL	DX	301	-	-	33/110/110/110	-
153	PC1	EB	301	-	-	13/57/57/57	-
150	CDL	Dn	501	-	-	38/110/110/110	-
150	CDL	El	903	-	-	38/110/110/110	-
150	CDL	DJ	307	-	-	34/110/110/110	-
167	UQ8	Ed	202	-	-	9/51/75/75	0/1/1/1
153	PC1	Di	1104	-	-	19/57/57/57	-
150	CDL	EL	901	-	-	45/110/110/110	-
155	3PE	G	401	-	-	8/54/54/54	-
153	PC1	DC	603	-	-	14/57/57/57	-
150	CDL	AC	801	-	-	37/110/110/110	-
150	CDL	EL	902	-	-	44/110/110/110	-
150	CDL	c	506	-	-	38/110/110/110	-
150	CDL	C	504	-	-	39/110/110/110	-
150	CDL	Ed	205	-	-	30/110/110/110	-
150	CDL	Du	402	-	-	33/110/110/110	-
168	HEM	c	505	87	-	1/12/54/54	-
151	UDP	A0	603	152	-	7/16/32/32	0/2/2/2
150	CDL	Dc	608	-	-	27/110/110/110	-
153	PC1	c	507	-	-	19/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Dj	402	-	-	34/110/110/110	-
153	PC1	Dc	602	-	-	16/57/57/57	-
150	CDL	BL	301	-	-	21/110/110/110	-
153	PC1	D	402	-	-	18/57/57/57	-
150	CDL	Dc	601	-	-	37/110/110/110	-
150	CDL	DM	502	-	-	24/110/110/110	-
155	3PE	Em	901	-	-	15/54/54/54	-
159	SF4	AD	501	14	-	-	0/6/5/5
158	FES	BI	201	52	-	-	0/1/1/1
150	CDL	Di	1101	-	-	40/110/110/110	-
150	CDL	BE	201	-	-	29/110/110/110	-
155	3PE	Dd	703	-	-	18/54/54/54	-
150	CDL	Dg	201	-	-	46/110/110/110	-
153	PC1	AL	303	-	-	9/57/57/57	-
155	3PE	DC	607	-	-	13/54/54/54	-
155	3PE	DX	303	-	-	18/54/54/54	-
158	FES	Ef	503	127	-	-	0/1/1/1
150	CDL	AC	802	-	-	34/110/110/110	-
158	FES	E	302	89	-	-	0/1/1/1
153	PC1	Dv	406	-	-	13/57/57/57	-
153	PC1	A0	605	-	-	13/57/57/57	-
153	PC1	Eb	301	-	-	12/57/57/57	-
150	CDL	El	901	-	-	42/110/110/110	-
169	HEA	DA	703	97	3/3/16/16	9/32/76/76	-
158	FES	EF	201	127	-	-	0/1/1/1
150	CDL	DQ	1501	-	-	31/110/110/110	-
153	PC1	El	904	-	-	10/57/57/57	-
167	UQ8	EN	1205	-	-	15/51/75/75	0/1/1/1
150	CDL	ED	601	-	-	32/110/110/110	-
153	PC1	Dv	404	-	-	11/57/57/57	-
155	3PE	Dr	401	-	-	15/54/54/54	-
155	3PE	EM	901	-	-	13/54/54/54	-
155	3PE	DJ	301	-	-	15/54/54/54	-
153	PC1	A	1201	-	-	13/57/57/57	-
153	PC1	DQ	1503	-	-	11/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Ei	401	-	-	26/110/110/110	-
153	PC1	EN	1203	-	-	16/57/57/57	-
153	PC1	K	502	-	-	12/57/57/57	-
156	LPP	DN	505	-	-	1/45/45/45	-
153	PC1	DC	602	-	-	15/57/57/57	-
168	HEM	c	504	87	-	2/12/54/54	-
150	CDL	DJ	302	-	-	29/110/110/110	-
157	ADP	AQ	201	-	-	2/12/32/32	0/3/3/3
158	FES	CB	1000	75	-	-	0/1/1/1
153	PC1	AC	804	-	-	12/57/57/57	-
158	FES	AB	801	12	-	-	0/1/1/1
153	PC1	Da	706	-	-	16/57/57/57	-
153	PC1	DX	305	-	-	11/57/57/57	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	CE	401	HEC	C2B-C3B	10.60	1.51	1.40
166	D	401	HEC	C3C-C2C	7.13	1.48	1.40
166	d	802	HEC	C2B-C3B	6.80	1.47	1.40
166	D	401	HEC	C2B-C3B	6.73	1.47	1.40
166	d	802	HEC	C3C-C2C	6.71	1.47	1.40
169	Da	702	HEA	C3A-C2A	6.50	1.49	1.40
169	DA	702	HEA	C3A-C2A	6.40	1.49	1.40
169	Da	703	HEA	C3A-C2A	6.28	1.49	1.40
166	CE	401	HEC	C3C-C2C	6.27	1.47	1.40
169	DA	703	HEA	C3A-C2A	6.17	1.48	1.40
169	DA	702	HEA	C3B-C2B	5.55	1.47	1.34
169	Da	702	HEA	C3B-C2B	5.50	1.47	1.34
169	DA	703	HEA	C3B-C2B	5.46	1.47	1.34
169	Da	703	HEA	C3B-C2B	5.40	1.46	1.34
169	DA	702	HEA	C3C-C2C	5.21	1.47	1.40
169	Da	703	HEA	C3C-C2C	5.20	1.47	1.40
169	Da	702	HEA	C3C-C2C	5.18	1.47	1.40
169	DA	703	HEA	C3C-C2C	5.14	1.47	1.40
169	DA	703	HEA	CHC-C4B	5.02	1.47	1.35
169	Da	702	HEA	CHC-C4B	4.97	1.47	1.35
169	DA	702	HEA	CHC-C4B	4.96	1.47	1.35
169	Da	703	HEA	CHC-C4B	4.93	1.47	1.35
169	Da	702	HEA	C3D-C2D	4.90	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	Da	703	HEA	C3D-C2D	4.89	1.47	1.36
169	DA	703	HEA	C3D-C2D	4.89	1.47	1.36
169	DA	703	HEA	CHD-C1D	4.87	1.47	1.35
169	DA	702	HEA	C3D-C2D	4.85	1.47	1.36
169	Da	702	HEA	CHD-C1D	4.83	1.47	1.35
169	DA	702	HEA	CHD-C1D	4.82	1.47	1.35
169	Da	703	HEA	CHD-C1D	4.82	1.47	1.35
166	CE	401	HEC	C4B-C3B	4.32	1.50	1.43
168	c	504	HEM	C3C-C2C	-4.18	1.34	1.40
168	c	505	HEM	C3C-C2C	-4.13	1.34	1.40
168	C	501	HEM	C3C-C2C	-4.10	1.34	1.40
168	Ed	201	HEM	C3C-C2C	-4.09	1.34	1.40
168	ED	602	HEM	C3C-C2C	-4.02	1.34	1.40
168	C	502	HEM	C3C-C2C	-4.01	1.34	1.40
166	CE	401	HEC	C2A-C3A	3.85	1.49	1.37
166	CE	401	HEC	C3A-C4A	3.84	1.51	1.42
168	Ed	201	HEM	C3C-CAC	3.69	1.55	1.47
168	c	504	HEM	C3C-CAC	3.66	1.55	1.47
168	ED	602	HEM	C3C-CAC	3.64	1.55	1.47
168	c	505	HEM	C3C-CAC	3.61	1.55	1.47
168	C	501	HEM	C3C-CAC	3.61	1.55	1.47
168	C	502	HEM	C3C-CAC	3.61	1.55	1.47
166	CE	401	HEC	C2A-C1A	3.56	1.50	1.42
166	D	401	HEC	C3D-C2D	3.43	1.47	1.37
166	d	802	HEC	C3D-C2D	3.41	1.47	1.37
169	Da	702	HEA	C2A-C1A	3.38	1.50	1.42
166	d	802	HEC	C2A-C3A	3.34	1.47	1.37
166	D	401	HEC	C2A-C3A	3.29	1.47	1.37
169	DA	702	HEA	C2A-C1A	3.27	1.50	1.42
166	D	401	HEC	C3C-C4C	3.24	1.48	1.43
169	Da	703	HEA	C2A-C1A	3.18	1.49	1.42
166	d	802	HEC	C3C-C4C	3.17	1.48	1.43
169	DA	703	HEA	C2A-C1A	3.16	1.49	1.42
166	d	802	HEC	C4B-C3B	3.12	1.48	1.43
169	DA	703	HEA	FE-NB	3.04	2.11	1.96
169	Da	703	HEA	FE-NB	3.03	2.11	1.96
166	D	401	HEC	C4B-C3B	3.03	1.48	1.43
169	Da	702	HEA	FE-NB	3.00	2.11	1.96
169	DA	702	HEA	FE-NB	2.99	2.11	1.96
169	DA	703	HEA	FE-ND	2.99	2.11	1.96
169	Da	703	HEA	FE-ND	2.99	2.11	1.96
166	CE	401	HEC	C3D-C2D	2.96	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	D	401	HEC	C2A-C1A	2.95	1.49	1.42
169	Da	702	HEA	FE-ND	2.94	2.11	1.96
169	DA	703	HEA	C4B-C3B	2.92	1.49	1.44
169	DA	702	HEA	FE-ND	2.91	2.11	1.96
168	c	505	HEM	CAB-C3B	2.90	1.55	1.47
169	Da	703	HEA	C4B-C3B	2.89	1.49	1.44
168	ED	602	HEM	CAB-C3B	2.89	1.55	1.47
168	c	504	HEM	CAB-C3B	2.88	1.55	1.47
168	Ed	201	HEM	CAB-C3B	2.88	1.55	1.47
168	C	501	HEM	CAB-C3B	2.88	1.55	1.47
168	C	502	HEM	CAB-C3B	2.86	1.55	1.47
166	D	401	HEC	C1D-CHD	2.82	1.48	1.41
166	d	802	HEC	C2A-C1A	2.81	1.48	1.42
166	CE	401	HEC	C1B-CHB	2.81	1.48	1.41
169	DA	702	HEA	C4B-C3B	2.80	1.49	1.44
169	DA	702	HEA	C1D-ND	-2.79	1.35	1.40
169	Da	703	HEA	C1D-ND	-2.78	1.35	1.40
169	DA	703	HEA	C1D-ND	-2.76	1.35	1.40
169	Da	702	HEA	C1D-ND	-2.76	1.35	1.40
166	D	401	HEC	C3A-C4A	2.75	1.48	1.42
169	Da	702	HEA	C4B-C3B	2.72	1.49	1.44
166	d	802	HEC	C3A-C4A	2.69	1.48	1.42
169	Da	702	HEA	C4B-NB	-2.68	1.35	1.40
166	d	802	HEC	C1D-CHD	2.65	1.48	1.41
169	DA	702	HEA	C4B-NB	-2.63	1.35	1.40
166	D	401	HEC	C4D-CHA	2.57	1.48	1.41
166	d	802	HEC	C1C-CHC	2.56	1.48	1.41
166	D	401	HEC	C1C-CHC	2.56	1.48	1.41
166	d	802	HEC	C4D-CHA	2.52	1.48	1.41
169	DA	703	HEA	C4B-NB	-2.50	1.36	1.40
169	DA	703	HEA	C1C-CHC	2.49	1.47	1.41
169	Da	703	HEA	C1C-CHC	2.49	1.47	1.41
169	Da	703	HEA	C4B-NB	-2.48	1.36	1.40
169	Da	702	HEA	C4C-CHD	2.47	1.47	1.41
169	Da	702	HEA	C1C-CHC	2.47	1.47	1.41
169	DA	703	HEA	C4D-C3D	2.42	1.49	1.45
169	DA	702	HEA	C1C-CHC	2.42	1.47	1.41
169	DA	703	HEA	C4C-CHD	2.41	1.47	1.41
169	DA	702	HEA	C4C-CHD	2.40	1.47	1.41
169	Da	703	HEA	C4C-CHD	2.39	1.47	1.41
169	Da	703	HEA	C4D-C3D	2.37	1.49	1.45
166	CE	401	HEC	CMB-C2B	2.37	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	d	802	HEC	C1B-CHB	2.24	1.47	1.41
169	DA	702	HEA	CHB-C1B	2.22	1.47	1.41
169	Da	702	HEA	C1D-C2D	2.22	1.48	1.44
169	DA	702	HEA	C1D-C2D	2.22	1.48	1.44
169	Da	702	HEA	C4D-C3D	2.21	1.48	1.45
169	DA	703	HEA	CHA-C4D	2.20	1.47	1.41
166	D	401	HEC	C1B-CHB	2.20	1.47	1.41
169	Da	703	HEA	CHB-C1B	2.19	1.47	1.41
169	Da	703	HEA	CHA-C4D	2.18	1.47	1.41
169	DA	703	HEA	C1D-C2D	2.18	1.48	1.44
169	Da	703	HEA	C1D-C2D	2.16	1.48	1.44
169	Da	702	HEA	CHB-C1B	2.16	1.47	1.41
169	Da	703	HEA	C1B-C2B	2.15	1.48	1.44
169	Da	702	HEA	CHA-C4D	2.15	1.47	1.41
169	DA	702	HEA	C1B-C2B	2.13	1.48	1.44
169	DA	703	HEA	CHB-C1B	2.11	1.47	1.41
169	Da	702	HEA	C1B-C2B	2.09	1.48	1.44
169	DA	702	HEA	C4D-C3D	2.09	1.48	1.45
169	DA	702	HEA	CHA-C4D	2.08	1.47	1.41
169	DA	703	HEA	C1B-C2B	2.07	1.48	1.44
166	CE	401	HEC	C1D-CHD	2.04	1.46	1.41
168	C	501	HEM	CAA-C2A	2.03	1.55	1.52
168	C	502	HEM	CMB-C2B	2.00	1.55	1.50

All (356) 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	6.04	116.21	110.36
169	DA	703	HEA	C3D-C4D-ND	6.00	116.17	110.36
169	Da	702	HEA	C3D-C4D-ND	5.91	116.08	110.36
169	Da	703	HEA	C3D-C4D-ND	5.89	116.06	110.36
166	d	802	HEC	CMB-C2B-C3B	5.66	132.48	125.82
169	DA	703	HEA	C2D-C1D-ND	5.38	116.21	109.84
169	Da	703	HEA	C2D-C1D-ND	5.33	116.16	109.84
169	DA	703	HEA	C2B-C1B-NB	5.32	116.26	109.88
166	CE	401	HEC	CMC-C2C-C3C	5.31	132.06	125.82
166	d	802	HEC	C1D-C2D-C3D	-5.29	103.31	107.00
169	Da	702	HEA	C2B-C1B-NB	5.28	116.20	109.88
169	DA	702	HEA	C2D-C1D-ND	5.28	116.09	109.84
169	Da	703	HEA	C2B-C1B-NB	5.24	116.16	109.88
169	Da	702	HEA	C2D-C1D-ND	5.21	116.02	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
169	Da	702	HEA	C3B-C4B-NB	5.21	116.01	109.84
169	DA	702	HEA	C3B-C4B-NB	5.19	115.99	109.84
169	Da	703	HEA	C3B-C4B-NB	5.19	115.99	109.84
169	DA	702	HEA	C2B-C1B-NB	5.17	116.08	109.88
169	DA	703	HEA	C3B-C4B-NB	5.03	115.80	109.84
166	D	401	HEC	C1D-C2D-C3D	-5.03	103.50	107.00
166	D	401	HEC	CMC-C2C-C3C	5.02	131.73	125.82
166	d	802	HEC	CMC-C2C-C3C	4.90	131.58	125.82
169	DA	702	HEA	C1D-C2D-C3D	-4.18	102.56	106.96
169	Da	702	HEA	C1D-C2D-C3D	-4.10	102.64	106.96
166	CE	401	HEC	C1D-C2D-C3D	-4.10	104.14	107.00
169	DA	702	HEA	C3C-C4C-NC	4.10	114.51	109.21
169	DA	703	HEA	C3C-C4C-NC	4.06	114.46	109.21
169	Da	702	HEA	C3C-C4C-NC	4.05	114.45	109.21
169	Da	703	HEA	C3C-C4C-NC	4.05	114.44	109.21
169	DA	703	HEA	C1D-C2D-C3D	-4.01	102.74	106.96
169	Da	703	HEA	C1D-C2D-C3D	-4.00	102.75	106.96
167	El	906	UQ8	C7-C8-C9	3.89	133.27	126.79
169	DA	703	HEA	C13-C12-C11	-3.78	108.67	114.35
166	CE	401	HEC	CMB-C2B-C3B	3.74	130.21	125.82
169	Da	703	HEA	CMC-C2C-C3C	3.63	131.47	124.68
167	EL	905	UQ8	C7-C8-C9	3.62	132.81	126.79
169	Da	702	HEA	C1B-C2B-C3B	-3.53	102.58	106.80
167	El	906	UQ8	C8-C7-C6	3.50	121.47	112.05
169	Da	702	HEA	CMC-C2C-C3C	3.49	131.22	124.68
169	DA	702	HEA	CMC-C2C-C3C	3.49	131.21	124.68
169	DA	703	HEA	C1B-C2B-C3B	-3.45	102.67	106.80
169	DA	703	HEA	CMC-C2C-C3C	3.41	131.05	124.68
169	DA	702	HEA	C1B-C2B-C3B	-3.40	102.73	106.80
168	Ed	201	HEM	C4D-ND-C1D	3.36	108.55	105.07
169	Da	703	HEA	C27-C19-C20	3.33	120.88	115.27
169	Da	703	HEA	C1B-C2B-C3B	-3.33	102.82	106.80
169	DA	703	HEA	C26-C15-C16	3.23	120.70	115.27
168	ED	602	HEM	C4D-ND-C1D	3.19	108.37	105.07
169	DA	703	HEA	CHB-C1B-C2B	-3.15	120.06	124.98
169	DA	703	HEA	C4D-C3D-C2D	-3.15	102.31	106.90
169	DA	702	HEA	CHA-C4D-C3D	-3.15	120.21	124.84
169	Da	703	HEA	C4D-C3D-C2D	-3.10	102.38	106.90
168	c	505	HEM	C4D-ND-C1D	3.08	108.26	105.07
169	Da	702	HEA	C4D-C3D-C2D	-3.03	102.48	106.90
167	C	511	UQ8	C7-C8-C9	3.03	131.83	126.79
167	EL	905	UQ8	C8-C7-C6	3.03	120.20	112.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
169	DA	702	HEA	C4D-C3D-C2D	-3.02	102.50	106.90
168	C	501	HEM	C4D-ND-C1D	3.00	108.18	105.07
167	Ed	202	UQ8	C7-C8-C9	2.99	131.78	126.79
168	C	502	HEM	C4D-ND-C1D	2.98	108.16	105.07
168	c	504	HEM	C4D-ND-C1D	2.97	108.14	105.07
169	Da	702	HEA	CHA-C4D-C3D	-2.97	120.47	124.84
168	c	505	HEM	C1B-NB-C4B	2.97	108.14	105.07
169	Da	703	HEA	CHB-C1B-C2B	-2.95	120.38	124.98
166	CE	401	HEC	CMA-C3A-C2A	2.94	130.49	124.94
150	Di	1101	CDL	CB2-C1-CA2	-2.91	104.22	112.79
167	ED	603	UQ8	C7-C8-C9	2.91	131.63	126.79
169	DA	702	HEA	C4B-C3B-C2B	-2.89	102.47	107.41
169	Da	703	HEA	C4B-C3B-C2B	-2.89	102.48	107.41
150	EA	301	CDL	CB2-C1-CA2	-2.89	104.29	112.79
169	DA	703	HEA	C27-C19-C20	2.88	120.12	115.27
168	Ed	201	HEM	C4C-CHD-C1D	2.88	126.36	122.56
169	Da	703	HEA	C13-C12-C11	-2.87	110.03	114.35
150	BT	204	CDL	CB2-C1-CA2	-2.87	104.35	112.79
169	Da	702	HEA	CHB-C1B-C2B	-2.86	120.51	124.98
168	C	502	HEM	C1B-NB-C4B	2.85	108.02	105.07
169	DA	702	HEA	CHB-C1B-C2B	-2.85	120.53	124.98
150	C	507	CDL	CB2-C1-CA2	-2.83	104.46	112.79
150	DV	401	CDL	CB2-C1-CA2	-2.81	104.51	112.79
151	A0	603	UDP	PA-O3A-PB	-2.81	123.18	132.83
169	Da	702	HEA	C4B-C3B-C2B	-2.81	102.62	107.41
169	DA	703	HEA	C4B-C3B-C2B	-2.80	102.62	107.41
167	Ds	404	UQ8	C7-C8-C9	2.78	131.43	126.79
150	BL	301	CDL	CB2-C1-CA2	-2.78	104.60	112.79
150	Dv	403	CDL	CB2-C1-CA2	-2.78	104.61	112.79
150	El	901	CDL	CB2-C1-CA2	-2.77	104.63	112.79
169	Da	703	HEA	CAD-C3D-C4D	2.77	129.50	124.66
169	DA	703	HEA	CAD-C3D-C4D	2.76	129.48	124.66
150	AA	901	CDL	CB2-C1-CA2	-2.76	104.67	112.79
166	d	802	HEC	CBA-CAA-C2A	-2.75	107.97	112.60
168	C	501	HEM	C1B-NB-C4B	2.75	107.91	105.07
168	ED	602	HEM	C4C-CHD-C1D	2.74	126.18	122.56
169	Da	702	HEA	OMA-CMA-C3A	-2.74	118.94	124.91
169	Da	703	HEA	C26-C15-C16	2.74	119.88	115.27
167	c	510	UQ8	C8-C7-C6	2.73	119.40	112.05
150	BC	302	CDL	CB2-C1-CA2	-2.72	104.79	112.79
168	ED	602	HEM	C1B-NB-C4B	2.71	107.88	105.07
150	DN	503	CDL	CB2-C1-CA2	-2.71	104.82	112.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	Ek	201	CDL	CB2-C1-CA2	-2.70	104.85	112.79
150	DU	402	CDL	CB2-C1-CA2	-2.68	104.91	112.79
150	ES	1101	CDL	CB2-C1-CA2	-2.67	104.92	112.79
168	c	504	HEM	C1B-NB-C4B	2.67	107.83	105.07
150	ED	604	CDL	CB2-C1-CA2	-2.66	104.95	112.79
164	CA	702	FAD	P-O3P-PA	-2.66	123.69	132.83
150	DD	706	CDL	CB2-C1-CA2	-2.66	104.97	112.79
167	DS	403	UQ8	C7-C8-C9	2.66	131.21	126.79
150	DX	301	CDL	CB2-C1-CA2	-2.65	104.98	112.79
150	AC	801	CDL	CB2-C1-CA2	-2.65	104.98	112.79
150	Dg	202	CDL	CB2-C1-CA2	-2.65	104.99	112.79
150	EK	201	CDL	CB2-C1-CA2	-2.65	105.00	112.79
150	Dj	403	CDL	CB2-C1-CA2	-2.64	105.01	112.79
167	C	512	UQ8	C7-C8-C9	2.64	131.19	126.79
150	DU	404	CDL	CB2-C1-CA2	-2.63	105.06	112.79
150	Dd	706	CDL	CB2-C1-CA2	-2.62	105.07	112.79
150	DR	402	CDL	CB2-C1-CA2	-2.62	105.08	112.79
150	Eg	101	CDL	CB2-C1-CA2	-2.62	105.09	112.79
150	Do	501	CDL	CB2-C1-CA2	-2.61	105.11	112.79
168	c	504	HEM	C4B-CHC-C1C	2.61	126.00	122.56
150	h	501	CDL	CB2-C1-CA2	-2.60	105.12	112.79
150	Eb	302	CDL	CB2-C1-CA2	-2.60	105.13	112.79
167	C	511	UQ8	C8-C7-C6	2.60	119.06	112.05
150	Da	709	CDL	CB2-C1-CA2	-2.60	105.14	112.79
150	Ds	402	CDL	CB2-C1-CA2	-2.60	105.15	112.79
150	DA	706	CDL	CB2-C1-CA2	-2.59	105.15	112.79
169	Da	703	HEA	CHA-C4D-C3D	-2.59	121.03	124.84
150	DS	401	CDL	CB2-C1-CA2	-2.58	105.18	112.79
169	DA	703	HEA	CHA-C4D-C3D	-2.58	121.04	124.84
150	CC	305	CDL	CB2-C1-CA2	-2.58	105.19	112.79
150	DO	501	CDL	CB2-C1-CA2	-2.58	105.20	112.79
150	BT	202	CDL	CB2-C1-CA2	-2.57	105.21	112.79
150	Dc	601	CDL	CB2-C1-CA2	-2.57	105.23	112.79
169	Da	702	HEA	C13-C14-C15	-2.57	121.47	127.66
150	BE	201	CDL	CB2-C1-CA2	-2.57	105.23	112.79
167	EL	905	UQ8	C17-C18-C19	-2.56	121.49	127.66
150	CG	302	CDL	CB2-C1-CA2	-2.56	105.25	112.79
150	DV	403	CDL	CB2-C1-CA2	-2.56	105.26	112.79
150	Dn	502	CDL	CB2-C1-CA2	-2.56	105.26	112.79
168	Ed	201	HEM	C1B-NB-C4B	2.56	107.71	105.07
150	c	502	CDL	CB2-C1-CA2	-2.56	105.27	112.79
150	Dq	1403	CDL	CB2-C1-CA2	-2.56	105.27	112.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	DI	302	CDL	CB2-C1-CA2	-2.55	105.27	112.79
150	DD	704	CDL	CB2-C1-CA2	-2.55	105.27	112.79
150	DC	601	CDL	CB2-C1-CA2	-2.55	105.28	112.79
150	BG	201	CDL	CB2-C1-CA2	-2.55	105.28	112.79
150	E	301	CDL	CB2-C1-CA2	-2.54	105.31	112.79
169	Da	703	HEA	CMB-C2B-C1B	2.54	128.91	125.04
150	Dx	1204	CDL	CB2-C1-CA2	-2.54	105.32	112.79
150	DV	402	CDL	CB2-C1-CA2	-2.54	105.32	112.79
150	Dm	502	CDL	CB2-C1-CA2	-2.53	105.33	112.79
150	AC	802	CDL	CB2-C1-CA2	-2.53	105.35	112.79
150	DH	202	CDL	CB2-C1-CA2	-2.53	105.35	112.79
169	Da	703	HEA	CHD-C1D-C2D	-2.53	119.73	126.72
167	C	511	UQ8	C17-C18-C19	-2.52	121.59	127.66
150	Dr	403	CDL	CB2-C1-CA2	-2.52	105.38	112.79
167	Ed	202	UQ8	C8-C7-C6	2.51	118.82	112.05
150	Du	403	CDL	CB2-C1-CA2	-2.51	105.40	112.79
150	EL	901	CDL	CB2-C1-CA2	-2.51	105.40	112.79
169	Da	703	HEA	CAD-CBD-CGD	-2.51	108.20	113.60
150	CC	304	CDL	CB2-C1-CA2	-2.51	105.41	112.79
150	En	1201	CDL	CB2-C1-CA2	-2.50	105.42	112.79
169	DA	702	HEA	C13-C14-C15	-2.50	121.63	127.66
150	Dn	506	CDL	CB2-C1-CA2	-2.50	105.43	112.79
150	DQ	1502	CDL	CB2-C1-CA2	-2.50	105.44	112.79
150	Dq	1401	CDL	CB2-C1-CA2	-2.50	105.44	112.79
168	Ed	201	HEM	C4B-CHC-C1C	2.50	125.85	122.56
167	c	510	UQ8	C17-C18-C19	-2.50	121.65	127.66
150	Dh	201	CDL	CB2-C1-CA2	-2.49	105.45	112.79
150	DZ	501	CDL	CB2-C1-CA2	-2.49	105.46	112.79
150	Ea	502	CDL	CB2-C1-CA2	-2.48	105.47	112.79
150	CJ	201	CDL	CB2-C1-CA2	-2.48	105.49	112.79
150	Dj	404	CDL	CB2-C1-CA2	-2.48	105.49	112.79
150	A0	601	CDL	CB2-C1-CA2	-2.48	105.49	112.79
150	c	509	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	H	1302	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	Dn	503	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	Dx	1201	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	DM	501	CDL	CB2-C1-CA2	-2.47	105.51	112.79
150	DN	507	CDL	CB2-C1-CA2	-2.47	105.51	112.79
169	DA	703	HEA	CMD-C2D-C1D	2.47	128.80	125.04
150	DS	404	CDL	CB2-C1-CA2	-2.47	105.52	112.79
150	Dj	401	CDL	CB2-C1-CA2	-2.46	105.55	112.79
169	DA	703	HEA	CHD-C1D-C2D	-2.46	119.92	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	B1	402	CDL	CB2-C1-CA2	-2.46	105.56	112.79
150	DN	506	CDL	CB2-C1-CA2	-2.46	105.56	112.79
150	B0	101	CDL	CB2-C1-CA2	-2.46	105.56	112.79
168	Ed	201	HEM	C3D-C4D-ND	-2.46	107.43	110.17
150	DH	201	CDL	CB2-C1-CA2	-2.45	105.57	112.79
169	Da	703	HEA	C25-C23-C24	2.45	120.02	114.60
167	CC	303	UQ8	C7-C8-C9	2.45	130.87	126.79
168	C	501	HEM	C4C-CHD-C1D	2.45	125.79	122.56
150	DQ	1504	CDL	CB2-C1-CA2	-2.44	105.60	112.79
169	Da	702	HEA	CHD-C1D-C2D	-2.44	119.96	126.72
150	c	501	CDL	CB2-C1-CA2	-2.44	105.60	112.79
169	DA	702	HEA	C25-C23-C24	2.44	120.00	114.60
169	DA	702	HEA	CHD-C1D-C2D	-2.44	119.96	126.72
150	DU	401	CDL	CB2-C1-CA2	-2.44	105.60	112.79
169	Da	703	HEA	C4B-NB-C1B	-2.44	102.56	105.07
150	BY	201	CDL	CB2-C1-CA2	-2.44	105.61	112.79
169	DA	703	HEA	C25-C23-C24	2.44	119.99	114.60
150	DJ	305	CDL	CB2-C1-CA2	-2.43	105.63	112.79
150	DN	502	CDL	CB2-C1-CA2	-2.43	105.64	112.79
150	AP	301	CDL	CB2-C1-CA2	-2.43	105.64	112.79
150	Du	401	CDL	CB2-C1-CA2	-2.43	105.64	112.79
150	Ds	405	CDL	CB2-C1-CA2	-2.43	105.65	112.79
167	EN	1205	UQ8	C17-C18-C19	-2.43	121.82	127.66
169	DA	703	HEA	C1D-ND-C4D	-2.43	102.57	105.07
169	Da	702	HEA	C25-C23-C24	2.42	119.95	114.60
150	Ds	406	CDL	CB2-C1-CA2	-2.42	105.67	112.79
169	Da	702	HEA	C27-C19-C20	2.42	119.34	115.27
150	EB	302	CDL	CB2-C1-CA2	-2.41	105.68	112.79
150	EN	1202	CDL	CB2-C1-CA2	-2.41	105.69	112.79
150	Di	1103	CDL	CB2-C1-CA2	-2.41	105.71	112.79
150	CD	302	CDL	CB2-C1-CA2	-2.41	105.71	112.79
150	DA	709	CDL	CB2-C1-CA2	-2.41	105.71	112.79
150	Dv	401	CDL	CB2-C1-CA2	-2.40	105.72	112.79
167	ED	603	UQ8	C8-C7-C6	2.40	118.52	112.05
169	Da	702	HEA	C4B-NB-C1B	-2.40	102.59	105.07
150	Ea	501	CDL	CB2-C1-CA2	-2.40	105.73	112.79
150	DG	202	CDL	CB2-C1-CA2	-2.39	105.75	112.79
169	DA	702	HEA	C27-C19-C20	2.39	119.29	115.27
150	Dn	501	CDL	CB2-C1-CA2	-2.39	105.76	112.79
150	CD	301	CDL	CB2-C1-CA2	-2.39	105.77	112.79
168	c	504	HEM	C4C-CHD-C1D	2.38	125.69	122.56
169	DA	702	HEA	CMD-C2D-C1D	2.37	128.65	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	Du	402	CDL	CB2-C1-CA2	-2.37	105.82	112.79
150	EI	401	CDL	CB2-C1-CA2	-2.37	105.82	112.79
150	Dm	501	CDL	CB2-C1-CA2	-2.36	105.83	112.79
150	Dd	702	CDL	CB2-C1-CA2	-2.36	105.84	112.79
150	DS	405	CDL	CB2-C1-CA2	-2.36	105.85	112.79
169	DA	702	HEA	C1D-ND-C4D	-2.36	102.64	105.07
169	DA	703	HEA	C4B-NB-C1B	-2.36	102.64	105.07
150	DU	403	CDL	CB2-C1-CA2	-2.36	105.85	112.79
150	Dr	402	CDL	CB2-C1-CA2	-2.36	105.85	112.79
150	Ed	204	CDL	CB2-C1-CA2	-2.36	105.85	112.79
150	Eh	1601	CDL	CB2-C1-CA2	-2.35	105.86	112.79
150	EO	202	CDL	CB2-C1-CA2	-2.35	105.87	112.79
150	ED	601	CDL	CB2-C1-CA2	-2.35	105.88	112.79
168	Ed	201	HEM	CAD-CBD-CGD	-2.35	108.55	113.60
150	C	506	CDL	CB2-C1-CA2	-2.35	105.88	112.79
150	EH	1601	CDL	CB2-C1-CA2	-2.35	105.89	112.79
150	EN	1201	CDL	CB2-C1-CA2	-2.34	105.89	112.79
150	BC	301	CDL	CB2-C1-CA2	-2.34	105.90	112.79
150	Ep	701	CDL	CB2-C1-CA2	-2.34	105.90	112.79
157	AQ	201	ADP	C5-C6-N6	2.34	123.91	120.35
150	El	903	CDL	CB2-C1-CA2	-2.34	105.91	112.79
150	DG	201	CDL	CB2-C1-CA2	-2.34	105.91	112.79
169	Da	703	HEA	C1D-ND-C4D	-2.34	102.66	105.07
169	DA	703	HEA	CAD-CBD-CGD	-2.33	108.59	113.60
157	A8	401	ADP	C5-C6-N6	2.33	123.89	120.35
150	B0	102	CDL	CB2-C1-CA2	-2.33	105.93	112.79
150	DX	307	CDL	CB2-C1-CA2	-2.33	105.94	112.79
169	DA	703	HEA	C13-C14-C15	-2.33	122.06	127.66
167	CC	303	UQ8	C11-C9-C8	-2.33	116.41	121.12
150	Dj	407	CDL	CB2-C1-CA2	-2.32	105.95	112.79
167	En	1202	UQ8	C7-C8-C9	2.32	130.65	126.79
150	DM	502	CDL	CB2-C1-CA2	-2.32	105.97	112.79
150	Dh	202	CDL	CB2-C1-CA2	-2.31	105.98	112.79
150	Ei	401	CDL	CB2-C1-CA2	-2.31	105.98	112.79
173	Er	201	ATP	C5-C6-N6	2.31	123.86	120.35
169	Da	702	HEA	CMD-C2D-C1D	2.31	128.56	125.04
164	CA	702	FAD	C5A-C6A-N6A	2.30	123.85	120.35
150	Dg	201	CDL	CB2-C1-CA2	-2.30	106.02	112.79
169	DA	703	HEA	CMB-C2B-C1B	2.30	128.54	125.04
154	A1	401	NDP	C5A-C6A-N6A	2.30	123.84	120.35
173	ER	201	ATP	C5-C6-N6	2.29	123.83	120.35
167	El	906	UQ8	C17-C18-C19	-2.29	122.14	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
168	C	502	HEM	C3D-C4D-ND	-2.29	107.62	110.17
167	EN	1205	UQ8	C7-C8-C9	2.29	130.60	126.79
150	Eu	101	CDL	CB2-C1-CA2	-2.29	106.06	112.79
166	D	401	HEC	CBA-CAA-C2A	-2.28	108.76	112.60
168	ED	602	HEM	C3B-C2B-C1B	2.28	108.18	106.49
167	CC	303	UQ8	C8-C7-C6	2.28	118.18	112.05
168	C	501	HEM	C3B-C2B-C1B	2.28	108.17	106.49
150	DJ	303	CDL	CB2-C1-CA2	-2.27	106.09	112.79
150	DJ	302	CDL	CB2-C1-CA2	-2.27	106.10	112.79
169	Da	703	HEA	CMD-C2D-C1D	2.27	128.50	125.04
150	Ed	205	CDL	CB2-C1-CA2	-2.27	106.11	112.79
156	A6	301	LPP	P1-O5-C6	-2.27	112.04	118.30
168	c	505	HEM	C3D-C4D-ND	-2.27	107.64	110.17
150	C	505	CDL	CB2-C1-CA2	-2.27	106.12	112.79
169	DA	702	HEA	C4B-NB-C1B	-2.27	102.73	105.07
150	CG	301	CDL	CB2-C1-CA2	-2.27	106.12	112.79
150	EL	903	CDL	CB2-C1-CA2	-2.26	106.12	112.79
150	DQ	1501	CDL	CB2-C1-CA2	-2.26	106.15	112.79
150	Dq	1402	CDL	CB2-C1-CA2	-2.25	106.17	112.79
150	Ds	401	CDL	CB2-C1-CA2	-2.24	106.19	112.79
150	DX	306	CDL	CB2-C1-CA2	-2.24	106.20	112.79
150	Dd	705	CDL	CB2-C1-CA2	-2.24	106.20	112.79
168	ED	602	HEM	C3D-C4D-ND	-2.24	107.68	110.17
169	Da	702	HEA	CAD-C3D-C4D	2.23	128.56	124.66
167	Ed	202	UQ8	C21-C19-C18	2.23	125.64	121.12
169	Da	702	HEA	C1D-ND-C4D	-2.22	102.78	105.07
150	Dc	608	CDL	CB2-C1-CA2	-2.22	106.25	112.79
150	Dv	402	CDL	CB2-C1-CA2	-2.22	106.25	112.79
151	A0	603	UDP	O3B-PB-O3A	2.22	112.08	104.64
150	BV	201	CDL	CB2-C1-CA2	-2.22	106.27	112.79
168	Ed	201	HEM	C3B-C2B-C1B	2.21	108.13	106.49
169	DA	702	HEA	CMB-C2B-C1B	2.21	128.41	125.04
150	Dj	405	CDL	CB2-C1-CA2	-2.20	106.30	112.79
169	Da	702	HEA	C17-C18-C19	-2.20	122.36	127.66
150	AF	401	CDL	CB2-C1-CA2	-2.20	106.31	112.79
150	H	1301	CDL	CB2-C1-CA2	-2.19	106.34	112.79
168	C	501	HEM	C4B-CHC-C1C	2.19	125.45	122.56
150	ED	605	CDL	CB2-C1-CA2	-2.19	106.35	112.79
166	CE	401	HEC	CBA-CAA-C2A	-2.18	108.92	112.60
166	d	802	HEC	CMA-C3A-C2A	2.18	129.06	124.94
150	AF	402	CDL	CB2-C1-CA2	-2.18	106.37	112.79
168	ED	602	HEM	C4B-CHC-C1C	2.17	125.43	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	Dy	301	CDL	CB2-C1-CA2	-2.17	106.40	112.79
169	DA	702	HEA	CHC-C4B-C3B	-2.17	120.22	125.80
169	Da	702	HEA	CHC-C4B-C3B	-2.16	120.23	125.80
169	Da	702	HEA	CMB-C2B-C1B	2.16	128.32	125.04
168	c	504	HEM	CBA-CAA-C2A	-2.15	108.95	112.62
150	C	504	CDL	CB2-C1-CA2	-2.15	106.47	112.79
169	DA	702	HEA	C26-C15-C16	2.14	118.86	115.27
150	Dj	402	CDL	CB2-C1-CA2	-2.13	106.51	112.79
168	ED	602	HEM	CBA-CAA-C2A	-2.13	108.99	112.62
150	DJ	307	CDL	CB2-C1-CA2	-2.12	106.56	112.79
169	Da	703	HEA	OMA-CMA-C3A	-2.11	120.31	124.91
150	DY	301	CDL	CB2-C1-CA2	-2.11	106.58	112.79
150	DD	703	CDL	CB2-C1-CA2	-2.11	106.59	112.79
168	c	504	HEM	C3B-C2B-C1B	2.10	108.05	106.49
169	Da	703	HEA	C16-C17-C18	-2.10	104.97	111.88
168	Ed	201	HEM	C2D-C1D-ND	-2.10	107.36	109.88
150	AA	908	CDL	CB2-C1-CA2	-2.10	106.61	112.79
169	Da	702	HEA	C26-C15-C16	2.10	118.80	115.27
169	DA	702	HEA	CAD-C3D-C4D	2.10	128.33	124.66
150	A0	602	CDL	CB2-C1-CA2	-2.10	106.62	112.79
169	DA	702	HEA	C17-C18-C19	-2.09	122.62	127.66
168	ED	602	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
173	Er	201	ATP	PB-O3B-PG	2.08	139.98	132.83
150	DR	403	CDL	CB2-C1-CA2	-2.08	106.66	112.79
150	c	506	CDL	CB2-C1-CA2	-2.08	106.66	112.79
167	CC	303	UQ8	C17-C18-C19	-2.08	122.65	127.66
169	DA	703	HEA	CAA-CBA-CGA	-2.08	107.94	113.76
166	D	401	HEC	CMA-C3A-C2A	2.07	128.85	124.94
169	Da	703	HEA	CHC-C4B-C3B	-2.07	120.47	125.80
167	C	512	UQ8	C8-C7-C6	2.06	117.61	112.05
168	c	505	HEM	C3B-C2B-C1B	2.06	108.02	106.49
173	ER	201	ATP	PB-O3B-PG	2.06	139.88	132.83
169	DA	703	HEA	C16-C17-C18	-2.05	105.13	111.88
150	h	501	CDL	OB6-CB4-CB6	-2.05	100.96	108.40
167	ED	603	UQ8	C21-C19-C18	2.05	125.27	121.12
169	DA	702	HEA	OMA-CMA-C3A	-2.04	120.46	124.91
150	DJ	304	CDL	CB2-C1-CA2	-2.04	106.78	112.79
150	EL	902	CDL	CB2-C1-CA2	-2.03	106.81	112.79
150	Dv	401	CDL	OA6-CA4-CA6	-2.02	101.08	108.40
169	Da	702	HEA	CAA-CBA-CGA	-2.02	108.09	113.76
150	g	801	CDL	CB2-C1-CA2	-2.02	106.85	112.79
150	BC	302	CDL	OA6-CA4-CA6	-2.02	101.10	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
167	En	1202	UQ8	C17-C18-C19	-2.01	122.81	127.66
150	El	902	CDL	CB2-C1-CA2	-2.01	106.86	112.79
168	C	501	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
168	C	501	HEM	C3D-C4D-ND	-2.01	107.93	110.17
167	C	512	UQ8	C17-C18-C19	-2.00	122.84	127.66

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
169	DA	702	HEA	NB
169	DA	702	HEA	NA
169	DA	702	HEA	ND
169	DA	703	HEA	NB
169	DA	703	HEA	NA
169	DA	703	HEA	ND
169	Da	702	HEA	NB
169	Da	702	HEA	NA
169	Da	702	HEA	ND
169	Da	703	HEA	NB
169	Da	703	HEA	NA
169	Da	703	HEA	ND

All (7630) 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-OB5
150	A0	601	CDL	CB3-OB5-PB2-OB3
150	A0	601	CDL	CB3-OB5-PB2-OB4
150	A0	601	CDL	C51-CB5-OB6-CB4
150	A0	602	CDL	CA3-OA5-PA1-OA3
150	A0	602	CDL	C1-CB2-OB2-PB2
150	A0	602	CDL	CB3-OB5-PB2-OB2
150	A0	602	CDL	CB3-OB5-PB2-OB3
150	A0	602	CDL	OB5-CB3-CB4-OB6
150	A0	602	CDL	C51-CB5-OB6-CB4
150	A1	402	CDL	CB2-C1-CA2-OA2
150	A1	402	CDL	O1-C1-CB2-OB2
150	A1	402	CDL	CA3-OA5-PA1-OA2
150	A1	402	CDL	CA3-OA5-PA1-OA3
150	A1	402	CDL	CA3-OA5-PA1-OA4
150	A1	402	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AA	901	CDL	C51-CB5-OB6-CB4
150	AA	908	CDL	C11-CA5-OA6-CA4
150	AA	908	CDL	C51-CB5-OB6-CB4
150	AC	801	CDL	CA3-OA5-PA1-OA2
150	AC	801	CDL	CA3-OA5-PA1-OA3
150	AC	801	CDL	CA3-OA5-PA1-OA4
150	AC	801	CDL	CB2-OB2-PB2-OB3
150	AC	801	CDL	CB2-OB2-PB2-OB5
150	AC	801	CDL	CB3-OB5-PB2-OB3
150	AC	801	CDL	CB3-OB5-PB2-OB4
150	AC	802	CDL	CB2-OB2-PB2-OB3
150	AC	802	CDL	CB2-OB2-PB2-OB4
150	AC	802	CDL	CB3-OB5-PB2-OB4
150	AF	401	CDL	CA3-OA5-PA1-OA2
150	AF	401	CDL	CA3-OA5-PA1-OA3
150	AF	401	CDL	CA3-OA5-PA1-OA4
150	AF	401	CDL	OB7-CB5-OB6-CB4
150	AF	402	CDL	CA2-OA2-PA1-OA3
150	AM	301	CDL	CA2-OA2-PA1-OA4
150	AM	301	CDL	C11-CA5-OA6-CA4
150	AM	301	CDL	CB2-OB2-PB2-OB3
150	AM	301	CDL	CB2-OB2-PB2-OB5
150	AP	301	CDL	CA3-OA5-PA1-OA2
150	AP	301	CDL	CA3-OA5-PA1-OA3
150	AP	301	CDL	CA3-OA5-PA1-OA4
150	AP	301	CDL	C11-CA5-OA6-CA4
150	AP	301	CDL	CB2-OB2-PB2-OB4
150	AP	301	CDL	C51-CB5-OB6-CB4
150	B0	101	CDL	CA2-OA2-PA1-OA4
150	B0	101	CDL	C11-CA5-OA6-CA4
150	B0	101	CDL	CB2-OB2-PB2-OB3
150	B0	101	CDL	CB2-OB2-PB2-OB4
150	B0	101	CDL	CB3-OB5-PB2-OB4
150	B0	101	CDL	OB7-CB5-OB6-CB4
150	B0	101	CDL	C51-CB5-OB6-CB4
150	B0	102	CDL	O1-C1-CB2-OB2
150	B0	102	CDL	CA2-C1-CB2-OB2
150	B0	102	CDL	OA6-CA4-CA6-OA8
150	B1	402	CDL	CA3-OA5-PA1-OA3
150	B1	402	CDL	CB2-OB2-PB2-OB3
150	B1	402	CDL	CB2-OB2-PB2-OB4
150	BC	302	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	BC	302	CDL	CA3-OA5-PA1-OA3
150	BC	302	CDL	CB2-OB2-PB2-OB3
150	BC	302	CDL	CB3-OB5-PB2-OB4
150	BE	201	CDL	O1-C1-CB2-OB2
150	BE	201	CDL	CA2-C1-CB2-OB2
150	BE	201	CDL	CA2-OA2-PA1-OA4
150	BE	201	CDL	CA3-OA5-PA1-OA3
150	BE	201	CDL	C11-CA5-OA6-CA4
150	BE	201	CDL	CB2-OB2-PB2-OB3
150	BE	201	CDL	CB2-OB2-PB2-OB5
150	BE	201	CDL	OB7-CB5-OB6-CB4
150	BG	201	CDL	CA2-OA2-PA1-OA3
150	BG	201	CDL	C11-CA5-OA6-CA4
150	BG	201	CDL	CB2-OB2-PB2-OB3
150	BG	201	CDL	CB3-OB5-PB2-OB3
150	BL	301	CDL	O1-C1-CA2-OA2
150	BL	301	CDL	CB3-OB5-PB2-OB3
150	BT	202	CDL	CA2-C1-CB2-OB2
150	BT	202	CDL	C11-CA5-OA6-CA4
150	BT	202	CDL	CB2-OB2-PB2-OB3
150	BT	202	CDL	CB2-OB2-PB2-OB4
150	BT	202	CDL	CB3-OB5-PB2-OB3
150	BT	202	CDL	CB3-OB5-PB2-OB4
150	BT	202	CDL	C51-CB5-OB6-CB4
150	BT	204	CDL	CA2-OA2-PA1-OA3
150	BT	204	CDL	CA3-OA5-PA1-OA3
150	BT	204	CDL	OA7-CA5-OA6-CA4
150	BT	204	CDL	CB2-OB2-PB2-OB3
150	BT	204	CDL	CB2-OB2-PB2-OB4
150	BT	204	CDL	CB2-OB2-PB2-OB5
150	BV	201	CDL	C51-CB5-OB6-CB4
150	BY	201	CDL	CB2-OB2-PB2-OB5
150	BY	201	CDL	CB4-CB3-OB5-PB2
150	BY	201	CDL	C51-CB5-OB6-CB4
150	CG	301	CDL	CA2-OA2-PA1-OA3
150	CG	301	CDL	CA2-OA2-PA1-OA4
150	CG	301	CDL	CA2-OA2-PA1-OA5
150	CG	301	CDL	CB2-OB2-PB2-OB3
150	CG	302	CDL	CA2-OA2-PA1-OA3
150	CG	302	CDL	CA2-OA2-PA1-OA4
150	CG	302	CDL	CA3-OA5-PA1-OA3
150	CG	302	CDL	C11-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	CG	302	CDL	C1-CB2-OB2-PB2
150	CJ	201	CDL	O1-C1-CA2-OA2
150	CC	304	CDL	CA2-OA2-PA1-OA3
150	CC	304	CDL	CB2-OB2-PB2-OB3
150	CC	304	CDL	OB6-CB4-CB6-OB8
150	CC	305	CDL	CB2-OB2-PB2-OB3
150	CC	305	CDL	CB2-OB2-PB2-OB4
150	CC	305	CDL	CB2-OB2-PB2-OB5
150	CC	305	CDL	CB3-OB5-PB2-OB2
150	CC	305	CDL	OB7-CB5-OB6-CB4
150	CD	301	CDL	CA2-OA2-PA1-OA4
150	CD	301	CDL	CA2-OA2-PA1-OA5
150	CD	301	CDL	CA3-OA5-PA1-OA4
150	CD	301	CDL	CB2-OB2-PB2-OB3
150	CD	301	CDL	CB2-OB2-PB2-OB4
150	CD	301	CDL	CB3-OB5-PB2-OB3
150	CD	302	CDL	CA3-OA5-PA1-OA2
150	CD	302	CDL	CA3-OA5-PA1-OA3
150	CD	302	CDL	CA4-CA3-OA5-PA1
150	CD	302	CDL	C11-CA5-OA6-CA4
150	CD	302	CDL	CB2-OB2-PB2-OB3
150	C	503	CDL	O1-C1-CA2-OA2
150	C	504	CDL	CA2-OA2-PA1-OA3
150	C	504	CDL	CA2-OA2-PA1-OA4
150	C	504	CDL	CA3-OA5-PA1-OA3
150	C	504	CDL	OA5-CA3-CA4-OA6
150	C	504	CDL	C1-CB2-OB2-PB2
150	C	504	CDL	CB2-OB2-PB2-OB3
150	C	505	CDL	CA3-OA5-PA1-OA2
150	C	505	CDL	CA3-OA5-PA1-OA3
150	C	505	CDL	CA3-OA5-PA1-OA4
150	C	505	CDL	C11-CA5-OA6-CA4
150	C	506	CDL	CA3-OA5-PA1-OA3
150	C	506	CDL	C11-CA5-OA6-CA4
150	C	506	CDL	CB3-OB5-PB2-OB3
150	C	506	CDL	CB3-OB5-PB2-OB4
150	C	506	CDL	C51-CB5-OB6-CB4
150	C	507	CDL	O1-C1-CB2-OB2
150	C	507	CDL	CA3-OA5-PA1-OA4
150	C	507	CDL	OA7-CA5-OA6-CA4
150	C	507	CDL	CB3-OB5-PB2-OB3
150	E	301	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	E	301	CDL	CA3-OA5-PA1-OA3
150	E	301	CDL	CA3-OA5-PA1-OA4
150	H	1301	CDL	C11-CA5-OA6-CA4
150	H	1301	CDL	CB2-OB2-PB2-OB3
150	H	1301	CDL	CB2-OB2-PB2-OB4
150	H	1301	CDL	CB3-OB5-PB2-OB3
150	H	1301	CDL	CB3-OB5-PB2-OB4
150	H	1302	CDL	CA2-C1-CB2-OB2
150	H	1302	CDL	CA2-OA2-PA1-OA3
150	H	1302	CDL	CA2-OA2-PA1-OA4
150	H	1302	CDL	OA7-CA5-OA6-CA4
150	H	1302	CDL	C11-CA5-OA6-CA4
150	H	1302	CDL	CB3-OB5-PB2-OB3
150	c	501	CDL	CA3-OA5-PA1-OA2
150	c	501	CDL	CA3-OA5-PA1-OA3
150	c	501	CDL	CA3-OA5-PA1-OA4
150	c	501	CDL	C11-CA5-OA6-CA4
150	c	501	CDL	CB2-OB2-PB2-OB3
150	c	501	CDL	CB2-OB2-PB2-OB4
150	c	502	CDL	CA2-OA2-PA1-OA4
150	c	502	CDL	CB2-OB2-PB2-OB3
150	c	502	CDL	CB2-OB2-PB2-OB4
150	c	502	CDL	CB2-OB2-PB2-OB5
150	c	506	CDL	CA2-C1-CB2-OB2
150	c	506	CDL	CA2-OA2-PA1-OA3
150	c	506	CDL	CA3-OA5-PA1-OA3
150	c	506	CDL	C11-CA5-OA6-CA4
150	c	506	CDL	CB2-OB2-PB2-OB3
150	c	509	CDL	CA2-OA2-PA1-OA3
150	c	509	CDL	CA2-OA2-PA1-OA4
150	c	509	CDL	CA2-OA2-PA1-OA5
150	c	509	CDL	C1-CB2-OB2-PB2
150	c	509	CDL	CB3-OB5-PB2-OB3
150	g	801	CDL	CA2-C1-CB2-OB2
150	g	801	CDL	CA2-OA2-PA1-OA3
150	g	801	CDL	CB2-OB2-PB2-OB3
150	g	801	CDL	OB6-CB4-CB6-OB8
150	g	801	CDL	C51-CB5-OB6-CB4
150	h	501	CDL	CB2-OB2-PB2-OB3
150	h	501	CDL	CB2-OB2-PB2-OB4
150	h	501	CDL	C51-CB5-OB6-CB4
150	DA	706	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DA	706	CDL	CB3-OB5-PB2-OB4
150	DA	709	CDL	CA3-OA5-PA1-OA3
150	DA	709	CDL	CA3-OA5-PA1-OA4
150	DA	709	CDL	C11-CA5-OA6-CA4
150	DC	601	CDL	CA2-OA2-PA1-OA4
150	DC	601	CDL	CA3-OA5-PA1-OA4
150	DC	601	CDL	CB2-OB2-PB2-OB4
150	DC	601	CDL	CB3-OB5-PB2-OB4
150	DD	703	CDL	CA3-OA5-PA1-OA4
150	DD	703	CDL	C11-CA5-OA6-CA4
150	DD	704	CDL	CB2-OB2-PB2-OB3
150	DD	705	CDL	CA2-OA2-PA1-OA3
150	DD	705	CDL	CA2-OA2-PA1-OA4
150	DD	705	CDL	CA3-OA5-PA1-OA3
150	DD	705	CDL	C51-CB5-OB6-CB4
150	DD	706	CDL	CA2-OA2-PA1-OA3
150	DD	706	CDL	CA2-OA2-PA1-OA4
150	DD	706	CDL	CA3-OA5-PA1-OA3
150	DD	706	CDL	CB3-OB5-PB2-OB3
150	DG	201	CDL	CB2-OB2-PB2-OB3
150	DG	201	CDL	CB3-OB5-PB2-OB2
150	DG	201	CDL	CB4-CB3-OB5-PB2
150	DG	201	CDL	C51-CB5-OB6-CB4
150	DG	202	CDL	CA2-OA2-PA1-OA4
150	DG	202	CDL	CB3-OB5-PB2-OB4
150	DH	201	CDL	CB2-C1-CA2-OA2
150	DH	201	CDL	CA3-OA5-PA1-OA3
150	DH	201	CDL	OA6-CA4-CA6-OA8
150	DH	202	CDL	CA3-OA5-PA1-OA2
150	DH	202	CDL	CA3-OA5-PA1-OA3
150	DH	202	CDL	CA3-OA5-PA1-OA4
150	DH	202	CDL	CB3-OB5-PB2-OB2
150	DH	202	CDL	CB3-OB5-PB2-OB3
150	DI	302	CDL	C11-CA5-OA6-CA4
150	DI	302	CDL	CB2-OB2-PB2-OB3
150	DI	302	CDL	CB2-OB2-PB2-OB4
150	DI	302	CDL	CB3-OB5-PB2-OB3
150	DI	302	CDL	C51-CB5-OB6-CB4
150	DJ	302	CDL	CA4-CA6-OA8-CA7
150	DJ	302	CDL	C1-CB2-OB2-PB2
150	DJ	302	CDL	CB2-OB2-PB2-OB3
150	DJ	302	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DJ	302	CDL	C51-CB5-OB6-CB4
150	DJ	303	CDL	C1-CA2-OA2-PA1
150	DJ	303	CDL	CB2-OB2-PB2-OB5
150	DJ	303	CDL	CB3-OB5-PB2-OB4
150	DJ	304	CDL	CA2-OA2-PA1-OA3
150	DJ	304	CDL	CA2-OA2-PA1-OA4
150	DJ	304	CDL	CA2-OA2-PA1-OA5
150	DJ	304	CDL	C11-CA5-OA6-CA4
150	DJ	305	CDL	O1-C1-CA2-OA2
150	DJ	305	CDL	CB2-C1-CA2-OA2
150	DJ	305	CDL	CA3-OA5-PA1-OA4
150	DJ	305	CDL	OA7-CA5-OA6-CA4
150	DJ	307	CDL	OA6-CA4-CA6-OA8
150	DJ	307	CDL	CB3-OB5-PB2-OB4
150	DJ	307	CDL	OB5-CB3-CB4-OB6
150	DJ	307	CDL	OB7-CB5-OB6-CB4
150	DJ	307	CDL	C51-CB5-OB6-CB4
150	DM	501	CDL	C1-CA2-OA2-PA1
150	DM	501	CDL	CA2-OA2-PA1-OA3
150	DM	501	CDL	CB2-OB2-PB2-OB3
150	DM	501	CDL	CB2-OB2-PB2-OB4
150	DM	501	CDL	OB7-CB5-OB6-CB4
150	DM	501	CDL	C51-CB5-OB6-CB4
150	DN	502	CDL	CA2-OA2-PA1-OA3
150	DN	502	CDL	CA2-OA2-PA1-OA4
150	DN	502	CDL	CA2-OA2-PA1-OA5
150	DN	502	CDL	CA3-OA5-PA1-OA3
150	DN	502	CDL	CA3-OA5-PA1-OA4
150	DN	502	CDL	CB2-OB2-PB2-OB3
150	DN	503	CDL	CA2-OA2-PA1-OA3
150	DN	503	CDL	CA2-OA2-PA1-OA4
150	DN	503	CDL	CA2-OA2-PA1-OA5
150	DN	503	CDL	CB2-OB2-PB2-OB4
150	DN	506	CDL	CB3-OB5-PB2-OB3
150	DN	506	CDL	C51-CB5-OB6-CB4
150	DN	507	CDL	C1-CA2-OA2-PA1
150	DN	507	CDL	CA2-OA2-PA1-OA4
150	DN	507	CDL	CA3-OA5-PA1-OA3
150	DN	507	CDL	CA3-OA5-PA1-OA4
150	DN	507	CDL	C11-CA5-OA6-CA4
150	DN	507	CDL	CB3-OB5-PB2-OB2
150	DN	507	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DO	501	CDL	CA3-OA5-PA1-OA2
150	DO	501	CDL	CA3-OA5-PA1-OA3
150	DO	501	CDL	C11-CA5-OA6-CA4
150	DO	501	CDL	CB2-OB2-PB2-OB3
150	DO	501	CDL	CB3-OB5-PB2-OB2
150	DO	501	CDL	CB3-OB5-PB2-OB3
150	DO	501	CDL	C51-CB5-OB6-CB4
150	DQ	1501	CDL	CA3-OA5-PA1-OA3
150	DQ	1501	CDL	CA3-OA5-PA1-OA4
150	DQ	1502	CDL	CA2-OA2-PA1-OA3
150	DQ	1502	CDL	CA3-OA5-PA1-OA2
150	DQ	1502	CDL	CA3-OA5-PA1-OA3
150	DQ	1502	CDL	CA3-OA5-PA1-OA4
150	DQ	1502	CDL	CB3-OB5-PB2-OB2
150	DQ	1502	CDL	CB3-OB5-PB2-OB3
150	DQ	1504	CDL	OA5-CA3-CA4-OA6
150	DQ	1504	CDL	OA7-CA5-OA6-CA4
150	DR	402	CDL	CA3-OA5-PA1-OA3
150	DR	402	CDL	CA3-OA5-PA1-OA4
150	DR	402	CDL	CB2-OB2-PB2-OB3
150	DR	402	CDL	CB2-OB2-PB2-OB4
150	DR	402	CDL	CB2-OB2-PB2-OB5
150	DR	402	CDL	OB6-CB4-CB6-OB8
150	DR	403	CDL	OB6-CB4-CB6-OB8
150	DS	401	CDL	CA2-OA2-PA1-OA3
150	DS	401	CDL	CB4-CB3-OB5-PB2
150	DS	404	CDL	CB3-OB5-PB2-OB2
150	DS	404	CDL	CB3-OB5-PB2-OB3
150	DS	404	CDL	CB3-OB5-PB2-OB4
150	DS	404	CDL	C51-CB5-OB6-CB4
150	DS	405	CDL	CA2-OA2-PA1-OA3
150	DS	405	CDL	CA2-OA2-PA1-OA4
150	DS	405	CDL	CB2-OB2-PB2-OB3
150	DS	405	CDL	CB3-OB5-PB2-OB3
150	DS	405	CDL	CB3-OB5-PB2-OB4
150	DU	401	CDL	CA2-OA2-PA1-OA3
150	DU	401	CDL	CA2-OA2-PA1-OA4
150	DU	401	CDL	CB2-OB2-PB2-OB3
150	DU	402	CDL	C11-CA5-OA6-CA4
150	DU	402	CDL	CB2-OB2-PB2-OB3
150	DU	402	CDL	CB2-OB2-PB2-OB4
150	DU	402	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DU	402	CDL	CB3-OB5-PB2-OB3
150	DU	402	CDL	CB3-OB5-PB2-OB4
150	DU	403	CDL	CB3-OB5-PB2-OB3
150	DU	404	CDL	CA3-OA5-PA1-OA3
150	DU	404	CDL	CA3-CA4-OA6-CA5
150	DU	404	CDL	CB2-OB2-PB2-OB3
150	DU	404	CDL	CB2-OB2-PB2-OB4
150	DV	401	CDL	CA3-OA5-PA1-OA3
150	DV	401	CDL	CA3-OA5-PA1-OA4
150	DV	401	CDL	OA7-CA5-OA6-CA4
150	DV	401	CDL	C51-CB5-OB6-CB4
150	DV	402	CDL	CA3-OA5-PA1-OA4
150	DV	403	CDL	O1-C1-CA2-OA2
150	DV	403	CDL	CA2-OA2-PA1-OA4
150	DV	403	CDL	CA3-OA5-PA1-OA3
150	DV	403	CDL	CB3-OB5-PB2-OB3
150	DV	403	CDL	C51-CB5-OB6-CB4
150	DX	301	CDL	CA2-OA2-PA1-OA5
150	DX	301	CDL	CB2-OB2-PB2-OB3
150	DX	301	CDL	CB2-OB2-PB2-OB4
150	DX	301	CDL	CB2-OB2-PB2-OB5
150	DX	306	CDL	CA3-OA5-PA1-OA3
150	DX	306	CDL	CA4-CA3-OA5-PA1
150	DX	306	CDL	OA7-CA5-OA6-CA4
150	DX	306	CDL	C11-CA5-OA6-CA4
150	DX	306	CDL	CB2-OB2-PB2-OB3
150	DX	306	CDL	CB3-OB5-PB2-OB4
150	DX	307	CDL	CA2-OA2-PA1-OA4
150	DY	301	CDL	CA3-OA5-PA1-OA3
150	DY	301	CDL	CA3-OA5-PA1-OA4
150	DY	301	CDL	C11-CA5-OA6-CA4
150	DY	301	CDL	CB2-OB2-PB2-OB3
150	DY	301	CDL	OB6-CB4-CB6-OB8
150	DY	301	CDL	C51-CB5-OB6-CB4
150	EA	301	CDL	CA2-OA2-PA1-OA3
150	EA	301	CDL	CA2-OA2-PA1-OA4
150	EA	301	CDL	CA2-OA2-PA1-OA5
150	EA	301	CDL	OA9-CA7-OA8-CA6
150	EA	301	CDL	CB2-OB2-PB2-OB3
150	EA	301	CDL	CB2-OB2-PB2-OB4
150	EB	302	CDL	CA3-OA5-PA1-OA3
150	EB	302	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EB	302	CDL	C11-CA5-OA6-CA4
150	EB	302	CDL	CB2-OB2-PB2-OB3
150	EB	302	CDL	CB2-OB2-PB2-OB4
150	EB	302	CDL	CB3-OB5-PB2-OB3
150	EB	302	CDL	OB7-CB5-OB6-CB4
150	ED	601	CDL	O1-C1-CA2-OA2
150	ED	601	CDL	CA2-OA2-PA1-OA3
150	ED	601	CDL	CA2-OA2-PA1-OA5
150	ED	601	CDL	CA3-OA5-PA1-OA3
150	ED	601	CDL	OA7-CA5-OA6-CA4
150	ED	601	CDL	C11-CA5-OA6-CA4
150	ED	601	CDL	CB3-OB5-PB2-OB3
150	ED	604	CDL	C11-CA5-OA6-CA4
150	ED	605	CDL	CA3-OA5-PA1-OA2
150	ED	605	CDL	CA3-OA5-PA1-OA3
150	ED	605	CDL	CA3-OA5-PA1-OA4
150	ED	605	CDL	CB2-OB2-PB2-OB3
150	ED	605	CDL	CB3-OB5-PB2-OB4
150	EH	1601	CDL	C11-CA5-OA6-CA4
150	EH	1601	CDL	CB3-OB5-PB2-OB3
150	EH	1601	CDL	C51-CB5-OB6-CB4
150	EI	401	CDL	CB3-OB5-PB2-OB3
150	EK	201	CDL	CA2-OA2-PA1-OA3
150	EK	201	CDL	CA2-OA2-PA1-OA4
150	EK	201	CDL	CA2-OA2-PA1-OA5
150	EK	201	CDL	CA3-OA5-PA1-OA3
150	EL	902	CDL	C11-CA5-OA6-CA4
150	EL	902	CDL	CB2-OB2-PB2-OB3
150	EL	902	CDL	CB2-OB2-PB2-OB4
150	EL	902	CDL	CB3-OB5-PB2-OB2
150	EL	902	CDL	CB3-OB5-PB2-OB3
150	EL	902	CDL	CB3-OB5-PB2-OB4
150	EL	903	CDL	CA2-OA2-PA1-OA4
150	EL	903	CDL	CB2-OB2-PB2-OB3
150	EL	903	CDL	CB2-OB2-PB2-OB4
150	EL	903	CDL	CB3-OB5-PB2-OB3
150	EL	903	CDL	CB3-OB5-PB2-OB4
150	EN	1201	CDL	O1-C1-CA2-OA2
150	EN	1201	CDL	CA2-OA2-PA1-OA4
150	EN	1202	CDL	CA3-OA5-PA1-OA4
150	EN	1202	CDL	CB3-OB5-PB2-OB3
150	EN	1202	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EO	202	CDL	C11-CA5-OA6-CA4
150	EO	202	CDL	CB2-OB2-PB2-OB3
150	EO	202	CDL	C51-CB5-OB6-CB4
150	ES	1101	CDL	CA2-OA2-PA1-OA5
150	ES	1101	CDL	CB3-OB5-PB2-OB2
150	ES	1101	CDL	CB3-OB5-PB2-OB3
150	ES	1101	CDL	OB5-CB3-CB4-OB6
150	Da	709	CDL	CA2-OA2-PA1-OA3
150	Da	709	CDL	CA3-OA5-PA1-OA4
150	Da	709	CDL	OA7-CA5-OA6-CA4
150	Da	709	CDL	C11-CA5-OA6-CA4
150	Da	709	CDL	CB3-OB5-PB2-OB3
150	Da	709	CDL	CB3-OB5-PB2-OB4
150	Dc	601	CDL	CA2-OA2-PA1-OA4
150	Dc	601	CDL	CB2-OB2-PB2-OB4
150	Dc	601	CDL	CB3-OB5-PB2-OB4
150	Dc	608	CDL	O1-C1-CB2-OB2
150	Dc	608	CDL	OA7-CA5-OA6-CA4
150	Dc	608	CDL	C11-CA5-OA6-CA4
150	Dc	608	CDL	CB2-OB2-PB2-OB5
150	Dc	608	CDL	CB3-OB5-PB2-OB2
150	Dc	608	CDL	CB3-OB5-PB2-OB3
150	Dc	608	CDL	CB3-OB5-PB2-OB4
150	Dd	702	CDL	C1-CA2-OA2-PA1
150	Dd	702	CDL	CA3-OA5-PA1-OA3
150	Dd	702	CDL	CA3-OA5-PA1-OA4
150	Dd	702	CDL	C11-CA5-OA6-CA4
150	Dd	704	CDL	O1-C1-CA2-OA2
150	Dd	704	CDL	CB2-C1-CA2-OA2
150	Dd	704	CDL	C1-CB2-OB2-PB2
150	Dd	705	CDL	CA3-OA5-PA1-OA4
150	Dd	706	CDL	CA2-C1-CB2-OB2
150	Dd	706	CDL	CA2-OA2-PA1-OA4
150	Dg	201	CDL	CB2-C1-CA2-OA2
150	Dg	201	CDL	CA2-OA2-PA1-OA4
150	Dg	201	CDL	OA7-CA5-OA6-CA4
150	Dg	201	CDL	C11-CA5-OA6-CA4
150	Dg	201	CDL	CB3-OB5-PB2-OB2
150	Dg	201	CDL	CB4-CB3-OB5-PB2
150	Dg	202	CDL	CA2-OA2-PA1-OA3
150	Dg	202	CDL	CA2-OA2-PA1-OA4
150	Dg	202	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dh	201	CDL	CB2-C1-CA2-OA2
150	Dh	201	CDL	CA3-OA5-PA1-OA3
150	Dh	201	CDL	OA6-CA4-CA6-OA8
150	Dh	201	CDL	CB2-OB2-PB2-OB3
150	Dh	201	CDL	CB2-OB2-PB2-OB5
150	Dh	202	CDL	CA3-OA5-PA1-OA3
150	Dh	202	CDL	CA3-OA5-PA1-OA4
150	Dh	202	CDL	CB2-OB2-PB2-OB3
150	Dh	202	CDL	CB2-OB2-PB2-OB4
150	Dh	202	CDL	CB3-OB5-PB2-OB2
150	Dh	202	CDL	CB3-OB5-PB2-OB3
150	Di	1101	CDL	CB3-OB5-PB2-OB4
150	Di	1103	CDL	C11-CA5-OA6-CA4
150	Di	1103	CDL	CB3-OB5-PB2-OB2
150	Di	1103	CDL	OB7-CB5-OB6-CB4
150	Di	1103	CDL	C51-CB5-OB6-CB4
150	Dj	401	CDL	CA2-OA2-PA1-OA3
150	Dj	401	CDL	CA2-OA2-PA1-OA4
150	Dj	401	CDL	CB2-OB2-PB2-OB3
150	Dj	401	CDL	CB3-OB5-PB2-OB3
150	Dj	401	CDL	CB3-OB5-PB2-OB4
150	Dj	401	CDL	OB7-CB5-OB6-CB4
150	Dj	401	CDL	C51-CB5-OB6-CB4
150	Dj	402	CDL	CB2-C1-CA2-OA2
150	Dj	402	CDL	C11-CA5-OA6-CA4
150	Dj	402	CDL	CB3-OB5-PB2-OB4
150	Dj	403	CDL	CA2-OA2-PA1-OA4
150	Dj	403	CDL	CA3-OA5-PA1-OA2
150	Dj	403	CDL	CA3-OA5-PA1-OA3
150	Dj	403	CDL	CA3-OA5-PA1-OA4
150	Dj	403	CDL	OB5-CB3-CB4-OB6
150	Dj	404	CDL	CA3-OA5-PA1-OA2
150	Dj	404	CDL	CA3-OA5-PA1-OA3
150	Dj	404	CDL	CA3-OA5-PA1-OA4
150	Dj	404	CDL	OA7-CA5-OA6-CA4
150	Dj	404	CDL	CB3-OB5-PB2-OB2
150	Dj	404	CDL	C51-CB5-OB6-CB4
150	Dj	405	CDL	OA7-CA5-OA6-CA4
150	Dj	405	CDL	CB2-OB2-PB2-OB3
150	Dj	405	CDL	CB2-OB2-PB2-OB5
150	Dj	407	CDL	OA6-CA4-CA6-OA8
150	Dj	407	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dm	501	CDL	CA3-OA5-PA1-OA4
150	Dm	501	CDL	C1-CB2-OB2-PB2
150	Dm	501	CDL	CB2-OB2-PB2-OB4
150	Dm	501	CDL	C51-CB5-OB6-CB4
150	Dm	502	CDL	CA2-OA2-PA1-OA3
150	Dm	502	CDL	CA3-OA5-PA1-OA3
150	Dm	502	CDL	CA3-OA5-PA1-OA4
150	Dm	502	CDL	C11-CA5-OA6-CA4
150	Dn	501	CDL	CA2-OA2-PA1-OA3
150	Dn	501	CDL	CA2-OA2-PA1-OA4
150	Dn	501	CDL	CA2-OA2-PA1-OA5
150	Dn	502	CDL	CA3-OA5-PA1-OA2
150	Dn	502	CDL	CA3-OA5-PA1-OA3
150	Dn	502	CDL	CA3-OA5-PA1-OA4
150	Dn	502	CDL	CA4-CA3-OA5-PA1
150	Dn	503	CDL	CA2-OA2-PA1-OA3
150	Dn	503	CDL	CA2-OA2-PA1-OA5
150	Dn	503	CDL	CA3-OA5-PA1-OA2
150	Dn	503	CDL	CA3-OA5-PA1-OA3
150	Dn	506	CDL	CB3-OB5-PB2-OB3
150	Dn	506	CDL	OB7-CB5-OB6-CB4
150	Dn	506	CDL	C51-CB5-OB6-CB4
150	Do	501	CDL	CA2-OA2-PA1-OA4
150	Do	501	CDL	CA3-OA5-PA1-OA3
150	Do	501	CDL	CA3-OA5-PA1-OA4
150	Do	501	CDL	CB3-OB5-PB2-OB2
150	Do	501	CDL	C51-CB5-OB6-CB4
150	Dq	1401	CDL	OA7-CA5-OA6-CA4
150	Dq	1401	CDL	CB3-OB5-PB2-OB2
150	Dq	1401	CDL	C51-CB5-OB6-CB4
150	Dq	1402	CDL	CA2-OA2-PA1-OA5
150	Dq	1402	CDL	CA3-OA5-PA1-OA3
150	Dq	1402	CDL	CA3-OA5-PA1-OA4
150	Dq	1403	CDL	CB3-OB5-PB2-OB3
150	Dr	402	CDL	CA3-OA5-PA1-OA4
150	Dr	402	CDL	CB2-OB2-PB2-OB4
150	Dr	403	CDL	OB6-CB4-CB6-OB8
150	Ds	401	CDL	CA3-OA5-PA1-OA4
150	Ds	401	CDL	CB3-OB5-PB2-OB3
150	Ds	401	CDL	C51-CB5-OB6-CB4
150	Ds	402	CDL	CA2-OA2-PA1-OA3
150	Ds	402	CDL	CB4-CB3-OB5-PB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ds	405	CDL	CB3-OB5-PB2-OB2
150	Ds	405	CDL	CB3-OB5-PB2-OB3
150	Ds	405	CDL	CB3-OB5-PB2-OB4
150	Ds	405	CDL	C51-CB5-OB6-CB4
150	Ds	406	CDL	CA2-OA2-PA1-OA3
150	Ds	406	CDL	CA3-OA5-PA1-OA3
150	Ds	406	CDL	CB2-OB2-PB2-OB3
150	Ds	406	CDL	CB3-OB5-PB2-OB3
150	Du	401	CDL	C1-CA2-OA2-PA1
150	Du	401	CDL	CA2-OA2-PA1-OA3
150	Du	401	CDL	CA3-OA5-PA1-OA3
150	Du	401	CDL	CB2-OB2-PB2-OB3
150	Du	401	CDL	CB2-OB2-PB2-OB4
150	Du	401	CDL	CB2-OB2-PB2-OB5
150	Du	402	CDL	CA2-OA2-PA1-OA5
150	Du	402	CDL	CA3-OA5-PA1-OA3
150	Du	402	CDL	CB3-OB5-PB2-OB2
150	Du	402	CDL	CB3-OB5-PB2-OB3
150	Du	402	CDL	CB3-OB5-PB2-OB4
150	Du	403	CDL	CB3-OB5-PB2-OB3
150	Dv	401	CDL	CA3-OA5-PA1-OA2
150	Dv	401	CDL	CA3-OA5-PA1-OA3
150	Dv	401	CDL	CA3-OA5-PA1-OA4
150	Dv	401	CDL	OA7-CA5-OA6-CA4
150	Dv	401	CDL	CB2-OB2-PB2-OB4
150	Dv	402	CDL	CA3-OA5-PA1-OA2
150	Dv	402	CDL	CA3-OA5-PA1-OA3
150	Dv	402	CDL	CA3-OA5-PA1-OA4
150	Dv	402	CDL	CB2-OB2-PB2-OB3
150	Dv	403	CDL	CB3-OB5-PB2-OB2
150	Dv	403	CDL	CB3-OB5-PB2-OB3
150	Dv	403	CDL	OB5-CB3-CB4-OB6
150	Dv	403	CDL	C51-CB5-OB6-CB4
150	Dx	1201	CDL	CA2-OA2-PA1-OA3
150	Dx	1201	CDL	CA2-OA2-PA1-OA4
150	Dx	1201	CDL	CA2-OA2-PA1-OA5
150	Dx	1201	CDL	CB2-OB2-PB2-OB4
150	Dx	1204	CDL	OB5-CB3-CB4-OB6
150	Dx	1204	CDL	C51-CB5-OB6-CB4
150	Dy	301	CDL	CA3-OA5-PA1-OA2
150	Dy	301	CDL	CA3-OA5-PA1-OA3
150	Dy	301	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dy	301	CDL	C11-CA5-OA6-CA4
150	Dy	301	CDL	C51-CB5-OB6-CB4
150	Ea	501	CDL	CA2-OA2-PA1-OA3
150	Ea	501	CDL	CA2-OA2-PA1-OA5
150	Ea	501	CDL	CB2-OB2-PB2-OB3
150	Ea	502	CDL	C11-CA5-OA6-CA4
150	Ea	502	CDL	CB2-OB2-PB2-OB3
150	Eb	302	CDL	O1-C1-CA2-OA2
150	Eb	302	CDL	CA2-OA2-PA1-OA5
150	Eb	302	CDL	CB2-OB2-PB2-OB4
150	Eb	302	CDL	CB3-OB5-PB2-OB4
150	Eb	302	CDL	OB7-CB5-OB6-CB4
150	Ed	204	CDL	CA2-OA2-PA1-OA3
150	Ed	204	CDL	CA2-OA2-PA1-OA5
150	Ed	204	CDL	CA3-OA5-PA1-OA3
150	Ed	204	CDL	CA3-OA5-PA1-OA4
150	Ed	204	CDL	C11-CA5-OA6-CA4
150	Ed	204	CDL	OA9-CA7-OA8-CA6
150	Ed	204	CDL	CB2-OB2-PB2-OB3
150	Ed	204	CDL	CB2-OB2-PB2-OB4
150	Ed	204	CDL	CB2-OB2-PB2-OB5
150	Ed	205	CDL	CA3-OA5-PA1-OA3
150	Ed	205	CDL	CA3-OA5-PA1-OA4
150	Ed	205	CDL	CB3-OB5-PB2-OB3
150	Eg	101	CDL	O1-C1-CA2-OA2
150	Eg	101	CDL	CA2-OA2-PA1-OA3
150	Eg	101	CDL	CA2-OA2-PA1-OA5
150	Eg	101	CDL	C11-CA5-OA6-CA4
150	Eh	1601	CDL	CA2-OA2-PA1-OA3
150	Eh	1601	CDL	CA2-OA2-PA1-OA5
150	Eh	1601	CDL	C11-CA5-OA6-CA4
150	Eh	1601	CDL	CB3-OB5-PB2-OB3
150	Ei	401	CDL	CA2-OA2-PA1-OA4
150	Ei	401	CDL	C11-CA5-OA6-CA4
150	Ei	401	CDL	CB3-OB5-PB2-OB4
150	Ei	401	CDL	CB4-CB3-OB5-PB2
150	Ek	201	CDL	CA2-OA2-PA1-OA3
150	Ek	201	CDL	CA2-OA2-PA1-OA4
150	Ek	201	CDL	CA2-OA2-PA1-OA5
150	Ek	201	CDL	CA3-OA5-PA1-OA2
150	Ek	201	CDL	CA3-OA5-PA1-OA3
150	Ek	201	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ek	201	CDL	OA7-CA5-OA6-CA4
150	Ek	201	CDL	C11-CA5-OA6-CA4
150	El	901	CDL	CA3-OA5-PA1-OA4
150	El	901	CDL	OB6-CB4-CB6-OB8
150	El	901	CDL	C51-CB5-OB6-CB4
150	El	902	CDL	CA2-C1-CB2-OB2
150	El	902	CDL	C1-CB2-OB2-PB2
150	El	902	CDL	CB3-OB5-PB2-OB2
150	El	902	CDL	CB3-OB5-PB2-OB3
150	El	902	CDL	CB3-OB5-PB2-OB4
150	El	903	CDL	CA2-OA2-PA1-OA4
150	El	903	CDL	CA3-OA5-PA1-OA4
150	El	903	CDL	C1-CB2-OB2-PB2
150	El	903	CDL	CB2-OB2-PB2-OB3
150	El	903	CDL	CB3-OB5-PB2-OB2
150	El	903	CDL	CB3-OB5-PB2-OB3
150	El	903	CDL	CB3-OB5-PB2-OB4
150	El	903	CDL	C51-CB5-OB6-CB4
150	En	1201	CDL	O1-C1-CA2-OA2
150	En	1201	CDL	CA2-OA2-PA1-OA5
150	En	1201	CDL	CB2-OB2-PB2-OB5
150	Ep	701	CDL	CB2-C1-CA2-OA2
150	Ep	701	CDL	C1-CA2-OA2-PA1
150	Eu	101	CDL	CB2-OB2-PB2-OB3
150	Eu	101	CDL	CB2-OB2-PB2-OB5
151	A0	603	UDP	C5'-O5'-PA-O2A
153	A0	605	PC1	C1-O11-P-O12
153	A0	605	PC1	C1-O11-P-O14
153	A0	605	PC1	C1-O11-P-O13
153	A1	403	PC1	O11-C1-C2-O21
153	A1	403	PC1	O22-C21-O21-C2
153	A2	402	PC1	C22-C21-O21-C2
153	A6	303	PC1	C11-O13-P-O14
153	A9	601	PC1	O13-C11-C12-N
153	A9	603	PC1	C11-O13-P-O14
153	A9	603	PC1	C1-O11-P-O12
153	A9	603	PC1	O22-C21-O21-C2
153	A9	603	PC1	C22-C21-O21-C2
153	AA	904	PC1	C22-C21-O21-C2
153	AA	905	PC1	C11-O13-P-O12
153	AA	905	PC1	C11-O13-P-O14
153	AA	905	PC1	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AA	905	PC1	C1-O11-P-O13
153	AA	905	PC1	O13-C11-C12-N
153	AA	906	PC1	C11-O13-P-O14
153	AA	907	PC1	C1-O11-P-O12
153	AA	907	PC1	C1-O11-P-O14
153	AA	907	PC1	C1-O11-P-O13
153	AA	907	PC1	O13-C11-C12-N
153	AA	907	PC1	C2-C1-O11-P
153	AC	804	PC1	C11-O13-P-O14
153	AC	804	PC1	C11-O13-P-O11
153	AH	301	PC1	C11-O13-P-O14
153	AJ	501	PC1	C1-O11-P-O12
153	AJ	501	PC1	C1-O11-P-O14
153	AJ	501	PC1	C1-O11-P-O13
153	AJ	501	PC1	O13-C11-C12-N
153	AL	303	PC1	O13-C11-C12-N
153	AL	303	PC1	O22-C21-O21-C2
153	AM	302	PC1	C11-O13-P-O12
153	AM	302	PC1	C1-O11-P-O12
153	AM	302	PC1	C1-O11-P-O14
153	AM	302	PC1	C1-O11-P-O13
153	AQ	202	PC1	C11-O13-P-O14
153	AQ	202	PC1	C1-O11-P-O14
153	AU	202	PC1	O21-C2-C3-O31
153	B1	401	PC1	C11-O13-P-O14
153	B1	401	PC1	C1-O11-P-O12
153	B1	401	PC1	C1-O11-P-O14
153	B1	401	PC1	C2-C1-O11-P
153	B1	401	PC1	O21-C2-C3-O31
153	B1	403	PC1	C11-O13-P-O14
153	B1	403	PC1	C11-O13-P-O11
153	BG	202	PC1	C11-O13-P-O12
153	BG	202	PC1	C12-C11-O13-P
153	BG	202	PC1	O13-C11-C12-N
153	BS	1301	PC1	C11-O13-P-O12
153	BS	1301	PC1	C11-O13-P-O11
153	BS	1301	PC1	C1-O11-P-O14
153	BS	1301	PC1	O22-C21-O21-C2
153	BS	1301	PC1	C22-C21-O21-C2
153	BS	1302	PC1	C11-O13-P-O12
153	BS	1302	PC1	C1-O11-P-O12
153	BS	1302	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	BT	203	PC1	C11-O13-P-O14
153	BT	203	PC1	C1-O11-P-O12
153	BT	203	PC1	C1-O11-P-O14
153	BT	203	PC1	C1-O11-P-O13
153	BT	203	PC1	O22-C21-O21-C2
153	BT	203	PC1	C22-C21-O21-C2
153	CC	302	PC1	C1-O11-P-O12
153	CC	302	PC1	C1-O11-P-O14
153	CC	302	PC1	O21-C2-C3-O31
153	A	1201	PC1	C11-O13-P-O14
153	A	1201	PC1	C11-O13-P-O11
153	C	509	PC1	C11-O13-P-O12
153	C	509	PC1	C11-O13-P-O14
153	C	509	PC1	C12-C11-O13-P
153	C	509	PC1	O13-C11-C12-N
153	C	509	PC1	O22-C21-O21-C2
153	C	509	PC1	C22-C21-O21-C2
153	C	510	PC1	C11-O13-P-O14
153	D	402	PC1	C11-O13-P-O14
153	E	303	PC1	C11-O13-P-O14
153	E	303	PC1	C22-C21-O21-C2
153	K	501	PC1	C11-O13-P-O14
153	K	501	PC1	C1-O11-P-O14
153	K	501	PC1	C1-O11-P-O13
153	K	501	PC1	O13-C11-C12-N
153	K	502	PC1	C11-O13-P-O12
153	K	502	PC1	C22-C21-O21-C2
153	c	503	PC1	O13-C11-C12-N
153	c	503	PC1	O22-C21-O21-C2
153	c	503	PC1	C22-C21-O21-C2
153	c	507	PC1	O13-C11-C12-N
153	c	508	PC1	C22-C21-O21-C2
153	d	801	PC1	C1-O11-P-O14
153	e	1101	PC1	C11-O13-P-O14
153	e	1101	PC1	C11-O13-P-O11
153	g	802	PC1	C11-O13-P-O12
153	g	802	PC1	C1-O11-P-O14
153	g	802	PC1	C22-C21-O21-C2
153	k	301	PC1	C11-O13-P-O11
153	k	301	PC1	O13-C11-C12-N
153	DA	707	PC1	C11-O13-P-O14
153	DA	708	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	DB	702	PC1	O22-C21-O21-C2
153	DC	602	PC1	C11-O13-P-O14
153	DC	602	PC1	C1-O11-P-O12
153	DC	602	PC1	C1-O11-P-O14
153	DC	603	PC1	O13-C11-C12-N
153	DC	604	PC1	C11-O13-P-O12
153	DC	604	PC1	C11-O13-P-O14
153	DC	604	PC1	C11-O13-P-O11
153	DC	605	PC1	C22-C21-O21-C2
153	DC	608	PC1	C11-O13-P-O12
153	DC	608	PC1	O22-C21-O21-C2
153	DC	608	PC1	C22-C21-O21-C2
153	DI	303	PC1	C1-O11-P-O12
153	DI	303	PC1	C1-O11-P-O14
153	DI	303	PC1	C1-O11-P-O13
153	DJ	306	PC1	C11-O13-P-O12
153	DJ	306	PC1	C11-O13-P-O14
153	DS	406	PC1	C11-O13-P-O14
153	DS	406	PC1	C11-O13-P-O11
153	DS	406	PC1	C1-O11-P-O12
153	DS	406	PC1	C1-O11-P-O14
153	DS	406	PC1	C12-C11-O13-P
153	DV	404	PC1	C11-O13-P-O12
153	DV	406	PC1	C11-O13-P-O12
153	DV	406	PC1	C11-O13-P-O14
153	DV	406	PC1	C1-O11-P-O12
153	DV	406	PC1	C1-O11-P-O14
153	DX	305	PC1	C22-C21-O21-C2
153	DX	308	PC1	O13-C11-C12-N
153	DY	302	PC1	O13-C11-C12-N
153	DY	302	PC1	O22-C21-O21-C2
153	EB	301	PC1	C11-O13-P-O11
153	EB	301	PC1	C1-O11-P-O14
153	EB	303	PC1	O13-C11-C12-N
153	EN	1203	PC1	C11-O13-P-O14
153	EN	1203	PC1	O21-C2-C3-O31
153	EO	201	PC1	C12-C11-O13-P
153	EO	201	PC1	O13-C11-C12-N
153	EO	204	PC1	C11-O13-P-O12
153	EO	204	PC1	C1-O11-P-O12
153	EO	205	PC1	C11-O13-P-O12
153	EO	205	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	EO	205	PC1	C11-O13-P-O11
153	EO	205	PC1	C22-C21-O21-C2
153	EO	206	PC1	C11-O13-P-O12
153	EO	206	PC1	C11-O13-P-O14
153	EO	206	PC1	C11-O13-P-O11
153	EO	206	PC1	C22-C21-O21-C2
153	Da	706	PC1	C11-O13-P-O14
153	Da	706	PC1	O21-C2-C3-O31
153	Da	707	PC1	C1-O11-P-O12
153	Da	707	PC1	C1-O11-P-O14
153	Da	707	PC1	C1-O11-P-O13
153	Da	707	PC1	O13-C11-C12-N
153	Db	702	PC1	C11-O13-P-O12
153	Db	702	PC1	C22-C21-O21-C2
153	Dc	602	PC1	C1-O11-P-O12
153	Dc	602	PC1	C1-O11-P-O14
153	Dc	602	PC1	C1-O11-P-O13
153	Dc	604	PC1	C1-O11-P-O12
153	Dc	604	PC1	C1-O11-P-O14
153	Dc	605	PC1	C11-O13-P-O14
153	Dc	605	PC1	C1-O11-P-O14
153	Dc	605	PC1	O22-C21-O21-C2
153	Dc	605	PC1	C22-C21-O21-C2
153	Dc	609	PC1	C11-O13-P-O12
153	Dc	609	PC1	O22-C21-O21-C2
153	Dc	609	PC1	C22-C21-O21-C2
153	Dg	203	PC1	C22-C21-O21-C2
153	Di	1104	PC1	C1-O11-P-O14
153	Dj	406	PC1	C11-O13-P-O12
153	Dj	406	PC1	C1-O11-P-O14
153	Dj	406	PC1	C1-O11-P-O13
153	Ds	407	PC1	O21-C2-C3-O31
153	Dv	405	PC1	C11-O13-P-O14
153	Dv	405	PC1	C11-O13-P-O11
153	Dv	405	PC1	C1-O11-P-O12
153	Dv	405	PC1	C1-O11-P-O14
153	Dv	405	PC1	C1-O11-P-O13
153	Dv	407	PC1	C11-O13-P-O12
153	Dv	407	PC1	C11-O13-P-O14
153	Dv	407	PC1	C1-O11-P-O12
153	Dx	1203	PC1	C1-O11-P-O12
153	Dx	1203	PC1	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dx	1203	PC1	O13-C11-C12-N
153	Dx	1203	PC1	O11-C1-C2-O21
153	Dx	1205	PC1	C11-O13-P-O14
153	Dy	302	PC1	O13-C11-C12-N
153	Dy	302	PC1	O22-C21-O21-C2
153	Eb	301	PC1	C1-O11-P-O14
153	Eb	303	PC1	O13-C11-C12-N
153	Ef	501	PC1	C11-O13-P-O14
153	Ef	501	PC1	C1-O11-P-O12
153	El	904	PC1	C11-O13-P-O12
153	El	904	PC1	C1-O11-P-O12
153	Eo	201	PC1	C12-C11-O13-P
153	Eo	201	PC1	O13-C11-C12-N
153	Eo	204	PC1	C11-O13-P-O12
153	Eo	204	PC1	C11-O13-P-O14
153	Eo	204	PC1	C22-C21-O21-C2
153	Eo	205	PC1	C11-O13-P-O12
153	Eo	205	PC1	C11-O13-P-O14
153	Eo	205	PC1	C22-C21-O21-C2
154	A1	401	NDP	C5B-O5B-PA-O1A
155	A2	401	3PE	O11-C1-C2-O21
155	A9	602	3PE	C1-O11-P-O12
155	AJ	502	3PE	C11-O13-P-O14
155	BA	301	3PE	C11-O13-P-O14
155	BP	201	3PE	C1-O11-P-O14
155	BT	201	3PE	C1-O11-P-O12
155	BT	201	3PE	C1-O11-P-O14
155	BT	201	3PE	C11-O13-P-O14
155	BT	201	3PE	C22-C21-O21-C2
155	CD	303	3PE	C1-O11-P-O12
155	CD	303	3PE	C1-O11-P-O14
155	C	513	3PE	C11-O13-P-O11
155	C	513	3PE	C11-O13-P-O12
155	C	513	3PE	C11-O13-P-O14
155	G	401	3PE	C1-O11-P-O14
155	G	401	3PE	C11-O13-P-O12
155	G	401	3PE	C11-O13-P-O14
155	DC	606	3PE	C1-O11-P-O12
155	DC	606	3PE	C1-O11-P-O14
155	DC	607	3PE	C11-O13-P-O14
155	DG	204	3PE	C11-O13-P-O12
155	DG	204	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DI	301	3PE	C1-O11-P-O14
155	DI	301	3PE	O21-C2-C3-O31
155	DJ	301	3PE	C1-O11-P-O12
155	DR	401	3PE	O21-C2-C3-O31
155	DS	402	3PE	C1-O11-P-O14
155	DS	402	3PE	C11-O13-P-O11
155	DX	302	3PE	C11-O13-P-O12
155	DX	302	3PE	C11-O13-P-O14
155	DX	302	3PE	O13-C11-C12-N
155	DX	303	3PE	C1-O11-P-O12
155	DX	303	3PE	C1-O11-P-O13
155	DX	303	3PE	C1-O11-P-O14
155	DX	303	3PE	C11-O13-P-O14
155	DX	304	3PE	C1-O11-P-O12
155	DX	304	3PE	C1-O11-P-O13
155	DX	304	3PE	C1-O11-P-O14
155	DX	304	3PE	C11-O13-P-O12
155	DX	304	3PE	C11-O13-P-O14
155	EL	904	3PE	C1-O11-P-O12
155	EL	904	3PE	C1-O11-P-O14
155	EL	904	3PE	C11-O13-P-O14
155	EM	901	3PE	C1-O11-P-O12
155	EM	901	3PE	C1-O11-P-O13
155	EM	901	3PE	C1-O11-P-O14
155	EN	1204	3PE	C11-O13-P-O12
155	EO	203	3PE	C1-O11-P-O12
155	EO	203	3PE	C1-O11-P-O14
155	Da	708	3PE	C1-O11-P-O12
155	Da	708	3PE	C1-O11-P-O14
155	Da	708	3PE	C11-O13-P-O14
155	Dc	607	3PE	C1-O11-P-O14
155	Dc	607	3PE	C11-O13-P-O11
155	Dc	607	3PE	C11-O13-P-O12
155	Dc	607	3PE	C11-O13-P-O14
155	Dd	703	3PE	C1-O11-P-O12
155	Dd	703	3PE	C11-O13-P-O14
155	Dg	204	3PE	C1-O11-P-O13
155	Di	1102	3PE	C1-O11-P-O13
155	Di	1102	3PE	C1-O11-P-O14
155	Di	1102	3PE	O21-C2-C3-O31
155	Dr	401	3PE	C1-O11-P-O13
155	Dr	404	3PE	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	Ds	403	3PE	C1-O11-P-O14
155	Ds	403	3PE	C11-O13-P-O11
155	Dx	1202	3PE	C1-O11-P-O12
155	Dx	1202	3PE	C1-O11-P-O14
155	Dx	1202	3PE	C11-O13-P-O14
155	Dx	1202	3PE	O21-C2-C3-O31
155	Dx	1202	3PE	C22-C21-O21-C2
155	Dx	1206	3PE	C1-O11-P-O12
155	Dx	1206	3PE	C1-O11-P-O13
155	Dx	1206	3PE	C1-O11-P-O14
155	Dx	1206	3PE	C11-O13-P-O11
155	Dx	1206	3PE	C11-O13-P-O12
155	Dx	1206	3PE	C11-O13-P-O14
155	Dx	1206	3PE	O13-C11-C12-N
155	Dx	1207	3PE	C1-O11-P-O14
155	Dx	1207	3PE	C11-O13-P-O12
155	Dx	1207	3PE	C11-O13-P-O14
155	Dx	1208	3PE	C1-O11-P-O12
155	Dx	1208	3PE	C1-O11-P-O13
155	Dx	1208	3PE	C1-O11-P-O14
155	Dx	1208	3PE	C11-O13-P-O12
155	El	905	3PE	C1-O11-P-O12
155	El	905	3PE	C11-O13-P-O14
155	Em	901	3PE	C1-O11-P-O12
155	Em	901	3PE	C1-O11-P-O13
155	Em	901	3PE	C1-O11-P-O14
155	Eo	202	3PE	O22-C21-O21-C2
155	Eo	202	3PE	C22-C21-O21-C2
155	Eo	203	3PE	C1-O11-P-O12
155	Eo	203	3PE	C1-O11-P-O13
155	Eo	203	3PE	C1-O11-P-O14
156	AA	902	LPP	C6-O5-P1-O2
156	AA	902	LPP	C6-O5-P1-O3
156	AA	902	LPP	C6-O5-P1-O4
156	DA	710	LPP	C6-O5-P1-O2
156	DA	710	LPP	C6-O5-P1-O3
156	DA	710	LPP	C6-O5-P1-O4
156	DN	504	LPP	C6-O5-P1-O2
156	DN	504	LPP	C6-O5-P1-O3
156	DN	504	LPP	C6-O5-P1-O4
156	Dn	504	LPP	C6-O5-P1-O2
156	Dn	504	LPP	C6-O5-P1-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
156	Dl	1101	LPP	C6-O5-P1-O2
156	Dl	1101	LPP	C6-O5-P1-O4
157	A8	401	ADP	PA-O3A-PB-O2B
161	AS	200	8Q1	C28-C29-C32-C34
161	AS	200	8Q1	C28-C29-C32-O33
161	AS	200	8Q1	C30-C29-C32-C34
161	AS	200	8Q1	C30-C29-C32-O33
161	AS	200	8Q1	C31-C29-C32-C34
161	AS	200	8Q1	C31-C29-C32-O33
161	AS	200	8Q1	C42-C43-S44-C1
164	CA	702	FAD	C5B-O5B-PA-O1A
164	CA	702	FAD	C5B-O5B-PA-O2A
164	CA	702	FAD	N10-C1'-C2'-O2'
164	CA	702	FAD	N10-C1'-C2'-C3'
164	CA	702	FAD	C5'-O5'-P-O1P
164	CA	702	FAD	C5'-O5'-P-O2P
164	CA	702	FAD	C5'-O5'-P-O3P
167	CC	303	UQ8	C12-C11-C9-C10
167	CC	303	UQ8	C12-C11-C9-C8
167	C	511	UQ8	C30-C29-C31-C32
167	C	511	UQ8	C28-C29-C31-C32
167	C	511	UQ8	C5-C6-C7-C8
167	C	512	UQ8	C9-C11-C12-C13
167	c	510	UQ8	C1-C6-C7-C8
167	c	510	UQ8	C5-C6-C7-C8
167	EL	905	UQ8	C30-C29-C31-C32
167	EL	905	UQ8	C28-C29-C31-C32
167	EL	905	UQ8	C1-C6-C7-C8
167	EL	905	UQ8	C5-C6-C7-C8
167	Ds	404	UQ8	C35-C34-C36-C37
167	Ds	404	UQ8	C33-C34-C36-C37
167	El	906	UQ8	C30-C29-C31-C32
167	El	906	UQ8	C28-C29-C31-C32
167	El	906	UQ8	C1-C6-C7-C8
167	El	906	UQ8	C5-C6-C7-C8
167	En	1202	UQ8	C25-C24-C26-C27
167	En	1202	UQ8	C23-C24-C26-C27
168	C	501	HEM	C1A-C2A-CAA-CBA
168	C	501	HEM	C3A-C2A-CAA-CBA
173	ER	201	ATP	C5'-O5'-PA-O2A
150	A0	602	CDL	OA9-CA7-OA8-CA6
150	AF	402	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	BG	201	CDL	OB9-CB7-OB8-CB6
150	CD	302	CDL	OA9-CA7-OA8-CA6
150	H	1301	CDL	OB9-CB7-OB8-CB6
150	DD	704	CDL	OA9-CA7-OA8-CA6
150	DV	402	CDL	OA9-CA7-OA8-CA6
150	EI	401	CDL	OA9-CA7-OA8-CA6
150	EK	201	CDL	OB9-CB7-OB8-CB6
150	EL	901	CDL	OB9-CB7-OB8-CB6
150	Dd	704	CDL	OA9-CA7-OA8-CA6
150	Dj	402	CDL	OA9-CA7-OA8-CA6
150	Dj	403	CDL	OA9-CA7-OA8-CA6
150	Dj	405	CDL	OB9-CB7-OB8-CB6
150	Dn	506	CDL	OA9-CA7-OA8-CA6
150	Du	402	CDL	OB9-CB7-OB8-CB6
150	Dv	403	CDL	OA9-CA7-OA8-CA6
150	Ei	401	CDL	OA9-CA7-OA8-CA6
153	AA	906	PC1	O32-C31-O31-C3
153	D	402	PC1	O32-C31-O31-C3
153	c	508	PC1	O32-C31-O31-C3
153	e	1101	PC1	O32-C31-O31-C3
153	DJ	306	PC1	O32-C31-O31-C3
153	EB	301	PC1	O32-C31-O31-C3
153	Dj	406	PC1	O32-C31-O31-C3
155	BT	201	3PE	O32-C31-O31-C3
150	DG	202	CDL	CA4-CA6-OA8-CA7
150	A0	602	CDL	C31-CA7-OA8-CA6
150	EA	301	CDL	C31-CA7-OA8-CA6
150	Dj	402	CDL	C31-CA7-OA8-CA6
150	Ei	401	CDL	C31-CA7-OA8-CA6
153	c	508	PC1	C32-C31-O31-C3
153	e	1101	PC1	C32-C31-O31-C3
153	EB	301	PC1	C32-C31-O31-C3
155	BT	201	3PE	C32-C31-O31-C3
150	A1	402	CDL	OB9-CB7-OB8-CB6
150	B0	102	CDL	OA9-CA7-OA8-CA6
150	B1	402	CDL	OB9-CB7-OB8-CB6
150	CG	301	CDL	OB9-CB7-OB8-CB6
150	C	506	CDL	OA9-CA7-OA8-CA6
150	H	1302	CDL	OA9-CA7-OA8-CA6
150	c	509	CDL	OB9-CB7-OB8-CB6
150	g	801	CDL	OA9-CA7-OA8-CA6
150	g	801	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DD	704	CDL	OB9-CB7-OB8-CB6
150	DG	201	CDL	OB9-CB7-OB8-CB6
150	DH	202	CDL	OB9-CB7-OB8-CB6
150	DJ	302	CDL	OB9-CB7-OB8-CB6
150	DJ	305	CDL	OB9-CB7-OB8-CB6
150	DJ	307	CDL	OA9-CA7-OA8-CA6
150	DN	502	CDL	OB9-CB7-OB8-CB6
150	DN	506	CDL	OA9-CA7-OA8-CA6
150	DS	401	CDL	OB9-CB7-OB8-CB6
150	DS	404	CDL	OA9-CA7-OA8-CA6
150	DS	405	CDL	OB9-CB7-OB8-CB6
150	DU	402	CDL	OB9-CB7-OB8-CB6
150	DV	403	CDL	OA9-CA7-OA8-CA6
150	DX	301	CDL	OA9-CA7-OA8-CA6
150	DX	306	CDL	OA9-CA7-OA8-CA6
150	ED	604	CDL	OA9-CA7-OA8-CA6
150	ED	604	CDL	OB9-CB7-OB8-CB6
150	EH	1601	CDL	OB9-CB7-OB8-CB6
150	EO	202	CDL	OB9-CB7-OB8-CB6
150	ES	1101	CDL	OA9-CA7-OA8-CA6
150	Dd	704	CDL	OB9-CB7-OB8-CB6
150	Dg	201	CDL	OB9-CB7-OB8-CB6
150	Dh	202	CDL	OB9-CB7-OB8-CB6
150	Dj	401	CDL	OB9-CB7-OB8-CB6
150	Dj	404	CDL	OB9-CB7-OB8-CB6
150	Dj	407	CDL	OA9-CA7-OA8-CA6
150	Dn	501	CDL	OB9-CB7-OB8-CB6
150	Dn	503	CDL	OB9-CB7-OB8-CB6
150	Dq	1401	CDL	OA9-CA7-OA8-CA6
150	Ds	406	CDL	OB9-CB7-OB8-CB6
150	Ea	502	CDL	OA9-CA7-OA8-CA6
150	El	902	CDL	OB9-CB7-OB8-CB6
150	Ep	701	CDL	OB9-CB7-OB8-CB6
150	Eu	101	CDL	OA9-CA7-OA8-CA6
153	AA	904	PC1	O32-C31-O31-C3
153	AA	907	PC1	O32-C31-O31-C3
153	B1	403	PC1	O32-C31-O31-C3
153	c	503	PC1	O32-C31-O31-C3
153	Eb	301	PC1	O32-C31-O31-C3
153	Ef	501	PC1	O32-C31-O31-C3
155	BA	301	3PE	O32-C31-O31-C3
155	CK	101	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	CD	303	3PE	O32-C31-O31-C3
155	C	513	3PE	O32-C31-O31-C3
155	Da	708	3PE	O32-C31-O31-C3
155	Dr	401	3PE	O32-C31-O31-C3
150	A0	601	CDL	OA7-CA5-OA6-CA4
150	A0	601	CDL	OB7-CB5-OB6-CB4
150	A0	602	CDL	OB7-CB5-OB6-CB4
150	AA	908	CDL	OA7-CA5-OA6-CA4
150	AA	908	CDL	OB7-CB5-OB6-CB4
150	AM	301	CDL	OA7-CA5-OA6-CA4
150	AP	301	CDL	OA7-CA5-OA6-CA4
150	AP	301	CDL	OB7-CB5-OB6-CB4
150	B0	101	CDL	OA7-CA5-OA6-CA4
150	BC	301	CDL	OA7-CA5-OA6-CA4
150	BE	201	CDL	OA7-CA5-OA6-CA4
150	BG	201	CDL	OA7-CA5-OA6-CA4
150	BL	301	CDL	OA7-CA5-OA6-CA4
150	BT	202	CDL	OA7-CA5-OA6-CA4
150	BT	202	CDL	OB7-CB5-OB6-CB4
150	BV	201	CDL	OB7-CB5-OB6-CB4
150	BY	201	CDL	OB7-CB5-OB6-CB4
150	CG	302	CDL	OA7-CA5-OA6-CA4
150	CD	302	CDL	OA7-CA5-OA6-CA4
150	C	505	CDL	OA7-CA5-OA6-CA4
150	C	506	CDL	OA7-CA5-OA6-CA4
150	C	506	CDL	OB7-CB5-OB6-CB4
150	H	1301	CDL	OA7-CA5-OA6-CA4
150	c	506	CDL	OA7-CA5-OA6-CA4
150	g	801	CDL	OB7-CB5-OB6-CB4
150	h	501	CDL	OB7-CB5-OB6-CB4
150	DA	709	CDL	OA7-CA5-OA6-CA4
150	DD	703	CDL	OA7-CA5-OA6-CA4
150	DD	705	CDL	OB7-CB5-OB6-CB4
150	DG	201	CDL	OB7-CB5-OB6-CB4
150	DI	302	CDL	OA7-CA5-OA6-CA4
150	DI	302	CDL	OB7-CB5-OB6-CB4
150	DJ	302	CDL	OB7-CB5-OB6-CB4
150	DJ	304	CDL	OA7-CA5-OA6-CA4
150	DJ	305	CDL	OB7-CB5-OB6-CB4
150	DM	502	CDL	OA7-CA5-OA6-CA4
150	DM	502	CDL	OB7-CB5-OB6-CB4
150	DN	506	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DN	507	CDL	OA7-CA5-OA6-CA4
150	DO	501	CDL	OA7-CA5-OA6-CA4
150	DO	501	CDL	OB7-CB5-OB6-CB4
150	DS	404	CDL	OA7-CA5-OA6-CA4
150	DU	402	CDL	OA7-CA5-OA6-CA4
150	DV	401	CDL	OB7-CB5-OB6-CB4
150	DV	403	CDL	OB7-CB5-OB6-CB4
150	DY	301	CDL	OA7-CA5-OA6-CA4
150	DY	301	CDL	OB7-CB5-OB6-CB4
150	EB	302	CDL	OA7-CA5-OA6-CA4
150	ED	604	CDL	OA7-CA5-OA6-CA4
150	EH	1601	CDL	OB7-CB5-OB6-CB4
150	EL	902	CDL	OA7-CA5-OA6-CA4
150	EL	903	CDL	OB7-CB5-OB6-CB4
150	EN	1202	CDL	OA7-CA5-OA6-CA4
150	EN	1202	CDL	OB7-CB5-OB6-CB4
150	EO	202	CDL	OB7-CB5-OB6-CB4
150	Dd	702	CDL	OA7-CA5-OA6-CA4
150	Dg	201	CDL	OB7-CB5-OB6-CB4
150	Di	1103	CDL	OA7-CA5-OA6-CA4
150	Dj	402	CDL	OA7-CA5-OA6-CA4
150	Dj	404	CDL	OB7-CB5-OB6-CB4
150	Dj	407	CDL	OB7-CB5-OB6-CB4
150	Dm	501	CDL	OB7-CB5-OB6-CB4
150	Dm	502	CDL	OA7-CA5-OA6-CA4
150	Dm	502	CDL	OB7-CB5-OB6-CB4
150	Do	501	CDL	OB7-CB5-OB6-CB4
150	Dq	1401	CDL	OB7-CB5-OB6-CB4
150	Du	401	CDL	OB7-CB5-OB6-CB4
150	Dv	403	CDL	OB7-CB5-OB6-CB4
150	Dx	1204	CDL	OB7-CB5-OB6-CB4
150	Dy	301	CDL	OB7-CB5-OB6-CB4
150	Ea	502	CDL	OA7-CA5-OA6-CA4
150	Eb	302	CDL	OA7-CA5-OA6-CA4
150	Ed	204	CDL	OA7-CA5-OA6-CA4
150	Eg	101	CDL	OA7-CA5-OA6-CA4
150	Ei	401	CDL	OA7-CA5-OA6-CA4
150	El	901	CDL	OB7-CB5-OB6-CB4
150	El	902	CDL	OB7-CB5-OB6-CB4
150	El	903	CDL	OB7-CB5-OB6-CB4
153	A2	402	PC1	O22-C21-O21-C2
153	AA	904	PC1	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AM	302	PC1	O22-C21-O21-C2
153	A	1201	PC1	O22-C21-O21-C2
153	E	303	PC1	O22-C21-O21-C2
153	K	502	PC1	O22-C21-O21-C2
153	c	508	PC1	O22-C21-O21-C2
153	DC	605	PC1	O22-C21-O21-C2
153	DG	203	PC1	O22-C21-O21-C2
153	DX	305	PC1	O22-C21-O21-C2
153	EO	205	PC1	O22-C21-O21-C2
153	EO	206	PC1	O22-C21-O21-C2
153	Db	702	PC1	O22-C21-O21-C2
153	Dg	203	PC1	O22-C21-O21-C2
153	Eo	204	PC1	O22-C21-O21-C2
153	Eo	205	PC1	O22-C21-O21-C2
155	BT	201	3PE	O22-C21-O21-C2
155	Dx	1202	3PE	O22-C21-O21-C2
150	Ds	405	CDL	OA9-CA7-OA8-CA6
150	Dg	202	CDL	CA4-CA6-OA8-CA7
150	AF	402	CDL	C71-CB7-OB8-CB6
150	B0	102	CDL	C31-CA7-OA8-CA6
150	BG	201	CDL	C71-CB7-OB8-CB6
150	CD	302	CDL	C31-CA7-OA8-CA6
150	H	1301	CDL	C71-CB7-OB8-CB6
150	H	1302	CDL	C31-CA7-OA8-CA6
150	DD	704	CDL	C31-CA7-OA8-CA6
150	DG	201	CDL	C71-CB7-OB8-CB6
150	DJ	302	CDL	C71-CB7-OB8-CB6
150	DJ	305	CDL	C71-CB7-OB8-CB6
150	DN	506	CDL	C31-CA7-OA8-CA6
150	DQ	1504	CDL	C71-CB7-OB8-CB6
150	DS	405	CDL	C71-CB7-OB8-CB6
150	DV	402	CDL	C31-CA7-OA8-CA6
150	DX	301	CDL	C31-CA7-OA8-CA6
150	ED	604	CDL	C71-CB7-OB8-CB6
150	EI	401	CDL	C31-CA7-OA8-CA6
150	EK	201	CDL	C71-CB7-OB8-CB6
150	EL	901	CDL	C71-CB7-OB8-CB6
150	EL	903	CDL	C71-CB7-OB8-CB6
150	ES	1101	CDL	C31-CA7-OA8-CA6
150	Da	709	CDL	C71-CB7-OB8-CB6
150	Dd	704	CDL	C31-CA7-OA8-CA6
150	Dd	704	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	201	CDL	C71-CB7-OB8-CB6
150	Dj	403	CDL	C31-CA7-OA8-CA6
150	Dj	405	CDL	C71-CB7-OB8-CB6
150	Dn	501	CDL	C71-CB7-OB8-CB6
150	Dn	506	CDL	C31-CA7-OA8-CA6
150	Dq	1401	CDL	C31-CA7-OA8-CA6
150	Ds	406	CDL	C71-CB7-OB8-CB6
150	Du	401	CDL	C31-CA7-OA8-CA6
150	Du	402	CDL	C71-CB7-OB8-CB6
150	Dv	403	CDL	C31-CA7-OA8-CA6
150	Ea	502	CDL	C31-CA7-OA8-CA6
150	Ed	204	CDL	C31-CA7-OA8-CA6
150	Eh	1601	CDL	C71-CB7-OB8-CB6
153	AA	904	PC1	C32-C31-O31-C3
153	AA	906	PC1	C32-C31-O31-C3
153	B1	403	PC1	C32-C31-O31-C3
153	D	402	PC1	C32-C31-O31-C3
153	E	303	PC1	C32-C31-O31-C3
153	DJ	306	PC1	C32-C31-O31-C3
153	Dj	406	PC1	C32-C31-O31-C3
155	BA	301	3PE	C32-C31-O31-C3
155	C	513	3PE	C32-C31-O31-C3
155	EN	1204	3PE	C32-C31-O31-C3
155	Da	708	3PE	C32-C31-O31-C3
155	Ds	408	3PE	C32-C31-O31-C3
150	AF	401	CDL	C51-CB5-OB6-CB4
150	BC	301	CDL	C11-CA5-OA6-CA4
150	BE	201	CDL	C51-CB5-OB6-CB4
150	BL	301	CDL	C11-CA5-OA6-CA4
150	BT	204	CDL	C11-CA5-OA6-CA4
150	CC	305	CDL	C51-CB5-OB6-CB4
150	C	507	CDL	C11-CA5-OA6-CA4
150	DJ	305	CDL	C11-CA5-OA6-CA4
150	DJ	305	CDL	C51-CB5-OB6-CB4
150	DM	502	CDL	C11-CA5-OA6-CA4
150	DM	502	CDL	C51-CB5-OB6-CB4
150	DQ	1504	CDL	C11-CA5-OA6-CA4
150	DS	404	CDL	C11-CA5-OA6-CA4
150	DV	401	CDL	C11-CA5-OA6-CA4
150	EB	302	CDL	C51-CB5-OB6-CB4
150	EL	903	CDL	C51-CB5-OB6-CB4
150	EN	1202	CDL	C11-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	201	CDL	C51-CB5-OB6-CB4
150	Dj	404	CDL	C11-CA5-OA6-CA4
150	Dj	405	CDL	C11-CA5-OA6-CA4
150	Dm	502	CDL	C51-CB5-OB6-CB4
150	Dq	1401	CDL	C11-CA5-OA6-CA4
150	Du	401	CDL	C51-CB5-OB6-CB4
150	Dv	401	CDL	C11-CA5-OA6-CA4
150	Eb	302	CDL	C11-CA5-OA6-CA4
150	Eb	302	CDL	C51-CB5-OB6-CB4
150	El	902	CDL	C51-CB5-OB6-CB4
153	A1	403	PC1	C22-C21-O21-C2
153	AL	303	PC1	C22-C21-O21-C2
153	AM	302	PC1	C22-C21-O21-C2
153	A	1201	PC1	C22-C21-O21-C2
153	DB	702	PC1	C22-C21-O21-C2
153	DG	203	PC1	C22-C21-O21-C2
153	DY	302	PC1	C22-C21-O21-C2
153	Dy	302	PC1	C22-C21-O21-C2
150	Dx	1201	CDL	OB9-CB7-OB8-CB6
150	DV	401	CDL	OA9-CA7-OA8-CA6
150	Dg	201	CDL	OA9-CA7-OA8-CA6
150	Di	1101	CDL	OB9-CB7-OB8-CB6
150	A1	402	CDL	C31-CA7-OA8-CA6
150	A1	402	CDL	C71-CB7-OB8-CB6
150	B1	402	CDL	C71-CB7-OB8-CB6
150	BT	204	CDL	C31-CA7-OA8-CA6
150	CG	301	CDL	C71-CB7-OB8-CB6
150	CJ	201	CDL	C31-CA7-OA8-CA6
150	C	503	CDL	C31-CA7-OA8-CA6
150	C	506	CDL	C31-CA7-OA8-CA6
150	c	509	CDL	C71-CB7-OB8-CB6
150	g	801	CDL	C31-CA7-OA8-CA6
150	g	801	CDL	C71-CB7-OB8-CB6
150	DD	704	CDL	C71-CB7-OB8-CB6
150	DH	202	CDL	C31-CA7-OA8-CA6
150	DH	202	CDL	C71-CB7-OB8-CB6
150	DJ	307	CDL	C31-CA7-OA8-CA6
150	DN	502	CDL	C71-CB7-OB8-CB6
150	DS	401	CDL	C71-CB7-OB8-CB6
150	DS	404	CDL	C31-CA7-OA8-CA6
150	DU	402	CDL	C71-CB7-OB8-CB6
150	DV	403	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DX	306	CDL	C31-CA7-OA8-CA6
150	EA	301	CDL	C71-CB7-OB8-CB6
150	ED	604	CDL	C31-CA7-OA8-CA6
150	EH	1601	CDL	C71-CB7-OB8-CB6
150	EN	1201	CDL	C71-CB7-OB8-CB6
150	EO	202	CDL	C71-CB7-OB8-CB6
150	Dh	202	CDL	C31-CA7-OA8-CA6
150	Dh	202	CDL	C71-CB7-OB8-CB6
150	Dj	401	CDL	C71-CB7-OB8-CB6
150	Dj	404	CDL	C71-CB7-OB8-CB6
150	Dj	407	CDL	C31-CA7-OA8-CA6
150	Dn	503	CDL	C71-CB7-OB8-CB6
150	Dr	402	CDL	C31-CA7-OA8-CA6
150	Ds	405	CDL	C31-CA7-OA8-CA6
150	Dv	401	CDL	C31-CA7-OA8-CA6
150	Dx	1204	CDL	C31-CA7-OA8-CA6
150	Eg	101	CDL	C31-CA7-OA8-CA6
150	Ek	201	CDL	C71-CB7-OB8-CB6
150	El	902	CDL	C71-CB7-OB8-CB6
150	Ep	701	CDL	C71-CB7-OB8-CB6
150	Eu	101	CDL	C31-CA7-OA8-CA6
153	A9	601	PC1	C32-C31-O31-C3
153	AA	907	PC1	C32-C31-O31-C3
153	c	503	PC1	C32-C31-O31-C3
153	c	507	PC1	C32-C31-O31-C3
153	DC	602	PC1	C32-C31-O31-C3
153	DC	604	PC1	C32-C31-O31-C3
153	Dc	604	PC1	C32-C31-O31-C3
153	Ds	407	PC1	C32-C31-O31-C3
153	Eb	301	PC1	C32-C31-O31-C3
153	Ef	501	PC1	C32-C31-O31-C3
155	CK	101	3PE	C32-C31-O31-C3
155	CD	303	3PE	C32-C31-O31-C3
155	Dr	401	3PE	C32-C31-O31-C3
150	AA	901	CDL	OB7-CB5-OB6-CB4
150	c	501	CDL	OA7-CA5-OA6-CA4
150	DS	404	CDL	OB7-CB5-OB6-CB4
150	EH	1601	CDL	OA7-CA5-OA6-CA4
150	EO	202	CDL	OA7-CA5-OA6-CA4
150	Ds	401	CDL	OB7-CB5-OB6-CB4
150	Ds	405	CDL	OB7-CB5-OB6-CB4
150	Dy	301	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Eh	1601	CDL	OA7-CA5-OA6-CA4
153	D	402	PC1	O22-C21-O21-C2
153	g	802	PC1	O22-C21-O21-C2
150	A1	402	CDL	OA9-CA7-OA8-CA6
150	CJ	201	CDL	OA9-CA7-OA8-CA6
150	CC	304	CDL	OB9-CB7-OB8-CB6
150	CD	301	CDL	OA9-CA7-OA8-CA6
150	C	503	CDL	OA9-CA7-OA8-CA6
150	DA	706	CDL	OB9-CB7-OB8-CB6
150	DH	202	CDL	OA9-CA7-OA8-CA6
150	DQ	1504	CDL	OA9-CA7-OA8-CA6
150	DQ	1504	CDL	OB9-CB7-OB8-CB6
150	EA	301	CDL	OB9-CB7-OB8-CB6
150	EL	903	CDL	OB9-CB7-OB8-CB6
150	Du	401	CDL	OA9-CA7-OA8-CA6
150	Dv	401	CDL	OA9-CA7-OA8-CA6
150	Dv	402	CDL	OA9-CA7-OA8-CA6
150	Ek	201	CDL	OB9-CB7-OB8-CB6
150	El	901	CDL	OB9-CB7-OB8-CB6
153	E	303	PC1	O32-C31-O31-C3
153	c	507	PC1	O32-C31-O31-C3
153	DC	604	PC1	O32-C31-O31-C3
153	EN	1203	PC1	O32-C31-O31-C3
153	Dc	602	PC1	O32-C31-O31-C3
153	Ds	407	PC1	O32-C31-O31-C3
155	EN	1204	3PE	O32-C31-O31-C3
155	EO	203	3PE	O32-C31-O31-C3
155	Ds	408	3PE	O32-C31-O31-C3
150	AA	908	CDL	O1-C1-CB2-OB2
150	AF	402	CDL	O1-C1-CB2-OB2
150	AM	301	CDL	O1-C1-CA2-OA2
150	B0	101	CDL	O1-C1-CB2-OB2
150	BC	302	CDL	O1-C1-CB2-OB2
150	CG	302	CDL	O1-C1-CA2-OA2
150	C	503	CDL	O1-C1-CB2-OB2
150	C	506	CDL	O1-C1-CB2-OB2
150	c	501	CDL	O1-C1-CA2-OA2
150	c	509	CDL	O1-C1-CA2-OA2
150	DA	709	CDL	O1-C1-CA2-OA2
150	DA	709	CDL	O1-C1-CB2-OB2
150	DD	703	CDL	O1-C1-CA2-OA2
150	DD	706	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DG	201	CDL	O1-C1-CA2-OA2
150	DH	202	CDL	O1-C1-CA2-OA2
150	DJ	303	CDL	O1-C1-CA2-OA2
150	DJ	307	CDL	O1-C1-CB2-OB2
150	DM	502	CDL	O1-C1-CB2-OB2
150	DN	507	CDL	O1-C1-CA2-OA2
150	DR	403	CDL	O1-C1-CA2-OA2
150	DU	403	CDL	O1-C1-CB2-OB2
150	DX	306	CDL	O1-C1-CA2-OA2
150	EB	302	CDL	O1-C1-CA2-OA2
150	ED	605	CDL	O1-C1-CB2-OB2
150	EH	1601	CDL	O1-C1-CB2-OB2
150	EK	201	CDL	O1-C1-CA2-OA2
150	Da	709	CDL	O1-C1-CA2-OA2
150	Dd	702	CDL	O1-C1-CA2-OA2
150	Dd	706	CDL	O1-C1-CB2-OB2
150	Dh	202	CDL	O1-C1-CA2-OA2
150	Dj	402	CDL	O1-C1-CA2-OA2
150	Dj	403	CDL	O1-C1-CB2-OB2
150	Dm	501	CDL	O1-C1-CB2-OB2
150	Dn	503	CDL	O1-C1-CA2-OA2
150	Dr	403	CDL	O1-C1-CA2-OA2
150	Du	403	CDL	O1-C1-CA2-OA2
150	Dv	401	CDL	O1-C1-CB2-OB2
150	Dv	402	CDL	O1-C1-CB2-OB2
150	Dv	403	CDL	O1-C1-CA2-OA2
150	Dx	1204	CDL	O1-C1-CA2-OA2
150	Ed	204	CDL	O1-C1-CB2-OB2
150	Ed	205	CDL	O1-C1-CB2-OB2
150	Ei	401	CDL	O1-C1-CA2-OA2
150	El	902	CDL	O1-C1-CA2-OA2
150	Eu	101	CDL	O1-C1-CA2-OA2
150	A0	601	CDL	C71-CB7-OB8-CB6
150	B0	102	CDL	C71-CB7-OB8-CB6
150	B1	402	CDL	C31-CA7-OA8-CA6
150	CD	301	CDL	C31-CA7-OA8-CA6
150	C	505	CDL	C31-CA7-OA8-CA6
150	DA	709	CDL	C31-CA7-OA8-CA6
150	DC	601	CDL	C71-CB7-OB8-CB6
150	ED	601	CDL	C31-CA7-OA8-CA6
150	EL	902	CDL	C71-CB7-OB8-CB6
150	Dc	601	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	201	CDL	C31-CA7-OA8-CA6
150	Dh	201	CDL	C71-CB7-OB8-CB6
150	Dq	1401	CDL	C71-CB7-OB8-CB6
150	Dx	1201	CDL	C71-CB7-OB8-CB6
150	El	901	CDL	C71-CB7-OB8-CB6
150	Ep	701	CDL	C31-CA7-OA8-CA6
153	DV	405	PC1	C32-C31-O31-C3
153	DX	308	PC1	C32-C31-O31-C3
153	EN	1203	PC1	C32-C31-O31-C3
153	Dc	602	PC1	C32-C31-O31-C3
150	A0	601	CDL	OB9-CB7-OB8-CB6
150	BT	204	CDL	OA9-CA7-OA8-CA6
150	EL	902	CDL	OB9-CB7-OB8-CB6
150	Da	709	CDL	OB9-CB7-OB8-CB6
150	Dc	601	CDL	OB9-CB7-OB8-CB6
150	Eh	1601	CDL	OB9-CB7-OB8-CB6
153	DC	602	PC1	O32-C31-O31-C3
150	AC	802	CDL	C11-CA5-OA6-CA4
150	C	503	CDL	C11-CA5-OA6-CA4
150	c	502	CDL	C11-CA5-OA6-CA4
150	DM	501	CDL	C11-CA5-OA6-CA4
150	DQ	1501	CDL	C11-CA5-OA6-CA4
150	DQ	1502	CDL	C11-CA5-OA6-CA4
150	DR	403	CDL	C11-CA5-OA6-CA4
150	DU	401	CDL	C11-CA5-OA6-CA4
150	DU	401	CDL	C51-CB5-OB6-CB4
150	DU	404	CDL	C11-CA5-OA6-CA4
150	EK	201	CDL	C11-CA5-OA6-CA4
150	EK	201	CDL	C51-CB5-OB6-CB4
150	ES	1101	CDL	C11-CA5-OA6-CA4
150	Dj	403	CDL	C11-CA5-OA6-CA4
150	Dj	407	CDL	C11-CA5-OA6-CA4
150	Dm	501	CDL	C11-CA5-OA6-CA4
150	Dn	503	CDL	C11-CA5-OA6-CA4
150	Do	501	CDL	C11-CA5-OA6-CA4
150	Dq	1402	CDL	C51-CB5-OB6-CB4
150	Dr	403	CDL	C11-CA5-OA6-CA4
150	Dv	401	CDL	C51-CB5-OB6-CB4
150	Eu	101	CDL	C11-CA5-OA6-CA4
153	AX	401	PC1	C22-C21-O21-C2
153	D	402	PC1	C22-C21-O21-C2
153	k	301	PC1	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dv	405	PC1	C22-C21-O21-C2
153	Dx	1209	PC1	C22-C21-O21-C2
155	DG	204	3PE	C22-C21-O21-C2
150	Dd	705	CDL	CA5-C11-C12-C13
153	A9	601	PC1	O32-C31-O31-C3
151	A0	603	UDP	C3'-C4'-C5'-O5'
164	CA	702	FAD	O4B-C4B-C5B-O5B
164	CA	702	FAD	C3B-C4B-C5B-O5B
150	CC	304	CDL	C71-CB7-OB8-CB6
150	DA	706	CDL	C71-CB7-OB8-CB6
150	DQ	1504	CDL	C31-CA7-OA8-CA6
150	DV	401	CDL	C31-CA7-OA8-CA6
150	Di	1101	CDL	C71-CB7-OB8-CB6
150	Dv	402	CDL	C31-CA7-OA8-CA6
155	EO	203	3PE	C32-C31-O31-C3
150	DM	501	CDL	OA7-CA5-OA6-CA4
150	DQ	1501	CDL	OA7-CA5-OA6-CA4
150	DU	401	CDL	OB7-CB5-OB6-CB4
150	EK	201	CDL	OA7-CA5-OA6-CA4
150	ES	1101	CDL	OA7-CA5-OA6-CA4
150	Dj	407	CDL	OA7-CA5-OA6-CA4
150	Do	501	CDL	OA7-CA5-OA6-CA4
150	Dr	403	CDL	OA7-CA5-OA6-CA4
150	Dv	401	CDL	OB7-CB5-OB6-CB4
150	DU	401	CDL	C1-CA2-OA2-PA1
150	Dg	201	CDL	C1-CA2-OA2-PA1
150	Di	1101	CDL	CB4-CB3-OB5-PB2
150	Dj	405	CDL	C1-CB2-OB2-PB2
150	Ea	501	CDL	C1-CB2-OB2-PB2
153	A0	605	PC1	C2-C1-O11-P
153	AU	201	PC1	C2-C1-O11-P
155	CD	303	3PE	C2-C1-O11-P
150	Dh	201	CDL	OB9-CB7-OB8-CB6
150	Dh	202	CDL	OA9-CA7-OA8-CA6
150	Dr	402	CDL	OA9-CA7-OA8-CA6
150	Dx	1204	CDL	OA9-CA7-OA8-CA6
153	DV	405	PC1	O32-C31-O31-C3
153	DX	308	PC1	O32-C31-O31-C3
153	Dc	604	PC1	O32-C31-O31-C3
167	C	511	UQ8	C40-C39-C41-C42
167	C	512	UQ8	C20-C19-C21-C22
167	DS	403	UQ8	C35-C34-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
167	EN	1205	UQ8	C25-C24-C26-C27
167	C	511	UQ8	C38-C39-C41-C42
167	C	512	UQ8	C18-C19-C21-C22
167	EN	1205	UQ8	C23-C24-C26-C27
150	B0	102	CDL	OB9-CB7-OB8-CB6
150	C	505	CDL	OA9-CA7-OA8-CA6
150	DA	709	CDL	OA9-CA7-OA8-CA6
150	DC	601	CDL	OB9-CB7-OB8-CB6
150	EN	1201	CDL	OB9-CB7-OB8-CB6
150	Dq	1401	CDL	OB9-CB7-OB8-CB6
150	Eg	101	CDL	OA9-CA7-OA8-CA6
167	C	511	UQ8	C34-C36-C37-C38
167	C	512	UQ8	C24-C26-C27-C28
167	ED	603	UQ8	C39-C41-C42-C43
167	En	1202	UQ8	C34-C36-C37-C38
167	En	1202	UQ8	C19-C21-C22-C23
169	DA	703	HEA	C15-C16-C17-C18
169	Da	703	HEA	C19-C20-C21-C22
150	B0	101	CDL	C71-CB7-OB8-CB6
150	C	505	CDL	C71-CB7-OB8-CB6
150	c	501	CDL	C31-CA7-OA8-CA6
150	DN	502	CDL	C31-CA7-OA8-CA6
150	DZ	501	CDL	C71-CB7-OB8-CB6
150	Dn	501	CDL	C31-CA7-OA8-CA6
153	CC	302	PC1	C32-C31-O31-C3
153	K	502	PC1	C32-C31-O31-C3
155	G	401	3PE	C32-C31-O31-C3
155	DJ	301	3PE	C32-C31-O31-C3
150	B1	402	CDL	OA9-CA7-OA8-CA6
150	ED	601	CDL	OA9-CA7-OA8-CA6
150	Ep	701	CDL	OA9-CA7-OA8-CA6
150	Dj	405	CDL	C51-CB5-OB6-CB4
150	Dr	402	CDL	C51-CB5-OB6-CB4
150	Ds	401	CDL	C11-CA5-OA6-CA4
150	El	902	CDL	C11-CA5-OA6-CA4
153	Da	707	PC1	C22-C21-O21-C2
155	A2	401	3PE	C22-C21-O21-C2
150	B0	101	CDL	CA2-C1-CB2-OB2
150	BC	301	CDL	CA2-C1-CB2-OB2
150	C	504	CDL	CA2-C1-CB2-OB2
150	C	507	CDL	CA2-C1-CB2-OB2
150	DA	709	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DD	706	CDL	CA2-C1-CB2-OB2
150	DG	201	CDL	CB2-C1-CA2-OA2
150	DJ	302	CDL	CB2-C1-CA2-OA2
150	DJ	307	CDL	CA2-C1-CB2-OB2
150	DM	502	CDL	CA2-C1-CB2-OB2
150	DN	507	CDL	CB2-C1-CA2-OA2
150	DS	401	CDL	CA2-C1-CB2-OB2
150	DV	403	CDL	CB2-C1-CA2-OA2
150	DY	301	CDL	CB2-C1-CA2-OA2
150	EB	302	CDL	CA2-C1-CB2-OB2
150	ED	604	CDL	CB2-C1-CA2-OA2
150	EL	902	CDL	CA2-C1-CB2-OB2
150	Dd	702	CDL	CB2-C1-CA2-OA2
150	Dj	407	CDL	CA2-C1-CB2-OB2
150	Dm	501	CDL	CA2-C1-CB2-OB2
150	Dv	402	CDL	CA2-C1-CB2-OB2
150	AC	802	CDL	OA7-CA5-OA6-CA4
150	DQ	1502	CDL	OA7-CA5-OA6-CA4
150	DR	403	CDL	OA7-CA5-OA6-CA4
150	EK	201	CDL	OB7-CB5-OB6-CB4
150	Dj	403	CDL	OA7-CA5-OA6-CA4
150	Eu	101	CDL	OA7-CA5-OA6-CA4
153	AX	401	PC1	O22-C21-O21-C2
153	k	301	PC1	O22-C21-O21-C2
153	Dv	405	PC1	O22-C21-O21-C2
153	Dx	1209	PC1	O22-C21-O21-C2
150	DN	502	CDL	OA9-CA7-OA8-CA6
150	DZ	501	CDL	OB9-CB7-OB8-CB6
153	K	502	PC1	O32-C31-O31-C3
155	G	401	3PE	O32-C31-O31-C3
155	DJ	301	3PE	O32-C31-O31-C3
150	A0	601	CDL	C31-CA7-OA8-CA6
150	AM	301	CDL	C31-CA7-OA8-CA6
150	BT	202	CDL	C71-CB7-OB8-CB6
150	CG	302	CDL	C31-CA7-OA8-CA6
150	CC	305	CDL	C31-CA7-OA8-CA6
150	c	501	CDL	C71-CB7-OB8-CB6
150	c	506	CDL	C31-CA7-OA8-CA6
150	DD	706	CDL	C71-CB7-OB8-CB6
150	DG	202	CDL	C31-CA7-OA8-CA6
150	DN	507	CDL	C31-CA7-OA8-CA6
150	DO	501	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DR	402	CDL	C31-CA7-OA8-CA6
150	DR	402	CDL	C71-CB7-OB8-CB6
150	ED	601	CDL	C71-CB7-OB8-CB6
150	EN	1202	CDL	C31-CA7-OA8-CA6
150	Da	709	CDL	C31-CA7-OA8-CA6
150	Dc	608	CDL	C71-CB7-OB8-CB6
150	Dg	202	CDL	C31-CA7-OA8-CA6
150	Dn	503	CDL	C31-CA7-OA8-CA6
150	Do	501	CDL	C31-CA7-OA8-CA6
150	Ea	501	CDL	C71-CB7-OB8-CB6
150	El	903	CDL	C71-CB7-OB8-CB6
153	AH	301	PC1	C32-C31-O31-C3
153	AQ	202	PC1	C32-C31-O31-C3
153	DA	707	PC1	C32-C31-O31-C3
153	DC	608	PC1	C32-C31-O31-C3
153	DQ	1503	PC1	C32-C31-O31-C3
153	Da	706	PC1	C32-C31-O31-C3
153	Dq	1404	PC1	C32-C31-O31-C3
153	Dv	406	PC1	C32-C31-O31-C3
153	Dx	1205	PC1	C32-C31-O31-C3
155	DC	607	3PE	C32-C31-O31-C3
155	DS	402	3PE	C32-C31-O31-C3
155	Dc	607	3PE	C32-C31-O31-C3
155	Dr	404	3PE	C32-C31-O31-C3
155	Ds	403	3PE	C32-C31-O31-C3
154	A1	401	NDP	O4D-C1D-N1N-C6N
153	DA	708	PC1	C3C-C3D-C3E-C3F
150	Dh	201	CDL	C38-C39-C40-C41
150	Dj	404	CDL	C77-C78-C79-C80
150	BL	301	CDL	OB5-CB3-CB4-OB6
150	DV	403	CDL	OB5-CB3-CB4-OB6
150	EB	302	CDL	OB5-CB3-CB4-OB6
153	DQ	1503	PC1	O11-C1-C2-O21
150	Dq	1402	CDL	C19-C20-C21-C22
153	d	801	PC1	C3E-C3F-C3G-C3H
153	Da	707	PC1	C3C-C3D-C3E-C3F
150	A1	402	CDL	O1-C1-CA2-OA2
150	BT	202	CDL	O1-C1-CB2-OB2
150	BT	204	CDL	O1-C1-CA2-OA2
150	c	506	CDL	O1-C1-CB2-OB2
150	g	801	CDL	O1-C1-CB2-OB2
150	DH	201	CDL	O1-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DQ	1501	CDL	O1-C1-CA2-OA2
150	DQ	1502	CDL	O1-C1-CA2-OA2
150	DX	301	CDL	O1-C1-CA2-OA2
150	DX	307	CDL	O1-C1-CA2-OA2
150	DZ	501	CDL	O1-C1-CA2-OA2
150	EL	902	CDL	O1-C1-CA2-OA2
150	EN	1202	CDL	O1-C1-CA2-OA2
150	Dh	201	CDL	O1-C1-CA2-OA2
150	Dj	405	CDL	O1-C1-CA2-OA2
150	Dj	407	CDL	O1-C1-CB2-OB2
150	Dy	301	CDL	O1-C1-CA2-OA2
150	Ea	501	CDL	O1-C1-CA2-OA2
150	Eh	1601	CDL	O1-C1-CA2-OA2
150	Ep	701	CDL	O1-C1-CA2-OA2
150	CG	301	CDL	OB6-CB4-CB6-OB8
150	DA	706	CDL	OA6-CA4-CA6-OA8
150	EL	901	CDL	OA6-CA4-CA6-OA8
150	Di	1101	CDL	OA6-CA4-CA6-OA8
150	Dr	402	CDL	OB6-CB4-CB6-OB8
150	Dy	301	CDL	OB6-CB4-CB6-OB8
153	DA	707	PC1	O21-C2-C3-O31
155	C	513	3PE	O21-C2-C3-O31
155	Da	708	3PE	O21-C2-C3-O31
150	A0	601	CDL	OA9-CA7-OA8-CA6
150	BT	202	CDL	OB9-CB7-OB8-CB6
150	CC	305	CDL	OA9-CA7-OA8-CA6
150	DG	202	CDL	OA9-CA7-OA8-CA6
150	DN	507	CDL	OA9-CA7-OA8-CA6
150	EN	1202	CDL	OA9-CA7-OA8-CA6
155	DS	402	3PE	O32-C31-O31-C3
167	Ed	202	UQ8	C35-C34-C36-C37
150	DA	706	CDL	C34-C35-C36-C37
150	DH	201	CDL	C38-C39-C40-C41
150	Di	1101	CDL	C34-C35-C36-C37
150	DU	401	CDL	OA7-CA5-OA6-CA4
150	Dm	501	CDL	OA7-CA5-OA6-CA4
150	Dn	503	CDL	OA7-CA5-OA6-CA4
155	DG	204	3PE	O22-C21-O21-C2
150	AF	402	CDL	C11-CA5-OA6-CA4
150	CG	302	CDL	C51-CB5-OB6-CB4
150	g	801	CDL	C11-CA5-OA6-CA4
150	DX	301	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EI	401	CDL	C11-CA5-OA6-CA4
150	Dh	202	CDL	C11-CA5-OA6-CA4
150	Ds	405	CDL	C11-CA5-OA6-CA4
155	Dg	204	3PE	C22-C21-O21-C2
150	Dg	201	CDL	C23-C24-C25-C26
150	h	501	CDL	CA5-C11-C12-C13
150	DS	404	CDL	CA5-C11-C12-C13
150	Ei	401	CDL	CA5-C11-C12-C13
150	c	506	CDL	OA9-CA7-OA8-CA6
150	DO	501	CDL	OA9-CA7-OA8-CA6
150	El	903	CDL	OB9-CB7-OB8-CB6
153	Da	706	PC1	O32-C31-O31-C3
155	DC	607	3PE	O32-C31-O31-C3
155	Dr	404	3PE	O32-C31-O31-C3
150	AA	908	CDL	C61-C62-C63-C64
150	DQ	1501	CDL	C19-C20-C21-C22
153	AA	905	PC1	C32-C31-O31-C3
155	DG	205	3PE	C32-C31-O31-C3
155	Em	901	3PE	C32-C31-O31-C3
166	CE	401	HEC	C2A-CAA-CBA-CGA
150	B0	101	CDL	CA5-C11-C12-C13
150	BC	302	CDL	CB5-C51-C52-C53
150	DN	503	CDL	CA5-C11-C12-C13
150	DU	404	CDL	CA5-C11-C12-C13
150	Dc	608	CDL	CA5-C11-C12-C13
150	Dg	202	CDL	CB7-C71-C72-C73
150	Dh	202	CDL	CA5-C11-C12-C13
150	Dm	501	CDL	CA5-C11-C12-C13
150	Du	403	CDL	CA5-C11-C12-C13
150	El	901	CDL	CA5-C11-C12-C13
150	DR	402	CDL	OA9-CA7-OA8-CA6
150	CG	302	CDL	OA9-CA7-OA8-CA6
155	Ds	403	3PE	O32-C31-O31-C3
150	A0	602	CDL	CA5-C11-C12-C13
150	AF	401	CDL	CA5-C11-C12-C13
150	B0	102	CDL	CA5-C11-C12-C13
150	C	507	CDL	CB5-C51-C52-C53
150	E	301	CDL	CA5-C11-C12-C13
150	H	1302	CDL	CA5-C11-C12-C13
150	DG	202	CDL	CA5-C11-C12-C13
150	DH	202	CDL	CA5-C11-C12-C13
150	DQ	1504	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DZ	501	CDL	CA5-C11-C12-C13
150	ED	601	CDL	CA5-C11-C12-C13
150	EH	1601	CDL	CA5-C11-C12-C13
150	Dc	601	CDL	CA5-C11-C12-C13
150	Dn	503	CDL	CA5-C11-C12-C13
150	Ds	405	CDL	CA5-C11-C12-C13
150	El	902	CDL	CA5-C11-C12-C13
155	EM	901	3PE	C21-C22-C23-C24
156	AA	902	LPP	C11-C12-C13-C14
151	A0	603	UDP	O4'-C4'-C5'-O5'
150	c	502	CDL	C31-CA7-OA8-CA6
150	DH	201	CDL	C71-CB7-OB8-CB6
150	DY	301	CDL	C31-CA7-OA8-CA6
150	Dd	706	CDL	C71-CB7-OB8-CB6
150	Dn	502	CDL	C31-CA7-OA8-CA6
153	A1	403	PC1	C32-C31-O31-C3
155	Dc	607	3PE	C2-C3-O31-C31
150	EO	202	CDL	C77-C78-C79-C80
150	C	503	CDL	OA7-CA5-OA6-CA4
150	c	502	CDL	OA7-CA5-OA6-CA4
150	DU	404	CDL	OA7-CA5-OA6-CA4
150	Dj	405	CDL	OB7-CB5-OB6-CB4
150	Dq	1402	CDL	OB7-CB5-OB6-CB4
150	AC	802	CDL	CA4-CA3-OA5-PA1
155	DG	205	3PE	C2-C1-O11-P
150	DZ	501	CDL	CB7-C71-C72-C73
150	EL	901	CDL	CA5-C11-C12-C13
150	Dq	1402	CDL	CA5-C11-C12-C13
150	Dy	301	CDL	CA5-C11-C12-C13
153	EO	201	PC1	C31-C32-C33-C34
156	A6	301	LPP	C11-C12-C13-C14
150	DJ	307	CDL	C11-CA5-OA6-CA4
150	Dc	601	CDL	C51-CB5-OB6-CB4
153	B1	401	PC1	C22-C21-O21-C2
150	AM	301	CDL	OA9-CA7-OA8-CA6
150	DR	402	CDL	OB9-CB7-OB8-CB6
150	Dc	608	CDL	OB9-CB7-OB8-CB6
150	Dn	503	CDL	OA9-CA7-OA8-CA6
150	Ea	501	CDL	OB9-CB7-OB8-CB6
153	AH	301	PC1	O32-C31-O31-C3
153	DA	707	PC1	O32-C31-O31-C3
153	DC	608	PC1	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dq	1404	PC1	O32-C31-O31-C3
153	Dx	1205	PC1	O32-C31-O31-C3
150	ED	601	CDL	OB9-CB7-OB8-CB6
150	Da	709	CDL	OA9-CA7-OA8-CA6
150	Do	501	CDL	OA9-CA7-OA8-CA6
153	AQ	202	PC1	O32-C31-O31-C3
153	DQ	1503	PC1	O32-C31-O31-C3
153	Dv	406	PC1	O32-C31-O31-C3
167	EN	1205	UQ8	C34-C36-C37-C38
167	EN	1205	UQ8	C19-C21-C22-C23
167	Ed	202	UQ8	C39-C41-C42-C43
167	El	906	UQ8	C14-C16-C17-C18
150	AA	908	CDL	CA5-C11-C12-C13
150	AC	801	CDL	CA5-C11-C12-C13
151	A0	603	UDP	O4'-C1'-N1-C2
150	C	504	CDL	O1-C1-CB2-OB2
150	C	505	CDL	O1-C1-CB2-OB2
150	H	1302	CDL	O1-C1-CB2-OB2
150	DD	705	CDL	O1-C1-CA2-OA2
150	DJ	302	CDL	O1-C1-CA2-OA2
150	DV	402	CDL	O1-C1-CB2-OB2
150	DY	301	CDL	O1-C1-CA2-OA2
150	EL	902	CDL	O1-C1-CB2-OB2
150	Dd	704	CDL	O1-C1-CB2-OB2
150	Dg	201	CDL	O1-C1-CA2-OA2
150	Ds	402	CDL	O1-C1-CB2-OB2
150	El	902	CDL	O1-C1-CB2-OB2
150	CG	302	CDL	OB7-CB5-OB6-CB4
150	Dr	402	CDL	OB7-CB5-OB6-CB4
150	Ds	401	CDL	OA7-CA5-OA6-CA4
150	Ds	405	CDL	OA7-CA5-OA6-CA4
150	El	902	CDL	OA7-CA5-OA6-CA4
153	Da	707	PC1	O22-C21-O21-C2
155	Ds	403	3PE	C2-C3-O31-C31
153	DI	303	PC1	C32-C31-O31-C3
155	Di	1102	3PE	C32-C31-O31-C3
150	ES	1101	CDL	C35-C36-C37-C38
150	B0	101	CDL	OB9-CB7-OB8-CB6
150	C	505	CDL	OB9-CB7-OB8-CB6
150	c	501	CDL	OA9-CA7-OA8-CA6
150	c	501	CDL	OB9-CB7-OB8-CB6
150	DD	706	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	202	CDL	OA9-CA7-OA8-CA6
150	Dn	501	CDL	OA9-CA7-OA8-CA6
153	A1	403	PC1	O32-C31-O31-C3
153	AA	905	PC1	O32-C31-O31-C3
153	CC	302	PC1	O32-C31-O31-C3
155	Dc	607	3PE	O32-C31-O31-C3
155	Em	901	3PE	O32-C31-O31-C3
150	DU	401	CDL	CA5-C11-C12-C13
150	DS	405	CDL	C38-C39-C40-C41
150	Dj	402	CDL	C54-C55-C56-C57
155	DG	205	3PE	O32-C31-O31-C3
150	c	501	CDL	C51-CB5-OB6-CB4
150	DD	705	CDL	C11-CA5-OA6-CA4
150	DH	202	CDL	C11-CA5-OA6-CA4
150	DJ	303	CDL	C11-CA5-OA6-CA4
150	DN	502	CDL	C11-CA5-OA6-CA4
150	Dq	1403	CDL	C11-CA5-OA6-CA4
155	Ds	408	3PE	C22-C21-O21-C2
155	Eo	203	3PE	C22-C21-O21-C2
150	AC	801	CDL	C34-C35-C36-C37
150	A0	601	CDL	CB3-OB5-PB2-OB2
150	A0	602	CDL	CA3-OA5-PA1-OA2
150	A1	402	CDL	CB2-OB2-PB2-OB5
150	AA	901	CDL	CA3-OA5-PA1-OA2
150	AA	901	CDL	CB2-OB2-PB2-OB5
150	AC	801	CDL	CB3-OB5-PB2-OB2
150	AC	802	CDL	CB2-OB2-PB2-OB5
150	AC	802	CDL	CB3-OB5-PB2-OB2
150	AM	301	CDL	CA2-OA2-PA1-OA5
150	AM	301	CDL	CB3-OB5-PB2-OB2
150	AP	301	CDL	CB2-OB2-PB2-OB5
150	B0	101	CDL	CA2-OA2-PA1-OA5
150	B0	101	CDL	CB2-OB2-PB2-OB5
150	B1	402	CDL	CA3-OA5-PA1-OA2
150	B1	402	CDL	CB2-OB2-PB2-OB5
150	BC	301	CDL	CA2-OA2-PA1-OA5
150	BC	302	CDL	CB2-OB2-PB2-OB5
150	BC	302	CDL	CB3-OB5-PB2-OB2
150	BE	201	CDL	CA2-OA2-PA1-OA5
150	BG	201	CDL	CA2-OA2-PA1-OA5
150	BT	202	CDL	CB2-OB2-PB2-OB5
150	BT	202	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	CG	301	CDL	CB2-OB2-PB2-OB5
150	CG	302	CDL	CA2-OA2-PA1-OA5
150	CG	302	CDL	CB3-OB5-PB2-OB2
150	CC	304	CDL	CA3-OA5-PA1-OA2
150	CC	305	CDL	CA3-OA5-PA1-OA2
150	CD	301	CDL	CA3-OA5-PA1-OA2
150	CD	301	CDL	CB2-OB2-PB2-OB5
150	CD	302	CDL	CB2-OB2-PB2-OB5
150	C	503	CDL	CA2-OA2-PA1-OA5
150	C	503	CDL	CA3-OA5-PA1-OA2
150	C	503	CDL	CB2-OB2-PB2-OB5
150	C	504	CDL	CA2-OA2-PA1-OA5
150	C	504	CDL	CA3-OA5-PA1-OA2
150	C	504	CDL	CB2-OB2-PB2-OB5
150	C	505	CDL	CA2-OA2-PA1-OA5
150	C	506	CDL	CB3-OB5-PB2-OB2
150	C	507	CDL	CA3-OA5-PA1-OA2
150	E	301	CDL	CA2-OA2-PA1-OA5
150	E	301	CDL	CB2-OB2-PB2-OB5
150	H	1301	CDL	CB2-OB2-PB2-OB5
150	H	1301	CDL	CB3-OB5-PB2-OB2
150	H	1302	CDL	CA2-OA2-PA1-OA5
150	H	1302	CDL	CA3-OA5-PA1-OA2
150	H	1302	CDL	CB3-OB5-PB2-OB2
150	c	501	CDL	CB2-OB2-PB2-OB5
150	h	501	CDL	CA2-OA2-PA1-OA5
150	h	501	CDL	CB2-OB2-PB2-OB5
150	DA	709	CDL	CA3-OA5-PA1-OA2
150	DC	601	CDL	CA3-OA5-PA1-OA2
150	DC	601	CDL	CB2-OB2-PB2-OB5
150	DC	601	CDL	CB3-OB5-PB2-OB2
150	DD	705	CDL	CA2-OA2-PA1-OA5
150	DD	706	CDL	CA2-OA2-PA1-OA5
150	DD	706	CDL	CA3-OA5-PA1-OA2
150	DD	706	CDL	CB3-OB5-PB2-OB2
150	DH	202	CDL	CB2-OB2-PB2-OB5
150	DI	302	CDL	CB2-OB2-PB2-OB5
150	DJ	302	CDL	CB3-OB5-PB2-OB2
150	DJ	305	CDL	CB2-OB2-PB2-OB5
150	DJ	307	CDL	CB2-OB2-PB2-OB5
150	DJ	307	CDL	CB3-OB5-PB2-OB2
150	DM	501	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DM	502	CDL	CA2-OA2-PA1-OA5
150	DM	502	CDL	CB2-OB2-PB2-OB5
150	DN	502	CDL	CA3-OA5-PA1-OA2
150	DN	502	CDL	CB3-OB5-PB2-OB2
150	DN	503	CDL	CB2-OB2-PB2-OB5
150	DN	506	CDL	CB3-OB5-PB2-OB2
150	DN	507	CDL	CA2-OA2-PA1-OA5
150	DN	507	CDL	CA3-OA5-PA1-OA2
150	DQ	1501	CDL	CA3-OA5-PA1-OA2
150	DQ	1504	CDL	CA2-OA2-PA1-OA5
150	DR	402	CDL	CA3-OA5-PA1-OA2
150	DR	403	CDL	CA2-OA2-PA1-OA5
150	DS	405	CDL	CA2-OA2-PA1-OA5
150	DS	405	CDL	CB3-OB5-PB2-OB2
150	DU	401	CDL	CA2-OA2-PA1-OA5
150	DU	401	CDL	CB2-OB2-PB2-OB5
150	DU	402	CDL	CB3-OB5-PB2-OB2
150	DU	403	CDL	CA2-OA2-PA1-OA5
150	DU	403	CDL	CB3-OB5-PB2-OB2
150	DU	404	CDL	CB2-OB2-PB2-OB5
150	DV	401	CDL	CA3-OA5-PA1-OA2
150	DV	402	CDL	CA3-OA5-PA1-OA2
150	DV	403	CDL	CA2-OA2-PA1-OA5
150	DV	403	CDL	CB2-OB2-PB2-OB5
150	DX	306	CDL	CA2-OA2-PA1-OA5
150	DX	306	CDL	CB3-OB5-PB2-OB2
150	DX	307	CDL	CA2-OA2-PA1-OA5
150	DY	301	CDL	CA3-OA5-PA1-OA2
150	DZ	501	CDL	CA2-OA2-PA1-OA5
150	EA	301	CDL	CB2-OB2-PB2-OB5
150	EB	302	CDL	CA3-OA5-PA1-OA2
150	EB	302	CDL	CB2-OB2-PB2-OB5
150	ED	604	CDL	CA3-OA5-PA1-OA2
150	ED	604	CDL	CB3-OB5-PB2-OB2
150	ED	605	CDL	CB3-OB5-PB2-OB2
150	EH	1601	CDL	CA2-OA2-PA1-OA5
150	EH	1601	CDL	CB3-OB5-PB2-OB2
150	EI	401	CDL	CB3-OB5-PB2-OB2
150	EL	902	CDL	CB2-OB2-PB2-OB5
150	EL	903	CDL	CB2-OB2-PB2-OB5
150	EL	903	CDL	CB3-OB5-PB2-OB2
150	EN	1201	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	ES	1101	CDL	CA3-OA5-PA1-OA2
150	Da	709	CDL	CB3-OB5-PB2-OB2
150	Dc	601	CDL	CA3-OA5-PA1-OA2
150	Dc	601	CDL	CB2-OB2-PB2-OB5
150	Dc	601	CDL	CB3-OB5-PB2-OB2
150	Dd	702	CDL	CA3-OA5-PA1-OA2
150	Dd	704	CDL	CB2-OB2-PB2-OB5
150	Dg	201	CDL	CA2-OA2-PA1-OA5
150	Dg	202	CDL	CA2-OA2-PA1-OA5
150	Dh	202	CDL	CA3-OA5-PA1-OA2
150	Dh	202	CDL	CB2-OB2-PB2-OB5
150	Di	1101	CDL	CB3-OB5-PB2-OB2
150	Dj	401	CDL	CA2-OA2-PA1-OA5
150	Dj	401	CDL	CB3-OB5-PB2-OB2
150	Dj	402	CDL	CA3-OA5-PA1-OA2
150	Dj	403	CDL	CA2-OA2-PA1-OA5
150	Dj	404	CDL	CA2-OA2-PA1-OA5
150	Dj	407	CDL	CA2-OA2-PA1-OA5
150	Dj	407	CDL	CB2-OB2-PB2-OB5
150	Dm	501	CDL	CA3-OA5-PA1-OA2
150	Dm	501	CDL	CB2-OB2-PB2-OB5
150	Dm	502	CDL	CA3-OA5-PA1-OA2
150	Dn	502	CDL	CB3-OB5-PB2-OB2
150	Dn	506	CDL	CB3-OB5-PB2-OB2
150	Do	501	CDL	CA3-OA5-PA1-OA2
150	Dq	1401	CDL	CA2-OA2-PA1-OA5
150	Dq	1402	CDL	CA3-OA5-PA1-OA2
150	Dq	1403	CDL	CA2-OA2-PA1-OA5
150	Dq	1403	CDL	CA3-OA5-PA1-OA2
150	Dr	402	CDL	CA3-OA5-PA1-OA2
150	Dr	402	CDL	CB2-OB2-PB2-OB5
150	Dr	403	CDL	CA2-OA2-PA1-OA5
150	Ds	401	CDL	CA3-OA5-PA1-OA2
150	Ds	406	CDL	CA2-OA2-PA1-OA5
150	Ds	406	CDL	CB3-OB5-PB2-OB2
150	Du	401	CDL	CA2-OA2-PA1-OA5
150	Du	401	CDL	CB3-OB5-PB2-OB2
150	Dv	401	CDL	CB2-OB2-PB2-OB5
150	Dv	403	CDL	CA2-OA2-PA1-OA5
150	Dv	403	CDL	CA3-OA5-PA1-OA2
150	Dv	403	CDL	CB2-OB2-PB2-OB5
150	Dx	1201	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dx	1201	CDL	CB3-OB5-PB2-OB2
150	Dx	1204	CDL	CA2-OA2-PA1-OA5
150	Dx	1204	CDL	CA3-OA5-PA1-OA2
150	Dx	1204	CDL	CB3-OB5-PB2-OB2
150	Ea	502	CDL	CA2-OA2-PA1-OA5
150	Ea	502	CDL	CB2-OB2-PB2-OB5
150	Eb	302	CDL	CB2-OB2-PB2-OB5
150	Eb	302	CDL	CB3-OB5-PB2-OB2
150	Ed	204	CDL	CA3-OA5-PA1-OA2
150	Ed	204	CDL	CB3-OB5-PB2-OB2
150	Ed	205	CDL	CA3-OA5-PA1-OA2
150	Eg	101	CDL	CB3-OB5-PB2-OB2
150	Eh	1601	CDL	CB3-OB5-PB2-OB2
150	Ei	401	CDL	CA2-OA2-PA1-OA5
150	Ei	401	CDL	CB3-OB5-PB2-OB2
150	El	903	CDL	CA2-OA2-PA1-OA5
150	El	903	CDL	CB2-OB2-PB2-OB5
150	Ep	701	CDL	CA3-OA5-PA1-OA2
150	Eu	101	CDL	CB3-OB5-PB2-OB2
153	A9	603	PC1	C11-O13-P-O11
153	AA	903	PC1	C1-O11-P-O13
153	AA	905	PC1	C11-O13-P-O11
153	AA	906	PC1	C11-O13-P-O11
153	AA	907	PC1	C11-O13-P-O11
153	AQ	202	PC1	C1-O11-P-O13
153	AU	201	PC1	C11-O13-P-O11
153	AU	201	PC1	C1-O11-P-O13
153	AX	401	PC1	C1-O11-P-O13
153	B1	401	PC1	C11-O13-P-O11
153	B1	401	PC1	C1-O11-P-O13
153	B1	403	PC1	C1-O11-P-O13
153	BG	202	PC1	C11-O13-P-O11
153	BS	1301	PC1	C1-O11-P-O13
153	BS	1302	PC1	C11-O13-P-O11
153	CC	302	PC1	C1-O11-P-O13
153	C	508	PC1	C11-O13-P-O11
153	C	508	PC1	C1-O11-P-O13
153	C	509	PC1	C11-O13-P-O11
153	C	510	PC1	C11-O13-P-O11
153	K	501	PC1	C11-O13-P-O11
153	K	502	PC1	C11-O13-P-O11
153	c	508	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	d	801	PC1	C1-O11-P-O13
153	g	802	PC1	C11-O13-P-O11
153	DA	708	PC1	C1-O11-P-O13
153	DB	702	PC1	C11-O13-P-O11
153	DC	602	PC1	C11-O13-P-O11
153	DC	602	PC1	C1-O11-P-O13
153	DC	603	PC1	C11-O13-P-O11
153	DC	604	PC1	C1-O11-P-O13
153	DC	605	PC1	C1-O11-P-O13
153	DC	608	PC1	C11-O13-P-O11
153	DI	303	PC1	C11-O13-P-O11
153	DJ	306	PC1	C11-O13-P-O11
153	DJ	306	PC1	C1-O11-P-O13
153	DQ	1503	PC1	C11-O13-P-O11
153	DS	406	PC1	C1-O11-P-O13
153	DV	404	PC1	C11-O13-P-O11
153	DV	405	PC1	C11-O13-P-O11
153	DV	406	PC1	C11-O13-P-O11
153	DV	406	PC1	C1-O11-P-O13
153	DX	305	PC1	C11-O13-P-O11
153	DX	308	PC1	C1-O11-P-O13
153	EB	301	PC1	C1-O11-P-O13
153	EO	201	PC1	C11-O13-P-O11
153	EO	204	PC1	C11-O13-P-O11
153	EO	204	PC1	C1-O11-P-O13
153	Da	706	PC1	C11-O13-P-O11
153	Db	702	PC1	C11-O13-P-O11
153	Dc	602	PC1	C11-O13-P-O11
153	Dc	603	PC1	C11-O13-P-O11
153	Dc	604	PC1	C11-O13-P-O11
153	Dc	604	PC1	C1-O11-P-O13
153	Dc	605	PC1	C1-O11-P-O13
153	Dc	609	PC1	C11-O13-P-O11
153	Di	1104	PC1	C11-O13-P-O11
153	Di	1104	PC1	C1-O11-P-O13
153	Dj	406	PC1	C11-O13-P-O11
153	Dq	1404	PC1	C11-O13-P-O11
153	Dv	406	PC1	C11-O13-P-O11
153	Dv	407	PC1	C11-O13-P-O11
153	Dv	407	PC1	C1-O11-P-O13
153	Dx	1203	PC1	C1-O11-P-O13
153	Ef	501	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	El	904	PC1	C11-O13-P-O11
153	El	904	PC1	C1-O11-P-O13
153	Eo	201	PC1	C11-O13-P-O11
153	Eo	204	PC1	C11-O13-P-O11
153	Eo	205	PC1	C11-O13-P-O11
155	A9	602	3PE	C1-O11-P-O13
155	AJ	502	3PE	C11-O13-P-O11
155	BA	301	3PE	C11-O13-P-O11
155	BT	201	3PE	C1-O11-P-O13
155	CD	303	3PE	C1-O11-P-O13
155	G	401	3PE	C11-O13-P-O11
155	DC	606	3PE	C1-O11-P-O13
155	DC	607	3PE	C11-O13-P-O11
155	DG	204	3PE	C1-O11-P-O13
155	DG	204	3PE	C11-O13-P-O11
155	DI	301	3PE	C1-O11-P-O13
155	DJ	301	3PE	C1-O11-P-O13
155	DS	402	3PE	C1-O11-P-O13
155	DX	302	3PE	C11-O13-P-O11
155	DX	303	3PE	C11-O13-P-O11
155	DX	304	3PE	C11-O13-P-O11
155	EL	904	3PE	C1-O11-P-O13
155	EL	904	3PE	C11-O13-P-O11
155	EN	1204	3PE	C11-O13-P-O11
155	EO	203	3PE	C1-O11-P-O13
155	Da	708	3PE	C1-O11-P-O13
155	Dd	703	3PE	C1-O11-P-O13
155	Ds	403	3PE	C1-O11-P-O13
155	Dx	1202	3PE	C1-O11-P-O13
155	Dx	1202	3PE	C11-O13-P-O11
155	Dx	1207	3PE	C1-O11-P-O13
155	Dx	1207	3PE	C11-O13-P-O11
155	El	905	3PE	C1-O11-P-O13
155	El	905	3PE	C11-O13-P-O11
150	Dm	502	CDL	CB7-C71-C72-C73
155	EN	1204	3PE	C21-C22-C23-C24
150	C	507	CDL	C71-CB7-OB8-CB6
150	DV	403	CDL	C71-CB7-OB8-CB6
150	Dx	1204	CDL	C71-CB7-OB8-CB6
150	En	1201	CDL	C71-CB7-OB8-CB6
153	Di	1104	PC1	C32-C31-O31-C3
155	A2	401	3PE	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	BV	201	CDL	CA5-C11-C12-C13
150	DM	502	CDL	CB7-C71-C72-C73
150	Dx	1201	CDL	CA5-C11-C12-C13
150	A0	601	CDL	CA2-C1-CB2-OB2
150	AA	908	CDL	CA2-C1-CB2-OB2
150	c	501	CDL	CB2-C1-CA2-OA2
150	c	509	CDL	CB2-C1-CA2-OA2
150	DD	705	CDL	CB2-C1-CA2-OA2
150	DR	403	CDL	CB2-C1-CA2-OA2
150	DV	402	CDL	CA2-C1-CB2-OB2
150	DX	306	CDL	CB2-C1-CA2-OA2
150	EH	1601	CDL	CA2-C1-CB2-OB2
150	EN	1202	CDL	CB2-C1-CA2-OA2
150	Dd	704	CDL	CA2-C1-CB2-OB2
150	Dr	403	CDL	CB2-C1-CA2-OA2
150	Ds	401	CDL	CB2-C1-CA2-OA2
150	Ds	402	CDL	CA2-C1-CB2-OB2
150	Ei	401	CDL	CB2-C1-CA2-OA2
150	Eu	101	CDL	CB2-C1-CA2-OA2
150	AF	402	CDL	OA7-CA5-OA6-CA4
150	c	501	CDL	OB7-CB5-OB6-CB4
150	g	801	CDL	OA7-CA5-OA6-CA4
150	DD	705	CDL	OA7-CA5-OA6-CA4
150	DH	202	CDL	OA7-CA5-OA6-CA4
150	DJ	303	CDL	OA7-CA5-OA6-CA4
150	DJ	307	CDL	OA7-CA5-OA6-CA4
150	DN	502	CDL	OA7-CA5-OA6-CA4
150	DX	301	CDL	OB7-CB5-OB6-CB4
150	DZ	501	CDL	OB7-CB5-OB6-CB4
150	EI	401	CDL	OA7-CA5-OA6-CA4
150	Dc	601	CDL	OB7-CB5-OB6-CB4
150	Dh	202	CDL	OA7-CA5-OA6-CA4
150	Dq	1403	CDL	OA7-CA5-OA6-CA4
153	B1	401	PC1	O22-C21-O21-C2
155	A2	401	3PE	O22-C21-O21-C2
155	Dg	204	3PE	O22-C21-O21-C2
155	Ds	408	3PE	O22-C21-O21-C2
155	Eo	203	3PE	O22-C21-O21-C2
167	CC	303	UQ8	C15-C14-C16-C17
150	DJ	304	CDL	C71-CB7-OB8-CB6
150	DJ	307	CDL	C71-CB7-OB8-CB6
150	Dc	601	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dm	502	CDL	C71-CB7-OB8-CB6
150	Ds	401	CDL	C31-CA7-OA8-CA6
150	Dv	403	CDL	C71-CB7-OB8-CB6
150	Ed	204	CDL	C71-CB7-OB8-CB6
153	A9	603	PC1	C32-C31-O31-C3
153	d	801	PC1	C32-C31-O31-C3
153	Dc	609	PC1	C32-C31-O31-C3
150	C	506	CDL	C20-C21-C22-C23
150	Dd	704	CDL	C38-C39-C40-C41
150	Ds	406	CDL	C38-C39-C40-C41
155	BA	301	3PE	C24-C25-C26-C27
150	BG	201	CDL	CA5-C11-C12-C13
150	c	502	CDL	C57-C58-C59-C60
150	c	509	CDL	C12-C13-C14-C15
150	DX	301	CDL	C14-C15-C16-C17
150	Ds	405	CDL	C77-C78-C79-C80
150	BG	201	CDL	C51-CB5-OB6-CB4
150	C	505	CDL	C51-CB5-OB6-CB4
150	DN	503	CDL	C11-CA5-OA6-CA4
150	DQ	1501	CDL	C51-CB5-OB6-CB4
150	DQ	1504	CDL	C51-CB5-OB6-CB4
150	DZ	501	CDL	C51-CB5-OB6-CB4
150	EL	902	CDL	C51-CB5-OB6-CB4
150	EL	903	CDL	C11-CA5-OA6-CA4
150	Dg	202	CDL	C11-CA5-OA6-CA4
150	Ds	402	CDL	C11-CA5-OA6-CA4
150	Du	403	CDL	C11-CA5-OA6-CA4
150	Dv	402	CDL	C11-CA5-OA6-CA4
150	El	903	CDL	C11-CA5-OA6-CA4
153	A0	605	PC1	C22-C21-O21-C2
153	A9	601	PC1	C22-C21-O21-C2
153	DA	708	PC1	C22-C21-O21-C2
150	AA	908	CDL	C73-C74-C75-C76
150	B1	402	CDL	C80-C81-C82-C83
150	BE	201	CDL	C11-C12-C13-C14
150	C	505	CDL	C23-C24-C25-C26
150	DA	709	CDL	C17-C18-C19-C20
150	DG	201	CDL	C14-C15-C16-C17
150	DG	202	CDL	C80-C81-C82-C83
150	DJ	307	CDL	C54-C55-C56-C57
150	DN	507	CDL	C16-C17-C18-C19
150	DO	501	CDL	C76-C77-C78-C79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DQ	1502	CDL	C51-C52-C53-C54
150	DU	402	CDL	C61-C62-C63-C64
150	Dd	704	CDL	C22-C23-C24-C25
150	Dj	403	CDL	C17-C18-C19-C20
150	Dm	501	CDL	C55-C56-C57-C58
150	Dn	503	CDL	C17-C18-C19-C20
150	Ds	401	CDL	C57-C58-C59-C60
150	Ds	402	CDL	C57-C58-C59-C60
150	Du	403	CDL	C11-C12-C13-C14
150	Ea	501	CDL	C39-C40-C41-C42
150	El	901	CDL	C55-C56-C57-C58
150	El	902	CDL	C37-C38-C39-C40
153	D	402	PC1	C39-C3A-C3B-C3C
153	c	508	PC1	C24-C25-C26-C27
153	DC	604	PC1	C3B-C3C-C3D-C3E
153	EB	301	PC1	C27-C28-C29-C2A
153	Dc	609	PC1	C3D-C3E-C3F-C3G
150	DH	201	CDL	OB9-CB7-OB8-CB6
150	Eh	1601	CDL	C31-CA7-OA8-CA6
150	A0	602	CDL	C57-C58-C59-C60
150	AA	901	CDL	C17-C18-C19-C20
150	AC	802	CDL	C32-C33-C34-C35
150	DJ	305	CDL	C12-C13-C14-C15
150	DS	401	CDL	C57-C58-C59-C60
150	DV	402	CDL	C54-C55-C56-C57
150	Dc	601	CDL	C13-C14-C15-C16
150	Dd	704	CDL	C75-C76-C77-C78
150	Dr	403	CDL	C13-C14-C15-C16
150	Ea	502	CDL	C13-C14-C15-C16
153	A6	302	PC1	C26-C27-C28-C29
153	AX	401	PC1	C3B-C3C-C3D-C3E
153	A	1201	PC1	C36-C37-C38-C39
150	h	501	CDL	CB3-CB4-OB6-CB5
150	DS	404	CDL	CB3-CB4-OB6-CB5
150	Ds	405	CDL	CB3-CB4-OB6-CB5
153	EO	205	PC1	C1-C2-O21-C21
150	C	505	CDL	OB7-CB5-OB6-CB4
150	DN	503	CDL	OA7-CA5-OA6-CA4
150	DQ	1501	CDL	OB7-CB5-OB6-CB4
150	DQ	1504	CDL	OB7-CB5-OB6-CB4
150	EL	903	CDL	OA7-CA5-OA6-CA4
150	Dg	202	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ds	402	CDL	OA7-CA5-OA6-CA4
150	Du	403	CDL	OA7-CA5-OA6-CA4
150	Dv	402	CDL	OA7-CA5-OA6-CA4
150	El	903	CDL	OA7-CA5-OA6-CA4
153	A0	605	PC1	O22-C21-O21-C2
150	C	504	CDL	CA7-C31-C32-C33
150	A0	601	CDL	C13-C14-C15-C16
150	A1	402	CDL	C40-C41-C42-C43
150	H	1301	CDL	C33-C34-C35-C36
150	DU	404	CDL	C11-C12-C13-C14
150	ED	605	CDL	C16-C17-C18-C19
150	EL	901	CDL	C37-C38-C39-C40
150	Da	709	CDL	C76-C77-C78-C79
150	Dd	705	CDL	C13-C14-C15-C16
150	Dn	501	CDL	C73-C74-C75-C76
150	Dn	506	CDL	C37-C38-C39-C40
150	Dq	1403	CDL	C51-C52-C53-C54
150	Dv	402	CDL	C54-C55-C56-C57
150	Ea	501	CDL	C42-C43-C44-C45
150	Ea	501	CDL	C77-C78-C79-C80
150	Eg	101	CDL	C16-C17-C18-C19
150	El	903	CDL	C74-C75-C76-C77
153	B1	403	PC1	C36-C37-C38-C39
153	EO	206	PC1	C3E-C3F-C3G-C3H
153	Eb	301	PC1	C27-C28-C29-C2A
150	CD	301	CDL	C1-CB2-OB2-PB2
150	CD	302	CDL	C1-CB2-OB2-PB2
150	DD	705	CDL	CA4-CA3-OA5-PA1
150	EK	201	CDL	C1-CA2-OA2-PA1
155	BP	201	3PE	C2-C1-O11-P
150	B1	402	CDL	C56-C57-C58-C59
150	BC	302	CDL	C34-C35-C36-C37
150	DJ	302	CDL	C35-C36-C37-C38
150	Dj	403	CDL	C55-C56-C57-C58
150	Dj	407	CDL	C55-C56-C57-C58
150	Ds	406	CDL	C11-C12-C13-C14
150	Ed	205	CDL	C51-C52-C53-C54
150	El	901	CDL	C80-C81-C82-C83
153	AJ	501	PC1	C3C-C3D-C3E-C3F
155	Dd	703	3PE	C25-C26-C27-C28
150	A0	601	CDL	O1-C1-CB2-OB2
150	DJ	307	CDL	O1-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	202	CDL	O1-C1-CA2-OA2
150	Dg	202	CDL	O1-C1-CB2-OB2
150	Dj	407	CDL	O1-C1-CA2-OA2
150	Dq	1403	CDL	O1-C1-CA2-OA2
150	Ds	401	CDL	O1-C1-CA2-OA2
150	Du	401	CDL	O1-C1-CB2-OB2
150	DG	201	CDL	C12-C13-C14-C15
150	Dg	201	CDL	C11-C12-C13-C14
150	Dq	1401	CDL	C13-C14-C15-C16
150	Dv	401	CDL	C54-C55-C56-C57
153	c	507	PC1	C24-C25-C26-C27
153	Dc	605	PC1	C29-C2A-C2B-C2C
150	C	503	CDL	CA5-C11-C12-C13
150	DH	201	CDL	CA5-C11-C12-C13
150	DV	401	CDL	CA5-C11-C12-C13
150	EN	1201	CDL	CA5-C11-C12-C13
153	Eo	201	PC1	C31-C32-C33-C34
150	EL	901	CDL	OB6-CB4-CB6-OB8
150	BC	302	CDL	C31-CA7-OA8-CA6
150	DJ	303	CDL	C71-CB7-OB8-CB6
150	DQ	1502	CDL	C71-CB7-OB8-CB6
153	AC	804	PC1	C32-C31-O31-C3
150	AA	908	CDL	C41-C42-C43-C44
150	C	503	CDL	C81-C82-C83-C84
150	DA	709	CDL	C16-C17-C18-C19
150	DI	302	CDL	C13-C14-C15-C16
150	DQ	1504	CDL	C11-C12-C13-C14
150	DS	404	CDL	C14-C15-C16-C17
150	DU	404	CDL	C33-C34-C35-C36
150	DV	401	CDL	C54-C55-C56-C57
150	DX	301	CDL	C11-C12-C13-C14
150	EL	903	CDL	C63-C64-C65-C66
150	Dg	201	CDL	C58-C59-C60-C61
150	Dj	407	CDL	C13-C14-C15-C16
150	Ds	406	CDL	C14-C15-C16-C17
150	Dx	1204	CDL	C19-C20-C21-C22
150	Eh	1601	CDL	C61-C62-C63-C64
150	El	902	CDL	C39-C40-C41-C42
153	k	301	PC1	C3D-C3E-C3F-C3G
153	DJ	306	PC1	C3D-C3E-C3F-C3G
153	Eo	204	PC1	C2C-C2D-C2E-C2F
155	BA	301	3PE	C2D-C2E-C2F-C2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dc	601	CDL	OA9-CA7-OA8-CA6
150	Dd	706	CDL	OB9-CB7-OB8-CB6
153	Dc	609	PC1	O32-C31-O31-C3
167	El	906	UQ8	C15-C14-C16-C17
150	B0	101	CDL	C52-C53-C54-C55
150	C	505	CDL	C21-C22-C23-C24
150	c	506	CDL	C36-C37-C38-C39
150	DJ	304	CDL	C62-C63-C64-C65
150	DN	502	CDL	C73-C74-C75-C76
150	DU	404	CDL	C80-C81-C82-C83
150	EL	901	CDL	C39-C40-C41-C42
150	Dj	403	CDL	C39-C40-C41-C42
150	Dq	1402	CDL	C12-C13-C14-C15
150	Dr	402	CDL	C51-C52-C53-C54
150	Dr	402	CDL	C57-C58-C59-C60
150	Ds	402	CDL	C61-C62-C63-C64
150	Ds	405	CDL	C14-C15-C16-C17
150	Dx	1201	CDL	C14-C15-C16-C17
150	Ed	205	CDL	C16-C17-C18-C19
153	Eo	205	PC1	C3E-C3F-C3G-C3H
156	AA	902	LPP	C17-C18-C19-C20
150	Dj	402	CDL	CA4-CA6-OA8-CA7
150	Dj	407	CDL	CA5-C11-C12-C13
150	Dv	401	CDL	CA5-C11-C12-C13
150	Ea	501	CDL	CB7-C71-C72-C73
150	CD	301	CDL	C61-C62-C63-C64
150	C	503	CDL	C41-C42-C43-C44
150	C	504	CDL	C53-C54-C55-C56
150	C	504	CDL	C55-C56-C57-C58
150	DA	706	CDL	C41-C42-C43-C44
150	DH	202	CDL	C21-C22-C23-C24
150	DI	302	CDL	C42-C43-C44-C45
150	DJ	303	CDL	C40-C41-C42-C43
150	DM	501	CDL	C55-C56-C57-C58
150	EA	301	CDL	C11-C12-C13-C14
150	EK	201	CDL	C40-C41-C42-C43
150	ES	1101	CDL	C13-C14-C15-C16
150	Di	1101	CDL	C41-C42-C43-C44
150	Di	1103	CDL	C71-C72-C73-C74
150	Dj	402	CDL	C62-C63-C64-C65
150	Du	402	CDL	C37-C38-C39-C40
150	Ek	201	CDL	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	CD	303	3PE	C27-C28-C29-C2A
150	c	502	CDL	OA9-CA7-OA8-CA6
150	DY	301	CDL	OA9-CA7-OA8-CA6
150	Dn	502	CDL	OA9-CA7-OA8-CA6
150	Dx	1204	CDL	OB9-CB7-OB8-CB6
155	A2	401	3PE	O32-C31-O31-C3
150	B0	102	CDL	C13-C14-C15-C16
150	BG	201	CDL	C34-C35-C36-C37
150	DM	502	CDL	C14-C15-C16-C17
150	DO	501	CDL	C32-C33-C34-C35
150	DU	402	CDL	C21-C22-C23-C24
150	DX	301	CDL	C19-C20-C21-C22
150	EN	1202	CDL	C57-C58-C59-C60
150	El	903	CDL	C20-C21-C22-C23
153	Dy	302	PC1	C2E-C2F-C2G-C2H
150	BG	201	CDL	OB7-CB5-OB6-CB4
150	DC	601	CDL	OB7-CB5-OB6-CB4
150	EL	902	CDL	OB7-CB5-OB6-CB4
150	Dh	201	CDL	OA7-CA5-OA6-CA4
150	Ea	501	CDL	OB7-CB5-OB6-CB4
153	A9	601	PC1	O22-C21-O21-C2
153	DA	708	PC1	O22-C21-O21-C2
150	AC	801	CDL	C51-CB5-OB6-CB4
150	DA	706	CDL	C51-CB5-OB6-CB4
150	DC	601	CDL	C51-CB5-OB6-CB4
150	Dc	601	CDL	C11-CA5-OA6-CA4
150	Dh	201	CDL	C11-CA5-OA6-CA4
150	Dn	501	CDL	C11-CA5-OA6-CA4
150	Dn	503	CDL	C51-CB5-OB6-CB4
150	Ea	501	CDL	C51-CB5-OB6-CB4
153	BG	202	PC1	C22-C21-O21-C2
150	CG	302	CDL	C20-C21-C22-C23
150	c	506	CDL	C56-C57-C58-C59
150	DC	601	CDL	C40-C41-C42-C43
150	DD	706	CDL	C75-C76-C77-C78
150	DN	503	CDL	C13-C14-C15-C16
150	ED	601	CDL	C17-C18-C19-C20
150	EK	201	CDL	C74-C75-C76-C77
150	EL	903	CDL	C81-C82-C83-C84
150	EO	202	CDL	C11-C12-C13-C14
150	ES	1101	CDL	C17-C18-C19-C20
150	Dd	705	CDL	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Di	1103	CDL	C74-C75-C76-C77
150	Eb	302	CDL	C20-C21-C22-C23
153	AA	904	PC1	C3D-C3E-C3F-C3G
153	DI	303	PC1	C27-C28-C29-C2A
153	EO	206	PC1	C3B-C3C-C3D-C3E
153	Dc	602	PC1	C3C-C3D-C3E-C3F
153	Dj	406	PC1	C3D-C3E-C3F-C3G
150	EA	301	CDL	CB7-C71-C72-C73
150	Dy	301	CDL	CB5-C51-C52-C53
150	AA	908	CDL	C59-C60-C61-C62
150	BY	201	CDL	C56-C57-C58-C59
150	CD	301	CDL	C72-C73-C74-C75
150	CD	302	CDL	C39-C40-C41-C42
150	CD	302	CDL	C61-C62-C63-C64
150	g	801	CDL	C11-C12-C13-C14
150	DD	704	CDL	C75-C76-C77-C78
150	DJ	302	CDL	C11-C12-C13-C14
150	DR	403	CDL	C11-C12-C13-C14
150	DR	403	CDL	C13-C14-C15-C16
150	DS	404	CDL	C75-C76-C77-C78
150	DV	403	CDL	C79-C80-C81-C82
150	DX	301	CDL	C38-C39-C40-C41
150	DX	306	CDL	C72-C73-C74-C75
150	EN	1201	CDL	C77-C78-C79-C80
150	Da	709	CDL	C14-C15-C16-C17
150	Di	1103	CDL	C37-C38-C39-C40
150	Di	1103	CDL	C42-C43-C44-C45
150	Di	1103	CDL	C77-C78-C79-C80
150	Dj	404	CDL	C11-C12-C13-C14
150	Dj	404	CDL	C16-C17-C18-C19
150	Ds	402	CDL	C74-C75-C76-C77
150	Ds	405	CDL	C20-C21-C22-C23
150	Du	402	CDL	C34-C35-C36-C37
150	Du	403	CDL	C80-C81-C82-C83
150	Dv	401	CDL	C80-C81-C82-C83
150	Dx	1201	CDL	C77-C78-C79-C80
150	Dx	1204	CDL	C40-C41-C42-C43
150	Eu	101	CDL	C11-C12-C13-C14
153	A9	603	PC1	C3C-C3D-C3E-C3F
153	AU	202	PC1	C3C-C3D-C3E-C3F
153	C	509	PC1	C35-C36-C37-C38
153	DB	702	PC1	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	DC	602	PC1	C3C-C3D-C3E-C3F
153	Dx	1205	PC1	C24-C25-C26-C27
155	DJ	301	3PE	C32-C33-C34-C35
156	EI	402	LPP	C34-C35-C36-C37
155	DS	402	3PE	C2-C3-O31-C31
150	DR	402	CDL	C61-C62-C63-C64
150	DS	401	CDL	C61-C62-C63-C64
150	DS	404	CDL	C20-C21-C22-C23
150	DX	307	CDL	C32-C33-C34-C35
150	DY	301	CDL	C12-C13-C14-C15
150	DY	301	CDL	C35-C36-C37-C38
150	EO	202	CDL	C16-C17-C18-C19
150	Dd	704	CDL	C63-C64-C65-C66
150	Dh	202	CDL	C37-C38-C39-C40
150	Dj	403	CDL	C13-C14-C15-C16
150	Du	401	CDL	C11-C12-C13-C14
150	Du	402	CDL	C14-C15-C16-C17
150	Dx	1204	CDL	C35-C36-C37-C38
153	C	508	PC1	C2B-C2C-C2D-C2E
153	k	301	PC1	C2E-C2F-C2G-C2H
153	DY	302	PC1	C2E-C2F-C2G-C2H
153	Dc	603	PC1	C2A-C2B-C2C-C2D
155	DC	607	3PE	O13-C11-C12-N
150	AA	908	CDL	C12-C13-C14-C15
150	AM	301	CDL	C82-C83-C84-C85
150	B0	101	CDL	C38-C39-C40-C41
150	B1	402	CDL	C34-C35-C36-C37
150	BC	302	CDL	C32-C33-C34-C35
150	c	509	CDL	C75-C76-C77-C78
150	DJ	303	CDL	C60-C61-C62-C63
150	DV	401	CDL	C57-C58-C59-C60
150	DX	307	CDL	C11-C12-C13-C14
150	ED	605	CDL	C11-C12-C13-C14
150	ED	605	CDL	C23-C24-C25-C26
150	Dj	405	CDL	C20-C21-C22-C23
150	Dn	506	CDL	C35-C36-C37-C38
150	Ds	405	CDL	C75-C76-C77-C78
150	Dx	1204	CDL	C60-C61-C62-C63
150	Ek	201	CDL	C74-C75-C76-C77
150	El	901	CDL	C23-C24-C25-C26
153	k	301	PC1	C35-C36-C37-C38
153	DS	406	PC1	C3B-C3C-C3D-C3E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dd	702	CDL	CB7-C71-C72-C73
150	Dr	402	CDL	CA7-C31-C32-C33
150	DJ	304	CDL	OB9-CB7-OB8-CB6
150	Ds	401	CDL	OA9-CA7-OA8-CA6
150	Dv	403	CDL	OB9-CB7-OB8-CB6
153	A9	603	PC1	O32-C31-O31-C3
153	d	801	PC1	O32-C31-O31-C3
150	AA	901	CDL	C23-C24-C25-C26
150	AA	901	CDL	C36-C37-C38-C39
150	AF	401	CDL	C63-C64-C65-C66
150	c	502	CDL	C73-C74-C75-C76
150	DD	704	CDL	C63-C64-C65-C66
150	DI	302	CDL	C71-C72-C73-C74
150	DV	403	CDL	C72-C73-C74-C75
150	Dh	202	CDL	C21-C22-C23-C24
150	Dh	202	CDL	C63-C64-C65-C66
150	Do	501	CDL	C77-C78-C79-C80
150	Du	403	CDL	C57-C58-C59-C60
150	Eh	1601	CDL	C20-C21-C22-C23
150	h	501	CDL	C71-CB7-OB8-CB6
150	AC	801	CDL	C55-C56-C57-C58
150	CC	305	CDL	C11-C12-C13-C14
150	DI	302	CDL	C37-C38-C39-C40
150	DI	302	CDL	C62-C63-C64-C65
150	DQ	1504	CDL	C17-C18-C19-C20
150	DS	401	CDL	C16-C17-C18-C19
150	DX	306	CDL	C36-C37-C38-C39
150	EB	302	CDL	C20-C21-C22-C23
150	EO	202	CDL	C63-C64-C65-C66
150	Ds	401	CDL	C37-C38-C39-C40
150	Ed	205	CDL	C11-C12-C13-C14
150	Eh	1601	CDL	C55-C56-C57-C58
150	Ek	201	CDL	C77-C78-C79-C80
150	El	901	CDL	C12-C13-C14-C15
150	El	903	CDL	C81-C82-C83-C84
155	Eo	202	3PE	C36-C37-C38-C39
150	AC	802	CDL	C13-C14-C15-C16
150	AF	402	CDL	C71-C72-C73-C74
150	C	507	CDL	C22-C23-C24-C25
150	DN	502	CDL	C57-C58-C59-C60
150	DN	507	CDL	C60-C61-C62-C63
150	EI	401	CDL	C61-C62-C63-C64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EL	903	CDL	C20-C21-C22-C23
150	EN	1202	CDL	C36-C37-C38-C39
150	Dc	601	CDL	C40-C41-C42-C43
150	Di	1103	CDL	C13-C14-C15-C16
150	Ea	501	CDL	C34-C35-C36-C37
153	DB	702	PC1	C3C-C3D-C3E-C3F
153	Di	1104	PC1	C27-C28-C29-C2A
155	BA	301	3PE	C34-C35-C36-C37
164	CA	702	FAD	O3'-C3'-C4'-C5'
153	DI	303	PC1	O32-C31-O31-C3
153	Di	1104	PC1	O32-C31-O31-C3
155	Di	1102	3PE	O32-C31-O31-C3
150	AC	802	CDL	C62-C63-C64-C65
150	AF	401	CDL	C61-C62-C63-C64
150	CG	301	CDL	C63-C64-C65-C66
150	CJ	201	CDL	C76-C77-C78-C79
150	H	1301	CDL	C80-C81-C82-C83
150	g	801	CDL	C79-C80-C81-C82
150	DD	705	CDL	C62-C63-C64-C65
150	DH	202	CDL	C37-C38-C39-C40
150	DJ	307	CDL	C82-C83-C84-C85
150	DV	401	CDL	C80-C81-C82-C83
150	EH	1601	CDL	C20-C21-C22-C23
150	EL	902	CDL	C38-C39-C40-C41
150	EN	1201	CDL	C17-C18-C19-C20
150	EN	1202	CDL	C23-C24-C25-C26
150	ES	1101	CDL	C55-C56-C57-C58
150	Da	709	CDL	C74-C75-C76-C77
150	Dd	706	CDL	C75-C76-C77-C78
150	Dn	501	CDL	C57-C58-C59-C60
150	Do	501	CDL	C32-C33-C34-C35
150	Do	501	CDL	C40-C41-C42-C43
150	Ds	401	CDL	C11-C12-C13-C14
150	Ds	401	CDL	C23-C24-C25-C26
150	Ds	402	CDL	C16-C17-C18-C19
150	Ds	405	CDL	C37-C38-C39-C40
150	Dv	403	CDL	C13-C14-C15-C16
150	Dv	403	CDL	C72-C73-C74-C75
150	Dx	1201	CDL	C20-C21-C22-C23
150	Dx	1204	CDL	C17-C18-C19-C20
150	Dy	301	CDL	C35-C36-C37-C38
150	Ed	205	CDL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Eg	101	CDL	C60-C61-C62-C63
150	Eg	101	CDL	C63-C64-C65-C66
150	Eh	1601	CDL	C23-C24-C25-C26
150	Ei	401	CDL	C61-C62-C63-C64
150	El	901	CDL	C37-C38-C39-C40
150	El	903	CDL	C56-C57-C58-C59
155	Ds	408	3PE	C27-C28-C29-C2A
150	A0	601	CDL	CA3-CA4-CA6-OA8
150	BV	201	CDL	CB3-CB4-CB6-OB8
150	DU	401	CDL	CA3-CA4-CA6-OA8
150	EL	902	CDL	CA3-CA4-CA6-OA8
150	Ds	402	CDL	CA3-CA4-CA6-OA8
153	DC	605	PC1	C1-C2-C3-O31
153	EO	205	PC1	C1-C2-C3-O31
155	EN	1204	3PE	C1-C2-C3-O31
150	Dn	501	CDL	OA7-CA5-OA6-CA4
150	C	507	CDL	C17-C18-C19-C20
150	c	506	CDL	C60-C61-C62-C63
150	DG	202	CDL	C14-C15-C16-C17
150	DQ	1504	CDL	C51-C52-C53-C54
150	DS	404	CDL	C37-C38-C39-C40
150	EK	201	CDL	C77-C78-C79-C80
150	Dd	704	CDL	C17-C18-C19-C20
150	Dv	401	CDL	C57-C58-C59-C60
150	Dv	403	CDL	C79-C80-C81-C82
150	Dv	403	CDL	C82-C83-C84-C85
150	Dx	1201	CDL	C74-C75-C76-C77
150	El	901	CDL	C61-C62-C63-C64
153	DC	603	PC1	C2A-C2B-C2C-C2D
150	Dh	201	CDL	CA5-C11-C12-C13
153	AC	804	PC1	C21-C22-C23-C24
150	AC	801	CDL	C54-C55-C56-C57
150	AC	802	CDL	C80-C81-C82-C83
150	DN	506	CDL	C35-C36-C37-C38
150	DX	306	CDL	C11-C12-C13-C14
150	Dc	601	CDL	C12-C13-C14-C15
150	Dn	506	CDL	C14-C15-C16-C17
150	Dq	1401	CDL	C17-C18-C19-C20
150	Eu	101	CDL	C36-C37-C38-C39
155	DX	302	3PE	C39-C3A-C3B-C3C
150	En	1201	CDL	OB9-CB7-OB8-CB6
150	Dj	401	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dr	403	CDL	C71-CB7-OB8-CB6
155	DR	401	3PE	C32-C31-O31-C3
167	c	510	UQ8	C28-C29-C31-C32
167	El	906	UQ8	C13-C14-C16-C17
150	A0	602	CDL	C11-CA5-OA6-CA4
150	h	501	CDL	C11-CA5-OA6-CA4
150	DC	601	CDL	C11-CA5-OA6-CA4
150	DV	402	CDL	C11-CA5-OA6-CA4
150	ED	605	CDL	C11-CA5-OA6-CA4
150	Dq	1402	CDL	C11-CA5-OA6-CA4
150	Ea	501	CDL	C11-CA5-OA6-CA4
153	Ef	501	PC1	C22-C21-O21-C2
155	AJ	502	3PE	C22-C21-O21-C2
155	DG	205	3PE	C22-C21-O21-C2
155	Dd	703	3PE	C22-C21-O21-C2
150	Dj	401	CDL	CA4-CA6-OA8-CA7
150	DA	709	CDL	C12-C13-C14-C15
150	DQ	1504	CDL	C34-C35-C36-C37
150	ED	605	CDL	C61-C62-C63-C64
150	EL	901	CDL	C61-C62-C63-C64
150	Dv	403	CDL	C17-C18-C19-C20
150	Dy	301	CDL	C82-C83-C84-C85
150	Ea	502	CDL	C74-C75-C76-C77
153	BS	1302	PC1	C36-C37-C38-C39
150	AC	802	CDL	C73-C74-C75-C76
150	BC	302	CDL	C12-C13-C14-C15
150	DC	601	CDL	C14-C15-C16-C17
150	DD	705	CDL	C36-C37-C38-C39
150	DM	501	CDL	C79-C80-C81-C82
150	DO	501	CDL	C40-C41-C42-C43
150	DV	403	CDL	C82-C83-C84-C85
150	DY	301	CDL	C82-C83-C84-C85
150	EL	901	CDL	C82-C83-C84-C85
150	EN	1201	CDL	C34-C35-C36-C37
150	EO	202	CDL	C31-C32-C33-C34
150	El	901	CDL	C39-C40-C41-C42
150	El	902	CDL	C34-C35-C36-C37
153	A9	601	PC1	C3B-C3C-C3D-C3E
155	EL	904	3PE	C26-C27-C28-C29
155	EN	1204	3PE	C38-C39-C3A-C3B
150	C	507	CDL	OB9-CB7-OB8-CB6
150	DV	403	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
156	EI	402	LPP	C11-C12-C13-C14
150	C	504	CDL	C43-C44-C45-C46
150	EL	901	CDL	C19-C20-C21-C22
150	Dj	401	CDL	C11-C12-C13-C14
150	El	902	CDL	C75-C76-C77-C78
153	C	508	PC1	C3D-C3E-C3F-C3G
150	CG	301	CDL	O1-C1-CB2-OB2
150	Dd	706	CDL	O1-C1-CA2-OA2
150	CC	304	CDL	C13-C14-C15-C16
150	DU	402	CDL	C14-C15-C16-C17
150	Dh	202	CDL	C74-C75-C76-C77
150	Di	1103	CDL	C80-C81-C82-C83
150	Dj	405	CDL	C37-C38-C39-C40
150	Dj	407	CDL	C82-C83-C84-C85
150	Dr	403	CDL	C34-C35-C36-C37
150	Ei	401	CDL	C12-C13-C14-C15
153	AQ	202	PC1	C26-C27-C28-C29
153	e	1101	PC1	C25-C26-C27-C28
155	Dx	1207	3PE	C3D-C3E-C3F-C3G
150	AA	901	CDL	C11-C12-C13-C14
150	DC	601	CDL	C80-C81-C82-C83
150	DH	202	CDL	C63-C64-C65-C66
150	DM	501	CDL	C81-C82-C83-C84
150	DR	403	CDL	C17-C18-C19-C20
150	DS	405	CDL	C58-C59-C60-C61
150	DS	405	CDL	C62-C63-C64-C65
150	EO	202	CDL	C37-C38-C39-C40
150	Dd	704	CDL	C82-C83-C84-C85
150	Ed	205	CDL	C61-C62-C63-C64
150	Eh	1601	CDL	C53-C54-C55-C56
150	El	903	CDL	C76-C77-C78-C79
153	c	507	PC1	C3C-C3D-C3E-C3F
150	DJ	307	CDL	OB9-CB7-OB8-CB6
150	Dm	502	CDL	OB9-CB7-OB8-CB6
150	Ed	204	CDL	OB9-CB7-OB8-CB6
150	BT	202	CDL	CA5-C11-C12-C13
150	CJ	201	CDL	CB2-C1-CA2-OA2
150	DS	404	CDL	CA2-C1-CB2-OB2
150	DX	301	CDL	CA2-C1-CB2-OB2
150	DX	307	CDL	CB2-C1-CA2-OA2
150	ED	601	CDL	CB2-C1-CA2-OA2
150	Dd	705	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	202	CDL	CB2-C1-CA2-OA2
150	Ea	502	CDL	CA2-C1-CB2-OB2
150	AA	908	CDL	C53-C54-C55-C56
150	AA	908	CDL	C60-C61-C62-C63
150	AC	802	CDL	C42-C43-C44-C45
150	CD	302	CDL	C51-C52-C53-C54
150	DD	703	CDL	C74-C75-C76-C77
150	DJ	307	CDL	C59-C60-C61-C62
150	EL	903	CDL	C56-C57-C58-C59
150	Dc	608	CDL	C57-C58-C59-C60
150	Dg	201	CDL	C63-C64-C65-C66
150	Dq	1402	CDL	C36-C37-C38-C39
150	Dx	1201	CDL	C11-C12-C13-C14
153	AL	303	PC1	C3C-C3D-C3E-C3F
150	AC	801	CDL	OB7-CB5-OB6-CB4
150	h	501	CDL	OA7-CA5-OA6-CA4
150	DA	706	CDL	OB7-CB5-OB6-CB4
150	DC	601	CDL	OA7-CA5-OA6-CA4
150	DJ	304	CDL	OB7-CB5-OB6-CB4
150	DV	402	CDL	OA7-CA5-OA6-CA4
150	ED	605	CDL	OA7-CA5-OA6-CA4
150	Dc	601	CDL	OA7-CA5-OA6-CA4
150	Dn	503	CDL	OB7-CB5-OB6-CB4
150	Dq	1402	CDL	OA7-CA5-OA6-CA4
150	Dq	1403	CDL	OB7-CB5-OB6-CB4
150	Ea	501	CDL	OA7-CA5-OA6-CA4
153	BG	202	PC1	O22-C21-O21-C2
153	Ef	501	PC1	O22-C21-O21-C2
155	DG	205	3PE	O22-C21-O21-C2
155	Dd	703	3PE	O22-C21-O21-C2
150	AP	301	CDL	C74-C75-C76-C77
150	BL	301	CDL	C21-C22-C23-C24
150	BY	201	CDL	C36-C37-C38-C39
150	H	1302	CDL	C59-C60-C61-C62
150	DG	201	CDL	C63-C64-C65-C66
150	Dn	506	CDL	C40-C41-C42-C43
150	Dr	403	CDL	C11-C12-C13-C14
150	Du	402	CDL	C12-C13-C14-C15
150	Dv	402	CDL	C13-C14-C15-C16
150	Ek	201	CDL	C53-C54-C55-C56
153	AA	903	PC1	C34-C35-C36-C37
153	BS	1302	PC1	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DX	303	3PE	C3D-C3E-C3F-C3G
155	Ds	408	3PE	C38-C39-C3A-C3B
150	AC	801	CDL	C1-CB2-OB2-PB2
150	DJ	305	CDL	C1-CB2-OB2-PB2
150	Dj	401	CDL	C1-CB2-OB2-PB2
150	Eh	1601	CDL	OA9-CA7-OA8-CA6
150	AC	802	CDL	C55-C56-C57-C58
150	AF	402	CDL	C37-C38-C39-C40
150	BT	204	CDL	C43-C44-C45-C46
150	BV	201	CDL	C37-C38-C39-C40
150	C	503	CDL	C32-C33-C34-C35
150	c	501	CDL	C13-C14-C15-C16
150	DD	705	CDL	C41-C42-C43-C44
150	DJ	305	CDL	C20-C21-C22-C23
150	DN	503	CDL	C41-C42-C43-C44
150	DS	404	CDL	C60-C61-C62-C63
150	DU	402	CDL	C56-C57-C58-C59
150	DZ	501	CDL	C38-C39-C40-C41
150	EL	901	CDL	C80-C81-C82-C83
150	EN	1201	CDL	C53-C54-C55-C56
150	Dj	405	CDL	C77-C78-C79-C80
150	Ds	405	CDL	C60-C61-C62-C63
150	Ea	501	CDL	C16-C17-C18-C19
150	Eb	302	CDL	C54-C55-C56-C57
150	Ek	201	CDL	C33-C34-C35-C36
150	El	902	CDL	C12-C13-C14-C15
150	El	902	CDL	C63-C64-C65-C66
150	Eu	101	CDL	C17-C18-C19-C20
153	DB	702	PC1	C32-C33-C34-C35
155	EN	1204	3PE	C27-C28-C29-C2A
150	DA	709	CDL	CA5-C11-C12-C13
150	DC	601	CDL	CA5-C11-C12-C13
150	DD	703	CDL	CA5-C11-C12-C13
150	B0	101	CDL	C40-C41-C42-C43
150	BE	201	CDL	C19-C20-C21-C22
150	C	506	CDL	C71-C72-C73-C74
150	DJ	307	CDL	C51-C52-C53-C54
150	DV	401	CDL	C39-C40-C41-C42
150	DV	403	CDL	C17-C18-C19-C20
150	DX	306	CDL	C17-C18-C19-C20
150	ED	605	CDL	C51-C52-C53-C54
150	Dd	705	CDL	C62-C63-C64-C65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dj	405	CDL	C41-C42-C43-C44
150	Dj	407	CDL	C59-C60-C61-C62
150	Ds	406	CDL	C62-C63-C64-C65
150	Dx	1201	CDL	C43-C44-C45-C46
150	Ed	204	CDL	C80-C81-C82-C83
150	En	1201	CDL	C82-C83-C84-C85
153	D	402	PC1	C3C-C3D-C3E-C3F
153	DC	605	PC1	C29-C2A-C2B-C2C
155	DC	606	3PE	C3E-C3F-C3G-C3H
155	Dx	1202	3PE	C36-C37-C38-C39
150	DD	705	CDL	C71-CB7-OB8-CB6
150	DV	401	CDL	C71-CB7-OB8-CB6
150	Dq	1403	CDL	C71-CB7-OB8-CB6
150	Ds	402	CDL	C71-CB7-OB8-CB6
150	Du	403	CDL	C71-CB7-OB8-CB6
153	AU	201	PC1	C32-C31-O31-C3
153	BG	202	PC1	C32-C31-O31-C3
153	EO	206	PC1	C32-C31-O31-C3
150	CC	304	CDL	C51-CB5-OB6-CB4
150	CD	302	CDL	C51-CB5-OB6-CB4
150	E	301	CDL	C51-CB5-OB6-CB4
150	DJ	304	CDL	C51-CB5-OB6-CB4
150	ED	605	CDL	C51-CB5-OB6-CB4
150	EN	1201	CDL	C11-CA5-OA6-CA4
150	Dd	702	CDL	C51-CB5-OB6-CB4
150	Dq	1403	CDL	C51-CB5-OB6-CB4
150	Ed	205	CDL	C11-CA5-OA6-CA4
150	Eh	1601	CDL	C51-CB5-OB6-CB4
150	Ek	201	CDL	C51-CB5-OB6-CB4
150	Ep	701	CDL	C11-CA5-OA6-CA4
155	El	905	3PE	C22-C21-O21-C2
150	AC	802	CDL	C60-C61-C62-C63
150	B0	102	CDL	C58-C59-C60-C61
150	BG	201	CDL	C60-C61-C62-C63
150	BT	202	CDL	C82-C83-C84-C85
150	h	501	CDL	C14-C15-C16-C17
150	DD	704	CDL	C82-C83-C84-C85
150	DI	302	CDL	C74-C75-C76-C77
150	DJ	305	CDL	C37-C38-C39-C40
150	DJ	305	CDL	C41-C42-C43-C44
150	DJ	307	CDL	C77-C78-C79-C80
150	DN	506	CDL	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DN	506	CDL	C40-C41-C42-C43
150	DV	403	CDL	C12-C13-C14-C15
150	DX	307	CDL	C20-C21-C22-C23
150	DZ	501	CDL	C34-C35-C36-C37
150	Dc	601	CDL	C80-C81-C82-C83
150	Dc	608	CDL	C42-C43-C44-C45
150	Dd	706	CDL	C80-C81-C82-C83
150	Dh	201	CDL	C56-C57-C58-C59
150	Dm	501	CDL	C11-C12-C13-C14
150	Du	401	CDL	C36-C37-C38-C39
150	Dv	401	CDL	C39-C40-C41-C42
150	Dv	402	CDL	C36-C37-C38-C39
150	Dv	402	CDL	C62-C63-C64-C65
150	Dx	1204	CDL	C56-C57-C58-C59
150	Ea	502	CDL	C81-C82-C83-C84
150	Eb	302	CDL	C34-C35-C36-C37
150	Eu	101	CDL	C63-C64-C65-C66
153	DX	305	PC1	C3D-C3E-C3F-C3G
155	BA	301	3PE	C25-C26-C27-C28
155	DS	402	3PE	C37-C38-C39-C3A
155	EL	904	3PE	C37-C38-C39-C3A
155	Dx	1202	3PE	C3C-C3D-C3E-C3F
156	Ed	203	LPP	C19-C20-C21-C22
150	BC	302	CDL	OA9-CA7-OA8-CA6
150	DJ	303	CDL	OB9-CB7-OB8-CB6
150	DQ	1502	CDL	OB9-CB7-OB8-CB6
150	Di	1103	CDL	CA7-C31-C32-C33
150	Ea	501	CDL	CA5-C11-C12-C13
150	DG	201	CDL	C56-C57-C58-C59
150	DN	503	CDL	C36-C37-C38-C39
150	Dn	501	CDL	C35-C36-C37-C38
150	Dr	402	CDL	C20-C21-C22-C23
150	Ds	406	CDL	C53-C54-C55-C56
155	DN	501	3PE	C28-C29-C2A-C2B
150	CG	302	CDL	C42-C43-C44-C45
150	DU	401	CDL	C36-C37-C38-C39
150	DX	307	CDL	C63-C64-C65-C66
150	Dr	403	CDL	C17-C18-C19-C20
153	c	507	PC1	C28-C29-C2A-C2B
153	k	301	PC1	C22-C23-C24-C25
153	Dv	406	PC1	C3C-C3D-C3E-C3F
155	Ds	403	3PE	C37-C38-C39-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
167	DS	403	UQ8	C33-C34-C36-C37
167	Ed	202	UQ8	C33-C34-C36-C37
150	h	501	CDL	OB9-CB7-OB8-CB6
150	Dj	401	CDL	OA9-CA7-OA8-CA6
150	Dr	403	CDL	OB9-CB7-OB8-CB6
153	AC	804	PC1	O32-C31-O31-C3
155	DR	401	3PE	O32-C31-O31-C3
150	CG	302	CDL	C78-C79-C80-C81
150	c	509	CDL	C43-C44-C45-C46
150	DJ	304	CDL	C40-C41-C42-C43
150	DQ	1502	CDL	C75-C76-C77-C78
150	DS	405	CDL	C53-C54-C55-C56
150	DV	402	CDL	C81-C82-C83-C84
150	EN	1201	CDL	C39-C40-C41-C42
150	EO	202	CDL	C62-C63-C64-C65
150	Dg	201	CDL	C44-C45-C46-C47
150	Dn	503	CDL	C56-C57-C58-C59
150	Dn	506	CDL	C56-C57-C58-C59
150	Ds	406	CDL	C55-C56-C57-C58
150	Dx	1204	CDL	C36-C37-C38-C39
150	Eg	101	CDL	C81-C82-C83-C84
150	Eh	1601	CDL	C57-C58-C59-C60
150	El	901	CDL	C33-C34-C35-C36
150	El	901	CDL	C51-C52-C53-C54
153	AC	804	PC1	C29-C2A-C2B-C2C
150	A0	602	CDL	OA7-CA5-OA6-CA4
150	A1	402	CDL	OA7-CA5-OA6-CA4
150	c	506	CDL	OB7-CB5-OB6-CB4
150	DH	201	CDL	OA7-CA5-OA6-CA4
150	DU	403	CDL	OA7-CA5-OA6-CA4
150	DX	307	CDL	OB7-CB5-OB6-CB4
150	Du	401	CDL	OA7-CA5-OA6-CA4
150	El	901	CDL	OA7-CA5-OA6-CA4
153	DX	308	PC1	O22-C21-O21-C2
153	Dq	1404	PC1	O22-C21-O21-C2
155	AJ	502	3PE	O22-C21-O21-C2
155	C	513	3PE	O22-C21-O21-C2
155	DN	501	3PE	O22-C21-O21-C2
150	BY	201	CDL	CA5-C11-C12-C13
150	DR	403	CDL	CA7-C31-C32-C33
150	Ea	501	CDL	CA7-C31-C32-C33
155	Em	901	3PE	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	BT	204	CDL	C71-CB7-OB8-CB6
150	C	504	CDL	C71-CB7-OB8-CB6
150	DN	507	CDL	C71-CB7-OB8-CB6
150	DX	306	CDL	C71-CB7-OB8-CB6
150	ED	605	CDL	C71-CB7-OB8-CB6
150	Du	401	CDL	C71-CB7-OB8-CB6
150	Du	402	CDL	C31-CA7-OA8-CA6
153	A6	303	PC1	C32-C31-O31-C3
153	BS	1301	PC1	C32-C31-O31-C3
153	Da	707	PC1	C32-C31-O31-C3
155	AJ	502	3PE	C32-C31-O31-C3
150	A1	402	CDL	C82-C83-C84-C85
150	BT	204	CDL	C83-C84-C85-C86
150	CC	305	CDL	C58-C59-C60-C61
150	DA	709	CDL	C40-C41-C42-C43
150	DN	507	CDL	C55-C56-C57-C58
150	DQ	1504	CDL	C40-C41-C42-C43
150	DR	403	CDL	C12-C13-C14-C15
150	DS	405	CDL	C55-C56-C57-C58
150	Dj	404	CDL	C31-C32-C33-C34
150	Dn	506	CDL	C82-C83-C84-C85
150	Dq	1401	CDL	C40-C41-C42-C43
150	Dr	403	CDL	C12-C13-C14-C15
150	En	1201	CDL	C21-C22-C23-C24
153	D	402	PC1	C25-C26-C27-C28
150	A0	602	CDL	C40-C41-C42-C43
150	B0	101	CDL	C13-C14-C15-C16
150	C	505	CDL	C75-C76-C77-C78
150	DA	706	CDL	C17-C18-C19-C20
150	DN	506	CDL	C56-C57-C58-C59
150	DV	403	CDL	C53-C54-C55-C56
150	ED	604	CDL	C80-C81-C82-C83
150	EK	201	CDL	C53-C54-C55-C56
150	Eh	1601	CDL	C83-C84-C85-C86
150	En	1201	CDL	C17-C18-C19-C20
153	A0	605	PC1	C2C-C2D-C2E-C2F
153	AQ	202	PC1	C2B-C2C-C2D-C2E
153	Dx	1209	PC1	C3D-C3E-C3F-C3G
150	C	503	CDL	C79-C80-C81-C82
150	h	501	CDL	C71-C72-C73-C74
150	DG	201	CDL	C53-C54-C55-C56
150	DH	201	CDL	C56-C57-C58-C59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DN	507	CDL	C80-C81-C82-C83
150	DX	301	CDL	C74-C75-C76-C77
150	DY	301	CDL	C79-C80-C81-C82
150	EB	302	CDL	C34-C35-C36-C37
150	EK	201	CDL	C33-C34-C35-C36
150	ES	1101	CDL	C23-C24-C25-C26
150	ES	1101	CDL	C60-C61-C62-C63
150	Di	1101	CDL	C17-C18-C19-C20
150	Dj	401	CDL	C37-C38-C39-C40
150	Dj	403	CDL	C60-C61-C62-C63
150	Dy	301	CDL	C43-C44-C45-C46
150	Eh	1601	CDL	C81-C82-C83-C84
153	AQ	202	PC1	C3C-C3D-C3E-C3F
153	E	303	PC1	C3C-C3D-C3E-C3F
153	EO	206	PC1	C3C-C3D-C3E-C3F
153	Eo	204	PC1	C3A-C3B-C3C-C3D
150	Eh	1601	CDL	CA5-C11-C12-C13
150	Ek	201	CDL	CA5-C11-C12-C13
153	B1	403	PC1	C31-C32-C33-C34
150	AC	801	CDL	C78-C79-C80-C81
150	B0	102	CDL	C43-C44-C45-C46
150	CC	305	CDL	C36-C37-C38-C39
150	DD	704	CDL	C17-C18-C19-C20
150	DD	706	CDL	C23-C24-C25-C26
150	DJ	302	CDL	C17-C18-C19-C20
150	DJ	302	CDL	C39-C40-C41-C42
150	DJ	305	CDL	C77-C78-C79-C80
150	DQ	1504	CDL	C57-C58-C59-C60
150	DU	404	CDL	C23-C24-C25-C26
150	DX	301	CDL	C12-C13-C14-C15
150	DX	307	CDL	C43-C44-C45-C46
150	EL	901	CDL	C33-C34-C35-C36
150	EN	1201	CDL	C21-C22-C23-C24
150	Da	709	CDL	C16-C17-C18-C19
150	Dd	705	CDL	C40-C41-C42-C43
150	Dj	407	CDL	C51-C52-C53-C54
150	Ds	406	CDL	C58-C59-C60-C61
150	En	1201	CDL	C39-C40-C41-C42
153	A6	302	PC1	C3C-C3D-C3E-C3F
153	BG	202	PC1	C35-C36-C37-C38
153	DC	608	PC1	C2C-C2D-C2E-C2F
153	EO	205	PC1	C3A-C3B-C3C-C3D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Ds	407	PC1	C2B-C2C-C2D-C2E
155	AJ	502	3PE	C3E-C3F-C3G-C3H
155	DN	501	3PE	C25-C26-C27-C28
155	DS	402	3PE	C39-C3A-C3B-C3C
155	Dr	404	3PE	C3E-C3F-C3G-C3H
155	Ds	408	3PE	C35-C36-C37-C38
155	Dx	1208	3PE	C27-C28-C29-C2A
150	CG	301	CDL	C53-C54-C55-C56
150	DJ	304	CDL	C19-C20-C21-C22
150	DQ	1504	CDL	C61-C62-C63-C64
150	DR	402	CDL	C82-C83-C84-C85
150	DX	301	CDL	C61-C62-C63-C64
150	DX	306	CDL	C63-C64-C65-C66
150	DZ	501	CDL	C16-C17-C18-C19
150	EH	1601	CDL	C83-C84-C85-C86
150	Dh	202	CDL	C71-C72-C73-C74
150	Dj	402	CDL	C16-C17-C18-C19
150	Dj	402	CDL	C52-C53-C54-C55
150	Dx	1204	CDL	C76-C77-C78-C79
153	AC	804	PC1	C2E-C2F-C2G-C2H
153	K	502	PC1	C3D-C3E-C3F-C3G
153	DV	405	PC1	C3C-C3D-C3E-C3F
153	Dj	406	PC1	C22-C23-C24-C25
155	DG	205	3PE	C3E-C3F-C3G-C3H
153	Eo	204	PC1	C32-C31-O31-C3
150	BG	201	CDL	C53-C54-C55-C56
150	c	506	CDL	C17-C18-C19-C20
150	c	506	CDL	C20-C21-C22-C23
150	DH	202	CDL	C42-C43-C44-C45
150	DJ	302	CDL	C82-C83-C84-C85
150	DJ	304	CDL	C33-C34-C35-C36
150	DN	502	CDL	C35-C36-C37-C38
150	DQ	1504	CDL	C36-C37-C38-C39
150	EL	902	CDL	C83-C84-C85-C86
150	Dd	704	CDL	C11-C12-C13-C14
150	Dj	402	CDL	C58-C59-C60-C61
150	Dj	404	CDL	C19-C20-C21-C22
150	Dj	405	CDL	C11-C12-C13-C14
150	Dv	402	CDL	C81-C82-C83-C84
150	Dy	301	CDL	C79-C80-C81-C82
150	En	1201	CDL	C54-C55-C56-C57
153	AA	903	PC1	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	EN	1203	PC1	C2B-C2C-C2D-C2E
153	Di	1104	PC1	C3A-C3B-C3C-C3D
155	Eo	202	3PE	C3C-C3D-C3E-C3F
150	DR	402	CDL	CA7-C31-C32-C33
153	A1	403	PC1	C31-C32-C33-C34
150	A1	402	CDL	C11-CA5-OA6-CA4
150	A1	402	CDL	C51-CB5-OB6-CB4
150	AC	801	CDL	C11-CA5-OA6-CA4
150	AM	301	CDL	C51-CB5-OB6-CB4
150	B0	102	CDL	C51-CB5-OB6-CB4
150	BC	302	CDL	C11-CA5-OA6-CA4
150	CJ	201	CDL	C51-CB5-OB6-CB4
150	CD	301	CDL	C51-CB5-OB6-CB4
150	c	506	CDL	C51-CB5-OB6-CB4
150	DD	703	CDL	C51-CB5-OB6-CB4
150	DD	704	CDL	C11-CA5-OA6-CA4
150	DH	201	CDL	C11-CA5-OA6-CA4
150	DN	506	CDL	C11-CA5-OA6-CA4
150	DQ	1502	CDL	C51-CB5-OB6-CB4
150	DS	401	CDL	C11-CA5-OA6-CA4
150	DS	405	CDL	C51-CB5-OB6-CB4
150	DU	403	CDL	C11-CA5-OA6-CA4
150	DX	307	CDL	C51-CB5-OB6-CB4
150	Dd	705	CDL	C11-CA5-OA6-CA4
150	Dd	705	CDL	C51-CB5-OB6-CB4
150	Ds	402	CDL	C51-CB5-OB6-CB4
150	Ds	406	CDL	C51-CB5-OB6-CB4
150	Du	401	CDL	C11-CA5-OA6-CA4
150	Du	402	CDL	C11-CA5-OA6-CA4
150	El	901	CDL	C11-CA5-OA6-CA4
153	A6	303	PC1	C22-C21-O21-C2
153	AA	905	PC1	C22-C21-O21-C2
153	AU	202	PC1	C22-C21-O21-C2
153	c	507	PC1	C22-C21-O21-C2
153	e	1101	PC1	C22-C21-O21-C2
153	DS	406	PC1	C22-C21-O21-C2
153	DX	308	PC1	C22-C21-O21-C2
153	Dq	1404	PC1	C22-C21-O21-C2
153	Dx	1203	PC1	C22-C21-O21-C2
155	CD	303	3PE	C22-C21-O21-C2
155	C	513	3PE	C22-C21-O21-C2
155	DC	606	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DN	501	3PE	C22-C21-O21-C2
155	DX	303	3PE	C22-C21-O21-C2
155	EO	203	3PE	C22-C21-O21-C2
155	Dc	606	3PE	C22-C21-O21-C2
155	Dx	1207	3PE	C22-C21-O21-C2
150	AA	908	CDL	OA5-CA3-CA4-OA6
150	BT	202	CDL	OB5-CB3-CB4-OB6
150	CD	302	CDL	OB5-CB3-CB4-OB6
150	DX	301	CDL	OB5-CB3-CB4-OB6
150	ED	605	CDL	OB5-CB3-CB4-OB6
150	EH	1601	CDL	OA5-CA3-CA4-OA6
150	Du	401	CDL	OA5-CA3-CA4-OA6
150	Ed	205	CDL	OB5-CB3-CB4-OB6
153	Dq	1404	PC1	O11-C1-C2-O21
150	AA	908	CDL	C38-C39-C40-C41
150	AA	908	CDL	C82-C83-C84-C85
150	DC	601	CDL	C33-C34-C35-C36
150	DG	201	CDL	C13-C14-C15-C16
150	DM	501	CDL	C58-C59-C60-C61
150	DN	506	CDL	C82-C83-C84-C85
150	DR	403	CDL	C41-C42-C43-C44
150	DV	402	CDL	C23-C24-C25-C26
150	EL	902	CDL	C63-C64-C65-C66
150	EL	902	CDL	C74-C75-C76-C77
150	Dv	403	CDL	C53-C54-C55-C56
150	Dx	1204	CDL	C32-C33-C34-C35
150	Eg	101	CDL	C42-C43-C44-C45
153	DC	602	PC1	C3D-C3E-C3F-C3G
155	DX	303	3PE	C26-C27-C28-C29
155	Eo	202	3PE	C2C-C2D-C2E-C2F
156	AL	304	LPP	C20-C21-C22-C23
156	Dn	504	LPP	C31-C32-C33-C34
150	BT	204	CDL	C36-C37-C38-C39
150	DO	501	CDL	C15-C16-C17-C18
150	Dj	401	CDL	C53-C54-C55-C56
150	Ep	701	CDL	C11-C12-C13-C14
153	Db	702	PC1	C27-C28-C29-C2A
150	AM	301	CDL	OB7-CB5-OB6-CB4
150	B0	102	CDL	OB7-CB5-OB6-CB4
150	CD	302	CDL	OB7-CB5-OB6-CB4
150	E	301	CDL	OB7-CB5-OB6-CB4
150	DQ	1502	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DS	401	CDL	OA7-CA5-OA6-CA4
150	DS	405	CDL	OB7-CB5-OB6-CB4
150	ED	605	CDL	OB7-CB5-OB6-CB4
150	EN	1201	CDL	OA7-CA5-OA6-CA4
150	Dd	702	CDL	OB7-CB5-OB6-CB4
150	Dd	705	CDL	OA7-CA5-OA6-CA4
150	Dd	705	CDL	OB7-CB5-OB6-CB4
150	Ds	406	CDL	OB7-CB5-OB6-CB4
150	Ed	205	CDL	OA7-CA5-OA6-CA4
150	Ek	201	CDL	OB7-CB5-OB6-CB4
153	e	1101	PC1	O22-C21-O21-C2
155	CD	303	3PE	O22-C21-O21-C2
155	DC	606	3PE	O22-C21-O21-C2
155	EO	203	3PE	O22-C21-O21-C2
155	El	905	3PE	O22-C21-O21-C2
150	DY	301	CDL	C57-C58-C59-C60
150	DZ	501	CDL	C77-C78-C79-C80
150	EA	301	CDL	C81-C82-C83-C84
150	EI	401	CDL	C11-C12-C13-C14
150	Dn	502	CDL	C12-C13-C14-C15
156	AC	803	LPP	C39-C40-C41-C42
150	AF	402	CDL	OB6-CB4-CB6-OB8
150	c	502	CDL	OB6-CB4-CB6-OB8
150	DA	709	CDL	OA6-CA4-CA6-OA8
150	DD	703	CDL	OB6-CB4-CB6-OB8
150	DJ	304	CDL	OB6-CB4-CB6-OB8
150	Da	709	CDL	OA6-CA4-CA6-OA8
150	Dg	201	CDL	OA6-CA4-CA6-OA8
150	Dn	503	CDL	OB6-CB4-CB6-OB8
150	En	1201	CDL	OA6-CA4-CA6-OA8
153	AA	907	PC1	O21-C2-C3-O31
153	DV	406	PC1	O21-C2-C3-O31
153	EO	205	PC1	O21-C2-C3-O31
155	DN	501	3PE	O21-C2-C3-O31
156	AC	803	LPP	O9-C7-C8-O27
150	DV	402	CDL	C36-C37-C38-C39
150	DX	306	CDL	C40-C41-C42-C43
150	EA	301	CDL	C13-C14-C15-C16
150	EH	1601	CDL	C81-C82-C83-C84
150	Dj	401	CDL	C82-C83-C84-C85
153	BS	1301	PC1	C2C-C2D-C2E-C2F
153	d	801	PC1	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	EO	205	PC1	C33-C34-C35-C36
155	EN	1204	3PE	C35-C36-C37-C38
155	Dx	1202	3PE	C2C-C2D-C2E-C2F
153	BG	202	PC1	O32-C31-O31-C3
150	AF	402	CDL	C39-C40-C41-C42
150	DD	705	CDL	C82-C83-C84-C85
150	DG	201	CDL	C31-C32-C33-C34
150	DJ	303	CDL	C13-C14-C15-C16
150	DJ	304	CDL	C51-C52-C53-C54
150	DS	404	CDL	C17-C18-C19-C20
150	DV	403	CDL	C13-C14-C15-C16
150	ES	1101	CDL	C79-C80-C81-C82
150	Dr	402	CDL	C60-C61-C62-C63
150	Dv	402	CDL	C23-C24-C25-C26
150	Dx	1204	CDL	C20-C21-C22-C23
150	El	902	CDL	C78-C79-C80-C81
153	A9	601	PC1	C23-C24-C25-C26
153	B1	401	PC1	C2E-C2F-C2G-C2H
155	El	905	3PE	C26-C27-C28-C29
155	Eo	202	3PE	C27-C28-C29-C2A
167	c	510	UQ8	C30-C29-C31-C32
150	A1	402	CDL	CB7-C71-C72-C73
167	CC	303	UQ8	C13-C14-C16-C17
150	AM	301	CDL	C11-C12-C13-C14
150	DN	507	CDL	C42-C43-C44-C45
150	DU	403	CDL	C36-C37-C38-C39
150	Dv	403	CDL	C12-C13-C14-C15
150	Ed	204	CDL	C76-C77-C78-C79
155	Ds	403	3PE	C39-C3A-C3B-C3C
155	Dx	1202	3PE	C27-C28-C29-C2A
156	EI	402	LPP	C20-C21-C22-C23
150	EK	201	CDL	CA4-CA6-OA8-CA7
150	DG	202	CDL	C51-C52-C53-C54
150	DX	307	CDL	C14-C15-C16-C17
150	Dd	705	CDL	C82-C83-C84-C85
150	Dx	1204	CDL	C54-C55-C56-C57
153	BS	1301	PC1	C34-C35-C36-C37
153	E	303	PC1	C33-C34-C35-C36
153	DI	303	PC1	C2C-C2D-C2E-C2F
155	Dr	404	3PE	C22-C23-C24-C25
156	EI	402	LPP	C15-C16-C17-C18
150	AC	801	CDL	C76-C77-C78-C79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DJ	302	CDL	C53-C54-C55-C56
150	DJ	303	CDL	C14-C15-C16-C17
150	Dc	608	CDL	C60-C61-C62-C63
150	Dg	202	CDL	C17-C18-C19-C20
150	Dq	1403	CDL	C38-C39-C40-C41
150	Dr	402	CDL	C82-C83-C84-C85
150	Dv	403	CDL	C43-C44-C45-C46
153	DJ	306	PC1	C22-C23-C24-C25
153	Da	707	PC1	C3E-C3F-C3G-C3H
153	Db	702	PC1	C32-C33-C34-C35
153	Di	1104	PC1	C2C-C2D-C2E-C2F
153	Eo	201	PC1	C3B-C3C-C3D-C3E
155	BT	201	3PE	C3D-C3E-C3F-C3G
155	EM	901	3PE	C26-C27-C28-C29
155	Dc	607	3PE	C34-C35-C36-C37
155	Dx	1207	3PE	C26-C27-C28-C29
150	DM	501	CDL	C71-CB7-OB8-CB6
150	Ed	205	CDL	C71-CB7-OB8-CB6
150	AC	801	CDL	C19-C20-C21-C22
150	Ds	405	CDL	C17-C18-C19-C20
150	Dv	402	CDL	C75-C76-C77-C78
153	DA	707	PC1	C24-C25-C26-C27
153	EO	204	PC1	C3C-C3D-C3E-C3F
150	BT	204	CDL	OB9-CB7-OB8-CB6
150	DD	705	CDL	OB9-CB7-OB8-CB6
150	DV	401	CDL	OB9-CB7-OB8-CB6
150	Dq	1403	CDL	OB9-CB7-OB8-CB6
150	Ds	402	CDL	OB9-CB7-OB8-CB6
150	Du	403	CDL	OB9-CB7-OB8-CB6
153	AU	201	PC1	O32-C31-O31-C3
153	EO	206	PC1	O32-C31-O31-C3
150	A1	402	CDL	OB7-CB5-OB6-CB4
150	AC	801	CDL	OA7-CA5-OA6-CA4
150	CC	304	CDL	OB7-CB5-OB6-CB4
150	CD	301	CDL	OB7-CB5-OB6-CB4
150	DD	703	CDL	OB7-CB5-OB6-CB4
150	DD	704	CDL	OA7-CA5-OA6-CA4
150	DG	201	CDL	OA7-CA5-OA6-CA4
150	DN	506	CDL	OA7-CA5-OA6-CA4
150	Du	402	CDL	OA7-CA5-OA6-CA4
150	Eh	1601	CDL	OB7-CB5-OB6-CB4
150	Ep	701	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AA	905	PC1	O22-C21-O21-C2
153	Dx	1203	PC1	O22-C21-O21-C2
155	DX	303	3PE	O22-C21-O21-C2
155	Dc	606	3PE	O22-C21-O21-C2
155	Dx	1207	3PE	O22-C21-O21-C2
150	DG	201	CDL	C11-CA5-OA6-CA4
150	Dx	1201	CDL	C11-CA5-OA6-CA4
155	DJ	301	3PE	C22-C21-O21-C2
150	BT	204	CDL	C37-C38-C39-C40
150	CD	302	CDL	C12-C13-C14-C15
150	DQ	1501	CDL	C43-C44-C45-C46
150	Dg	202	CDL	C35-C36-C37-C38
150	Ds	405	CDL	C16-C17-C18-C19
150	Dv	401	CDL	C21-C22-C23-C24
153	B1	401	PC1	C3B-C3C-C3D-C3E
155	El	905	3PE	C3E-C3F-C3G-C3H
155	Em	901	3PE	C2A-C2B-C2C-C2D
156	DN	504	LPP	C35-C36-C37-C38
150	A0	602	CDL	CA2-OA2-PA1-OA5
150	BG	201	CDL	CB3-OB5-PB2-OB2
150	g	801	CDL	CA2-OA2-PA1-OA5
150	g	801	CDL	CB2-OB2-PB2-OB5
150	DA	706	CDL	CB3-OB5-PB2-OB2
150	DC	601	CDL	CA2-OA2-PA1-OA5
150	DD	703	CDL	CA3-OA5-PA1-OA2
150	DD	703	CDL	CB2-OB2-PB2-OB5
150	DD	704	CDL	CB2-OB2-PB2-OB5
150	DG	202	CDL	CA2-OA2-PA1-OA5
150	DG	202	CDL	CB3-OB5-PB2-OB2
150	DI	302	CDL	CB3-OB5-PB2-OB2
150	DJ	305	CDL	CA3-OA5-PA1-OA2
150	DM	501	CDL	CA2-OA2-PA1-OA5
150	DN	502	CDL	CB2-OB2-PB2-OB5
150	DU	401	CDL	CB3-OB5-PB2-OB2
150	DV	403	CDL	CA3-OA5-PA1-OA2
150	DY	301	CDL	CB2-OB2-PB2-OB5
150	ED	601	CDL	CB2-OB2-PB2-OB5
150	EK	201	CDL	CA3-OA5-PA1-OA2
150	EL	901	CDL	CB2-OB2-PB2-OB5
150	EL	903	CDL	CA2-OA2-PA1-OA5
150	EN	1202	CDL	CA3-OA5-PA1-OA2
150	Dd	706	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Di	1101	CDL	CB2-OB2-PB2-OB5
150	Dj	401	CDL	CB2-OB2-PB2-OB5
150	Dj	402	CDL	CB3-OB5-PB2-OB2
150	Dj	403	CDL	CB2-OB2-PB2-OB5
150	Dn	501	CDL	CA3-OA5-PA1-OA2
150	Dq	1403	CDL	CB3-OB5-PB2-OB2
150	Du	402	CDL	CA3-OA5-PA1-OA2
150	Du	403	CDL	CB3-OB5-PB2-OB2
150	Dv	402	CDL	CB3-OB5-PB2-OB2
150	El	901	CDL	CA3-OA5-PA1-OA2
150	El	902	CDL	CB2-OB2-PB2-OB5
150	El	903	CDL	CA3-OA5-PA1-OA2
153	AM	302	PC1	C11-O13-P-O11
153	BG	202	PC1	C1-O11-P-O13
153	D	402	PC1	C11-O13-P-O11
153	DA	707	PC1	C11-O13-P-O11
153	DX	308	PC1	C11-O13-P-O11
153	EN	1203	PC1	C11-O13-P-O11
153	Dx	1203	PC1	C11-O13-P-O11
153	Eb	301	PC1	C1-O11-P-O13
155	BT	201	3PE	C11-O13-P-O11
155	DJ	301	3PE	C11-O13-P-O11
155	Dd	703	3PE	C11-O13-P-O11
155	Dx	1208	3PE	C11-O13-P-O11
150	BG	201	CDL	C13-C14-C15-C16
150	DQ	1501	CDL	C36-C37-C38-C39
150	DS	401	CDL	C80-C81-C82-C83
150	DZ	501	CDL	C12-C13-C14-C15
150	Dc	608	CDL	C21-C22-C23-C24
150	Dg	201	CDL	C83-C84-C85-C86
150	Dj	403	CDL	C23-C24-C25-C26
150	Do	501	CDL	C15-C16-C17-C18
150	Dr	403	CDL	C54-C55-C56-C57
155	EM	901	3PE	C2A-C2B-C2C-C2D
150	C	504	CDL	CA5-C11-C12-C13
150	DD	703	CDL	CB7-C71-C72-C73
150	DG	201	CDL	CA4-CA3-OA5-PA1
150	DH	202	CDL	C1-CB2-OB2-PB2
150	EL	902	CDL	C1-CB2-OB2-PB2
150	ES	1101	CDL	CA4-CA3-OA5-PA1
150	Ds	401	CDL	C1-CA2-OA2-PA1
153	Da	706	PC1	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DG	201	CDL	C58-C59-C60-C61
150	Dh	202	CDL	C42-C43-C44-C45
150	Dq	1403	CDL	C75-C76-C77-C78
150	Eu	101	CDL	C72-C73-C74-C75
153	c	507	PC1	C2E-C2F-C2G-C2H
155	AJ	502	3PE	O32-C31-O31-C3
153	AA	903	PC1	C32-C31-O31-C3
153	C	508	PC1	C32-C31-O31-C3
150	A0	602	CDL	OB5-CB3-CB4-CB6
150	AM	301	CDL	OA5-CA3-CA4-CA6
150	BC	301	CDL	OA5-CA3-CA4-CA6
150	CD	301	CDL	OA5-CA3-CA4-CA6
150	C	505	CDL	OB5-CB3-CB4-CB6
150	c	502	CDL	OA5-CA3-CA4-CA6
150	DA	706	CDL	OB5-CB3-CB4-CB6
150	DC	601	CDL	OB5-CB3-CB4-CB6
150	DG	201	CDL	OA5-CA3-CA4-CA6
150	DJ	307	CDL	OB5-CB3-CB4-CB6
150	DU	404	CDL	OB5-CB3-CB4-CB6
150	ED	601	CDL	OB5-CB3-CB4-CB6
150	ED	604	CDL	OB5-CB3-CB4-CB6
150	EI	401	CDL	OB5-CB3-CB4-CB6
150	ES	1101	CDL	OB5-CB3-CB4-CB6
150	Dc	601	CDL	OB5-CB3-CB4-CB6
150	Dd	705	CDL	OA5-CA3-CA4-CA6
150	Dn	502	CDL	OB5-CB3-CB4-CB6
150	Do	501	CDL	OA5-CA3-CA4-CA6
150	Dq	1401	CDL	OB5-CB3-CB4-CB6
150	Dq	1403	CDL	OB5-CB3-CB4-CB6
150	Ds	406	CDL	OB5-CB3-CB4-CB6
153	A1	403	PC1	O11-C1-C2-C3
153	AA	905	PC1	O11-C1-C2-C3
153	AJ	501	PC1	O11-C1-C2-C3
153	AU	201	PC1	O11-C1-C2-C3
153	B1	403	PC1	O11-C1-C2-C3
153	C	509	PC1	O11-C1-C2-C3
153	D	402	PC1	O11-C1-C2-C3
153	EN	1203	PC1	O11-C1-C2-C3
153	Dc	603	PC1	O11-C1-C2-C3
153	Di	1104	PC1	O11-C1-C2-C3
155	A2	401	3PE	O11-C1-C2-C3
155	Dc	606	3PE	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	CC	305	CDL	C52-C53-C54-C55
150	Dc	601	CDL	C33-C34-C35-C36
150	Dg	202	CDL	C63-C64-C65-C66
150	Ds	401	CDL	C32-C33-C34-C35
150	Ds	402	CDL	C22-C23-C24-C25
153	AA	904	PC1	C3F-C3G-C3H-C3I
151	A0	603	UDP	O4'-C1'-N1-C6
150	Dg	202	CDL	CA5-C11-C12-C13
150	BY	201	CDL	C20-C21-C22-C23
150	DS	404	CDL	C12-C13-C14-C15
150	Dn	502	CDL	C41-C42-C43-C44
150	Ea	501	CDL	C12-C13-C14-C15
150	En	1201	CDL	C53-C54-C55-C56
153	Dc	609	PC1	C2C-C2D-C2E-C2F
153	Dx	1203	PC1	C2B-C2C-C2D-C2E
155	BT	201	3PE	C35-C36-C37-C38
155	DX	304	3PE	C27-C28-C29-C2A
150	DM	502	CDL	CA4-CA6-OA8-CA7
150	EH	1601	CDL	CA4-CA6-OA8-CA7
150	CG	302	CDL	C52-C53-C54-C55
150	DS	404	CDL	C57-C58-C59-C60
150	Dy	301	CDL	C56-C57-C58-C59
150	En	1201	CDL	C34-C35-C36-C37
153	A	1201	PC1	C3B-C3C-C3D-C3E
153	DC	603	PC1	C35-C36-C37-C38
153	Eo	201	PC1	C25-C26-C27-C28
156	DN	504	LPP	C31-C32-C33-C34
150	CG	302	CDL	C72-C73-C74-C75
150	c	506	CDL	C58-C59-C60-C61
150	DN	507	CDL	C12-C13-C14-C15
150	EB	302	CDL	C57-C58-C59-C60
150	EH	1601	CDL	C73-C74-C75-C76
150	EI	401	CDL	C76-C77-C78-C79
150	EL	901	CDL	C55-C56-C57-C58
150	Dj	404	CDL	C18-C19-C20-C21
150	Dm	501	CDL	C82-C83-C84-C85
150	Dn	506	CDL	C43-C44-C45-C46
153	DQ	1503	PC1	C34-C35-C36-C37
153	EO	205	PC1	C2D-C2E-C2F-C2G
156	DN	504	LPP	C37-C38-C39-C40
150	BT	204	CDL	CA5-C11-C12-C13
150	DR	402	CDL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EL	901	CDL	C23-C24-C25-C26
150	Di	1101	CDL	C75-C76-C77-C78
150	Ds	406	CDL	C12-C13-C14-C15
150	El	903	CDL	C61-C62-C63-C64
153	Dx	1209	PC1	C24-C25-C26-C27
150	DQ	1501	CDL	C71-CB7-OB8-CB6
150	A1	402	CDL	CA2-C1-CB2-OB2
150	C	503	CDL	CB2-C1-CA2-OA2
150	DJ	303	CDL	CB2-C1-CA2-OA2
150	EN	1201	CDL	CB2-C1-CA2-OA2
150	Eb	302	CDL	CB2-C1-CA2-OA2
150	Ds	402	CDL	OB7-CB5-OB6-CB4
150	AA	901	CDL	C82-C83-C84-C85
150	CJ	201	CDL	C79-C80-C81-C82
150	CJ	201	CDL	C81-C82-C83-C84
150	C	505	CDL	C11-C12-C13-C14
150	DR	402	CDL	C33-C34-C35-C36
150	DV	403	CDL	C43-C44-C45-C46
150	ED	601	CDL	C56-C57-C58-C59
150	EL	902	CDL	C36-C37-C38-C39
150	Dj	403	CDL	C58-C59-C60-C61
150	Dn	506	CDL	C36-C37-C38-C39
153	AU	201	PC1	C23-C24-C25-C26
153	B1	403	PC1	C2C-C2D-C2E-C2F
153	EO	201	PC1	C3B-C3C-C3D-C3E
153	Dv	406	PC1	C2D-C2E-C2F-C2G
150	BT	202	CDL	C73-C74-C75-C76
150	CD	302	CDL	C20-C21-C22-C23
150	DA	709	CDL	C42-C43-C44-C45
150	DR	403	CDL	C54-C55-C56-C57
150	DU	402	CDL	C42-C43-C44-C45
150	DV	401	CDL	C21-C22-C23-C24
150	Dg	201	CDL	C17-C18-C19-C20
150	Dg	201	CDL	C52-C53-C54-C55
150	Dq	1402	CDL	C17-C18-C19-C20
150	Dr	403	CDL	C41-C42-C43-C44
150	Ds	405	CDL	C76-C77-C78-C79
150	Eu	101	CDL	C40-C41-C42-C43
153	Da	706	PC1	C24-C25-C26-C27
153	Dq	1404	PC1	C34-C35-C36-C37
153	El	904	PC1	C3C-C3D-C3E-C3F
150	AF	401	CDL	C11-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	C	504	CDL	C51-CB5-OB6-CB4
150	DU	402	CDL	C51-CB5-OB6-CB4
150	DX	306	CDL	C51-CB5-OB6-CB4
155	Dc	607	3PE	C22-C21-O21-C2
150	DX	306	CDL	OB9-CB7-OB8-CB6
150	Du	401	CDL	OB9-CB7-OB8-CB6
150	Du	402	CDL	OA9-CA7-OA8-CA6
153	A6	303	PC1	O32-C31-O31-C3
153	BS	1301	PC1	O32-C31-O31-C3
150	AA	901	CDL	C60-C61-C62-C63
150	DV	401	CDL	C43-C44-C45-C46
150	DV	402	CDL	C13-C14-C15-C16
150	Do	501	CDL	C76-C77-C78-C79
150	Ea	501	CDL	C11-C12-C13-C14
155	El	905	3PE	C37-C38-C39-C3A
153	DI	303	PC1	C11-C12-N-C14
150	AF	401	CDL	CA3-CA4-CA6-OA8
150	AM	301	CDL	CB3-CB4-CB6-OB8
150	AP	301	CDL	CA3-CA4-CA6-OA8
150	B0	102	CDL	CA3-CA4-CA6-OA8
150	BC	302	CDL	CB3-CB4-CB6-OB8
150	BG	201	CDL	CA3-CA4-CA6-OA8
150	BG	201	CDL	CB3-CB4-CB6-OB8
150	E	301	CDL	CA3-CA4-CA6-OA8
150	c	509	CDL	CA3-CA4-CA6-OA8
150	DG	202	CDL	CB3-CB4-CB6-OB8
150	DI	302	CDL	CA3-CA4-CA6-OA8
150	DJ	303	CDL	CA3-CA4-CA6-OA8
150	DJ	303	CDL	CB3-CB4-CB6-OB8
150	DM	501	CDL	CA3-CA4-CA6-OA8
150	DN	507	CDL	CB3-CB4-CB6-OB8
150	DR	402	CDL	CA3-CA4-CA6-OA8
150	DR	402	CDL	CB3-CB4-CB6-OB8
150	DS	401	CDL	CA3-CA4-CA6-OA8
150	DS	401	CDL	C76-C77-C78-C79
150	DU	402	CDL	C11-C12-C13-C14
150	DX	306	CDL	CB3-CB4-CB6-OB8
150	DX	307	CDL	CA3-CA4-CA6-OA8
150	DY	301	CDL	CA3-CA4-CA6-OA8
150	EI	401	CDL	CA3-CA4-CA6-OA8
150	EK	201	CDL	CA3-CA4-CA6-OA8
150	EL	902	CDL	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EL	902	CDL	CB3-CB4-CB6-OB8
150	EO	202	CDL	CB3-CB4-CB6-OB8
150	Dc	601	CDL	C14-C15-C16-C17
150	Dc	608	CDL	CA3-CA4-CA6-OA8
150	Dd	702	CDL	CA3-CA4-CA6-OA8
150	Dd	704	CDL	CB3-CB4-CB6-OB8
150	Dg	201	CDL	CB3-CB4-CB6-OB8
150	Dh	201	CDL	CA3-CA4-CA6-OA8
150	Di	1103	CDL	CA3-CA4-CA6-OA8
150	Dj	401	CDL	CA3-CA4-CA6-OA8
150	Dm	502	CDL	CA3-CA4-CA6-OA8
150	Dn	501	CDL	CA3-CA4-CA6-OA8
150	Dr	403	CDL	CB3-CB4-CB6-OB8
150	Dv	403	CDL	CA3-CA4-CA6-OA8
150	Dv	403	CDL	C40-C41-C42-C43
150	Dx	1201	CDL	CA3-CA4-CA6-OA8
150	Eb	302	CDL	CB3-CB4-CB6-OB8
150	Eh	1601	CDL	C14-C15-C16-C17
150	Eh	1601	CDL	CB3-CB4-CB6-OB8
150	Ei	401	CDL	CA3-CA4-CA6-OA8
150	El	901	CDL	CB3-CB4-CB6-OB8
150	El	902	CDL	CA3-CA4-CA6-OA8
153	A2	402	PC1	C1-C2-C3-O31
153	A6	303	PC1	C1-C2-C3-O31
153	BT	203	PC1	C1-C2-C3-O31
153	C	508	PC1	C1-C2-C3-O31
153	C	509	PC1	C1-C2-C3-O31
153	K	501	PC1	C1-C2-C3-O31
153	d	801	PC1	C1-C2-C3-O31
153	g	802	PC1	C1-C2-C3-O31
153	DA	708	PC1	C1-C2-C3-O31
153	DC	608	PC1	C1-C2-C3-O31
153	DX	308	PC1	C1-C2-C3-O31
153	DY	302	PC1	C1-C2-C3-O31
153	EN	1203	PC1	C1-C2-C3-O31
153	EO	206	PC1	C1-C2-C3-O31
153	Dc	605	PC1	C1-C2-C3-O31
153	Ds	407	PC1	C1-C2-C3-O31
153	Dv	404	PC1	C1-C2-C3-O31
153	Dy	302	PC1	C1-C2-C3-O31
153	Ef	501	PC1	C33-C34-C35-C36
153	Eo	201	PC1	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	C	513	3PE	C1-C2-C3-O31
155	DR	401	3PE	C1-C2-C3-O31
155	DX	304	3PE	C1-C2-C3-O31
155	DX	304	3PE	C39-C3A-C3B-C3C
155	EL	904	3PE	C3E-C3F-C3G-C3H
155	EM	901	3PE	C1-C2-C3-O31
155	Da	708	3PE	C28-C29-C2A-C2B
155	Dx	1202	3PE	C1-C2-C3-O31
155	Em	901	3PE	C26-C27-C28-C29
156	DA	710	LPP	C40-C41-C42-C43
156	Dn	504	LPP	C37-C38-C39-C40
150	c	506	CDL	C13-C14-C15-C16
150	DQ	1502	CDL	C38-C39-C40-C41
150	Dd	704	CDL	C12-C13-C14-C15
150	Eg	101	CDL	C79-C80-C81-C82
153	A6	302	PC1	C28-C29-C2A-C2B
153	DJ	306	PC1	C37-C38-C39-C3A
153	DV	404	PC1	C3B-C3C-C3D-C3E
167	CC	303	UQ8	C1-C6-C7-C8
167	C	511	UQ8	C1-C6-C7-C8
150	DQ	1504	CDL	CB4-CB6-OB8-CB7
150	DX	307	CDL	CA4-CA6-OA8-CA7
150	BC	301	CDL	C35-C36-C37-C38
150	DM	501	CDL	C14-C15-C16-C17
150	DV	401	CDL	C18-C19-C20-C21
150	EL	902	CDL	C79-C80-C81-C82
150	Da	709	CDL	C18-C19-C20-C21
150	Da	709	CDL	C21-C22-C23-C24
150	Dj	401	CDL	C13-C14-C15-C16
150	Eg	101	CDL	C11-C12-C13-C14
153	C	508	PC1	C38-C39-C3A-C3B
153	DI	303	PC1	C3A-C3B-C3C-C3D
155	Dx	1208	3PE	C39-C3A-C3B-C3C
150	c	501	CDL	C19-C20-C21-C22
150	EL	903	CDL	C77-C78-C79-C80
150	Dj	404	CDL	C61-C62-C63-C64
155	DI	301	3PE	C35-C36-C37-C38
150	Dv	401	CDL	C72-C71-CB7-OB8
150	CC	305	CDL	CB5-C51-C52-C53
150	DJ	304	CDL	CA5-C11-C12-C13
150	Ds	402	CDL	CB5-C51-C52-C53
150	C	504	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AA	901	CDL	C22-C23-C24-C25
150	DH	202	CDL	C34-C35-C36-C37
150	Dj	404	CDL	C63-C64-C65-C66
150	Dr	402	CDL	C13-C14-C15-C16
150	Dr	403	CDL	C35-C36-C37-C38
150	Dx	1201	CDL	C38-C39-C40-C41
153	DC	608	PC1	C3D-C3E-C3F-C3G
153	Dv	404	PC1	C3F-C3G-C3H-C3I
167	CC	303	UQ8	C39-C41-C42-C43
150	AP	301	CDL	C60-C61-C62-C63
150	c	502	CDL	C14-C15-C16-C17
150	DH	202	CDL	C73-C74-C75-C76
150	DU	401	CDL	C60-C61-C62-C63
150	DV	402	CDL	C62-C63-C64-C65
150	EN	1202	CDL	C37-C38-C39-C40
150	Dd	702	CDL	C32-C33-C34-C35
150	Dn	503	CDL	C83-C84-C85-C86
153	A9	601	PC1	C2D-C2E-C2F-C2G
153	C	509	PC1	C2E-C2F-C2G-C2H
153	D	402	PC1	C2B-C2C-C2D-C2E
156	AL	304	LPP	C40-C41-C42-C43
150	CD	301	CDL	CB4-CB6-OB8-CB7
150	h	501	CDL	CA4-CA6-OA8-CA7
150	DD	703	CDL	C23-C24-C25-C26
150	DX	301	CDL	C35-C36-C37-C38
150	Dv	401	CDL	C18-C19-C20-C21
153	EB	301	PC1	C36-C37-C38-C39
153	Dg	203	PC1	C3D-C3E-C3F-C3G
153	Eo	204	PC1	C3F-C3G-C3H-C3I
155	AJ	502	3PE	C2B-C2C-C2D-C2E
164	CA	702	FAD	O3'-C3'-C4'-O4'
150	ED	605	CDL	OB9-CB7-OB8-CB6
153	Da	707	PC1	O32-C31-O31-C3
153	AA	906	PC1	C21-C22-C23-C24
150	C	507	CDL	C14-C15-C16-C17
150	DH	202	CDL	C51-C52-C53-C54
150	EH	1601	CDL	C78-C79-C80-C81
150	Dd	704	CDL	C20-C21-C22-C23
150	Du	401	CDL	C60-C61-C62-C63
150	El	902	CDL	C52-C53-C54-C55
153	Dc	604	PC1	C3F-C3G-C3H-C3I
150	B1	402	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dx	1204	CDL	C11-CA5-OA6-CA4
153	AA	906	PC1	C22-C21-O21-C2
150	DS	405	CDL	C43-C44-C45-C46
150	Du	402	CDL	C19-C20-C21-C22
167	DS	403	UQ8	C30-C29-C31-C32
167	Ds	404	UQ8	C30-C29-C31-C32
150	AC	801	CDL	C62-C63-C64-C65
150	Dd	702	CDL	C37-C38-C39-C40
150	Dx	1201	CDL	C32-C33-C34-C35
153	Db	702	PC1	C2C-C2D-C2E-C2F
155	DC	607	3PE	C25-C26-C27-C28
167	DS	403	UQ8	C28-C29-C31-C32
157	A8	401	ADP	PA-O3A-PB-O1B
157	AQ	201	ADP	PA-O3A-PB-O1B
150	ES	1101	CDL	CA5-C11-C12-C13
150	CD	301	CDL	C71-CB7-OB8-CB6
150	Dm	501	CDL	C71-CB7-OB8-CB6
150	Ds	402	CDL	C31-CA7-OA8-CA6
153	Dc	603	PC1	C32-C31-O31-C3
150	DJ	302	CDL	C37-C38-C39-C40
150	DV	402	CDL	C75-C76-C77-C78
150	Dg	201	CDL	C19-C20-C21-C22
153	DV	404	PC1	C3F-C3G-C3H-C3I
153	Dv	404	PC1	C2A-C2B-C2C-C2D
150	A0	601	CDL	C11-C12-C13-C14
150	DN	506	CDL	C36-C37-C38-C39
150	DO	501	CDL	C11-C12-C13-C14
150	DS	404	CDL	C16-C17-C18-C19
150	DU	401	CDL	C13-C14-C15-C16
150	DY	301	CDL	C56-C57-C58-C59
150	EO	202	CDL	C53-C54-C55-C56
150	Dj	403	CDL	C34-C35-C36-C37
150	Ds	402	CDL	C11-C12-C13-C14
153	DA	707	PC1	C29-C2A-C2B-C2C
153	DX	305	PC1	C24-C25-C26-C27
150	AC	802	CDL	CA6-CA4-OA6-CA5
150	CD	302	CDL	CA3-CA4-OA6-CA5
150	c	501	CDL	CB6-CB4-OB6-CB5
150	DJ	305	CDL	CB6-CB4-OB6-CB5
150	DN	503	CDL	CA6-CA4-OA6-CA5
150	DQ	1502	CDL	CB6-CB4-OB6-CB5
150	Dj	405	CDL	CB6-CB4-OB6-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dq	1403	CDL	CB6-CB4-OB6-CB5
150	Dx	1204	CDL	CB6-CB4-OB6-CB5
150	El	903	CDL	CA3-CA4-OA6-CA5
153	A	1201	PC1	C3-C2-O21-C21
153	k	301	PC1	C3-C2-O21-C21
153	Eo	204	PC1	C1-C2-O21-C21
155	BT	201	3PE	C1-C2-O21-C21
153	AU	202	PC1	O22-C21-O21-C2
150	DH	202	CDL	C44-C45-C46-C47
150	DR	402	CDL	C20-C21-C22-C23
150	EN	1202	CDL	C32-C33-C34-C35
150	Dj	401	CDL	C39-C40-C41-C42
153	C	510	PC1	C28-C29-C2A-C2B
153	DB	702	PC1	C2D-C2E-C2F-C2G
153	DB	702	PC1	C2E-C2F-C2G-C2H
153	Dg	203	PC1	C28-C29-C2A-C2B
153	Dv	405	PC1	C3B-C3C-C3D-C3E
153	El	904	PC1	C3B-C3C-C3D-C3E
150	BV	201	CDL	C17-C18-C19-C20
150	c	509	CDL	C41-C42-C43-C44
150	DD	705	CDL	C84-C85-C86-C87
150	DN	506	CDL	C43-C44-C45-C46
150	EI	401	CDL	C20-C21-C22-C23
150	EL	901	CDL	C42-C43-C44-C45
150	Dd	706	CDL	C20-C21-C22-C23
150	Dg	202	CDL	C14-C15-C16-C17
150	Dj	404	CDL	C53-C54-C55-C56
150	Dq	1402	CDL	C53-C54-C55-C56
153	Eo	204	PC1	C33-C34-C35-C36
150	EI	401	CDL	C1-CA2-OA2-PA1
156	Dn	504	LPP	C6-O5-P1-O3
156	Dl	1101	LPP	C6-O5-P1-O3
150	AA	908	CDL	C39-C40-C41-C42
150	B0	101	CDL	C15-C16-C17-C18
150	C	505	CDL	C38-C39-C40-C41
150	DN	506	CDL	C14-C15-C16-C17
150	Dn	502	CDL	C19-C20-C21-C22
150	Dv	403	CDL	C41-C42-C43-C44
150	Eb	302	CDL	C57-C58-C59-C60
153	B1	403	PC1	C2D-C2E-C2F-C2G
153	c	503	PC1	C3C-C3D-C3E-C3F
153	c	503	PC1	C3D-C3E-C3F-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dc	603	PC1	C35-C36-C37-C38
155	Ds	408	3PE	C3E-C3F-C3G-C3H
150	CG	302	CDL	C71-CB7-OB8-CB6
150	DD	703	CDL	C31-CA7-OA8-CA6
150	DJ	302	CDL	C31-CA7-OA8-CA6
150	DJ	303	CDL	C31-CA7-OA8-CA6
150	DV	402	CDL	C71-CB7-OB8-CB6
153	A	1201	PC1	C32-C31-O31-C3
155	DI	301	3PE	C32-C31-O31-C3
150	AA	901	CDL	OA5-CA3-CA4-OA6
150	AF	402	CDL	OA5-CA3-CA4-OA6
150	AM	301	CDL	OA5-CA3-CA4-OA6
150	B1	402	CDL	OB5-CB3-CB4-OB6
150	DC	601	CDL	OB5-CB3-CB4-OB6
150	DJ	307	CDL	OA5-CA3-CA4-OA6
150	DU	404	CDL	OB5-CB3-CB4-OB6
150	Dj	402	CDL	OB5-CB3-CB4-OB6
150	Dq	1401	CDL	OA5-CA3-CA4-OA6
150	Eb	302	CDL	OA5-CA3-CA4-OA6
150	Eb	302	CDL	OB5-CB3-CB4-OB6
153	A9	601	PC1	O11-C1-C2-O21
153	AA	903	PC1	O11-C1-C2-O21
153	AA	905	PC1	O11-C1-C2-O21
153	c	503	PC1	O11-C1-C2-O21
153	DB	702	PC1	O11-C1-C2-O21
153	DX	308	PC1	O11-C1-C2-O21
153	EN	1203	PC1	O11-C1-C2-O21
155	Ds	403	3PE	O11-C1-C2-O21
150	B1	402	CDL	C76-C77-C78-C79
150	BT	204	CDL	C44-C45-C46-C47
150	DS	401	CDL	C72-C73-C74-C75
150	ES	1101	CDL	C72-C73-C74-C75
150	Dd	705	CDL	C84-C85-C86-C87
150	Ds	405	CDL	C57-C58-C59-C60
150	Dv	401	CDL	C14-C15-C16-C17
153	DV	404	PC1	C2A-C2B-C2C-C2D
155	EN	1204	3PE	C3E-C3F-C3G-C3H
150	DM	502	CDL	C19-C20-C21-C22
150	Ds	406	CDL	C43-C44-C45-C46
153	DV	405	PC1	C2D-C2E-C2F-C2G
155	DC	607	3PE	C34-C35-C36-C37
150	El	901	CDL	O1-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DM	501	CDL	OB9-CB7-OB8-CB6
150	DN	507	CDL	OB9-CB7-OB8-CB6
150	Ed	205	CDL	OB9-CB7-OB8-CB6
153	AA	903	PC1	O32-C31-O31-C3
153	Eo	204	PC1	O32-C31-O31-C3
150	Dj	401	CDL	C17-C18-C19-C20
150	BV	201	CDL	CB5-C51-C52-C53
150	DU	402	CDL	CA5-C11-C12-C13
155	Di	1102	3PE	C35-C36-C37-C38
150	Ek	201	CDL	CA4-CA6-OA8-CA7
150	A0	601	CDL	OA6-CA4-CA6-OA8
150	A1	402	CDL	OA6-CA4-CA6-OA8
150	AM	301	CDL	OB6-CB4-CB6-OB8
150	BC	302	CDL	OB6-CB4-CB6-OB8
150	BG	201	CDL	OA6-CA4-CA6-OA8
150	c	509	CDL	OB6-CB4-CB6-OB8
150	DD	704	CDL	OA6-CA4-CA6-OA8
150	EN	1201	CDL	OA6-CA4-CA6-OA8
150	Dm	502	CDL	OA6-CA4-CA6-OA8
153	C	509	PC1	O21-C2-C3-O31
153	DA	708	PC1	O21-C2-C3-O31
153	DS	406	PC1	O21-C2-C3-O31
153	DX	308	PC1	O21-C2-C3-O31
155	EN	1204	3PE	O21-C2-C3-O31
150	DU	403	CDL	C12-C13-C14-C15
150	DY	301	CDL	C14-C15-C16-C17
150	DZ	501	CDL	C73-C74-C75-C76
150	Do	501	CDL	C11-C12-C13-C14
153	c	507	PC1	C39-C3A-C3B-C3C
153	DG	203	PC1	C28-C29-C2A-C2B
153	Dj	406	PC1	C37-C38-C39-C3A
150	BC	302	CDL	OA7-CA5-OA6-CA4
150	CJ	201	CDL	OB7-CB5-OB6-CB4
153	c	507	PC1	O22-C21-O21-C2
153	C	508	PC1	O32-C31-O31-C3
150	B1	402	CDL	C77-C78-C79-C80
150	C	503	CDL	C55-C56-C57-C58
150	C	506	CDL	C44-C45-C46-C47
150	H	1301	CDL	C38-C39-C40-C41
150	DV	403	CDL	C40-C41-C42-C43
150	Dh	201	CDL	C12-C13-C14-C15
150	Dn	501	CDL	C76-C77-C78-C79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	D	402	PC1	C3F-C3G-C3H-C3I
153	DG	203	PC1	C26-C27-C28-C29
153	Db	702	PC1	C2A-C2B-C2C-C2D
156	Dn	504	LPP	C35-C36-C37-C38
150	A0	602	CDL	C13-C14-C15-C16
150	A1	402	CDL	C84-C85-C86-C87
150	AP	301	CDL	C14-C15-C16-C17
150	B1	402	CDL	C11-C12-C13-C14
150	CG	302	CDL	C73-C74-C75-C76
150	C	504	CDL	C75-C76-C77-C78
150	DQ	1504	CDL	C53-C54-C55-C56
150	Dd	702	CDL	C23-C24-C25-C26
150	Ei	401	CDL	C20-C21-C22-C23
155	Dc	607	3PE	C25-C26-C27-C28
167	Ds	404	UQ8	C28-C29-C31-C32
150	CJ	201	CDL	C73-C74-C75-C76
150	DI	302	CDL	C79-C80-C81-C82
150	Dj	401	CDL	C35-C36-C37-C38
150	Dm	501	CDL	C81-C82-C83-C84
153	Db	702	PC1	C2E-C2F-C2G-C2H
155	DS	402	3PE	C2B-C2C-C2D-C2E
155	Di	1102	3PE	C39-C3A-C3B-C3C
150	AA	901	CDL	C81-C82-C83-C84
150	B0	101	CDL	C18-C19-C20-C21
150	BY	201	CDL	C76-C77-C78-C79
150	E	301	CDL	C14-C15-C16-C17
150	DI	302	CDL	C19-C20-C21-C22
150	DM	501	CDL	C82-C83-C84-C85
150	DV	402	CDL	C11-C12-C13-C14
150	EB	302	CDL	C55-C56-C57-C58
150	Dn	502	CDL	C36-C37-C38-C39
153	EO	205	PC1	C2E-C2F-C2G-C2H
153	Da	706	PC1	C29-C2A-C2B-C2C
153	Eb	301	PC1	C36-C37-C38-C39
150	c	509	CDL	C31-CA7-OA8-CA6
150	Dm	502	CDL	C31-CA7-OA8-CA6
150	El	901	CDL	C31-CA7-OA8-CA6
153	DS	406	PC1	C32-C31-O31-C3
153	Dv	405	PC1	C32-C31-O31-C3
155	Dx	1202	3PE	C32-C31-O31-C3
150	Dg	201	CDL	C56-C57-C58-C59
150	Dh	202	CDL	C44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	BT	203	PC1	C33-C34-C35-C36
153	DB	702	PC1	C2B-C2C-C2D-C2E
153	DC	604	PC1	C3F-C3G-C3H-C3I
150	B1	402	CDL	C55-C56-C57-C58
150	DM	501	CDL	C77-C78-C79-C80
150	Dc	608	CDL	C20-C21-C22-C23
150	Do	501	CDL	C12-C13-C14-C15
153	AH	301	PC1	C3C-C3D-C3E-C3F
153	DS	406	PC1	C3F-C3G-C3H-C3I
153	EO	204	PC1	C3B-C3C-C3D-C3E
153	Dc	605	PC1	C3F-C3G-C3H-C3I
150	BG	201	CDL	C11-C12-C13-C14
150	CJ	201	CDL	C17-C18-C19-C20
150	C	505	CDL	C72-C73-C74-C75
150	DJ	305	CDL	C22-C23-C24-C25
150	DU	403	CDL	C14-C15-C16-C17
150	Dc	601	CDL	C36-C37-C38-C39
153	EO	201	PC1	C2B-C2C-C2D-C2E
153	Dv	405	PC1	C3F-C3G-C3H-C3I
150	DD	706	CDL	CA4-CA6-OA8-CA7
150	DD	705	CDL	CA2-C1-CB2-OB2
150	Dy	301	CDL	CA2-C1-CB2-OB2
153	A6	303	PC1	O22-C21-O21-C2
150	CG	301	CDL	C11-CA5-OA6-CA4
150	DN	502	CDL	C51-CB5-OB6-CB4
150	DX	307	CDL	C11-CA5-OA6-CA4
155	Dx	1206	3PE	C22-C21-O21-C2
150	AF	402	CDL	C20-C21-C22-C23
150	c	501	CDL	C12-C13-C14-C15
150	DA	706	CDL	C15-C16-C17-C18
150	DJ	303	CDL	C84-C85-C86-C87
150	DR	402	CDL	C84-C85-C86-C87
150	DS	404	CDL	C76-C77-C78-C79
150	DV	402	CDL	C82-C83-C84-C85
150	Dr	402	CDL	C59-C60-C61-C62
150	Ep	701	CDL	C84-C85-C86-C87
155	Dd	703	3PE	C35-C36-C37-C38
150	AF	402	CDL	C31-CA7-OA8-CA6
150	DS	401	CDL	C31-CA7-OA8-CA6
150	DU	401	CDL	C31-CA7-OA8-CA6
150	ED	605	CDL	C31-CA7-OA8-CA6
150	Dj	402	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dy	301	CDL	C31-CA7-OA8-CA6
150	En	1201	CDL	C31-CA7-OA8-CA6
150	Eu	101	CDL	C71-CB7-OB8-CB6
150	DS	401	CDL	C11-C12-C13-C14
150	Dg	201	CDL	C12-C13-C14-C15
150	Dj	403	CDL	CA5-C11-C12-C13
150	Do	501	CDL	C20-C21-C22-C23
156	Dl	1101	LPP	C41-C42-C43-C44
169	DA	703	HEA	C4D-C3D-CAD-CBD
169	Da	703	HEA	C4D-C3D-CAD-CBD
150	Ds	402	CDL	OA9-CA7-OA8-CA6
150	DN	506	CDL	C20-C21-C22-C23
150	DR	402	CDL	C13-C14-C15-C16
150	DV	403	CDL	C41-C42-C43-C44
150	Ds	405	CDL	C42-C43-C44-C45
150	Dv	402	CDL	C82-C83-C84-C85
153	DX	308	PC1	C2B-C2C-C2D-C2E
150	Dd	706	CDL	CA4-CA6-OA8-CA7
150	A1	402	CDL	OA5-CA3-CA4-CA6
150	AA	901	CDL	OA5-CA3-CA4-CA6
150	BC	302	CDL	OB5-CB3-CB4-CB6
150	CG	301	CDL	OA5-CA3-CA4-CA6
150	CC	304	CDL	OA5-CA3-CA4-CA6
150	C	503	CDL	OB5-CB3-CB4-CB6
150	DQ	1502	CDL	OB5-CB3-CB4-CB6
150	DQ	1504	CDL	OA5-CA3-CA4-CA6
150	DQ	1504	CDL	OB5-CB3-CB4-CB6
150	DS	405	CDL	OB5-CB3-CB4-CB6
150	DU	401	CDL	OB5-CB3-CB4-CB6
150	DX	307	CDL	OB5-CB3-CB4-CB6
150	DZ	501	CDL	OB5-CB3-CB4-CB6
150	EA	301	CDL	OA5-CA3-CA4-CA6
150	EB	302	CDL	OA5-CA3-CA4-CA6
150	ED	604	CDL	OA5-CA3-CA4-CA6
150	EL	901	CDL	OB5-CB3-CB4-CB6
150	Di	1101	CDL	OB5-CB3-CB4-CB6
150	Di	1103	CDL	OB5-CB3-CB4-CB6
150	Dn	502	CDL	OA5-CA3-CA4-CA6
150	Dn	503	CDL	OB5-CB3-CB4-CB6
150	Ds	402	CDL	OB5-CB3-CB4-CB6
150	Du	401	CDL	OB5-CB3-CB4-CB6
150	Du	403	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dx	1204	CDL	OB5-CB3-CB4-CB6
150	Ea	501	CDL	OB5-CB3-CB4-CB6
150	Eb	302	CDL	OA5-CA3-CA4-CA6
150	El	901	CDL	OA5-CA3-CA4-CA6
153	A9	601	PC1	O11-C1-C2-C3
153	AA	903	PC1	O11-C1-C2-C3
153	DQ	1503	PC1	O11-C1-C2-C3
153	Dq	1404	PC1	O11-C1-C2-C3
153	Dx	1203	PC1	O11-C1-C2-C3
155	BP	201	3PE	O11-C1-C2-C3
155	Da	708	3PE	O11-C1-C2-C3
155	Dr	404	3PE	O11-C1-C2-C3
155	Dx	1207	3PE	O11-C1-C2-C3
150	DJ	304	CDL	C16-C17-C18-C19
150	Dn	502	CDL	C11-C12-C13-C14
150	Dr	402	CDL	C84-C85-C86-C87
150	Ds	402	CDL	C77-C78-C79-C80
153	Eo	204	PC1	C2A-C2B-C2C-C2D
150	c	509	CDL	CA5-C11-C12-C13
155	DN	501	3PE	O13-C11-C12-N
155	Dg	204	3PE	O13-C11-C12-N
150	Dh	201	CDL	C19-C20-C21-C22
150	C	504	CDL	C31-CA7-OA8-CA6
150	Dg	202	CDL	C71-CB7-OB8-CB6
150	Dv	401	CDL	C71-CB7-OB8-CB6
150	Dv	402	CDL	C71-CB7-OB8-CB6
153	Dc	603	PC1	O32-C31-O31-C3
150	DQ	1501	CDL	C12-C13-C14-C15
150	DU	403	CDL	C15-C16-C17-C18
167	C	511	UQ8	C25-C24-C26-C27
169	DA	702	HEA	C26-C15-C16-C17
169	Da	702	HEA	C26-C15-C16-C17
150	Dn	501	CDL	CB7-C71-C72-C73
150	C	506	CDL	C12-C13-C14-C15
150	c	506	CDL	C15-C16-C17-C18
150	EL	901	CDL	C44-C45-C46-C47
150	Du	401	CDL	C71-C72-C73-C74
150	BC	301	CDL	O1-C1-CB2-OB2
150	Dx	1201	CDL	OA7-CA5-OA6-CA4
153	DS	406	PC1	O22-C21-O21-C2
150	DQ	1501	CDL	OB9-CB7-OB8-CB6
150	Dh	202	CDL	C51-C52-C53-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DI	301	3PE	C39-C3A-C3B-C3C
164	CA	702	FAD	C2'-C3'-C4'-O4'
150	DH	202	CDL	C53-C54-C55-C56
150	EB	302	CDL	C12-C13-C14-C15
150	Dd	702	CDL	C20-C21-C22-C23
150	Dj	407	CDL	C77-C78-C79-C80
150	Ds	405	CDL	C12-C13-C14-C15
153	CC	302	PC1	C35-C36-C37-C38
150	CD	301	CDL	C11-CA5-OA6-CA4
150	AF	401	CDL	C31-CA7-OA8-CA6
150	DU	403	CDL	C31-CA7-OA8-CA6
150	Ed	205	CDL	C31-CA7-OA8-CA6
153	AM	302	PC1	C32-C31-O31-C3
153	DY	302	PC1	C32-C31-O31-C3
153	Db	702	PC1	C32-C31-O31-C3
153	DC	604	PC1	O21-C21-C22-C23
150	Dd	704	CDL	CA5-C11-C12-C13
150	C	504	CDL	C24-C25-C26-C27
150	Dm	501	CDL	C58-C59-C60-C61
153	EO	205	PC1	C2B-C2C-C2D-C2E
155	Ds	403	3PE	C2B-C2C-C2D-C2E
150	A0	602	CDL	C1-CA2-OA2-PA1
150	A1	402	CDL	CB4-CB3-OB5-PB2
150	AF	401	CDL	C1-CB2-OB2-PB2
150	B0	102	CDL	CA4-CA3-OA5-PA1
150	CG	301	CDL	C1-CB2-OB2-PB2
150	C	507	CDL	C1-CA2-OA2-PA1
150	DD	704	CDL	CB4-CB3-OB5-PB2
150	DS	405	CDL	C1-CA2-OA2-PA1
150	DU	404	CDL	C1-CB2-OB2-PB2
150	ED	604	CDL	CA4-CA3-OA5-PA1
150	EI	401	CDL	CB4-CB3-OB5-PB2
150	EO	202	CDL	CA4-CA3-OA5-PA1
150	Dh	202	CDL	C1-CB2-OB2-PB2
150	Di	1101	CDL	CA4-CA3-OA5-PA1
150	Eg	101	CDL	C1-CA2-OA2-PA1
150	Eu	101	CDL	CA4-CA3-OA5-PA1
153	A	1201	PC1	C2-C1-O11-P
153	DA	707	PC1	C2-C1-O11-P
155	BA	301	3PE	C2-C1-O11-P
150	CC	304	CDL	C40-C41-C42-C43
150	DM	502	CDL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DM	502	CDL	C52-C53-C54-C55
150	DN	503	CDL	C14-C15-C16-C17
150	DS	401	CDL	C22-C23-C24-C25
153	BS	1301	PC1	C3E-C3F-C3G-C3H
150	B0	101	CDL	C31-C32-C33-C34
150	DD	704	CDL	C60-C61-C62-C63
150	DS	404	CDL	C42-C43-C44-C45
150	DV	403	CDL	C31-C32-C33-C34
150	EL	903	CDL	C61-C62-C63-C64
150	Di	1103	CDL	C19-C20-C21-C22
150	Dn	506	CDL	C11-C12-C13-C14
150	Dx	1204	CDL	C64-C65-C66-C67
153	BG	202	PC1	C23-C24-C25-C26
156	EI	402	LPP	C18-C19-C20-C21
150	El	901	CDL	CB5-C51-C52-C53
150	Dm	501	CDL	OB9-CB7-OB8-CB6
150	CG	301	CDL	C71-C72-C73-C74
150	DH	201	CDL	C63-C64-C65-C66
150	AA	908	CDL	C31-CA7-OA8-CA6
150	DD	705	CDL	C31-CA7-OA8-CA6
150	DU	401	CDL	C71-CB7-OB8-CB6
150	EL	901	CDL	C31-CA7-OA8-CA6
150	Dm	501	CDL	C31-CA7-OA8-CA6
153	B1	401	PC1	C32-C31-O31-C3
153	DC	603	PC1	C32-C31-O31-C3
150	DH	201	CDL	C21-C22-C23-C24
150	Dr	402	CDL	C75-C76-C77-C78
150	Ep	701	CDL	C60-C61-C62-C63
150	AA	908	CDL	CA3-CA4-CA6-OA8
150	BE	201	CDL	CB3-CB4-CB6-OB8
150	BV	201	CDL	CA3-CA4-CA6-OA8
150	CD	301	CDL	CB3-CB4-CB6-OB8
150	C	504	CDL	CB3-CB4-CB6-OB8
150	C	505	CDL	CA3-CA4-CA6-OA8
150	c	506	CDL	CA3-CA4-CA6-OA8
150	g	801	CDL	CB3-CB4-CB6-OB8
150	h	501	CDL	CA3-CA4-CA6-OA8
150	DA	706	CDL	CA3-CA4-CA6-OA8
150	DA	706	CDL	CB3-CB4-CB6-OB8
150	DA	709	CDL	CA3-CA4-CA6-OA8
150	DD	705	CDL	CA3-CA4-CA6-OA8
150	DH	201	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DJ	304	CDL	CB3-CB4-CB6-OB8
150	DJ	307	CDL	CA3-CA4-CA6-OA8
150	DR	403	CDL	CB3-CB4-CB6-OB8
150	ED	605	CDL	CA3-CA4-CA6-OA8
150	Da	709	CDL	CA3-CA4-CA6-OA8
150	Dc	601	CDL	CA3-CA4-CA6-OA8
150	Dg	201	CDL	CA3-CA4-CA6-OA8
150	Dg	202	CDL	CB3-CB4-CB6-OB8
150	Di	1101	CDL	CB3-CB4-CB6-OB8
150	Dj	407	CDL	CA3-CA4-CA6-OA8
150	Dr	402	CDL	CA3-CA4-CA6-OA8
150	Ed	205	CDL	CA3-CA4-CA6-OA8
153	A6	302	PC1	C1-C2-C3-O31
153	AA	906	PC1	C1-C2-C3-O31
153	AA	907	PC1	C1-C2-C3-O31
153	B1	401	PC1	C1-C2-C3-O31
153	BS	1301	PC1	C1-C2-C3-O31
153	CC	302	PC1	C1-C2-C3-O31
153	C	510	PC1	C1-C2-C3-O31
153	DA	707	PC1	C1-C2-C3-O31
153	DS	406	PC1	C1-C2-C3-O31
153	DV	404	PC1	C1-C2-C3-O31
153	DV	406	PC1	C1-C2-C3-O31
153	Da	706	PC1	C1-C2-C3-O31
153	Dc	609	PC1	C1-C2-C3-O31
155	BA	301	3PE	C1-C2-C3-O31
155	CC	301	3PE	C1-C2-C3-O31
155	DN	501	3PE	C1-C2-C3-O31
155	EL	904	3PE	C1-C2-C3-O31
155	Da	708	3PE	C1-C2-C3-O31
155	El	905	3PE	C1-C2-C3-O31
155	Em	901	3PE	C1-C2-C3-O31
156	AC	803	LPP	C6-C7-C8-O27
150	B1	402	CDL	OB7-CB5-OB6-CB4
155	DJ	301	3PE	O22-C21-O21-C2
150	DD	705	CDL	C40-C41-C42-C43
150	Ea	502	CDL	C11-C12-C13-C14
153	DC	608	PC1	C3C-C3D-C3E-C3F
153	Dg	203	PC1	C26-C27-C28-C29
150	DY	301	CDL	CA5-C11-C12-C13
150	CG	302	CDL	OB9-CB7-OB8-CB6
150	DV	402	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	B0	102	CDL	C15-C16-C17-C18
150	C	505	CDL	C76-C77-C78-C79
150	Da	709	CDL	C39-C40-C41-C42
150	Dg	201	CDL	C72-C73-C74-C75
153	Dc	603	PC1	C3D-C3E-C3F-C3G
155	DI	301	3PE	C38-C39-C3A-C3B
155	Dc	607	3PE	C2F-C2G-C2H-C2I
150	Dj	403	CDL	C11-C12-C13-C14
153	DB	702	PC1	C38-C39-C3A-C3B
153	DC	603	PC1	C2C-C2D-C2E-C2F
150	CD	301	CDL	OB9-CB7-OB8-CB6
167	ED	603	UQ8	C40-C39-C41-C42
169	DA	702	HEA	C14-C15-C16-C17
150	DJ	304	CDL	C59-C60-C61-C62
150	ES	1101	CDL	C58-C59-C60-C61
153	AQ	202	PC1	C28-C29-C2A-C2B
150	Dd	702	CDL	C14-C15-C16-C17
150	Dd	706	CDL	C77-C78-C79-C80
150	Dj	402	CDL	C51-C52-C53-C54
153	Eo	205	PC1	C3B-C3C-C3D-C3E
150	AF	402	CDL	CA2-OA2-PA1-OA5
150	B0	101	CDL	CA3-OA5-PA1-OA2
150	B0	101	CDL	CB3-OB5-PB2-OB2
150	BE	201	CDL	CA3-OA5-PA1-OA2
150	BT	204	CDL	CA2-OA2-PA1-OA5
150	BY	201	CDL	CA3-OA5-PA1-OA2
150	c	506	CDL	CA3-OA5-PA1-OA2
150	DX	306	CDL	CA3-OA5-PA1-OA2
150	Dd	705	CDL	CA3-OA5-PA1-OA2
150	Di	1103	CDL	CB2-OB2-PB2-OB5
150	Dj	402	CDL	CA2-OA2-PA1-OA5
150	Du	402	CDL	CB2-OB2-PB2-OB5
150	Ed	205	CDL	CB3-OB5-PB2-OB2
153	A6	303	PC1	C11-O13-P-O11
153	A9	603	PC1	C1-O11-P-O13
153	d	801	PC1	C11-O13-P-O11
153	g	802	PC1	C1-O11-P-O13
153	EB	303	PC1	C1-O11-P-O13
155	BP	201	3PE	C1-O11-P-O13
155	G	401	3PE	C1-O11-P-O13
155	DG	205	3PE	C1-O11-P-O13
150	DG	201	CDL	CA5-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DD	703	CDL	OA9-CA7-OA8-CA6
153	A	1201	PC1	O32-C31-O31-C3
150	AP	301	CDL	C12-C13-C14-C15
150	El	903	CDL	C79-C80-C81-C82
153	DS	406	PC1	C32-C33-C34-C35
155	DC	606	3PE	C2A-C2B-C2C-C2D
150	C	503	CDL	C37-C38-C39-C40
150	c	501	CDL	C79-C80-C81-C82
150	DU	401	CDL	C20-C21-C22-C23
150	Dq	1401	CDL	C34-C35-C36-C37
150	Ep	701	CDL	C44-C45-C46-C47
150	BC	302	CDL	OA5-CA3-CA4-OA6
150	CD	301	CDL	OA5-CA3-CA4-OA6
150	C	505	CDL	OB5-CB3-CB4-OB6
150	c	506	CDL	OA5-CA3-CA4-OA6
150	DA	706	CDL	OB5-CB3-CB4-OB6
150	DD	703	CDL	OA5-CA3-CA4-OA6
150	DG	202	CDL	OB5-CB3-CB4-OB6
150	DU	401	CDL	OA5-CA3-CA4-OA6
150	EA	301	CDL	OA5-CA3-CA4-OA6
150	ED	601	CDL	OB5-CB3-CB4-OB6
150	Dc	601	CDL	OB5-CB3-CB4-OB6
150	Dd	705	CDL	OA5-CA3-CA4-OA6
150	Dj	407	CDL	OB5-CB3-CB4-OB6
150	Dm	501	CDL	OA5-CA3-CA4-OA6
150	Dn	502	CDL	OA5-CA3-CA4-OA6
150	Dq	1401	CDL	OB5-CB3-CB4-OB6
150	Ds	406	CDL	OB5-CB3-CB4-OB6
150	Dy	301	CDL	OA5-CA3-CA4-OA6
150	Ep	701	CDL	OA5-CA3-CA4-OA6
153	A6	302	PC1	O11-C1-C2-O21
153	A9	603	PC1	O11-C1-C2-O21
153	AA	907	PC1	O11-C1-C2-O21
153	BG	202	PC1	O11-C1-C2-O21
153	D	402	PC1	O11-C1-C2-O21
153	DI	303	PC1	O11-C1-C2-O21
153	Eo	201	PC1	O11-C1-C2-O21
155	DX	302	3PE	O11-C1-C2-O21
155	Dc	607	3PE	O22-C21-O21-C2
155	Dd	703	3PE	C32-C31-O31-C3
150	Di	1103	CDL	C55-C56-C57-C58
161	AS	200	8Q1	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DJ	302	CDL	OA9-CA7-OA8-CA6
150	DJ	303	CDL	OA9-CA7-OA8-CA6
155	DI	301	3PE	O32-C31-O31-C3
150	DV	401	CDL	CB5-C51-C52-C53
150	EL	903	CDL	CA7-C31-C32-C33
150	C	506	CDL	C24-C25-C26-C27
150	Dq	1401	CDL	C35-C36-C37-C38
153	Dx	1205	PC1	C3D-C3E-C3F-C3G
150	BV	201	CDL	C72-C71-CB7-OB8
150	CD	301	CDL	C32-C31-CA7-OA8
153	Dv	406	PC1	O31-C31-C32-C33
150	DD	706	CDL	C44-C45-C46-C47
150	Dn	506	CDL	C84-C85-C86-C87
153	DA	707	PC1	C37-C38-C39-C3A
153	DC	603	PC1	C3D-C3E-C3F-C3G
155	Dx	1206	3PE	C2F-C2G-C2H-C2I
150	c	509	CDL	OA9-CA7-OA8-CA6
150	El	901	CDL	OA9-CA7-OA8-CA6
150	AM	301	CDL	C37-C38-C39-C40
150	CG	302	CDL	C14-C15-C16-C17
150	C	505	CDL	C19-C20-C21-C22
150	DD	704	CDL	C11-C12-C13-C14
153	C	509	PC1	C3E-C3F-C3G-C3H
167	Ed	202	UQ8	C2-C3-O3-C3M
150	Dr	402	CDL	CB7-C71-C72-C73
150	DU	404	CDL	C13-C14-C15-C16
150	AF	401	CDL	OA6-CA4-CA6-OA8
150	BE	201	CDL	OB6-CB4-CB6-OB8
150	BT	204	CDL	OB6-CB4-CB6-OB8
150	BV	201	CDL	OB6-CB4-CB6-OB8
150	BY	201	CDL	OA6-CA4-CA6-OA8
150	CD	301	CDL	OB6-CB4-CB6-OB8
150	DJ	303	CDL	OA6-CA4-CA6-OA8
150	DM	501	CDL	OA6-CA4-CA6-OA8
150	DS	401	CDL	OA6-CA4-CA6-OA8
150	DU	401	CDL	OA6-CA4-CA6-OA8
150	DX	307	CDL	OA6-CA4-CA6-OA8
150	ED	604	CDL	OA6-CA4-CA6-OA8
150	EI	401	CDL	OA6-CA4-CA6-OA8
150	EL	902	CDL	OA6-CA4-CA6-OA8
150	EL	902	CDL	OB6-CB4-CB6-OB8
150	Dc	608	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dd	702	CDL	OB6-CB4-CB6-OB8
150	Dd	704	CDL	OA6-CA4-CA6-OA8
150	Dg	202	CDL	OB6-CB4-CB6-OB8
150	Di	1103	CDL	OA6-CA4-CA6-OA8
150	Dj	401	CDL	OA6-CA4-CA6-OA8
150	Dn	501	CDL	OA6-CA4-CA6-OA8
150	Ds	402	CDL	OA6-CA4-CA6-OA8
150	Dy	301	CDL	OA6-CA4-CA6-OA8
150	Eh	1601	CDL	OB6-CB4-CB6-OB8
150	Ei	401	CDL	OA6-CA4-CA6-OA8
150	El	902	CDL	OA6-CA4-CA6-OA8
153	A2	402	PC1	O21-C2-C3-O31
153	A6	302	PC1	O21-C2-C3-O31
153	AA	903	PC1	O21-C2-C3-O31
153	BS	1301	PC1	O21-C2-C3-O31
153	C	508	PC1	O21-C2-C3-O31
153	K	501	PC1	O21-C2-C3-O31
153	d	801	PC1	O21-C2-C3-O31
153	EO	206	PC1	O21-C2-C3-O31
153	Dy	302	PC1	O21-C2-C3-O31
155	BA	301	3PE	O21-C2-C3-O31
155	CC	301	3PE	O21-C2-C3-O31
155	DC	607	3PE	O21-C2-C3-O31
155	DX	304	3PE	O21-C2-C3-O31
155	Dc	607	3PE	O21-C2-C3-O31
155	Dr	401	3PE	O21-C2-C3-O31
155	Em	901	3PE	O21-C2-C3-O31
150	AC	801	CDL	C71-CB7-OB8-CB6
153	A0	605	PC1	C32-C31-O31-C3
153	Dy	302	PC1	C32-C31-O31-C3
153	c	507	PC1	O21-C21-C22-C23
150	DN	503	CDL	C11-C12-C13-C14
150	DU	402	CDL	C60-C61-C62-C63
150	Di	1101	CDL	C77-C78-C79-C80
150	Eb	302	CDL	C37-C38-C39-C40
150	Dc	608	CDL	C51-CB5-OB6-CB4
150	Eu	101	CDL	C51-CB5-OB6-CB4
153	d	801	PC1	C22-C21-O21-C2
150	Dm	501	CDL	C76-C77-C78-C79
153	DC	602	PC1	C3F-C3G-C3H-C3I
150	DD	703	CDL	CB2-C1-CA2-OA2
150	Ds	405	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dv	401	CDL	CA2-C1-CB2-OB2
150	Ed	204	CDL	CA2-C1-CB2-OB2
150	El	901	CDL	CA2-C1-CB2-OB2
167	ED	603	UQ8	C24-C26-C27-C28
150	AC	801	CDL	C39-C40-C41-C42
150	DR	403	CDL	C37-C38-C39-C40
150	DS	405	CDL	C14-C15-C16-C17
150	El	901	CDL	C36-C37-C38-C39
150	AF	401	CDL	OA7-CA5-OA6-CA4
150	CG	301	CDL	OA7-CA5-OA6-CA4
150	CC	305	CDL	OA7-CA5-OA6-CA4
150	C	504	CDL	OB7-CB5-OB6-CB4
150	DN	502	CDL	OB7-CB5-OB6-CB4
150	DU	402	CDL	OB7-CB5-OB6-CB4
150	DX	306	CDL	OB7-CB5-OB6-CB4
150	DX	307	CDL	OA7-CA5-OA6-CA4
150	Dx	1204	CDL	OA7-CA5-OA6-CA4
153	AA	906	PC1	O22-C21-O21-C2
155	Dx	1206	3PE	O22-C21-O21-C2
167	EN	1205	UQ8	C40-C39-C41-C42
167	ED	603	UQ8	C38-C39-C41-C42
169	Da	702	HEA	C14-C15-C16-C17
150	DA	706	CDL	C75-C76-C77-C78
150	DA	706	CDL	C77-C78-C79-C80
150	EL	902	CDL	C52-C53-C54-C55
150	EL	903	CDL	C43-C44-C45-C46
150	Dg	202	CDL	C80-C81-C82-C83
150	Ds	402	CDL	C80-C81-C82-C83
150	El	903	CDL	C23-C24-C25-C26
153	Dc	603	PC1	C2C-C2D-C2E-C2F
153	Dg	203	PC1	O31-C31-C32-C33
150	DQ	1501	CDL	CB5-C51-C52-C53
150	DA	706	CDL	C55-C56-C57-C58
150	DG	201	CDL	C17-C18-C19-C20
150	EN	1201	CDL	C40-C41-C42-C43
150	Ea	501	CDL	C44-C45-C46-C47
153	Eo	205	PC1	C29-C2A-C2B-C2C
150	DG	202	CDL	C72-C73-C74-C75
150	Eh	1601	CDL	C73-C74-C75-C76
153	AA	905	PC1	C3B-C3C-C3D-C3E
153	Db	702	PC1	C38-C39-C3A-C3B
150	AA	901	CDL	CA4-CA3-OA5-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AC	802	CDL	CB4-CB3-OB5-PB2
150	AP	301	CDL	C1-CA2-OA2-PA1
150	AP	301	CDL	CB4-CB3-OB5-PB2
150	BG	201	CDL	C1-CB2-OB2-PB2
150	BL	301	CDL	CA4-CA3-OA5-PA1
150	C	506	CDL	C1-CB2-OB2-PB2
150	c	501	CDL	CB4-CB3-OB5-PB2
150	c	502	CDL	C1-CA2-OA2-PA1
150	DA	706	CDL	CB4-CB3-OB5-PB2
150	DN	503	CDL	CA4-CA3-OA5-PA1
150	DN	507	CDL	CA4-CA3-OA5-PA1
150	DR	402	CDL	CA4-CA3-OA5-PA1
150	DV	402	CDL	C1-CA2-OA2-PA1
150	DX	307	CDL	C1-CB2-OB2-PB2
150	DZ	501	CDL	C1-CB2-OB2-PB2
150	EA	301	CDL	CA4-CA3-OA5-PA1
150	EN	1202	CDL	C1-CA2-OA2-PA1
150	Dj	403	CDL	CA4-CA3-OA5-PA1
150	Dj	404	CDL	C1-CB2-OB2-PB2
150	Dj	404	CDL	CB4-CB3-OB5-PB2
150	Dn	502	CDL	C1-CB2-OB2-PB2
150	Dn	506	CDL	C1-CB2-OB2-PB2
150	Du	402	CDL	C1-CA2-OA2-PA1
150	Du	403	CDL	C1-CA2-OA2-PA1
150	Dv	401	CDL	C1-CA2-OA2-PA1
150	Dv	402	CDL	C1-CB2-OB2-PB2
150	Dx	1204	CDL	CA4-CA3-OA5-PA1
150	Ea	502	CDL	CA4-CA3-OA5-PA1
150	Ed	204	CDL	C1-CA2-OA2-PA1
150	Eh	1601	CDL	C1-CA2-OA2-PA1
150	Ek	201	CDL	C1-CA2-OA2-PA1
150	El	902	CDL	CA4-CA3-OA5-PA1
153	AC	804	PC1	C2-C1-O11-P
153	C	508	PC1	C2-C1-O11-P
153	C	509	PC1	C2-C1-O11-P
153	Db	702	PC1	C2-C1-O11-P
155	DG	204	3PE	C2-C1-O11-P
155	Dc	607	3PE	C2-C1-O11-P
150	Dm	502	CDL	OA9-CA7-OA8-CA6
153	DS	406	PC1	O32-C31-O31-C3
153	Dv	405	PC1	O32-C31-O31-C3
155	Dx	1202	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AC	802	CDL	C38-C39-C40-C41
150	B1	402	CDL	C32-C33-C34-C35
150	CD	301	CDL	C37-C38-C39-C40
150	DG	202	CDL	C34-C35-C36-C37
150	DS	404	CDL	C11-C12-C13-C14
150	DU	404	CDL	C17-C18-C19-C20
150	Ds	405	CDL	C11-C12-C13-C14
153	AA	904	PC1	C11-C12-N-C13
153	EO	205	PC1	C11-C12-N-C13
153	Di	1104	PC1	C11-C12-N-C14
150	Dx	1204	CDL	CA7-C31-C32-C33
150	g	801	CDL	C13-C14-C15-C16
150	DG	202	CDL	C35-C36-C37-C38
150	Dd	705	CDL	C44-C45-C46-C47
150	Di	1103	CDL	C33-C34-C35-C36
150	Dr	402	CDL	C34-C35-C36-C37
153	BT	203	PC1	C3B-C3C-C3D-C3E
155	DR	401	3PE	C35-C36-C37-C38
156	EI	402	LPP	C38-C39-C40-C41
150	BE	201	CDL	C42-C43-C44-C45
150	DN	507	CDL	C38-C39-C40-C41
150	EL	903	CDL	C84-C85-C86-C87
150	Dh	201	CDL	C31-CA7-OA8-CA6
150	EL	901	CDL	C11-C12-C13-C14
153	Da	706	PC1	C37-C38-C39-C3A
168	C	502	HEM	C3D-CAD-CBD-CGD
150	CD	301	CDL	OA7-CA5-OA6-CA4
150	Dn	502	CDL	OA7-CA5-OA6-CA4
150	Eu	101	CDL	OB7-CB5-OB6-CB4
150	CC	305	CDL	C11-CA5-OA6-CA4
150	DS	405	CDL	C11-CA5-OA6-CA4
150	DZ	501	CDL	C11-CA5-OA6-CA4
150	Dn	502	CDL	C11-CA5-OA6-CA4
153	C	510	PC1	C22-C21-O21-C2
155	EL	904	3PE	C22-C21-O21-C2
150	BY	201	CDL	C11-C12-C13-C14
150	EL	901	CDL	C12-C13-C14-C15
150	Da	709	CDL	C40-C41-C42-C43
150	Dj	403	CDL	C79-C80-C81-C82
153	DA	708	PC1	C3E-C3F-C3G-C3H
150	A0	602	CDL	C14-C15-C16-C17
150	DN	502	CDL	C76-C77-C78-C79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dd	704	CDL	C23-C24-C25-C26
150	Dd	706	CDL	C44-C45-C46-C47
150	Dj	403	CDL	C63-C64-C65-C66
150	DG	201	CDL	C24-C25-C26-C27
150	DU	402	CDL	C20-C21-C22-C23
150	Dh	201	CDL	C21-C22-C23-C24
164	CA	702	FAD	P-O3P-PA-O5B
150	AF	401	CDL	C64-C65-C66-C67
150	DG	202	CDL	C63-C64-C65-C66
150	DI	302	CDL	C33-C34-C35-C36
150	Eb	302	CDL	C12-C13-C14-C15
153	Dc	602	PC1	C3D-C3E-C3F-C3G
156	Dl	1101	LPP	C39-C40-C41-C42
150	DS	401	CDL	OA9-CA7-OA8-CA6
150	ED	605	CDL	OA9-CA7-OA8-CA6
153	Dc	602	PC1	C3F-C3G-C3H-C3I
156	Dl	1101	LPP	C18-C19-C20-C21
150	AC	801	CDL	OA5-CA3-CA4-CA6
150	B0	101	CDL	OA5-CA3-CA4-CA6
150	BC	302	CDL	OA5-CA3-CA4-CA6
150	BL	301	CDL	OB5-CB3-CB4-CB6
150	BY	201	CDL	OA5-CA3-CA4-CA6
150	CG	302	CDL	OB5-CB3-CB4-CB6
150	CD	302	CDL	OB5-CB3-CB4-CB6
150	E	301	CDL	OB5-CB3-CB4-CB6
150	DS	401	CDL	OB5-CB3-CB4-CB6
150	DZ	501	CDL	OA5-CA3-CA4-CA6
150	EB	302	CDL	OB5-CB3-CB4-CB6
150	Dj	403	CDL	OB5-CB3-CB4-CB6
150	Dm	501	CDL	OA5-CA3-CA4-CA6
150	Dv	403	CDL	OB5-CB3-CB4-CB6
150	Ep	701	CDL	OA5-CA3-CA4-CA6
150	Eu	101	CDL	OA5-CA3-CA4-CA6
153	A6	302	PC1	O11-C1-C2-C3
153	AA	904	PC1	O11-C1-C2-C3
153	AA	907	PC1	O11-C1-C2-C3
153	AL	303	PC1	O11-C1-C2-C3
153	BG	202	PC1	O11-C1-C2-C3
153	K	501	PC1	O11-C1-C2-C3
153	DB	702	PC1	O11-C1-C2-C3
153	DI	303	PC1	O11-C1-C2-C3
153	Dg	203	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DS	402	3PE	O11-C1-C2-C3
156	AC	803	LPP	O5-C6-C7-C8
150	Ed	205	CDL	O1-C1-CA2-OA2
150	BC	302	CDL	C11-C12-C13-C14
150	c	502	CDL	C34-C35-C36-C37
150	DN	506	CDL	C11-C12-C13-C14
150	DU	403	CDL	C44-C45-C46-C47
150	Ds	402	CDL	C78-C79-C80-C81
150	Ep	701	CDL	C80-C81-C82-C83
153	k	301	PC1	C2C-C2D-C2E-C2F
150	DU	401	CDL	OA9-CA7-OA8-CA6
150	Dj	402	CDL	OB9-CB7-OB8-CB6
150	A0	602	CDL	C37-C38-C39-C40
150	BT	202	CDL	C37-C38-C39-C40
150	DG	201	CDL	C42-C43-C44-C45
150	DJ	304	CDL	C13-C14-C15-C16
150	DQ	1502	CDL	C12-C13-C14-C15
155	Di	1102	3PE	C38-C39-C3A-C3B
156	Dn	505	LPP	C35-C36-C37-C38
150	DU	403	CDL	C84-C85-C86-C87
150	Di	1103	CDL	C16-C17-C18-C19
150	Dj	402	CDL	C57-C58-C59-C60
155	DS	402	3PE	C27-C28-C29-C2A
150	Dc	608	CDL	OB7-CB5-OB6-CB4
150	C	506	CDL	CB7-C71-C72-C73
150	EL	902	CDL	CA5-C11-C12-C13
150	BG	201	CDL	C31-CA7-OA8-CA6
150	AA	908	CDL	C40-C41-C42-C43
150	c	501	CDL	C60-C61-C62-C63
150	DR	402	CDL	C42-C43-C44-C45
150	AA	901	CDL	C32-C31-CA7-OA8
150	BC	302	CDL	C32-C31-CA7-OA8
150	Dg	202	CDL	OB9-CB7-OB8-CB6
150	Dy	301	CDL	OA9-CA7-OA8-CA6
155	CD	303	3PE	C2C-C2D-C2E-C2F
155	Di	1102	3PE	C34-C35-C36-C37
150	Ds	406	CDL	C11-CA5-OA6-CA4
150	DI	302	CDL	C16-C17-C18-C19
156	AC	803	LPP	C6-O5-P1-O2
156	AC	803	LPP	C6-O5-P1-O4
150	Dd	704	CDL	C74-C75-C76-C77
150	Dn	503	CDL	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	DS	406	PC1	C29-C2A-C2B-C2C
153	Db	702	PC1	C3E-C3F-C3G-C3H
153	DI	303	PC1	C11-C12-N-C13
150	CC	305	CDL	C71-CB7-OB8-CB6
150	DU	403	CDL	C71-CB7-OB8-CB6
153	AX	401	PC1	C32-C31-O31-C3
153	EO	205	PC1	C32-C31-O31-C3
150	DN	506	CDL	C16-C17-C18-C19
150	DO	501	CDL	C77-C78-C79-C80
150	EL	902	CDL	C13-C14-C15-C16
150	AC	801	CDL	C37-C38-C39-C40
150	CG	301	CDL	C32-C33-C34-C35
150	DN	507	CDL	C73-C74-C75-C76
150	ED	601	CDL	C20-C21-C22-C23
150	Dh	202	CDL	C53-C54-C55-C56
153	e	1101	PC1	C3C-C3D-C3E-C3F
150	A1	402	CDL	C20-C21-C22-C23
150	c	501	CDL	C84-C85-C86-C87
150	Eh	1601	CDL	C40-C41-C42-C43
153	EO	205	PC1	C2A-C2B-C2C-C2D
150	AP	301	CDL	CA3-CA4-OA6-CA5
150	DC	601	CDL	CB6-CB4-OB6-CB5
150	DG	201	CDL	CB3-CB4-OB6-CB5
150	DJ	304	CDL	CB3-CB4-OB6-CB5
150	DN	502	CDL	CB6-CB4-OB6-CB5
150	DO	501	CDL	CB6-CB4-OB6-CB5
150	DZ	501	CDL	CB6-CB4-OB6-CB5
150	EA	301	CDL	CA6-CA4-OA6-CA5
150	EB	302	CDL	CA6-CA4-OA6-CA5
150	Dg	201	CDL	CB3-CB4-OB6-CB5
150	Dj	404	CDL	CB3-CB4-OB6-CB5
150	Dn	501	CDL	CB6-CB4-OB6-CB5
150	Dn	502	CDL	CA6-CA4-OA6-CA5
150	Du	403	CDL	CA3-CA4-OA6-CA5
153	AA	906	PC1	C3-C2-O21-C21
153	CC	302	PC1	C1-C2-O21-C21
153	DS	406	PC1	C1-C2-O21-C21
155	Dx	1202	3PE	C1-C2-O21-C21
155	Eo	203	3PE	C3-C2-O21-C21
150	DZ	501	CDL	OA7-CA5-OA6-CA4
150	AF	402	CDL	C78-C79-C80-C81
150	DS	405	CDL	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DU	401	CDL	C32-C33-C34-C35
150	El	901	CDL	C32-C33-C34-C35
150	BL	301	CDL	C20-C21-C22-C23
150	DG	201	CDL	C44-C45-C46-C47
150	EN	1201	CDL	C14-C15-C16-C17
150	Dh	202	CDL	C34-C35-C36-C37
153	k	301	PC1	C37-C38-C39-C3A
155	A9	602	3PE	C2F-C2G-C2H-C2I
150	En	1201	CDL	OA9-CA7-OA8-CA6
150	CD	302	CDL	C71-CB7-OB8-CB6
150	DD	703	CDL	C71-CB7-OB8-CB6
153	DC	605	PC1	C32-C31-O31-C3
167	ED	603	UQ8	C35-C34-C36-C37
150	Dg	201	CDL	C75-C76-C77-C78
167	EN	1205	UQ8	C38-C39-C41-C42
150	AC	802	CDL	C44-C45-C46-C47
150	DM	501	CDL	C40-C41-C42-C43
150	DX	307	CDL	C42-C43-C44-C45
155	Da	708	3PE	C3A-C3B-C3C-C3D
155	Dc	607	3PE	C3B-C3C-C3D-C3E
150	CJ	201	CDL	CB5-C51-C52-C53
150	DI	302	CDL	CA7-C31-C32-C33
150	AC	802	CDL	CA3-CA4-CA6-OA8
150	AF	401	CDL	CB4-CB3-OB5-PB2
150	AF	402	CDL	CB3-CB4-CB6-OB8
150	CC	304	CDL	CB3-CB4-CB6-OB8
150	CD	302	CDL	CA3-CA4-CA6-OA8
150	h	501	CDL	CB3-CB4-CB6-OB8
150	DA	706	CDL	CA4-CA3-OA5-PA1
150	DC	601	CDL	CA3-CA4-CA6-OA8
150	DG	201	CDL	C1-CB2-OB2-PB2
150	DH	202	CDL	CB3-CB4-CB6-OB8
150	DJ	305	CDL	CB3-CB4-CB6-OB8
150	DN	502	CDL	CA3-CA4-CA6-OA8
150	EA	301	CDL	CB3-CB4-CB6-OB8
150	EK	201	CDL	CB4-CB3-OB5-PB2
150	EL	901	CDL	CA3-CA4-CA6-OA8
150	Dd	705	CDL	C1-CB2-OB2-PB2
150	Dh	202	CDL	CB3-CB4-CB6-OB8
150	Di	1101	CDL	CA3-CA4-CA6-OA8
150	Di	1101	CDL	C1-CB2-OB2-PB2
150	Dj	405	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dn	502	CDL	C1-CA2-OA2-PA1
150	Du	402	CDL	CB3-CB4-CB6-OB8
150	Dv	403	CDL	CB4-CB3-OB5-PB2
150	Dx	1201	CDL	C1-CB2-OB2-PB2
150	Dy	301	CDL	CA3-CA4-CA6-OA8
150	Eu	101	CDL	CB3-CB4-CB6-OB8
153	AU	202	PC1	C1-C2-C3-O31
153	Dv	405	PC1	C1-C2-C3-O31
155	DC	606	3PE	C1-C2-C3-O31
155	DI	301	3PE	C1-C2-C3-O31
155	Dc	607	3PE	C1-C2-C3-O31
155	Di	1102	3PE	C1-C2-C3-O31
155	Dr	401	3PE	C1-C2-C3-O31
153	A0	605	PC1	O32-C31-O31-C3
153	Dy	302	PC1	O32-C31-O31-C3
150	DN	507	CDL	C51-CB5-OB6-CB4
150	B0	101	CDL	C60-C61-C62-C63
150	Dn	506	CDL	C16-C17-C18-C19
153	EO	201	PC1	C25-C26-C27-C28
150	BC	301	CDL	OA5-CA3-CA4-OA6
150	BC	302	CDL	OB5-CB3-CB4-OB6
150	CG	301	CDL	OA5-CA3-CA4-OA6
150	C	503	CDL	OB5-CB3-CB4-OB6
150	C	505	CDL	OA5-CA3-CA4-OA6
150	DG	201	CDL	OA5-CA3-CA4-OA6
150	DI	302	CDL	OB5-CB3-CB4-OB6
150	DS	401	CDL	OB5-CB3-CB4-OB6
150	DU	401	CDL	OB5-CB3-CB4-OB6
150	DX	306	CDL	OA5-CA3-CA4-OA6
150	EH	1601	CDL	OB5-CB3-CB4-OB6
150	EI	401	CDL	OB5-CB3-CB4-OB6
150	EL	901	CDL	OB5-CB3-CB4-OB6
150	EL	903	CDL	OA5-CA3-CA4-OA6
150	EN	1202	CDL	OA5-CA3-CA4-OA6
150	EO	202	CDL	OA5-CA3-CA4-OA6
150	Dj	402	CDL	OA5-CA3-CA4-OA6
150	Dj	405	CDL	OB5-CB3-CB4-OB6
150	Dm	501	CDL	OB5-CB3-CB4-OB6
150	Do	501	CDL	OA5-CA3-CA4-OA6
150	Du	403	CDL	OB5-CB3-CB4-OB6
150	Dv	403	CDL	OA5-CA3-CA4-OA6
150	El	901	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	El	903	CDL	OB5-CB3-CB4-OB6
150	Eu	101	CDL	OA5-CA3-CA4-OA6
153	AA	904	PC1	O11-C1-C2-O21
153	BS	1302	PC1	O11-C1-C2-O21
153	E	303	PC1	O11-C1-C2-O21
153	K	501	PC1	O11-C1-C2-O21
153	DG	203	PC1	O11-C1-C2-O21
153	Di	1104	PC1	O11-C1-C2-O21
155	DS	402	3PE	O11-C1-C2-O21
155	Da	708	3PE	O11-C1-C2-O21
155	Dg	204	3PE	O11-C1-C2-O21
155	Dr	404	3PE	O11-C1-C2-O21
155	Dx	1207	3PE	O11-C1-C2-O21
150	DV	401	CDL	C72-C71-CB7-OB8
150	En	1201	CDL	C12-C11-CA5-OA6
153	DV	405	PC1	O31-C31-C32-C33
150	Eg	101	CDL	C73-C74-C75-C76
150	c	506	CDL	C21-C22-C23-C24
150	DU	401	CDL	C11-C12-C13-C14
150	EL	901	CDL	C51-C52-C53-C54
150	EL	902	CDL	C84-C85-C86-C87
153	A0	605	PC1	C3C-C3D-C3E-C3F
153	C	508	PC1	C26-C27-C28-C29
153	Dv	405	PC1	C29-C2A-C2B-C2C
150	AC	801	CDL	OB9-CB7-OB8-CB6
150	C	504	CDL	C17-C18-C19-C20
150	BC	302	CDL	CA2-C1-CB2-OB2
150	Dy	301	CDL	CB2-C1-CA2-OA2
150	Ed	204	CDL	CB2-C1-CA2-OA2
150	Eg	101	CDL	CB2-C1-CA2-OA2
150	En	1201	CDL	CB2-C1-CA2-OA2
150	BV	201	CDL	O1-C1-CA2-OA2
150	CD	301	CDL	O1-C1-CB2-OB2
150	DS	405	CDL	OA7-CA5-OA6-CA4
150	Ds	406	CDL	OA7-CA5-OA6-CA4
153	d	801	PC1	O22-C21-O21-C2
155	EL	904	3PE	O22-C21-O21-C2
150	Ea	501	CDL	CA4-CA6-OA8-CA7
157	AQ	201	ADP	PA-O3A-PB-O2B
150	EI	401	CDL	C52-C51-CB5-OB6
153	A0	605	PC1	O31-C31-C32-C33
150	BT	202	CDL	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dn	506	CDL	C60-C61-C62-C63
150	AF	401	CDL	OA9-CA7-OA8-CA6
150	AF	402	CDL	OA9-CA7-OA8-CA6
150	EL	901	CDL	OA9-CA7-OA8-CA6
150	Dv	402	CDL	OB9-CB7-OB8-CB6
150	Ed	205	CDL	OA9-CA7-OA8-CA6
153	AM	302	PC1	O32-C31-O31-C3
153	B1	401	PC1	O32-C31-O31-C3
153	Db	702	PC1	O32-C31-O31-C3
150	C	505	CDL	C73-C74-C75-C76
150	DH	202	CDL	C74-C75-C76-C77
150	DO	501	CDL	C20-C21-C22-C23
150	Dg	202	CDL	C42-C43-C44-C45
153	B1	401	PC1	C33-C34-C35-C36
155	DN	501	3PE	C3A-C3B-C3C-C3D
150	DD	706	CDL	C39-C40-C41-C42
150	DX	301	CDL	C16-C17-C18-C19
150	Di	1101	CDL	C82-C83-C84-C85
150	AC	801	CDL	OB6-CB4-CB6-OB8
150	AP	301	CDL	OA6-CA4-CA6-OA8
150	BG	201	CDL	OB6-CB4-CB6-OB8
150	CC	304	CDL	OA6-CA4-CA6-OA8
150	C	504	CDL	OB6-CB4-CB6-OB8
150	C	506	CDL	OA6-CA4-CA6-OA8
150	H	1301	CDL	OB6-CB4-CB6-OB8
150	DA	706	CDL	OB6-CB4-CB6-OB8
150	DD	703	CDL	OA6-CA4-CA6-OA8
150	DG	202	CDL	OB6-CB4-CB6-OB8
150	DJ	302	CDL	OB6-CB4-CB6-OB8
150	DJ	303	CDL	OB6-CB4-CB6-OB8
150	DN	506	CDL	OB6-CB4-CB6-OB8
150	DN	507	CDL	OA6-CA4-CA6-OA8
150	DN	507	CDL	OB6-CB4-CB6-OB8
150	DQ	1501	CDL	OA6-CA4-CA6-OA8
150	DQ	1501	CDL	OB6-CB4-CB6-OB8
150	DR	402	CDL	OA6-CA4-CA6-OA8
150	DU	401	CDL	OB6-CB4-CB6-OB8
150	DX	306	CDL	OB6-CB4-CB6-OB8
150	DY	301	CDL	OA6-CA4-CA6-OA8
150	ED	605	CDL	OB6-CB4-CB6-OB8
150	Dd	702	CDL	OA6-CA4-CA6-OA8
150	Dd	706	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Di	1101	CDL	OB6-CB4-CB6-OB8
150	Dn	506	CDL	OB6-CB4-CB6-OB8
150	Ds	401	CDL	OB6-CB4-CB6-OB8
150	Eb	302	CDL	OB6-CB4-CB6-OB8
150	Ed	205	CDL	OB6-CB4-CB6-OB8
150	Eg	101	CDL	OA6-CA4-CA6-OA8
150	Ek	201	CDL	OA6-CA4-CA6-OA8
150	Ep	701	CDL	OB6-CB4-CB6-OB8
153	A6	303	PC1	O21-C2-C3-O31
153	AA	906	PC1	O21-C2-C3-O31
153	BT	203	PC1	O21-C2-C3-O31
153	DV	404	PC1	O21-C2-C3-O31
153	DY	302	PC1	O21-C2-C3-O31
153	Dc	609	PC1	O21-C2-C3-O31
153	Dv	404	PC1	O21-C2-C3-O31
153	Eo	204	PC1	O21-C2-C3-O31
155	EL	904	3PE	O21-C2-C3-O31
155	Dx	1208	3PE	O21-C2-C3-O31
155	El	905	3PE	O21-C2-C3-O31
155	Eo	202	3PE	O21-C2-C3-O31
150	BG	201	CDL	C74-C75-C76-C77
150	BG	201	CDL	C75-C76-C77-C78
150	BT	204	CDL	C71-C72-C73-C74
150	c	509	CDL	C17-C18-C19-C20
150	EA	301	CDL	C60-C61-C62-C63
150	Dx	1204	CDL	C72-C73-C74-C75
150	El	902	CDL	C13-C14-C15-C16
153	AA	905	PC1	C3D-C3E-C3F-C3G
150	DN	502	CDL	CB7-C71-C72-C73
150	DD	705	CDL	OA9-CA7-OA8-CA6
150	DU	401	CDL	OB9-CB7-OB8-CB6
150	Dm	501	CDL	OA9-CA7-OA8-CA6
150	Dv	401	CDL	OB9-CB7-OB8-CB6
150	Eu	101	CDL	OB9-CB7-OB8-CB6
153	AX	401	PC1	O32-C31-O31-C3
153	DC	603	PC1	O32-C31-O31-C3
155	Dd	703	3PE	O32-C31-O31-C3
150	BT	202	CDL	C15-C16-C17-C18
150	DX	306	CDL	C32-C33-C34-C35
150	EA	301	CDL	C37-C38-C39-C40
150	ED	601	CDL	C12-C13-C14-C15
153	AA	904	PC1	C11-C12-N-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Di	1104	PC1	C11-C12-N-C13
154	A1	401	NDP	C5B-O5B-PA-O3
173	ER	201	ATP	C5'-O5'-PA-O3A
150	B1	402	CDL	C17-C18-C19-C20
150	DX	301	CDL	C33-C34-C35-C36
150	El	902	CDL	C44-C45-C46-C47
150	EL	901	CDL	C11-CA5-OA6-CA4
150	DQ	1501	CDL	C53-C54-C55-C56
150	En	1201	CDL	C40-C41-C42-C43
150	AA	908	CDL	OA9-CA7-OA8-CA6
150	C	504	CDL	OA9-CA7-OA8-CA6
150	DU	403	CDL	OA9-CA7-OA8-CA6
153	DY	302	PC1	O32-C31-O31-C3
150	AP	301	CDL	C13-C14-C15-C16
150	H	1301	CDL	C11-C12-C13-C14
150	Ds	402	CDL	C82-C83-C84-C85
150	Eh	1601	CDL	C18-C19-C20-C21
150	Eh	1601	CDL	C74-C75-C76-C77
150	DN	507	CDL	OB7-CB5-OB6-CB4
150	EL	901	CDL	OA7-CA5-OA6-CA4
153	C	510	PC1	O22-C21-O21-C2
150	H	1302	CDL	C15-C16-C17-C18
150	DM	501	CDL	C59-C60-C61-C62
150	DN	502	CDL	C12-C13-C14-C15
150	DQ	1502	CDL	C60-C61-C62-C63
150	DR	402	CDL	C41-C42-C43-C44
150	Ed	204	CDL	C13-C14-C15-C16
153	AA	906	PC1	C3E-C3F-C3G-C3H
153	DB	702	PC1	C3B-C3C-C3D-C3E
150	BG	201	CDL	OA9-CA7-OA8-CA6
150	DM	502	CDL	CA5-C11-C12-C13
150	BE	201	CDL	C15-C16-C17-C18
150	DJ	304	CDL	C75-C76-C77-C78
150	DN	506	CDL	C59-C60-C61-C62
150	DQ	1501	CDL	C17-C18-C19-C20
150	DR	402	CDL	C34-C35-C36-C37
150	c	502	CDL	C37-C38-C39-C40
153	A9	601	PC1	C3D-C3E-C3F-C3G
153	DC	603	PC1	C3B-C3C-C3D-C3E
150	AC	802	CDL	C72-C71-CB7-OB8
150	Dn	506	CDL	C20-C21-C22-C23
153	Ef	501	PC1	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	CC	305	CDL	OB9-CB7-OB8-CB6
150	Dh	201	CDL	OA9-CA7-OA8-CA6
150	DH	201	CDL	C19-C20-C21-C22
169	DA	703	HEA	C2D-C3D-CAD-CBD
169	Da	703	HEA	C2D-C3D-CAD-CBD
150	c	506	CDL	C62-C63-C64-C65
150	DH	202	CDL	C20-C21-C22-C23
150	DH	202	CDL	C52-C53-C54-C55
150	EN	1201	CDL	C13-C14-C15-C16
150	Eb	302	CDL	C55-C56-C57-C58
153	Eo	205	PC1	C3C-C3D-C3E-C3F
150	BT	204	CDL	C74-C75-C76-C77
150	CJ	201	CDL	C44-C45-C46-C47
150	ED	604	CDL	C74-C75-C76-C77
150	Dg	201	CDL	C21-C22-C23-C24
153	k	301	PC1	C36-C37-C38-C39
150	BC	301	CDL	CA5-C11-C12-C13
150	EL	903	CDL	C31-CA7-OA8-CA6
153	DX	305	PC1	C32-C31-O31-C3
150	Dj	404	CDL	C55-C56-C57-C58
150	BC	301	CDL	CB2-OB2-PB2-OB5
150	BG	201	CDL	CB2-OB2-PB2-OB5
150	BT	204	CDL	CA3-OA5-PA1-OA2
150	CJ	201	CDL	CA2-OA2-PA1-OA5
150	CC	304	CDL	CB2-OB2-PB2-OB5
150	C	506	CDL	CA2-OA2-PA1-OA5
150	c	502	CDL	CA2-OA2-PA1-OA5
150	c	506	CDL	CA2-OA2-PA1-OA5
150	DA	706	CDL	CA2-OA2-PA1-OA5
150	DA	709	CDL	CB2-OB2-PB2-OB5
150	DD	705	CDL	CB3-OB5-PB2-OB2
150	DH	201	CDL	CA3-OA5-PA1-OA2
150	DJ	302	CDL	CB2-OB2-PB2-OB5
150	DJ	303	CDL	CB3-OB5-PB2-OB2
150	DQ	1502	CDL	CA2-OA2-PA1-OA5
150	DS	401	CDL	CA2-OA2-PA1-OA5
150	DS	401	CDL	CB3-OB5-PB2-OB2
150	DV	403	CDL	CB3-OB5-PB2-OB2
150	DX	306	CDL	CB2-OB2-PB2-OB5
150	ED	605	CDL	CB2-OB2-PB2-OB5
150	EO	202	CDL	CB3-OB5-PB2-OB2
150	Da	709	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Da	709	CDL	CA3-OA5-PA1-OA2
150	Dc	601	CDL	CA2-OA2-PA1-OA5
150	Do	501	CDL	CA2-OA2-PA1-OA5
150	Ds	402	CDL	CA2-OA2-PA1-OA5
150	Ds	402	CDL	CB3-OB5-PB2-OB2
153	AH	301	PC1	C11-O13-P-O11
153	AU	202	PC1	C11-O13-P-O11
153	BT	203	PC1	C11-O13-P-O11
153	Dc	605	PC1	C11-O13-P-O11
153	Dx	1205	PC1	C11-O13-P-O11
153	Eb	301	PC1	C11-O13-P-O11
155	Da	708	3PE	C11-O13-P-O11
155	Ds	408	3PE	C11-O13-P-O11
150	DD	705	CDL	C59-C60-C61-C62
150	DD	706	CDL	C13-C14-C15-C16
153	Dv	404	PC1	C3B-C3C-C3D-C3E
150	Dn	502	CDL	O1-C1-CB2-OB2
150	Dj	404	CDL	C62-C63-C64-C65
155	DC	607	3PE	C3B-C3C-C3D-C3E
150	BG	201	CDL	CB4-CB3-OB5-PB2
150	BY	201	CDL	C1-CB2-OB2-PB2
150	CG	302	CDL	CB4-CB3-OB5-PB2
150	CC	304	CDL	C1-CB2-OB2-PB2
150	c	506	CDL	CB4-CB3-OB5-PB2
150	DD	703	CDL	C1-CA2-OA2-PA1
150	DD	704	CDL	C1-CB2-OB2-PB2
150	DG	201	CDL	C1-CA2-OA2-PA1
150	DM	501	CDL	CB4-CB3-OB5-PB2
150	DN	506	CDL	C1-CB2-OB2-PB2
150	DQ	1504	CDL	C1-CA2-OA2-PA1
150	DR	403	CDL	CA4-CA3-OA5-PA1
150	DR	403	CDL	C1-CB2-OB2-PB2
150	DX	301	CDL	CA4-CA3-OA5-PA1
150	EL	903	CDL	C1-CB2-OB2-PB2
150	EO	202	CDL	C1-CB2-OB2-PB2
150	EO	202	CDL	CB4-CB3-OB5-PB2
150	Dg	201	CDL	CA4-CA3-OA5-PA1
150	Dm	501	CDL	CA4-CA3-OA5-PA1
150	Ds	406	CDL	C1-CA2-OA2-PA1
150	Dv	403	CDL	C1-CA2-OA2-PA1
150	Ei	401	CDL	C1-CB2-OB2-PB2
150	Ek	201	CDL	CB4-CB3-OB5-PB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	El	901	CDL	C1-CA2-OA2-PA1
153	CC	302	PC1	C2-C1-O11-P
155	Da	708	3PE	C2-C1-O11-P
156	DN	504	LPP	C7-C6-O5-P1
150	DA	706	CDL	C82-C83-C84-C85
150	DN	502	CDL	C77-C78-C79-C80
150	DS	404	CDL	C77-C78-C79-C80
150	DV	402	CDL	C12-C13-C14-C15
150	Dd	706	CDL	C56-C57-C58-C59
150	Dm	502	CDL	C11-C12-C13-C14
155	Dc	606	3PE	C29-C2A-C2B-C2C
150	DU	403	CDL	OB9-CB7-OB8-CB6
153	EO	205	PC1	O32-C31-O31-C3
150	A0	601	CDL	CB2-OB2-PB2-OB4
150	A0	602	CDL	CA2-OA2-PA1-OA4
150	A0	602	CDL	CA3-OA5-PA1-OA4
150	A1	402	CDL	CB2-OB2-PB2-OB3
150	A1	402	CDL	CB3-OB5-PB2-OB4
150	AA	901	CDL	CA3-OA5-PA1-OA3
150	AA	901	CDL	CA3-OA5-PA1-OA4
150	AA	901	CDL	CB2-OB2-PB2-OB3
150	AM	301	CDL	CA2-OA2-PA1-OA3
150	AM	301	CDL	CB3-OB5-PB2-OB3
150	AP	301	CDL	CB2-OB2-PB2-OB3
150	B0	101	CDL	CB3-OB5-PB2-OB3
150	B1	402	CDL	CA3-OA5-PA1-OA4
150	BC	301	CDL	CA2-OA2-PA1-OA3
150	BC	302	CDL	CB2-OB2-PB2-OB4
150	BG	201	CDL	CA2-OA2-PA1-OA4
150	BG	201	CDL	CB3-OB5-PB2-OB4
150	BT	204	CDL	CA2-OA2-PA1-OA4
150	CG	301	CDL	CB2-OB2-PB2-OB4
150	CG	302	CDL	CA3-OA5-PA1-OA4
150	CG	302	CDL	CB3-OB5-PB2-OB3
150	CC	304	CDL	CA2-OA2-PA1-OA4
150	CC	305	CDL	CA3-OA5-PA1-OA3
150	CD	301	CDL	CA2-OA2-PA1-OA3
150	CD	301	CDL	CA3-OA5-PA1-OA3
150	CD	301	CDL	CB3-OB5-PB2-OB4
150	CD	302	CDL	CB2-OB2-PB2-OB4
150	C	503	CDL	CA2-OA2-PA1-OA3
150	C	503	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	C	503	CDL	CA3-OA5-PA1-OA4
150	C	503	CDL	CB2-OB2-PB2-OB3
150	C	504	CDL	CA3-OA5-PA1-OA4
150	C	504	CDL	CB2-OB2-PB2-OB4
150	C	505	CDL	CA2-OA2-PA1-OA3
150	C	506	CDL	CA3-OA5-PA1-OA4
150	C	507	CDL	CA2-OA2-PA1-OA4
150	C	507	CDL	CA3-OA5-PA1-OA3
150	C	507	CDL	CB3-OB5-PB2-OB4
150	E	301	CDL	CA2-OA2-PA1-OA3
150	E	301	CDL	CB2-OB2-PB2-OB3
150	H	1302	CDL	CA3-OA5-PA1-OA3
150	c	502	CDL	CA2-OA2-PA1-OA3
150	c	506	CDL	CB2-OB2-PB2-OB4
150	g	801	CDL	CA2-OA2-PA1-OA4
150	g	801	CDL	CB2-OB2-PB2-OB4
150	h	501	CDL	CA2-OA2-PA1-OA3
150	DA	706	CDL	CA2-OA2-PA1-OA4
150	DA	706	CDL	CB3-OB5-PB2-OB3
150	DC	601	CDL	CA2-OA2-PA1-OA3
150	DC	601	CDL	CA3-OA5-PA1-OA3
150	DC	601	CDL	CB2-OB2-PB2-OB3
150	DC	601	CDL	CB3-OB5-PB2-OB3
150	DD	703	CDL	CA3-OA5-PA1-OA3
150	DD	706	CDL	CB3-OB5-PB2-OB4
150	DG	202	CDL	CA2-OA2-PA1-OA3
150	DG	202	CDL	CB3-OB5-PB2-OB3
150	DH	202	CDL	CB2-OB2-PB2-OB3
150	DI	302	CDL	CB3-OB5-PB2-OB4
150	DJ	302	CDL	CB3-OB5-PB2-OB3
150	DJ	303	CDL	CB3-OB5-PB2-OB3
150	DJ	305	CDL	CA3-OA5-PA1-OA3
150	DJ	305	CDL	CB2-OB2-PB2-OB3
150	DJ	307	CDL	CB2-OB2-PB2-OB3
150	DJ	307	CDL	CB3-OB5-PB2-OB3
150	DM	501	CDL	CA2-OA2-PA1-OA4
150	DM	502	CDL	CA2-OA2-PA1-OA4
150	DM	502	CDL	CB2-OB2-PB2-OB3
150	DN	502	CDL	CB3-OB5-PB2-OB4
150	DN	506	CDL	CB3-OB5-PB2-OB4
150	DN	507	CDL	CA2-OA2-PA1-OA3
150	DO	501	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DQ	1504	CDL	CA2-OA2-PA1-OA3
150	DR	403	CDL	CA2-OA2-PA1-OA3
150	DS	405	CDL	CB2-OB2-PB2-OB4
150	DU	401	CDL	CB2-OB2-PB2-OB4
150	DU	403	CDL	CA2-OA2-PA1-OA4
150	DU	403	CDL	CB3-OB5-PB2-OB4
150	DV	402	CDL	CA3-OA5-PA1-OA3
150	DV	403	CDL	CA2-OA2-PA1-OA3
150	DV	403	CDL	CB2-OB2-PB2-OB3
150	DV	403	CDL	CB2-OB2-PB2-OB4
150	DX	306	CDL	CA2-OA2-PA1-OA3
150	DY	301	CDL	CB2-OB2-PB2-OB4
150	DZ	501	CDL	CA2-OA2-PA1-OA3
150	ED	601	CDL	CB2-OB2-PB2-OB4
150	ED	604	CDL	CA3-OA5-PA1-OA3
150	ED	604	CDL	CB3-OB5-PB2-OB3
150	ED	605	CDL	CB2-OB2-PB2-OB4
150	EH	1601	CDL	CA2-OA2-PA1-OA3
150	EH	1601	CDL	CB3-OB5-PB2-OB4
150	EI	401	CDL	CB3-OB5-PB2-OB4
150	EK	201	CDL	CA3-OA5-PA1-OA4
150	EL	901	CDL	CB2-OB2-PB2-OB4
150	EL	903	CDL	CA2-OA2-PA1-OA3
150	EN	1202	CDL	CA3-OA5-PA1-OA3
150	EN	1202	CDL	CB3-OB5-PB2-OB4
150	EO	202	CDL	CB2-OB2-PB2-OB4
150	ES	1101	CDL	CA2-OA2-PA1-OA4
150	ES	1101	CDL	CA3-OA5-PA1-OA3
150	Da	709	CDL	CA2-OA2-PA1-OA4
150	Da	709	CDL	CA3-OA5-PA1-OA3
150	Dc	601	CDL	CA2-OA2-PA1-OA3
150	Dc	601	CDL	CA3-OA5-PA1-OA3
150	Dc	601	CDL	CA3-OA5-PA1-OA4
150	Dc	601	CDL	CB2-OB2-PB2-OB3
150	Dd	704	CDL	CB2-OB2-PB2-OB3
150	Dd	705	CDL	CA3-OA5-PA1-OA3
150	Dd	706	CDL	CA2-OA2-PA1-OA3
150	Dg	201	CDL	CA2-OA2-PA1-OA3
150	Di	1101	CDL	CB3-OB5-PB2-OB3
150	Di	1103	CDL	CB3-OB5-PB2-OB4
150	Dj	402	CDL	CA3-OA5-PA1-OA4
150	Dj	402	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dj	403	CDL	CA2-OA2-PA1-OA3
150	Dj	403	CDL	CB2-OB2-PB2-OB3
150	Dj	403	CDL	CB2-OB2-PB2-OB4
150	Dj	404	CDL	CA2-OA2-PA1-OA3
150	Dj	404	CDL	CB3-OB5-PB2-OB4
150	Dj	407	CDL	CA2-OA2-PA1-OA4
150	Dj	407	CDL	CB2-OB2-PB2-OB3
150	Dm	501	CDL	CA3-OA5-PA1-OA3
150	Dn	501	CDL	CA3-OA5-PA1-OA3
150	Dn	501	CDL	CA3-OA5-PA1-OA4
150	Dn	502	CDL	CB3-OB5-PB2-OB3
150	Dn	506	CDL	CB3-OB5-PB2-OB4
150	Do	501	CDL	CA2-OA2-PA1-OA3
150	Do	501	CDL	CB3-OB5-PB2-OB3
150	Dq	1401	CDL	CA2-OA2-PA1-OA3
150	Dq	1402	CDL	CB3-OB5-PB2-OB3
150	Dq	1403	CDL	CA2-OA2-PA1-OA3
150	Dq	1403	CDL	CA3-OA5-PA1-OA3
150	Dq	1403	CDL	CB2-OB2-PB2-OB3
150	Dr	402	CDL	CA3-OA5-PA1-OA3
150	Dr	403	CDL	CA2-OA2-PA1-OA3
150	Dr	403	CDL	CA2-OA2-PA1-OA4
150	Ds	401	CDL	CA3-OA5-PA1-OA3
150	Ds	401	CDL	CB3-OB5-PB2-OB4
150	Ds	406	CDL	CA2-OA2-PA1-OA4
150	Ds	406	CDL	CA3-OA5-PA1-OA4
150	Ds	406	CDL	CB2-OB2-PB2-OB4
150	Ds	406	CDL	CB3-OB5-PB2-OB4
150	Du	401	CDL	CA2-OA2-PA1-OA4
150	Du	401	CDL	CA3-OA5-PA1-OA4
150	Du	401	CDL	CB3-OB5-PB2-OB3
150	Du	401	CDL	CB3-OB5-PB2-OB4
150	Du	402	CDL	CA2-OA2-PA1-OA4
150	Du	403	CDL	CB3-OB5-PB2-OB4
150	Dv	401	CDL	CB2-OB2-PB2-OB3
150	Dv	402	CDL	CB2-OB2-PB2-OB4
150	Dv	403	CDL	CA2-OA2-PA1-OA3
150	Dv	403	CDL	CA3-OA5-PA1-OA3
150	Dv	403	CDL	CB2-OB2-PB2-OB3
150	Dv	403	CDL	CB2-OB2-PB2-OB4
150	Dx	1201	CDL	CB2-OB2-PB2-OB3
150	Dx	1201	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dx	1201	CDL	CB3-OB5-PB2-OB4
150	Dx	1204	CDL	CA2-OA2-PA1-OA3
150	Dx	1204	CDL	CA2-OA2-PA1-OA4
150	Dx	1204	CDL	CA3-OA5-PA1-OA3
150	Dx	1204	CDL	CA3-OA5-PA1-OA4
150	Dx	1204	CDL	CB3-OB5-PB2-OB3
150	Ea	501	CDL	CB2-OB2-PB2-OB4
150	Ea	502	CDL	CA2-OA2-PA1-OA3
150	Ea	502	CDL	CA2-OA2-PA1-OA4
150	Ea	502	CDL	CB2-OB2-PB2-OB4
150	Eb	302	CDL	CB2-OB2-PB2-OB3
150	Eb	302	CDL	CB3-OB5-PB2-OB3
150	Ed	204	CDL	CB3-OB5-PB2-OB3
150	Eg	101	CDL	CB3-OB5-PB2-OB3
150	Eh	1601	CDL	CB3-OB5-PB2-OB4
150	Ei	401	CDL	CB3-OB5-PB2-OB3
150	El	901	CDL	CA3-OA5-PA1-OA3
150	El	902	CDL	CB2-OB2-PB2-OB4
150	El	903	CDL	CA2-OA2-PA1-OA3
150	El	903	CDL	CA3-OA5-PA1-OA3
150	El	903	CDL	CB2-OB2-PB2-OB4
150	En	1201	CDL	CA2-OA2-PA1-OA4
150	En	1201	CDL	CB2-OB2-PB2-OB4
150	Ep	701	CDL	CA3-OA5-PA1-OA3
150	Eu	101	CDL	CB3-OB5-PB2-OB4
153	A9	603	PC1	C1-O11-P-O14
153	AA	903	PC1	C1-O11-P-O14
153	AA	907	PC1	C11-O13-P-O12
153	AA	907	PC1	C11-O13-P-O14
153	AM	302	PC1	C11-O13-P-O14
153	AQ	202	PC1	C1-O11-P-O12
153	AU	201	PC1	C11-O13-P-O12
153	AU	201	PC1	C11-O13-P-O14
153	AU	201	PC1	C1-O11-P-O14
153	AX	401	PC1	C1-O11-P-O14
153	B1	401	PC1	C11-O13-P-O12
153	B1	403	PC1	C1-O11-P-O14
153	BG	202	PC1	C1-O11-P-O14
153	BS	1301	PC1	C11-O13-P-O14
153	BS	1301	PC1	C1-O11-P-O12
153	BS	1302	PC1	C1-O11-P-O14
153	C	508	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	C	508	PC1	C1-O11-P-O14
153	K	501	PC1	C11-O13-P-O12
153	K	502	PC1	C11-O13-P-O14
153	c	508	PC1	C11-O13-P-O14
153	d	801	PC1	C1-O11-P-O12
153	k	301	PC1	C11-O13-P-O12
153	DB	702	PC1	C11-O13-P-O12
153	DB	702	PC1	C11-O13-P-O14
153	DC	602	PC1	C11-O13-P-O12
153	DC	603	PC1	C11-O13-P-O14
153	DC	604	PC1	C1-O11-P-O12
153	DC	604	PC1	C1-O11-P-O14
153	DC	605	PC1	C1-O11-P-O12
153	DI	303	PC1	C11-O13-P-O12
153	DI	303	PC1	C11-O13-P-O14
153	DJ	306	PC1	C1-O11-P-O14
153	DQ	1503	PC1	C11-O13-P-O14
153	DV	404	PC1	C11-O13-P-O14
153	DV	405	PC1	C11-O13-P-O14
153	DX	305	PC1	C11-O13-P-O12
153	DX	305	PC1	C11-O13-P-O14
153	DX	305	PC1	C1-O11-P-O12
153	DX	308	PC1	C1-O11-P-O14
153	EB	301	PC1	C11-O13-P-O12
153	EB	301	PC1	C1-O11-P-O12
153	EN	1203	PC1	C11-O13-P-O12
153	EO	201	PC1	C11-O13-P-O14
153	EO	205	PC1	C11-C12-N-C15
153	Db	702	PC1	C11-O13-P-O14
153	Dc	602	PC1	C11-O13-P-O12
153	Dc	602	PC1	C11-O13-P-O14
153	Dc	603	PC1	C11-O13-P-O14
153	Dc	604	PC1	C11-O13-P-O14
153	Dc	605	PC1	C1-O11-P-O12
153	Di	1104	PC1	C11-O13-P-O12
153	Di	1104	PC1	C11-O13-P-O14
153	Di	1104	PC1	C1-O11-P-O12
153	Dj	406	PC1	C11-O13-P-O14
153	Dq	1404	PC1	C11-O13-P-O14
153	Dv	406	PC1	C11-O13-P-O14
153	Dv	407	PC1	C1-O11-P-O14
153	Dy	302	PC1	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Eb	301	PC1	C1-O11-P-O12
153	Ef	501	PC1	C1-O11-P-O14
153	Eo	201	PC1	C11-O13-P-O14
153	Eo	204	PC1	C11-C12-N-C13
154	A1	401	NDP	C5B-O5B-PA-O2A
155	AJ	502	3PE	C11-O13-P-O12
155	BA	301	3PE	C11-O13-P-O12
155	BP	201	3PE	C1-O11-P-O12
155	BT	201	3PE	C11-O13-P-O12
155	DC	607	3PE	C11-O13-P-O12
155	DG	204	3PE	C1-O11-P-O12
155	DG	204	3PE	C1-O11-P-O14
155	DG	205	3PE	C1-O11-P-O12
155	DJ	301	3PE	C11-O13-P-O12
155	DS	402	3PE	C1-O11-P-O12
155	DS	402	3PE	C11-O13-P-O12
155	DX	303	3PE	C11-O13-P-O12
155	EL	904	3PE	C11-O13-P-O12
155	Dg	204	3PE	C1-O11-P-O12
155	Dr	401	3PE	C1-O11-P-O12
155	Dr	404	3PE	C1-O11-P-O12
155	Ds	403	3PE	C1-O11-P-O12
155	Ds	403	3PE	C11-O13-P-O12
155	Dx	1207	3PE	C1-O11-P-O12
155	Dx	1208	3PE	C11-O13-P-O14
155	El	905	3PE	C11-O13-P-O12
155	Eo	203	3PE	C11-O13-P-O12
155	Eo	203	3PE	C11-O13-P-O14
173	ER	201	ATP	C5'-O5'-PA-O1A
150	DJ	303	CDL	CA5-C11-C12-C13
150	EL	902	CDL	C78-C79-C80-C81
150	Dc	601	CDL	C79-C80-C81-C82
150	Do	501	CDL	C80-C81-C82-C83
155	Dg	204	3PE	C2A-C2B-C2C-C2D
156	Dn	505	LPP	C38-C39-C40-C41
150	EL	902	CDL	C31-CA7-OA8-CA6
153	C	509	PC1	C32-C31-O31-C3
153	DA	708	PC1	C32-C31-O31-C3
150	AF	402	CDL	OB5-CB3-CB4-CB6
150	B1	402	CDL	OA5-CA3-CA4-CA6
150	BT	202	CDL	OA5-CA3-CA4-CA6
150	C	504	CDL	OA5-CA3-CA4-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	c	501	CDL	OA5-CA3-CA4-CA6
150	c	509	CDL	OA5-CA3-CA4-CA6
150	DD	704	CDL	OB5-CB3-CB4-CB6
150	DN	506	CDL	OB5-CB3-CB4-CB6
150	DO	501	CDL	OA5-CA3-CA4-CA6
150	ED	605	CDL	OB5-CB3-CB4-CB6
150	EH	1601	CDL	OB5-CB3-CB4-CB6
150	EL	903	CDL	OA5-CA3-CA4-CA6
150	Dd	704	CDL	OA5-CA3-CA4-CA6
150	Dd	706	CDL	OB5-CB3-CB4-CB6
150	Dj	401	CDL	OA5-CA3-CA4-CA6
153	AH	301	PC1	O11-C1-C2-C3
153	BS	1302	PC1	O11-C1-C2-C3
153	c	503	PC1	O11-C1-C2-C3
153	DG	203	PC1	O11-C1-C2-C3
155	DX	302	3PE	O11-C1-C2-C3
155	Dd	703	3PE	O11-C1-C2-C3
155	Dg	204	3PE	O11-C1-C2-C3
155	Ds	403	3PE	O11-C1-C2-C3
167	Ds	404	UQ8	C39-C41-C42-C43
150	A1	402	CDL	C15-C16-C17-C18
150	DN	506	CDL	C13-C14-C15-C16
150	EL	903	CDL	C23-C24-C25-C26
150	Dg	202	CDL	C31-C32-C33-C34
150	Ds	401	CDL	C36-C37-C38-C39
150	Du	401	CDL	C37-C38-C39-C40
150	Dv	401	CDL	C43-C44-C45-C46
155	EL	904	3PE	C2B-C2C-C2D-C2E
150	CD	302	CDL	OB9-CB7-OB8-CB6
150	BT	204	CDL	C60-C61-C62-C63
150	DC	601	CDL	C79-C80-C81-C82
150	Dn	506	CDL	C18-C19-C20-C21
150	H	1302	CDL	C34-C35-C36-C37
150	EO	202	CDL	C18-C19-C20-C21
150	Dn	501	CDL	C77-C78-C79-C80
150	Ds	405	CDL	C72-C73-C74-C75
150	Ds	406	CDL	C33-C34-C35-C36
153	AJ	501	PC1	C2F-C2G-C2H-C2I
153	c	507	PC1	C3E-C3F-C3G-C3H
153	Dx	1205	PC1	C25-C26-C27-C28
167	Ds	404	UQ8	C5-C4-O4-C4M
150	BT	204	CDL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DD	706	CDL	C80-C81-C82-C83
150	DS	401	CDL	C74-C75-C76-C77
150	DZ	501	CDL	C11-C12-C13-C14
153	A9	603	PC1	C12-C11-O13-P
153	DB	702	PC1	C12-C11-O13-P
153	Db	702	PC1	C12-C11-O13-P
153	Dv	405	PC1	C12-C11-O13-P
153	Dx	1203	PC1	C12-C11-O13-P
155	BP	201	3PE	C12-C11-O13-P
155	CC	301	3PE	C12-C11-O13-P
155	C	513	3PE	C12-C11-O13-P
155	DI	301	3PE	C12-C11-O13-P
155	DX	302	3PE	C12-C11-O13-P
155	Dg	204	3PE	C12-C11-O13-P
155	Di	1102	3PE	C12-C11-O13-P
155	Dx	1206	3PE	C12-C11-O13-P
150	Dg	201	CDL	CA5-C11-C12-C13
150	AF	402	CDL	C43-C44-C45-C46
150	BT	204	CDL	C42-C43-C44-C45
150	CD	302	CDL	C19-C20-C21-C22
150	EL	902	CDL	C17-C18-C19-C20
153	AA	907	PC1	C22-C23-C24-C25
153	EB	301	PC1	C3C-C3D-C3E-C3F
153	Ef	501	PC1	C26-C27-C28-C29
153	DC	605	PC1	O32-C31-O31-C3
150	AA	901	CDL	C63-C64-C65-C66
153	DG	203	PC1	C3B-C3C-C3D-C3E
150	E	301	CDL	C16-C17-C18-C19
150	DM	501	CDL	C62-C63-C64-C65
153	DG	203	PC1	C23-C24-C25-C26
150	AP	301	CDL	CB7-C71-C72-C73
150	BT	204	CDL	CB5-C51-C52-C53
150	Dd	702	CDL	CA5-C11-C12-C13
153	EN	1203	PC1	C3C-C3D-C3E-C3F
155	Ds	403	3PE	C27-C28-C29-C2A
150	Eb	302	CDL	C31-CA7-OA8-CA6
150	Du	402	CDL	CA2-C1-CB2-OB2
150	Dx	1201	CDL	OB7-CB5-OB6-CB4
150	A0	602	CDL	C39-C40-C41-C42
150	DJ	304	CDL	C74-C75-C76-C77
150	Dh	201	CDL	C63-C64-C65-C66
150	Dr	402	CDL	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ei	401	CDL	C76-C77-C78-C79
153	EO	201	PC1	C32-C33-C34-C35
150	AF	402	CDL	OB5-CB3-CB4-OB6
150	B1	402	CDL	OA5-CA3-CA4-OA6
150	BY	201	CDL	OA5-CA3-CA4-OA6
150	CJ	201	CDL	OB5-CB3-CB4-OB6
150	E	301	CDL	OB5-CB3-CB4-OB6
150	c	502	CDL	OA5-CA3-CA4-OA6
150	DD	705	CDL	OB5-CB3-CB4-OB6
150	DM	501	CDL	OB5-CB3-CB4-OB6
150	DO	501	CDL	OA5-CA3-CA4-OA6
150	DQ	1502	CDL	OB5-CB3-CB4-OB6
150	DQ	1504	CDL	OB5-CB3-CB4-OB6
150	DS	405	CDL	OB5-CB3-CB4-OB6
150	DV	403	CDL	OA5-CA3-CA4-OA6
150	DX	307	CDL	OB5-CB3-CB4-OB6
150	EB	302	CDL	OA5-CA3-CA4-OA6
150	ED	604	CDL	OA5-CA3-CA4-OA6
150	ED	604	CDL	OB5-CB3-CB4-OB6
150	Da	709	CDL	OB5-CB3-CB4-OB6
150	Dj	401	CDL	OA5-CA3-CA4-OA6
150	Dn	502	CDL	OB5-CB3-CB4-OB6
150	Dq	1403	CDL	OB5-CB3-CB4-OB6
150	Ds	402	CDL	OB5-CB3-CB4-OB6
150	Du	401	CDL	OB5-CB3-CB4-OB6
150	Eg	101	CDL	OB5-CB3-CB4-OB6
150	Eh	1601	CDL	OA5-CA3-CA4-OA6
153	AH	301	PC1	O11-C1-C2-O21
153	AJ	501	PC1	O11-C1-C2-O21
153	AL	303	PC1	O11-C1-C2-O21
153	AQ	202	PC1	O11-C1-C2-O21
153	B1	403	PC1	O11-C1-C2-O21
153	C	509	PC1	O11-C1-C2-O21
153	c	507	PC1	O11-C1-C2-O21
153	Db	702	PC1	O11-C1-C2-O21
153	Dc	603	PC1	O11-C1-C2-O21
153	Dg	203	PC1	O11-C1-C2-O21
155	AJ	502	3PE	O11-C1-C2-O21
155	BP	201	3PE	O11-C1-C2-O21
155	Dc	606	3PE	O11-C1-C2-O21
155	Dd	703	3PE	O11-C1-C2-O21
156	AC	803	LPP	O5-C6-C7-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
168	C	501	HEM	C2A-CAA-CBA-CGA
150	C	504	CDL	C41-C42-C43-C44
150	C	506	CDL	C11-C12-C13-C14
150	DO	501	CDL	C36-C37-C38-C39
150	DQ	1504	CDL	C13-C14-C15-C16
150	Da	709	CDL	C22-C23-C24-C25
150	Di	1103	CDL	C57-C58-C59-C60
150	Dn	502	CDL	C84-C85-C86-C87
150	Dq	1402	CDL	C78-C79-C80-C81
150	Dq	1403	CDL	C12-C13-C14-C15
150	AC	802	CDL	C61-C62-C63-C64
150	ED	604	CDL	C12-C13-C14-C15
150	E	301	CDL	C18-C19-C20-C21
153	A2	402	PC1	C37-C38-C39-C3A
153	AA	907	PC1	C37-C38-C39-C3A
155	BP	201	3PE	C36-C37-C38-C39
150	Dx	1201	CDL	C51-CB5-OB6-CB4
153	Dx	1205	PC1	C22-C21-O21-C2
150	DX	307	CDL	C78-C79-C80-C81
150	EN	1202	CDL	C11-C12-C13-C14
150	Dj	401	CDL	C36-C37-C38-C39
150	Du	402	CDL	C57-C58-C59-C60
155	DS	402	3PE	C34-C35-C36-C37
150	DD	703	CDL	OB9-CB7-OB8-CB6
150	DR	403	CDL	O1-C1-CB2-OB2
150	Dm	502	CDL	O1-C1-CB2-OB2
150	C	506	CDL	C34-C35-C36-C37
150	DX	301	CDL	C24-C25-C26-C27
150	Dh	202	CDL	C80-C81-C82-C83
150	Ds	405	CDL	C58-C59-C60-C61
150	El	902	CDL	C83-C84-C85-C86
153	EB	303	PC1	C2E-C2F-C2G-C2H
153	EO	201	PC1	C29-C2A-C2B-C2C
153	Dc	605	PC1	C3E-C3F-C3G-C3H
153	EN	1203	PC1	C11-C12-N-C13
153	Eo	204	PC1	C11-C12-N-C15
150	c	509	CDL	C11-C12-C13-C14
150	g	801	CDL	C37-C38-C39-C40
150	Du	403	CDL	C61-C62-C63-C64
155	DJ	301	3PE	C35-C36-C37-C38
150	DU	404	CDL	CA4-CA6-OA8-CA7
156	Dl	1101	LPP	O27-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	CG	301	CDL	CB3-CB4-CB6-OB8
150	DD	704	CDL	C16-C17-C18-C19
150	DH	201	CDL	CB3-CB4-CB6-OB8
150	DJ	303	CDL	C57-C58-C59-C60
150	DN	502	CDL	CB3-CB4-CB6-OB8
150	DY	301	CDL	CB3-CB4-CB6-OB8
150	Dc	601	CDL	C34-C35-C36-C37
150	Dh	201	CDL	CB3-CB4-CB6-OB8
150	Dn	501	CDL	CB3-CB4-CB6-OB8
150	Dy	301	CDL	CB3-CB4-CB6-OB8
153	A2	402	PC1	O13-C11-C12-N
153	A9	603	PC1	O13-C11-C12-N
153	AA	906	PC1	O13-C11-C12-N
153	AH	301	PC1	O13-C11-C12-N
153	AQ	202	PC1	O13-C11-C12-N
153	AU	201	PC1	O13-C11-C12-N
153	AU	202	PC1	O13-C11-C12-N
153	B1	403	PC1	O13-C11-C12-N
153	CC	302	PC1	O13-C11-C12-N
153	K	502	PC1	O13-C11-C12-N
153	d	801	PC1	O13-C11-C12-N
153	e	1101	PC1	O13-C11-C12-N
153	g	802	PC1	O13-C11-C12-N
153	DB	702	PC1	O13-C11-C12-N
153	DC	604	PC1	O13-C11-C12-N
153	DS	406	PC1	O13-C11-C12-N
153	DV	405	PC1	O13-C11-C12-N
153	EO	204	PC1	O13-C11-C12-N
153	Db	702	PC1	O13-C11-C12-N
153	Dc	604	PC1	O13-C11-C12-N
153	Dc	605	PC1	O13-C11-C12-N
153	Dg	203	PC1	C23-C24-C25-C26
153	Dv	405	PC1	O13-C11-C12-N
153	Dv	406	PC1	O13-C11-C12-N
153	Ef	501	PC1	C1-C2-C3-O31
153	El	904	PC1	O13-C11-C12-N
155	Dx	1208	3PE	C1-C2-C3-O31
150	BE	201	CDL	OA6-CA4-CA6-OA8
150	BL	301	CDL	OB6-CB4-CB6-OB8
150	BV	201	CDL	OA6-CA4-CA6-OA8
150	CD	302	CDL	OA6-CA4-CA6-OA8
150	H	1302	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	c	509	CDL	OA6-CA4-CA6-OA8
150	h	501	CDL	OA6-CA4-CA6-OA8
150	DD	706	CDL	OB6-CB4-CB6-OB8
150	DI	302	CDL	OA6-CA4-CA6-OA8
150	DN	502	CDL	OA6-CA4-CA6-OA8
150	DN	502	CDL	OB6-CB4-CB6-OB8
150	DX	301	CDL	OB6-CB4-CB6-OB8
150	DZ	501	CDL	OA6-CA4-CA6-OA8
150	ED	601	CDL	OA6-CA4-CA6-OA8
150	ED	605	CDL	OA6-CA4-CA6-OA8
150	EK	201	CDL	OA6-CA4-CA6-OA8
150	EN	1202	CDL	OB6-CB4-CB6-OB8
150	EO	202	CDL	OB6-CB4-CB6-OB8
150	Dd	704	CDL	OB6-CB4-CB6-OB8
150	Dg	201	CDL	OB6-CB4-CB6-OB8
150	Dh	201	CDL	OB6-CB4-CB6-OB8
150	Dh	202	CDL	OB6-CB4-CB6-OB8
150	Dj	401	CDL	OB6-CB4-CB6-OB8
150	Dj	402	CDL	OB6-CB4-CB6-OB8
150	Dj	404	CDL	OA6-CA4-CA6-OA8
150	Dn	501	CDL	OB6-CB4-CB6-OB8
150	Dq	1402	CDL	OA6-CA4-CA6-OA8
150	Dr	402	CDL	OA6-CA4-CA6-OA8
153	A1	403	PC1	O21-C2-C3-O31
153	C	510	PC1	O21-C2-C3-O31
153	g	802	PC1	O21-C2-C3-O31
153	DC	605	PC1	O21-C2-C3-O31
153	DC	608	PC1	O21-C2-C3-O31
153	Dc	604	PC1	O21-C2-C3-O31
153	Dc	605	PC1	O21-C2-C3-O31
153	Eo	201	PC1	O21-C2-C3-O31
155	EM	901	3PE	O21-C2-C3-O31
150	AA	908	CDL	C33-C34-C35-C36
150	EL	901	CDL	C78-C79-C80-C81
150	Dx	1201	CDL	C73-C74-C75-C76
150	El	902	CDL	C79-C80-C81-C82
150	C	504	CDL	C40-C41-C42-C43
150	DD	706	CDL	C84-C85-C86-C87
153	Db	702	PC1	C3B-C3C-C3D-C3E
150	EA	301	CDL	CA5-C11-C12-C13
168	C	502	HEM	C4D-C3D-CAD-CBD
150	E	301	CDL	C75-C76-C77-C78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	c	501	CDL	C80-C81-C82-C83
150	Di	1101	CDL	C55-C56-C57-C58
150	B0	101	CDL	C75-C76-C77-C78
150	Dn	506	CDL	C74-C75-C76-C77
150	Eh	1601	CDL	C13-C14-C15-C16
153	c	503	PC1	C24-C25-C26-C27
150	AC	801	CDL	C1-CA2-OA2-PA1
150	DD	705	CDL	CB4-CB3-OB5-PB2
150	DM	501	CDL	C1-CB2-OB2-PB2
150	Dr	402	CDL	CA4-CA3-OA5-PA1
150	Eg	101	CDL	CB4-CB3-OB5-PB2
150	DU	401	CDL	C37-C38-C39-C40
150	EL	902	CDL	OA9-CA7-OA8-CA6
153	DA	708	PC1	O32-C31-O31-C3
150	DN	503	CDL	C31-CA7-OA8-CA6
150	Dd	705	CDL	C71-CB7-OB8-CB6
150	AF	402	CDL	C12-C13-C14-C15
150	C	504	CDL	C77-C78-C79-C80
150	c	502	CDL	C60-C61-C62-C63
150	DG	202	CDL	C31-C32-C33-C34
150	DH	202	CDL	C36-C37-C38-C39
150	Dm	501	CDL	C52-C51-CB5-OB6
150	DH	202	CDL	C80-C81-C82-C83
150	DN	503	CDL	C57-C58-C59-C60
150	DZ	501	CDL	C39-C40-C41-C42
150	ES	1101	CDL	C11-C12-C13-C14
150	Dr	402	CDL	C71-C72-C73-C74
150	Dx	1204	CDL	C44-C45-C46-C47
153	Eb	303	PC1	C2E-C2F-C2G-C2H
153	C	509	PC1	O32-C31-O31-C3
153	DX	305	PC1	O32-C31-O31-C3
150	C	506	CDL	C80-C81-C82-C83
150	H	1301	CDL	C20-C21-C22-C23
150	DU	402	CDL	C17-C18-C19-C20
150	Dm	501	CDL	C40-C41-C42-C43
150	Do	501	CDL	C36-C37-C38-C39
153	DI	303	PC1	C35-C36-C37-C38
155	BA	301	3PE	C26-C27-C28-C29
150	A1	402	CDL	C80-C81-C82-C83
150	C	504	CDL	C73-C74-C75-C76
150	DY	301	CDL	C17-C18-C19-C20
150	Dn	502	CDL	C57-C58-C59-C60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Du	403	CDL	C40-C41-C42-C43
153	k	301	PC1	C33-C34-C35-C36
155	El	905	3PE	C22-C23-C24-C25
167	CC	303	UQ8	C14-C16-C17-C18
167	C	511	UQ8	C24-C26-C27-C28
167	EN	1205	UQ8	C14-C16-C17-C18
150	AC	802	CDL	C51-C52-C53-C54
150	ED	601	CDL	C35-C36-C37-C38
153	A6	302	PC1	C36-C37-C38-C39
153	A9	603	PC1	C24-C25-C26-C27
153	AM	302	PC1	C3C-C3D-C3E-C3F
153	Eo	201	PC1	C2B-C2C-C2D-C2E
150	EL	903	CDL	OA9-CA7-OA8-CA6
150	AC	801	CDL	C63-C64-C65-C66
150	DS	404	CDL	C72-C73-C74-C75
150	DU	404	CDL	C20-C21-C22-C23
150	Dh	201	CDL	C77-C78-C79-C80
150	El	903	CDL	C43-C44-C45-C46
150	En	1201	CDL	C44-C45-C46-C47
155	Di	1102	3PE	C32-C33-C34-C35
150	C	507	CDL	C16-C17-C18-C19
150	DZ	501	CDL	C43-C44-C45-C46
150	AP	301	CDL	CA5-C11-C12-C13
153	AJ	501	PC1	C21-C22-C23-C24
153	AA	904	PC1	C11-C12-N-C15
153	DI	303	PC1	C11-C12-N-C15
153	Di	1104	PC1	C11-C12-N-C15
150	CD	301	CDL	C74-C75-C76-C77
150	DR	402	CDL	C73-C74-C75-C76
150	EL	901	CDL	C77-C78-C79-C80
150	Eb	302	CDL	C14-C15-C16-C17
153	DV	405	PC1	C3B-C3C-C3D-C3E
153	Ds	407	PC1	C3C-C3D-C3E-C3F
150	DQ	1504	CDL	C32-C33-C34-C35
150	EK	201	CDL	C34-C35-C36-C37
150	Dx	1201	CDL	C36-C37-C38-C39
153	AA	906	PC1	C3B-C3C-C3D-C3E
153	Dc	609	PC1	C2B-C2C-C2D-C2E
150	DU	403	CDL	O1-C1-CA2-OA2
150	Dq	1402	CDL	O1-C1-CA2-OA2
150	El	901	CDL	O1-C1-CB2-OB2
150	Dd	706	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	E	301	CDL	C55-C56-C57-C58
150	H	1302	CDL	C14-C15-C16-C17
150	c	506	CDL	C61-C62-C63-C64
150	DO	501	CDL	C80-C81-C82-C83
153	Dc	603	PC1	C34-C35-C36-C37
167	EL	905	UQ8	C2-C3-O3-C3M
167	EL	905	UQ8	C5-C4-O4-C4M
167	EN	1205	UQ8	C2-C3-O3-C3M
167	Ds	404	UQ8	C2-C3-O3-C3M
150	c	506	CDL	C71-C72-C73-C74
150	Di	1101	CDL	C15-C16-C17-C18
150	Dn	501	CDL	C12-C13-C14-C15
150	Dx	1201	CDL	C71-C72-C73-C74
150	DR	403	CDL	OB9-CB7-OB8-CB6
150	c	506	CDL	C34-C35-C36-C37
150	c	509	CDL	C44-C45-C46-C47
150	DD	706	CDL	C34-C35-C36-C37
150	EA	301	CDL	C64-C65-C66-C67
150	Dg	202	CDL	C13-C14-C15-C16
150	AC	801	CDL	C14-C15-C16-C17
150	DO	501	CDL	C71-C72-C73-C74
150	EO	202	CDL	C58-C59-C60-C61
150	Dn	502	CDL	C73-C74-C75-C76
150	El	901	CDL	C40-C41-C42-C43
153	D	402	PC1	C3E-C3F-C3G-C3H
150	DJ	307	CDL	C72-C71-CB7-OB8
150	c	506	CDL	C73-C74-C75-C76
150	DQ	1501	CDL	C81-C82-C83-C84
150	DU	403	CDL	C52-C53-C54-C55
150	A1	402	CDL	CB6-CB4-OB6-CB5
150	AA	908	CDL	CB3-CB4-OB6-CB5
150	AM	301	CDL	CB3-CB4-OB6-CB5
150	BY	201	CDL	CB6-CB4-OB6-CB5
150	CG	302	CDL	CB6-CB4-OB6-CB5
150	CC	305	CDL	CA6-CA4-OA6-CA5
150	CD	301	CDL	CB3-CB4-OB6-CB5
150	H	1302	CDL	CA6-CA4-OA6-CA5
150	c	509	CDL	CA3-CA4-OA6-CA5
150	c	509	CDL	CA6-CA4-OA6-CA5
150	DD	704	CDL	CB3-CB4-OB6-CB5
150	DS	401	CDL	CB3-CB4-OB6-CB5
150	DV	401	CDL	CB6-CB4-OB6-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dc	601	CDL	CB6-CB4-OB6-CB5
150	Dd	704	CDL	CB3-CB4-OB6-CB5
150	Ds	402	CDL	CB3-CB4-OB6-CB5
150	Dv	401	CDL	CB6-CB4-OB6-CB5
150	Ea	501	CDL	CB6-CB4-OB6-CB5
150	Ea	502	CDL	CA6-CA4-OA6-CA5
150	Eb	302	CDL	CA6-CA4-OA6-CA5
150	Eh	1601	CDL	CB3-CB4-OB6-CB5
153	A1	403	PC1	C1-C2-O21-C21
153	AM	302	PC1	C3-C2-O21-C21
153	DC	608	PC1	C1-C2-O21-C21
153	EO	206	PC1	C1-C2-O21-C21
153	Dc	605	PC1	C3-C2-O21-C21
153	Dv	405	PC1	C1-C2-O21-C21
155	BP	201	3PE	C3-C2-O21-C21
155	DC	606	3PE	C1-C2-O21-C21
155	EO	203	3PE	C1-C2-O21-C21
155	Dr	401	3PE	C1-C2-O21-C21
150	BT	204	CDL	OB5-CB3-CB4-CB6
150	DD	706	CDL	OA5-CA3-CA4-CA6
150	DN	507	CDL	OA5-CA3-CA4-CA6
150	DO	501	CDL	OB5-CB3-CB4-CB6
150	DV	403	CDL	OB5-CB3-CB4-CB6
150	Da	709	CDL	OB5-CB3-CB4-CB6
150	Dd	706	CDL	OA5-CA3-CA4-CA6
150	Ea	501	CDL	OA5-CA3-CA4-CA6
150	Eg	101	CDL	OA5-CA3-CA4-CA6
150	Eh	1601	CDL	OA5-CA3-CA4-CA6
153	AQ	202	PC1	O11-C1-C2-C3
153	c	507	PC1	O11-C1-C2-C3
150	DM	501	CDL	C54-C55-C56-C57
150	Dn	501	CDL	C40-C41-C42-C43
150	C	507	CDL	OB7-CB5-OB6-CB4
150	Di	1101	CDL	OB7-CB5-OB6-CB4
153	Dx	1205	PC1	O22-C21-O21-C2
150	DR	403	CDL	C71-CB7-OB8-CB6
150	Dq	1401	CDL	C32-C33-C34-C35
150	Dq	1401	CDL	C59-C60-C61-C62
150	ES	1101	CDL	CA7-C31-C32-C33
150	Dn	502	CDL	CA5-C11-C12-C13
150	BE	201	CDL	C51-C52-C53-C54
153	A	1201	PC1	C3C-C3D-C3E-C3F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Eb	303	PC1	C34-C35-C36-C37
150	BE	201	CDL	OA9-CA7-OA8-CA6
150	Dd	705	CDL	OB9-CB7-OB8-CB6
150	Eb	302	CDL	OA9-CA7-OA8-CA6
150	DR	402	CDL	C31-C32-C33-C34
150	Dh	202	CDL	C79-C80-C81-C82
153	AA	906	PC1	C2C-C2D-C2E-C2F
155	El	905	3PE	C33-C34-C35-C36
150	BG	201	CDL	C63-C64-C65-C66
150	DJ	304	CDL	C1-CB2-OB2-PB2
150	ES	1101	CDL	C1-CB2-OB2-PB2
150	Dg	201	CDL	C1-CB2-OB2-PB2
150	Do	501	CDL	C1-CA2-OA2-PA1
156	AC	803	LPP	C6-O5-P1-O3
150	AM	301	CDL	C75-C76-C77-C78
150	Dn	501	CDL	C78-C79-C80-C81
153	c	503	PC1	C29-C2A-C2B-C2C
155	Ds	403	3PE	C28-C29-C2A-C2B
150	BE	201	CDL	C31-CA7-OA8-CA6
150	BY	201	CDL	C71-CB7-OB8-CB6
150	DN	503	CDL	OA9-CA7-OA8-CA6
150	Ea	501	CDL	OB5-CB3-CB4-OB6
153	AM	302	PC1	O11-C1-C2-O21
153	AU	201	PC1	O11-C1-C2-O21
153	Dc	609	PC1	O11-C1-C2-O21
150	DG	202	CDL	C17-C18-C19-C20
150	DH	201	CDL	C17-C18-C19-C20
150	DN	506	CDL	C81-C82-C83-C84
150	Di	1103	CDL	C62-C63-C64-C65
153	EN	1203	PC1	C11-C12-N-C15
153	EO	205	PC1	C11-C12-N-C14
150	CG	302	CDL	C12-C13-C14-C15
150	DD	704	CDL	C14-C15-C16-C17
150	ED	601	CDL	C51-C52-C53-C54
150	Dj	401	CDL	C59-C60-C61-C62
150	Dq	1403	CDL	C78-C79-C80-C81
153	A9	603	PC1	C3D-C3E-C3F-C3G
153	C	510	PC1	C3B-C3C-C3D-C3E
155	BA	301	3PE	C2B-C2C-C2D-C2E
167	C	511	UQ8	C23-C24-C26-C27
150	BY	201	CDL	OB9-CB7-OB8-CB6
150	CD	301	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dc	603	PC1	C3B-C3C-C3D-C3E
168	C	502	HEM	C2D-C3D-CAD-CBD
156	AL	304	LPP	C14-C15-C16-C17
150	Ei	401	CDL	C52-C51-CB5-OB6
156	DA	710	LPP	O27-C29-C30-C31
150	AF	402	CDL	C77-C78-C79-C80
150	Ds	402	CDL	C55-C56-C57-C58
150	DD	704	CDL	C74-C75-C76-C77
150	Ds	401	CDL	C59-C60-C61-C62
150	Dx	1204	CDL	C57-C58-C59-C60
150	C	507	CDL	C51-CB5-OB6-CB4
150	Dd	706	CDL	C51-CB5-OB6-CB4
150	Di	1101	CDL	C51-CB5-OB6-CB4
150	Dd	706	CDL	C39-C40-C41-C42
150	El	901	CDL	C11-C12-C13-C14
150	El	901	CDL	C77-C78-C79-C80
167	El	906	UQ8	C39-C41-C42-C43
150	DH	201	CDL	C77-C78-C79-C80
150	EL	902	CDL	C12-C13-C14-C15
150	B1	402	CDL	OA6-CA4-CA6-OA8
150	C	507	CDL	OA6-CA4-CA6-OA8
150	DC	601	CDL	OA6-CA4-CA6-OA8
150	DG	201	CDL	OB6-CB4-CB6-OB8
150	DH	202	CDL	OB6-CB4-CB6-OB8
150	DN	503	CDL	OB6-CB4-CB6-OB8
150	Dc	601	CDL	OA6-CA4-CA6-OA8
150	Dq	1401	CDL	OA6-CA4-CA6-OA8
150	Du	402	CDL	OB6-CB4-CB6-OB8
150	Eu	101	CDL	OB6-CB4-CB6-OB8
150	BG	201	CDL	C71-C72-C73-C74
150	BV	201	CDL	C51-C52-C53-C54
150	DN	506	CDL	C84-C85-C86-C87
150	ED	605	CDL	C80-C81-C82-C83
153	c	503	PC1	C27-C28-C29-C2A
150	DU	404	CDL	C71-CB7-OB8-CB6
150	AA	901	CDL	CA2-OA2-PA1-OA5
150	AC	802	CDL	CA3-OA5-PA1-OA2
150	B0	102	CDL	CA2-OA2-PA1-OA5
150	B0	102	CDL	CB2-OB2-PB2-OB5
150	BL	301	CDL	CB3-OB5-PB2-OB2
150	BT	202	CDL	CA2-OA2-PA1-OA5
150	BV	201	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	BY	201	CDL	CA2-OA2-PA1-OA5
150	C	503	CDL	CB3-OB5-PB2-OB2
150	C	506	CDL	CA3-OA5-PA1-OA2
150	C	507	CDL	CA2-OA2-PA1-OA5
150	c	509	CDL	CB3-OB5-PB2-OB2
150	DD	705	CDL	CA3-OA5-PA1-OA2
150	DG	201	CDL	CB2-OB2-PB2-OB5
150	DH	201	CDL	CA2-OA2-PA1-OA5
150	DH	201	CDL	CB2-OB2-PB2-OB5
150	DI	302	CDL	CA2-OA2-PA1-OA5
150	DJ	302	CDL	CA2-OA2-PA1-OA5
150	DJ	307	CDL	CA2-OA2-PA1-OA5
150	DM	501	CDL	CA3-OA5-PA1-OA2
150	DQ	1501	CDL	CA2-OA2-PA1-OA5
150	DQ	1504	CDL	CB3-OB5-PB2-OB2
150	DS	405	CDL	CB2-OB2-PB2-OB5
150	DU	402	CDL	CA2-OA2-PA1-OA5
150	DU	404	CDL	CA3-OA5-PA1-OA2
150	DV	401	CDL	CB2-OB2-PB2-OB5
150	DV	402	CDL	CB3-OB5-PB2-OB2
150	DY	301	CDL	CA2-OA2-PA1-OA5
150	DY	301	CDL	CB3-OB5-PB2-OB2
150	EB	302	CDL	CA2-OA2-PA1-OA5
150	EB	302	CDL	CB3-OB5-PB2-OB2
150	ED	601	CDL	CA3-OA5-PA1-OA2
150	ED	601	CDL	CB3-OB5-PB2-OB2
150	ED	604	CDL	CA2-OA2-PA1-OA5
150	EI	401	CDL	CA2-OA2-PA1-OA5
150	EL	901	CDL	CA3-OA5-PA1-OA2
150	EL	901	CDL	CB3-OB5-PB2-OB2
150	EN	1201	CDL	CB2-OB2-PB2-OB5
150	EN	1202	CDL	CA2-OA2-PA1-OA5
150	EN	1202	CDL	CB2-OB2-PB2-OB5
150	Dd	705	CDL	CB3-OB5-PB2-OB2
150	Dg	201	CDL	CB2-OB2-PB2-OB5
150	Dg	202	CDL	CA3-OA5-PA1-OA2
150	Dh	201	CDL	CA2-OA2-PA1-OA5
150	Dh	201	CDL	CA3-OA5-PA1-OA2
150	Dj	403	CDL	CB3-OB5-PB2-OB2
150	Dm	501	CDL	CA2-OA2-PA1-OA5
150	Dm	502	CDL	CA2-OA2-PA1-OA5
150	Dm	502	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dn	501	CDL	CB2-OB2-PB2-OB5
150	Dn	501	CDL	CB3-OB5-PB2-OB2
150	Ds	401	CDL	CA2-OA2-PA1-OA5
150	Ds	401	CDL	CB2-OB2-PB2-OB5
150	Du	403	CDL	CA2-OA2-PA1-OA5
150	Du	403	CDL	CA3-OA5-PA1-OA2
150	Dy	301	CDL	CA2-OA2-PA1-OA5
150	Dy	301	CDL	CB3-OB5-PB2-OB2
150	Ei	401	CDL	CA3-OA5-PA1-OA2
150	Ep	701	CDL	CB2-OB2-PB2-OB5
150	Eu	101	CDL	CA2-OA2-PA1-OA5
153	A6	302	PC1	C11-O13-P-O11
153	A9	601	PC1	C1-O11-P-O13
153	AA	904	PC1	C1-O11-P-O13
153	AC	804	PC1	C1-O11-P-O13
153	D	402	PC1	C1-O11-P-O13
153	Dv	406	PC1	C1-O11-P-O13
153	Eb	303	PC1	C1-O11-P-O13
153	Ef	501	PC1	C11-O13-P-O11
155	BP	201	3PE	C11-O13-P-O11
155	DI	301	3PE	C11-O13-P-O11
155	DR	401	3PE	C1-O11-P-O13
155	DX	302	3PE	C1-O11-P-O13
155	Di	1102	3PE	C11-O13-P-O11
155	Ds	408	3PE	C1-O11-P-O13
155	Eo	202	3PE	C11-O13-P-O11
150	AF	401	CDL	C84-C85-C86-C87
150	BT	204	CDL	C12-C13-C14-C15
150	Dh	202	CDL	C52-C53-C54-C55
155	DG	205	3PE	C29-C2A-C2B-C2C
155	Ds	403	3PE	C34-C35-C36-C37
155	El	905	3PE	C2F-C2G-C2H-C2I
150	g	801	CDL	C39-C40-C41-C42
150	EN	1201	CDL	C12-C13-C14-C15
150	Di	1103	CDL	C76-C77-C78-C79
153	AA	906	PC1	C3D-C3E-C3F-C3G
150	H	1301	CDL	C14-C15-C16-C17
150	DR	403	CDL	C34-C35-C36-C37
150	Dh	202	CDL	C20-C21-C22-C23
153	Dy	302	PC1	C3B-C3C-C3D-C3E
156	DA	710	LPP	C18-C19-C20-C21
150	Du	403	CDL	CA4-CA6-OA8-CA7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DA	706	CDL	C63-C64-C65-C66
150	DM	502	CDL	C12-C13-C14-C15
150	EO	202	CDL	C71-C72-C73-C74
150	Dg	202	CDL	C75-C76-C77-C78
150	Dv	401	CDL	C78-C79-C80-C81
150	El	901	CDL	C18-C19-C20-C21
153	Dv	405	PC1	C32-C33-C34-C35
150	B0	101	CDL	CB3-CB4-CB6-OB8
150	BL	301	CDL	CB3-CB4-CB6-OB8
150	g	801	CDL	CA3-CA4-CA6-OA8
150	DO	501	CDL	CA3-CA4-CA6-OA8
150	EA	301	CDL	CA3-CA4-CA6-OA8
150	ED	601	CDL	CA3-CA4-CA6-OA8
150	Dr	402	CDL	CB3-CB4-CB6-OB8
153	A1	403	PC1	C1-C2-C3-O31
153	AM	302	PC1	C1-C2-C3-O31
167	Ed	202	UQ8	C40-C39-C41-C42
167	El	906	UQ8	C12-C11-C9-C10
150	Dn	502	CDL	C75-C76-C77-C78
150	DM	502	CDL	C60-C61-C62-C63
150	DV	403	CDL	C34-C35-C36-C37
153	E	303	PC1	C3D-C3E-C3F-C3G
153	d	801	PC1	C3B-C3C-C3D-C3E
150	c	509	CDL	C32-C31-CA7-OA8
153	AJ	501	PC1	O21-C21-C22-C23
150	CC	305	CDL	C12-C13-C14-C15
150	h	501	CDL	C57-C58-C59-C60
150	DM	501	CDL	C61-C62-C63-C64
150	Eu	101	CDL	C51-C52-C53-C54
150	Ed	205	CDL	C51-CB5-OB6-CB4
150	DU	403	CDL	C20-C21-C22-C23
150	Ep	701	CDL	C57-C58-C59-C60
150	C	506	CDL	CA5-C11-C12-C13
150	C	505	CDL	C14-C15-C16-C17
150	DC	601	CDL	C60-C61-C62-C63
150	DD	705	CDL	C37-C38-C39-C40
150	Du	403	CDL	C73-C74-C75-C76
167	C	511	UQ8	C5-C4-O4-C4M
167	DS	403	UQ8	C5-C4-O4-C4M
150	C	506	CDL	C23-C24-C25-C26
150	DD	705	CDL	C13-C14-C15-C16
150	Dd	704	CDL	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dj	403	CDL	C35-C36-C37-C38
153	AQ	202	PC1	C3B-C3C-C3D-C3E
153	C	508	PC1	C28-C29-C2A-C2B
150	EK	201	CDL	CA5-C11-C12-C13
155	CD	303	3PE	C21-C22-C23-C24
150	C	504	CDL	C11-C12-C13-C14
150	DD	706	CDL	C56-C57-C58-C59
150	DN	506	CDL	C18-C19-C20-C21
150	EN	1202	CDL	C12-C13-C14-C15
150	El	903	CDL	C84-C85-C86-C87
153	AL	303	PC1	C23-C24-C25-C26
153	Eo	201	PC1	C3F-C3G-C3H-C3I
150	Dn	506	CDL	C59-C60-C61-C62
153	AL	303	PC1	C29-C2A-C2B-C2C
153	c	503	PC1	C2A-C2B-C2C-C2D
150	DC	601	CDL	C31-CA7-OA8-CA6
153	AU	202	PC1	C32-C31-O31-C3
150	DI	302	CDL	O1-C1-CB2-OB2
150	A0	601	CDL	C1-CA2-OA2-PA1
150	AM	301	CDL	CB4-CB3-OB5-PB2
150	B1	402	CDL	C1-CA2-OA2-PA1
150	C	503	CDL	C1-CA2-OA2-PA1
150	c	502	CDL	CB4-CB3-OB5-PB2
150	DN	502	CDL	CB4-CB3-OB5-PB2
150	DV	401	CDL	C1-CA2-OA2-PA1
150	DV	401	CDL	CB4-CB3-OB5-PB2
150	DV	402	CDL	C1-CB2-OB2-PB2
150	DV	403	CDL	CB4-CB3-OB5-PB2
150	ED	601	CDL	C1-CB2-OB2-PB2
150	ED	605	CDL	C1-CB2-OB2-PB2
150	EL	902	CDL	CA4-CA3-OA5-PA1
150	Dd	702	CDL	CB4-CB3-OB5-PB2
150	Dd	704	CDL	CB4-CB3-OB5-PB2
150	Dm	501	CDL	C1-CA2-OA2-PA1
150	Dq	1401	CDL	C1-CA2-OA2-PA1
150	Dr	403	CDL	CA4-CA3-OA5-PA1
150	Dr	403	CDL	C1-CB2-OB2-PB2
150	Ea	501	CDL	CA4-CA3-OA5-PA1
153	AL	303	PC1	C2-C1-O11-P
155	DX	303	3PE	C2-C1-O11-P
155	Dd	703	3PE	C2-C1-O11-P
150	CC	304	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Eb	301	PC1	C3C-C3D-C3E-C3F
155	DI	301	3PE	C34-C35-C36-C37
169	DA	703	HEA	CAA-CBA-CGA-O1A
150	c	509	CDL	C35-C36-C37-C38
150	DS	404	CDL	C78-C79-C80-C81
153	DA	707	PC1	C35-C36-C37-C38
150	AM	301	CDL	CB4-CB6-OB8-CB7
150	Dv	401	CDL	C72-C71-CB7-OB9
150	C	504	CDL	C13-C14-C15-C16
150	Dq	1403	CDL	C59-C60-C61-C62
150	BL	301	CDL	CB2-C1-CA2-OA2
150	E	301	CDL	CA2-C1-CB2-OB2
150	DG	201	CDL	CA2-C1-CB2-OB2
150	DH	202	CDL	CA2-C1-CB2-OB2
150	Dc	608	CDL	CA2-C1-CB2-OB2
150	Dd	706	CDL	OA7-CA5-OA6-CA4
150	Dn	506	CDL	OA7-CA5-OA6-CA4
150	Ed	205	CDL	OB7-CB5-OB6-CB4
150	DN	502	CDL	C61-C62-C63-C64
150	Dc	608	CDL	C12-C13-C14-C15
155	Dx	1208	3PE	C2B-C2C-C2D-C2E
150	Dh	202	CDL	CB7-C71-C72-C73
150	Dn	503	CDL	CB5-C51-C52-C53
150	Dr	403	CDL	CB7-C71-C72-C73
150	A1	402	CDL	C11-C12-C13-C14
150	DS	404	CDL	C32-C33-C34-C35
150	DU	403	CDL	C33-C34-C35-C36
150	DV	403	CDL	C14-C15-C16-C17
150	Dn	503	CDL	C23-C24-C25-C26
150	C	503	CDL	C71-CB7-OB8-CB6
150	c	506	CDL	C71-CB7-OB8-CB6
150	EB	302	CDL	C31-CA7-OA8-CA6
150	Eg	101	CDL	C71-CB7-OB8-CB6
150	AC	802	CDL	C17-C18-C19-C20
150	DR	402	CDL	C43-C44-C45-C46
156	AA	902	LPP	C34-C35-C36-C37
150	DC	601	CDL	OA9-CA7-OA8-CA6
150	AM	301	CDL	C39-C40-C41-C42
150	DQ	1504	CDL	C75-C76-C77-C78
150	AC	801	CDL	C59-C60-C61-C62
150	DN	507	CDL	C53-C54-C55-C56
150	DS	404	CDL	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DU	401	CDL	C71-C72-C73-C74
150	Dc	608	CDL	C17-C18-C19-C20
150	Dx	1201	CDL	C57-C58-C59-C60
150	C	503	CDL	OB9-CB7-OB8-CB6
150	DU	404	CDL	OB9-CB7-OB8-CB6
150	DS	401	CDL	CB5-C51-C52-C53
150	B0	102	CDL	C17-C18-C19-C20
150	c	502	CDL	C19-C20-C21-C22
150	DJ	303	CDL	C20-C21-C22-C23
150	CC	305	CDL	OA5-CA3-CA4-CA6
150	CD	302	CDL	OA5-CA3-CA4-CA6
150	DV	403	CDL	OA5-CA3-CA4-CA6
150	Dv	402	CDL	OA5-CA3-CA4-CA6
153	DX	308	PC1	O11-C1-C2-C3
167	c	510	UQ8	C9-C11-C12-C13
150	EN	1201	CDL	C11-C12-C13-C14
150	EO	202	CDL	C59-C60-C61-C62
150	Dx	1201	CDL	C81-C82-C83-C84
153	K	501	PC1	C22-C23-C24-C25
155	Dr	401	3PE	O13-C11-C12-N
150	Eb	302	CDL	C32-C33-C34-C35
155	EN	1204	3PE	C36-C37-C38-C39
150	BV	201	CDL	OB5-CB3-CB4-OB6
150	C	503	CDL	OA5-CA3-CA4-OA6
150	DZ	501	CDL	OB5-CB3-CB4-OB6
153	A	1201	PC1	O11-C1-C2-O21
153	Ds	407	PC1	O11-C1-C2-O21
155	DG	205	3PE	O11-C1-C2-O21
167	c	510	UQ8	C26-C27-C28-C29
167	DS	403	UQ8	C31-C32-C33-C34
150	CJ	201	CDL	C72-C73-C74-C75
150	Dn	502	CDL	C74-C75-C76-C77
150	Du	402	CDL	C44-C45-C46-C47
153	AA	903	PC1	C23-C24-C25-C26
150	EB	302	CDL	OA9-CA7-OA8-CA6
150	DN	503	CDL	C44-C45-C46-C47
150	EL	902	CDL	C55-C56-C57-C58
150	Dh	201	CDL	C40-C41-C42-C43
153	AA	907	PC1	C29-C2A-C2B-C2C
150	DH	202	CDL	CB7-C71-C72-C73
150	DX	306	CDL	CA5-C11-C12-C13
150	Dc	608	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dg	202	CDL	C40-C41-C42-C43
150	Dj	401	CDL	C57-C58-C59-C60
150	Ds	405	CDL	C79-C80-C81-C82
150	DM	501	CDL	C12-C13-C14-C15
150	DX	301	CDL	C78-C79-C80-C81
153	A2	402	PC1	C3D-C3E-C3F-C3G
150	c	506	CDL	OB9-CB7-OB8-CB6
150	Eg	101	CDL	OB9-CB7-OB8-CB6
153	AU	202	PC1	O32-C31-O31-C3
150	CG	301	CDL	CA5-C11-C12-C13
150	BT	204	CDL	C24-C25-C26-C27
150	c	501	CDL	C24-C25-C26-C27
150	DJ	302	CDL	C33-C34-C35-C36
150	DX	301	CDL	C34-C35-C36-C37
153	DC	604	PC1	C27-C28-C29-C2A
150	AA	901	CDL	O1-C1-CA2-OA2
150	AC	802	CDL	O1-C1-CA2-OA2
150	DU	401	CDL	O1-C1-CB2-OB2
155	BP	201	3PE	O22-C21-O21-C2
150	A1	402	CDL	C17-C18-C19-C20
150	DA	709	CDL	C77-C78-C79-C80
150	Dn	503	CDL	C73-C74-C75-C76
150	Du	403	CDL	C13-C14-C15-C16
150	DH	201	CDL	C12-C13-C14-C15
150	DH	201	CDL	C60-C61-C62-C63
150	EH	1601	CDL	C64-C65-C66-C67
150	BE	201	CDL	CA5-C11-C12-C13
150	DH	201	CDL	CB5-C51-C52-C53
150	Dd	702	CDL	C80-C81-C82-C83
150	Ea	502	CDL	C37-C38-C39-C40
150	El	901	CDL	C19-C20-C21-C22
150	EL	902	CDL	C33-C34-C35-C36
150	Dh	202	CDL	C55-C56-C57-C58
155	A9	602	3PE	C2E-C2F-C2G-C2H
155	C	513	3PE	C33-C34-C35-C36
150	c	506	CDL	OA6-CA4-CA6-OA8
150	Ed	205	CDL	OA6-CA4-CA6-OA8
153	Dv	407	PC1	O21-C2-C3-O31
155	A2	401	3PE	O21-C2-C3-O31
150	BT	202	CDL	C59-C60-C61-C62
150	CG	301	CDL	C56-C57-C58-C59
150	DD	706	CDL	C76-C77-C78-C79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dv	405	PC1	O31-C31-C32-C33
167	C	512	UQ8	C31-C32-C33-C34
150	C	505	CDL	C57-C58-C59-C60
150	DX	306	CDL	C13-C14-C15-C16
150	EB	302	CDL	C11-C12-C13-C14
150	BY	201	CDL	CA4-CA3-OA5-PA1
150	CJ	201	CDL	CA4-CA3-OA5-PA1
150	DD	703	CDL	CB4-CB3-OB5-PB2
150	EL	901	CDL	CB4-CB3-OB5-PB2
150	Eh	1601	CDL	CB4-CB3-OB5-PB2
153	El	904	PC1	C2-C1-O11-P
156	Dn	505	LPP	C7-C6-O5-P1
160	AD	502	FMN	C4'-C5'-O5'-P
150	AC	802	CDL	C34-C35-C36-C37
150	DI	302	CDL	C73-C74-C75-C76
150	EO	202	CDL	C13-C14-C15-C16
150	H	1302	CDL	OB7-CB5-OB6-CB4
150	DJ	303	CDL	OB7-CB5-OB6-CB4
153	K	501	PC1	O22-C21-O21-C2
167	El	906	UQ8	C2-C3-O3-C3M
150	Dj	407	CDL	C72-C71-CB7-OB8
153	DC	608	PC1	O31-C31-C32-C33
150	Dy	301	CDL	C57-C58-C59-C60
150	El	902	CDL	C55-C56-C57-C58
155	Dx	1207	3PE	C3F-C3G-C3H-C3I
150	c	506	CDL	CA4-CA6-OA8-CA7
150	c	501	CDL	C22-C23-C24-C25
150	DZ	501	CDL	C19-C20-C21-C22
150	EK	201	CDL	C15-C16-C17-C18
150	EN	1201	CDL	C62-C63-C64-C65
150	EO	202	CDL	C40-C41-C42-C43
155	Di	1102	3PE	C3A-C3B-C3C-C3D
169	Da	703	HEA	CAA-CBA-CGA-O1A
167	DS	403	UQ8	C40-C39-C41-C42
167	Ds	404	UQ8	C40-C39-C41-C42
150	A1	402	CDL	C71-C72-C73-C74
150	Dg	201	CDL	C18-C19-C20-C21
150	Dm	502	CDL	C38-C39-C40-C41
153	Dg	203	PC1	C3F-C3G-C3H-C3I
150	BT	204	CDL	C11-C12-C13-C14
150	Dq	1401	CDL	C71-C72-C73-C74
155	Dr	404	3PE	C29-C2A-C2B-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	AJ	502	3PE	O21-C21-C22-C23
150	H	1301	CDL	C39-C40-C41-C42
150	DX	301	CDL	C17-C18-C19-C20
153	D	402	PC1	C24-C25-C26-C27
155	DR	401	3PE	C3D-C3E-C3F-C3G
168	C	502	HEM	CAA-CBA-CGA-O1A
161	AS	200	8Q1	O40-C39-N41-C42
150	AC	801	CDL	C79-C80-C81-C82
150	CG	302	CDL	C77-C78-C79-C80
150	C	503	CDL	C73-C74-C75-C76
150	C	506	CDL	C63-C64-C65-C66
150	Dj	401	CDL	C12-C13-C14-C15
150	Du	403	CDL	C84-C85-C86-C87
150	Dv	402	CDL	C12-C13-C14-C15
156	DA	710	LPP	C17-C18-C19-C20
150	CC	304	CDL	C43-C44-C45-C46
150	DJ	304	CDL	C34-C35-C36-C37
150	DJ	305	CDL	C14-C15-C16-C17
150	Di	1101	CDL	C62-C63-C64-C65
150	Dn	502	CDL	C61-C62-C63-C64
150	CJ	201	CDL	CA3-CA4-CA6-OA8
150	C	503	CDL	CB3-CB4-CB6-OB8
150	c	502	CDL	CB2-C1-CA2-OA2
150	Dd	702	CDL	CA2-C1-CB2-OB2
150	Dd	706	CDL	CB3-CB4-CB6-OB8
150	Dj	404	CDL	CA3-CA4-CA6-OA8
150	Ds	402	CDL	CB3-CB4-CB6-OB8
150	Ds	405	CDL	CB3-CB4-CB6-OB8
153	AA	905	PC1	C1-C2-C3-O31
153	Dv	407	PC1	C1-C2-C3-O31
153	Eo	204	PC1	C1-C2-C3-O31
155	Ds	403	3PE	C1-C2-C3-O31
153	CC	302	PC1	O22-C21-O21-C2
150	BC	302	CDL	C36-C37-C38-C39
150	DQ	1501	CDL	C54-C55-C56-C57
150	Ds	405	CDL	C82-C83-C84-C85
150	Eg	101	CDL	C22-C23-C24-C25
150	ED	605	CDL	CB7-C71-C72-C73
150	BT	202	CDL	C16-C17-C18-C19
150	Ea	502	CDL	C60-C61-C62-C63
150	AA	901	CDL	C13-C14-C15-C16
150	DC	601	CDL	C77-C78-C79-C80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DJ	307	CDL	C15-C16-C17-C18
150	DJ	307	CDL	C57-C58-C59-C60
150	DQ	1501	CDL	O1-C1-CB2-OB2
150	DI	302	CDL	C57-C58-C59-C60
150	DQ	1502	CDL	C78-C79-C80-C81
150	H	1301	CDL	C37-C38-C39-C40
150	DN	507	CDL	C81-C82-C83-C84
150	Dq	1402	CDL	C21-C22-C23-C24
153	AU	202	PC1	C3B-C3C-C3D-C3E
153	Eo	201	PC1	C33-C34-C35-C36
150	BC	301	CDL	C11-C12-C13-C14
150	C	503	CDL	C52-C53-C54-C55
153	A2	402	PC1	C33-C34-C35-C36
155	DX	303	3PE	C3F-C3G-C3H-C3I
150	El	902	CDL	CB4-CB6-OB8-CB7
150	Dr	403	CDL	CA7-C31-C32-C33
150	Ed	204	CDL	CA5-C11-C12-C13
150	AF	402	CDL	C51-C52-C53-C54
150	BC	301	CDL	C71-C72-C73-C74
150	c	502	CDL	C32-C33-C34-C35
150	DY	301	CDL	C20-C21-C22-C23
150	Dj	403	CDL	C44-C45-C46-C47
150	Dq	1401	CDL	C60-C61-C62-C63
150	Dr	402	CDL	C74-C75-C76-C77
150	c	501	CDL	CA6-CA4-OA6-CA5
150	DJ	307	CDL	CB6-CB4-OB6-CB5
150	DN	506	CDL	CA3-CA4-OA6-CA5
150	DQ	1504	CDL	CA6-CA4-OA6-CA5
150	EK	201	CDL	CB3-CB4-OB6-CB5
150	EO	202	CDL	CB3-CB4-OB6-CB5
150	EO	202	CDL	CB6-CB4-OB6-CB5
150	Da	709	CDL	CA3-CA4-OA6-CA5
150	Dg	201	CDL	CA3-CA4-OA6-CA5
150	Dn	506	CDL	CA3-CA4-OA6-CA5
150	Do	501	CDL	CB3-CB4-OB6-CB5
150	Do	501	CDL	CB6-CB4-OB6-CB5
150	Dq	1401	CDL	CA6-CA4-OA6-CA5
150	Dq	1402	CDL	CA6-CA4-OA6-CA5
150	Du	403	CDL	CB3-CB4-OB6-CB5
150	Dv	401	CDL	CB3-CB4-OB6-CB5
153	A1	403	PC1	C3-C2-O21-C21
153	AQ	202	PC1	C1-C2-O21-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	C	508	PC1	C3-C2-O21-C21
153	Db	702	PC1	C1-C2-O21-C21
153	Dc	609	PC1	C1-C2-O21-C21
153	Dc	609	PC1	C3-C2-O21-C21
153	Eo	205	PC1	C1-C2-O21-C21
153	Eo	205	PC1	C3-C2-O21-C21
167	C	512	UQ8	C35-C34-C36-C37
167	EN	1205	UQ8	C12-C11-C9-C10
167	En	1202	UQ8	C35-C34-C36-C37
150	Dh	201	CDL	C17-C18-C19-C20
150	Di	1101	CDL	C63-C64-C65-C66
150	Dn	501	CDL	C52-C53-C54-C55
150	Dy	301	CDL	C15-C16-C17-C18
153	AU	202	PC1	C3E-C3F-C3G-C3H
153	EN	1203	PC1	C11-C12-N-C14
153	Eo	204	PC1	C11-C12-N-C14
150	DD	706	CDL	OB7-CB5-OB6-CB4
153	DQ	1503	PC1	O22-C21-O21-C2
153	K	501	PC1	C22-C21-O21-C2
150	DH	202	CDL	C79-C80-C81-C82
150	EN	1202	CDL	C33-C34-C35-C36
150	Dv	402	CDL	C11-C12-C13-C14
155	DJ	301	3PE	C3C-C3D-C3E-C3F
150	DX	301	CDL	CA7-C31-C32-C33
150	CG	301	CDL	C20-C21-C22-C23
150	c	501	CDL	C57-C58-C59-C60
150	Dq	1403	CDL	C60-C61-C62-C63
150	A1	402	CDL	CB3-OB5-PB2-OB2
150	AC	802	CDL	CA2-OA2-PA1-OA5
150	H	1302	CDL	CB2-OB2-PB2-OB5
150	DJ	304	CDL	CB3-OB5-PB2-OB2
150	Dj	405	CDL	CA2-OA2-PA1-OA5
150	Ds	406	CDL	CA3-OA5-PA1-OA2
150	Du	401	CDL	CA3-OA5-PA1-OA2
150	Dv	402	CDL	CB2-OB2-PB2-OB5
155	Dr	401	3PE	C11-O13-P-O11
167	EL	905	UQ8	C4-C3-O3-C3M
150	AA	901	CDL	C19-C20-C21-C22
150	DS	404	CDL	C82-C83-C84-C85
153	DC	604	PC1	C26-C27-C28-C29
153	Dv	406	PC1	O21-C21-C22-C23
150	DX	307	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
169	DA	703	HEA	CAA-CBA-CGA-O2A
169	Da	703	HEA	CAD-CBD-CGD-O1D
150	DR	403	CDL	C52-C53-C54-C55
150	ES	1101	CDL	C78-C79-C80-C81
150	A0	602	CDL	C12-C13-C14-C15
150	AM	301	CDL	C32-C33-C34-C35
150	ES	1101	CDL	C40-C41-C42-C43
150	Du	402	CDL	C80-C81-C82-C83
150	Ep	701	CDL	C20-C21-C22-C23
150	Eu	101	CDL	C13-C14-C15-C16
150	Dn	503	CDL	CB4-CB3-OB5-PB2
155	DI	301	3PE	C2-C1-O11-P
156	AA	902	LPP	C7-C6-O5-P1
150	Dj	401	CDL	C18-C19-C20-C21
150	Dj	402	CDL	C44-C45-C46-C47
150	H	1301	CDL	OA5-CA3-CA4-OA6
150	DJ	305	CDL	OA5-CA3-CA4-OA6
150	EL	901	CDL	OA5-CA3-CA4-OA6
150	Di	1103	CDL	OB5-CB3-CB4-OB6
150	Dy	301	CDL	OB5-CB3-CB4-OB6
153	DC	608	PC1	O11-C1-C2-O21
155	El	905	3PE	O11-C1-C2-O21
150	A0	602	CDL	C42-C43-C44-C45
150	AP	301	CDL	C11-C12-C13-C14
150	EH	1601	CDL	C13-C14-C15-C16
150	EL	901	CDL	C53-C54-C55-C56
150	Di	1103	CDL	C32-C33-C34-C35
150	Ek	201	CDL	C15-C16-C17-C18
150	DM	501	CDL	OB5-CB3-CB4-CB6
150	DX	306	CDL	OA5-CA3-CA4-CA6
150	ES	1101	CDL	OA5-CA3-CA4-CA6
150	Dj	405	CDL	OB5-CB3-CB4-CB6
150	Do	501	CDL	OB5-CB3-CB4-CB6
150	Eg	101	CDL	OB5-CB3-CB4-CB6
153	e	1101	PC1	O11-C1-C2-C3
153	Db	702	PC1	O11-C1-C2-C3
153	Ds	407	PC1	O11-C1-C2-C3
155	El	905	3PE	O11-C1-C2-C3
150	BC	301	CDL	C13-C14-C15-C16
150	c	502	CDL	C75-C76-C77-C78
150	Dj	402	CDL	C20-C21-C22-C23
150	Eb	302	CDL	C61-C62-C63-C64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AA	906	PC1	C2F-C2G-C2H-C2I
150	Dy	301	CDL	C77-C78-C79-C80
167	C	512	UQ8	C15-C14-C16-C17
150	c	501	CDL	C73-C74-C75-C76
153	k	301	PC1	C23-C24-C25-C26
150	DX	307	CDL	CA5-C11-C12-C13
150	DQ	1504	CDL	O1-C1-CB2-OB2
150	DU	404	CDL	O1-C1-CA2-OA2
150	Dj	404	CDL	O1-C1-CB2-OB2
150	BT	204	CDL	C82-C83-C84-C85
150	DM	501	CDL	C17-C18-C19-C20
150	DS	404	CDL	C18-C19-C20-C21
153	BT	203	PC1	C32-C31-O31-C3
166	CE	401	HEC	CAD-CBD-CGD-O1D
166	CE	401	HEC	CAD-CBD-CGD-O2D
169	DA	703	HEA	CAD-CBD-CGD-O1D
169	DA	703	HEA	CAD-CBD-CGD-O2D
169	Da	702	HEA	CAD-CBD-CGD-O1D
150	DR	402	CDL	C24-C25-C26-C27
155	BT	201	3PE	C23-C24-C25-C26
150	CG	302	CDL	C54-C55-C56-C57
153	AC	804	PC1	C2F-C2G-C2H-C2I
156	Dn	505	LPP	C37-C38-C39-C40
150	EL	901	CDL	OB7-CB5-OB6-CB4
153	Di	1104	PC1	O22-C21-O21-C2
155	Dr	401	3PE	O22-C21-O21-C2
150	DN	507	CDL	C20-C21-C22-C23
150	DS	405	CDL	C78-C79-C80-C81
150	Dd	704	CDL	C59-C60-C61-C62
150	Dr	403	CDL	C62-C63-C64-C65
150	B1	402	CDL	C12-C13-C14-C15
150	c	502	CDL	C40-C41-C42-C43
150	Dd	706	CDL	C34-C35-C36-C37
150	Dj	401	CDL	C60-C61-C62-C63
150	Dj	407	CDL	C32-C33-C34-C35
150	Dq	1401	CDL	C39-C40-C41-C42
150	Dq	1401	CDL	C74-C75-C76-C77
153	BT	203	PC1	O32-C31-O31-C3
150	B0	102	CDL	OB6-CB4-CB6-OB8
150	DQ	1504	CDL	OA6-CA4-CA6-OA8
150	EL	903	CDL	OB6-CB4-CB6-OB8
150	Dd	705	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	D	402	PC1	O21-C2-C3-O31
153	e	1101	PC1	O21-C2-C3-O31
153	Da	707	PC1	O21-C2-C3-O31
153	Ef	501	PC1	O21-C2-C3-O31
155	DC	606	3PE	O21-C2-C3-O31
150	BL	301	CDL	C42-C43-C44-C45
150	BY	201	CDL	C40-C41-C42-C43
150	c	509	CDL	C54-C55-C56-C57
150	Dd	705	CDL	C38-C39-C40-C41
150	Du	401	CDL	C32-C33-C34-C35
150	En	1201	CDL	C14-C15-C16-C17
150	EL	902	CDL	CB4-CB6-OB8-CB7
166	d	802	HEC	CAA-CBA-CGA-O2A
169	Da	702	HEA	CAD-CBD-CGD-O2D
150	DX	307	CDL	OB9-CB7-OB8-CB6
150	DQ	1504	CDL	C72-C73-C74-C75
150	EL	902	CDL	C44-C45-C46-C47
150	Eg	101	CDL	C12-C13-C14-C15
167	EN	1205	UQ8	C11-C12-C13-C14
153	B1	403	PC1	C37-C38-C39-C3A
156	Dl	1101	LPP	C17-C18-C19-C20
150	BL	301	CDL	C71-C72-C73-C74
155	EL	904	3PE	C2F-C2G-C2H-C2I
150	C	505	CDL	CA2-C1-CB2-OB2
150	C	506	CDL	CA2-C1-CB2-OB2
150	DJ	303	CDL	CA2-C1-CB2-OB2
169	Da	703	HEA	CAA-CBA-CGA-O2A
169	Da	703	HEA	CAD-CBD-CGD-O2D
150	DN	503	CDL	CA4-CA6-OA8-CA7
150	DN	502	CDL	C52-C53-C54-C55
150	BV	201	CDL	C13-C14-C15-C16
155	BT	201	3PE	C29-C2A-C2B-C2C
167	DS	403	UQ8	C38-C39-C41-C42
155	Ds	403	3PE	C3E-C3F-C3G-C3H
150	Ds	405	CDL	C18-C19-C20-C21
150	DU	403	CDL	C17-C18-C19-C20
150	DC	601	CDL	C36-C37-C38-C39
155	EM	901	3PE	C25-C26-C27-C28
168	C	502	HEM	CAA-CBA-CGA-O2A
150	c	509	CDL	C32-C33-C34-C35
150	A0	601	CDL	CA4-CA3-OA5-PA1
153	DB	702	PC1	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Eb	303	PC1	C2-C1-O11-P
155	BP	201	3PE	C22-C21-O21-C2
156	Dn	504	LPP	C7-C6-O5-P1
150	DH	201	CDL	C18-C19-C20-C21
153	Dc	605	PC1	O32-C31-O31-C3
150	Dm	502	CDL	O1-C1-CA2-OA2
150	AF	402	CDL	C76-C77-C78-C79
150	DM	502	CDL	C74-C75-C76-C77
150	Dn	502	CDL	C42-C43-C44-C45
150	Dq	1401	CDL	C57-C58-C59-C60
153	Dv	406	PC1	C3B-C3C-C3D-C3E
155	DX	302	3PE	C2B-C2C-C2D-C2E
150	En	1201	CDL	C77-C78-C79-C80
153	DB	702	PC1	O32-C31-O31-C3
150	AC	801	CDL	C41-C42-C43-C44
153	EO	201	PC1	C28-C29-C2A-C2B
150	DM	501	CDL	C52-C51-CB5-OB6
150	Dh	202	CDL	C72-C71-CB7-OB8
153	DS	406	PC1	O31-C31-C32-C33
153	Dc	609	PC1	O31-C31-C32-C33
150	H	1301	CDL	CA3-CA4-CA6-OA8
150	DC	601	CDL	CB3-CB4-CB6-OB8
150	DN	503	CDL	CA3-CA4-CA6-OA8
150	DX	307	CDL	CB3-CB4-CB6-OB8
150	DZ	501	CDL	CA3-CA4-CA6-OA8
150	Dd	705	CDL	CA3-CA4-CA6-OA8
150	Dj	402	CDL	CB3-CB4-CB6-OB8
150	Dq	1403	CDL	CB3-CB4-CB6-OB8
150	Ea	501	CDL	CB3-CB4-CB6-OB8
153	e	1101	PC1	C1-C2-C3-O31
153	g	802	PC1	C38-C39-C3A-C3B
153	Da	707	PC1	C1-C2-C3-O31
150	AF	402	CDL	C79-C80-C81-C82
150	C	504	CDL	C16-C17-C18-C19
150	DJ	303	CDL	C11-C12-C13-C14
150	DQ	1501	CDL	C51-C52-C53-C54
150	ED	601	CDL	C80-C81-C82-C83
150	Dd	705	CDL	C59-C60-C61-C62
150	Di	1101	CDL	C61-C62-C63-C64
150	Dy	301	CDL	C51-C52-C53-C54
155	DX	304	3PE	C35-C36-C37-C38
155	Dr	401	3PE	C3D-C3E-C3F-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dc	605	PC1	C32-C31-O31-C3
150	AC	801	CDL	C73-C74-C75-C76
150	B0	102	CDL	C32-C33-C34-C35
150	C	505	CDL	C71-C72-C73-C74
150	ES	1101	CDL	C44-C45-C46-C47
167	ED	603	UQ8	C25-C24-C26-C27
167	EN	1205	UQ8	C15-C14-C16-C17
167	En	1202	UQ8	C30-C29-C31-C32
169	Da	703	HEA	C27-C19-C20-C21
150	CJ	201	CDL	C51-C52-C53-C54
150	DQ	1501	CDL	C38-C39-C40-C41
150	Du	402	CDL	C39-C40-C41-C42
155	DR	401	3PE	C3F-C3G-C3H-C3I
155	DX	303	3PE	C32-C33-C34-C35
155	Ds	408	3PE	C36-C37-C38-C39
167	Ds	404	UQ8	C38-C39-C41-C42
167	Ed	202	UQ8	C38-C39-C41-C42
167	En	1202	UQ8	C33-C34-C36-C37
150	C	505	CDL	C13-C14-C15-C16
150	Dj	402	CDL	C21-C22-C23-C24
150	Ds	405	CDL	C40-C41-C42-C43
150	Dx	1204	CDL	C14-C15-C16-C17
155	Em	901	3PE	C25-C26-C27-C28
150	Dn	506	CDL	C11-CA5-OA6-CA4
150	Dm	502	CDL	C59-C60-C61-C62
153	Eo	205	PC1	C3D-C3E-C3F-C3G
155	DI	301	3PE	C3A-C3B-C3C-C3D
167	Ds	404	UQ8	C31-C32-C33-C34
150	BL	301	CDL	C11-C12-C13-C14
150	E	301	CDL	C11-C12-C13-C14
150	H	1302	CDL	C36-C37-C38-C39
150	DD	706	CDL	C11-C12-C13-C14
150	DV	402	CDL	C77-C78-C79-C80
150	Dg	202	CDL	C78-C79-C80-C81
150	Dj	404	CDL	C60-C61-C62-C63
150	Dq	1402	CDL	C32-C33-C34-C35
153	c	503	PC1	C26-C27-C28-C29
153	DJ	306	PC1	C23-C24-C25-C26
153	Dg	203	PC1	O32-C31-O31-C3
153	Dc	604	PC1	O21-C21-C22-C23
150	BY	201	CDL	C80-C81-C82-C83
150	Ed	204	CDL	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	Dx	1206	3PE	C3A-C3B-C3C-C3D
150	AA	901	CDL	C80-C81-C82-C83
150	BC	302	CDL	C13-C14-C15-C16
150	BT	202	CDL	C78-C79-C80-C81
150	DA	706	CDL	C62-C63-C64-C65
150	EB	302	CDL	C61-C62-C63-C64
150	CG	302	CDL	OB5-CB3-CB4-OB6
150	Ed	204	CDL	OB5-CB3-CB4-OB6
153	C	510	PC1	O11-C1-C2-O21
168	c	504	HEM	C2D-C3D-CAD-CBD
150	DQ	1501	CDL	CA5-C11-C12-C13
150	En	1201	CDL	CB5-C51-C52-C53
150	EL	903	CDL	C41-C42-C43-C44
150	El	902	CDL	C17-C18-C19-C20
153	DC	605	PC1	C3B-C3C-C3D-C3E
155	Dx	1202	3PE	C26-C27-C28-C29
156	AC	803	LPP	O9-C11-C12-C13
167	ED	603	UQ8	C2-C3-O3-C3M
150	DU	402	CDL	C35-C36-C37-C38
150	Dq	1403	CDL	C77-C78-C79-C80
150	DI	302	CDL	CB5-C51-C52-C53
150	DS	405	CDL	CA7-C31-C32-C33
153	DA	707	PC1	O22-C21-O21-C2
150	AM	301	CDL	C51-C52-C53-C54
150	DA	706	CDL	C73-C74-C75-C76
150	DD	704	CDL	C13-C14-C15-C16
166	d	802	HEC	CAA-CBA-CGA-O1A
153	DQ	1503	PC1	C3D-C3E-C3F-C3G
155	Dd	703	3PE	C3C-C3D-C3E-C3F
150	DU	404	CDL	C57-C58-C59-C60
150	Dn	501	CDL	C83-C84-C85-C86
153	C	509	PC1	C2F-C2G-C2H-C2I
150	AA	908	CDL	OA5-CA3-CA4-CA6
150	BE	201	CDL	OA5-CA3-CA4-CA6
150	BT	202	CDL	OB5-CB3-CB4-CB6
150	DQ	1502	CDL	OA5-CA3-CA4-CA6
150	Dn	501	CDL	OB5-CB3-CB4-CB6
150	Dq	1403	CDL	OA5-CA3-CA4-CA6
150	Dv	401	CDL	OB5-CB3-CB4-CB6
150	Ed	205	CDL	OB5-CB3-CB4-CB6
153	A9	603	PC1	O11-C1-C2-C3
153	C	508	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	k	301	PC1	O11-C1-C2-C3
153	Eo	201	PC1	O11-C1-C2-C3
155	DG	204	3PE	O11-C1-C2-C3
153	CC	302	PC1	O31-C31-C32-C33
167	c	510	UQ8	C12-C11-C9-C10
169	DA	703	HEA	C27-C19-C20-C21
153	DQ	1503	PC1	C22-C21-O21-C2
161	AS	200	8Q1	O33-C32-C34-O35
167	EL	905	UQ8	C39-C41-C42-C43
167	EL	905	UQ8	C14-C16-C17-C18
150	AF	401	CDL	C40-C41-C42-C43
150	Dm	501	CDL	C62-C63-C64-C65
150	Ea	501	CDL	C62-C63-C64-C65
155	DG	204	3PE	C2A-C2B-C2C-C2D
167	C	512	UQ8	C33-C34-C36-C37
167	ED	603	UQ8	C33-C34-C36-C37
150	DU	402	CDL	C31-CA7-OA8-CA6
150	Dn	502	CDL	C71-CB7-OB8-CB6
150	BV	201	CDL	C44-C45-C46-C47
150	DG	202	CDL	C71-C72-C73-C74
150	DI	302	CDL	C60-C61-C62-C63
150	DM	501	CDL	C84-C85-C86-C87
150	DV	402	CDL	C44-C45-C46-C47
150	Dj	405	CDL	C22-C23-C24-C25
150	Dv	403	CDL	C31-C32-C33-C34
155	EO	203	3PE	C2F-C2G-C2H-C2I
150	DC	601	CDL	C34-C35-C36-C37
150	DN	502	CDL	C83-C84-C85-C86
150	EN	1201	CDL	C54-C55-C56-C57
150	DJ	307	CDL	C32-C31-CA7-OA8
153	EO	204	PC1	O21-C21-C22-C23
150	DR	402	CDL	C76-C77-C78-C79
150	EA	301	CDL	C75-C76-C77-C78
150	H	1301	CDL	C1-CA2-OA2-PA1
150	ED	604	CDL	CB4-CB3-OB5-PB2
150	DR	403	CDL	C35-C36-C37-C38
150	Dh	201	CDL	C60-C61-C62-C63
150	Dn	501	CDL	C43-C44-C45-C46
155	BT	201	3PE	C34-C35-C36-C37
150	BT	202	CDL	OA6-CA4-CA6-OA8
150	Dx	1201	CDL	OA6-CA4-CA6-OA8
153	A9	601	PC1	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dv	405	PC1	O21-C2-C3-O31
150	C	503	CDL	CB5-C51-C52-C53
153	Db	702	PC1	C21-C22-C23-C24
150	Dd	702	CDL	C71-CB7-OB8-CB6
153	Dg	203	PC1	C32-C31-O31-C3
150	CJ	201	CDL	C77-C78-C79-C80
150	DU	403	CDL	C57-C58-C59-C60
150	Dv	401	CDL	C52-C53-C54-C55
150	BT	202	CDL	C64-C65-C66-C67
150	CC	305	CDL	C77-C78-C79-C80
150	DM	501	CDL	C44-C45-C46-C47
150	DS	401	CDL	C55-C56-C57-C58
150	Da	709	CDL	C43-C44-C45-C46
150	Ea	501	CDL	C33-C34-C35-C36
150	Ei	401	CDL	C12-C11-CA5-OA6
155	CC	301	3PE	O31-C31-C32-C33
155	DX	302	3PE	O21-C21-C22-C23
150	Dn	502	CDL	CA4-CA6-OA8-CA7
150	A0	602	CDL	C80-C81-C82-C83
150	c	502	CDL	C62-C63-C64-C65
150	DC	601	CDL	C54-C55-C56-C57
150	DI	302	CDL	C55-C56-C57-C58
150	Dv	402	CDL	C56-C57-C58-C59
150	E	301	CDL	C51-C52-C53-C54
150	DV	401	CDL	C14-C15-C16-C17
150	Dc	608	CDL	C22-C23-C24-C25
150	Dx	1201	CDL	C37-C38-C39-C40
173	Er	201	ATP	PG-O3B-PB-O3A
150	C	507	CDL	C34-C35-C36-C37
150	DH	201	CDL	C61-C62-C63-C64
150	EL	901	CDL	C83-C84-C85-C86
153	DV	406	PC1	C3D-C3E-C3F-C3G
167	C	511	UQ8	C36-C37-C38-C39
167	El	906	UQ8	C11-C12-C13-C14
150	BV	201	CDL	C76-C77-C78-C79
150	DX	306	CDL	C38-C39-C40-C41
150	DZ	501	CDL	C33-C34-C35-C36
150	EH	1601	CDL	C77-C78-C79-C80
150	Dq	1403	CDL	C44-C45-C46-C47
150	Dv	402	CDL	C43-C44-C45-C46
153	c	507	PC1	C3F-C3G-C3H-C3I
161	AS	200	8Q1	O33-C32-C34-N36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DD	704	CDL	CA5-C11-C12-C13
150	BC	301	CDL	C12-C11-CA5-OA6
150	BC	302	CDL	C72-C71-CB7-OB8
150	DN	506	CDL	C72-C71-CB7-OB8
150	Du	402	CDL	C32-C31-CA7-OA8
150	Eh	1601	CDL	C52-C51-CB5-OB6
155	BT	201	3PE	O21-C21-C22-C23
156	Dn	504	LPP	O27-C29-C30-C31
150	Di	1103	CDL	CB4-CB6-OB8-CB7
150	H	1302	CDL	C23-C24-C25-C26
150	h	501	CDL	C18-C19-C20-C21
167	EL	905	UQ8	C15-C14-C16-C17
167	EN	1205	UQ8	C35-C34-C36-C37
150	CC	305	CDL	C35-C36-C37-C38
150	C	504	CDL	C19-C20-C21-C22
150	DD	703	CDL	C38-C39-C40-C41
153	c	508	PC1	C38-C39-C3A-C3B
150	EK	201	CDL	CB3-OB5-PB2-OB2
150	Dh	202	CDL	CA2-OA2-PA1-OA5
150	Di	1103	CDL	CA2-OA2-PA1-OA5
150	Dr	403	CDL	CB2-OB2-PB2-OB5
153	A1	403	PC1	C1-O11-P-O13
153	AA	903	PC1	C11-O13-P-O11
153	c	507	PC1	C11-O13-P-O11
153	Dv	404	PC1	C1-O11-P-O13
155	DG	205	3PE	C11-O13-P-O11
167	C	512	UQ8	C13-C14-C16-C17
167	EN	1205	UQ8	C13-C14-C16-C17
167	EN	1205	UQ8	C12-C11-C9-C8
150	Do	501	CDL	C31-C32-C33-C34
150	Ep	701	CDL	C33-C34-C35-C36
150	DZ	501	CDL	C31-CA7-OA8-CA6
153	DB	702	PC1	C32-C31-O31-C3
150	B0	102	CDL	C12-C11-CA5-OA6
150	E	301	CDL	C32-C31-CA7-OA8
150	h	501	CDL	C52-C51-CB5-OB6
150	DQ	1502	CDL	C32-C31-CA7-OA8
150	Di	1103	CDL	C72-C71-CB7-OB8
153	EO	206	PC1	O21-C21-C22-C23
155	DJ	301	3PE	O21-C21-C22-C23
155	Di	1102	3PE	O21-C21-C22-C23
155	Dx	1207	3PE	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DN	502	CDL	C78-C79-C80-C81
150	DU	404	CDL	C40-C41-C42-C43
155	DX	304	3PE	C26-C27-C28-C29
155	Di	1102	3PE	C36-C37-C38-C39
150	DU	402	CDL	OA9-CA7-OA8-CA6
150	CG	302	CDL	C41-C42-C43-C44
150	DR	403	CDL	C71-C72-C73-C74
150	Du	401	CDL	C13-C14-C15-C16
153	D	402	PC1	C3D-C3E-C3F-C3G
153	K	502	PC1	C27-C28-C29-C2A
155	DC	607	3PE	C2F-C2G-C2H-C2I
155	EL	904	3PE	C34-C35-C36-C37
167	CC	303	UQ8	C5-C6-C7-C8
150	A0	602	CDL	C73-C74-C75-C76
150	DV	401	CDL	C78-C79-C80-C81
150	Dd	706	CDL	C63-C64-C65-C66
150	Dg	201	CDL	C51-C52-C53-C54
150	Dj	405	CDL	C32-C33-C34-C35
150	Dj	405	CDL	C53-C54-C55-C56
150	Dj	405	CDL	C61-C62-C63-C64
150	Dn	502	CDL	C38-C39-C40-C41
150	CC	304	CDL	C73-C74-C75-C76
150	DN	506	CDL	C74-C75-C76-C77
150	DQ	1504	CDL	C19-C20-C21-C22
150	DV	401	CDL	C52-C53-C54-C55
150	EA	301	CDL	C78-C79-C80-C81
155	DX	304	3PE	C2E-C2F-C2G-C2H
150	EB	302	CDL	O1-C1-CB2-OB2
150	Do	501	CDL	O1-C1-CB2-OB2
150	Dd	702	CDL	OB9-CB7-OB8-CB6
150	Dn	502	CDL	OB9-CB7-OB8-CB6
150	A1	402	CDL	C52-C51-CB5-OB6
150	B1	402	CDL	C72-C71-CB7-OB8
150	H	1302	CDL	C32-C31-CA7-OA8
150	DS	405	CDL	C32-C31-CA7-OA8
150	DU	403	CDL	C32-C31-CA7-OA8
150	Da	709	CDL	C12-C11-CA5-OA6
150	Dq	1403	CDL	C72-C71-CB7-OB8
153	BG	202	PC1	O21-C21-C22-C23
153	K	502	PC1	O31-C31-C32-C33
153	EO	205	PC1	O31-C31-C32-C33
153	Dv	404	PC1	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AC	802	CDL	C53-C54-C55-C56
150	ES	1101	CDL	C16-C17-C18-C19
150	Dg	202	CDL	C36-C37-C38-C39
150	BY	201	CDL	CB3-CB4-OB6-CB5
150	CC	305	CDL	CB6-CB4-OB6-CB5
150	C	507	CDL	CA6-CA4-OA6-CA5
150	DD	704	CDL	CA3-CA4-OA6-CA5
150	DM	501	CDL	CB6-CB4-OB6-CB5
150	DQ	1501	CDL	CA3-CA4-OA6-CA5
150	DV	401	CDL	CB3-CB4-OB6-CB5
150	EN	1202	CDL	CB6-CB4-OB6-CB5
150	Ds	401	CDL	CB6-CB4-OB6-CB5
150	Dv	401	CDL	CA6-CA4-OA6-CA5
150	Dv	403	CDL	CA6-CA4-OA6-CA5
150	Ek	201	CDL	CB3-CB4-OB6-CB5
153	AJ	501	PC1	C1-C2-O21-C21
153	C	508	PC1	C1-C2-O21-C21
153	EO	206	PC1	C3-C2-O21-C21
155	Dg	204	3PE	C1-C2-O21-C21
155	Dg	204	3PE	C3-C2-O21-C21
156	A6	301	LPP	C6-C7-O9-C11
150	Dd	706	CDL	C11-CA5-OA6-CA4
150	EN	1201	CDL	C80-C81-C82-C83
153	BG	202	PC1	C27-C28-C29-C2A
150	AC	802	CDL	OB7-CB5-OB6-CB4
150	E	301	CDL	OA7-CA5-OA6-CA4
150	DG	202	CDL	OB7-CB5-OB6-CB4
150	DU	403	CDL	OB7-CB5-OB6-CB4
150	AA	908	CDL	C34-C35-C36-C37
150	B1	402	CDL	C75-C76-C77-C78
150	Dx	1201	CDL	C75-C76-C77-C78
150	Ea	502	CDL	C44-C45-C46-C47
150	AA	901	CDL	C39-C40-C41-C42
150	CG	301	CDL	C51-C52-C53-C54
150	EL	901	CDL	C40-C41-C42-C43
150	EN	1202	CDL	C58-C59-C60-C61
150	BL	301	CDL	CA5-C11-C12-C13
150	BT	202	CDL	C32-C31-CA7-OA8
150	C	507	CDL	C72-C71-CB7-OB8
150	DJ	304	CDL	C12-C11-CA5-OA6
150	DM	502	CDL	C72-C71-CB7-OB8
150	Dj	401	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dj	402	CDL	C52-C51-CB5-OB6
150	Dj	407	CDL	C52-C51-CB5-OB6
150	Dr	403	CDL	C52-C51-CB5-OB6
153	BT	203	PC1	O31-C31-C32-C33
153	C	509	PC1	O31-C31-C32-C33
153	K	501	PC1	O31-C31-C32-C33
153	DA	707	PC1	O31-C31-C32-C33
153	Dc	603	PC1	O21-C21-C22-C23
153	Dq	1404	PC1	O21-C21-C22-C23
153	Dx	1205	PC1	O31-C31-C32-C33
155	A9	602	3PE	O21-C21-C22-C23
155	DG	204	3PE	O21-C21-C22-C23
155	DI	301	3PE	O21-C21-C22-C23
155	DX	303	3PE	O21-C21-C22-C23
155	Dc	607	3PE	O21-C21-C22-C23
155	Dd	703	3PE	O21-C21-C22-C23
155	Dg	204	3PE	O21-C21-C22-C23
155	Ds	403	3PE	O21-C21-C22-C23
156	AC	803	LPP	O27-C29-C30-C31
156	Dn	505	LPP	O27-C29-C30-C31
153	DC	604	PC1	O22-C21-C22-C23
150	DD	706	CDL	C20-C21-C22-C23
150	BC	301	CDL	C71-CB7-OB8-CB6
150	EH	1601	CDL	C62-C63-C64-C65
150	Di	1103	CDL	C79-C80-C81-C82
150	Dm	501	CDL	C78-C79-C80-C81
150	Dv	402	CDL	C78-C79-C80-C81
167	ED	603	UQ8	C12-C11-C9-C10
167	Ed	202	UQ8	C12-C11-C9-C10
167	En	1202	UQ8	C12-C11-C9-C10
150	C	507	CDL	C12-C13-C14-C15
150	DJ	307	CDL	C16-C17-C18-C19
150	DQ	1502	CDL	C73-C74-C75-C76
150	DR	402	CDL	C36-C37-C38-C39
150	Di	1101	CDL	C18-C19-C20-C21
155	DN	501	3PE	C36-C37-C38-C39
153	Dv	406	PC1	O32-C31-C32-C33
150	BE	201	CDL	C32-C31-CA7-OA8
150	C	507	CDL	C32-C31-CA7-OA8
150	H	1301	CDL	C52-C51-CB5-OB6
150	c	506	CDL	C72-C71-CB7-OB8
150	DS	404	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dn	506	CDL	C72-C71-CB7-OB8
150	El	902	CDL	C52-C51-CB5-OB6
153	AU	202	PC1	O31-C31-C32-C33
153	B1	401	PC1	O31-C31-C32-C33
153	DC	602	PC1	O21-C21-C22-C23
153	DC	603	PC1	O21-C21-C22-C23
155	DS	402	3PE	O21-C21-C22-C23
150	A0	602	CDL	C33-C34-C35-C36
150	DA	706	CDL	C71-C72-C73-C74
150	DI	302	CDL	C84-C85-C86-C87
156	AA	902	LPP	C31-C32-C33-C34
150	DD	703	CDL	C14-C15-C16-C17
150	DN	506	CDL	C60-C61-C62-C63
150	EL	903	CDL	C38-C39-C40-C41
150	Dh	202	CDL	C23-C24-C25-C26
150	Dv	403	CDL	C23-C24-C25-C26
153	EO	201	PC1	C23-C24-C25-C26
153	Dc	602	PC1	C2E-C2F-C2G-C2H
155	DI	301	3PE	C32-C33-C34-C35
155	DI	301	3PE	C36-C37-C38-C39
155	DS	402	3PE	C28-C29-C2A-C2B
150	AA	901	CDL	C1-CA2-OA2-PA1
150	CD	301	CDL	CA3-CA4-CA6-OA8
150	DD	703	CDL	CB3-CB4-CB6-OB8
150	DI	302	CDL	CB3-CB4-CB6-OB8
150	DU	403	CDL	C1-CB2-OB2-PB2
150	EB	302	CDL	CB3-CB4-CB6-OB8
150	ED	604	CDL	CA3-CA4-CA6-OA8
150	EL	901	CDL	CB3-CB4-CB6-OB8
150	Ds	401	CDL	CA3-CA4-CA6-OA8
150	Dx	1204	CDL	CB3-CB4-CB6-OB8
150	En	1201	CDL	CA3-CA4-CA6-OA8
155	A2	401	3PE	C1-C2-C3-O31
155	DC	607	3PE	C1-C2-C3-O31
155	Eo	202	3PE	C1-C2-C3-O31
166	CE	401	HEC	CAA-CBA-CGA-O2A
150	BC	301	CDL	C73-C74-C75-C76
150	BT	202	CDL	C55-C56-C57-C58
150	E	301	CDL	C19-C20-C21-C22
150	CD	301	CDL	C32-C31-CA7-OA9
150	BC	301	CDL	OB9-CB7-OB8-CB6
150	DD	706	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AC	802	CDL	C23-C24-C25-C26
153	d	801	PC1	C2B-C2C-C2D-C2E
153	EO	205	PC1	C3E-C3F-C3G-C3H
150	A1	402	CDL	OA5-CA3-CA4-OA6
150	CC	304	CDL	OA5-CA3-CA4-OA6
150	DD	704	CDL	OB5-CB3-CB4-OB6
150	DI	302	CDL	OA5-CA3-CA4-OA6
150	DS	404	CDL	OA5-CA3-CA4-OA6
150	DU	402	CDL	OB5-CB3-CB4-OB6
150	DY	301	CDL	OA5-CA3-CA4-OA6
150	Dn	503	CDL	OB5-CB3-CB4-OB6
153	C	508	PC1	O11-C1-C2-O21
150	g	801	CDL	C52-C51-CB5-OB6
150	DD	704	CDL	C52-C51-CB5-OB6
150	DH	202	CDL	C72-C71-CB7-OB8
150	Da	709	CDL	C52-C51-CB5-OB6
150	Di	1101	CDL	C72-C71-CB7-OB8
150	Dn	502	CDL	C32-C31-CA7-OA8
150	Ds	405	CDL	C12-C11-CA5-OA6
150	Eb	302	CDL	C72-C71-CB7-OB8
153	Da	706	PC1	O31-C31-C32-C33
153	El	904	PC1	O21-C21-C22-C23
150	DA	706	CDL	C61-C62-C63-C64
150	DQ	1502	CDL	C59-C60-C61-C62
150	C	506	CDL	C75-C76-C77-C78
150	H	1301	CDL	C57-C58-C59-C60
150	DJ	304	CDL	C20-C21-C22-C23
150	Ds	401	CDL	C12-C13-C14-C15
155	DX	302	3PE	C2C-C2D-C2E-C2F
150	DZ	501	CDL	OA9-CA7-OA8-CA6
150	CG	301	CDL	C23-C24-C25-C26
150	DJ	304	CDL	C53-C54-C55-C56
150	Dj	402	CDL	C56-C57-C58-C59
150	Dx	1204	CDL	C13-C14-C15-C16
150	Dx	1204	CDL	C84-C85-C86-C87
150	El	901	CDL	C73-C74-C75-C76
150	Dd	702	CDL	C31-CA7-OA8-CA6
150	Ep	701	CDL	C12-C13-C14-C15
150	Ed	205	CDL	CA5-C11-C12-C13
153	Dx	1205	PC1	C31-C32-C33-C34
150	AP	301	CDL	C32-C31-CA7-OA8
150	Ds	406	CDL	C32-C31-CA7-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ep	701	CDL	C12-C11-CA5-OA6
153	DV	404	PC1	O31-C31-C32-C33
153	Eb	301	PC1	O31-C31-C32-C33
155	EM	901	3PE	O21-C21-C22-C23
155	Eo	202	3PE	O31-C31-C32-C33
150	Dd	702	CDL	OA9-CA7-OA8-CA6
150	AC	801	CDL	C44-C45-C46-C47
150	BV	201	CDL	C42-C43-C44-C45
153	DB	702	PC1	C26-C27-C28-C29
153	Di	1104	PC1	C34-C35-C36-C37
150	A1	402	CDL	C37-C38-C39-C40
150	g	801	CDL	C75-C76-C77-C78
150	EO	202	CDL	C41-C42-C43-C44
150	Dh	201	CDL	C57-C58-C59-C60
150	Eb	302	CDL	C23-C24-C25-C26
150	EK	201	CDL	CB2-C1-CA2-OA2
150	BE	201	CDL	O1-C1-CA2-OA2
150	g	801	CDL	O1-C1-CA2-OA2
150	Di	1101	CDL	O1-C1-CB2-OB2
150	Du	402	CDL	C79-C80-C81-C82
153	DC	602	PC1	C2E-C2F-C2G-C2H
150	DJ	304	CDL	CA4-CA6-OA8-CA7
153	c	507	PC1	O22-C21-C22-C23
173	ER	201	ATP	PB-O3B-PG-O3G
166	CE	401	HEC	CAA-CBA-CGA-O1A
150	ED	605	CDL	C12-C11-CA5-OA6
150	Dm	501	CDL	C12-C11-CA5-OA6
150	Dv	403	CDL	C52-C51-CB5-OB6
150	El	901	CDL	C32-C31-CA7-OA8
153	A0	605	PC1	O21-C21-C22-C23
155	DJ	301	3PE	O31-C31-C32-C33
169	Da	703	HEA	C18-C19-C20-C21
150	A0	602	CDL	C51-C52-C53-C54
150	EH	1601	CDL	C11-C12-C13-C14
155	Dx	1208	3PE	C35-C36-C37-C38
155	Eo	202	3PE	C26-C27-C28-C29
150	DJ	303	CDL	C51-CB5-OB6-CB4
173	ER	201	ATP	PG-O3B-PB-O3A
150	BY	201	CDL	C17-C18-C19-C20
150	Dj	405	CDL	C44-C45-C46-C47
150	Dq	1401	CDL	C58-C59-C60-C61
150	Du	401	CDL	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ed	204	CDL	C53-C54-C55-C56
150	AM	301	CDL	OB5-CB3-CB4-CB6
150	CD	301	CDL	OB5-CB3-CB4-CB6
150	C	507	CDL	OB5-CB3-CB4-CB6
150	DJ	304	CDL	OB5-CB3-CB4-CB6
150	DM	502	CDL	OA5-CA3-CA4-CA6
150	DN	502	CDL	OB5-CB3-CB4-CB6
150	DR	403	CDL	OA5-CA3-CA4-CA6
150	DX	301	CDL	OB5-CB3-CB4-CB6
150	EH	1601	CDL	OA5-CA3-CA4-CA6
150	Dd	704	CDL	OB5-CB3-CB4-CB6
150	Du	401	CDL	OA5-CA3-CA4-CA6
150	Eh	1601	CDL	OB5-CB3-CB4-CB6
153	C	510	PC1	O11-C1-C2-C3
153	E	303	PC1	O11-C1-C2-C3
153	DC	603	PC1	O11-C1-C2-C3
155	AJ	502	3PE	O11-C1-C2-C3
150	E	301	CDL	C12-C13-C14-C15
150	Du	402	CDL	C17-C18-C19-C20
150	Ei	401	CDL	C84-C85-C86-C87
150	En	1201	CDL	C43-C44-C45-C46
150	A0	602	CDL	C72-C71-CB7-OB8
150	H	1301	CDL	C32-C31-CA7-OA8
150	DI	302	CDL	C72-C71-CB7-OB8
150	EN	1201	CDL	C52-C51-CB5-OB6
150	Dd	702	CDL	C72-C71-CB7-OB8
153	A6	302	PC1	O31-C31-C32-C33
153	AA	904	PC1	O21-C21-C22-C23
153	Dc	602	PC1	O21-C21-C22-C23
153	Eo	205	PC1	O21-C21-C22-C23
155	BA	301	3PE	O21-C21-C22-C23
155	DG	205	3PE	O21-C21-C22-C23
155	DX	303	3PE	O31-C31-C32-C33
155	Dx	1207	3PE	O31-C31-C32-C33
150	DI	302	CDL	C34-C35-C36-C37
150	DQ	1502	CDL	C37-C38-C39-C40
150	Dh	201	CDL	C20-C21-C22-C23
150	Dq	1401	CDL	C16-C17-C18-C19
150	Dq	1401	CDL	C51-C52-C53-C54
150	AA	908	CDL	OA6-CA4-CA6-OA8
150	E	301	CDL	OA6-CA4-CA6-OA8
150	h	501	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Da	709	CDL	OB6-CB4-CB6-OB8
150	Dn	502	CDL	OB6-CB4-CB6-OB8
150	Dq	1402	CDL	OB6-CB4-CB6-OB8
150	Dv	403	CDL	OA6-CA4-CA6-OA8
153	AC	804	PC1	O21-C2-C3-O31
153	AM	302	PC1	O21-C2-C3-O31
155	AJ	502	3PE	O21-C2-C3-O31
155	BT	201	3PE	O21-C2-C3-O31
150	DU	401	CDL	CB5-C51-C52-C53
150	DD	703	CDL	C20-C21-C22-C23
150	Dq	1402	CDL	C13-C14-C15-C16
150	Eu	101	CDL	C14-C15-C16-C17
155	A9	602	3PE	C29-C2A-C2B-C2C
150	Eg	101	CDL	C74-C75-C76-C77
150	Dn	501	CDL	OB7-CB5-OB6-CB4
150	AM	301	CDL	C32-C31-CA7-OA8
150	BT	204	CDL	C12-C11-CA5-OA6
150	DQ	1501	CDL	C72-C71-CB7-OB8
150	EL	903	CDL	C12-C11-CA5-OA6
150	Dd	705	CDL	C12-C11-CA5-OA6
150	Dj	402	CDL	C12-C11-CA5-OA6
150	Dn	503	CDL	C32-C31-CA7-OA8
150	Dq	1401	CDL	C32-C31-CA7-OA8
150	Dr	402	CDL	C52-C51-CB5-OB6
150	Ea	502	CDL	C52-C51-CB5-OB6
150	El	903	CDL	C32-C31-CA7-OA8
153	AJ	501	PC1	O31-C31-C32-C33
153	g	802	PC1	O21-C21-C22-C23
153	DC	608	PC1	O21-C21-C22-C23
153	EO	205	PC1	O21-C21-C22-C23
155	DG	205	3PE	O31-C31-C32-C33
155	Dx	1206	3PE	O21-C21-C22-C23
150	BV	201	CDL	C72-C71-CB7-OB9
150	H	1302	CDL	CB4-CB6-OB8-CB7
150	DZ	501	CDL	CA4-CA6-OA8-CA7
150	Dm	502	CDL	C19-C20-C21-C22
150	Du	402	CDL	C52-C53-C54-C55
150	Ek	201	CDL	C34-C35-C36-C37
155	CD	303	3PE	C32-C33-C34-C35
169	DA	702	HEA	CAD-CBD-CGD-O2D
151	A0	603	UDP	C5'-O5'-PA-O3A
154	A1	401	NDP	C2B-O2B-P2B-O3X

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
164	CA	702	FAD	C5B-O5B-PA-O3P
150	DN	507	CDL	C77-C78-C79-C80
150	DZ	501	CDL	C44-C45-C46-C47
150	Dn	502	CDL	C18-C19-C20-C21
155	DN	501	3PE	C2C-C2D-C2E-C2F
150	DI	302	CDL	C71-CB7-OB8-CB6
150	Di	1101	CDL	C16-C17-C18-C19
153	C	509	PC1	C25-C26-C27-C28
153	Di	1104	PC1	C22-C21-O21-C2
150	AF	402	CDL	C72-C71-CB7-OB8
150	BT	204	CDL	C32-C31-CA7-OA8
150	DD	705	CDL	C72-C71-CB7-OB8
150	Dd	705	CDL	C72-C71-CB7-OB8
150	Dj	407	CDL	C32-C31-CA7-OA8
150	Ea	502	CDL	C12-C11-CA5-OA6
150	Ek	201	CDL	C32-C31-CA7-OA8
153	AM	302	PC1	O21-C21-C22-C23
153	AM	302	PC1	O31-C31-C32-C33
153	DX	308	PC1	O31-C31-C32-C33
155	Dd	703	3PE	O31-C31-C32-C33
150	Dm	501	CDL	C84-C85-C86-C87
153	Dc	609	PC1	C3C-C3D-C3E-C3F
155	Dr	401	3PE	C3F-C3G-C3H-C3I
150	BT	202	CDL	C17-C18-C19-C20
150	Eh	1601	CDL	C21-C22-C23-C24
153	EO	206	PC1	C3D-C3E-C3F-C3G
150	Ed	205	CDL	CB7-C71-C72-C73
150	DX	301	CDL	C32-C33-C34-C35
150	Dv	402	CDL	C77-C78-C79-C80
167	EN	1205	UQ8	C33-C34-C36-C37
167	El	906	UQ8	C12-C11-C9-C8
167	En	1202	UQ8	C12-C11-C9-C8
150	DN	506	CDL	CA4-CA3-OA5-PA1
150	EL	902	CDL	CB4-CB3-OB5-PB2
150	Dj	407	CDL	C1-CA2-OA2-PA1
150	AC	801	CDL	C20-C21-C22-C23
150	ES	1101	CDL	C31-C32-C33-C34
150	El	901	CDL	C62-C63-C64-C65
153	BG	202	PC1	C34-C35-C36-C37
150	BL	301	CDL	C32-C31-CA7-OA8
150	DA	709	CDL	C72-C71-CB7-OB8
150	DJ	302	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DU	403	CDL	C52-C51-CB5-OB6
150	Dv	402	CDL	C72-C71-CB7-OB8
150	Dx	1204	CDL	C12-C11-CA5-OA6
150	Ea	502	CDL	C72-C71-CB7-OB8
155	EN	1204	3PE	O21-C21-C22-C23
150	Dn	503	CDL	C14-C15-C16-C17
161	AS	200	8Q1	C9-C10-C11-C12
155	BT	201	3PE	C31-C32-C33-C34
167	CC	303	UQ8	C9-C11-C12-C13
167	C	511	UQ8	C14-C16-C17-C18
167	C	511	UQ8	C9-C11-C12-C13
150	CC	304	CDL	C20-C21-C22-C23
150	ED	604	CDL	O1-C1-CA2-OA2
150	DD	705	CDL	C20-C21-C22-C23
150	DM	501	CDL	C13-C14-C15-C16
150	DQ	1501	CDL	C80-C81-C82-C83
150	EN	1201	CDL	C18-C19-C20-C21
167	Ds	404	UQ8	C3-C4-O4-C4M
167	Ed	202	UQ8	C4-C3-O3-C3M
154	A1	401	NDP	O4B-C4B-C5B-O5B
150	BY	201	CDL	CA7-C31-C32-C33
150	Dq	1402	CDL	CB5-C51-C52-C53
150	El	902	CDL	CB7-C71-C72-C73
150	CG	302	CDL	C56-C57-C58-C59
150	EH	1601	CDL	C14-C15-C16-C17
153	B1	403	PC1	C39-C3A-C3B-C3C
153	BG	202	PC1	C3E-C3F-C3G-C3H
153	C	508	PC1	C37-C38-C39-C3A
155	Dr	404	3PE	C28-C29-C2A-C2B
155	Eo	202	3PE	C38-C39-C3A-C3B
155	EM	901	3PE	C32-C31-O31-C3
150	c	509	CDL	C72-C71-CB7-OB8
150	DJ	304	CDL	C32-C31-CA7-OA8
150	DJ	304	CDL	C72-C71-CB7-OB8
150	Eu	101	CDL	C72-C71-CB7-OB8
153	Eo	201	PC1	O31-C31-C32-C33
153	DC	602	PC1	O22-C21-C22-C23
173	ER	201	ATP	PG-O3B-PB-O1B
150	c	506	CDL	C38-C39-C40-C41
150	DI	302	CDL	OB9-CB7-OB8-CB6
150	AA	908	CDL	C75-C76-C77-C78
150	DR	403	CDL	C62-C63-C64-C65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	EH	1601	CDL	C35-C36-C37-C38
150	Ds	406	CDL	C41-C42-C43-C44
153	Da	706	PC1	C2C-C2D-C2E-C2F
150	H	1302	CDL	C51-CB5-OB6-CB4
150	EL	901	CDL	C51-CB5-OB6-CB4
153	CC	302	PC1	C22-C21-O21-C2
153	DA	707	PC1	C22-C21-O21-C2
155	Dr	401	3PE	C22-C21-O21-C2
167	CC	303	UQ8	C26-C27-C28-C29
167	c	510	UQ8	C41-C42-C43-C44
167	El	906	UQ8	C36-C37-C38-C39
150	BE	201	CDL	C32-C31-CA7-OA9
150	C	507	CDL	C32-C31-CA7-OA9
150	c	506	CDL	C72-C71-CB7-OB9
150	Dj	402	CDL	C52-C51-CB5-OB7
150	Dn	506	CDL	C72-C71-CB7-OB9
153	DC	603	PC1	O22-C21-C22-C23
155	DS	402	3PE	O22-C21-C22-C23
150	C	505	CDL	C37-C38-C39-C40
150	c	501	CDL	C17-C18-C19-C20
150	DQ	1504	CDL	C55-C56-C57-C58
150	Dd	706	CDL	C23-C24-C25-C26
153	B1	403	PC1	C22-C23-C24-C25
150	CJ	201	CDL	C32-C31-CA7-OA8
150	ED	604	CDL	C72-C71-CB7-OB8
150	Ep	701	CDL	C52-C51-CB5-OB6
153	Dx	1203	PC1	O31-C31-C32-C33
150	AA	901	CDL	C64-C65-C66-C67
150	B0	101	CDL	C16-C17-C18-C19
150	DD	703	CDL	C73-C74-C75-C76
150	Dj	404	CDL	C71-C72-C73-C74
150	BE	201	CDL	C71-CB7-OB8-CB6
150	DS	405	CDL	C18-C19-C20-C21
150	EH	1601	CDL	C74-C75-C76-C77
150	Dj	404	CDL	C52-C53-C54-C55
150	Du	403	CDL	C15-C16-C17-C18
156	DN	505	LPP	C35-C36-C37-C38
150	AA	901	CDL	CB7-C71-C72-C73
150	DG	202	CDL	CA7-C31-C32-C33
164	CA	702	FAD	C2'-C3'-C4'-C5'
150	B1	402	CDL	C72-C71-CB7-OB9
150	DJ	304	CDL	C12-C11-CA5-OA7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DS	404	CDL	C12-C11-CA5-OA7
150	Dj	407	CDL	C52-C51-CB5-OB7
153	AU	202	PC1	O32-C31-C32-C33
153	BG	202	PC1	O22-C21-C22-C23
153	EO	205	PC1	O32-C31-C32-C33
155	Dx	1207	3PE	O22-C21-C22-C23
150	c	509	CDL	C51-C52-C53-C54
150	DQ	1502	CDL	C22-C23-C24-C25
167	c	510	UQ8	C40-C39-C41-C42
150	A0	602	CDL	C32-C33-C34-C35
150	Dg	202	CDL	C59-C60-C61-C62
150	Dn	506	CDL	C81-C82-C83-C84
150	Eg	101	CDL	C56-C57-C58-C59
150	En	1201	CDL	C32-C33-C34-C35
153	d	801	PC1	C22-C23-C24-C25
155	EM	901	3PE	O32-C31-O31-C3
167	c	510	UQ8	C12-C11-C9-C8
150	DU	401	CDL	C32-C31-CA7-OA8
150	DD	704	CDL	C40-C41-C42-C43
150	DN	507	CDL	C74-C75-C76-C77
150	Dq	1401	CDL	C11-C12-C13-C14
150	Dr	402	CDL	C54-C55-C56-C57
150	En	1201	CDL	C52-C53-C54-C55
150	DU	403	CDL	C52-C51-CB5-OB7
153	DA	707	PC1	O32-C31-C32-C33
153	Dg	203	PC1	O32-C31-C32-C33
155	BT	201	3PE	O22-C21-C22-C23
150	CC	305	CDL	C44-C45-C46-C47
150	g	801	CDL	C42-C43-C44-C45
150	Dh	201	CDL	C18-C19-C20-C21
155	Dx	1208	3PE	C2E-C2F-C2G-C2H
150	H	1301	CDL	C31-CA7-OA8-CA6
150	CD	301	CDL	C39-C40-C41-C42
150	ES	1101	CDL	C36-C37-C38-C39
150	Dg	201	CDL	C34-C35-C36-C37
150	Di	1101	CDL	C73-C74-C75-C76
150	Dq	1401	CDL	C19-C20-C21-C22
150	Dv	403	CDL	C34-C35-C36-C37
150	Dx	1201	CDL	C82-C83-C84-C85
153	EB	303	PC1	C34-C35-C36-C37
155	DN	501	3PE	C2D-C2E-C2F-C2G
155	Em	901	3PE	C3B-C3C-C3D-C3E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dj	403	CDL	CA2-C1-CB2-OB2
150	Du	401	CDL	CA2-C1-CB2-OB2
150	Du	401	CDL	C61-C62-C63-C64
150	E	301	CDL	C32-C31-CA7-OA9
150	DA	709	CDL	C72-C71-CB7-OB9
150	DD	704	CDL	C52-C51-CB5-OB7
150	Di	1103	CDL	C72-C71-CB7-OB9
150	Dn	502	CDL	C32-C31-CA7-OA9
150	Dr	403	CDL	C52-C51-CB5-OB7
153	C	509	PC1	O32-C31-C32-C33
155	DX	302	3PE	O22-C21-C22-C23
155	Di	1102	3PE	O22-C21-C22-C23
156	Dn	504	LPP	O28-C29-C30-C31
150	AF	402	CDL	C52-C51-CB5-OB6
150	Di	1101	CDL	C52-C51-CB5-OB6
150	c	501	CDL	C23-C24-C25-C26
150	DG	201	CDL	C34-C35-C36-C37
150	ES	1101	CDL	C83-C84-C85-C86
150	CD	302	CDL	C23-C24-C25-C26
150	g	801	CDL	C24-C25-C26-C27
150	DO	501	CDL	C23-C24-C25-C26
150	Dc	608	CDL	C59-C60-C61-C62
150	Di	1101	CDL	C53-C54-C55-C56
150	Ea	501	CDL	C43-C44-C45-C46
150	A1	402	CDL	C52-C51-CB5-OB7
150	B0	102	CDL	C12-C11-CA5-OA7
150	BC	301	CDL	C12-C11-CA5-OA7
150	BC	302	CDL	C72-C71-CB7-OB9
150	h	501	CDL	C52-C51-CB5-OB7
150	DM	502	CDL	C72-C71-CB7-OB9
150	ED	605	CDL	C12-C11-CA5-OA7
150	Dq	1403	CDL	C72-C71-CB7-OB9
150	Ds	406	CDL	C32-C31-CA7-OA9
150	Du	402	CDL	C32-C31-CA7-OA9
150	Eh	1601	CDL	C52-C51-CB5-OB7
150	Ei	401	CDL	C12-C11-CA5-OA7
150	Ep	701	CDL	C12-C11-CA5-OA7
153	DV	404	PC1	O32-C31-C32-C33
155	DG	204	3PE	O22-C21-C22-C23
155	DJ	301	3PE	O32-C31-C32-C33
155	Dd	703	3PE	O22-C21-C22-C23
155	Dg	204	3PE	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	c	502	CDL	CB3-CB4-CB6-OB8
150	DJ	302	CDL	CB3-CB4-CB6-OB8
150	DN	506	CDL	CA3-CA4-CA6-OA8
150	DQ	1502	CDL	CB3-CB4-CB6-OB8
150	DU	402	CDL	CB3-CB4-CB6-OB8
150	Ek	201	CDL	CB3-CB4-CB6-OB8
153	AA	903	PC1	C1-C2-C3-O31
153	c	503	PC1	C1-C2-C3-O31
153	DC	603	PC1	C1-C2-C3-O31
153	Dc	602	PC1	C1-C2-C3-O31
153	BG	202	PC1	O31-C31-C32-C33
150	BV	201	CDL	C11-C12-C13-C14
150	Ds	405	CDL	C34-C35-C36-C37
153	DA	707	PC1	C2C-C2D-C2E-C2F
153	DY	302	PC1	C3E-C3F-C3G-C3H
150	CG	302	CDL	CB2-OB2-PB2-OB5
150	CD	301	CDL	CB3-OB5-PB2-OB2
150	Ds	406	CDL	CB2-OB2-PB2-OB5
150	Ea	501	CDL	CB2-OB2-PB2-OB5
150	AC	801	CDL	C74-C75-C76-C77
150	DD	704	CDL	C51-C52-C53-C54
150	Ek	201	CDL	C11-C12-C13-C14
150	DU	402	CDL	O1-C1-CA2-OA2
150	ES	1101	CDL	O1-C1-CA2-OA2
150	C	507	CDL	CA5-C11-C12-C13
155	Da	708	3PE	C31-C32-C33-C34
150	C	507	CDL	C72-C71-CB7-OB9
150	H	1301	CDL	C52-C51-CB5-OB7
150	DN	506	CDL	C72-C71-CB7-OB9
150	Eb	302	CDL	C72-C71-CB7-OB9
150	El	902	CDL	C52-C51-CB5-OB7
153	EO	204	PC1	O22-C21-C22-C23
153	EO	206	PC1	O22-C21-C22-C23
155	A9	602	3PE	O22-C21-C22-C23
155	CC	301	3PE	O32-C31-C32-C33
155	DG	205	3PE	O32-C31-C32-C33
155	DI	301	3PE	O22-C21-C22-C23
155	EN	1204	3PE	O22-C21-C22-C23
156	AC	803	LPP	O28-C29-C30-C31
150	AF	401	CDL	C82-C83-C84-C85
150	CG	301	CDL	C72-C73-C74-C75
150	DJ	303	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	DN	507	CDL	C22-C23-C24-C25
150	DY	301	CDL	C77-C78-C79-C80
150	Da	709	CDL	C52-C53-C54-C55
150	Dc	601	CDL	C15-C16-C17-C18
150	Dq	1401	CDL	C12-C13-C14-C15
150	Eb	302	CDL	C33-C34-C35-C36
150	En	1201	CDL	C36-C37-C38-C39
150	DX	307	CDL	C39-C40-C41-C42
150	EB	302	CDL	C23-C24-C25-C26
150	Dd	705	CDL	C34-C35-C36-C37
150	Dj	401	CDL	C80-C81-C82-C83
150	Dj	404	CDL	C15-C16-C17-C18
153	K	502	PC1	C2E-C2F-C2G-C2H
156	EI	402	LPP	C21-C22-C23-C24
150	Dn	502	CDL	C52-C51-CB5-OB6
150	Ea	501	CDL	C32-C31-CA7-OA8
150	Ed	205	CDL	C12-C11-CA5-OA6
150	DJ	305	CDL	CB4-CB3-OB5-PB2
150	Dj	407	CDL	C1-CB2-OB2-PB2
150	Dq	1403	CDL	CA4-CA3-OA5-PA1
150	Ds	405	CDL	C1-CA2-OA2-PA1
153	EB	303	PC1	C2-C1-O11-P
153	EO	204	PC1	C2-C1-O11-P
155	A2	401	3PE	C2-C1-O11-P
150	A1	402	CDL	C31-C32-C33-C34
150	BG	201	CDL	C39-C40-C41-C42
150	Dj	407	CDL	C15-C16-C17-C18
150	Dm	501	CDL	C54-C55-C56-C57
150	Dj	401	CDL	C72-C71-CB7-OB9
150	Dm	501	CDL	C12-C11-CA5-OA7
150	Dv	403	CDL	C52-C51-CB5-OB7
150	Ea	502	CDL	C12-C11-CA5-OA7
150	Ea	502	CDL	C72-C71-CB7-OB9
150	El	901	CDL	C32-C31-CA7-OA9
155	DJ	301	3PE	O22-C21-C22-C23
155	Eo	202	3PE	O32-C31-C32-C33
150	ES	1101	CDL	C84-C85-C86-C87
150	Dn	506	CDL	C13-C14-C15-C16
150	BE	201	CDL	OB9-CB7-OB8-CB6
150	Dy	301	CDL	OB9-CB7-OB8-CB6
150	Dm	502	CDL	C60-C61-C62-C63
150	Do	501	CDL	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DS	402	3PE	C25-C26-C27-C28
150	A0	602	CDL	CA2-OA2-PA1-OA3
150	AC	802	CDL	CA2-OA2-PA1-OA3
150	AF	402	CDL	CB3-OB5-PB2-OB3
150	B0	101	CDL	CA3-OA5-PA1-OA3
150	B0	102	CDL	CA2-OA2-PA1-OA3
150	BV	201	CDL	CA2-OA2-PA1-OA3
150	BV	201	CDL	CA2-OA2-PA1-OA4
150	BY	201	CDL	CA3-OA5-PA1-OA3
150	BY	201	CDL	CB2-OB2-PB2-OB4
150	BY	201	CDL	CB3-OB5-PB2-OB4
150	CG	302	CDL	CB2-OB2-PB2-OB3
150	CC	305	CDL	CB3-OB5-PB2-OB4
150	C	505	CDL	CB3-OB5-PB2-OB4
150	C	507	CDL	CA2-OA2-PA1-OA3
150	H	1302	CDL	CB2-OB2-PB2-OB3
150	DD	703	CDL	CB2-OB2-PB2-OB3
150	DD	703	CDL	CB2-OB2-PB2-OB4
150	DG	202	CDL	CA3-OA5-PA1-OA3
150	DH	202	CDL	CA2-OA2-PA1-OA3
150	DI	302	CDL	CA2-OA2-PA1-OA3
150	DJ	303	CDL	CB2-OB2-PB2-OB4
150	DJ	304	CDL	CB3-OB5-PB2-OB3
150	DJ	307	CDL	CA2-OA2-PA1-OA3
150	DN	506	CDL	CA2-OA2-PA1-OA3
150	DU	401	CDL	CB3-OB5-PB2-OB3
150	DX	301	CDL	CB3-OB5-PB2-OB3
150	DY	301	CDL	CA2-OA2-PA1-OA3
150	EA	301	CDL	CB3-OB5-PB2-OB3
150	ED	601	CDL	CB2-OB2-PB2-OB3
150	EI	401	CDL	CA2-OA2-PA1-OA3
150	EL	901	CDL	CA3-OA5-PA1-OA3
150	EL	901	CDL	CB2-OB2-PB2-OB3
150	EL	901	CDL	CB3-OB5-PB2-OB3
150	Dd	702	CDL	CA2-OA2-PA1-OA3
150	Dh	201	CDL	CB3-OB5-PB2-OB3
150	Dh	202	CDL	CA2-OA2-PA1-OA3
150	Di	1101	CDL	CB2-OB2-PB2-OB3
150	Di	1101	CDL	CB2-OB2-PB2-OB4
150	Di	1103	CDL	CB2-OB2-PB2-OB3
150	Dj	405	CDL	CA2-OA2-PA1-OA3
150	Dj	405	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dm	502	CDL	CB2-OB2-PB2-OB3
150	Dn	501	CDL	CB3-OB5-PB2-OB3
150	Dn	506	CDL	CA2-OA2-PA1-OA3
150	Dq	1401	CDL	CA3-OA5-PA1-OA3
150	Dq	1401	CDL	CB3-OB5-PB2-OB4
150	Dq	1402	CDL	CA2-OA2-PA1-OA4
150	Dq	1402	CDL	CB3-OB5-PB2-OB4
150	Dq	1403	CDL	CB2-OB2-PB2-OB4
150	Du	402	CDL	CB2-OB2-PB2-OB3
150	Du	403	CDL	CA3-OA5-PA1-OA3
150	Dv	402	CDL	CB3-OB5-PB2-OB3
150	Dv	402	CDL	CB3-OB5-PB2-OB4
150	Dy	301	CDL	CB3-OB5-PB2-OB3
150	Ek	201	CDL	CB2-OB2-PB2-OB3
150	El	902	CDL	CB2-OB2-PB2-OB3
150	Ep	701	CDL	CB3-OB5-PB2-OB3
151	A0	603	UDP	C5'-O5'-PA-O1A
153	A9	603	PC1	C11-O13-P-O12
153	AA	903	PC1	C11-O13-P-O14
153	AA	906	PC1	C11-O13-P-O12
153	AC	804	PC1	C1-O11-P-O14
153	BG	202	PC1	C1-O11-P-O12
153	C	510	PC1	C11-O13-P-O12
153	E	303	PC1	C11-O13-P-O12
153	c	507	PC1	C11-O13-P-O14
153	d	801	PC1	C11-O13-P-O14
153	k	301	PC1	C1-O11-P-O14
153	DV	404	PC1	C1-O11-P-O14
153	DX	305	PC1	C1-O11-P-O14
153	DX	308	PC1	C11-O13-P-O14
153	EB	303	PC1	C1-O11-P-O14
153	EN	1203	PC1	C1-O11-P-O14
153	EO	205	PC1	C1-O11-P-O14
153	Da	706	PC1	C11-O13-P-O12
153	Dv	404	PC1	C11-O13-P-O14
153	Dv	404	PC1	C1-O11-P-O14
153	Dv	406	PC1	C1-O11-P-O14
153	Dx	1203	PC1	C11-O13-P-O12
153	Dx	1203	PC1	C11-O13-P-O14
153	Dx	1209	PC1	C11-O13-P-O14
153	Dy	302	PC1	C11-O13-P-O14
153	Dy	302	PC1	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Eb	303	PC1	C1-O11-P-O14
155	BP	201	3PE	C11-O13-P-O14
155	DR	401	3PE	C11-O13-P-O14
155	Ds	408	3PE	C11-O13-P-O14
155	Eo	202	3PE	C11-O13-P-O14
167	C	511	UQ8	C6-C7-C8-C9
173	Er	201	ATP	C5'-O5'-PA-O1A
150	Du	401	CDL	CB5-C51-C52-C53
155	EL	904	3PE	C31-C32-C33-C34
150	A0	602	CDL	C20-C21-C22-C23
150	DQ	1502	CDL	C44-C45-C46-C47
150	Dq	1402	CDL	C43-C44-C45-C46
153	Da	706	PC1	C3A-C3B-C3C-C3D
153	Dx	1205	PC1	C2B-C2C-C2D-C2E
150	AP	301	CDL	C32-C31-CA7-OA9
150	BT	202	CDL	C32-C31-CA7-OA9
150	BT	204	CDL	C32-C31-CA7-OA9
150	DQ	1502	CDL	C32-C31-CA7-OA9
150	DS	405	CDL	C32-C31-CA7-OA9
150	DU	403	CDL	C32-C31-CA7-OA9
150	Dv	402	CDL	C72-C71-CB7-OB9
150	Ep	701	CDL	C52-C51-CB5-OB7
153	A1	403	PC1	C2-C3-O31-C31
155	DX	303	3PE	O22-C21-C22-C23
155	Dc	607	3PE	O22-C21-C22-C23
150	B0	101	CDL	C52-C51-CB5-OB6
150	DD	706	CDL	C32-C31-CA7-OA8
150	Di	1101	CDL	OA5-CA3-CA4-CA6
150	Dj	403	CDL	OA5-CA3-CA4-CA6
150	Eb	302	CDL	OB5-CB3-CB4-CB6
150	El	903	CDL	OA5-CA3-CA4-CA6
153	A	1201	PC1	O11-C1-C2-C3
150	DJ	304	CDL	C82-C83-C84-C85
150	DX	307	CDL	C57-C58-C59-C60
150	Dq	1401	CDL	C72-C73-C74-C75
153	c	503	PC1	C2E-C2F-C2G-C2H
168	c	505	HEM	CAA-CBA-CGA-O2A
150	Di	1103	CDL	C23-C24-C25-C26
150	Dx	1201	CDL	C34-C35-C36-C37
153	DX	308	PC1	C2A-C2B-C2C-C2D
150	A0	601	CDL	CA5-C11-C12-C13
155	AJ	502	3PE	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DG	204	3PE	O13-C11-C12-N
155	Da	708	3PE	O13-C11-C12-N
150	A0	602	CDL	C72-C71-CB7-OB9
150	BL	301	CDL	C32-C31-CA7-OA9
150	CJ	201	CDL	C32-C31-CA7-OA9
150	DI	302	CDL	C72-C71-CB7-OB9
150	ED	604	CDL	C72-C71-CB7-OB9
150	Da	709	CDL	C12-C11-CA5-OA7
150	Eu	101	CDL	C72-C71-CB7-OB9
153	K	501	PC1	O32-C31-C32-C33
153	Dc	602	PC1	O22-C21-C22-C23
153	Dx	1205	PC1	O32-C31-C32-C33
156	Dn	505	LPP	O28-C29-C30-C31
150	DS	405	CDL	C41-C42-C43-C44
150	Dh	201	CDL	C32-C33-C34-C35
150	Dn	501	CDL	C82-C83-C84-C85
150	Dr	402	CDL	C41-C42-C43-C44
150	Dx	1204	CDL	C51-C52-C53-C54
153	BS	1301	PC1	C3C-C3D-C3E-C3F
150	BL	301	CDL	C72-C71-CB7-OB8
150	C	505	CDL	C32-C31-CA7-OA8
150	C	506	CDL	C32-C31-CA7-OA8
150	Da	709	CDL	C32-C31-CA7-OA8
150	Dd	706	CDL	C32-C31-CA7-OA8
150	Ds	402	CDL	C12-C11-CA5-OA6
150	El	903	CDL	C52-C51-CB5-OB6
155	BP	201	3PE	O21-C21-C22-C23
150	AF	401	CDL	CB4-CB6-OB8-CB7
155	BA	301	3PE	O22-C21-O21-C2
150	Du	403	CDL	C17-C18-C19-C20
150	Dy	301	CDL	C34-C35-C36-C37
153	DA	707	PC1	C2D-C2E-C2F-C2G
150	Dy	301	CDL	C71-CB7-OB8-CB6
150	AA	901	CDL	C32-C31-CA7-OA9
150	H	1302	CDL	C32-C31-CA7-OA9
150	Di	1101	CDL	C72-C71-CB7-OB9
150	Dx	1204	CDL	C12-C11-CA5-OA7
153	g	802	PC1	O22-C21-C22-C23
153	Da	706	PC1	O32-C31-C32-C33
153	Dc	603	PC1	O22-C21-C22-C23
155	Dx	1207	3PE	O32-C31-C32-C33
150	DN	502	CDL	C75-C76-C77-C78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Ep	701	CDL	C34-C35-C36-C37
150	CC	304	CDL	C18-C19-C20-C21
150	Ds	401	CDL	C33-C34-C35-C36
153	DA	707	PC1	C3A-C3B-C3C-C3D
169	DA	702	HEA	CAD-CBD-CGD-O1D
150	BT	202	CDL	C72-C71-CB7-OB8
153	AH	301	PC1	O21-C21-C22-C23
153	DQ	1503	PC1	O31-C31-C32-C33
153	Dx	1203	PC1	O21-C21-C22-C23
150	B0	101	CDL	C24-C25-C26-C27
150	B1	402	CDL	C51-C52-C53-C54
150	ES	1101	CDL	C37-C38-C39-C40
150	Da	709	CDL	C71-C72-C73-C74
150	Dn	501	CDL	C44-C45-C46-C47
150	El	902	CDL	C36-C37-C38-C39
153	CC	302	PC1	C3D-C3E-C3F-C3G
153	Dv	407	PC1	C3C-C3D-C3E-C3F
155	DX	302	3PE	C26-C27-C28-C29
150	BC	302	CDL	C32-C31-CA7-OA9
150	DI	302	CDL	CB4-CB6-OB8-CB7
150	DV	401	CDL	C72-C71-CB7-OB9
150	Dr	402	CDL	C52-C51-CB5-OB7
153	A0	605	PC1	O22-C21-C22-C23
153	Dv	404	PC1	O32-C31-C32-C33
155	BA	301	3PE	O22-C21-C22-C23
167	c	510	UQ8	C25-C24-C26-C27
150	BV	201	CDL	C21-C22-C23-C24
150	C	503	CDL	C14-C15-C16-C17
150	DJ	304	CDL	C38-C39-C40-C41
150	En	1201	CDL	C19-C20-C21-C22
156	AA	902	LPP	C35-C36-C37-C38
167	En	1202	UQ8	C16-C17-C18-C19
150	CG	301	CDL	C74-C75-C76-C77
150	h	501	CDL	C41-C42-C43-C44
153	Da	706	PC1	C2D-C2E-C2F-C2G
150	A1	402	CDL	CA3-CA4-OA6-CA5
150	Dd	704	CDL	CB6-CB4-OB6-CB5
150	Dj	404	CDL	CB6-CB4-OB6-CB5
150	Dr	403	CDL	CA3-CA4-OA6-CA5
150	Dy	301	CDL	CB3-CB4-OB6-CB5
153	A2	402	PC1	C12-C11-O13-P
153	A6	303	PC1	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AJ	501	PC1	C3-C2-O21-C21
153	AU	202	PC1	C12-C11-O13-P
153	AX	401	PC1	C1-C2-O21-C21
153	C	508	PC1	C12-C11-O13-P
153	E	303	PC1	C12-C11-O13-P
153	c	507	PC1	C12-C11-O13-P
153	d	801	PC1	C12-C11-O13-P
153	g	802	PC1	C12-C11-O13-P
153	DX	308	PC1	C12-C11-O13-P
153	EB	301	PC1	C12-C11-O13-P
153	EN	1203	PC1	C12-C11-O13-P
153	Eb	301	PC1	C12-C11-O13-P
155	A9	602	3PE	C12-C11-O13-P
155	BT	201	3PE	C12-C11-O13-P
155	CK	101	3PE	C12-C11-O13-P
155	DG	204	3PE	C12-C11-O13-P
155	DN	501	3PE	C12-C11-O13-P
155	Dx	1202	3PE	C12-C11-O13-P
169	DA	703	HEA	C3B-C11-C12-C13
150	H	1301	CDL	OA9-CA7-OA8-CA6
150	AM	301	CDL	C32-C31-CA7-OA9
150	g	801	CDL	C52-C51-CB5-OB7
150	DJ	302	CDL	C72-C71-CB7-OB9
150	DQ	1501	CDL	C72-C71-CB7-OB9
150	Da	709	CDL	C52-C51-CB5-OB7
150	Dj	402	CDL	C12-C11-CA5-OA7
150	Dn	503	CDL	C32-C31-CA7-OA9
150	Ds	405	CDL	C12-C11-CA5-OA7
150	El	903	CDL	C32-C31-CA7-OA9
153	B1	401	PC1	O32-C31-C32-C33
153	BT	203	PC1	O32-C31-C32-C33
153	DX	308	PC1	O32-C31-C32-C33
153	El	904	PC1	O22-C21-C22-C23
155	DG	205	3PE	O22-C21-C22-C23
155	EM	901	3PE	O22-C21-C22-C23
155	Ds	403	3PE	O22-C21-C22-C23
150	DS	401	CDL	C13-C14-C15-C16
150	DX	301	CDL	C59-C60-C61-C62
150	EB	302	CDL	C14-C15-C16-C17
150	Dq	1403	CDL	C37-C38-C39-C40
153	DV	404	PC1	C29-C2A-C2B-C2C
150	Dq	1402	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	DC	605	PC1	O21-C21-C22-C23
150	DN	503	CDL	O1-C1-CB2-OB2
150	DS	401	CDL	O1-C1-CB2-OB2
150	Di	1103	CDL	O1-C1-CB2-OB2
150	Du	403	CDL	O1-C1-CB2-OB2
150	AC	802	CDL	C72-C73-C74-C75
150	DG	201	CDL	C75-C76-C77-C78
150	Dg	201	CDL	C14-C15-C16-C17
155	Dr	401	3PE	C34-C35-C36-C37
150	DQ	1501	CDL	C32-C33-C34-C35
155	G	401	3PE	C34-C35-C36-C37
155	Dx	1207	3PE	C35-C36-C37-C38
150	Dq	1401	CDL	C32-C31-CA7-OA9
153	AA	904	PC1	O22-C21-C22-C23
153	AJ	501	PC1	O32-C31-C32-C33
153	AM	302	PC1	O22-C21-C22-C23
155	Dx	1206	3PE	O22-C21-C22-C23
150	EL	902	CDL	C72-C73-C74-C75
150	Dn	501	CDL	C75-C76-C77-C78
150	Dr	403	CDL	C40-C41-C42-C43
150	Dy	301	CDL	C20-C21-C22-C23
153	DV	404	PC1	C2D-C2E-C2F-C2G
153	A6	303	PC1	C11-C12-N-C15
150	C	503	CDL	C52-C51-CB5-OB6
150	DC	601	CDL	C72-C71-CB7-OB8
150	DG	201	CDL	C32-C31-CA7-OA8
150	DM	501	CDL	C12-C11-CA5-OA6
150	DN	502	CDL	C72-C71-CB7-OB8
150	DV	402	CDL	C52-C51-CB5-OB6
150	DV	402	CDL	C72-C71-CB7-OB8
150	DV	403	CDL	C52-C51-CB5-OB6
150	DZ	501	CDL	C12-C11-CA5-OA6
150	DZ	501	CDL	C32-C31-CA7-OA8
150	EK	201	CDL	C32-C31-CA7-OA8
150	Dc	601	CDL	C72-C71-CB7-OB8
150	Dd	706	CDL	C12-C11-CA5-OA6
150	Dg	201	CDL	C32-C31-CA7-OA8
150	Dj	405	CDL	C32-C31-CA7-OA8
150	Dn	503	CDL	C12-C11-CA5-OA6
150	Do	501	CDL	C72-C71-CB7-OB8
150	Dq	1402	CDL	C52-C51-CB5-OB6
150	Dv	401	CDL	C32-C31-CA7-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dv	401	CDL	C52-C51-CB5-OB6
150	Dv	402	CDL	C52-C51-CB5-OB6
150	Ep	701	CDL	C72-C71-CB7-OB8
153	A6	303	PC1	O31-C31-C32-C33
153	AA	906	PC1	O31-C31-C32-C33
153	C	510	PC1	O21-C21-C22-C23
153	Dc	605	PC1	O21-C21-C22-C23
155	Em	901	3PE	O21-C21-C22-C23
150	BL	301	CDL	C83-C84-C85-C86
150	DN	502	CDL	C82-C83-C84-C85
150	DV	402	CDL	C60-C61-C62-C63
150	Dj	405	CDL	C60-C61-C62-C63
150	Dr	402	CDL	C31-C32-C33-C34
150	Dv	403	CDL	C62-C63-C64-C65
156	Ed	203	LPP	C18-C19-C20-C21
150	EO	202	CDL	C52-C53-C54-C55
150	Dr	402	CDL	C44-C45-C46-C47
153	Dv	404	PC1	C29-C2A-C2B-C2C
155	BP	201	3PE	C37-C38-C39-C3A
150	Dj	403	CDL	CA7-C31-C32-C33
150	Dr	403	CDL	CA4-CA6-OA8-CA7
150	Ds	405	CDL	CB4-CB6-OB8-CB7
153	A6	302	PC1	O32-C31-C32-C33
153	DC	608	PC1	O22-C21-C22-C23
150	BC	301	CDL	C55-C56-C57-C58
150	DX	301	CDL	C62-C63-C64-C65
150	Eg	101	CDL	C20-C21-C22-C23
150	A0	601	CDL	C34-C35-C36-C37
150	c	501	CDL	C53-C54-C55-C56
150	EI	401	CDL	C84-C85-C86-C87
155	Dx	1207	3PE	C32-C33-C34-C35
150	B1	402	CDL	C12-C11-CA5-OA6
150	C	507	CDL	C52-C51-CB5-OB6
150	DA	706	CDL	C52-C51-CB5-OB6
150	DN	506	CDL	C32-C31-CA7-OA8
150	DS	404	CDL	C32-C31-CA7-OA8
150	DY	301	CDL	C72-C71-CB7-OB8
150	ED	605	CDL	C32-C31-CA7-OA8
150	ED	605	CDL	C72-C71-CB7-OB8
150	EI	401	CDL	C72-C71-CB7-OB8
150	ES	1101	CDL	C72-C71-CB7-OB8
150	Dn	501	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	Dn	506	CDL	C32-C31-CA7-OA8
150	Ds	405	CDL	C32-C31-CA7-OA8
150	Ds	405	CDL	C52-C51-CB5-OB6
150	Ed	205	CDL	C32-C31-CA7-OA8
153	A9	603	PC1	O31-C31-C32-C33
153	AA	907	PC1	O21-C21-C22-C23
153	DC	602	PC1	O31-C31-C32-C33
153	Dc	602	PC1	O31-C31-C32-C33
156	AA	902	LPP	O27-C29-C30-C31
167	C	512	UQ8	C36-C37-C38-C39
150	DU	401	CDL	CB2-C1-CA2-OA2
150	DG	202	CDL	C61-C62-C63-C64
150	Dq	1403	CDL	C22-C23-C24-C25
150	Ep	701	CDL	C79-C80-C81-C82
150	Eu	101	CDL	C38-C39-C40-C41
155	DS	402	3PE	C3E-C3F-C3G-C3H
150	B1	402	CDL	CB7-C71-C72-C73
150	h	501	CDL	CB7-C71-C72-C73
150	BT	204	CDL	C12-C11-CA5-OA7
150	Dd	702	CDL	C72-C71-CB7-OB9
150	Dd	705	CDL	C12-C11-CA5-OA7
150	Ea	502	CDL	C52-C51-CB5-OB7
153	EO	205	PC1	O22-C21-C22-C23
155	DX	303	3PE	O32-C31-C32-C33
150	CJ	201	CDL	OA7-CA5-OA6-CA4
153	DV	404	PC1	O22-C21-O21-C2
150	Da	709	CDL	C41-C42-C43-C44
150	Dm	501	CDL	C53-C54-C55-C56
150	El	903	CDL	C57-C58-C59-C60
150	El	903	CDL	C62-C63-C64-C65
150	DU	404	CDL	CB4-CB3-OB5-PB2
153	EB	301	PC1	C2-C1-O11-P
153	Eb	301	PC1	C2-C1-O11-P
150	g	801	CDL	CA4-CA6-OA8-CA7
167	C	511	UQ8	C15-C14-C16-C17
150	EL	903	CDL	C60-C61-C62-C63
150	Dy	301	CDL	C44-C45-C46-C47
150	CC	305	CDL	OA5-CA3-CA4-OA6
150	DZ	501	CDL	OA5-CA3-CA4-OA6
150	Di	1101	CDL	OB5-CB3-CB4-OB6
150	Dn	506	CDL	OA5-CA3-CA4-OA6
150	Dx	1204	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DG	204	3PE	O11-C1-C2-O21
155	Dr	401	3PE	O11-C1-C2-O21
156	A6	301	LPP	O5-C6-C7-O9
156	DN	504	LPP	O5-C6-C7-O9
167	En	1202	UQ8	C28-C29-C31-C32
150	AF	402	CDL	C72-C71-CB7-OB9
150	DD	706	CDL	C32-C31-CA7-OA9
150	DG	201	CDL	C32-C31-CA7-OA9
150	DV	402	CDL	C52-C51-CB5-OB7
150	EL	903	CDL	C12-C11-CA5-OA7
150	Di	1101	CDL	C52-C51-CB5-OB7
150	Dj	407	CDL	C32-C31-CA7-OA9
150	Dm	502	CDL	C12-C11-CA5-OA7
150	Ek	201	CDL	C32-C31-CA7-OA9
153	AA	906	PC1	O22-C21-C22-C23
153	AM	302	PC1	O32-C31-C32-C33
153	BG	202	PC1	O32-C31-C32-C33
153	DC	605	PC1	O22-C21-C22-C23
153	Eo	205	PC1	O22-C21-C22-C23
156	AA	902	LPP	O28-C29-C30-C31
150	c	502	CDL	C79-C80-C81-C82
150	DD	703	CDL	C37-C38-C39-C40
153	BT	203	PC1	C2B-C2C-C2D-C2E
150	BC	301	CDL	C52-C51-CB5-OB6
150	DN	503	CDL	C52-C51-CB5-OB6
150	DQ	1502	CDL	C72-C71-CB7-OB8
150	DR	403	CDL	C52-C51-CB5-OB6
150	DS	404	CDL	C52-C51-CB5-OB6
150	Dc	608	CDL	C32-C31-CA7-OA8
150	Dm	502	CDL	C12-C11-CA5-OA6
150	Dy	301	CDL	C72-C71-CB7-OB8
150	Eb	302	CDL	C12-C11-CA5-OA6
150	Eg	101	CDL	C12-C11-CA5-OA6
150	Ei	401	CDL	C72-C71-CB7-OB8
150	El	901	CDL	C72-C71-CB7-OB8
150	En	1201	CDL	C52-C51-CB5-OB6
153	A9	603	PC1	O21-C21-C22-C23
153	AA	906	PC1	O21-C21-C22-C23
153	AA	907	PC1	O31-C31-C32-C33
153	C	509	PC1	O21-C21-C22-C23
153	DG	203	PC1	O31-C31-C32-C33
153	Dc	609	PC1	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
155	DC	607	3PE	O21-C21-C22-C23
156	DN	504	LPP	O27-C29-C30-C31
150	BT	204	CDL	C57-C58-C59-C60
150	Du	403	CDL	C44-C45-C46-C47
150	Dv	402	CDL	C37-C38-C39-C40
153	Dx	1203	PC1	C2A-C2B-C2C-C2D
150	DH	202	CDL	C55-C56-C57-C58
150	DM	502	CDL	C59-C60-C61-C62
150	B0	101	CDL	C52-C51-CB5-OB7
150	H	1301	CDL	C32-C31-CA7-OA9
150	DJ	304	CDL	C32-C31-CA7-OA9
150	DU	401	CDL	C32-C31-CA7-OA9
150	DV	401	CDL	C52-C51-CB5-OB7
150	DV	402	CDL	C72-C71-CB7-OB9
150	ED	605	CDL	C72-C71-CB7-OB9
150	Dc	608	CDL	C32-C31-CA7-OA9
150	Dn	502	CDL	C52-C51-CB5-OB7
150	Dq	1402	CDL	C52-C51-CB5-OB7
150	Dv	402	CDL	C52-C51-CB5-OB7
150	Ed	205	CDL	C12-C11-CA5-OA7
150	Ep	701	CDL	C72-C71-CB7-OB9
168	c	504	HEM	C4D-C3D-CAD-CBD
150	A0	602	CDL	C55-C56-C57-C58
150	AA	901	CDL	C37-C38-C39-C40
150	AA	908	CDL	C64-C65-C66-C67
150	DX	306	CDL	C14-C15-C16-C17
150	DZ	501	CDL	C35-C36-C37-C38
150	EA	301	CDL	C56-C57-C58-C59
150	ED	601	CDL	C34-C35-C36-C37
150	Dy	301	CDL	C38-C39-C40-C41
150	AF	401	CDL	C72-C71-CB7-OB8
150	BC	302	CDL	C12-C11-CA5-OA6
150	DA	709	CDL	C12-C11-CA5-OA6
150	DO	501	CDL	C72-C71-CB7-OB8
150	Dm	501	CDL	C72-C71-CB7-OB8
153	DI	303	PC1	O21-C21-C22-C23
153	Eo	204	PC1	O21-C21-C22-C23
150	Da	709	CDL	C38-C39-C40-C41
153	AJ	501	PC1	C34-C35-C36-C37
153	C	509	PC1	C22-C23-C24-C25
167	EL	905	UQ8	C3-C4-O4-C4M
167	Ds	404	UQ8	C4-C3-O3-C3M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
150	AA	901	CDL	C32-C33-C34-C35
150	BC	302	CDL	C73-C74-C75-C76
150	CG	302	CDL	C71-C72-C73-C74
150	C	503	CDL	C33-C34-C35-C36
150	c	509	CDL	C20-C21-C22-C23
150	DH	202	CDL	C78-C79-C80-C81
150	DC	601	CDL	C72-C71-CB7-OB9
150	DJ	304	CDL	C72-C71-CB7-OB9
150	DM	501	CDL	C12-C11-CA5-OA7
150	EI	401	CDL	C72-C71-CB7-OB9
150	EN	1201	CDL	C52-C51-CB5-OB7
150	ES	1101	CDL	C72-C71-CB7-OB9
150	Dc	601	CDL	C72-C71-CB7-OB9
150	Dg	201	CDL	C32-C31-CA7-OA9
150	Dv	401	CDL	C52-C51-CB5-OB7
150	Ea	501	CDL	C32-C31-CA7-OA9
153	AA	907	PC1	O22-C21-C22-C23
153	AA	907	PC1	O32-C31-C32-C33
153	C	509	PC1	O22-C21-C22-C23
153	Dc	605	PC1	O22-C21-C22-C23
153	Dx	1203	PC1	O22-C21-C22-C23
155	Dd	703	3PE	O32-C31-C32-C33
155	Em	901	3PE	O22-C21-C22-C23
167	c	510	UQ8	C24-C26-C27-C28
167	Ed	202	UQ8	C24-C26-C27-C28
166	D	401	HEC	CAA-CBA-CGA-O2A
150	E	301	CDL	C11-CA5-OA6-CA4
150	DH	201	CDL	C14-C15-C16-C17
150	EL	901	CDL	C36-C37-C38-C39
150	EN	1202	CDL	C59-C60-C61-C62
150	DA	706	CDL	C39-C40-C41-C42
150	DD	704	CDL	C39-C40-C41-C42
150	BG	201	CDL	O1-C1-CA2-OA2
150	B0	102	CDL	C32-C31-CA7-OA8
150	BC	301	CDL	C32-C31-CA7-OA8
150	BT	202	CDL	C52-C51-CB5-OB6
150	CC	305	CDL	C12-C11-CA5-OA6
150	DD	704	CDL	C12-C11-CA5-OA6
150	DN	503	CDL	C32-C31-CA7-OA8
150	DV	401	CDL	C52-C51-CB5-OB6
150	Du	401	CDL	C32-C31-CA7-OA8
153	Ds	407	PC1	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Dx	1205	PC1	O21-C21-C22-C23
150	DJ	304	CDL	C52-C53-C54-C55
150	DV	402	CDL	C42-C43-C44-C45
150	Dh	201	CDL	C61-C62-C63-C64
150	Dv	402	CDL	C44-C45-C46-C47
150	DD	705	CDL	C72-C71-CB7-OB9
150	DN	502	CDL	C72-C71-CB7-OB9
150	DR	403	CDL	C52-C51-CB5-OB7
150	DY	301	CDL	C72-C71-CB7-OB9
150	Dd	705	CDL	C72-C71-CB7-OB9
150	El	903	CDL	C52-C51-CB5-OB7
153	A9	603	PC1	O32-C31-C32-C33
153	Dx	1203	PC1	O32-C31-C32-C33
168	C	501	HEM	C2D-C3D-CAD-CBD
169	Da	702	HEA	CAA-CBA-CGA-O1A
150	BT	202	CDL	C83-C84-C85-C86
150	C	504	CDL	C37-C38-C39-C40
153	Eo	204	PC1	C2F-C2G-C2H-C2I
155	DX	303	3PE	C38-C39-C3A-C3B
155	Em	901	3PE	C39-C3A-C3B-C3C
150	C	505	CDL	C12-C13-C14-C15
150	DR	402	CDL	C53-C54-C55-C56
150	EL	901	CDL	C73-C74-C75-C76
150	Dd	704	CDL	C57-C58-C59-C60
150	Do	501	CDL	C71-C72-C73-C74
150	C	507	CDL	C52-C51-CB5-OB7
150	DN	503	CDL	C52-C51-CB5-OB7
150	EK	201	CDL	C32-C31-CA7-OA9
150	Dn	503	CDL	C12-C11-CA5-OA7
150	Do	501	CDL	C72-C71-CB7-OB9
150	Dq	1402	CDL	C72-C71-CB7-OB9
150	Ds	405	CDL	C32-C31-CA7-OA9
150	En	1201	CDL	C52-C51-CB5-OB7
153	A9	603	PC1	O22-C21-C22-C23
155	Dx	1206	3PE	C2-C3-O31-C31
150	CJ	201	CDL	C31-C32-C33-C34
150	DJ	302	CDL	C80-C81-C82-C83
150	ED	605	CDL	C24-C25-C26-C27
150	EL	902	CDL	C15-C16-C17-C18
150	Ds	406	CDL	C34-C35-C36-C37
150	Dx	1204	CDL	C75-C76-C77-C78
153	A1	403	PC1	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	DJ	306	PC1	C28-C29-C2A-C2B
150	BT	204	CDL	C72-C71-CB7-OB8
150	DD	705	CDL	C52-C51-CB5-OB6
150	DX	307	CDL	C52-C51-CB5-OB6
150	ED	601	CDL	C52-C51-CB5-OB6
150	EL	903	CDL	C32-C31-CA7-OA8
150	Dx	1201	CDL	C52-C51-CB5-OB6
150	Ea	501	CDL	C72-C71-CB7-OB8
153	BS	1302	PC1	O21-C21-C22-C23
153	EB	301	PC1	O31-C31-C32-C33
155	Da	708	3PE	O31-C31-C32-C33

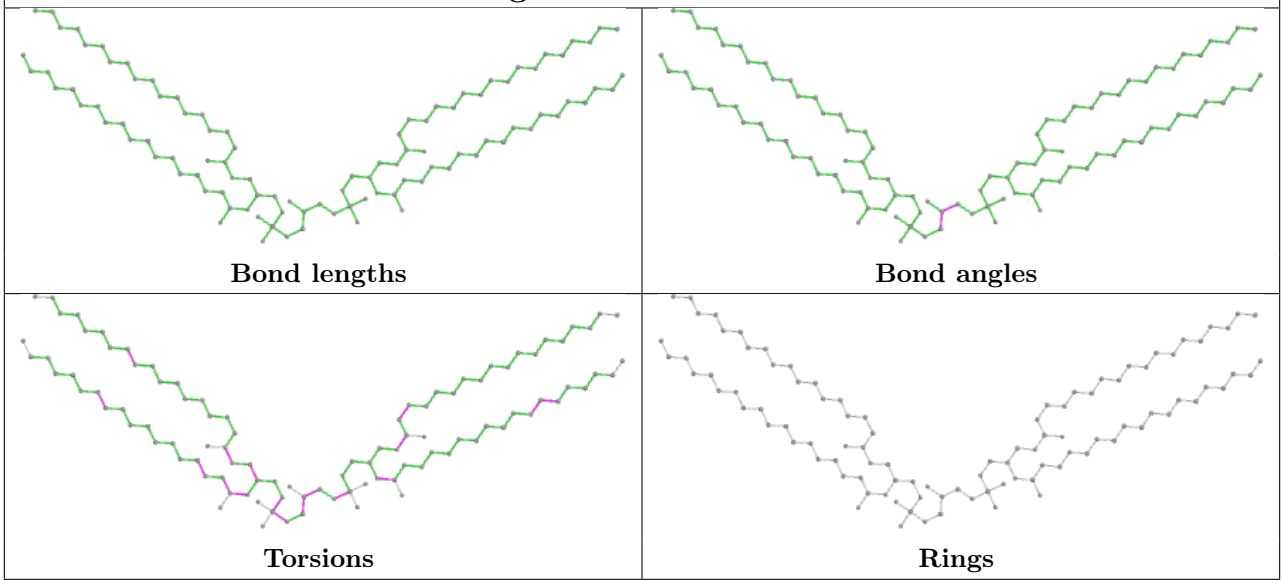
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
165	CB	1002	F3S	FE1-FE3-S1-S3
165	CB	1002	F3S	FE3-FE4-S3-S4

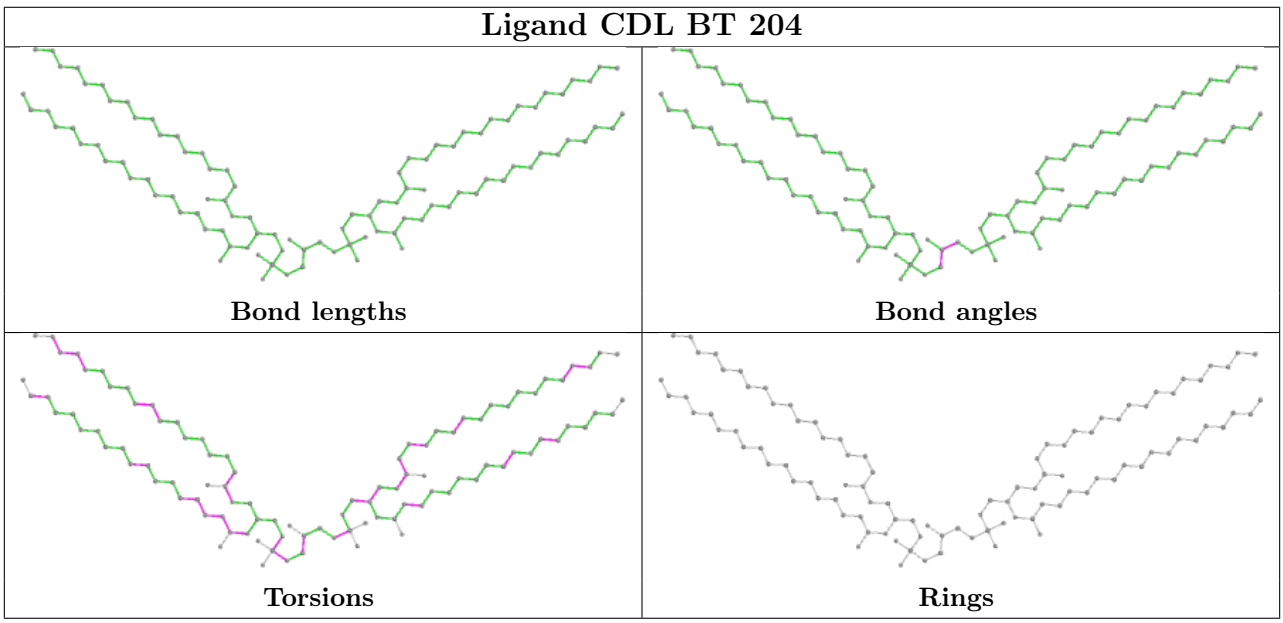
No monomer is involved in short contacts.

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.

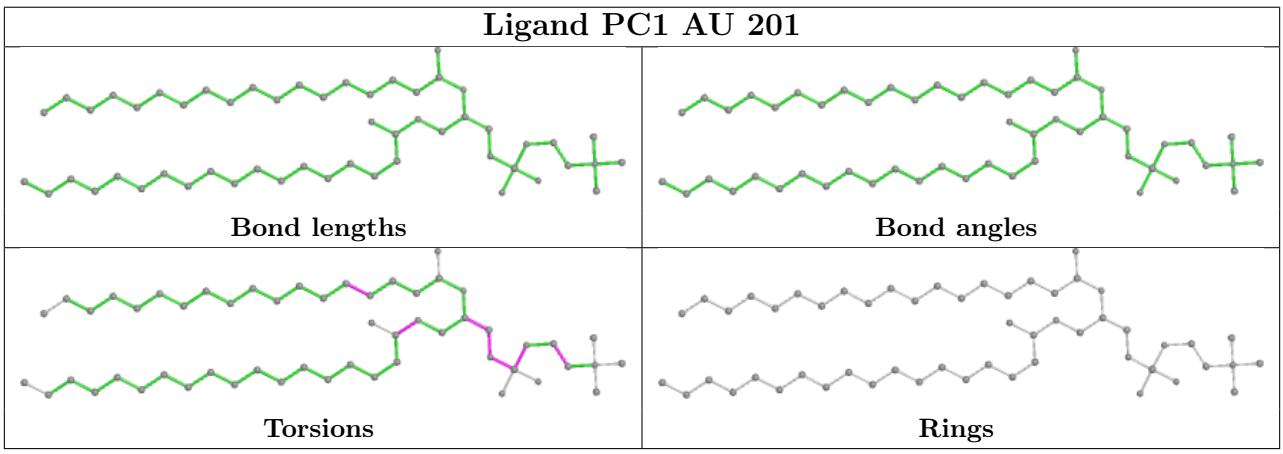
Ligand CDL Dm 502



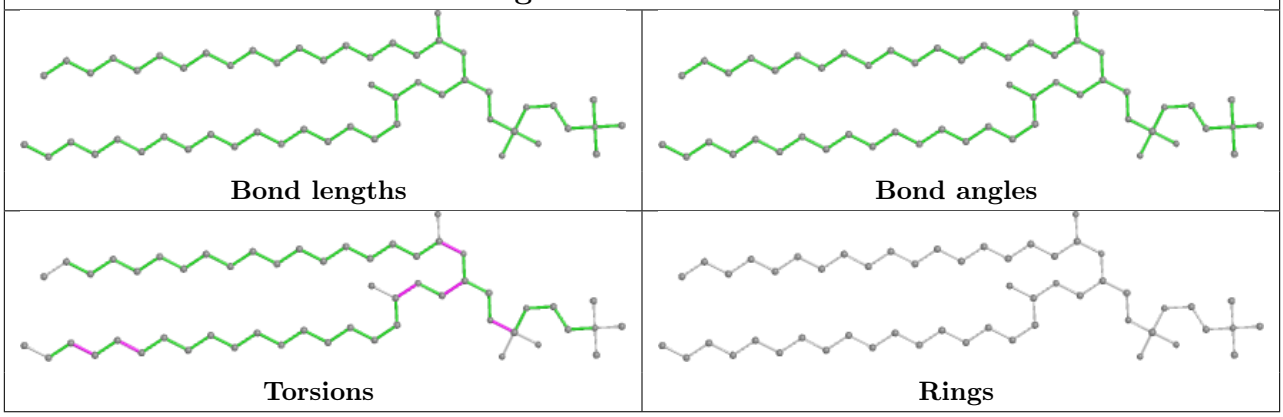
Ligand CDL BT 204



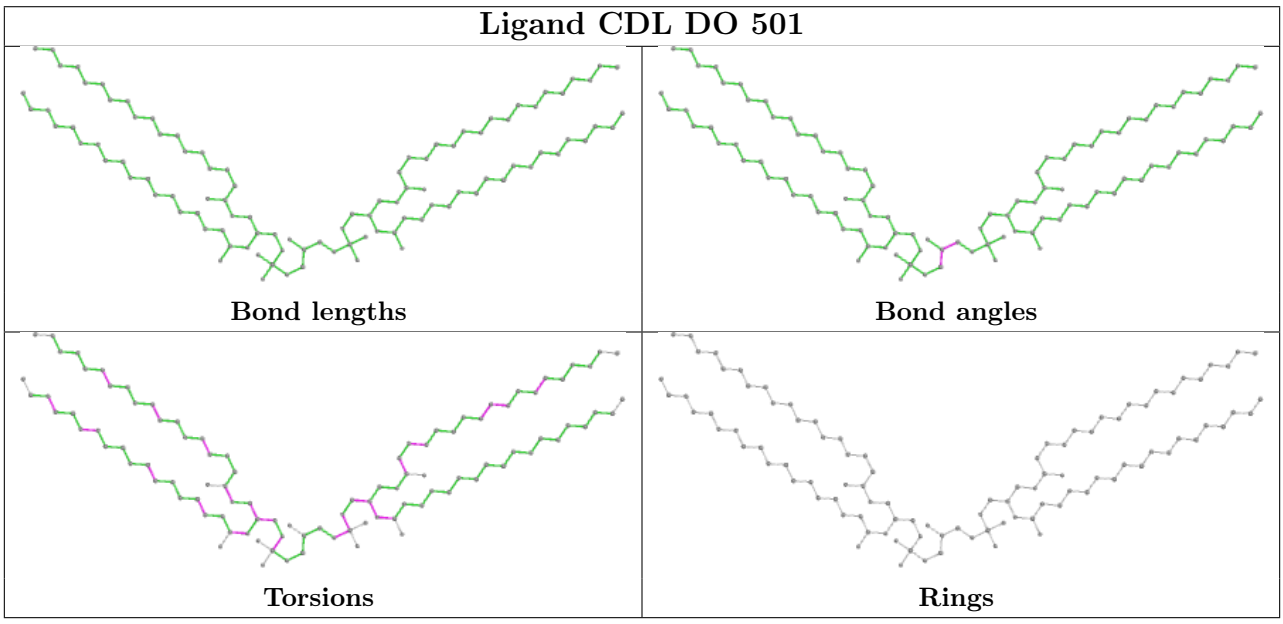
Ligand PC1 AU 201



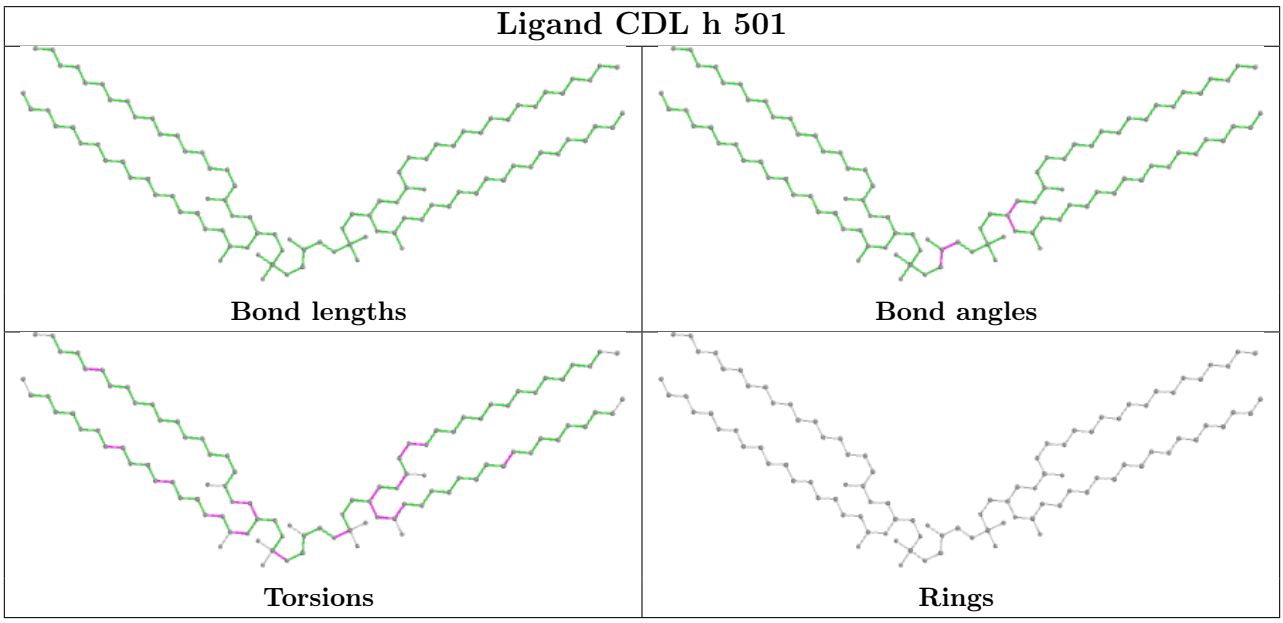
Ligand PC1 DA 708



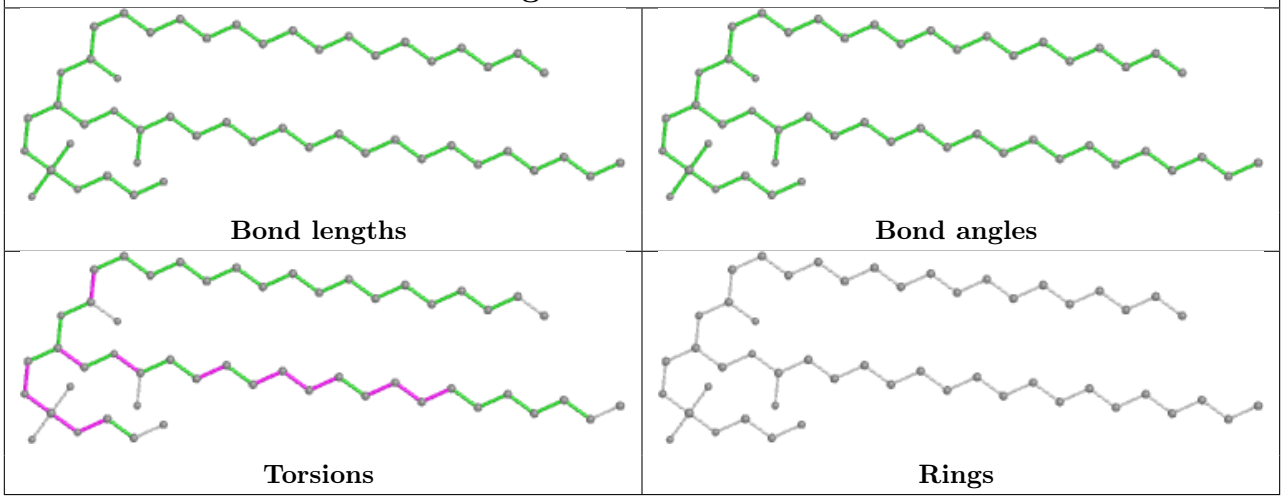
Ligand CDL DO 501



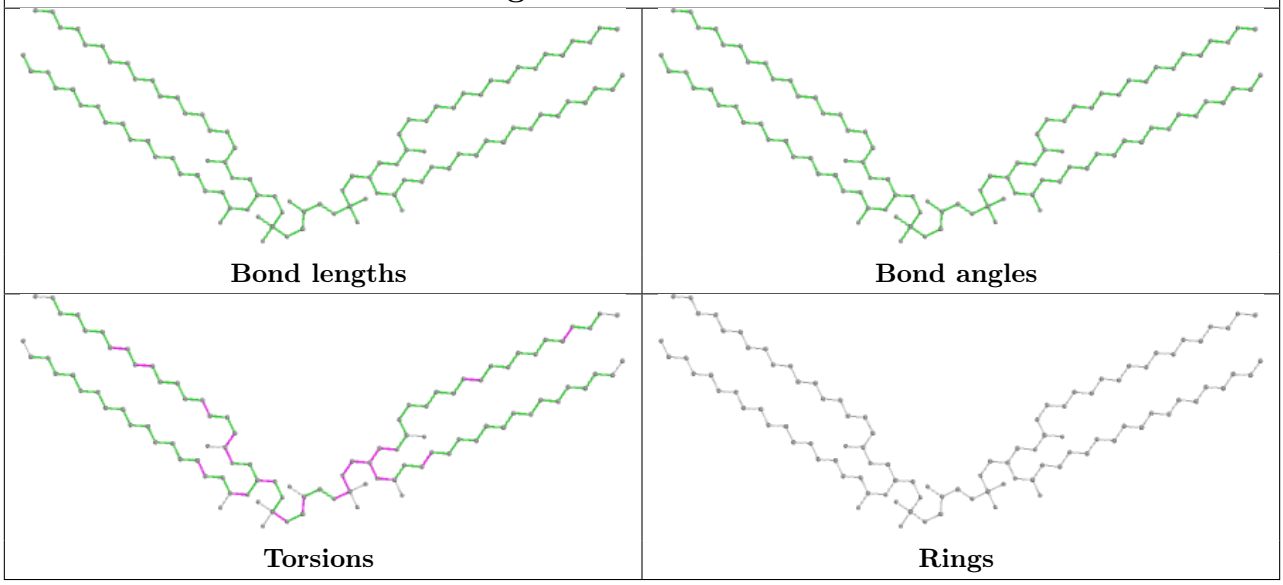
Ligand CDL h 501



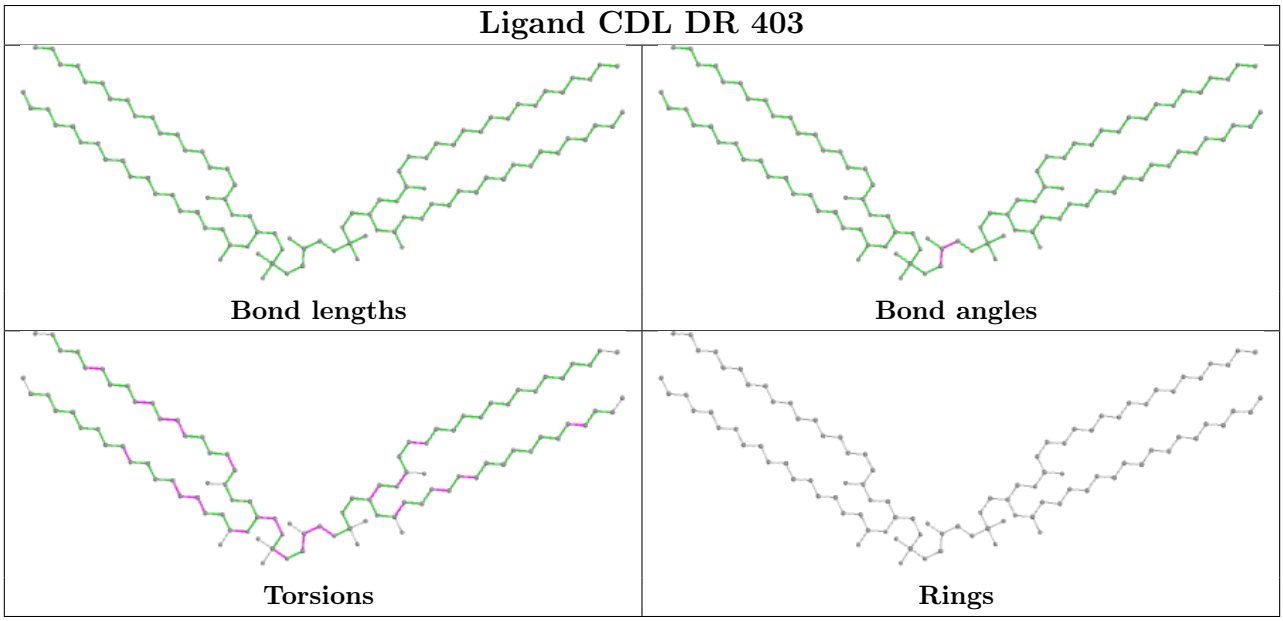
Ligand 3PE DI 301



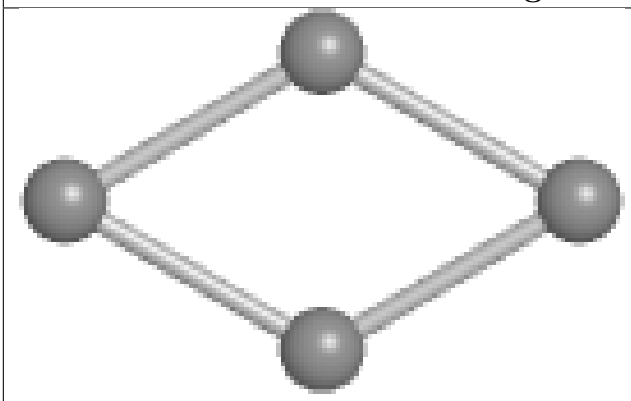
Ligand CDL AM 301



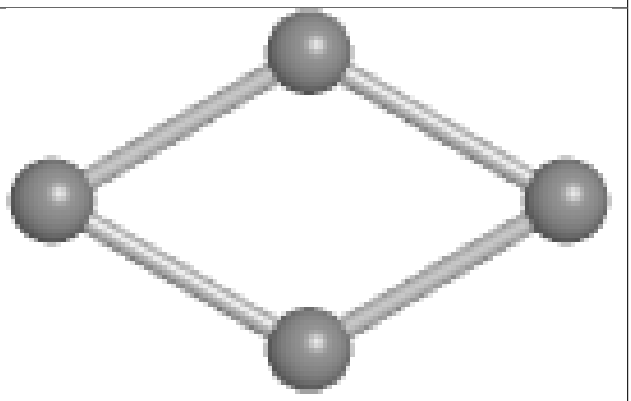
Ligand CDL DR 403



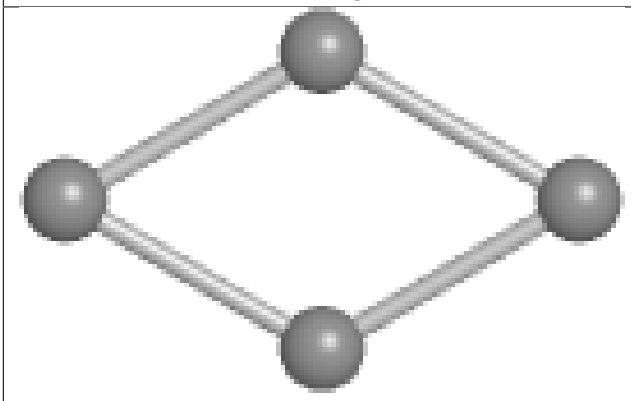
Ligand FES e 1102



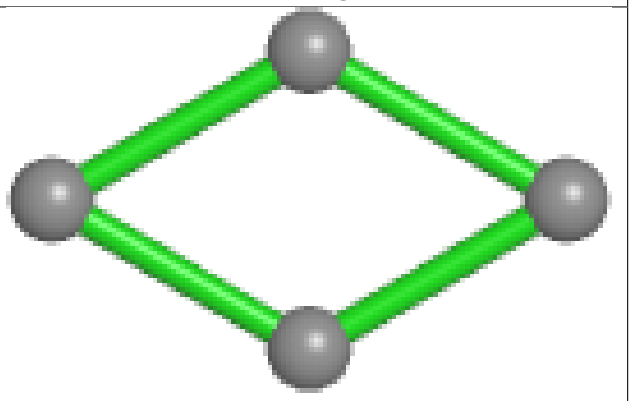
Bond lengths



Bond angles

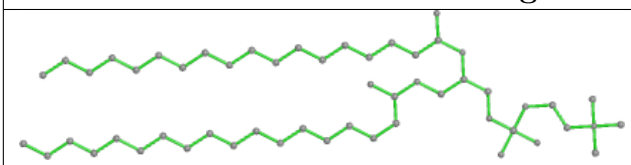


Torsions

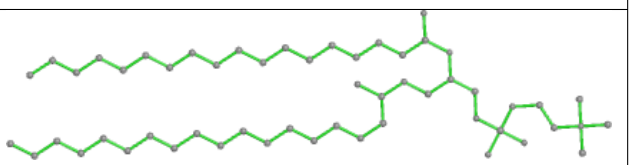


Rings

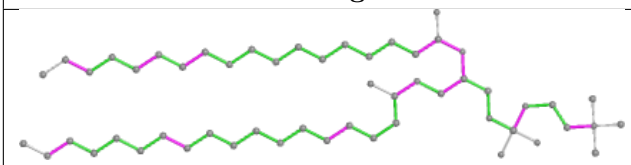
Ligand PC1 Eo 204



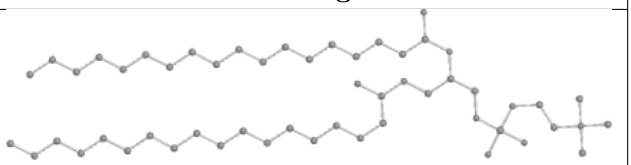
Bond lengths



Bond angles

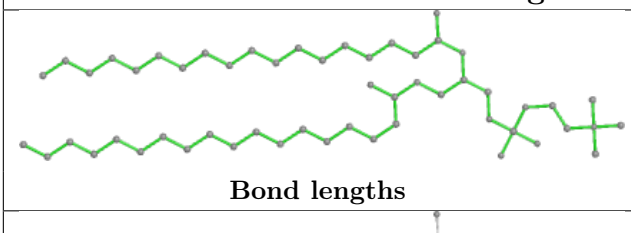


Torsions

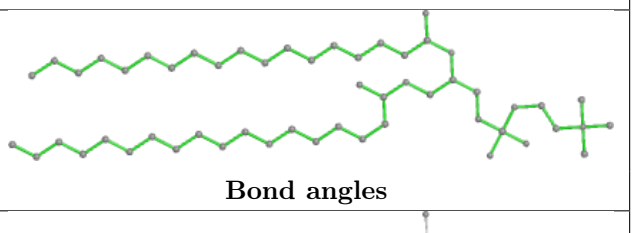


Rings

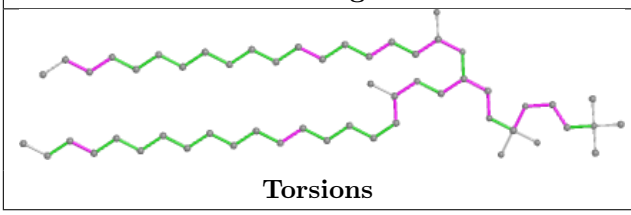
Ligand PC1 C 509



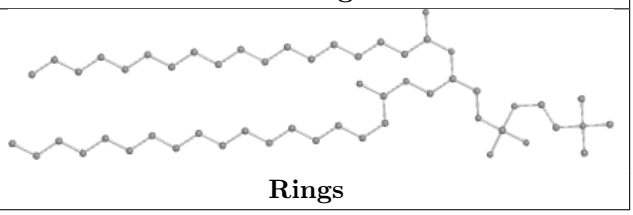
Bond lengths



Bond angles

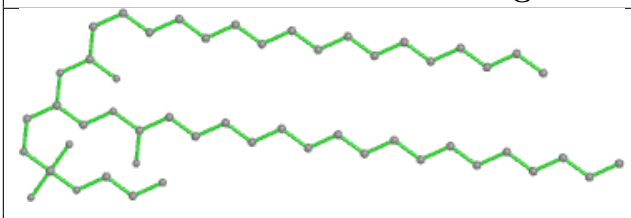


Torsions

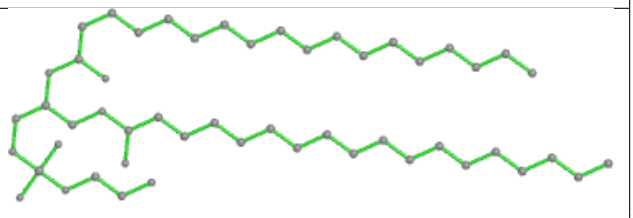


Rings

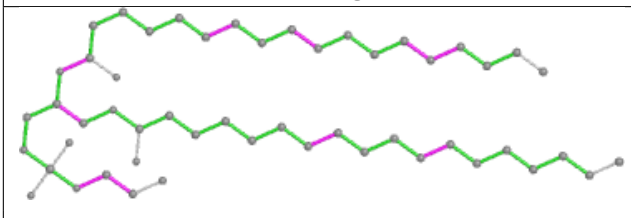
Ligand 3PE DN 501



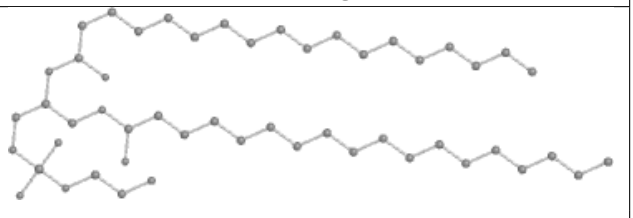
Bond lengths



Bond angles

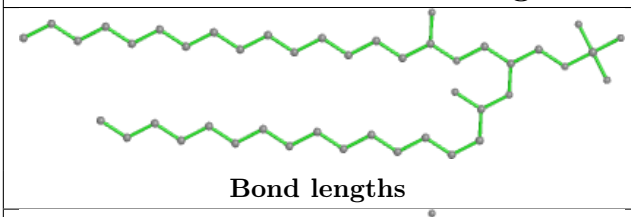


Torsions

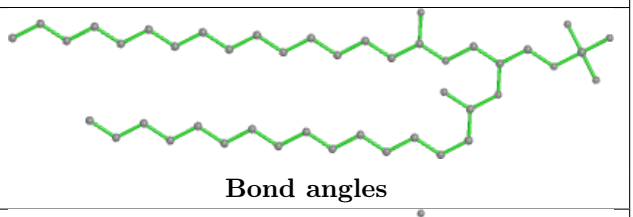


Rings

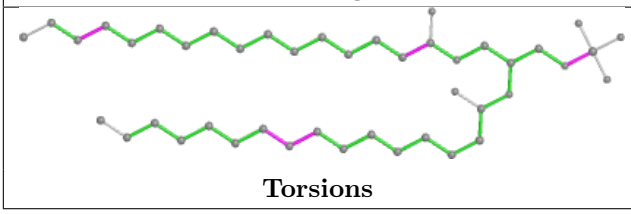
Ligand LPP DA 710



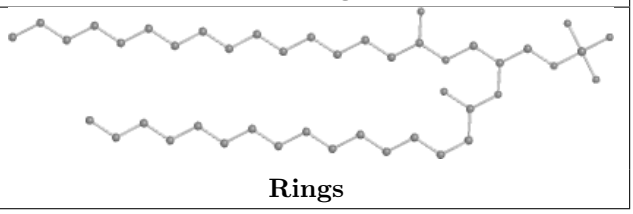
Bond lengths



Bond angles

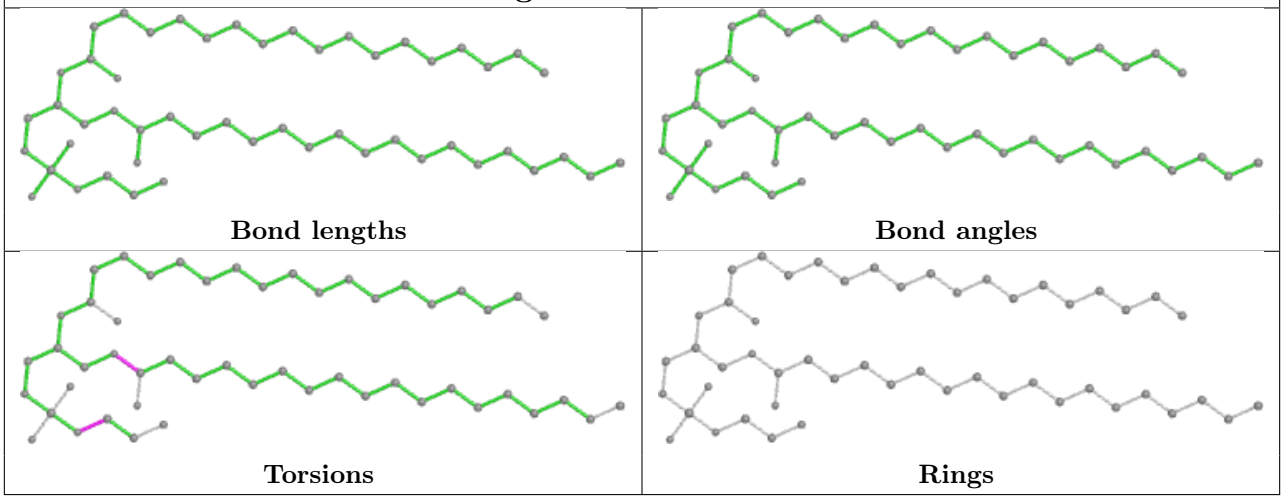


Torsions

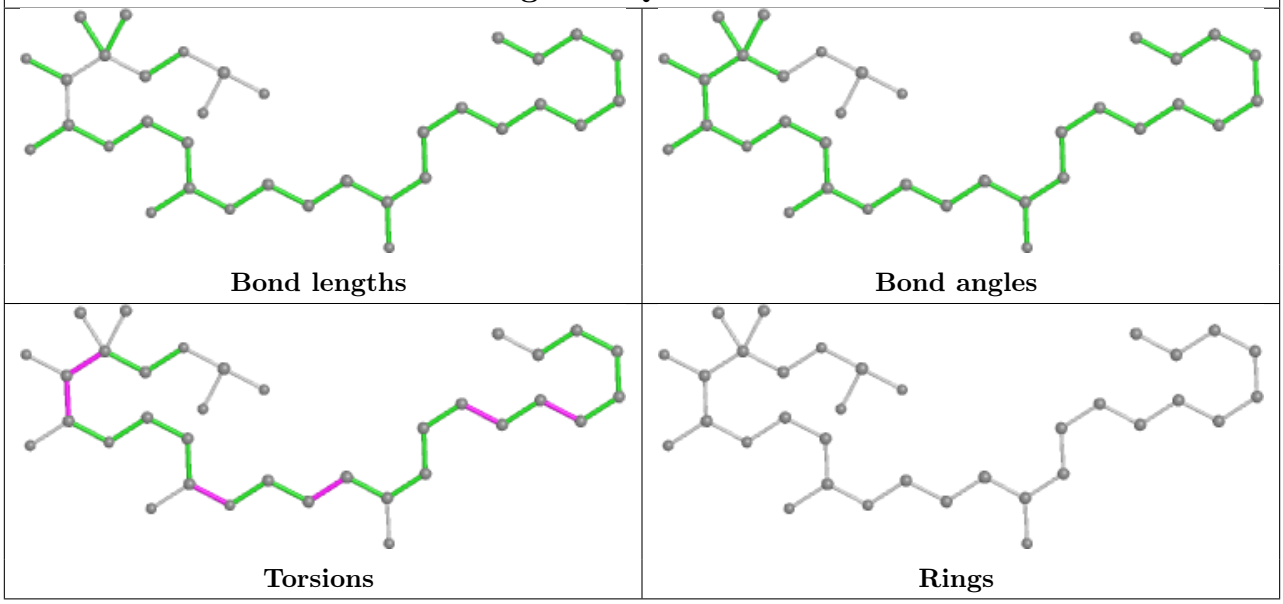


Rings

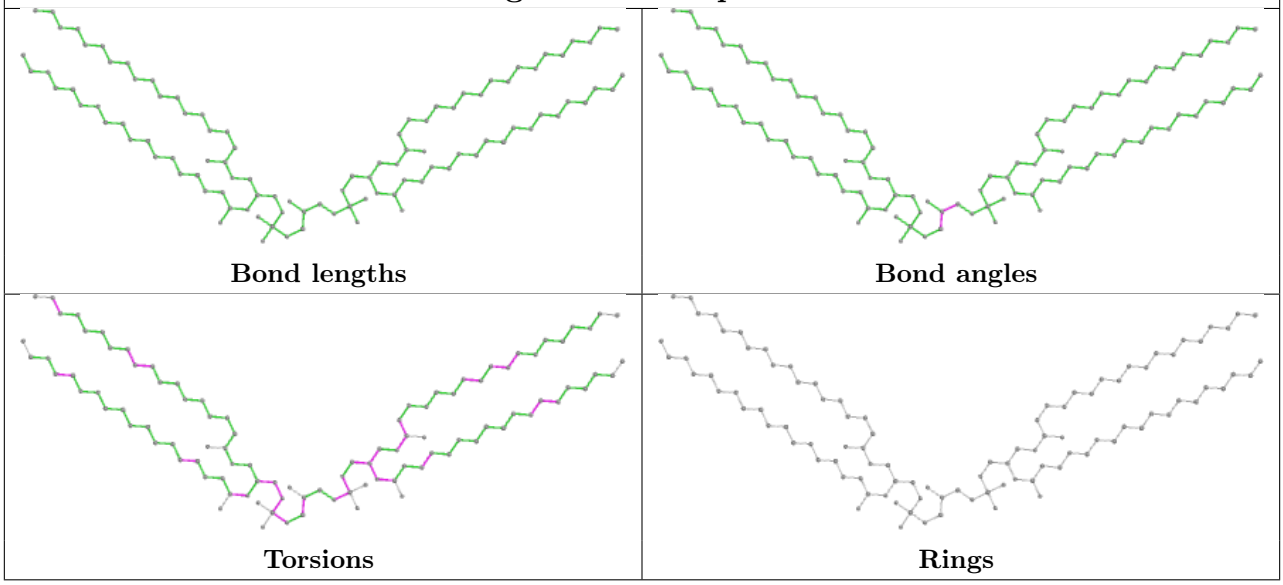
Ligand 3PE CK 101



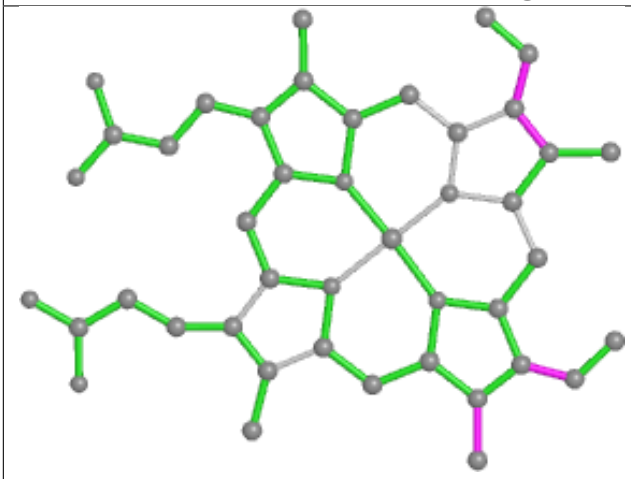
Ligand 8Q1 AS 200



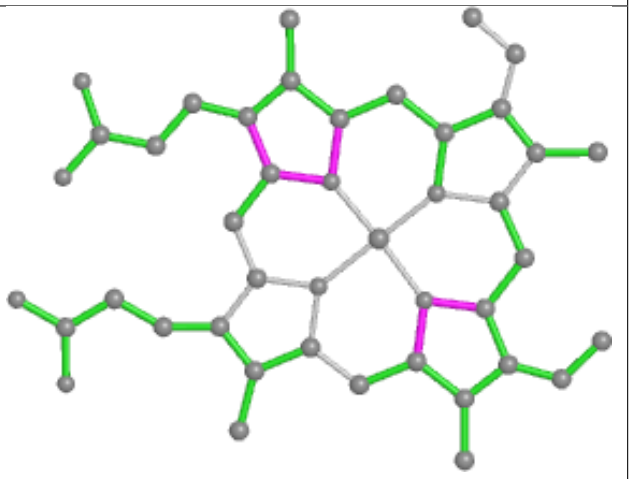
Ligand CDL Dq 1403



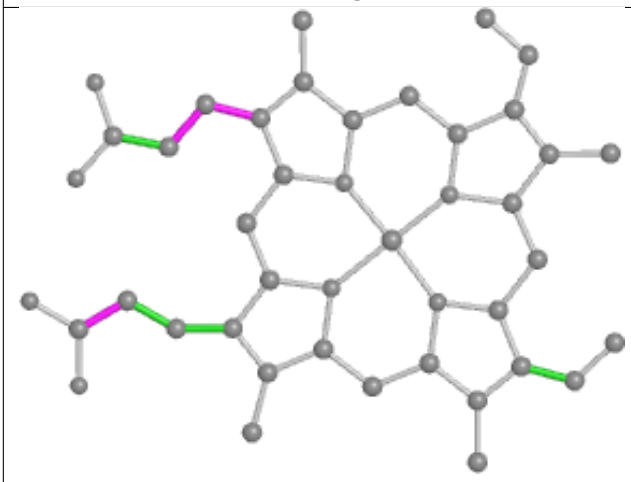
Ligand HEM C 502



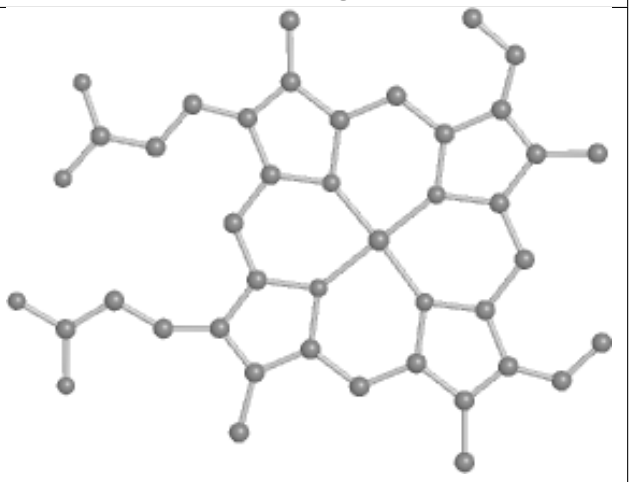
Bond lengths



Bond angles

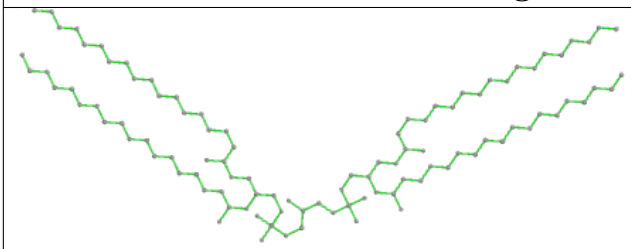


Torsions

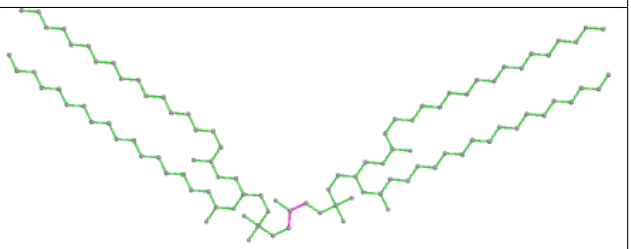


Rings

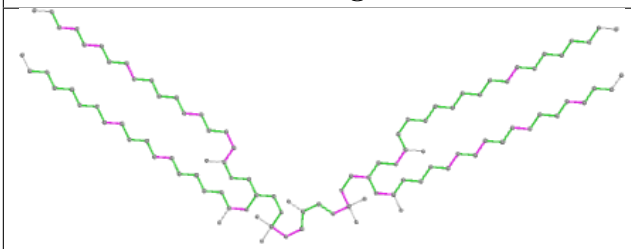
Ligand CDL DS 405



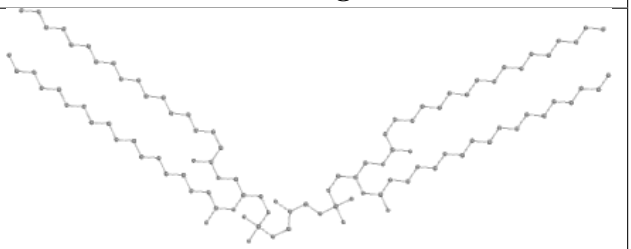
Bond lengths



Bond angles

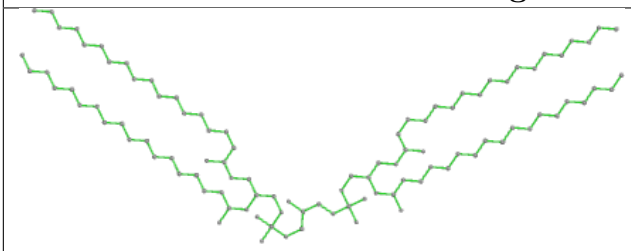


Torsions

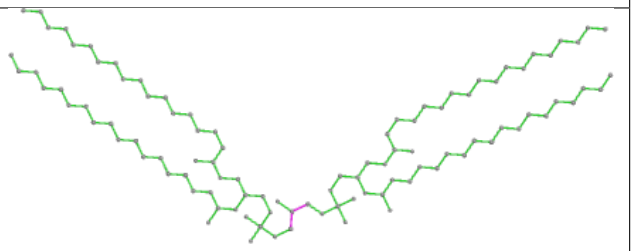


Rings

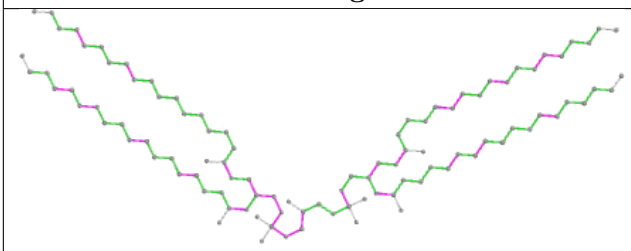
Ligand CDL DN 507



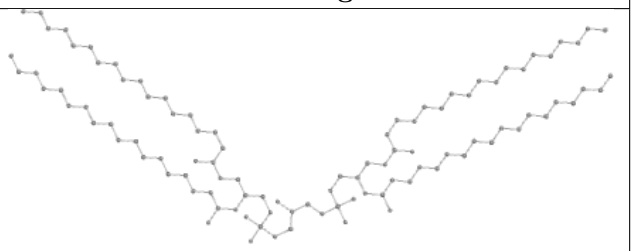
Bond lengths



Bond angles

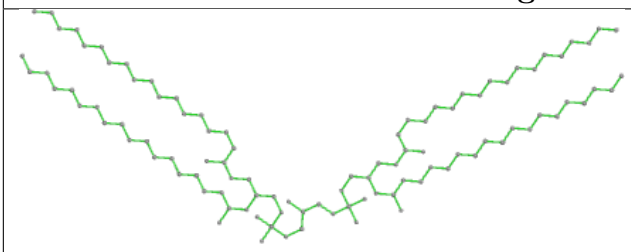


Torsions

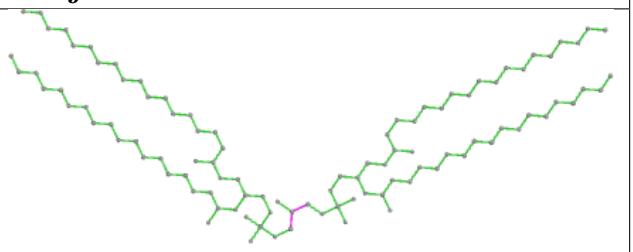


Rings

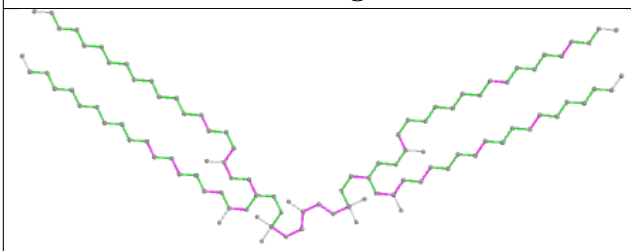
Ligand CDL Dj 407



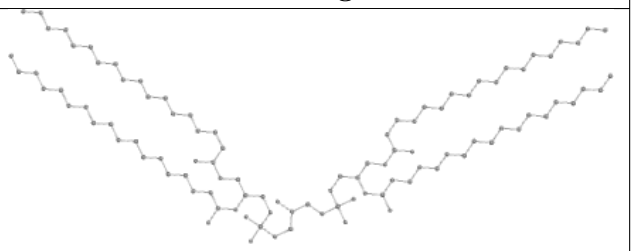
Bond lengths



Bond angles

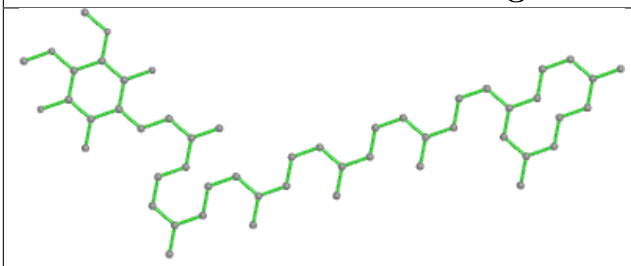


Torsions

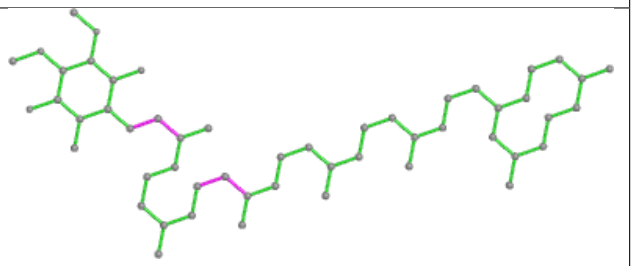


Rings

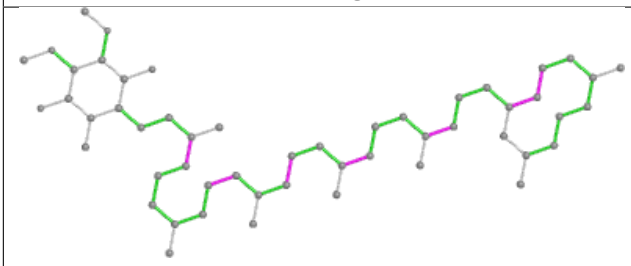
Ligand UQ8 En 1202



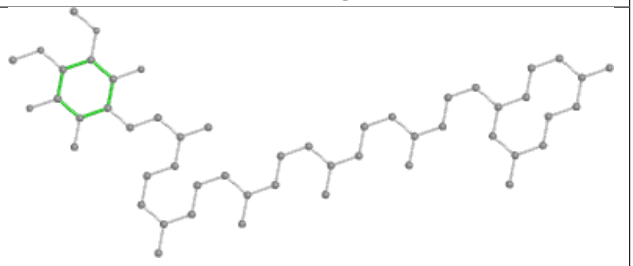
Bond lengths



Bond angles

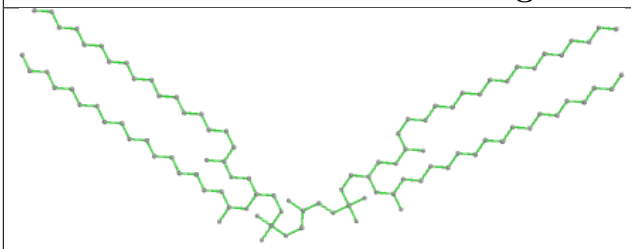


Torsions

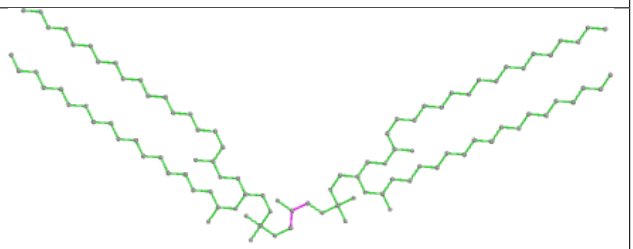


Rings

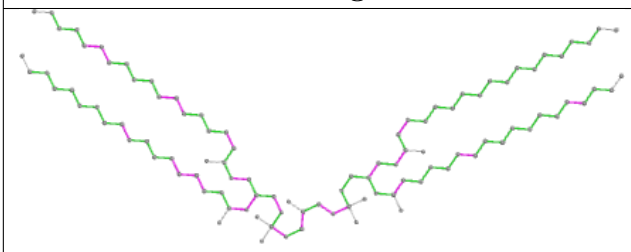
Ligand CDL Dr 403



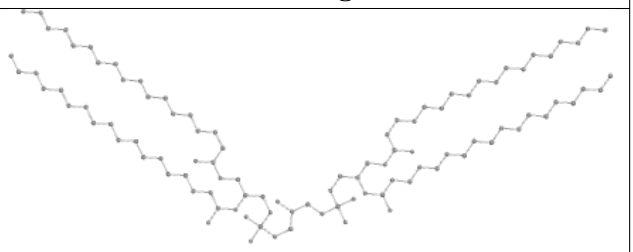
Bond lengths



Bond angles

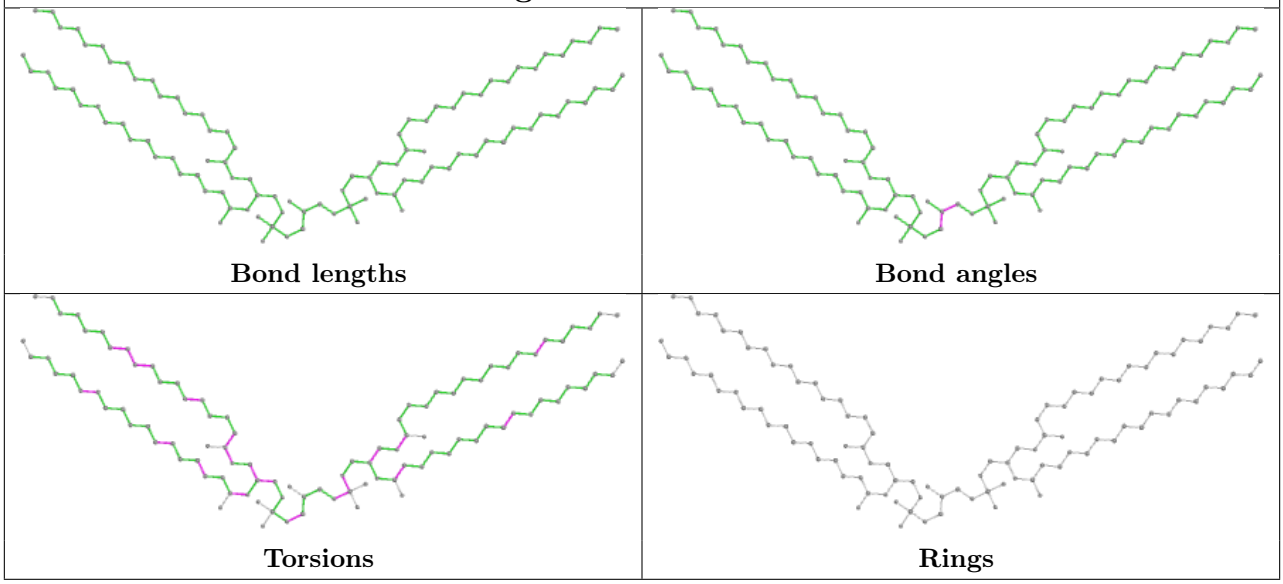


Torsions

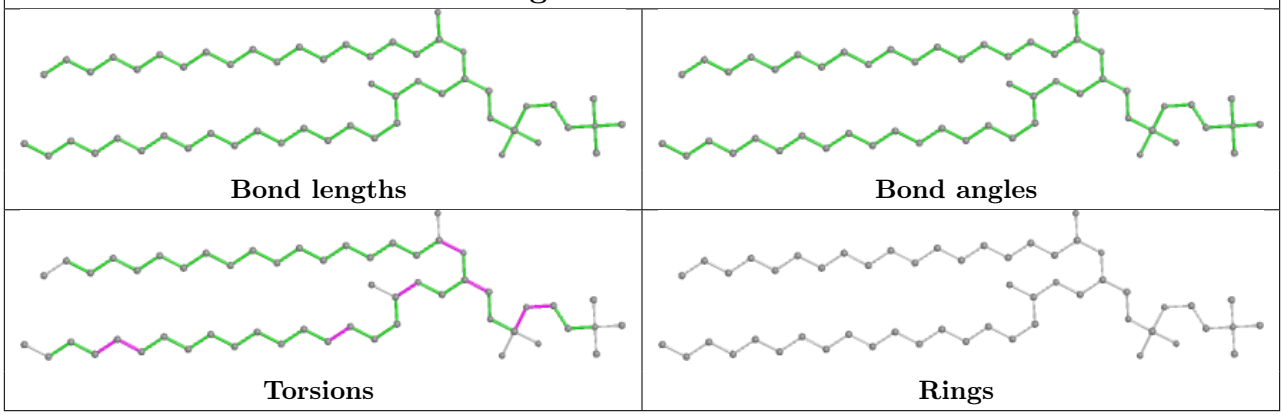


Rings

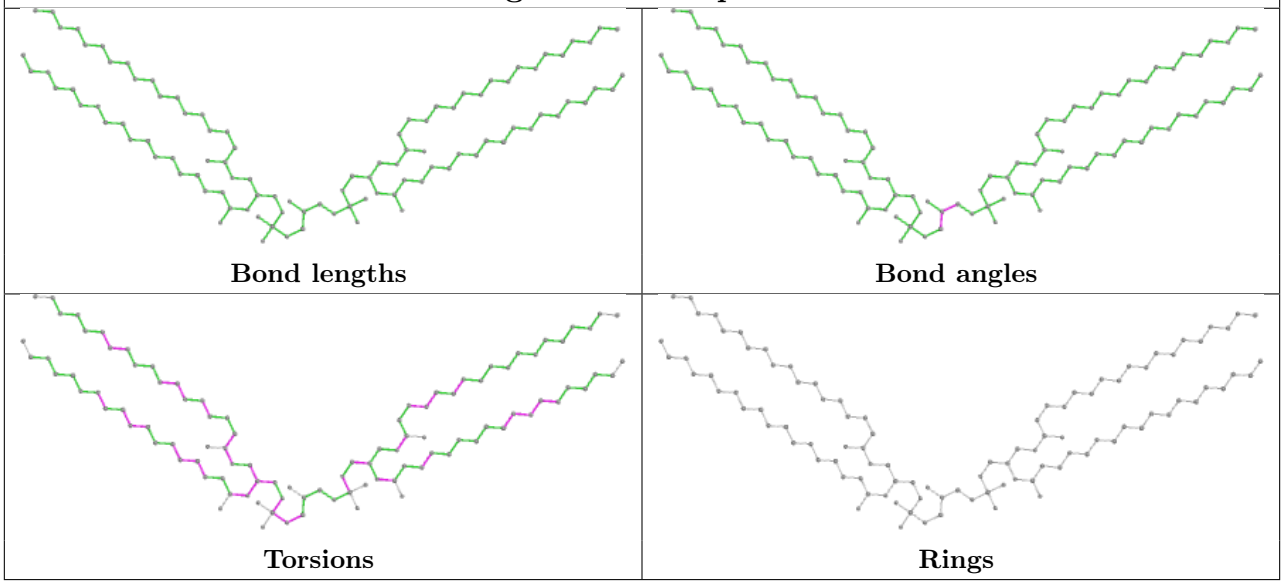
Ligand CDL H 1301



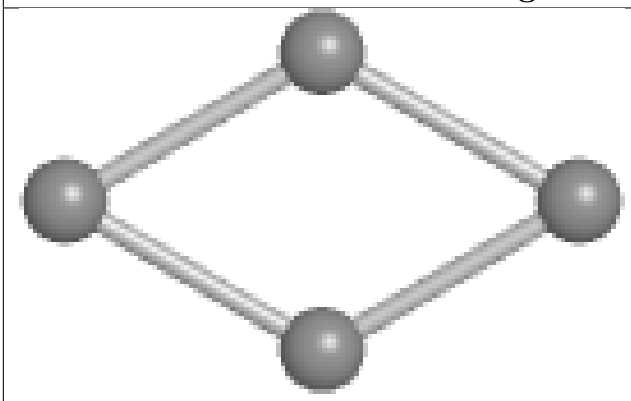
Ligand PC1 E 303



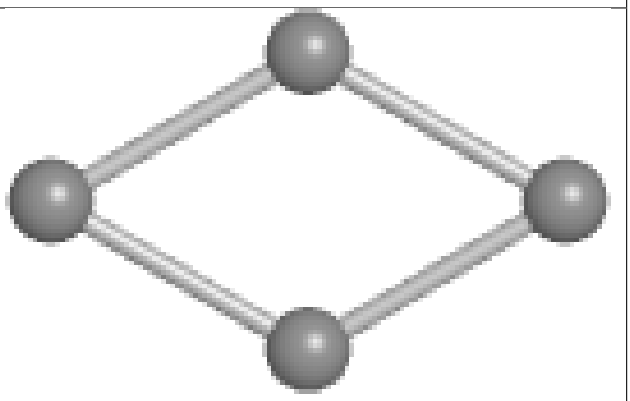
Ligand CDL Dq 1401



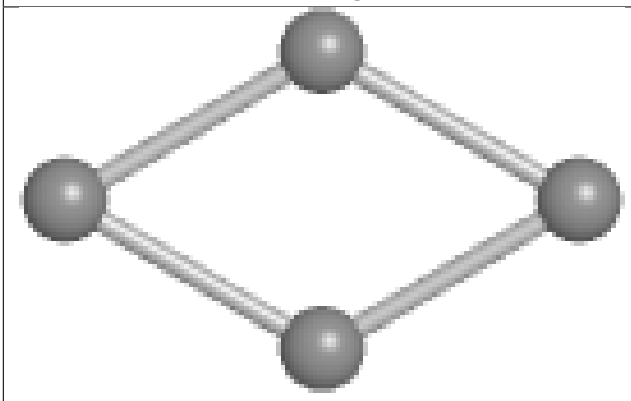
Ligand FES EF 202



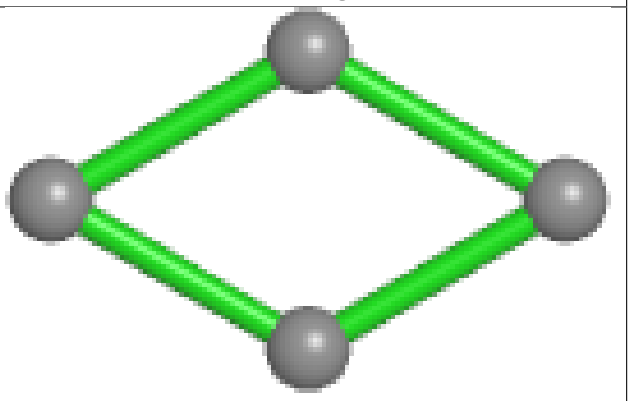
Bond lengths



Bond angles

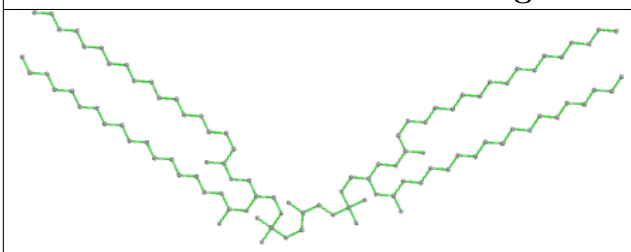


Torsions

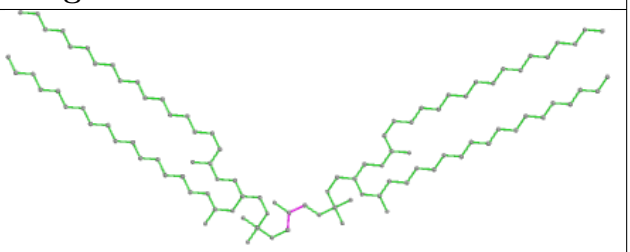


Rings

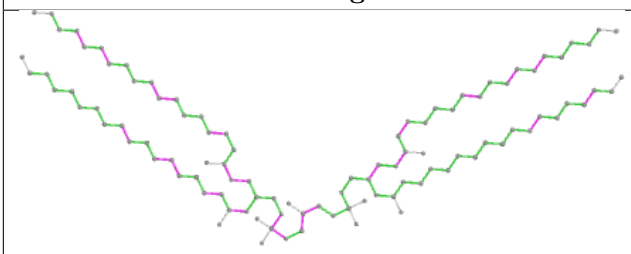
Ligand CDL Dg 202



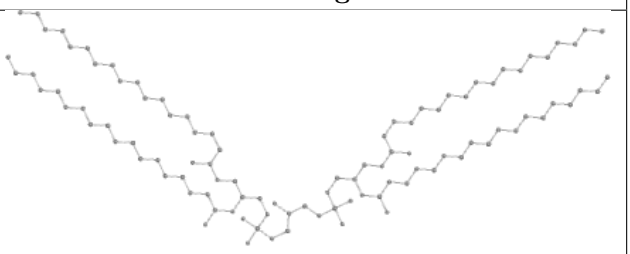
Bond lengths



Bond angles

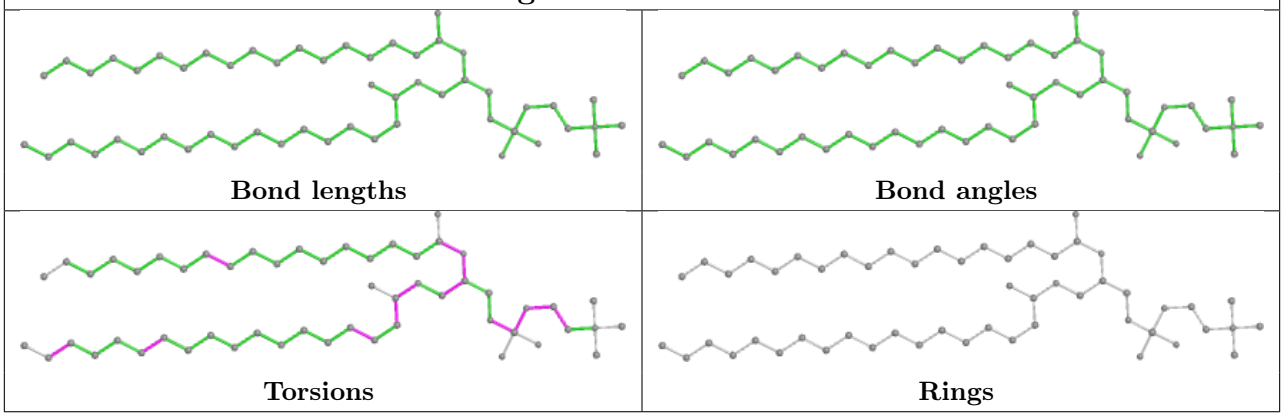


Torsions

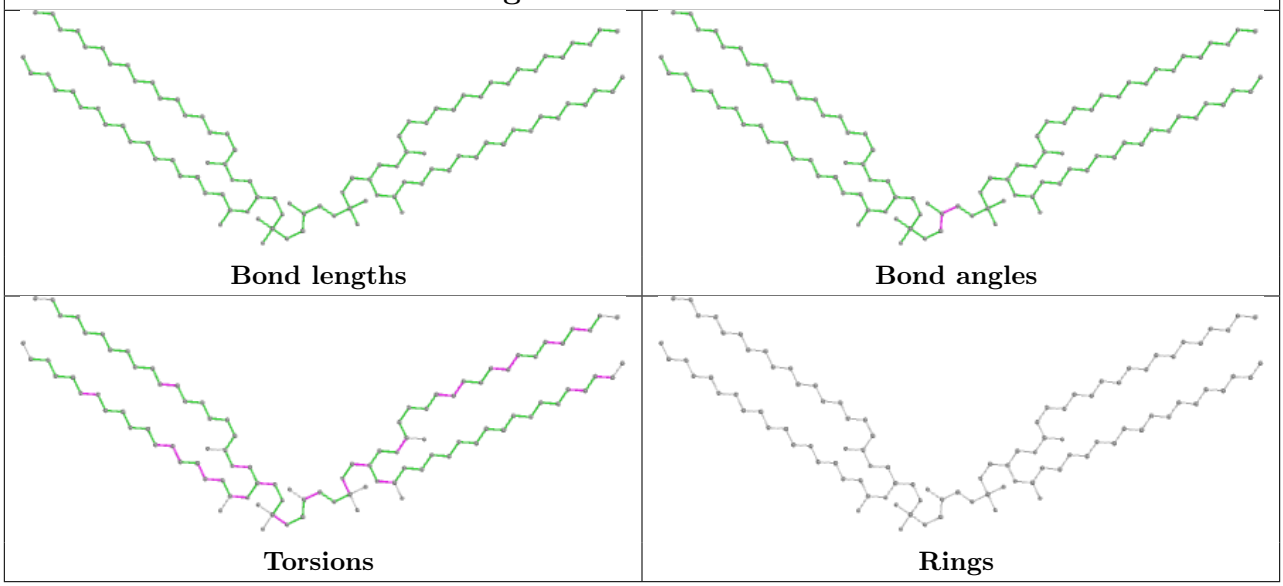


Rings

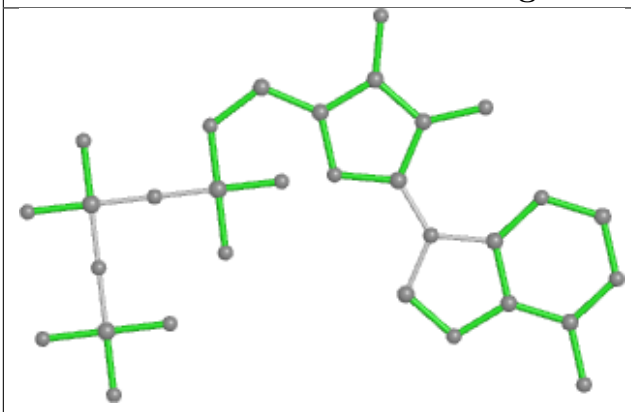
Ligand PC1 DS 406



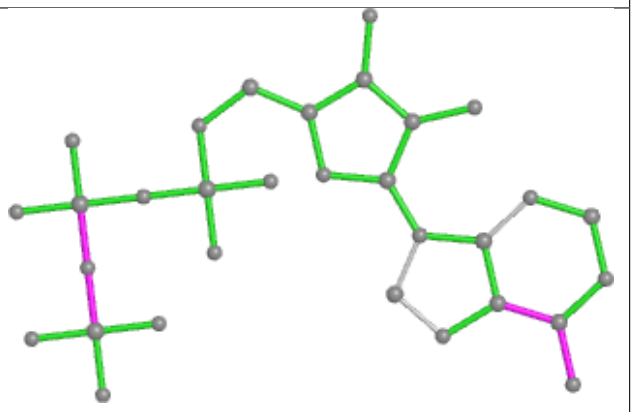
Ligand CDL EH 1601



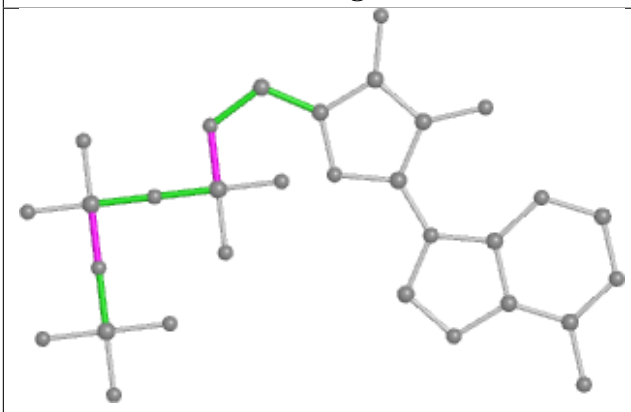
Ligand ATP Er 201



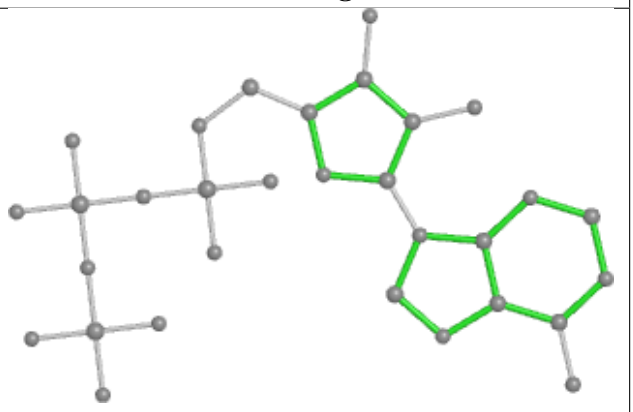
Bond lengths



Bond angles

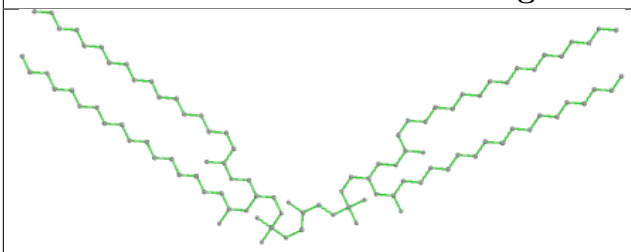


Torsions

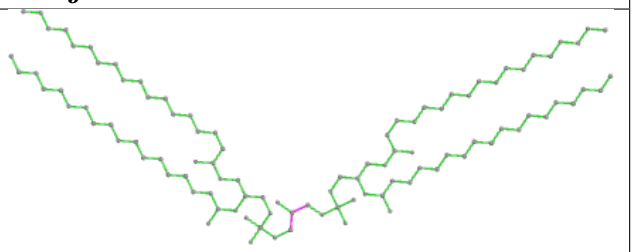


Rings

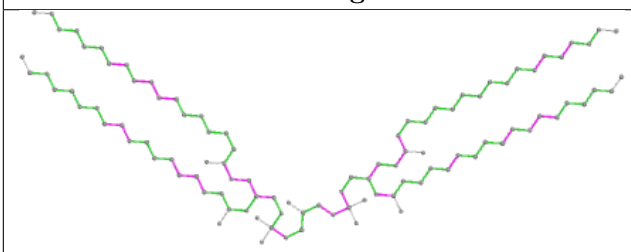
Ligand CDL Dj 401



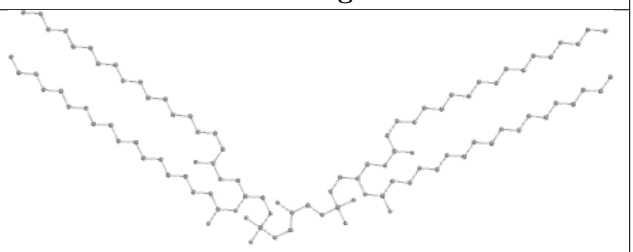
Bond lengths



Bond angles

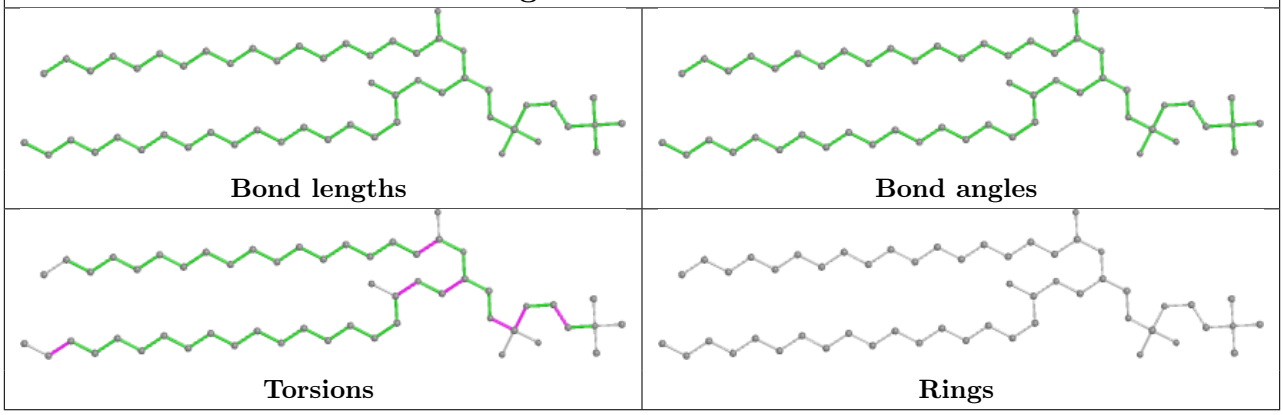


Torsions

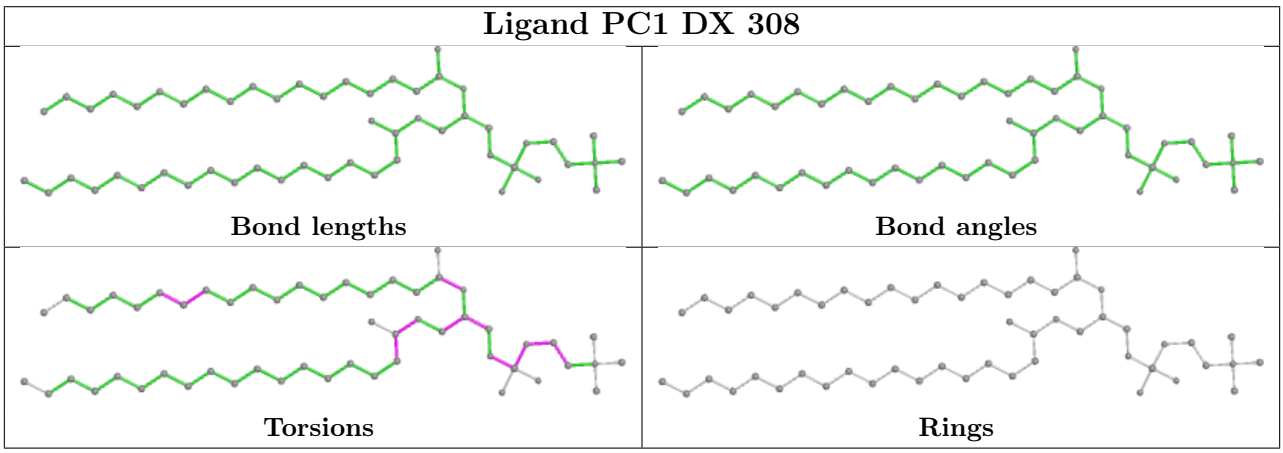


Rings

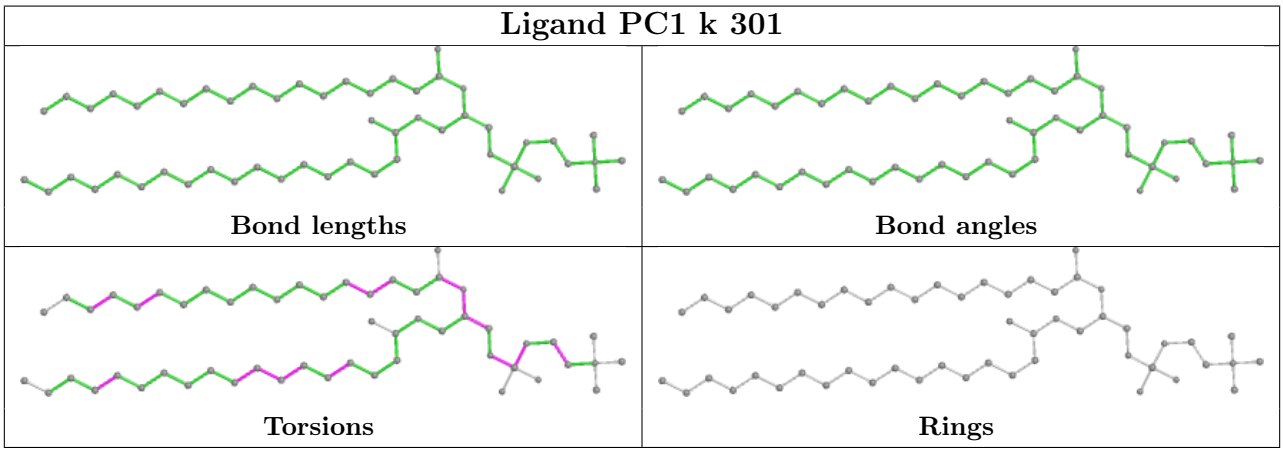
Ligand PC1 Dc 604



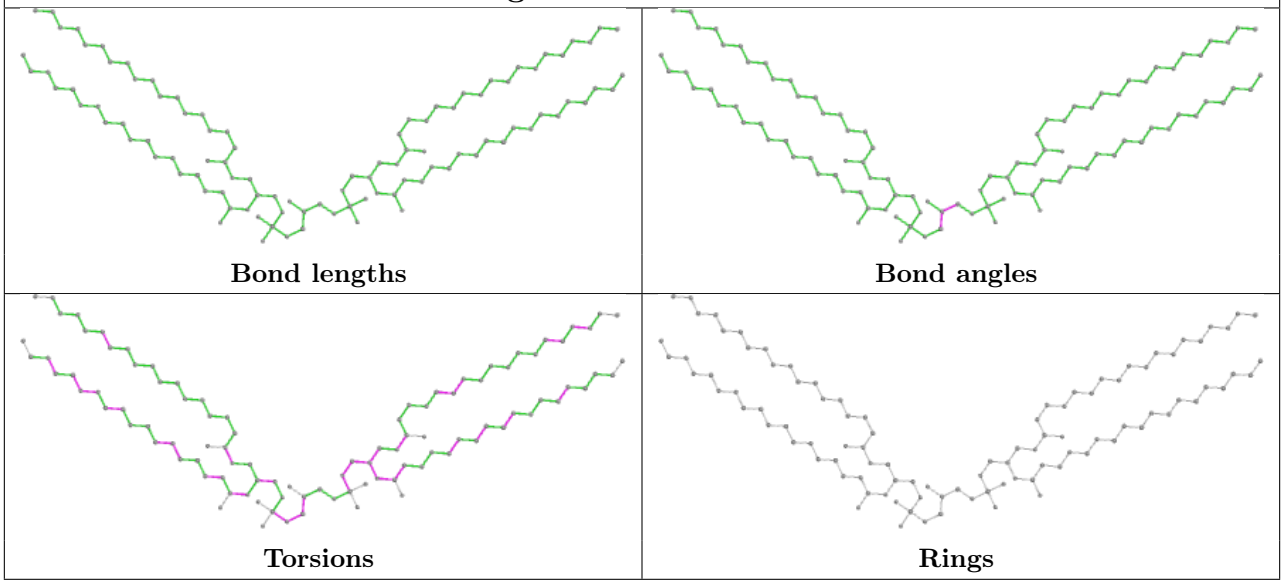
Ligand PC1 DX 308



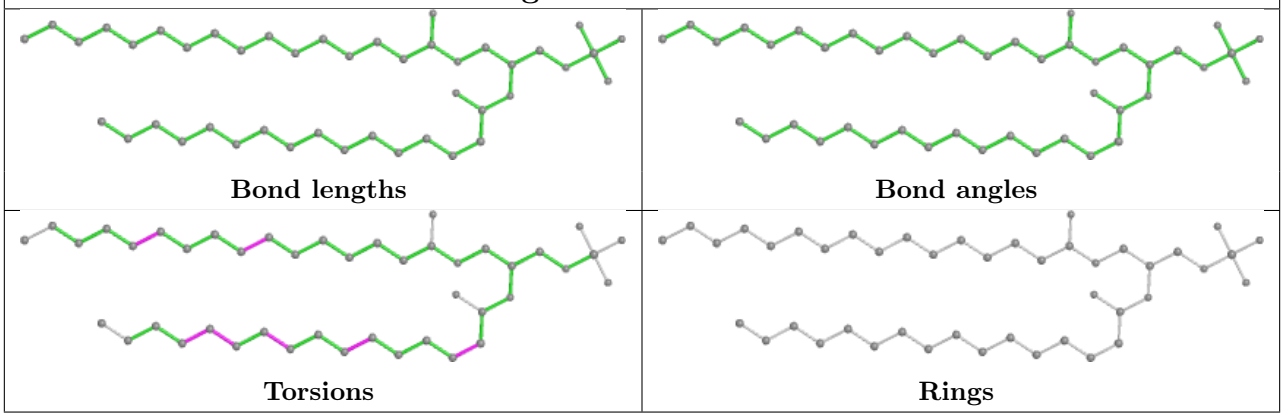
Ligand PC1 k 301



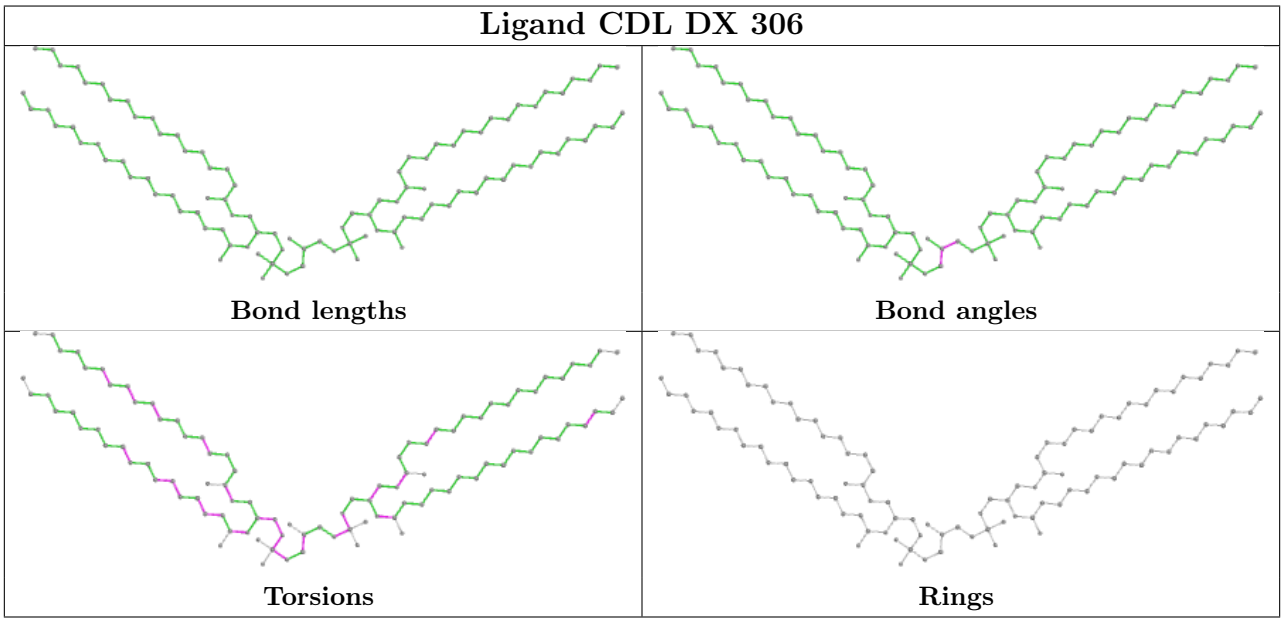
Ligand CDL Eh 1601



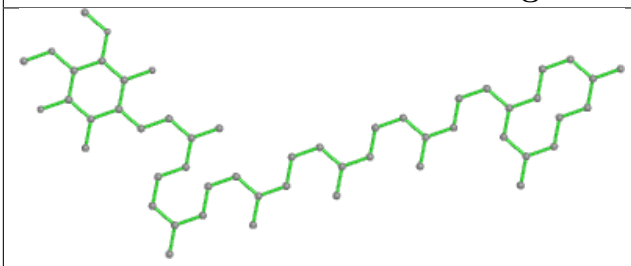
Ligand LPP EI 402



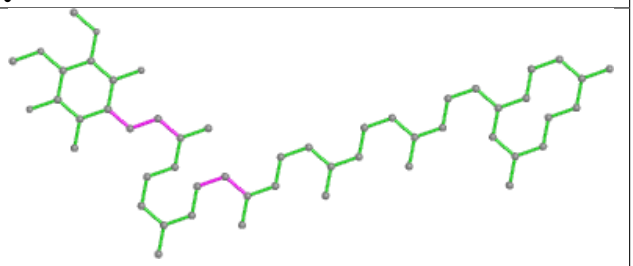
Ligand CDL DX 306



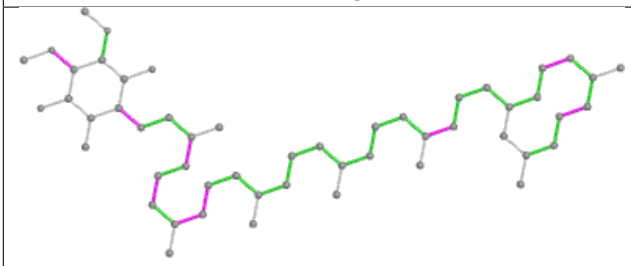
Ligand UQ8 El 906



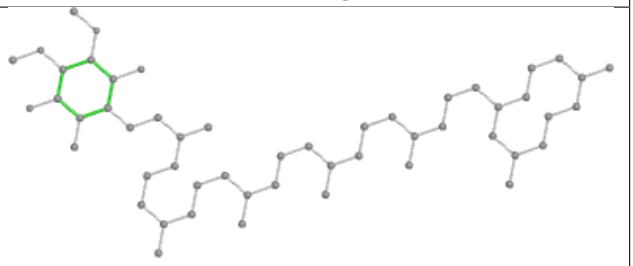
Bond lengths



Bond angles

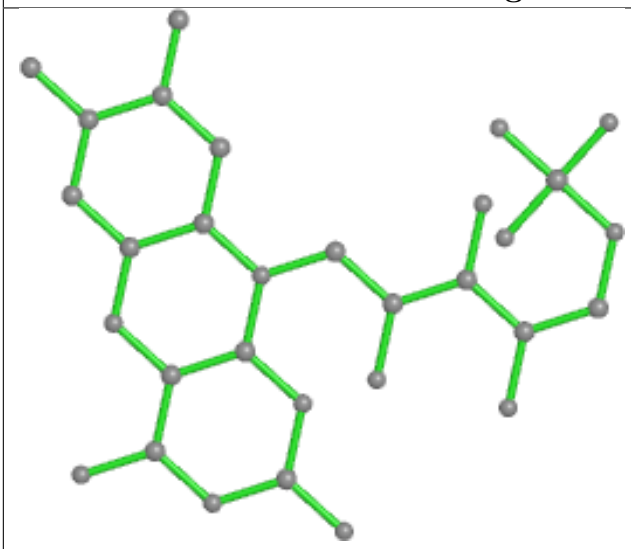


Torsions

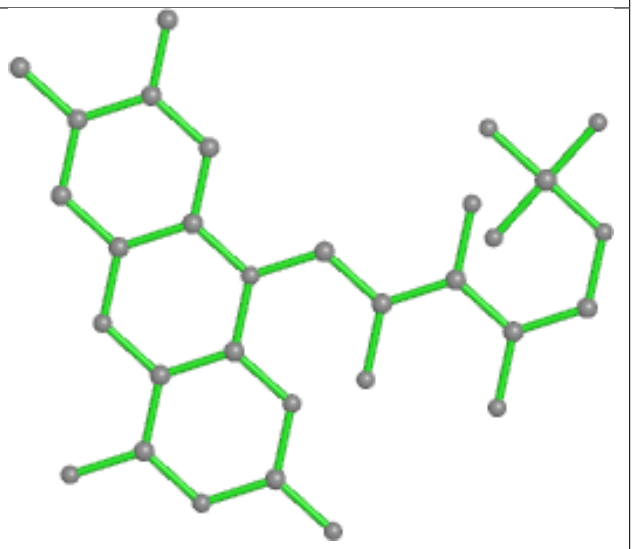


Rings

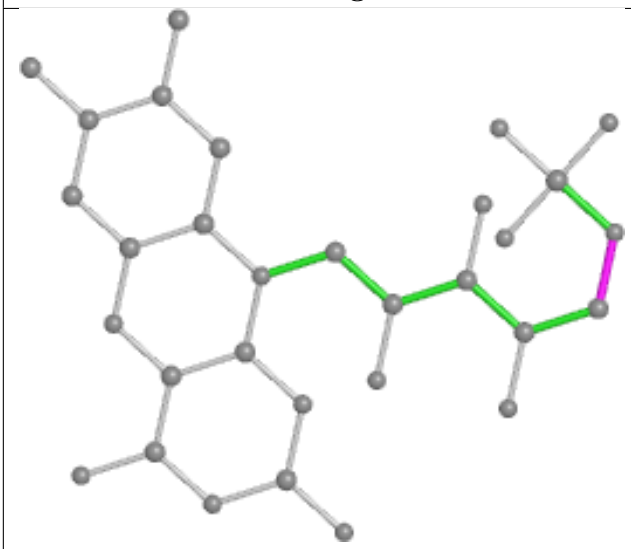
Ligand FMN AD 502



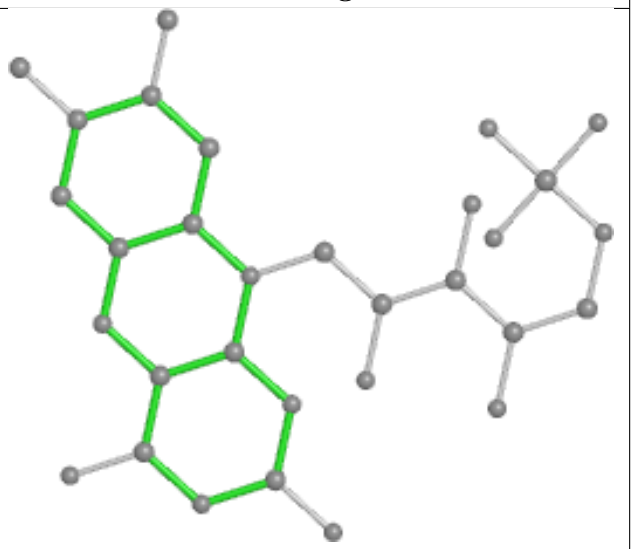
Bond lengths



Bond angles

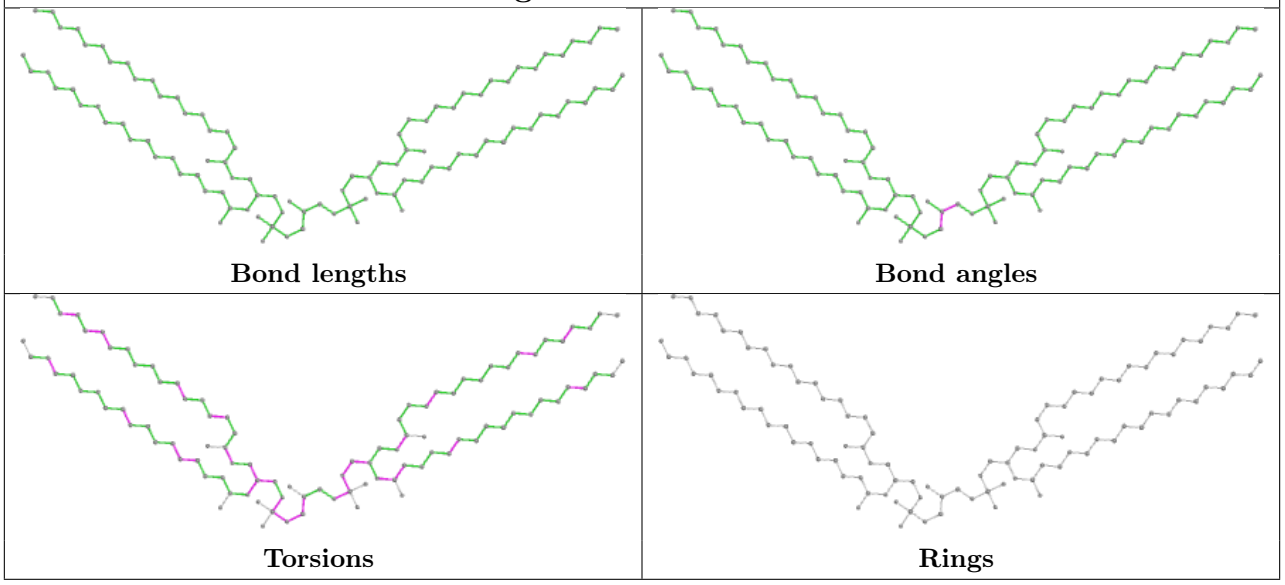


Torsions

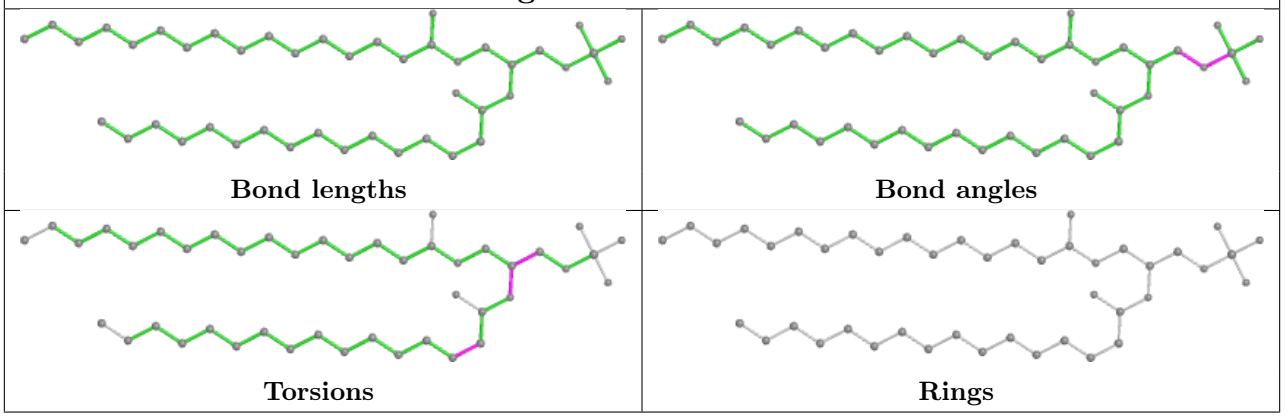


Rings

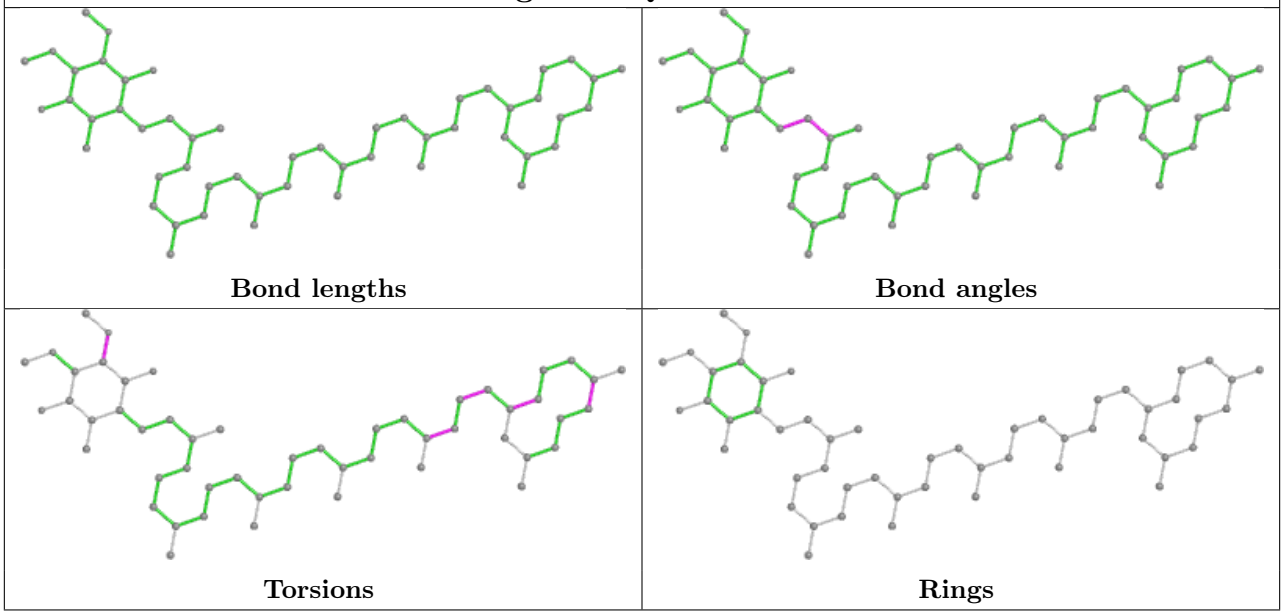
Ligand CDL Dv 403



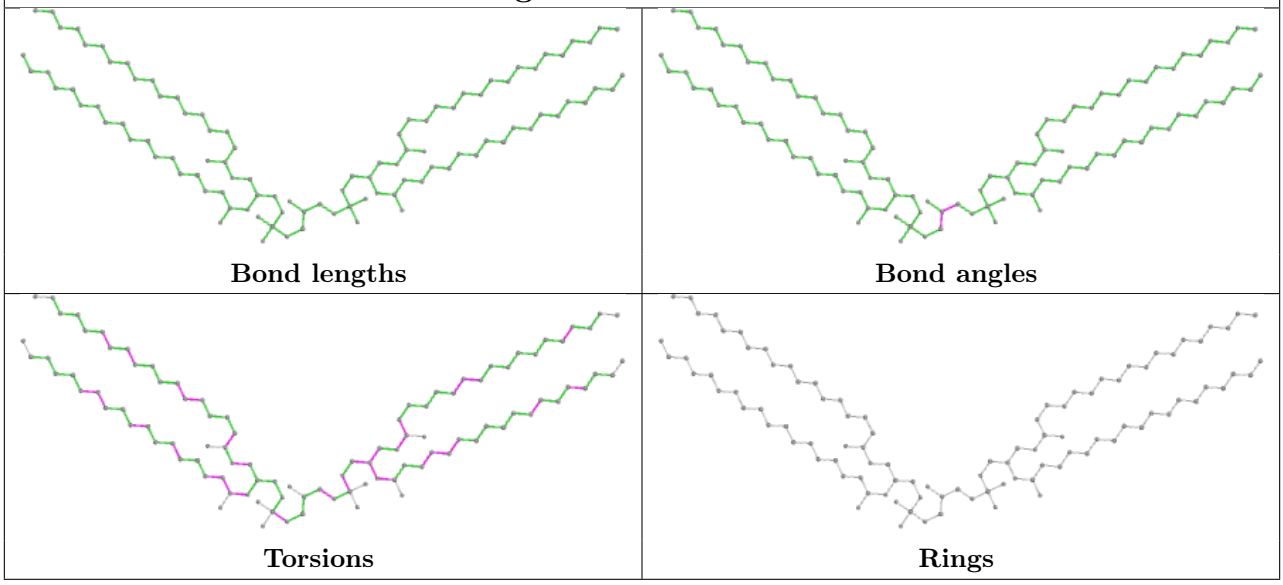
Ligand LPP A6 301



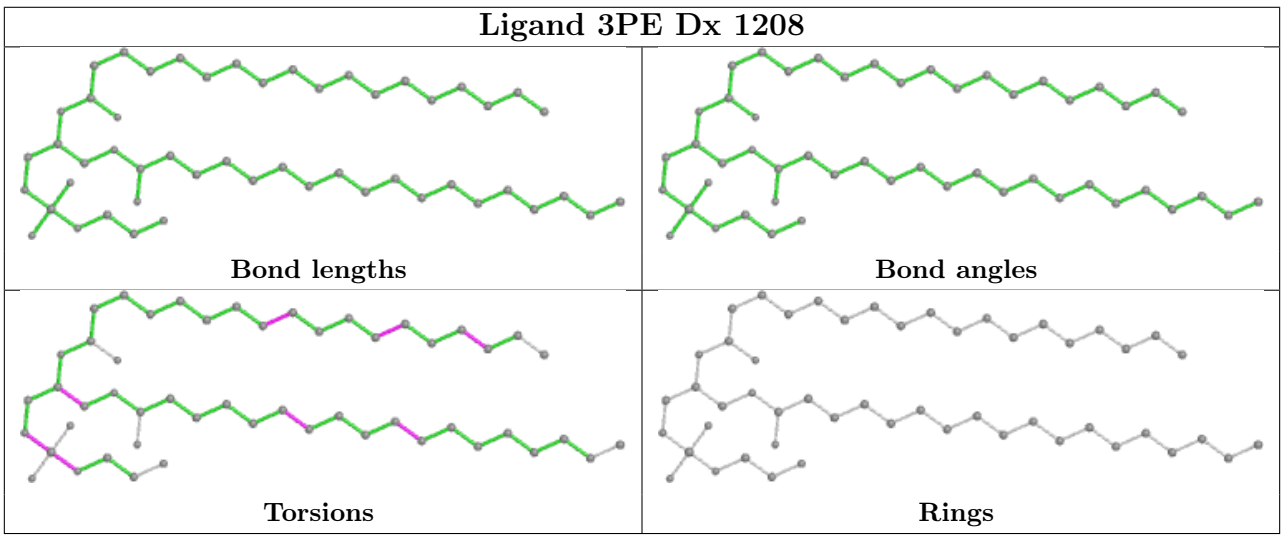
Ligand UQ8 DS 403



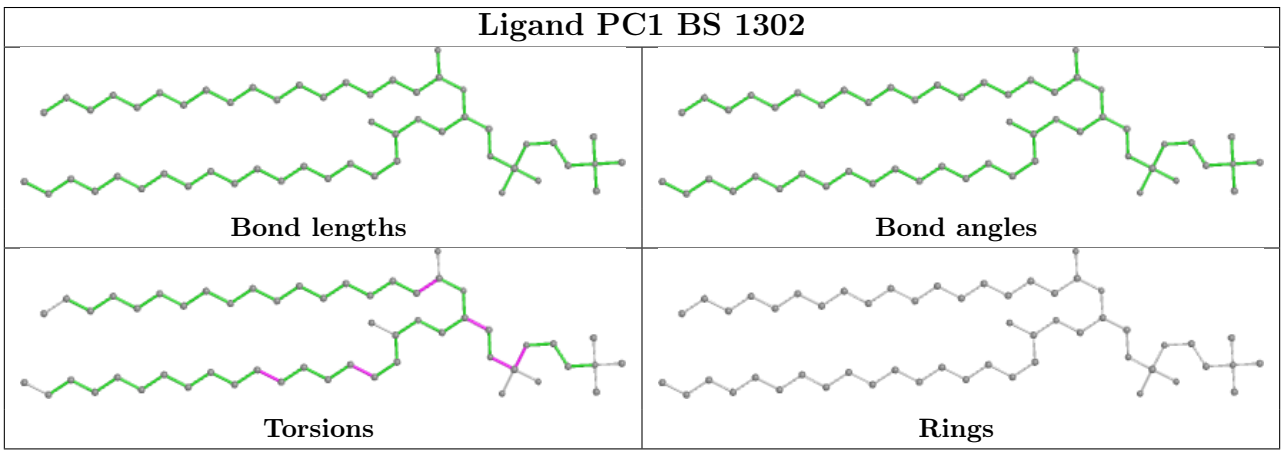
Ligand CDL DJ 304



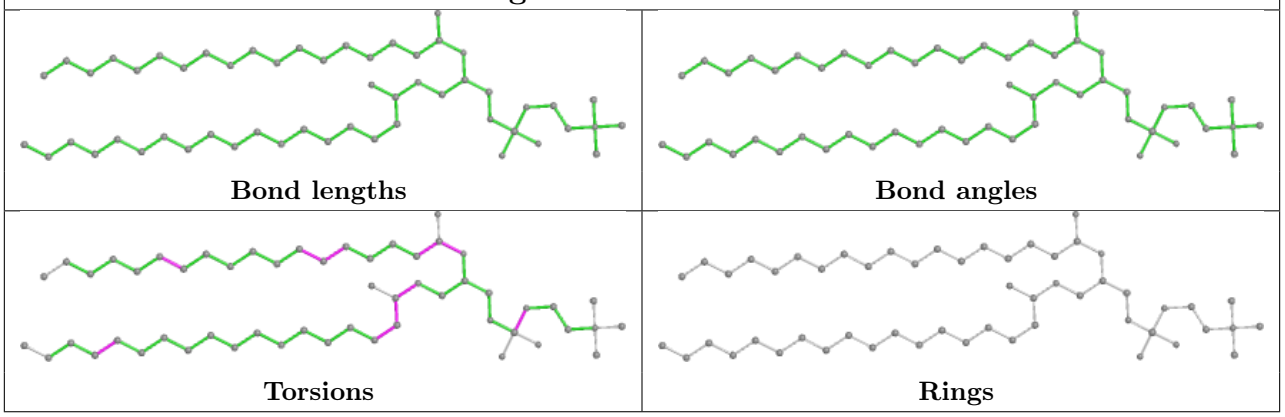
Ligand 3PE Dx 1208



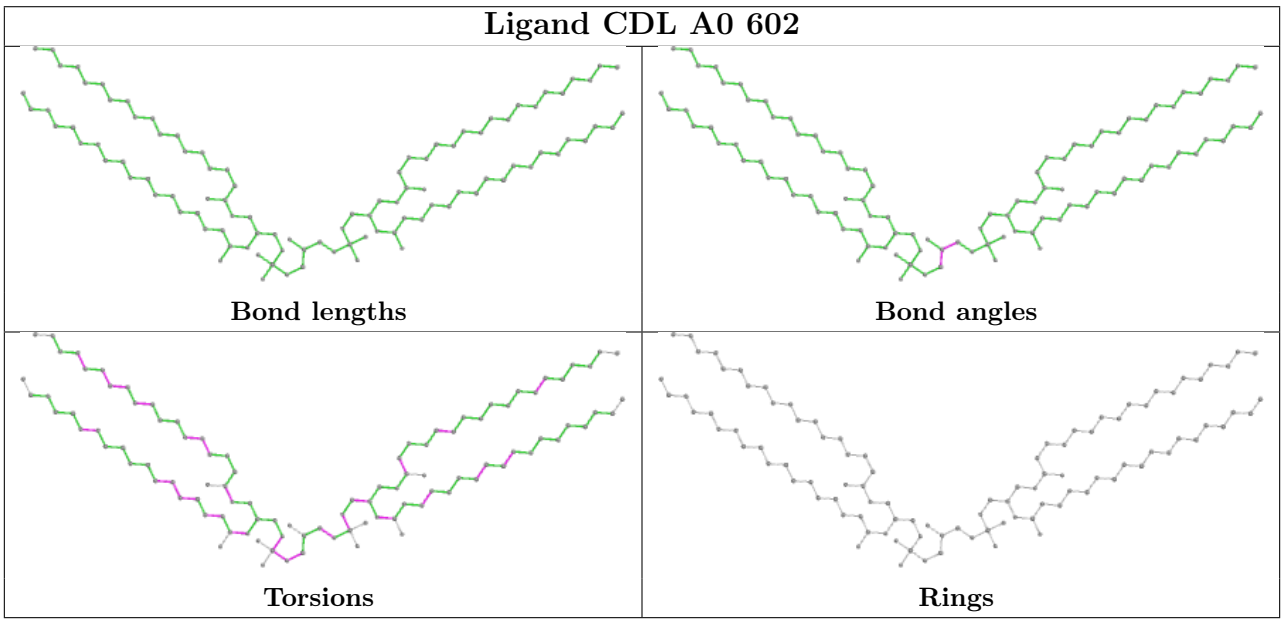
Ligand PC1 BS 1302



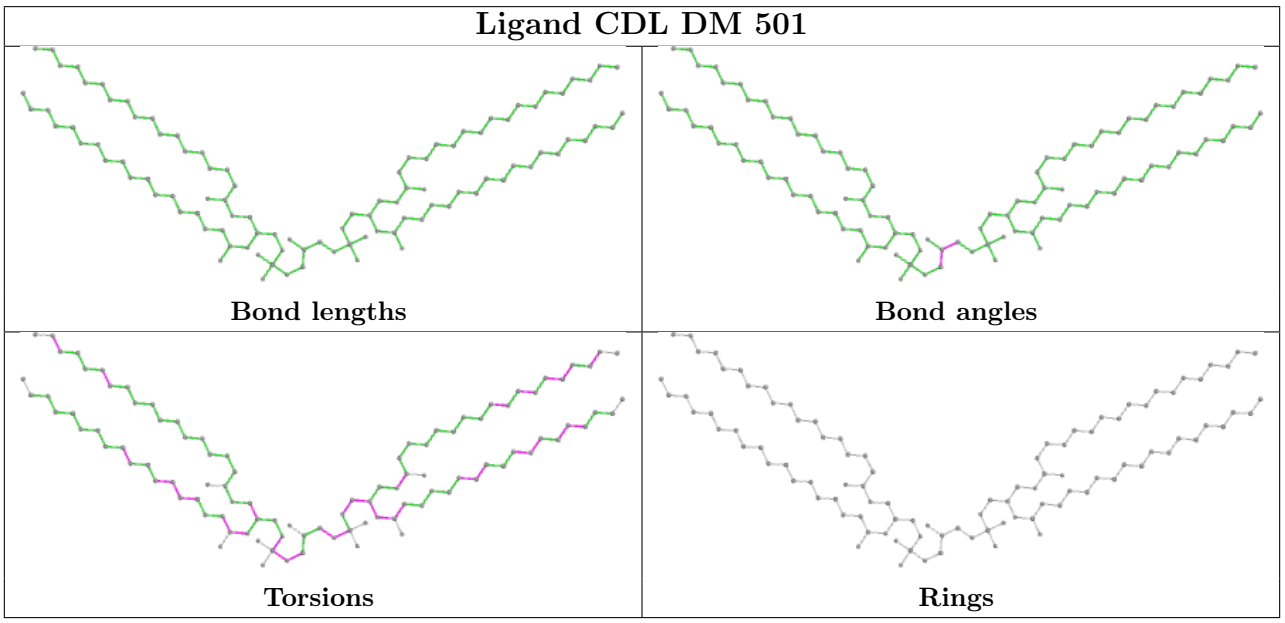
Ligand PC1 Dx 1205



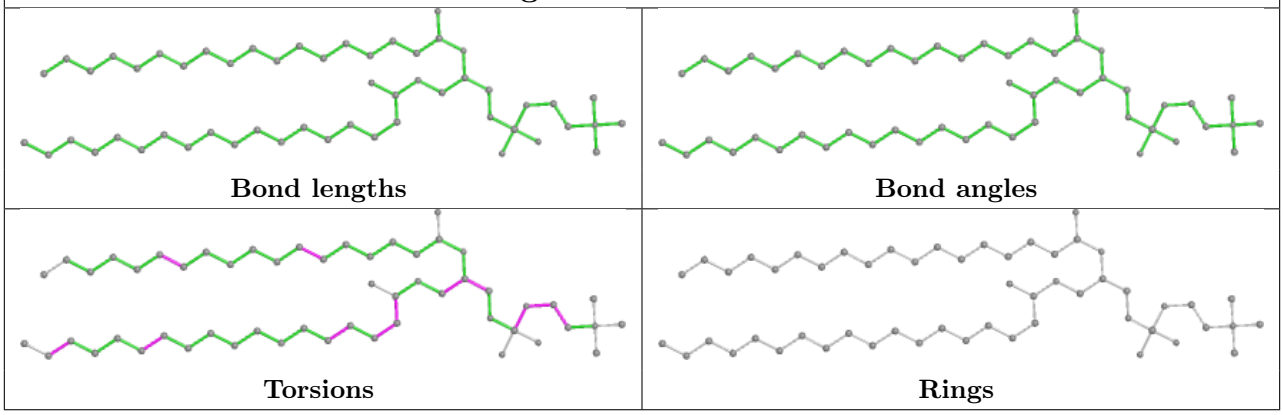
Ligand CDL A0 602



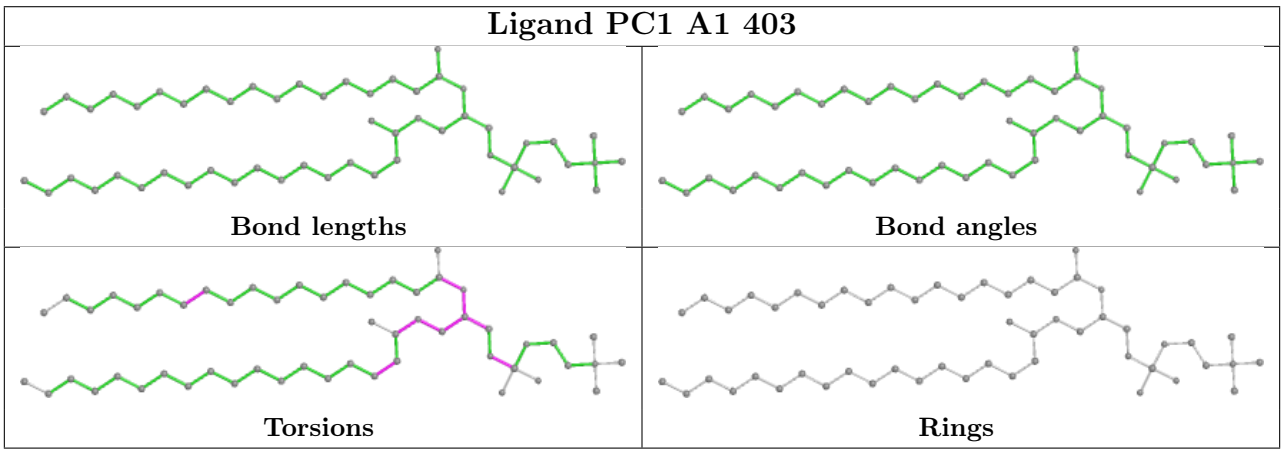
Ligand CDL DM 501



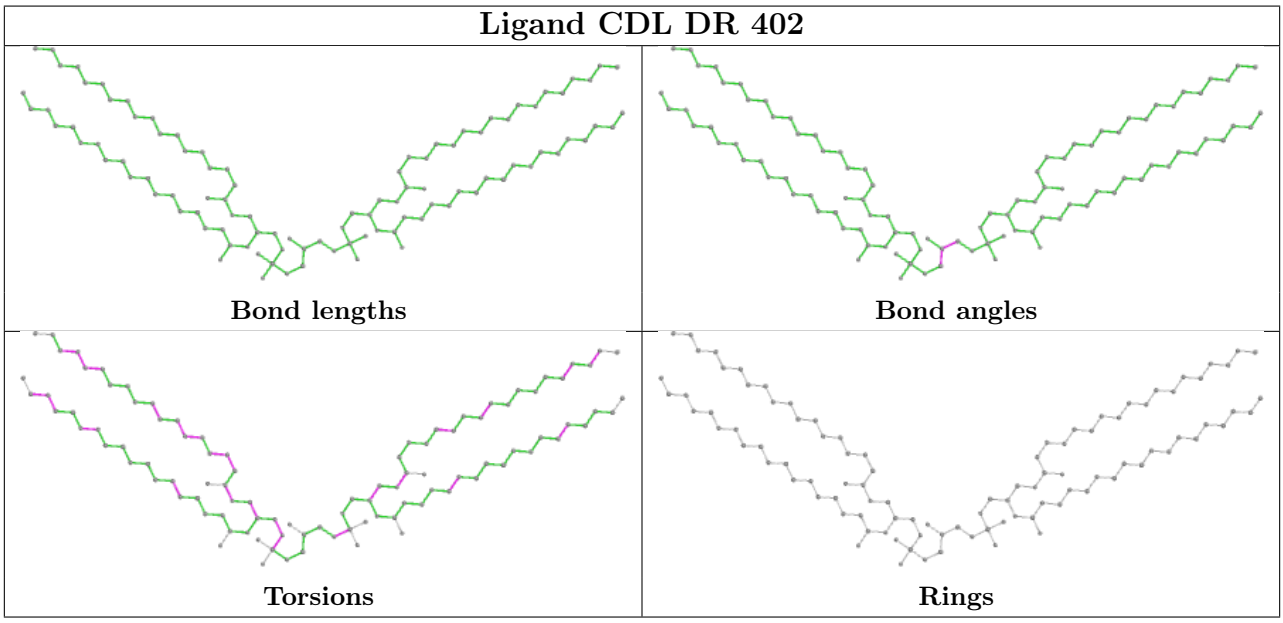
Ligand PC1 Eo 201



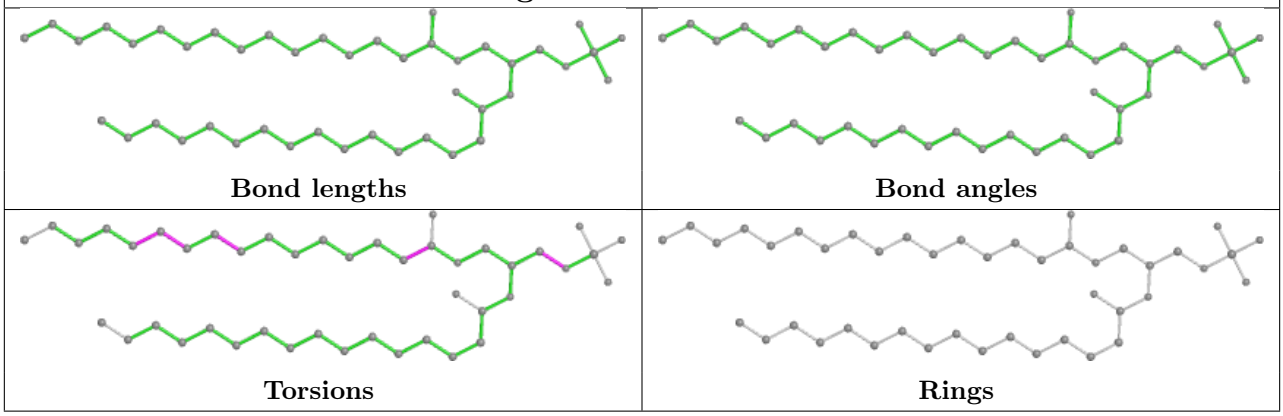
Ligand PC1 A1 403



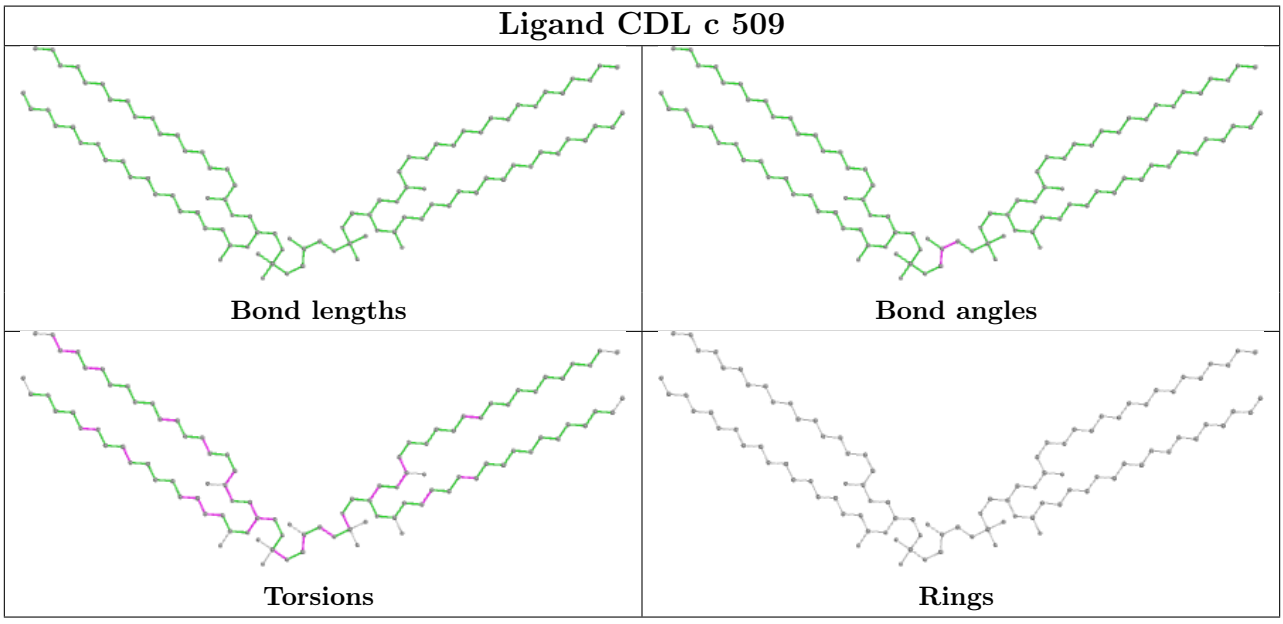
Ligand CDL DR 402



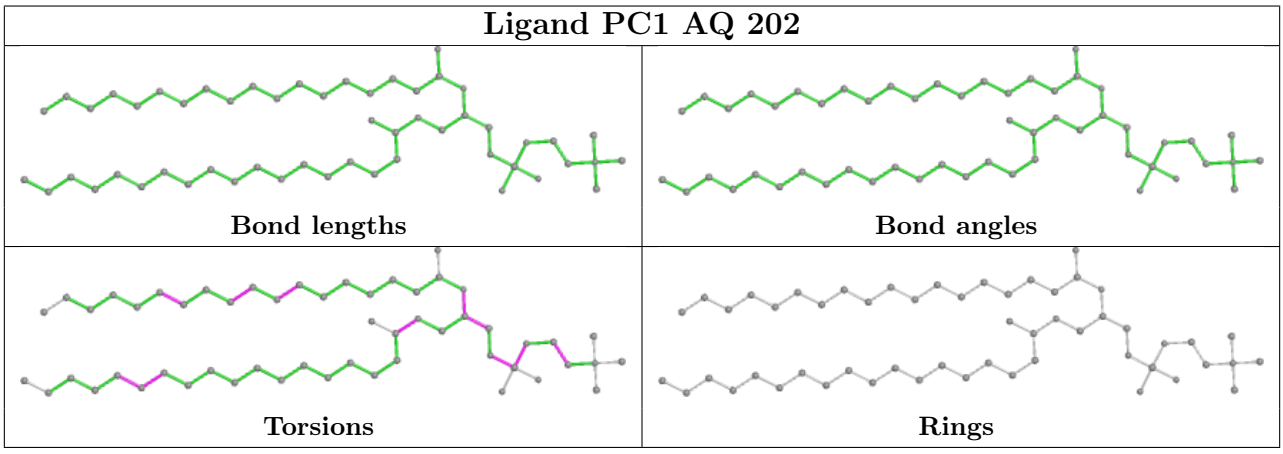
Ligand LPP Dn 505



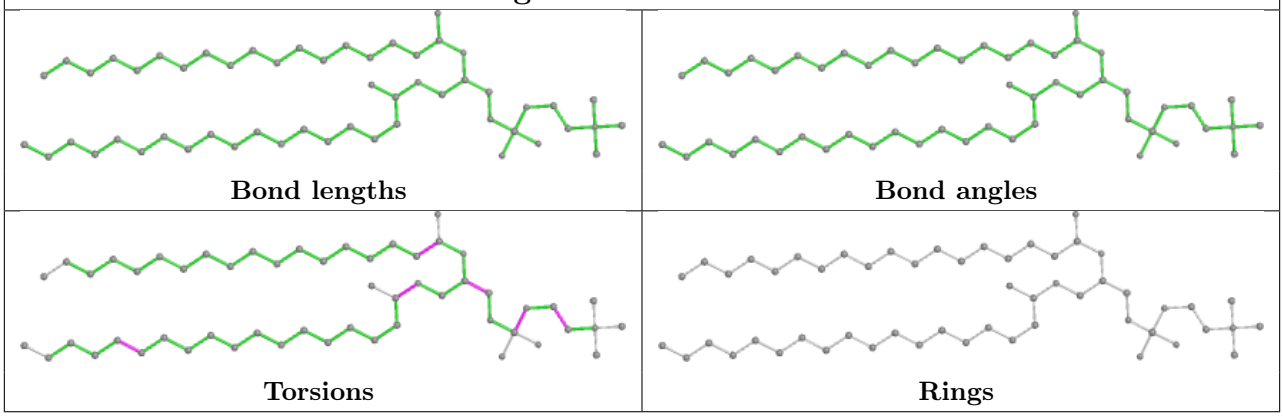
Ligand CDL c 509



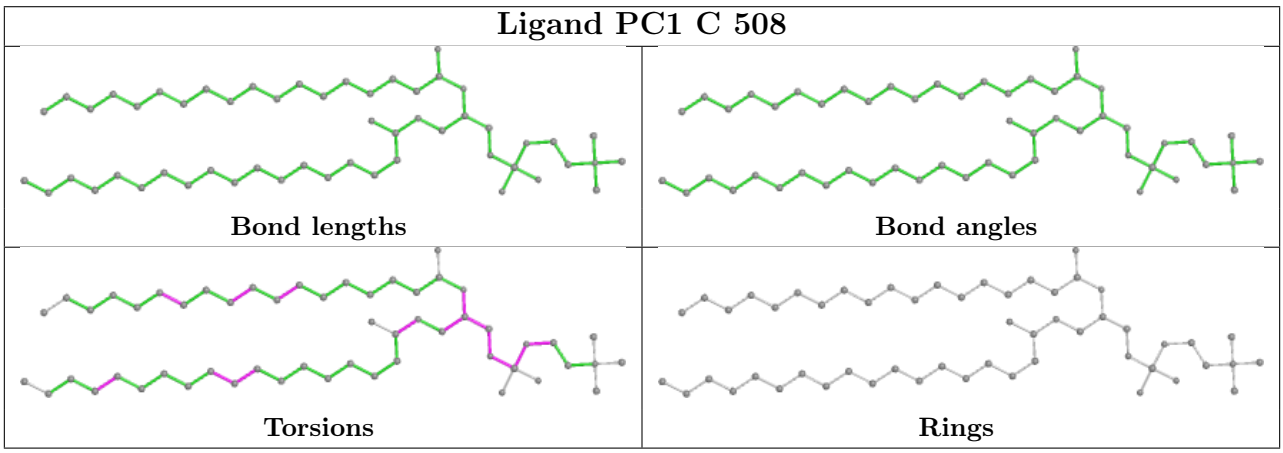
Ligand PC1 AQ 202



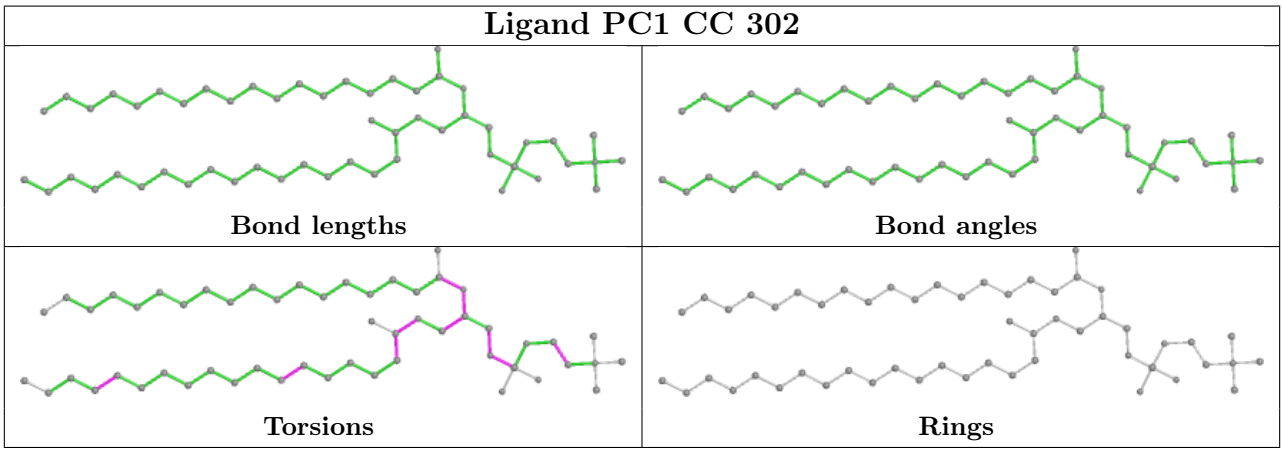
Ligand PC1 AH 301



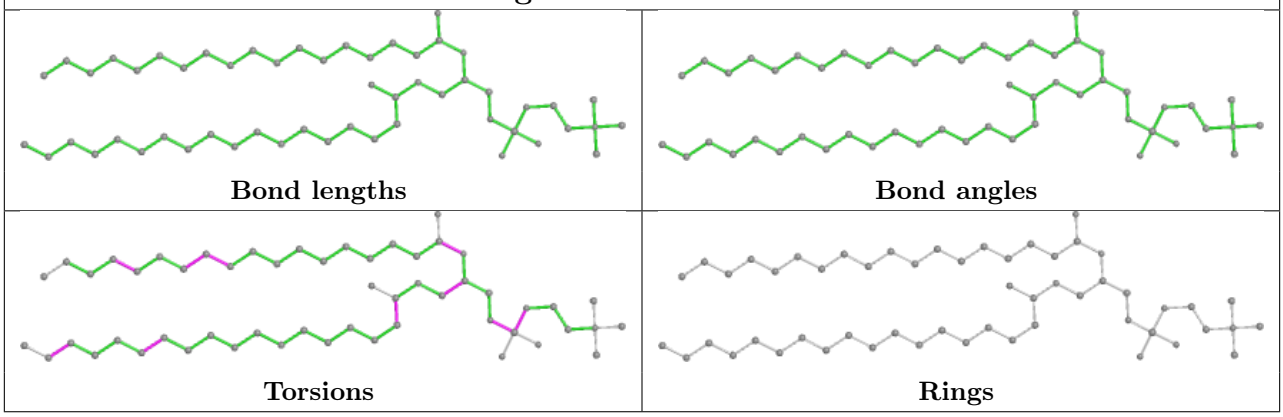
Ligand PC1 C 508



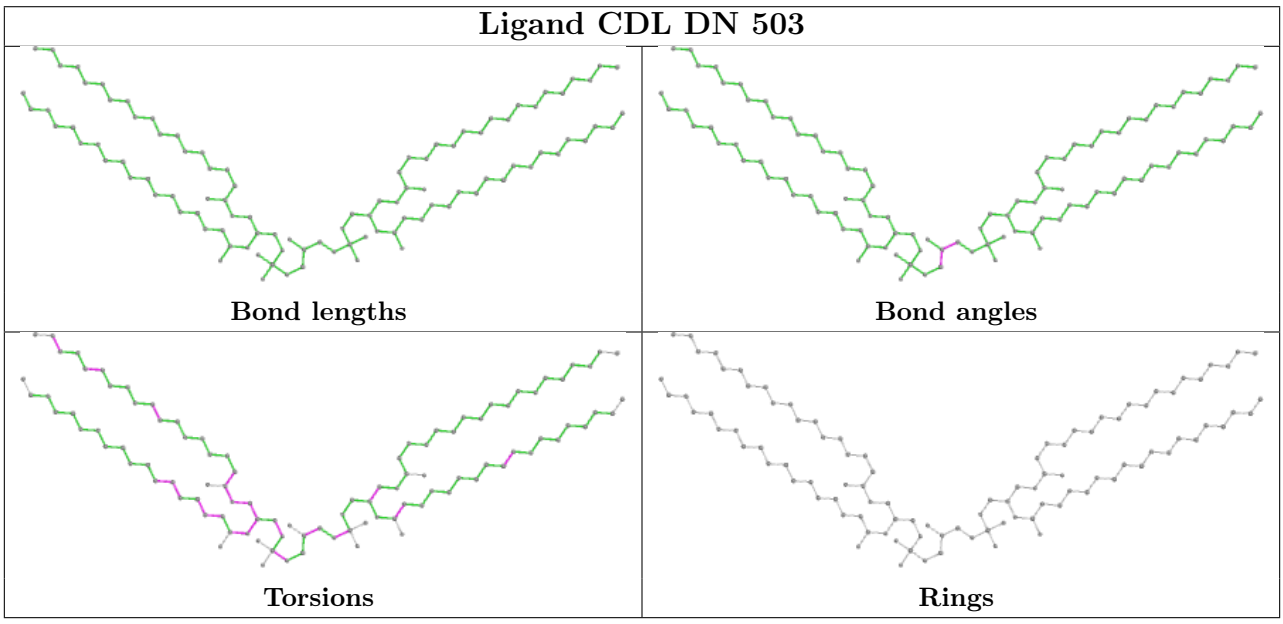
Ligand PC1 CC 302



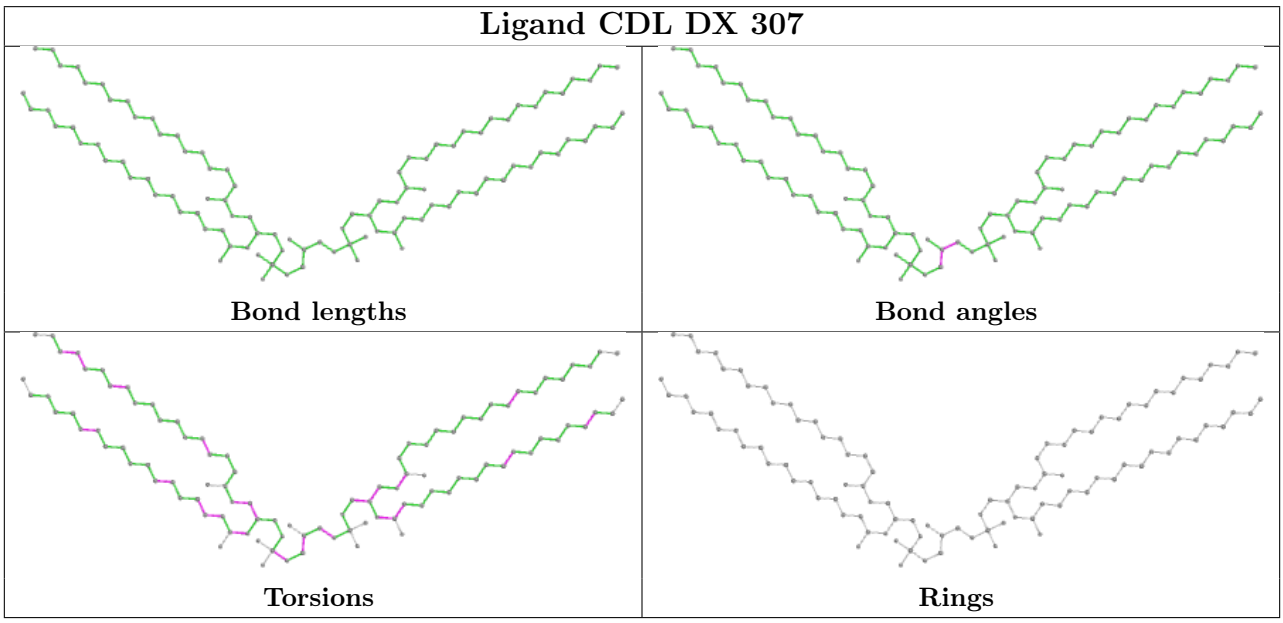
Ligand PC1 DV 404



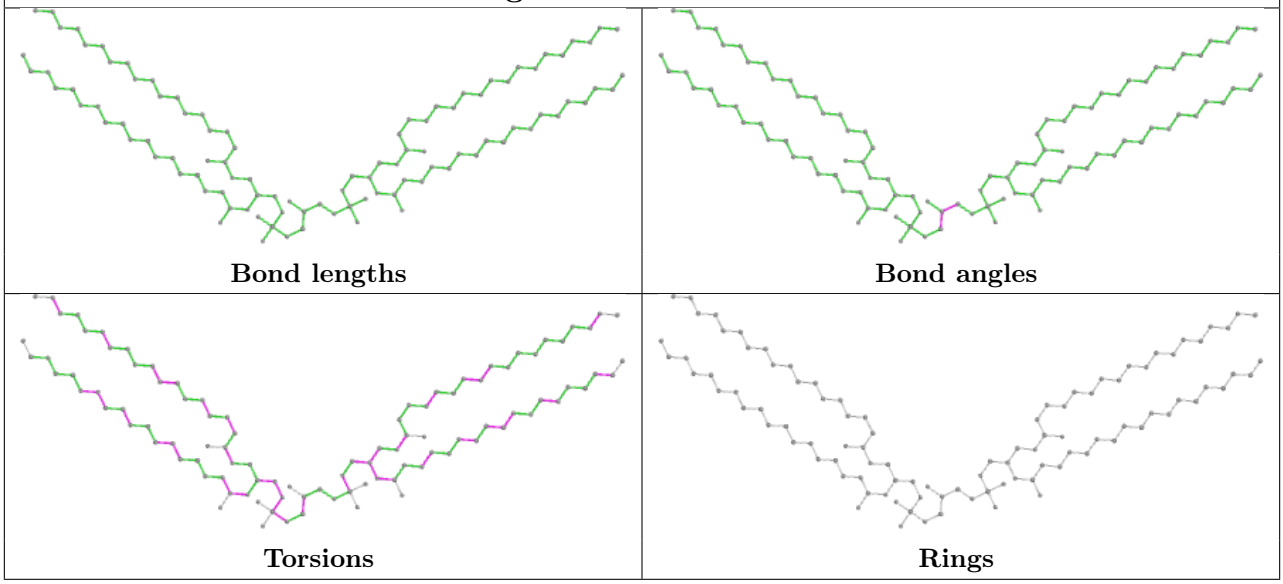
Ligand CDL DN 503



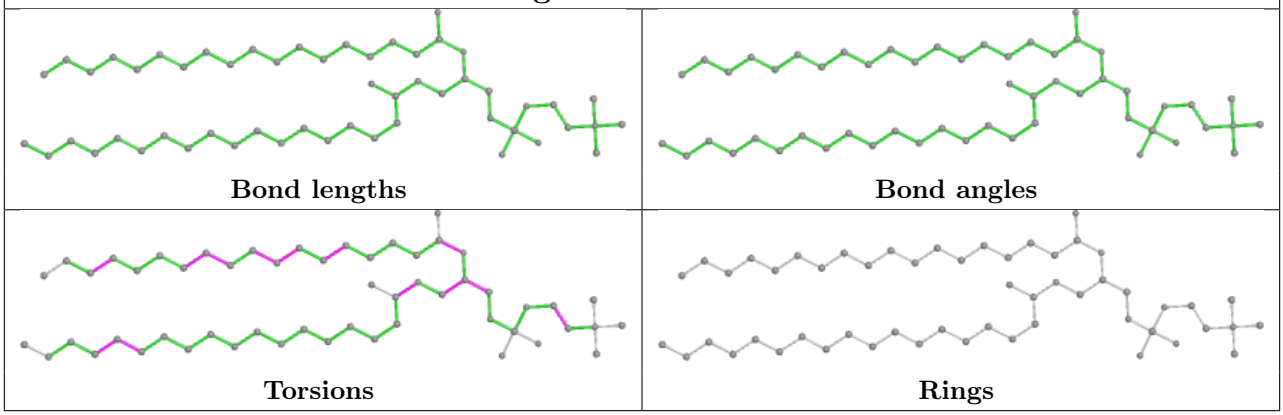
Ligand CDL DX 307



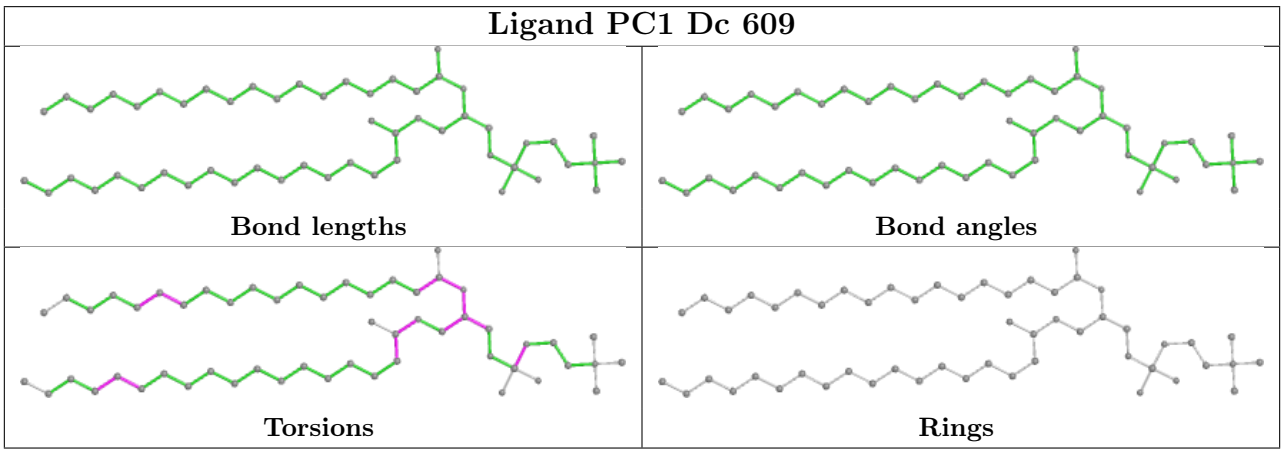
Ligand CDL Dx 1204



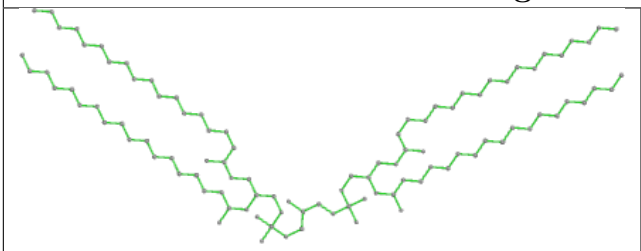
Ligand PC1 c 503



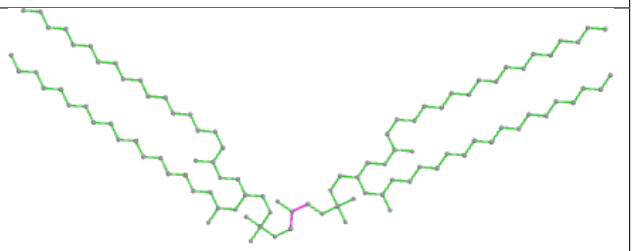
Ligand PC1 Dc 609



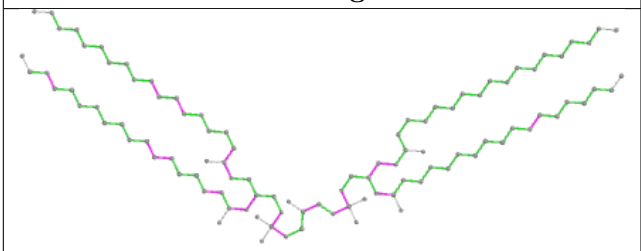
Ligand CDL H 1302



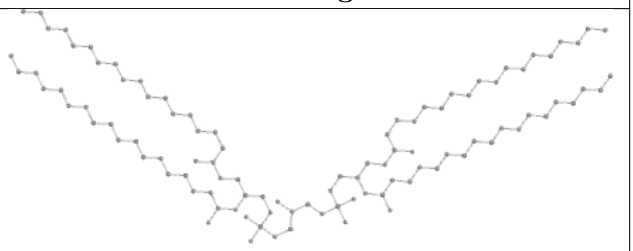
Bond lengths



Bond angles

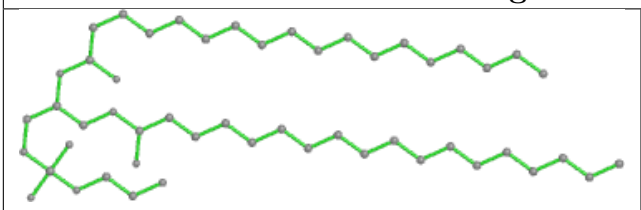


Torsions

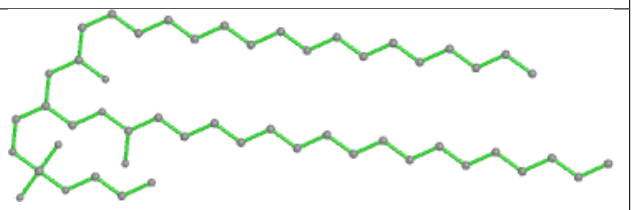


Rings

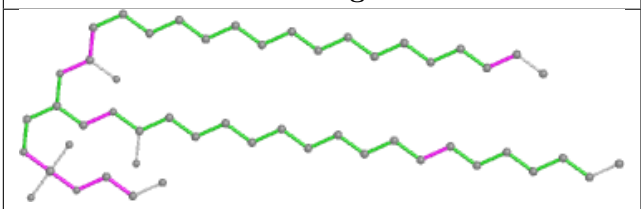
Ligand 3PE Dx 1206



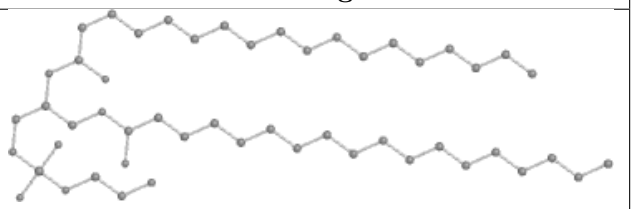
Bond lengths



Bond angles

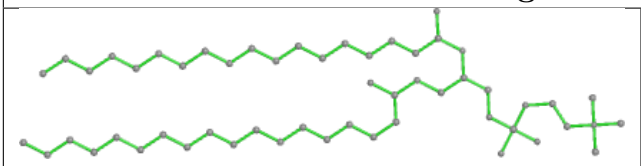


Torsions

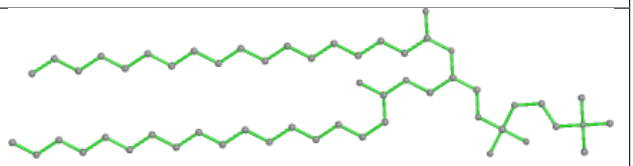


Rings

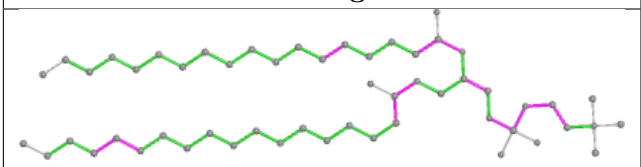
Ligand PC1 A9 603



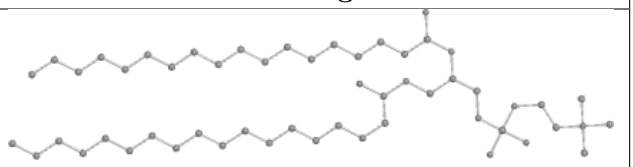
Bond lengths



Bond angles

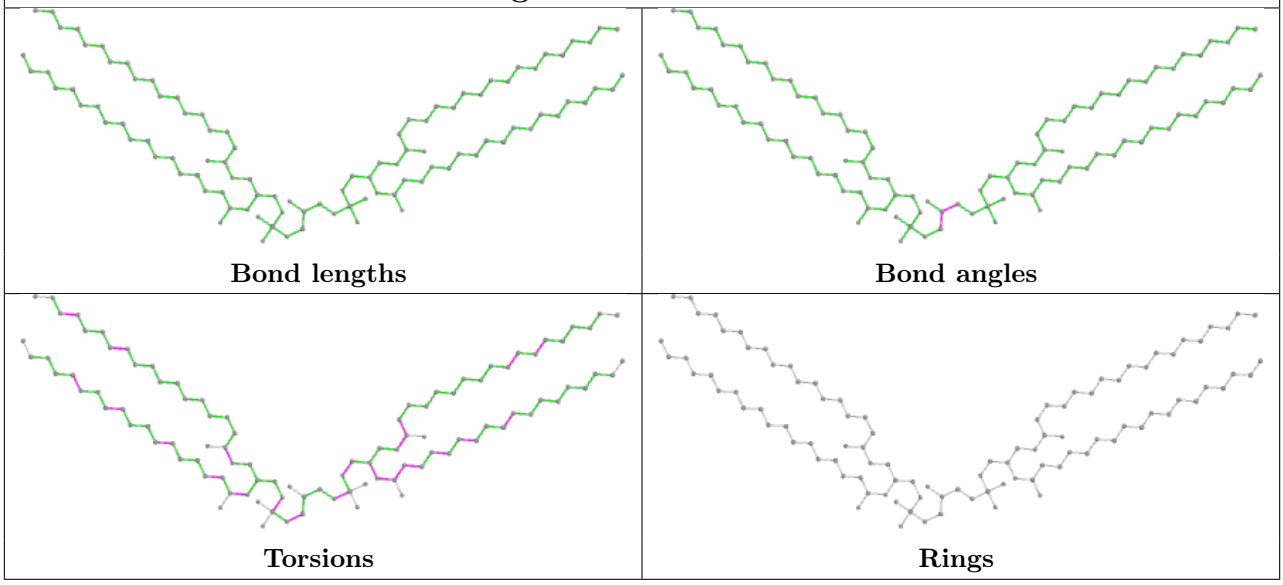


Torsions

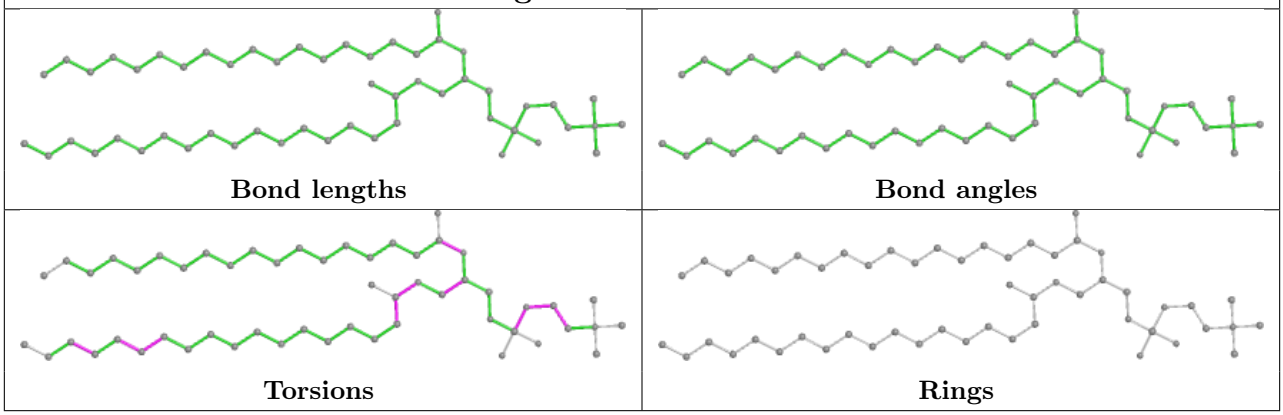


Rings

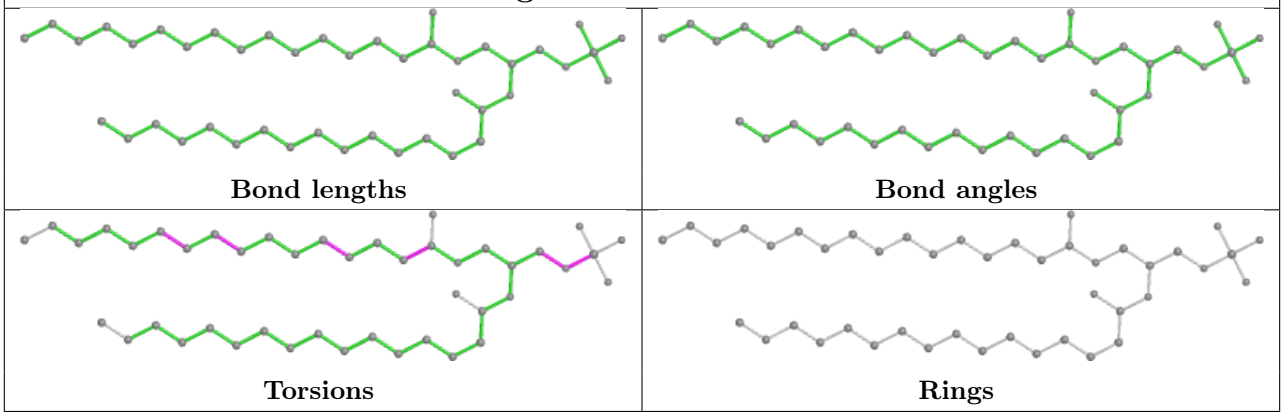
Ligand CDL DV 401



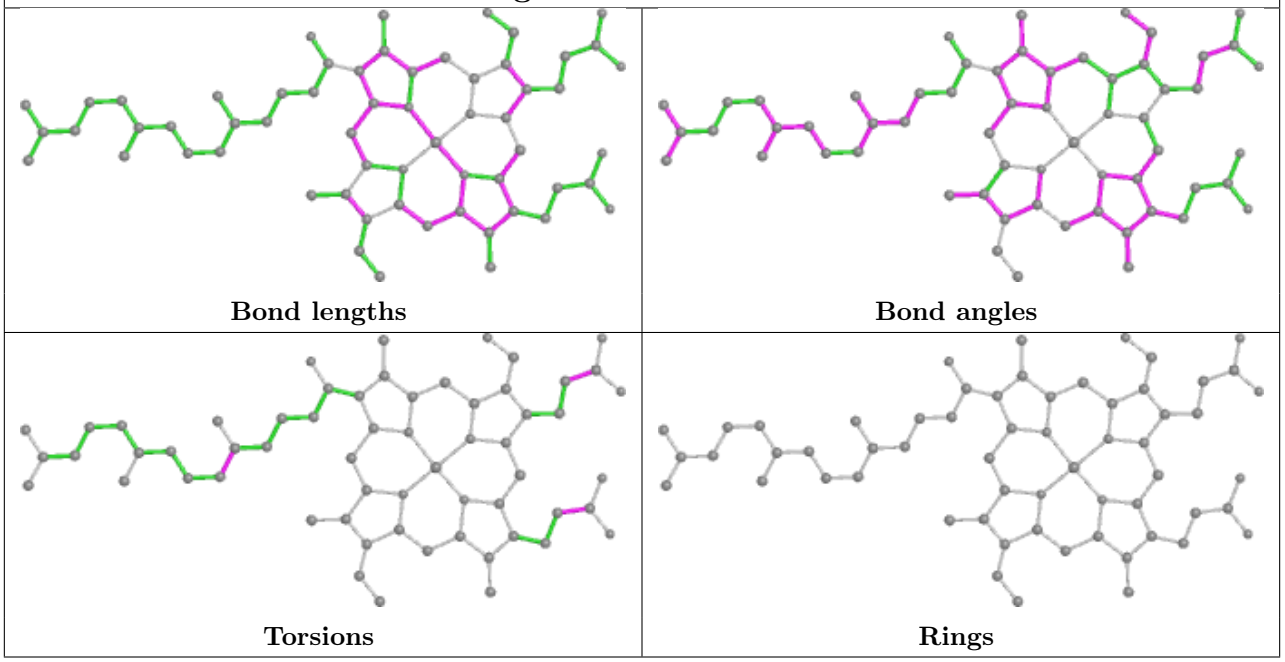
Ligand PC1 AU 202



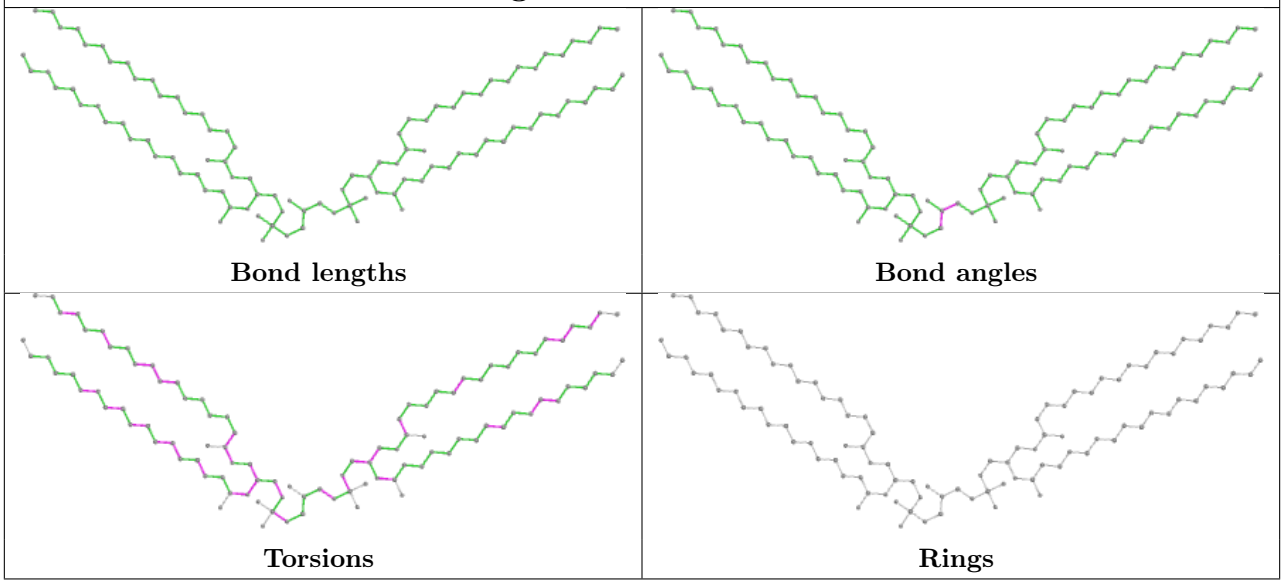
Ligand LPP Dn 504



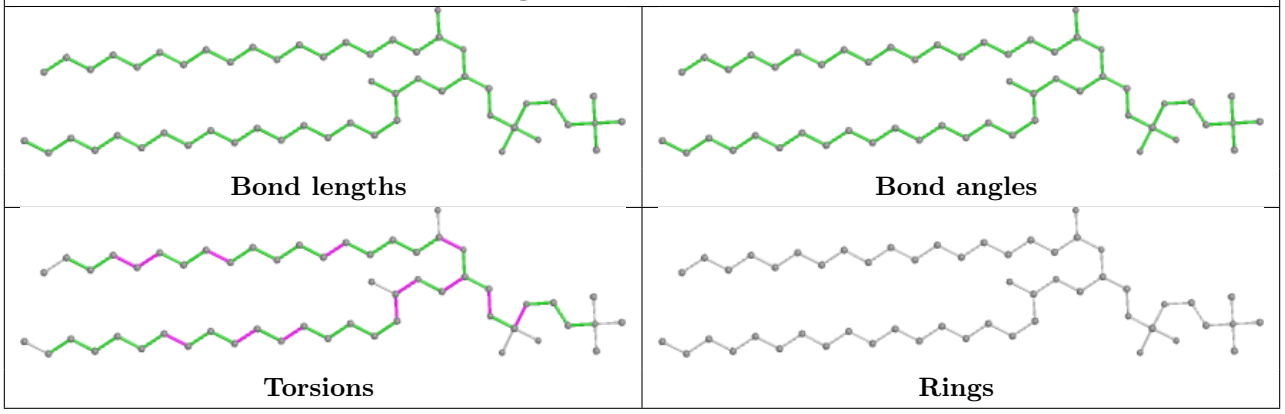
Ligand HEA Da 702



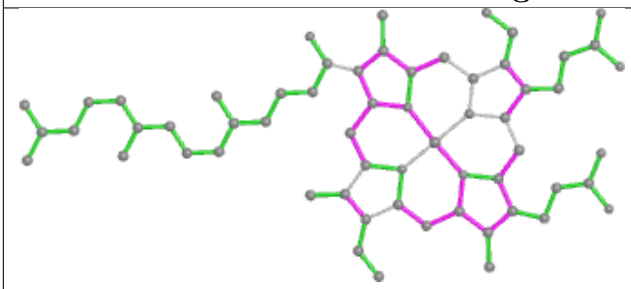
Ligand CDL DN 506



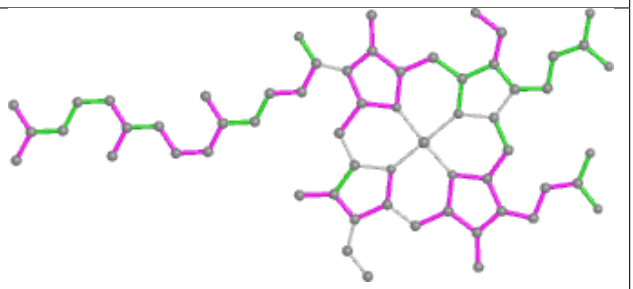
Ligand PC1 DA 707



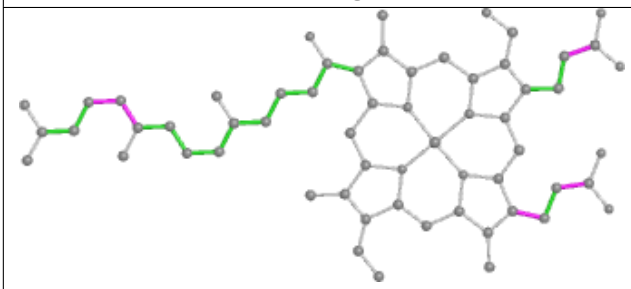
Ligand HEA Da 703



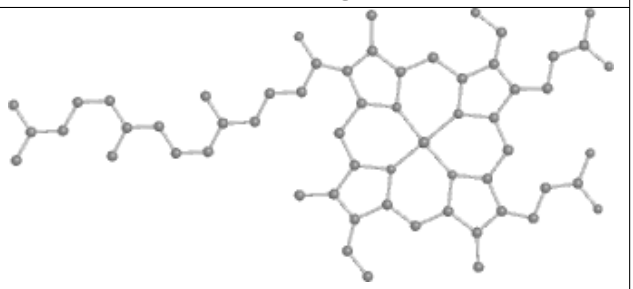
Bond lengths



Bond angles

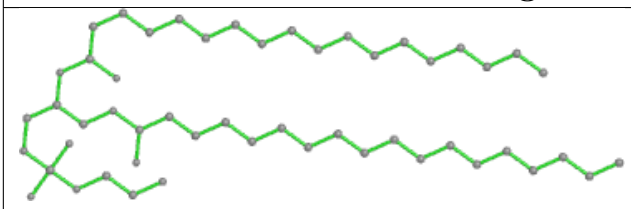


Torsions

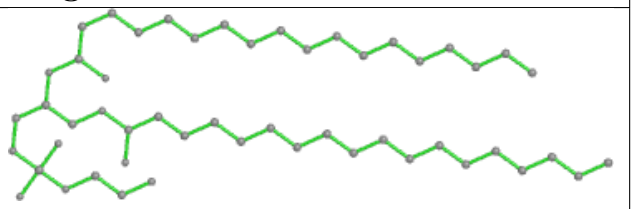


Rings

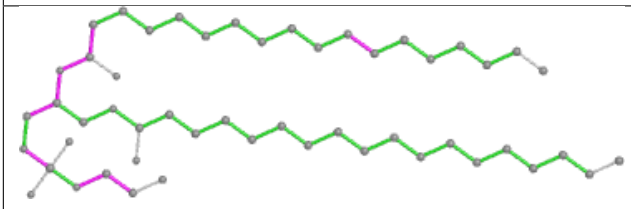
Ligand 3PE Dg 204



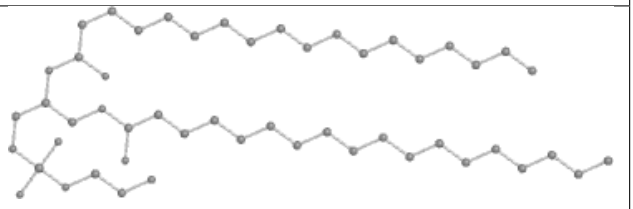
Bond lengths



Bond angles

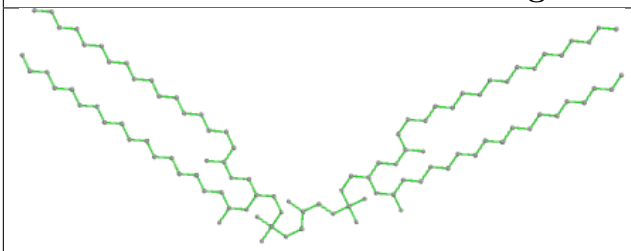


Torsions

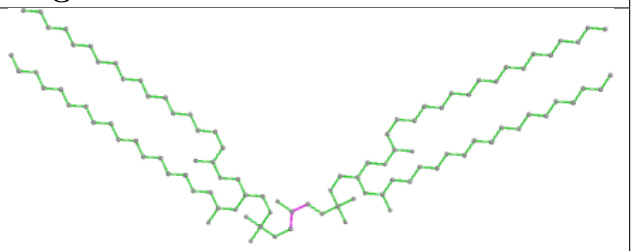


Rings

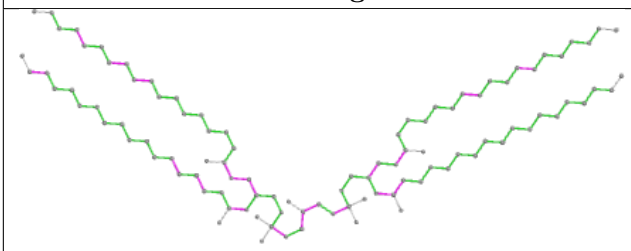
Ligand CDL g 801



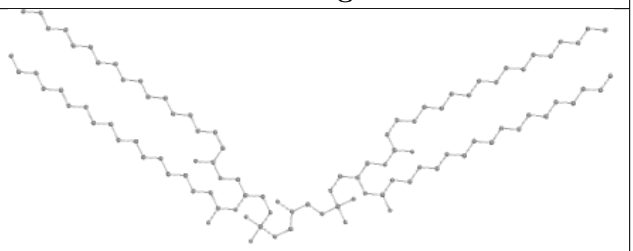
Bond lengths



Bond angles

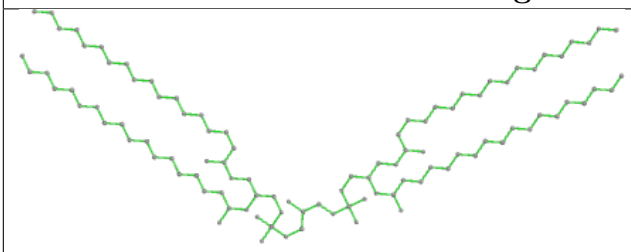


Torsions

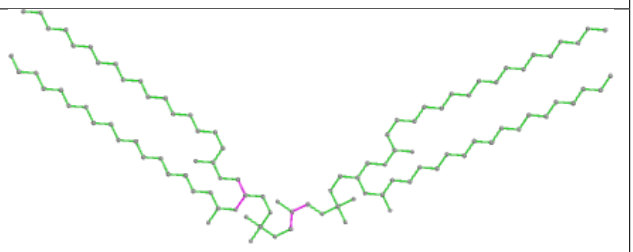


Rings

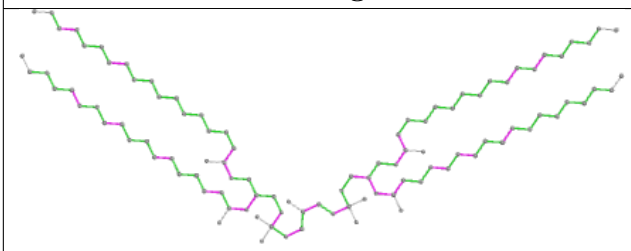
Ligand CDL Dv 401



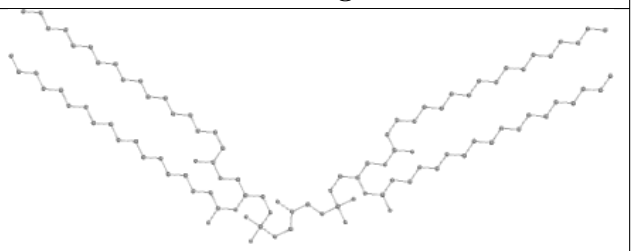
Bond lengths



Bond angles

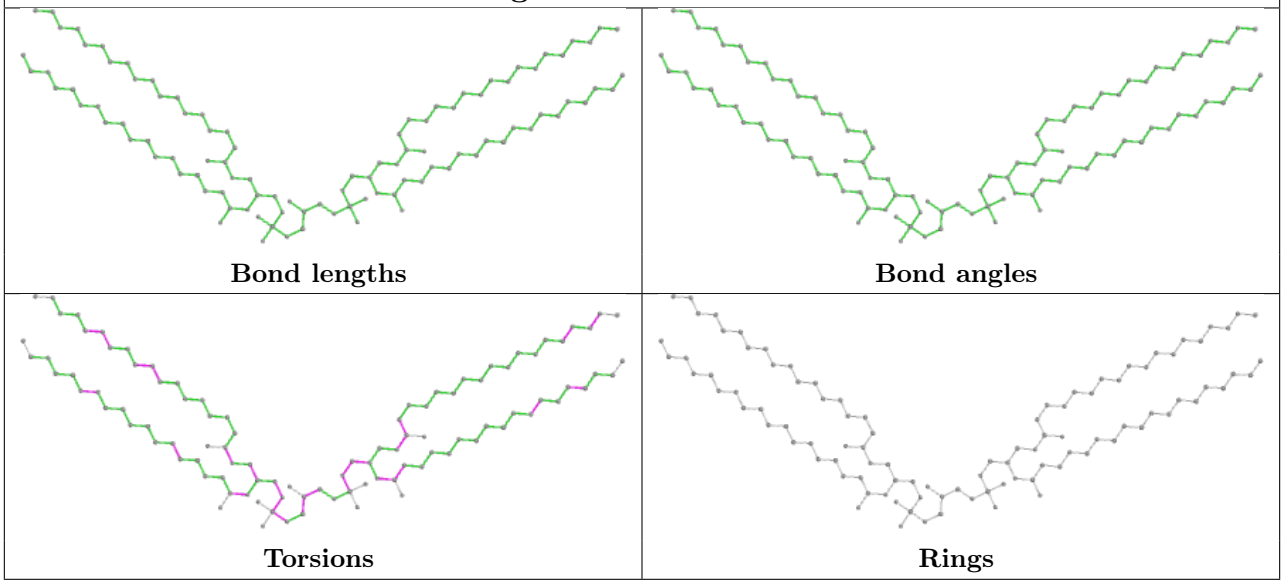


Torsions

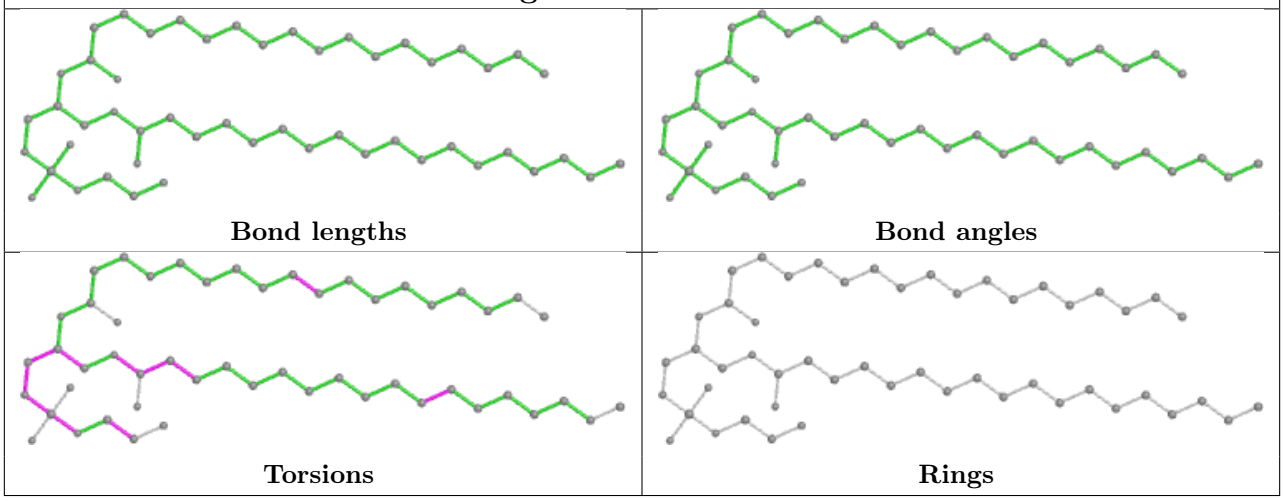


Rings

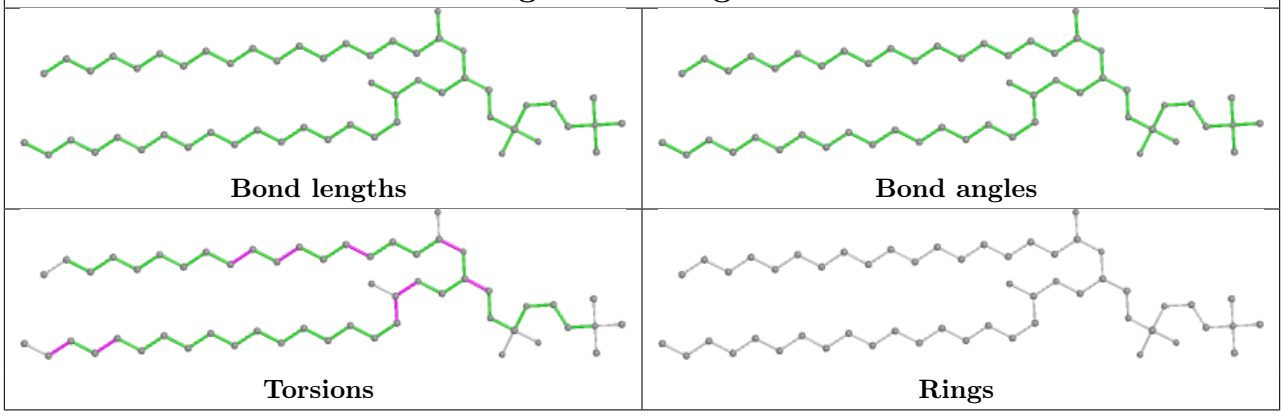
Ligand CDL DD 705



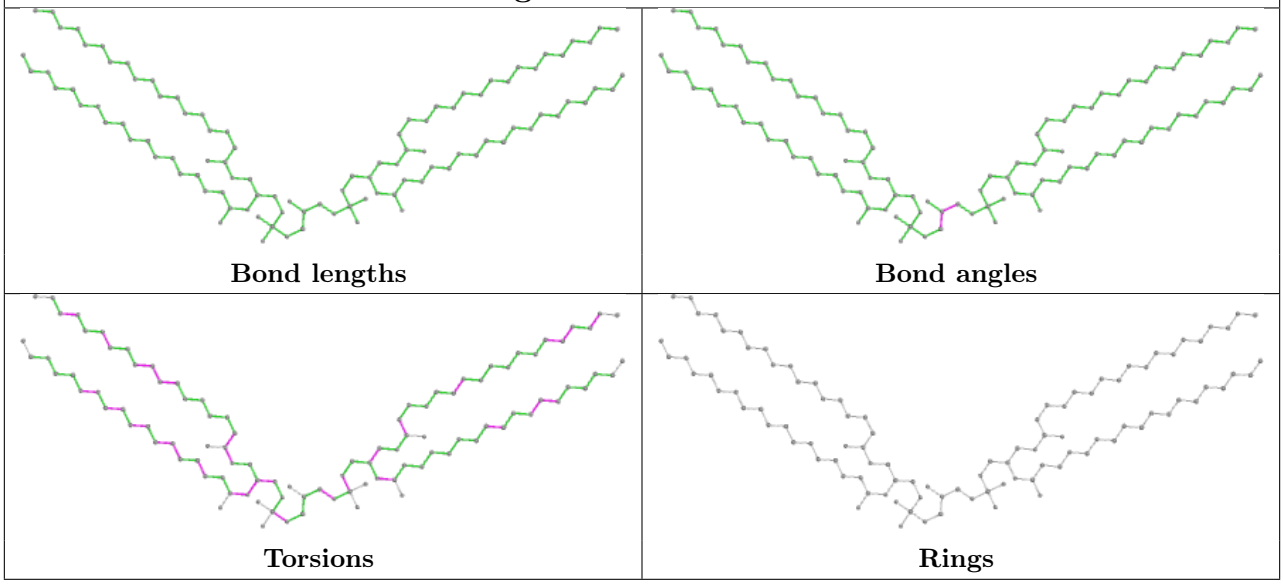
Ligand 3PE Da 708



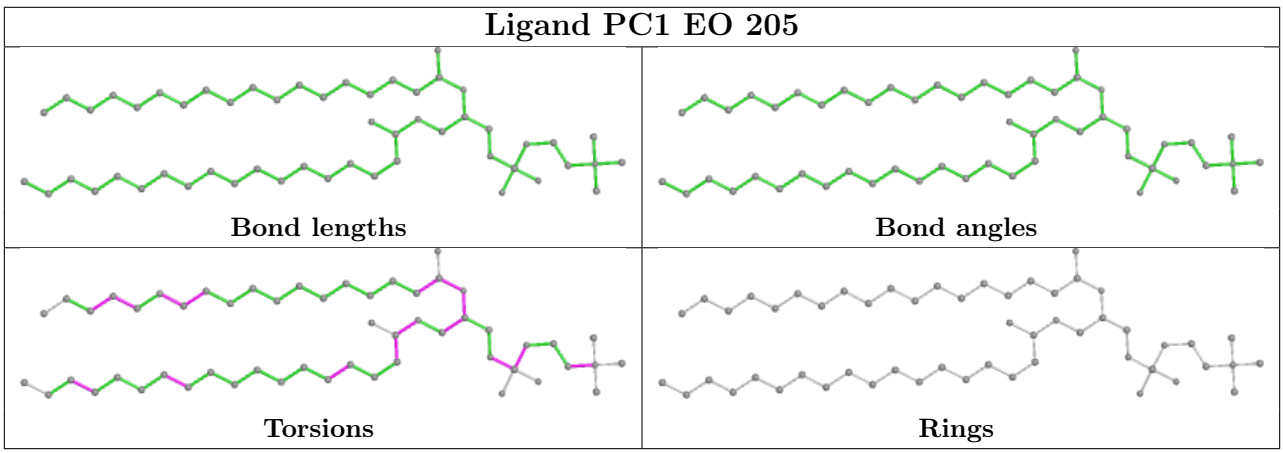
Ligand PC1 Dg 203



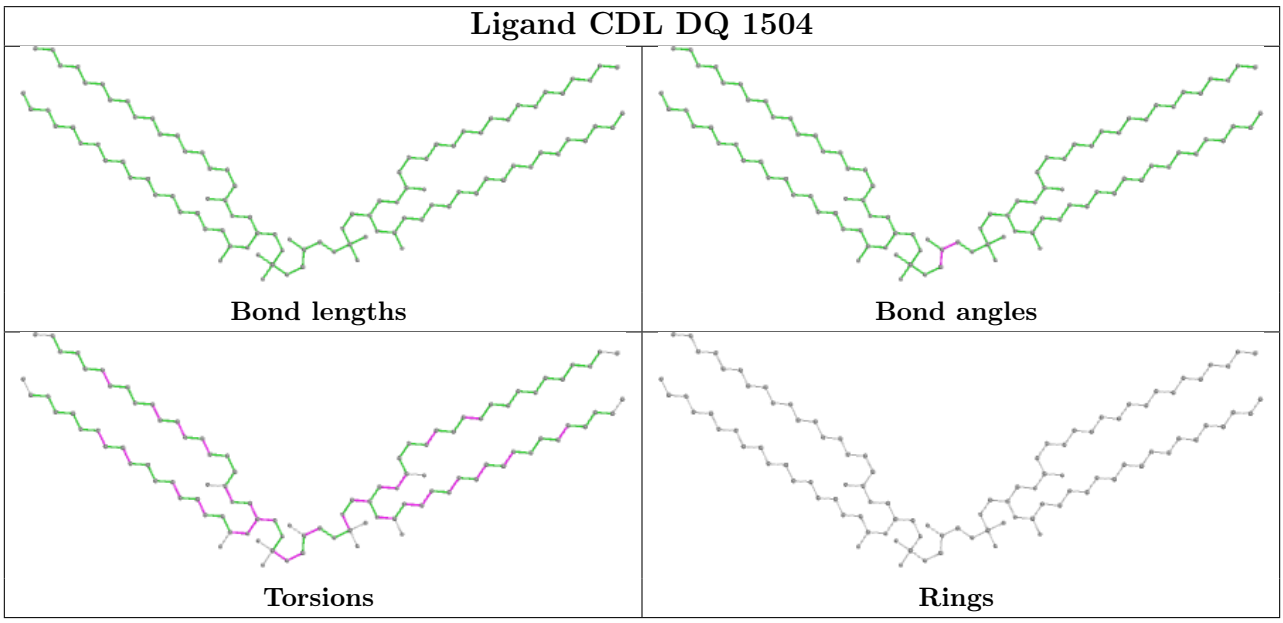
Ligand CDL Dn 506



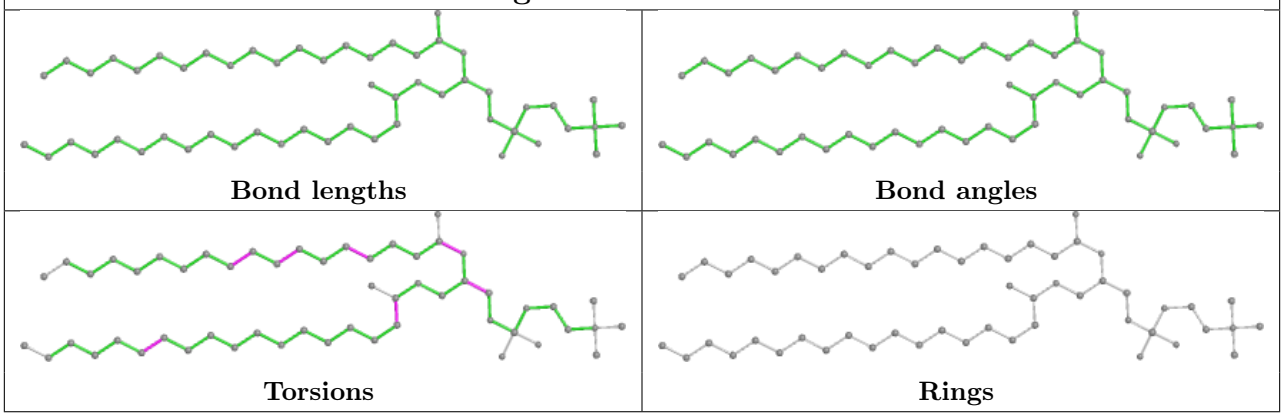
Ligand PC1 EO 205



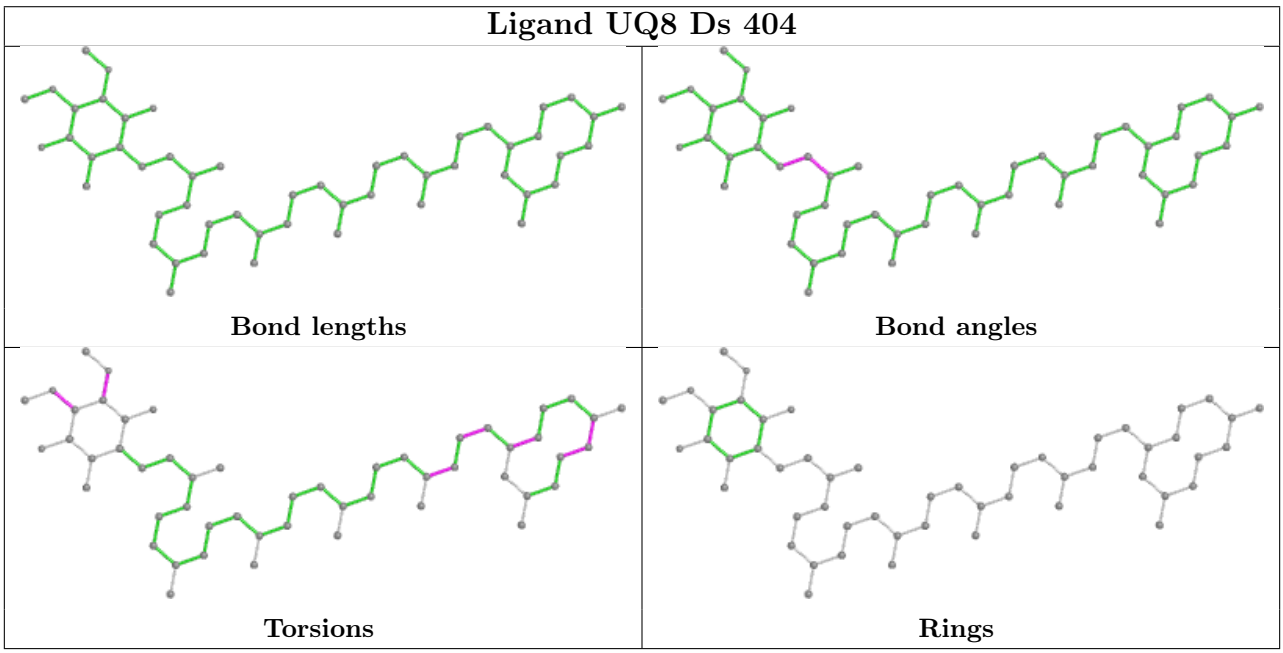
Ligand CDL DQ 1504



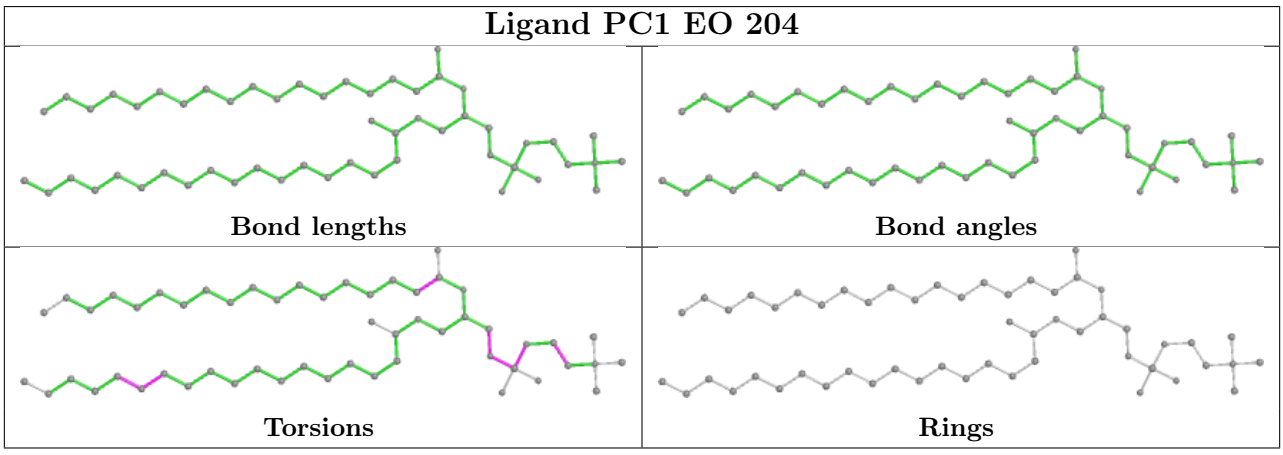
Ligand PC1 DG 203



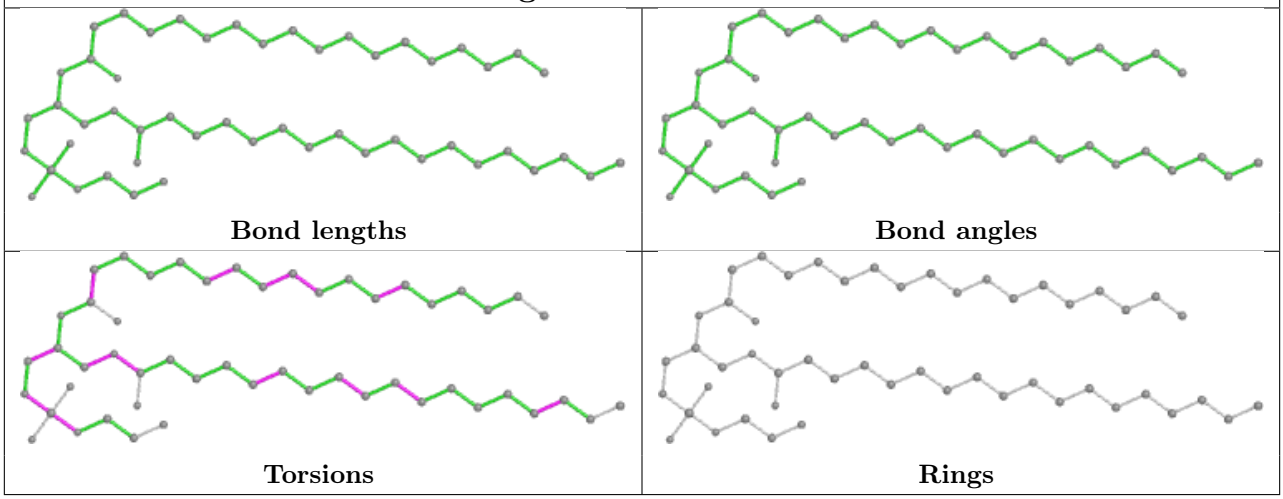
Ligand UQ8 Ds 404



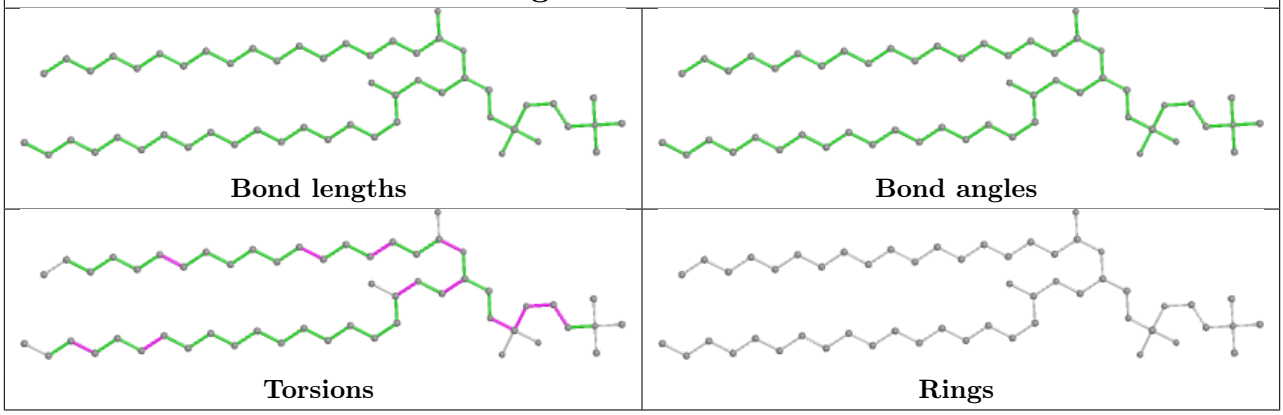
Ligand PC1 EO 204



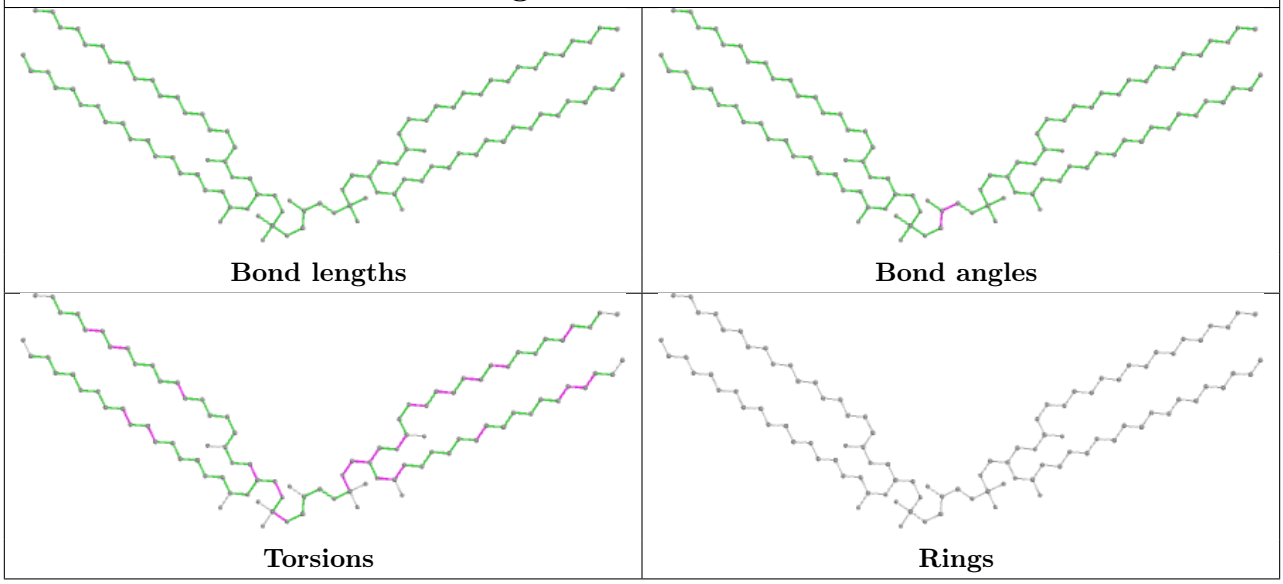
Ligand 3PE DS 402



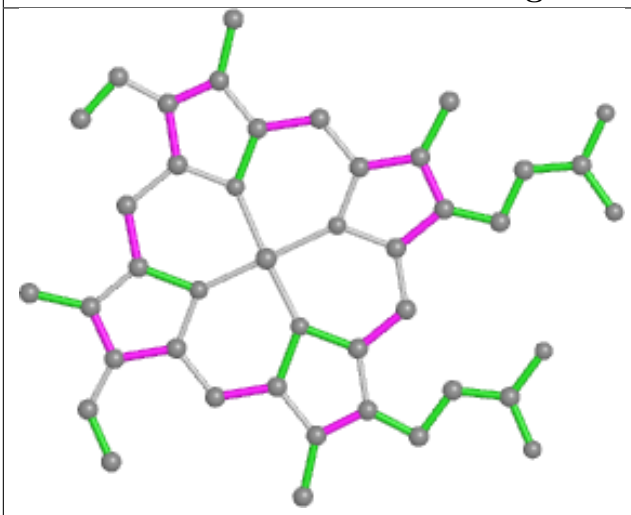
Ligand PC1 d 801



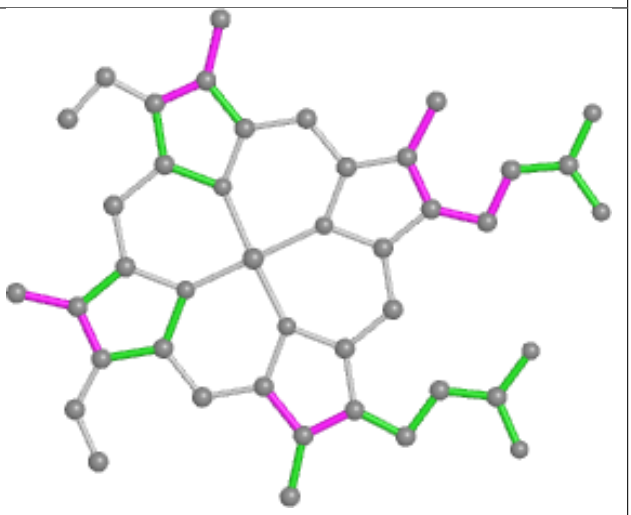
Ligand CDL DA 706



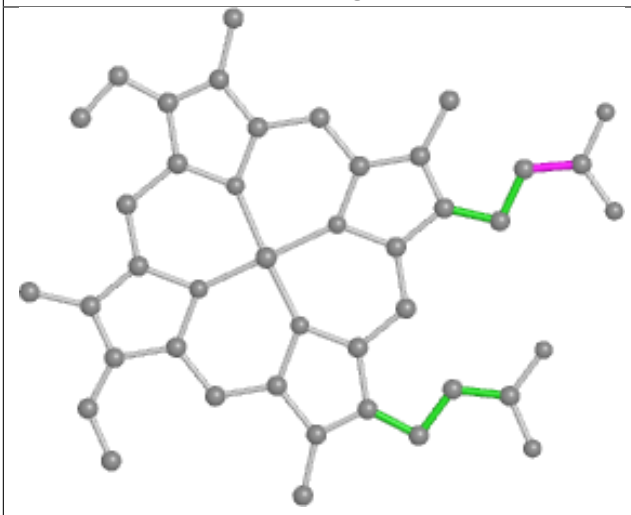
Ligand HEC d 802



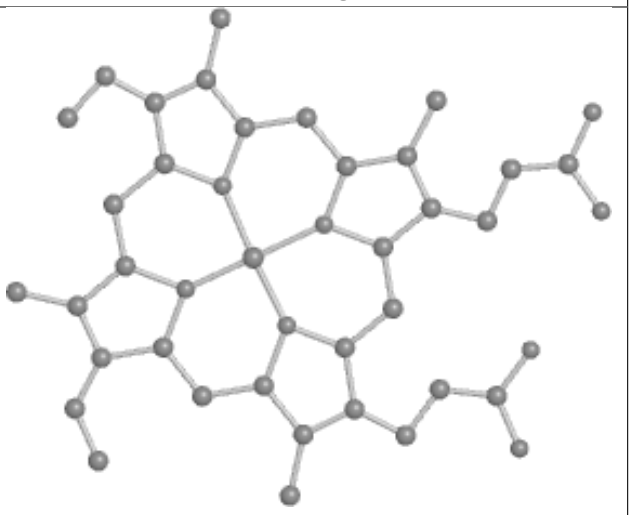
Bond lengths



Bond angles

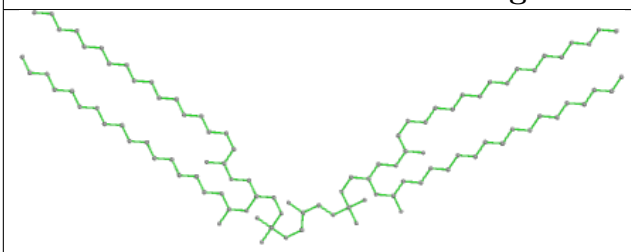


Torsions

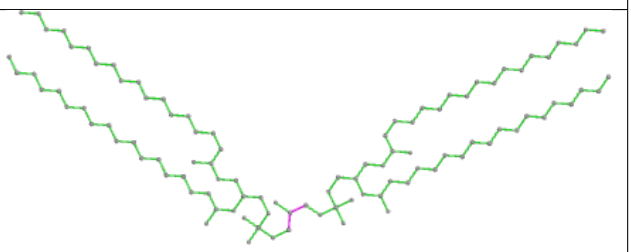


Rings

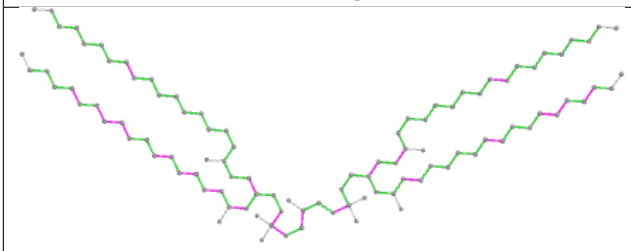
Ligand CDL DH 201



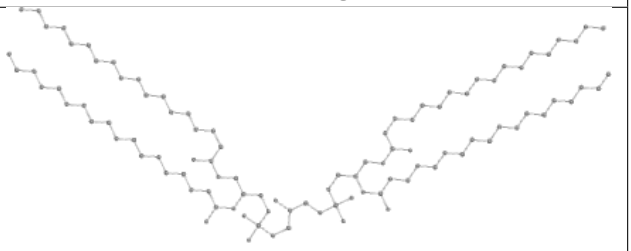
Bond lengths



Bond angles

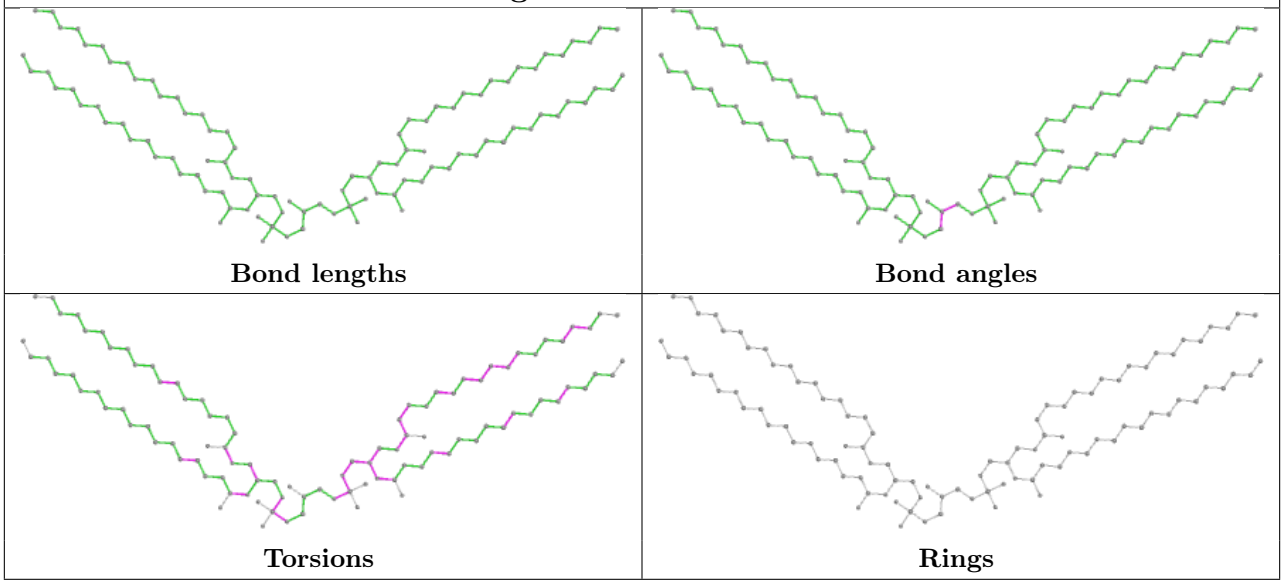


Torsions

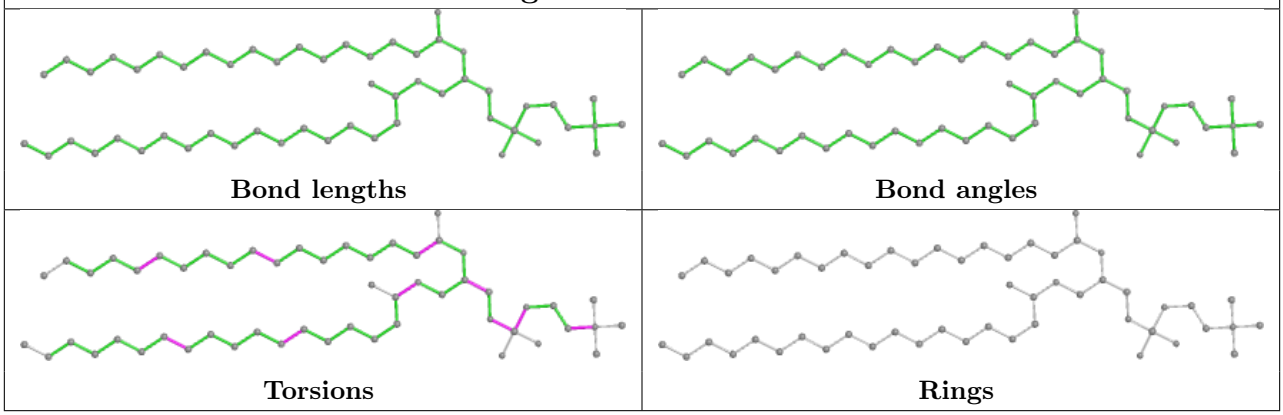


Rings

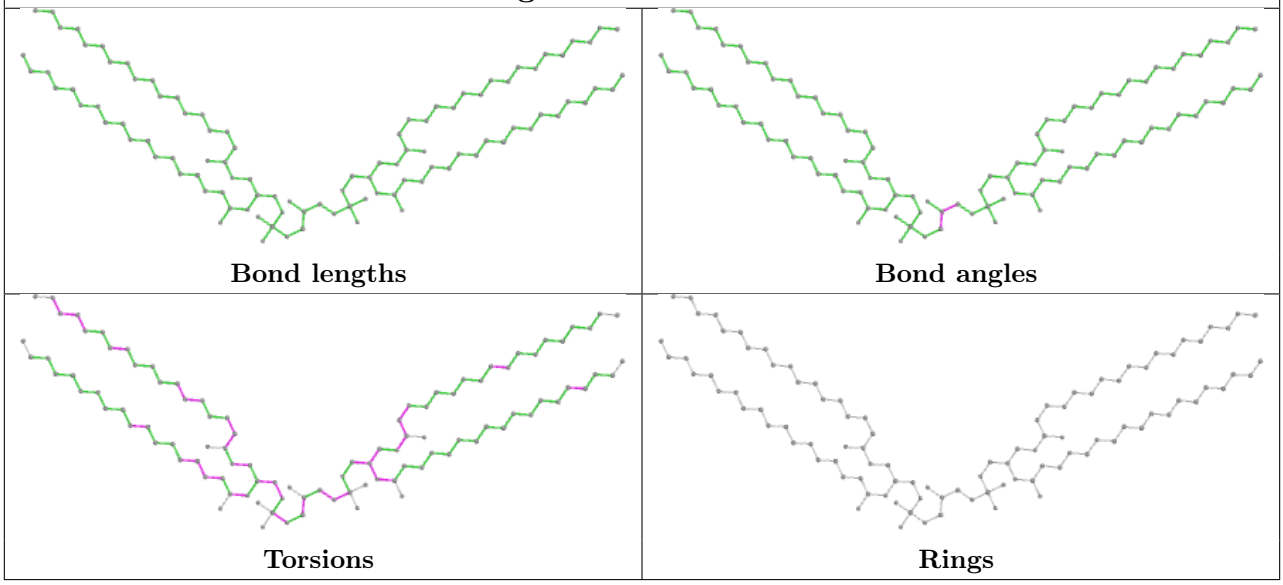
Ligand CDL DN 502



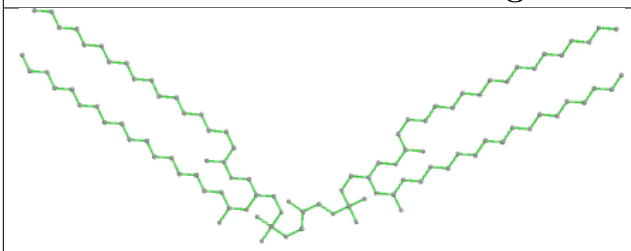
Ligand PC1 DI 303



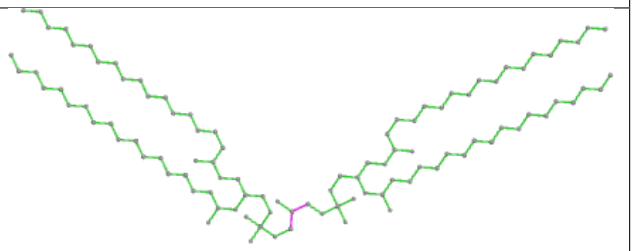
Ligand CDL Ea 501



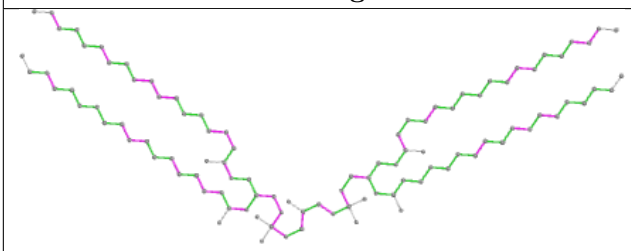
Ligand CDL ES 1101



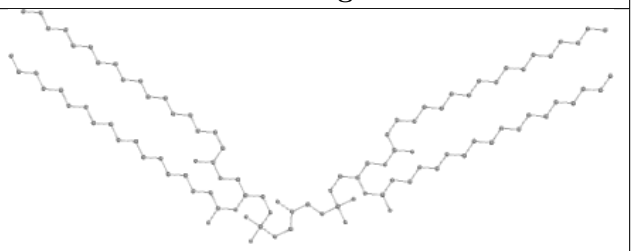
Bond lengths



Bond angles

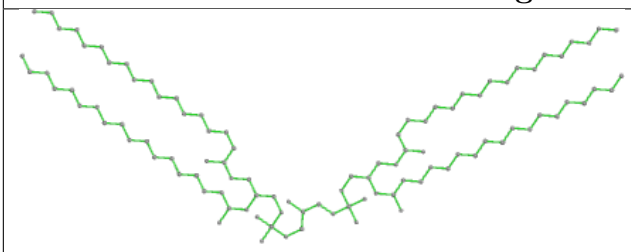


Torsions

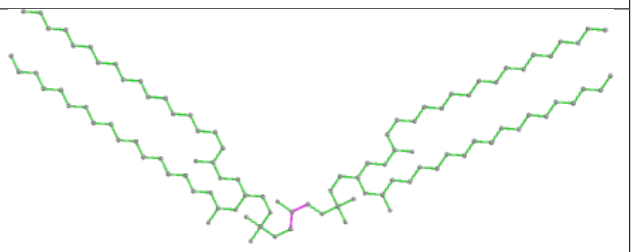


Rings

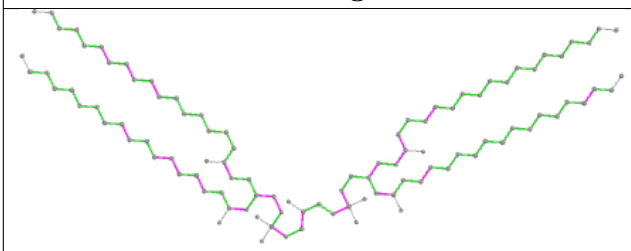
Ligand CDL Eu 101



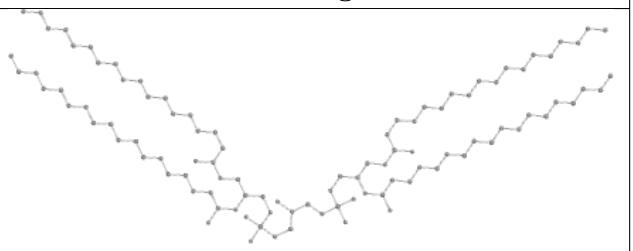
Bond lengths



Bond angles

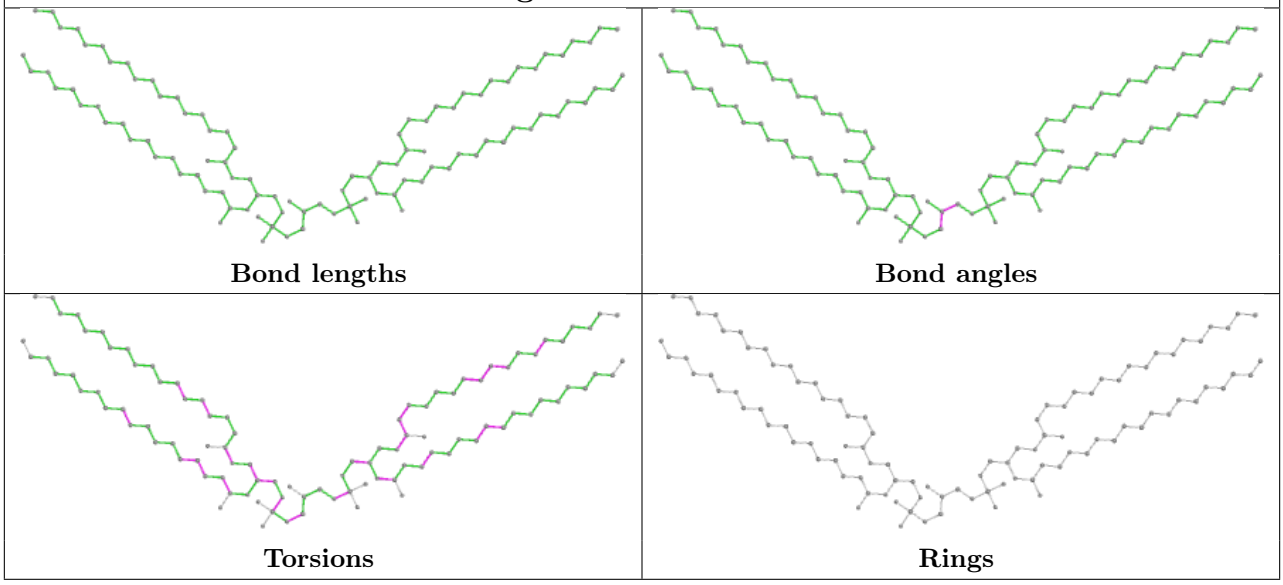


Torsions

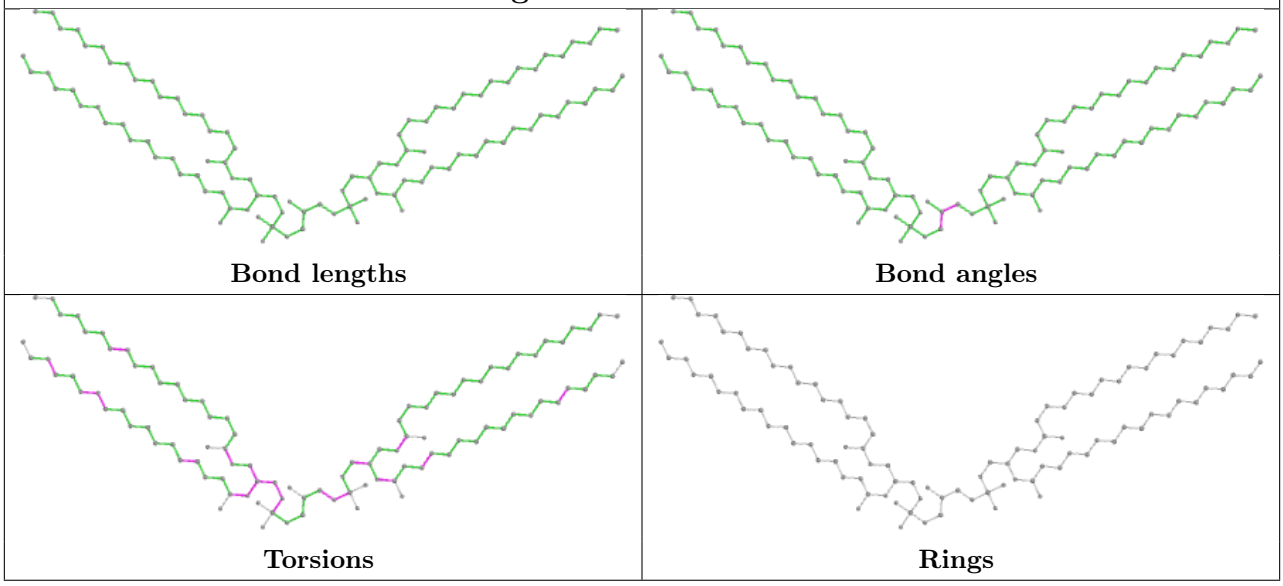


Rings

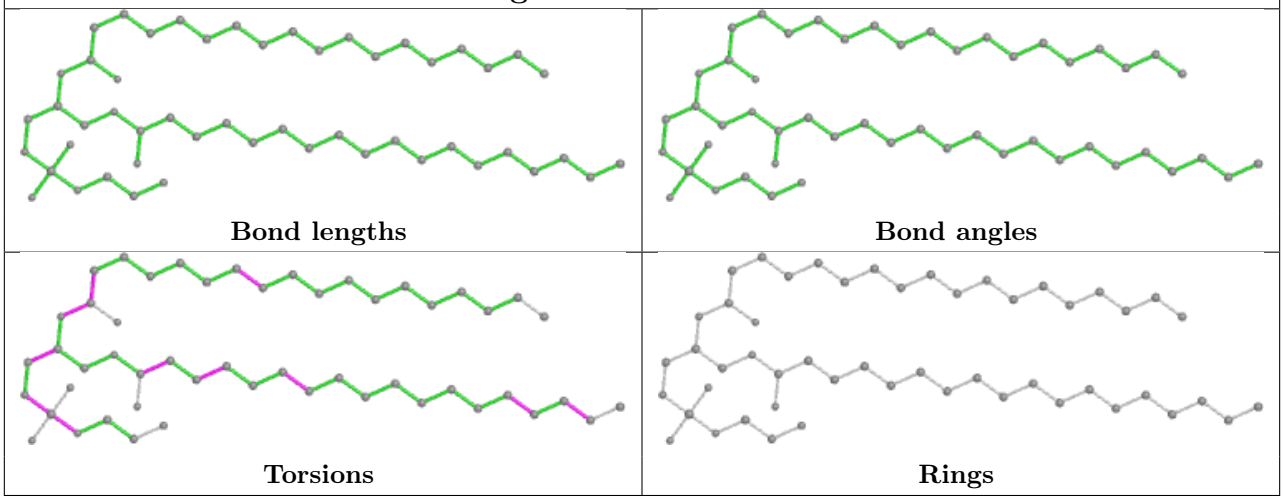
Ligand CDL B1 402



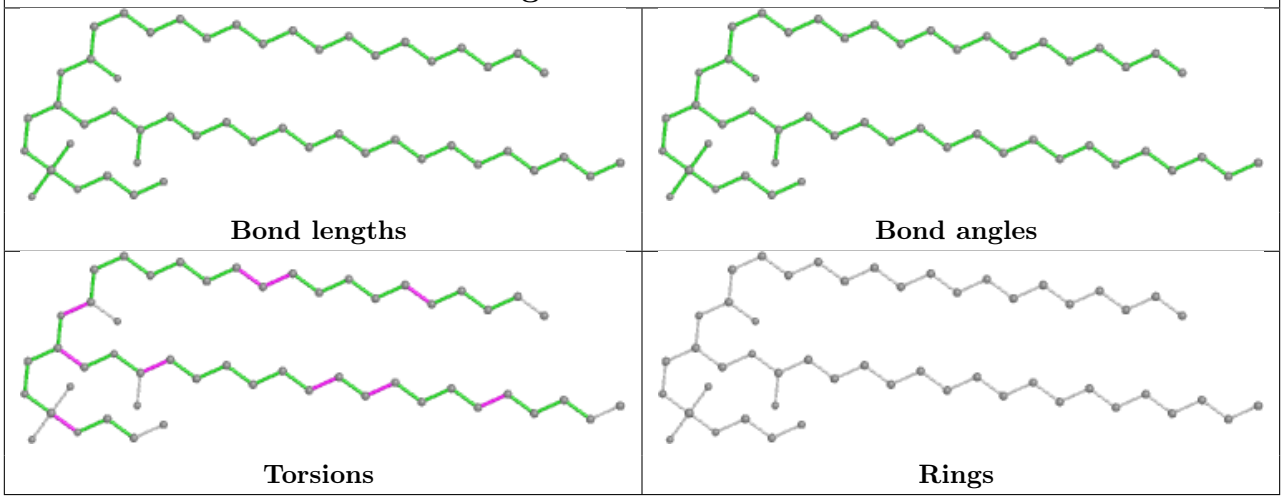
Ligand CDL CD 302



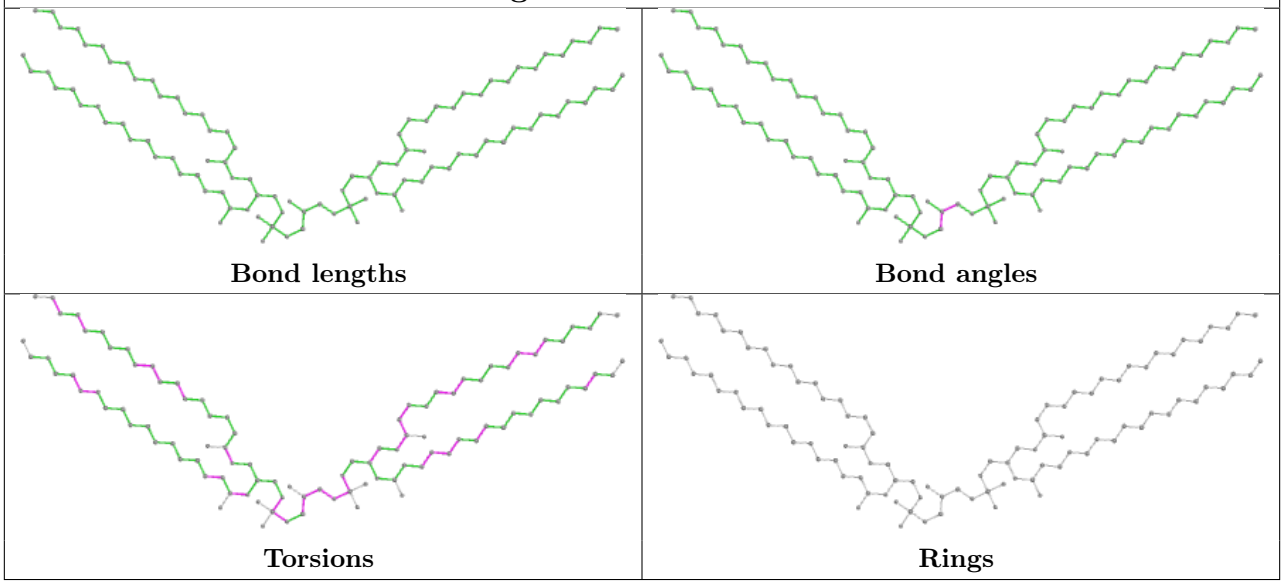
Ligand 3PE Dx 1207



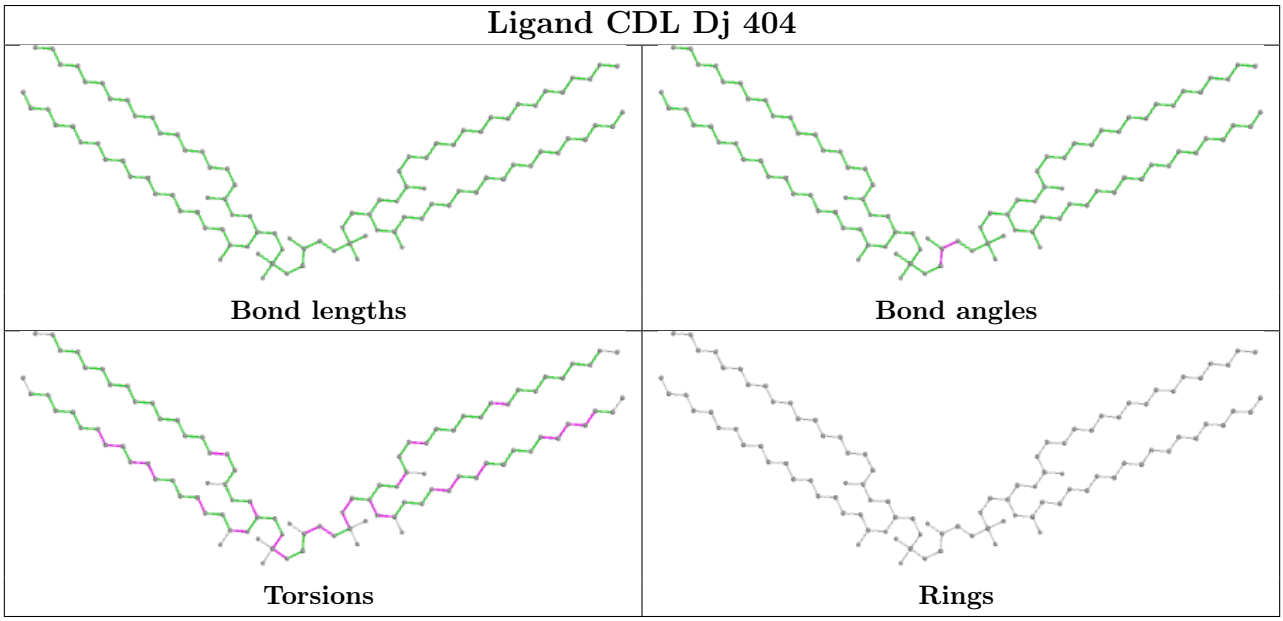
Ligand 3PE Eo 202



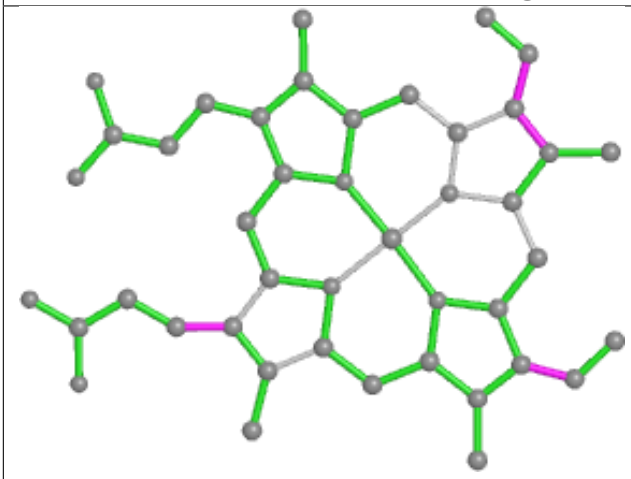
Ligand CDL DH 202



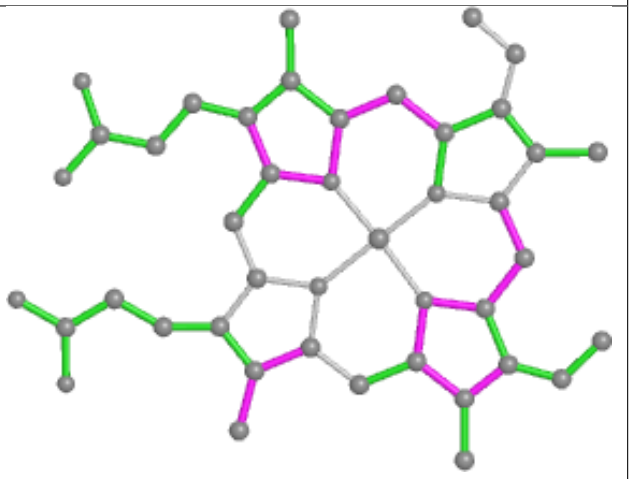
Ligand CDL Dj 404



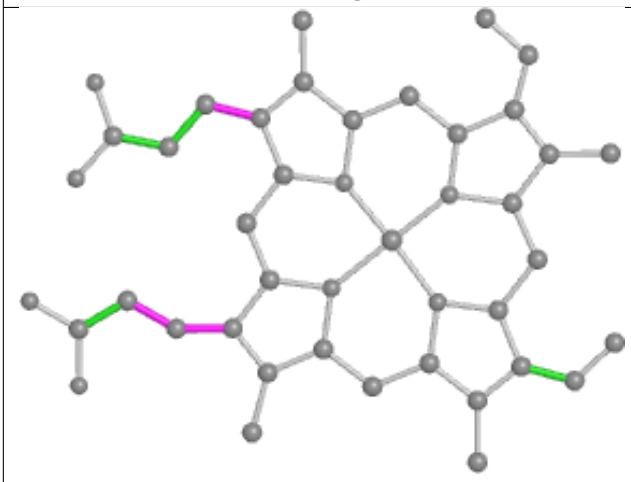
Ligand HEM C 501



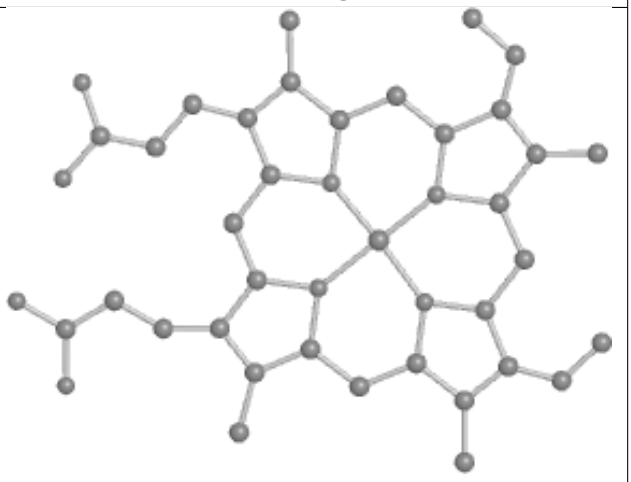
Bond lengths



Bond angles

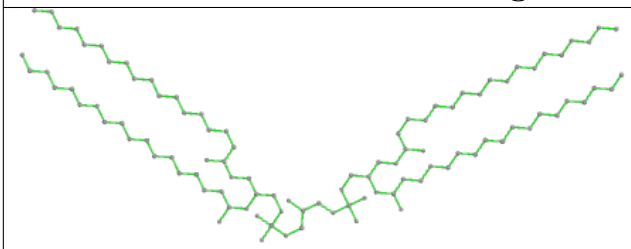


Torsions

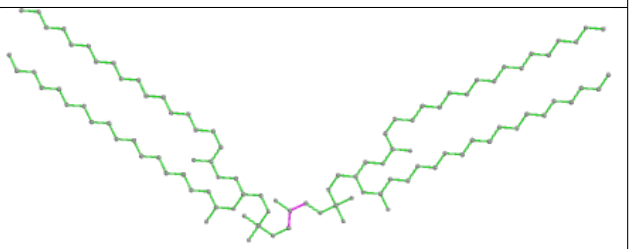


Rings

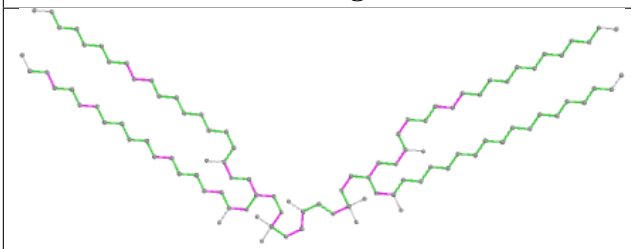
Ligand CDL DD 703



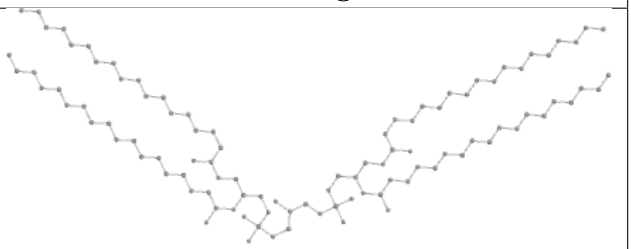
Bond lengths



Bond angles

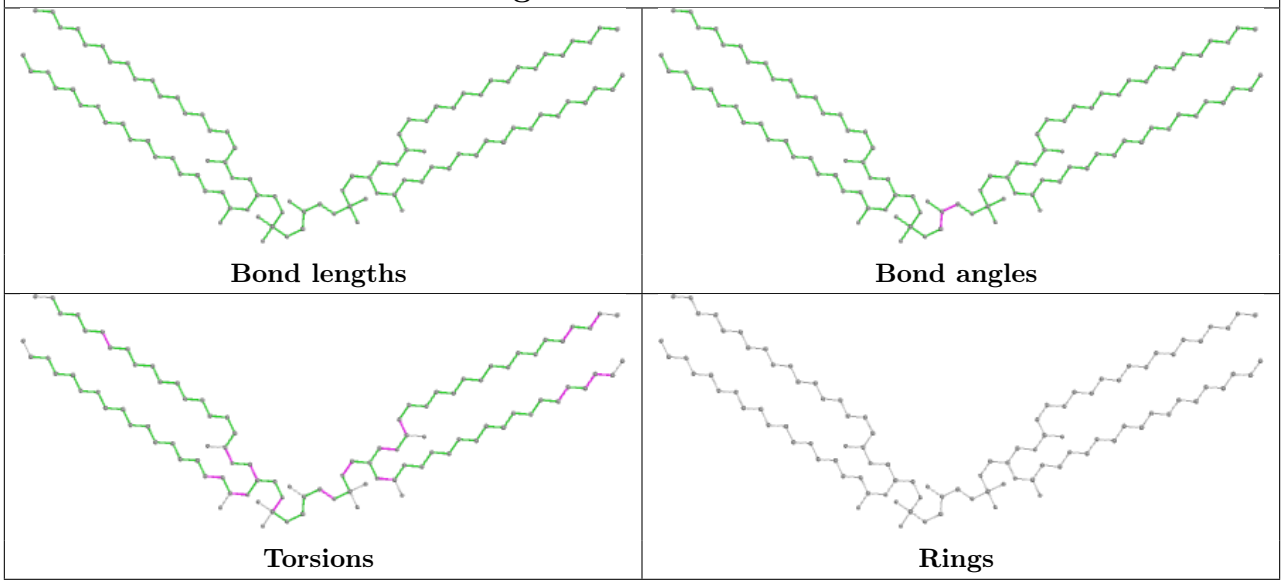


Torsions

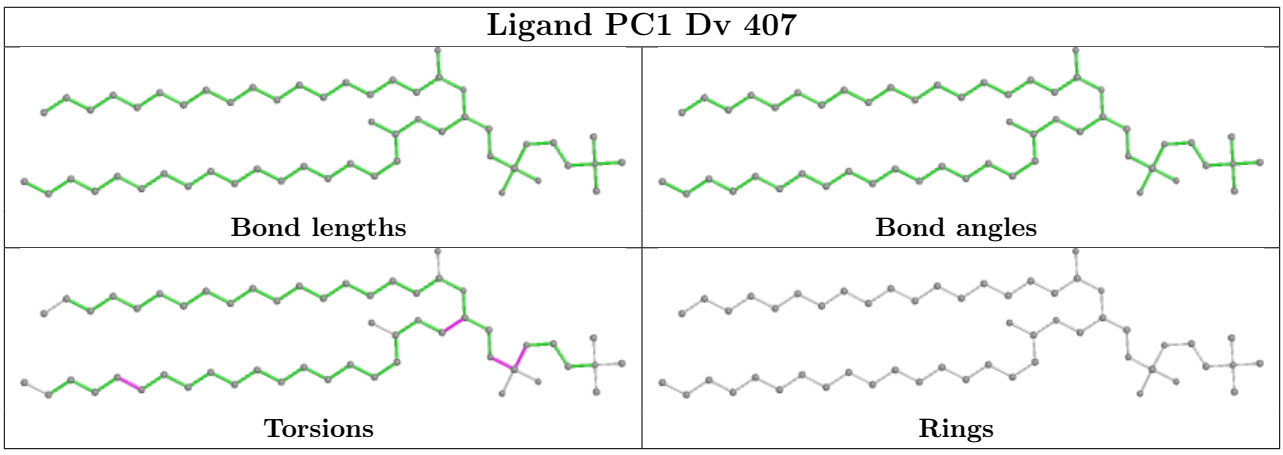


Rings

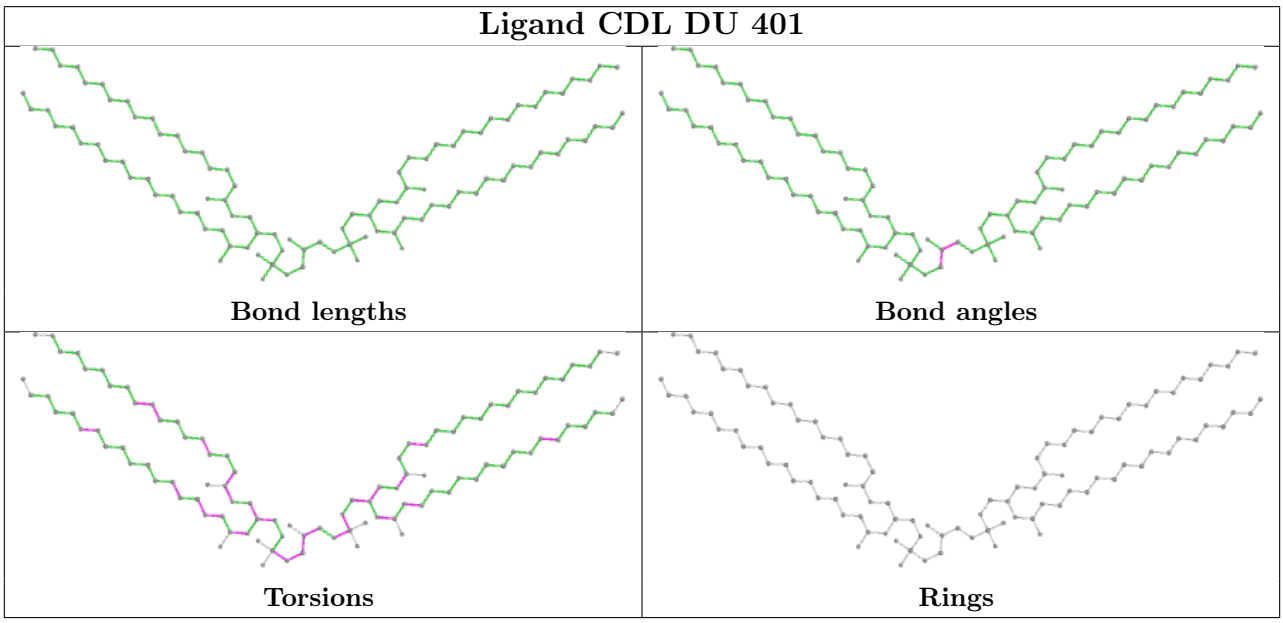
Ligand CDL AF 401



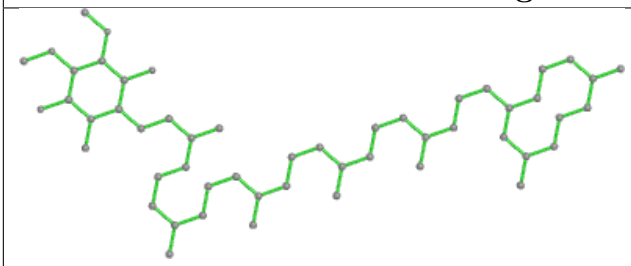
Ligand PC1 Dv 407



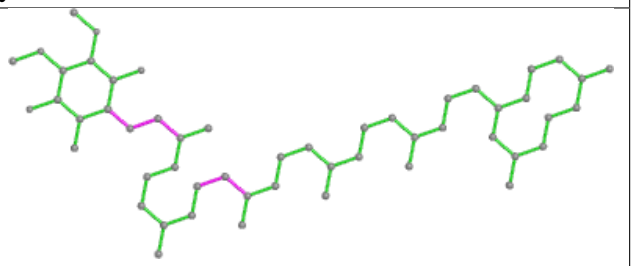
Ligand CDL DU 401



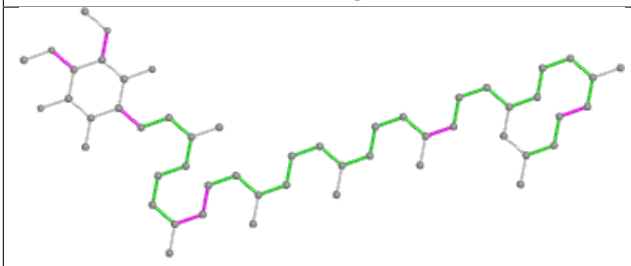
Ligand UQ8 EL 905



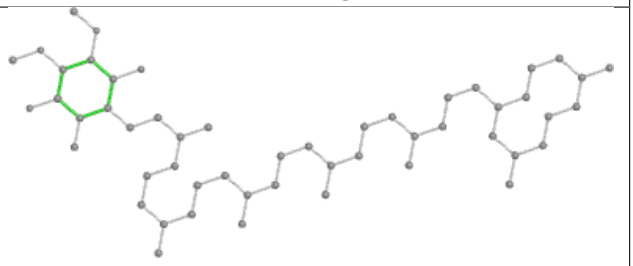
Bond lengths



Bond angles

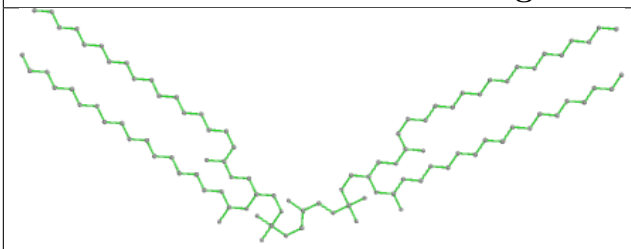


Torsions

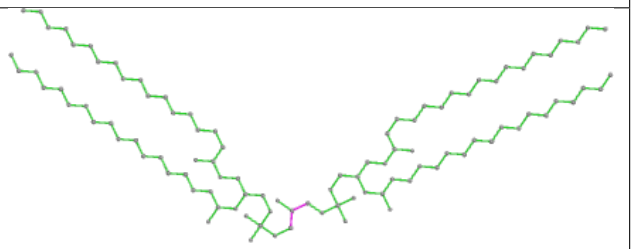


Rings

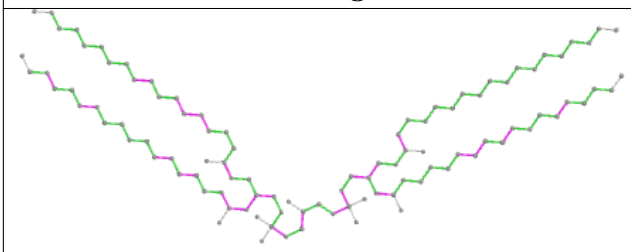
Ligand CDL Eb 302



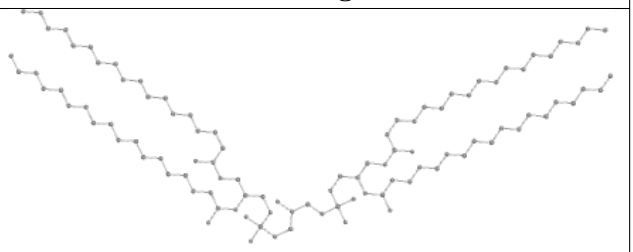
Bond lengths



Bond angles

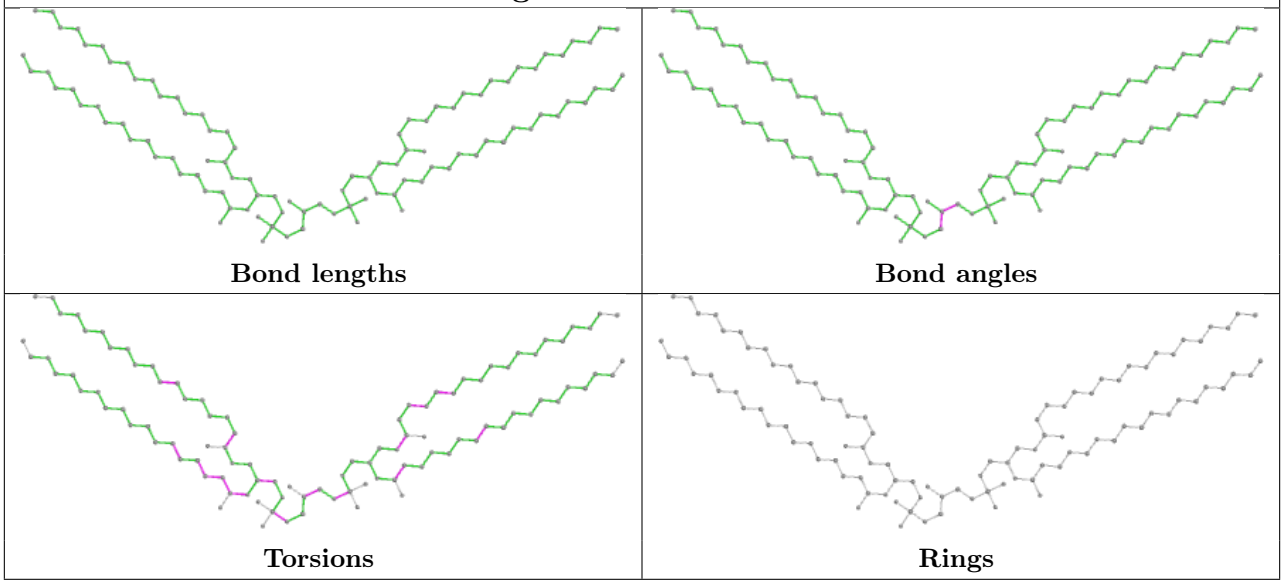


Torsions

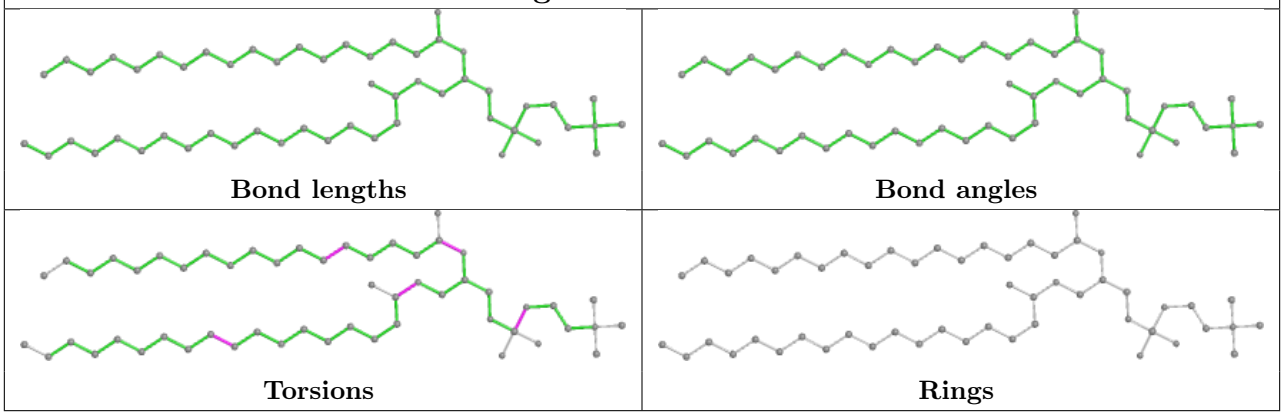


Rings

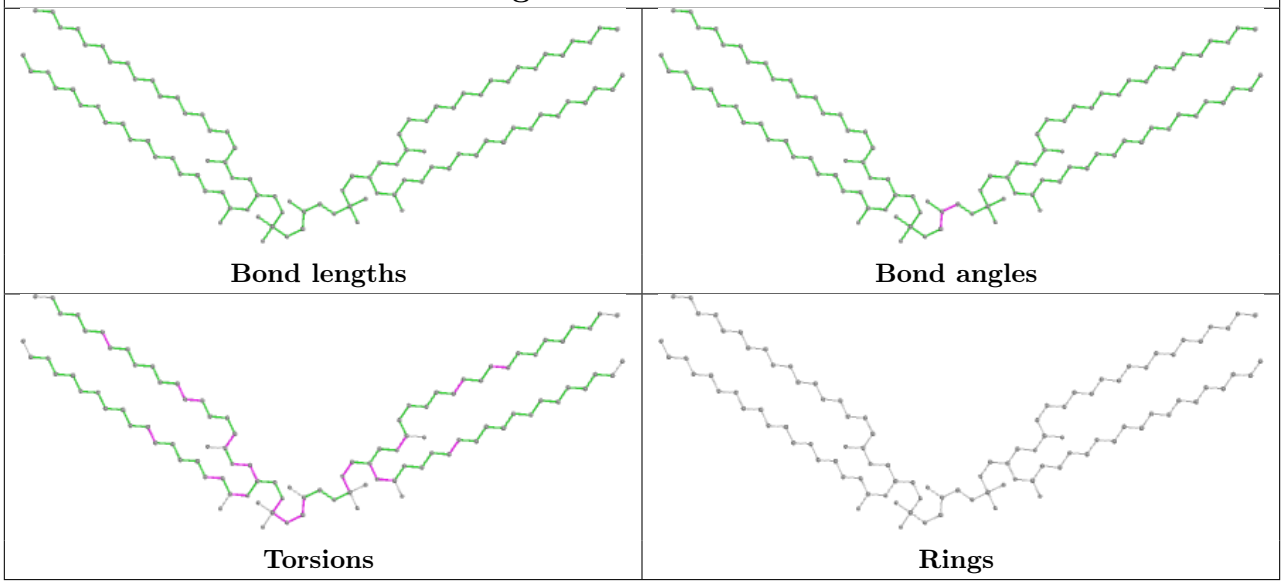
Ligand CDL BC 301



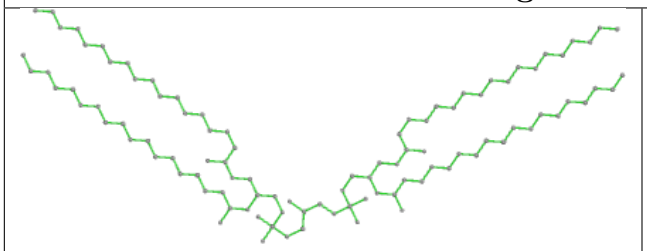
Ligand PC1 c 508



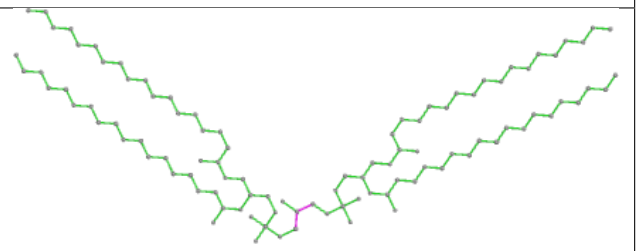
Ligand CDL EK 201



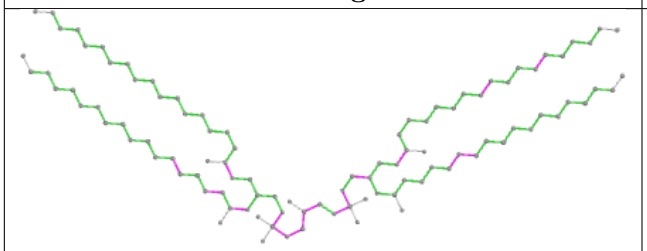
Ligand CDL Ed 204



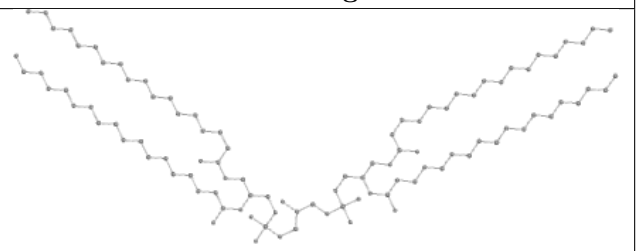
Bond lengths



Bond angles

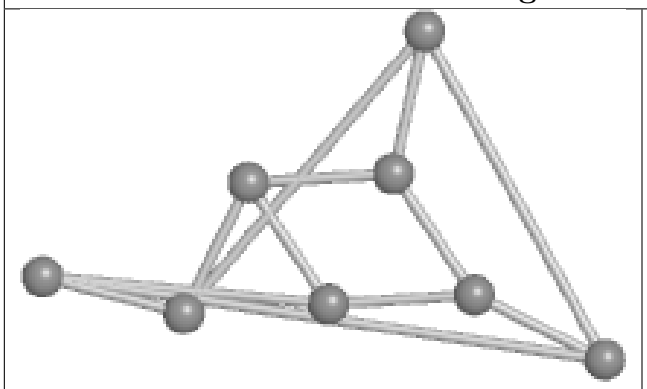


Torsions

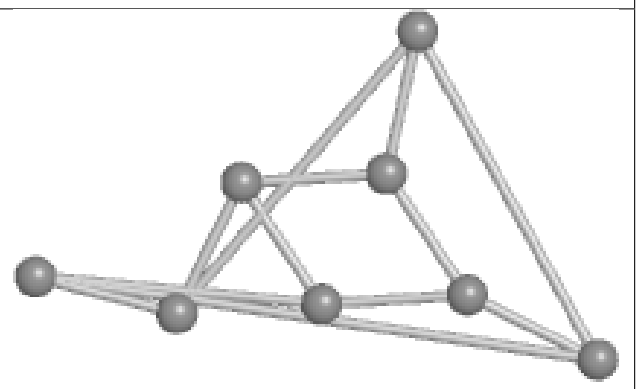


Rings

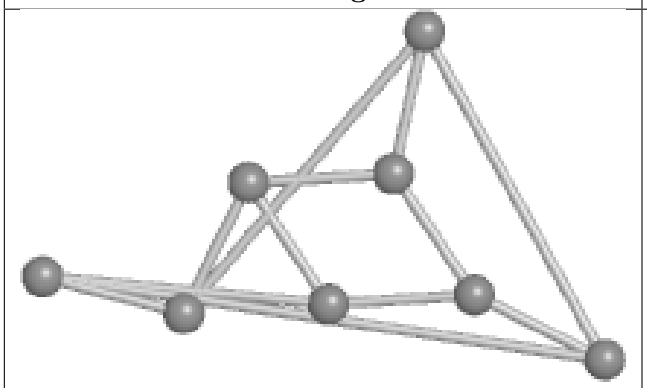
Ligand SF4 AB 803



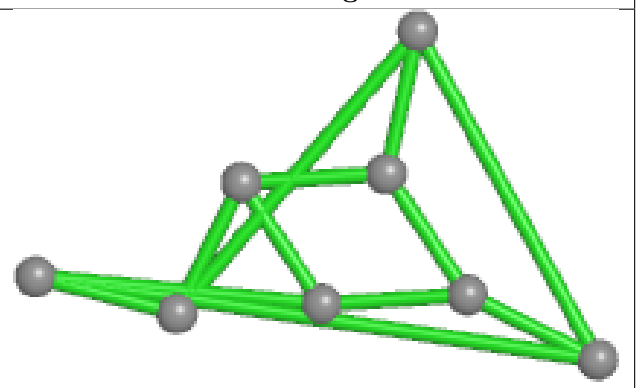
Bond lengths



Bond angles

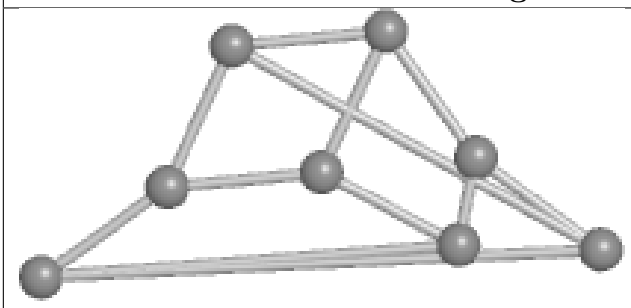


Torsions

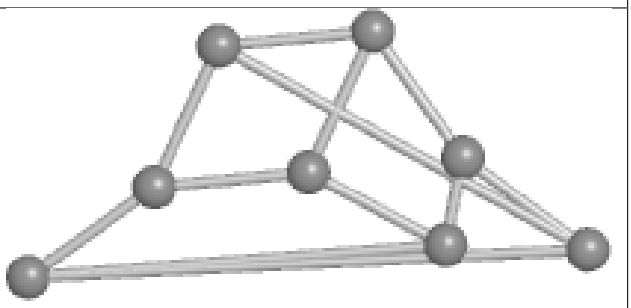


Rings

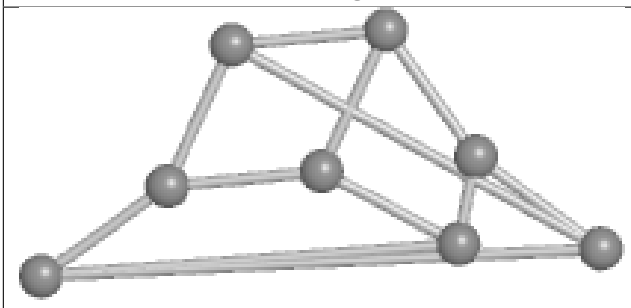
Ligand SF4 CB 1001



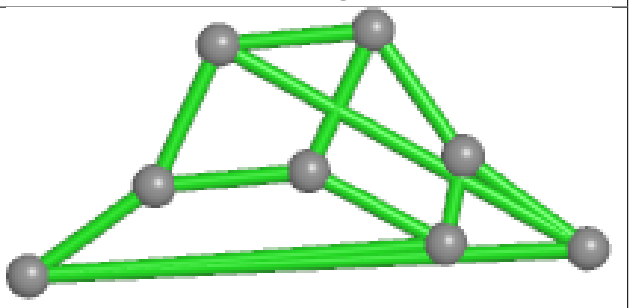
Bond lengths



Bond angles

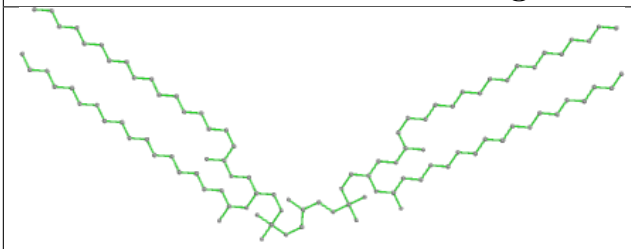


Torsions

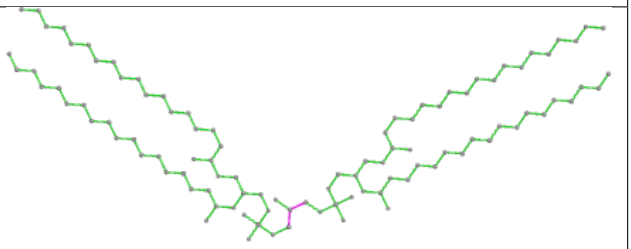


Rings

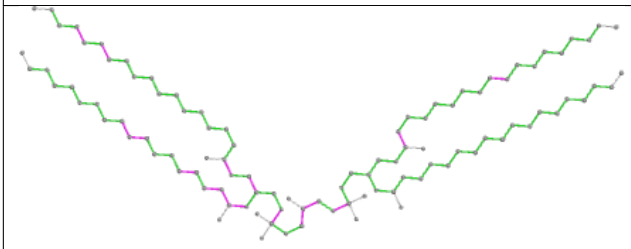
Ligand CDL DA 709



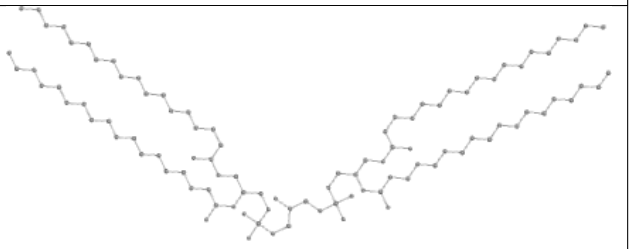
Bond lengths



Bond angles

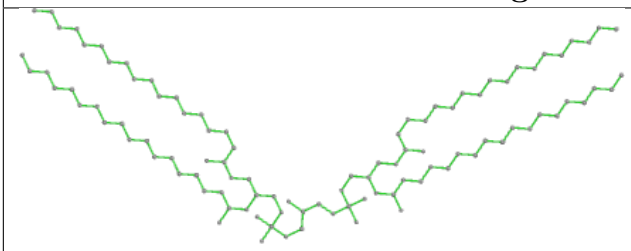


Torsions

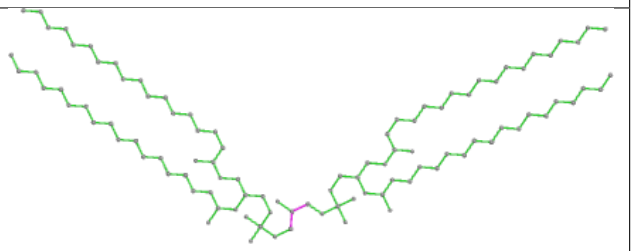


Rings

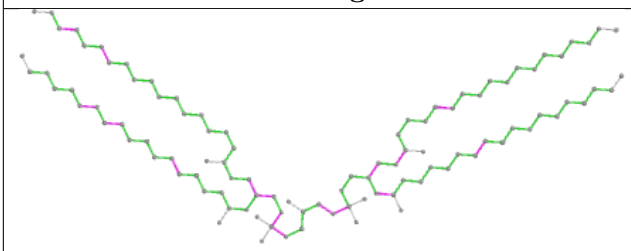
Ligand CDL CC 304



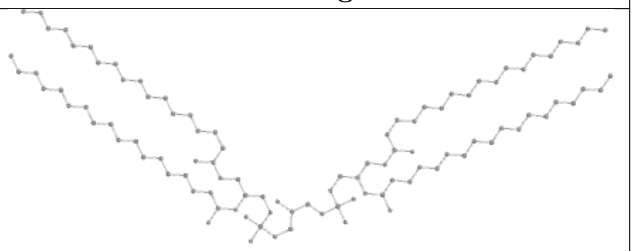
Bond lengths



Bond angles

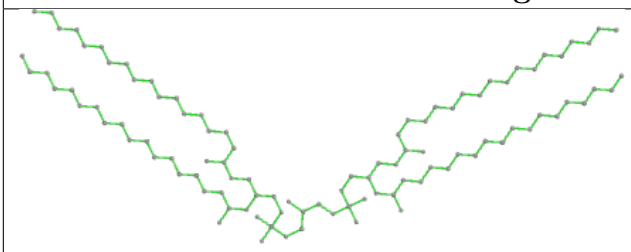


Torsions

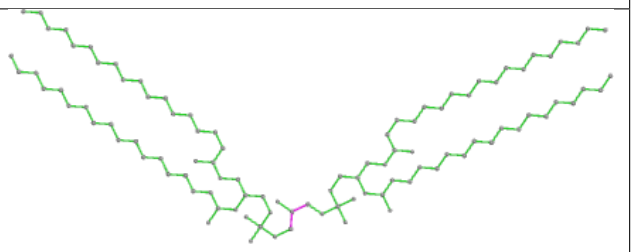


Rings

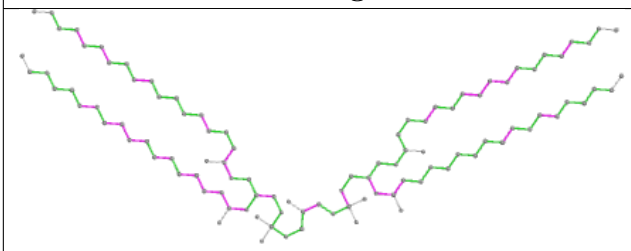
Ligand CDL DS 404



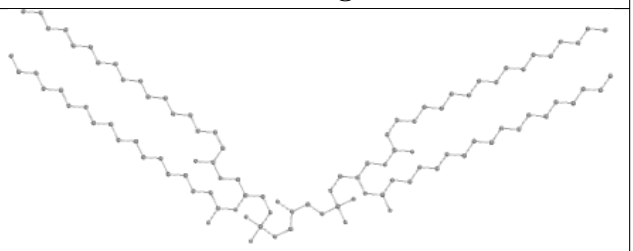
Bond lengths



Bond angles

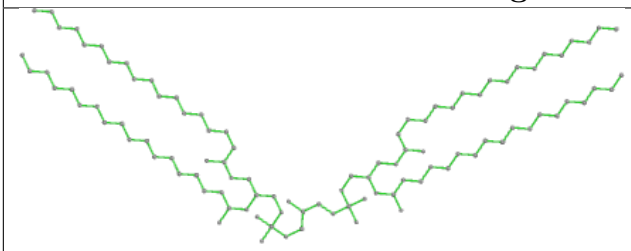


Torsions

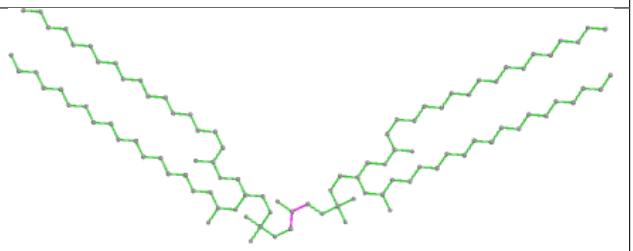


Rings

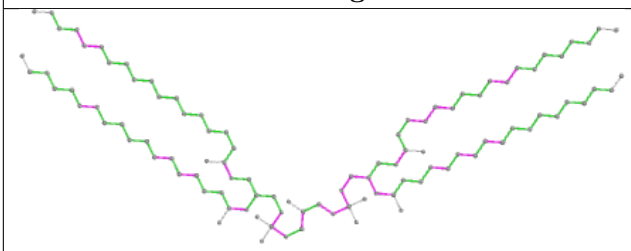
Ligand CDL CG 302



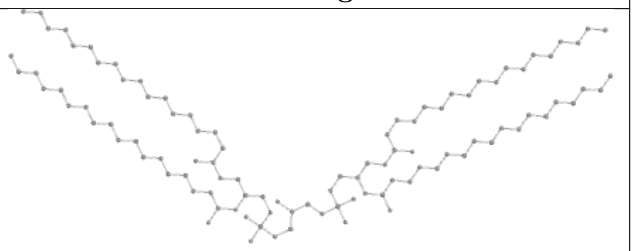
Bond lengths



Bond angles

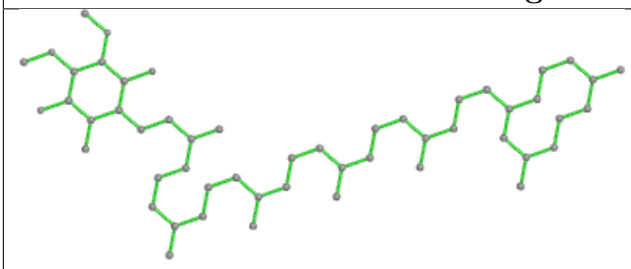


Torsions

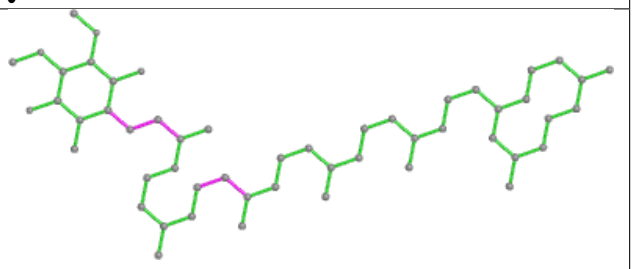


Rings

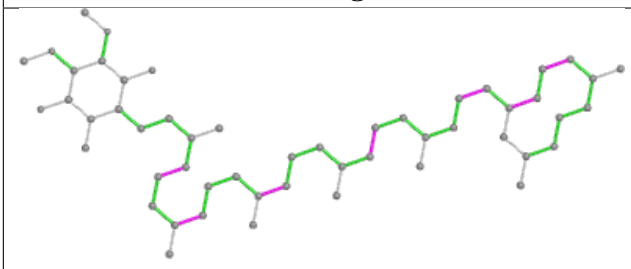
Ligand UQ8 C 512



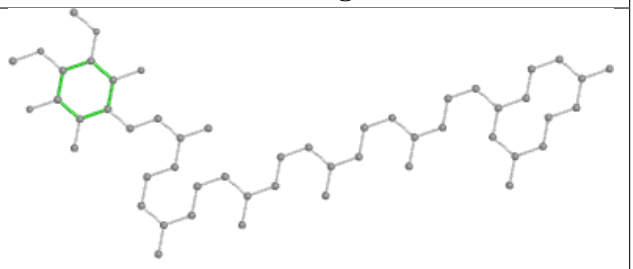
Bond lengths



Bond angles

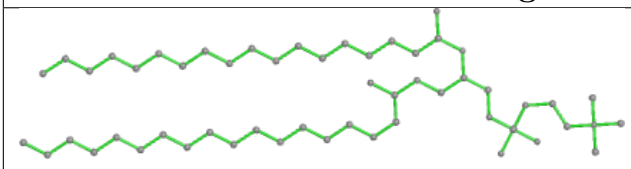


Torsions

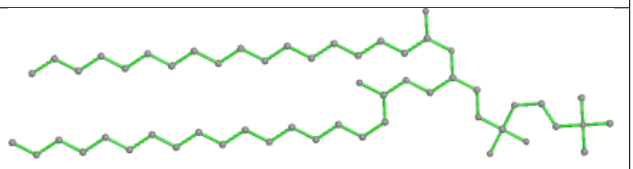


Rings

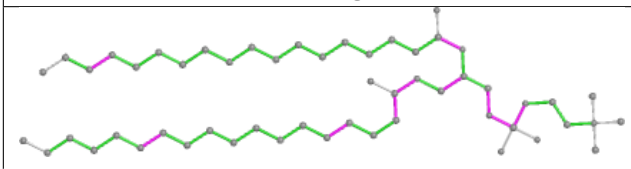
Ligand PC1 B1 401



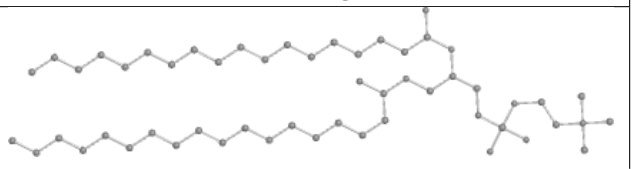
Bond lengths



Bond angles

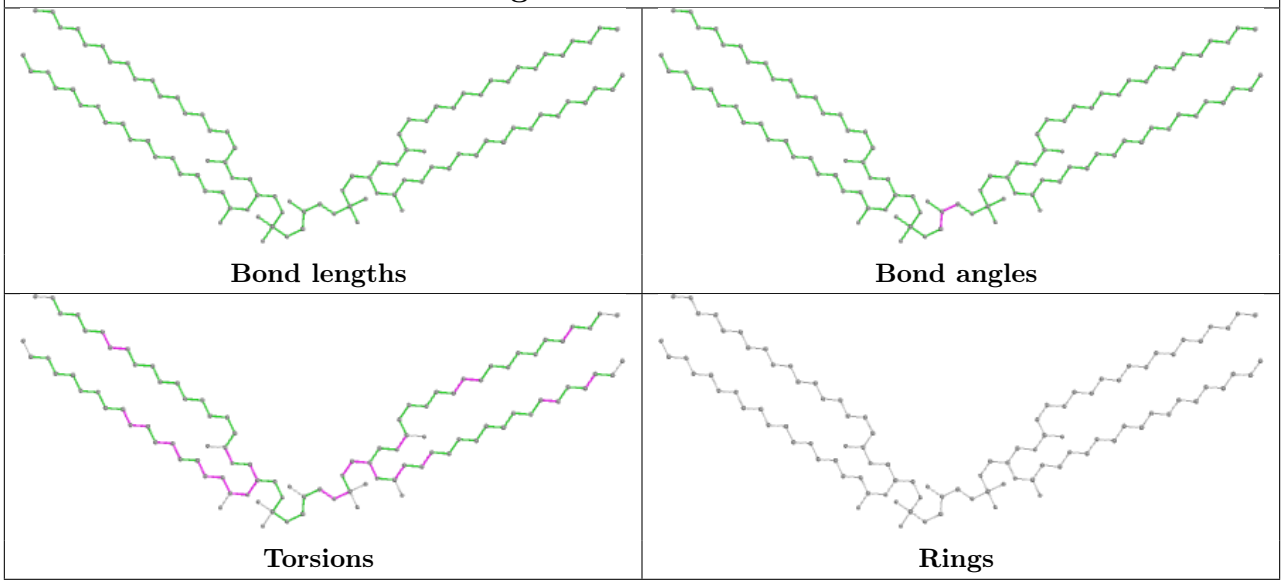


Torsions

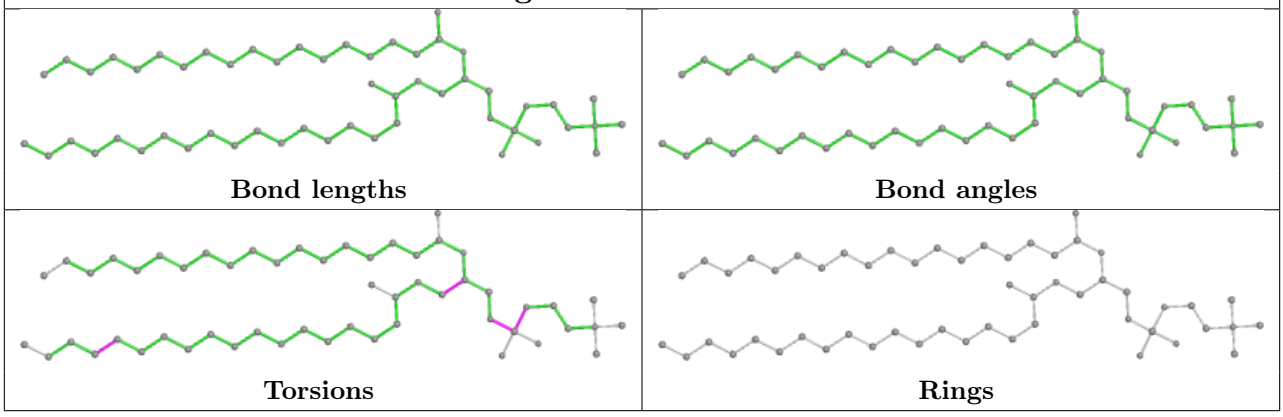


Rings

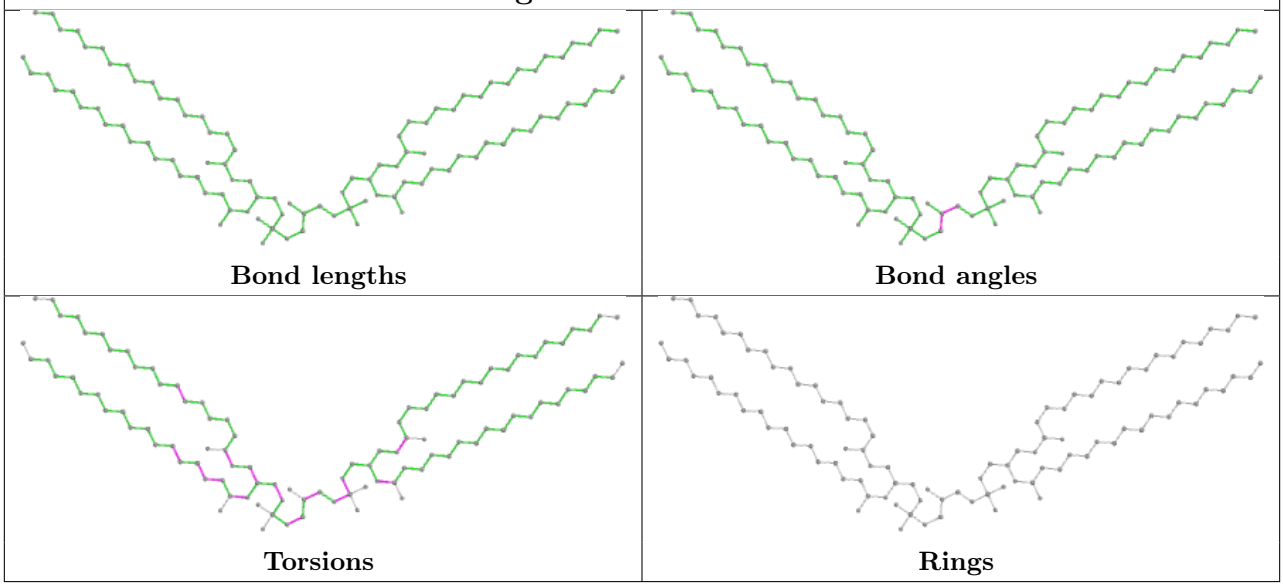
Ligand CDL DD 704



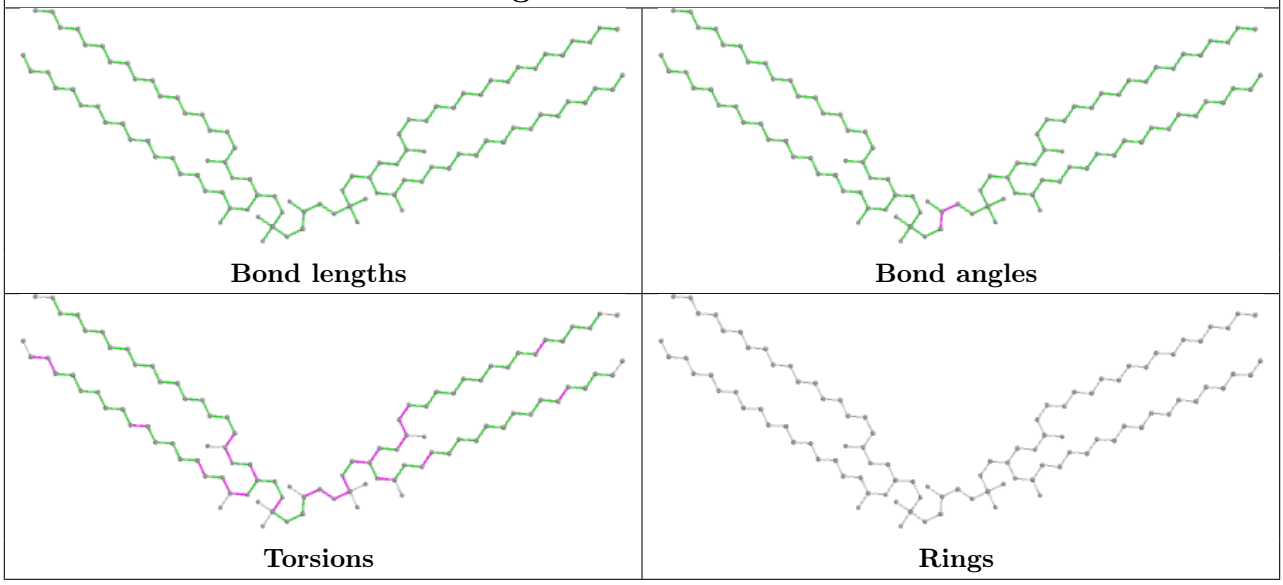
Ligand PC1 DV 406



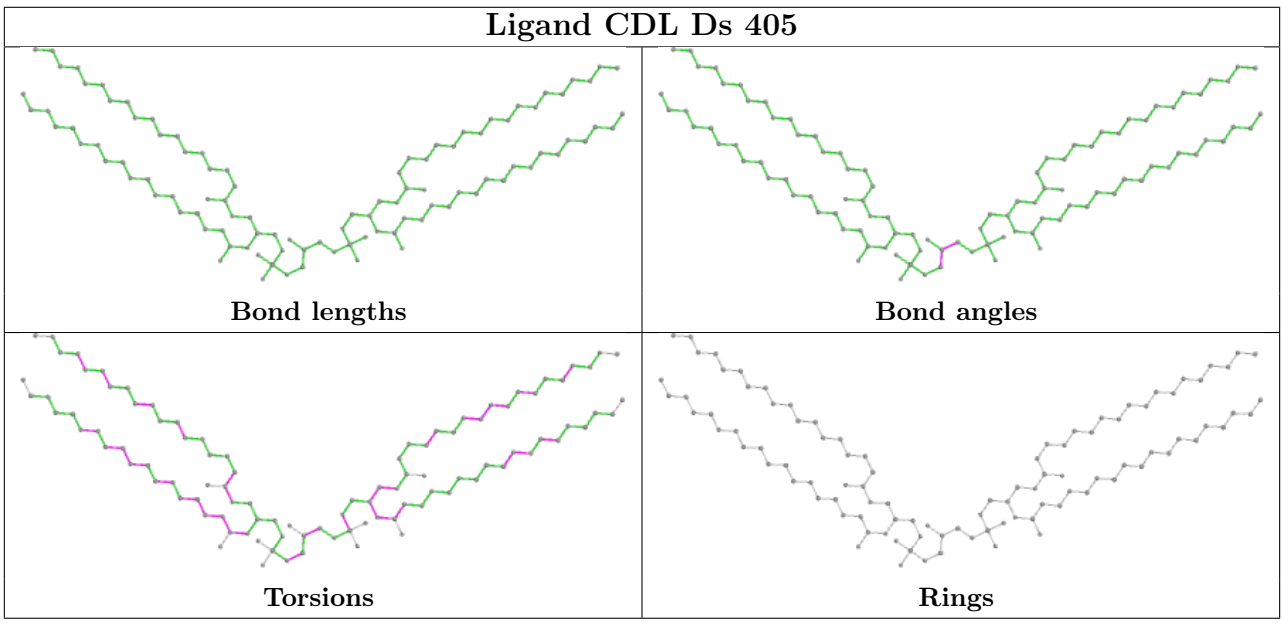
Ligand CDL A0 601



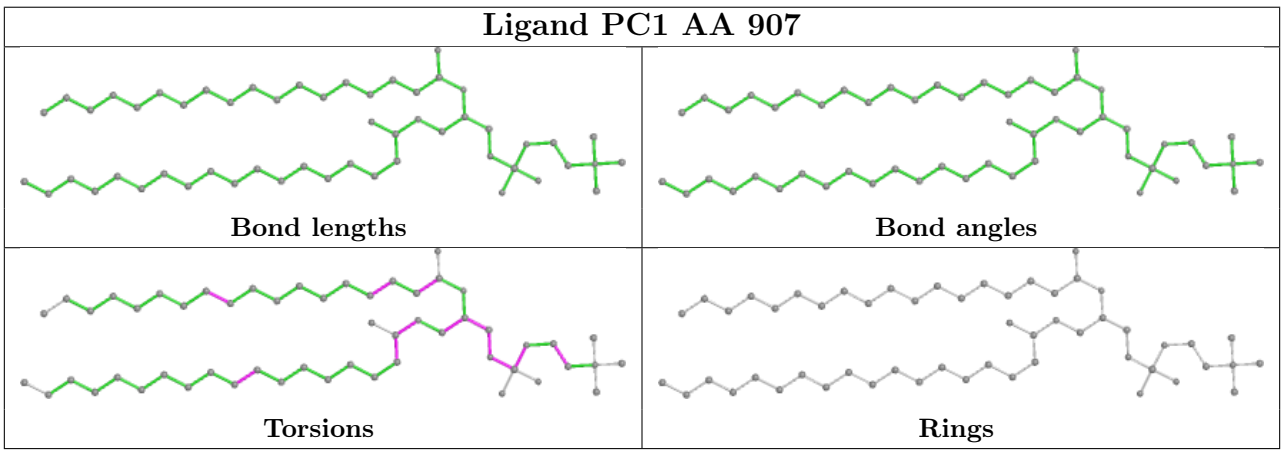
Ligand CDL ED 605



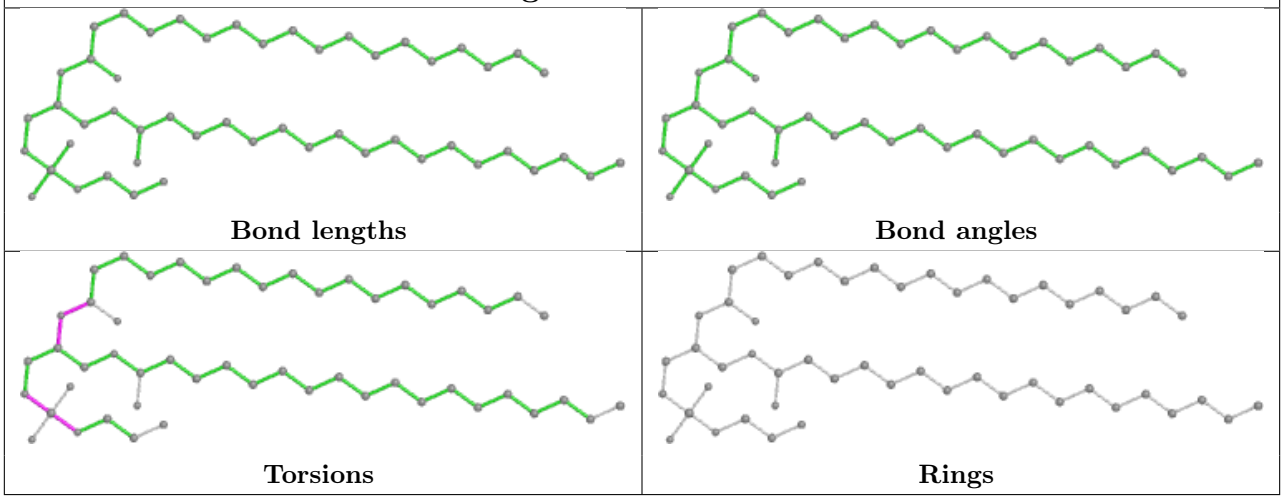
Ligand CDL Ds 405



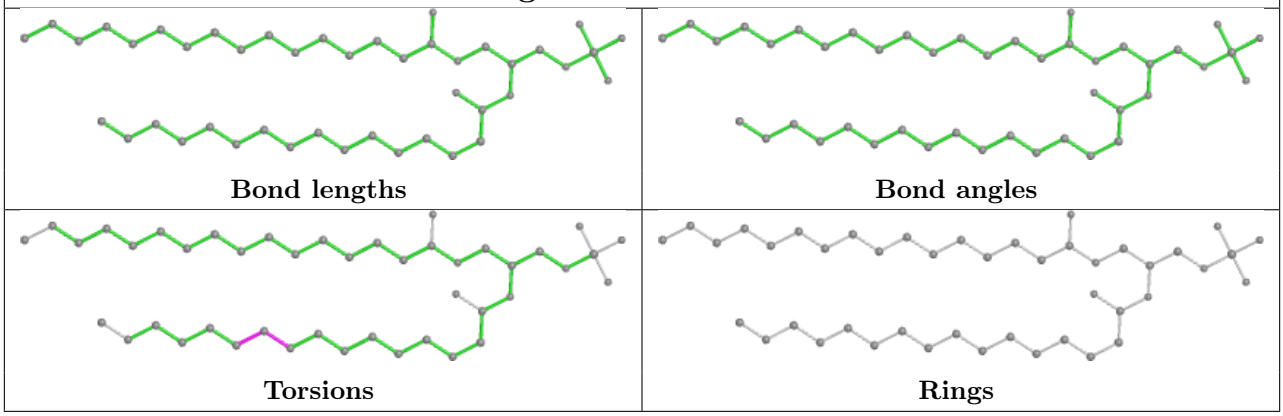
Ligand PC1 AA 907



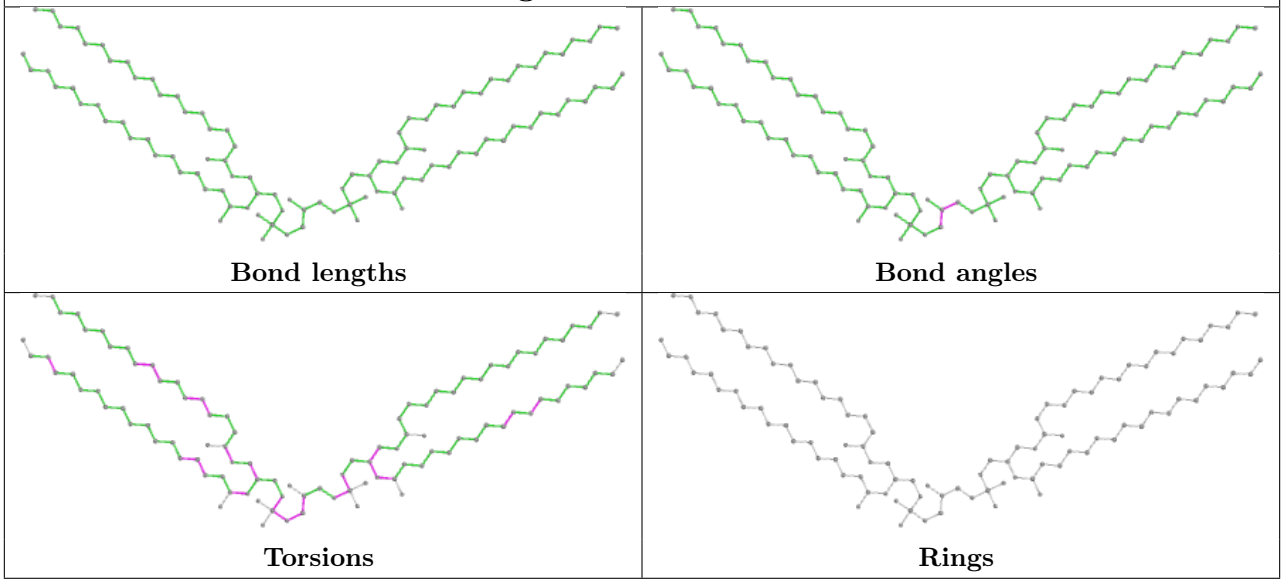
Ligand 3PE Eo 203



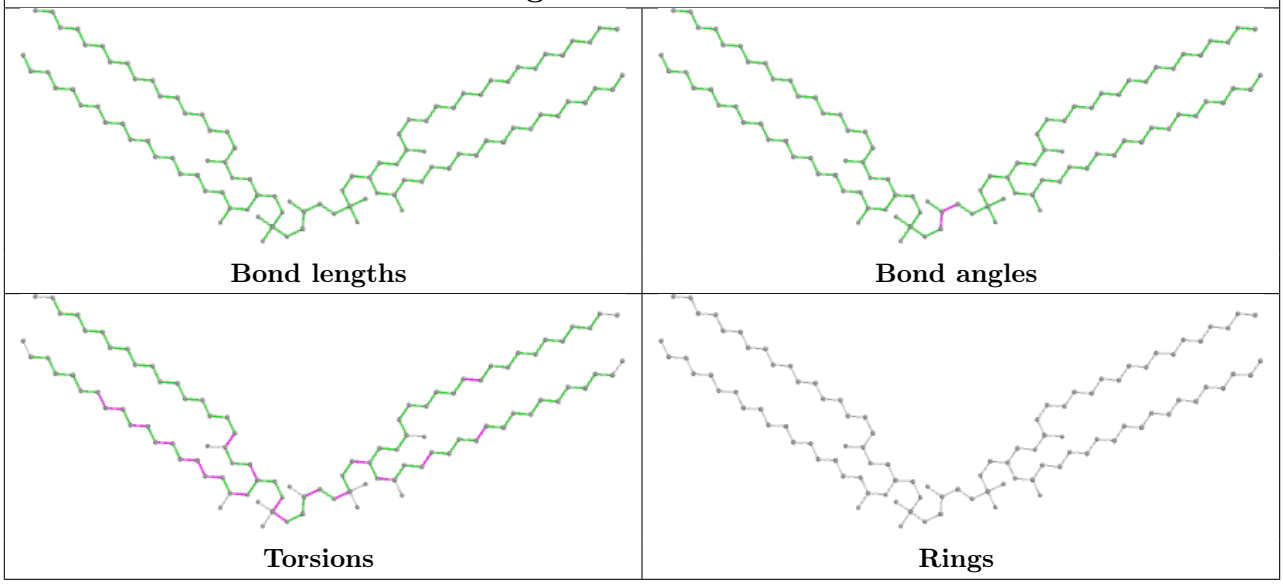
Ligand LPP Ed 203



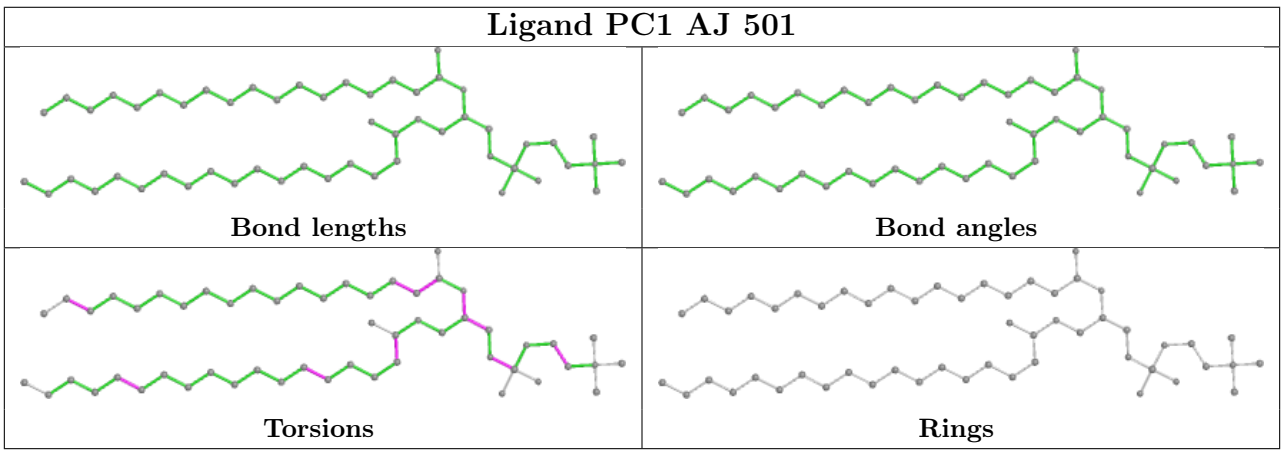
Ligand CDL Ds 401



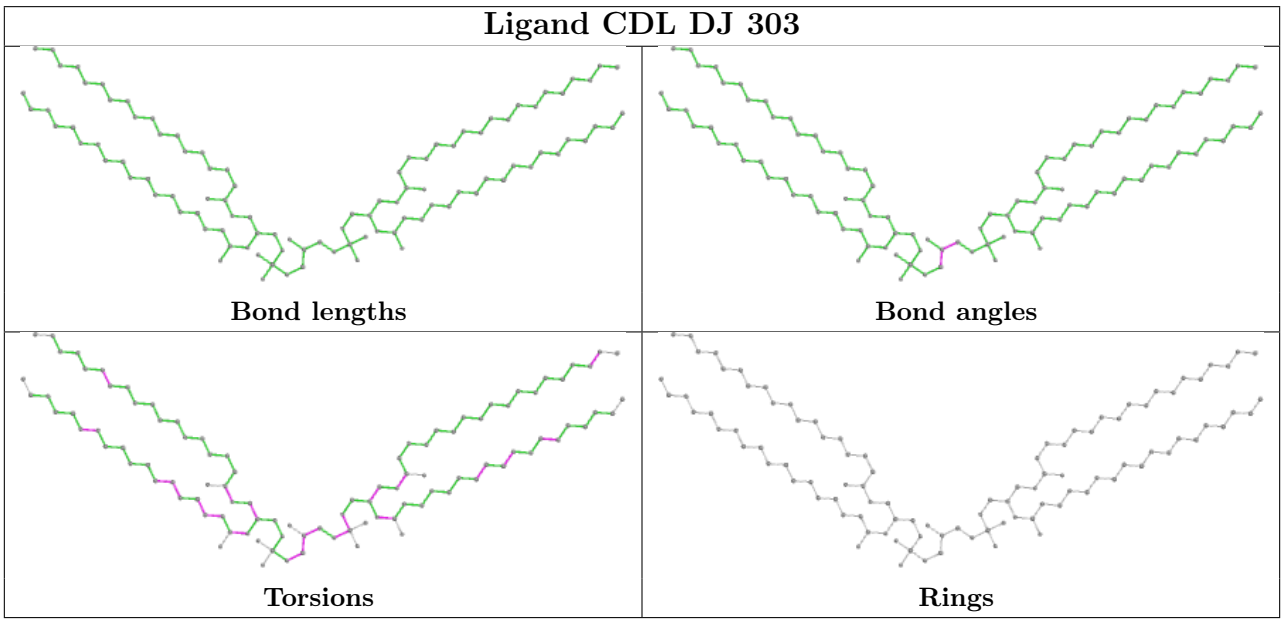
Ligand CDL E 301



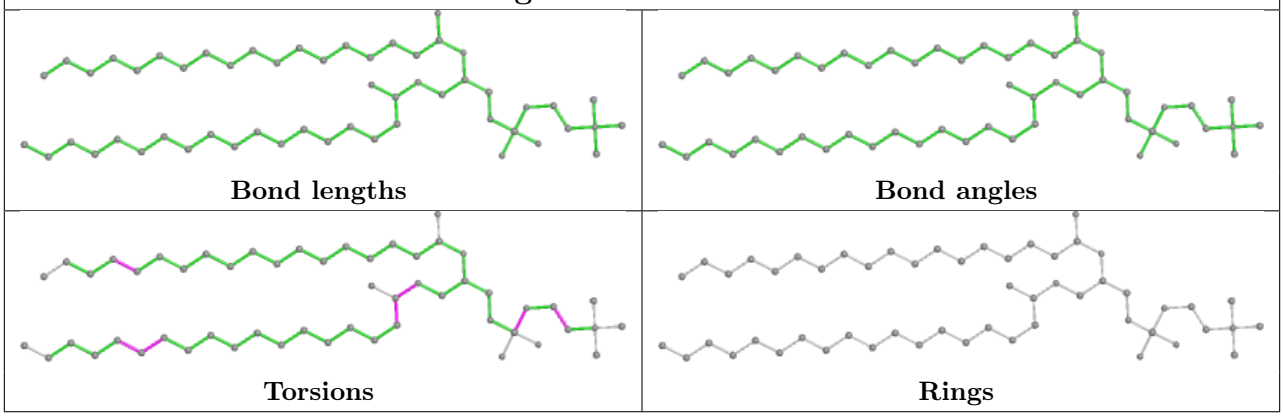
Ligand PC1 AJ 501



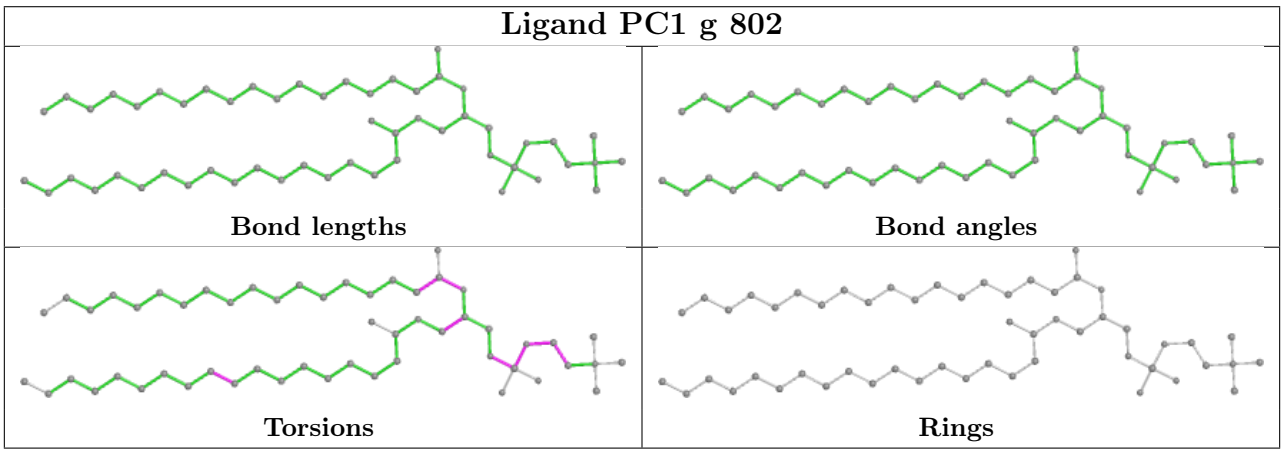
Ligand CDL DJ 303



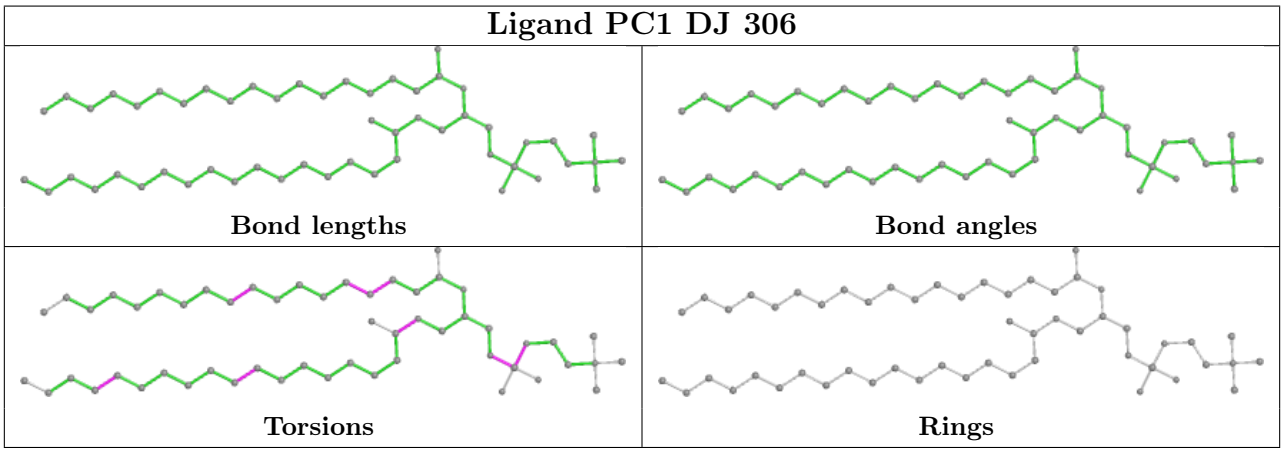
Ligand PC1 DV 405



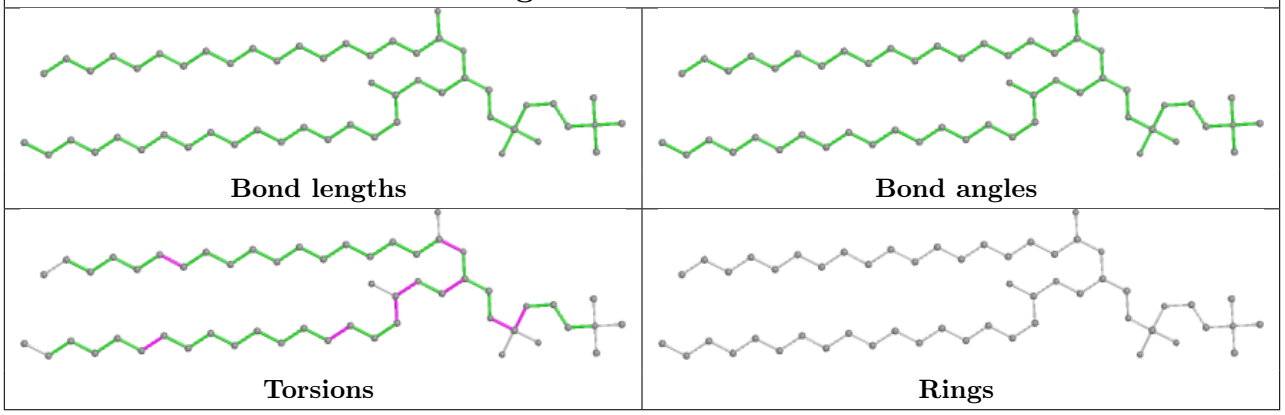
Ligand PC1 g 802



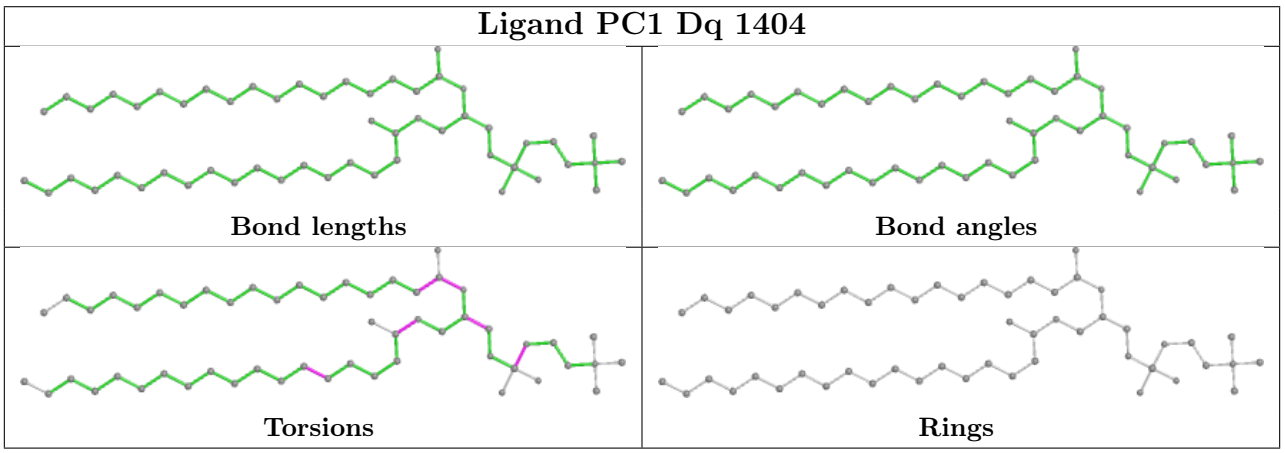
Ligand PC1 DJ 306



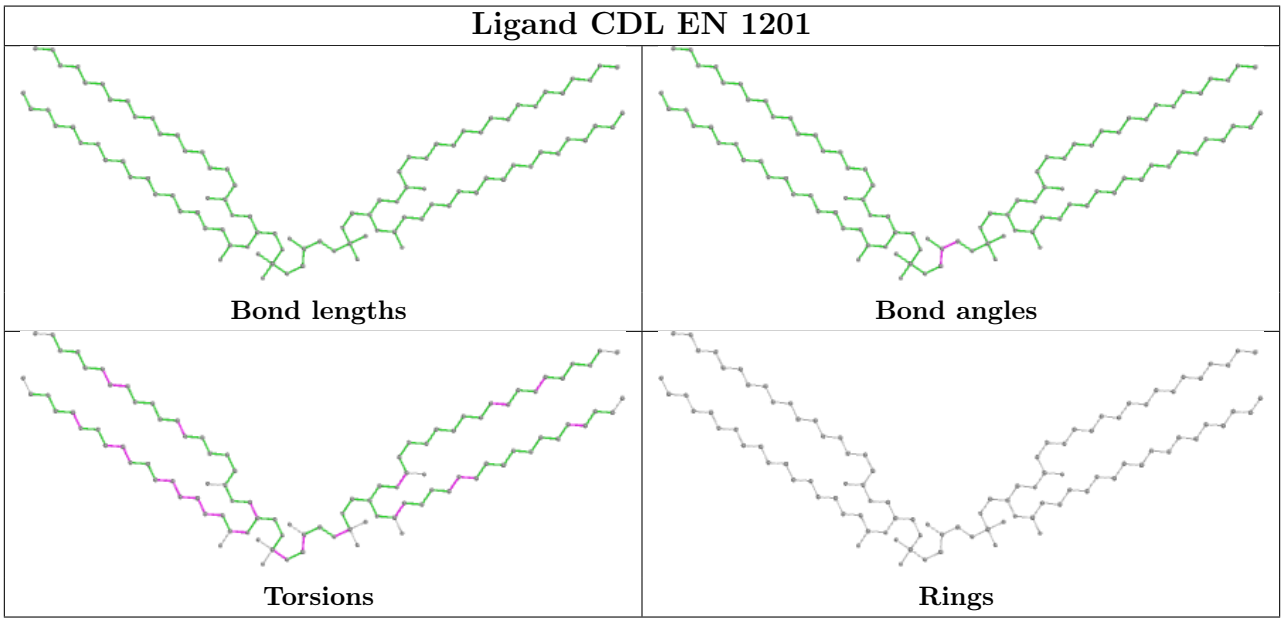
Ligand PC1 BT 203



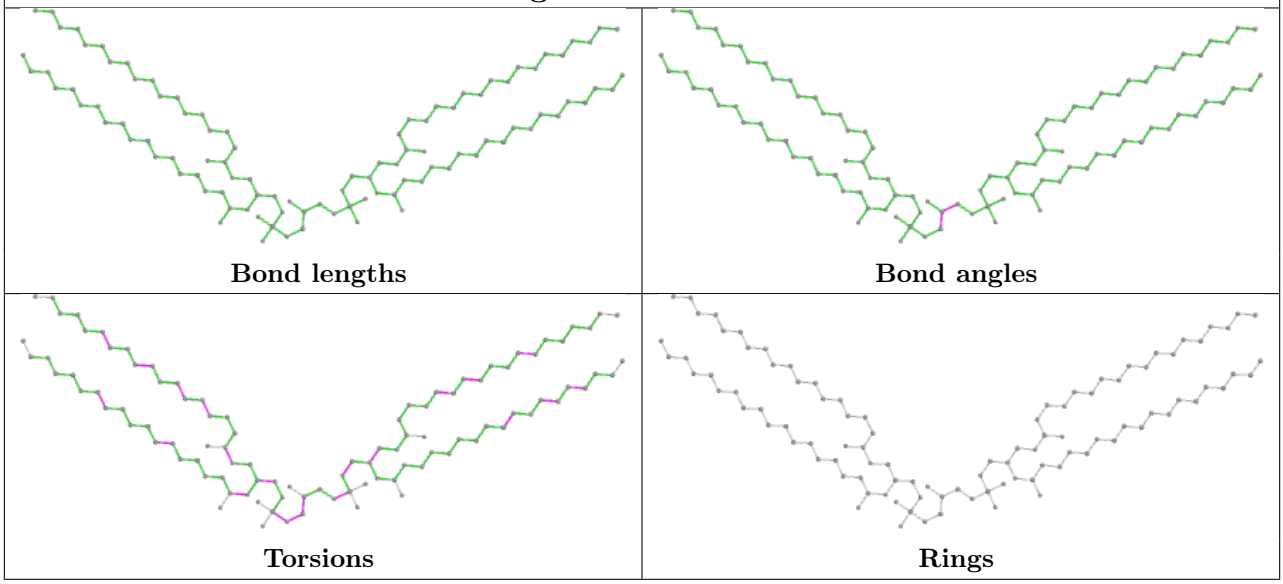
Ligand PC1 Dq 1404



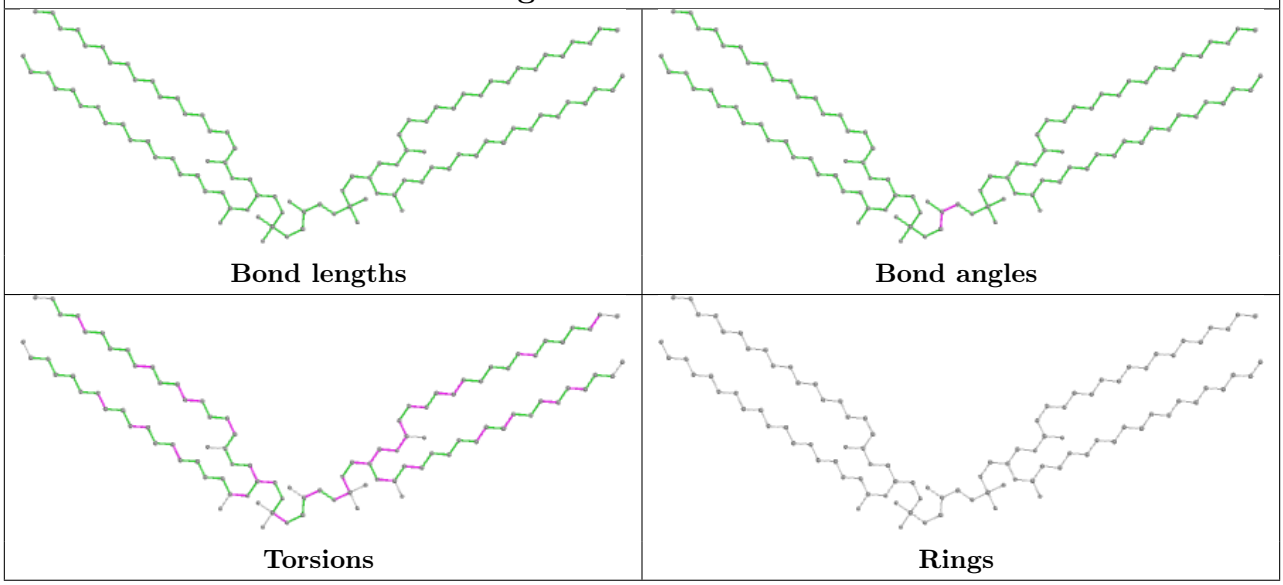
Ligand CDL EN 1201



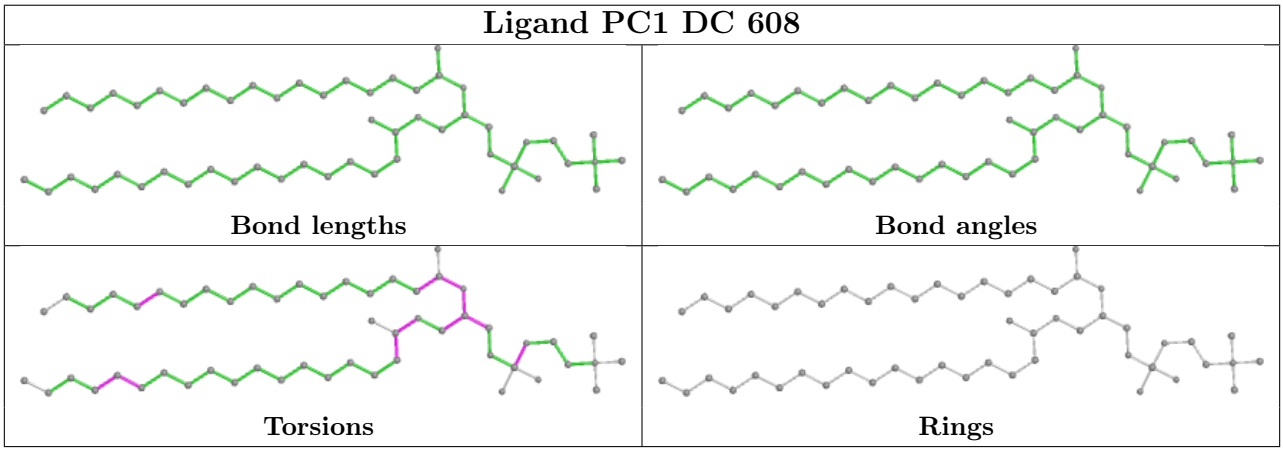
Ligand CDL c 502



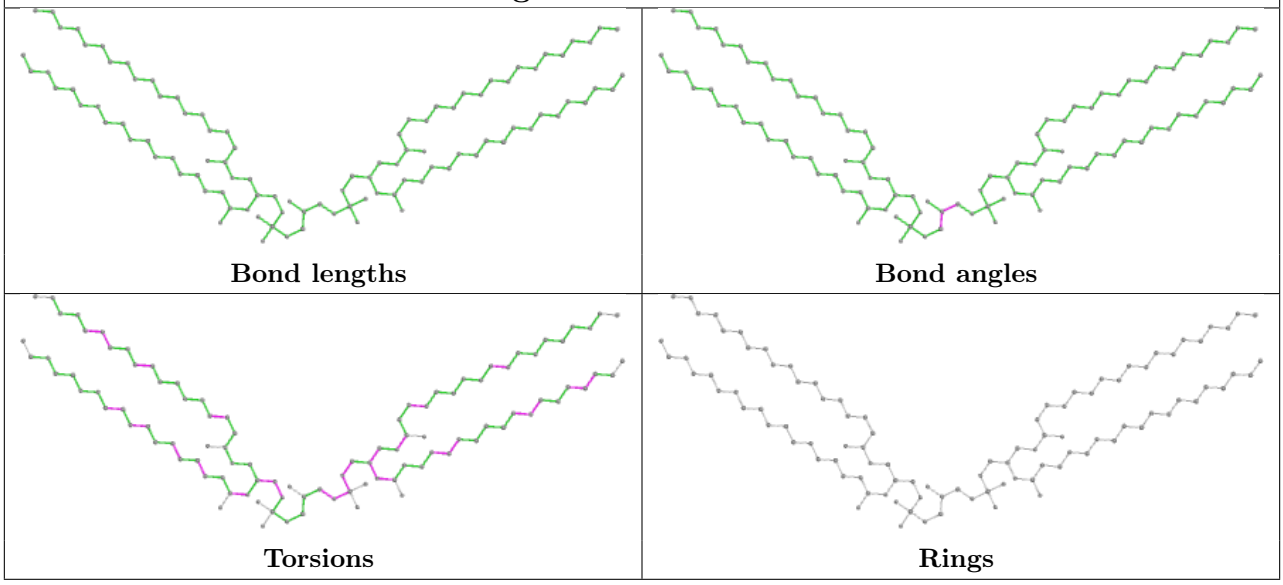
Ligand CDL DI 302



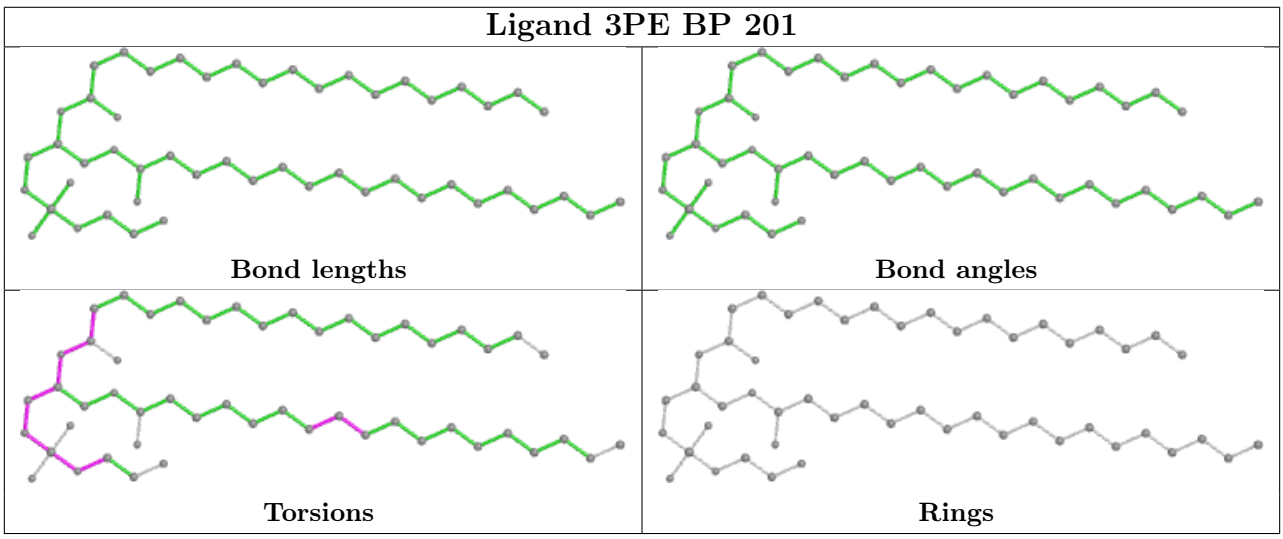
Ligand PC1 DC 608



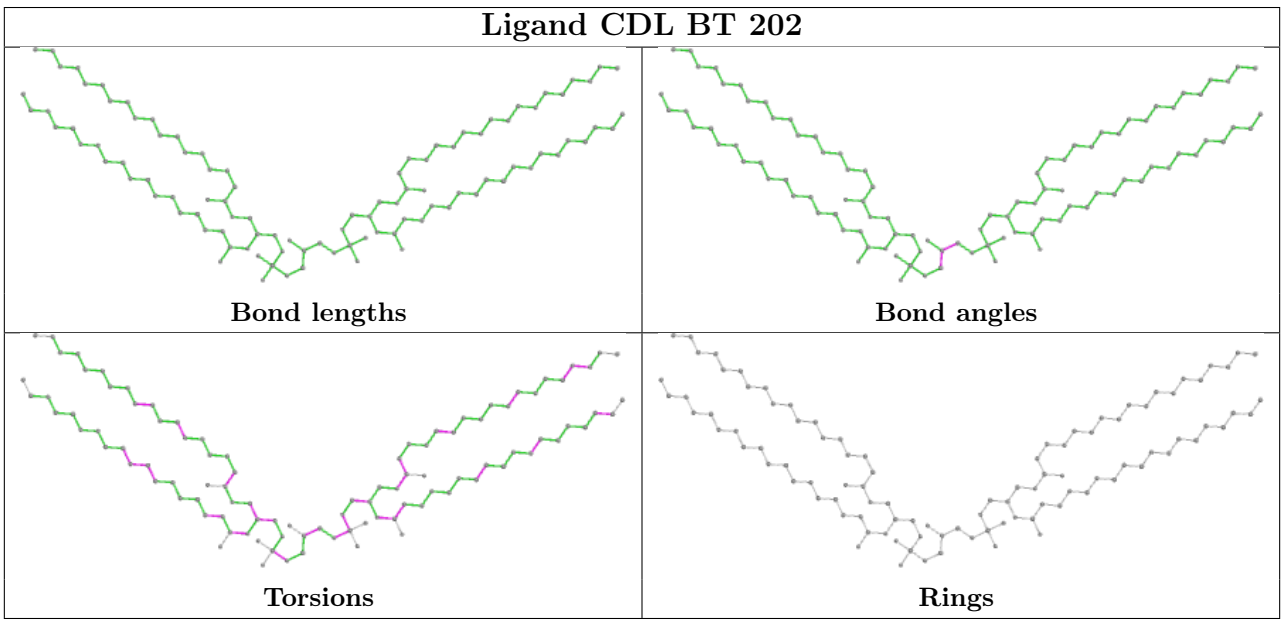
Ligand CDL EO 202



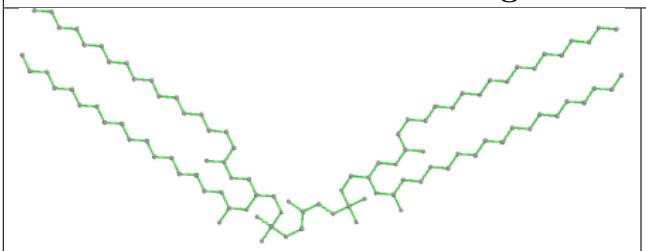
Ligand 3PE BP 201



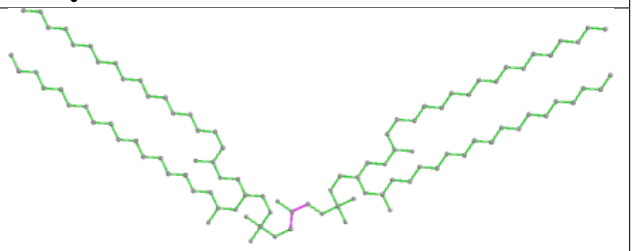
Ligand CDL BT 202



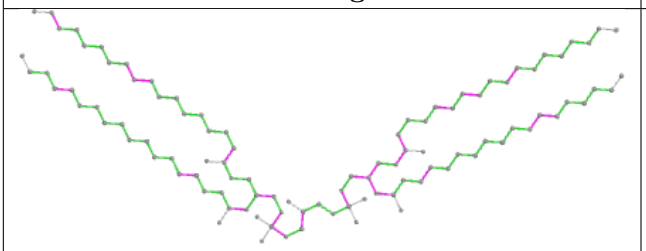
Ligand CDL DQ 1502



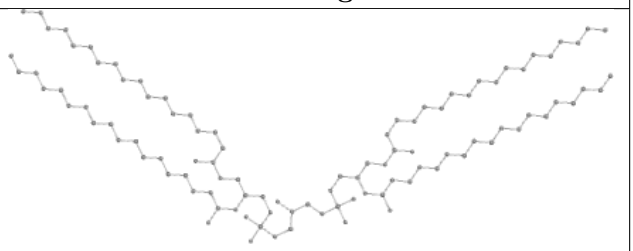
Bond lengths



Bond angles

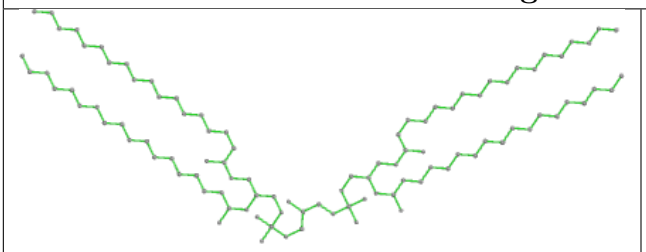


Torsions

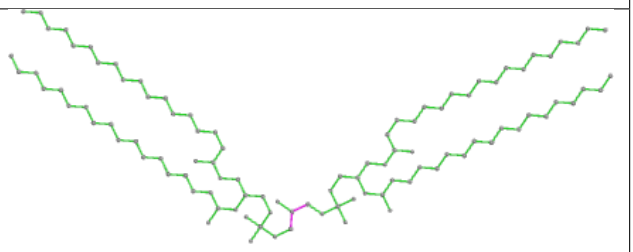


Rings

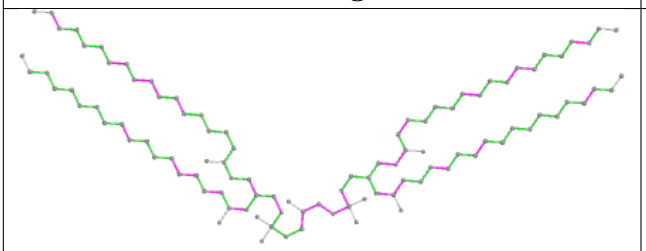
Ligand CDL El 902



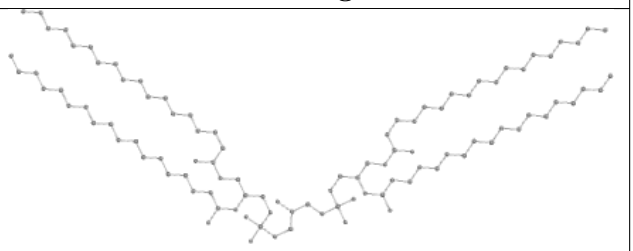
Bond lengths



Bond angles

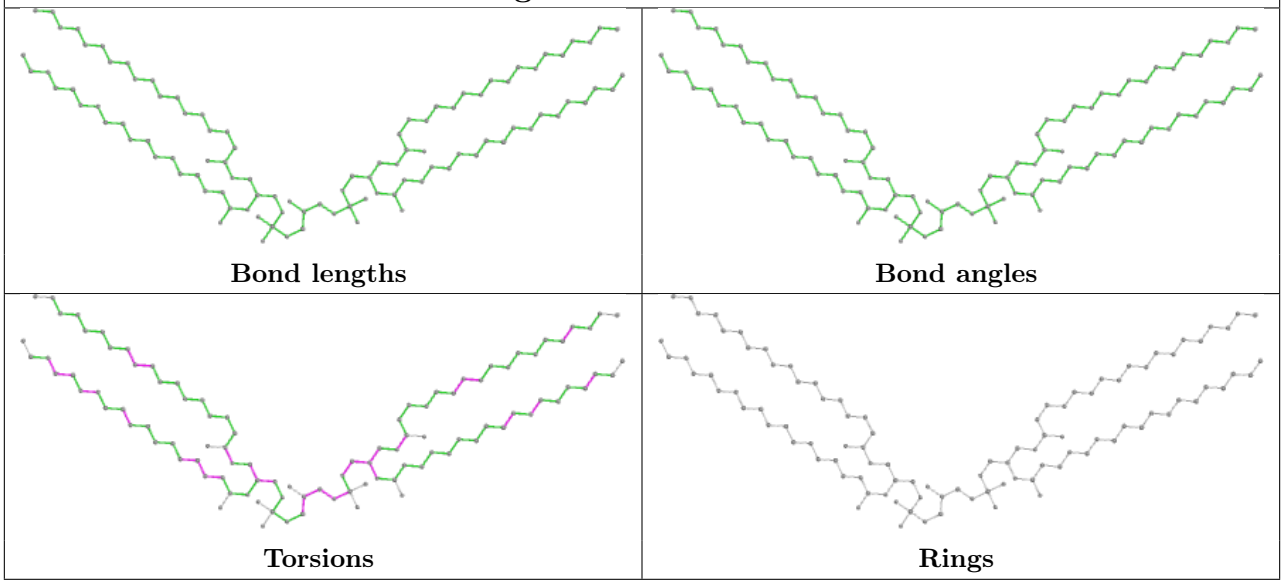


Torsions

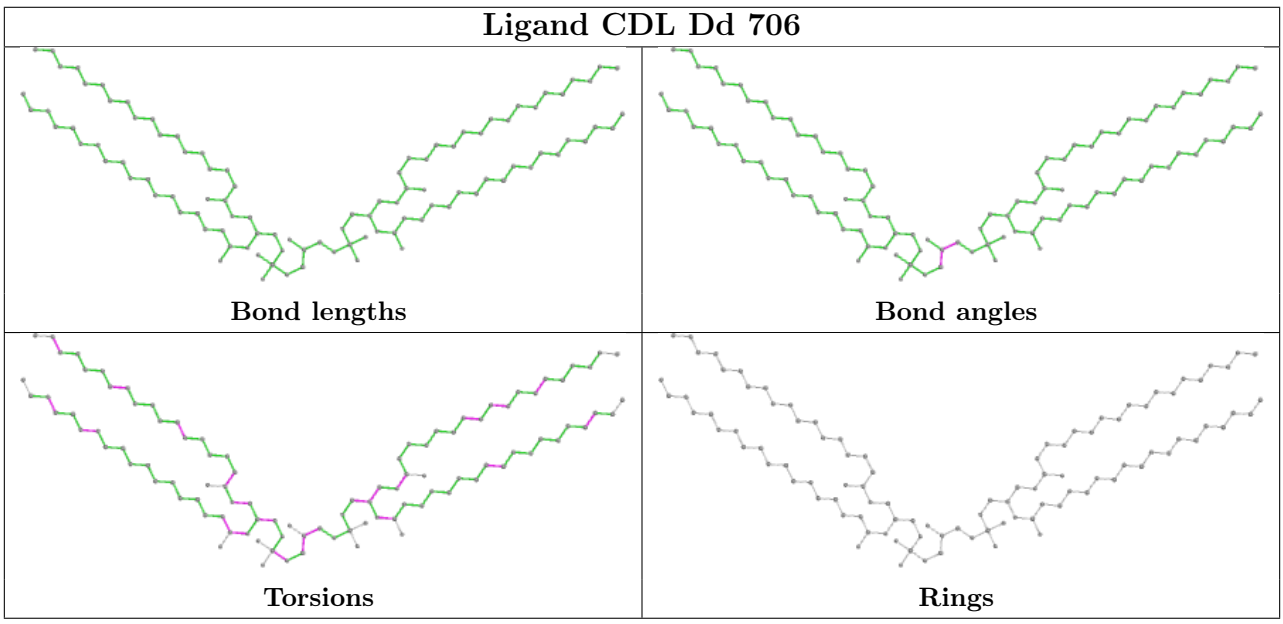


Rings

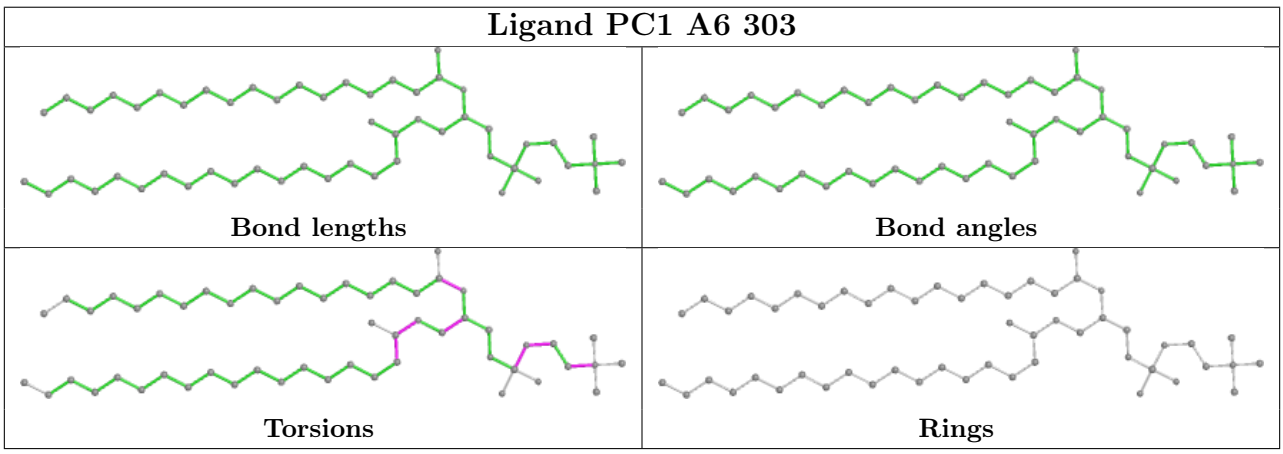
Ligand CDL Dd 704



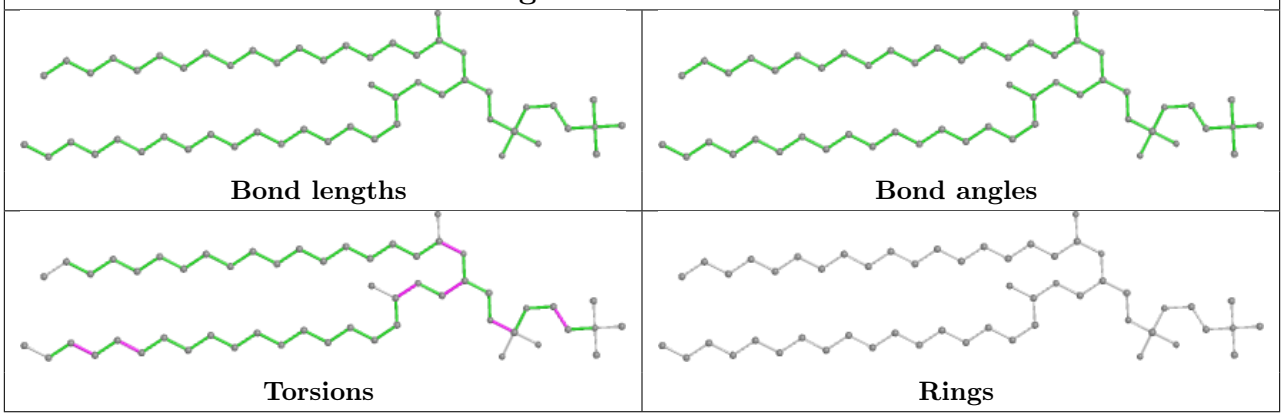
Ligand CDL Dd 706



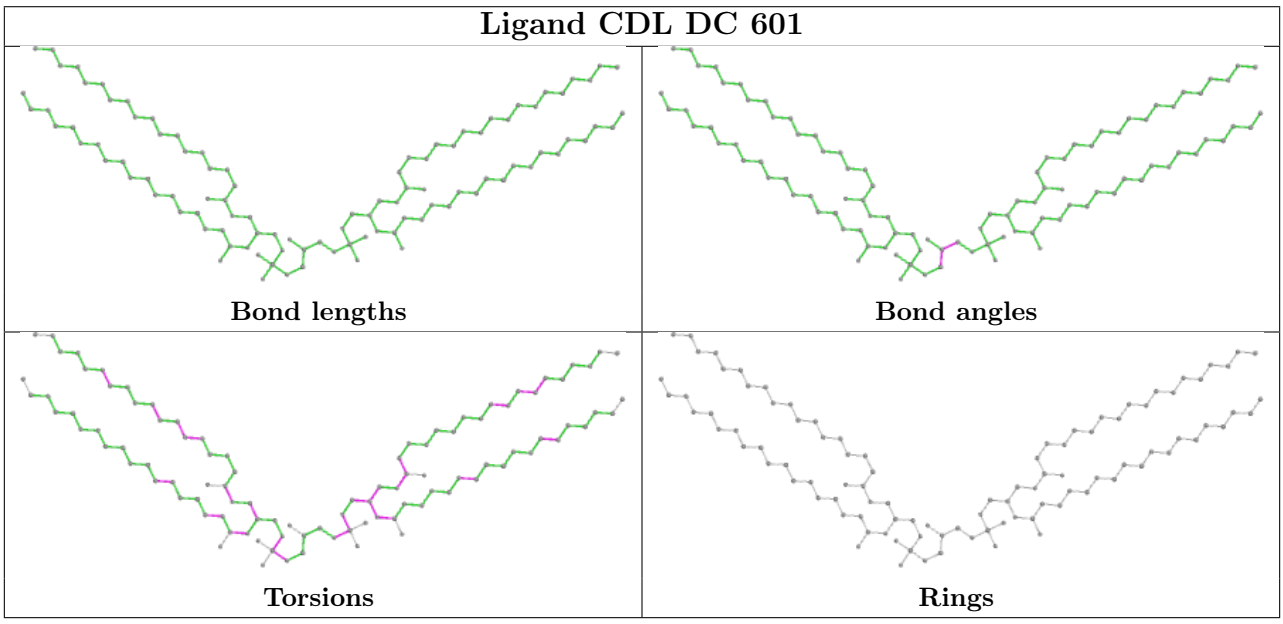
Ligand PC1 A6 303



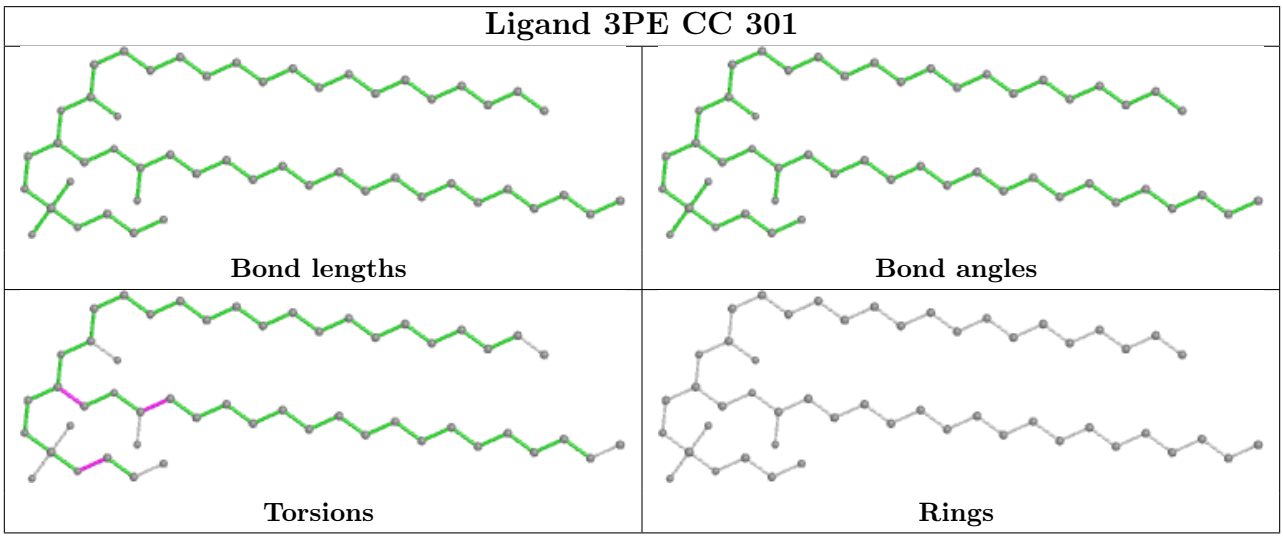
Ligand PC1 Da 707



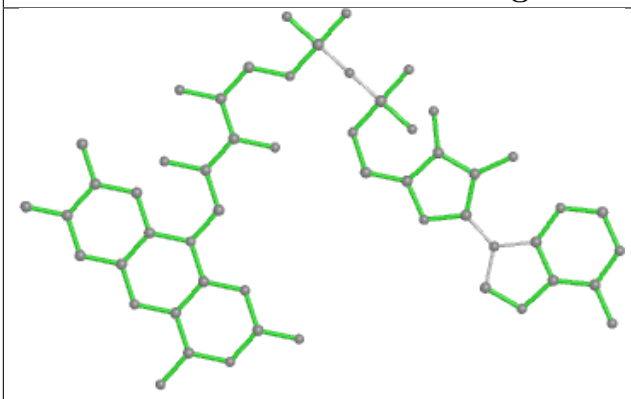
Ligand CDL DC 601



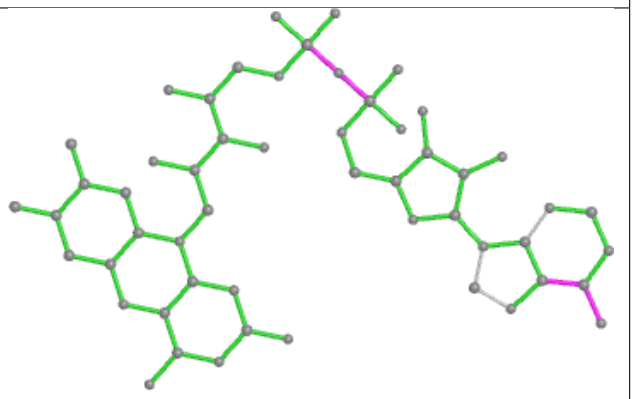
Ligand 3PE CC 301



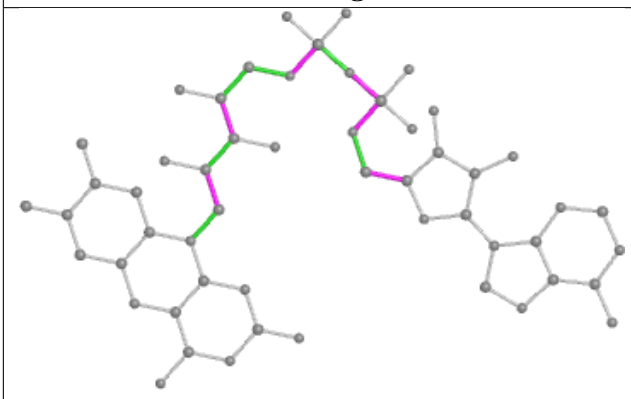
Ligand FAD CA 702



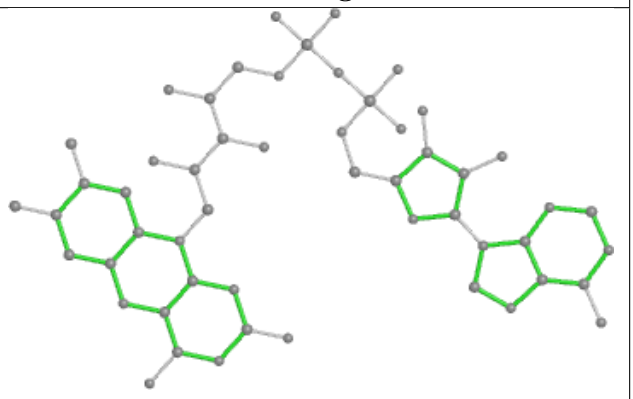
Bond lengths



Bond angles

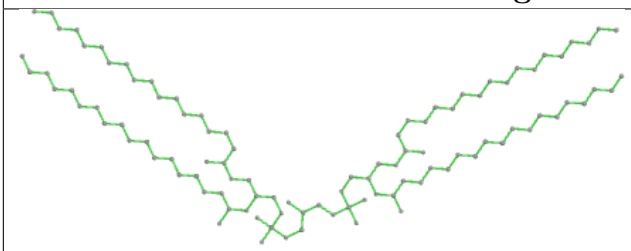


Torsions

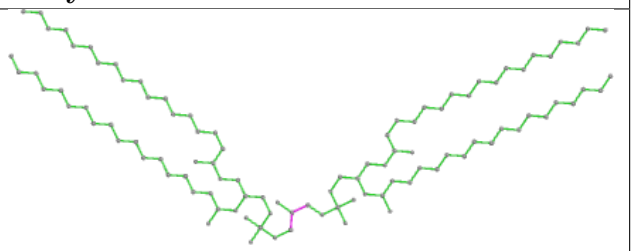


Rings

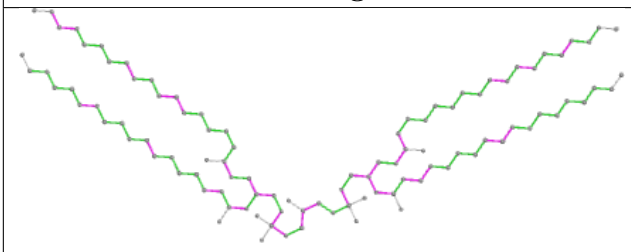
Ligand CDL Dy 301



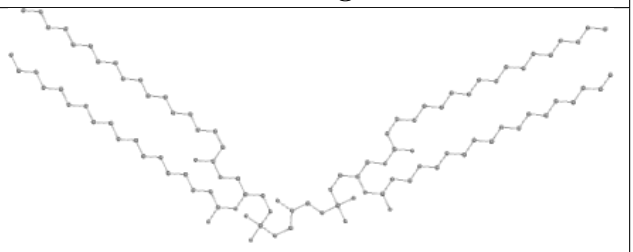
Bond lengths



Bond angles

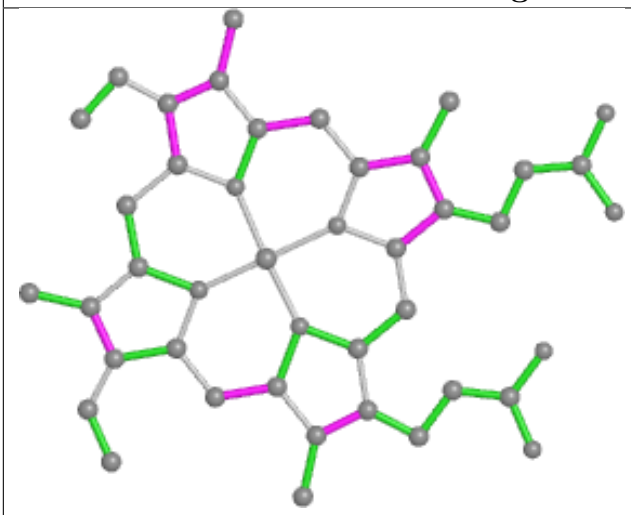


Torsions

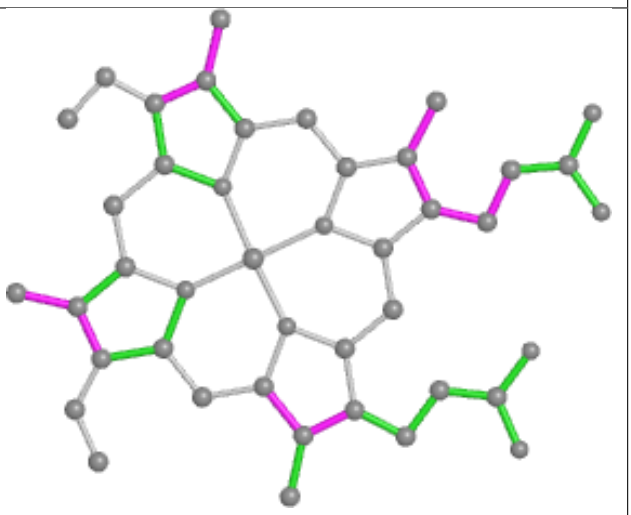


Rings

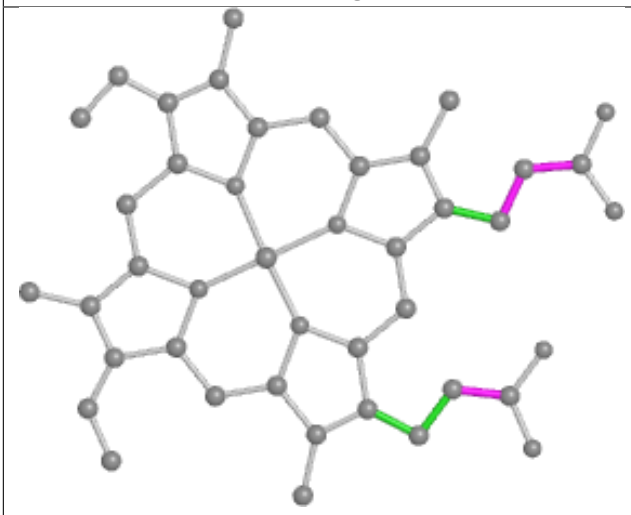
Ligand HEC CE 401



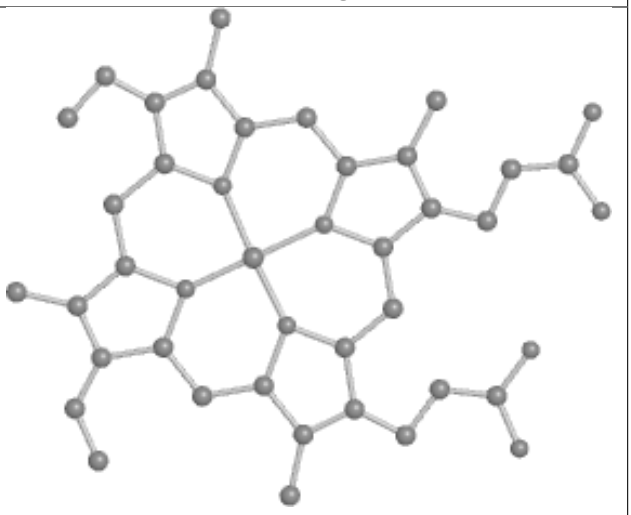
Bond lengths



Bond angles

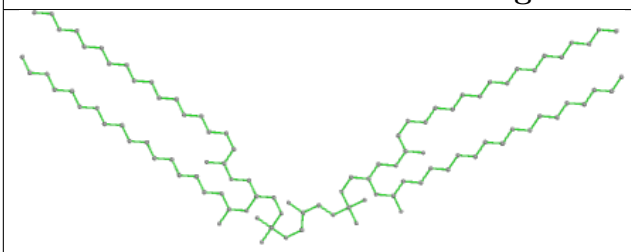


Torsions

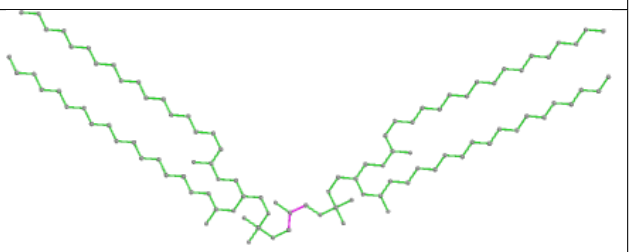


Rings

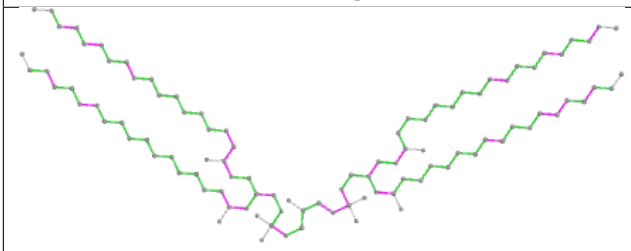
Ligand CDL EL 903



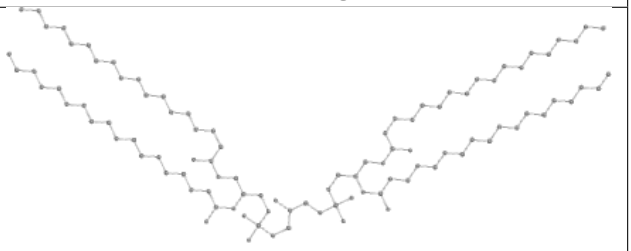
Bond lengths



Bond angles

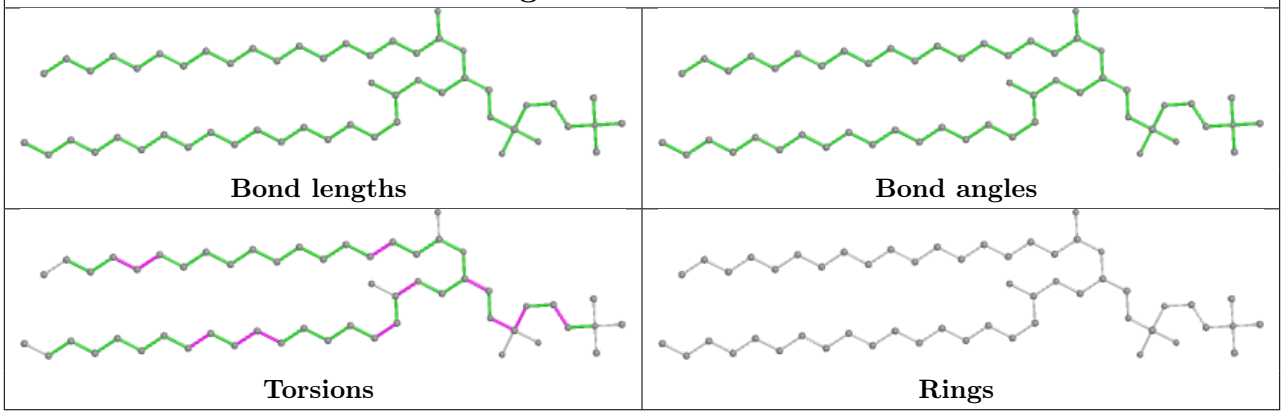


Torsions

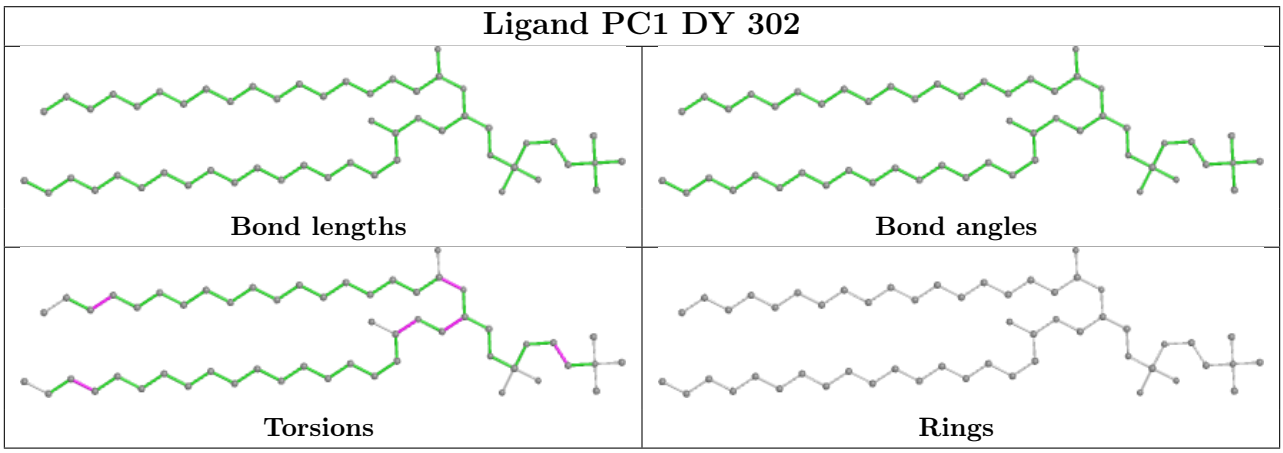


Rings

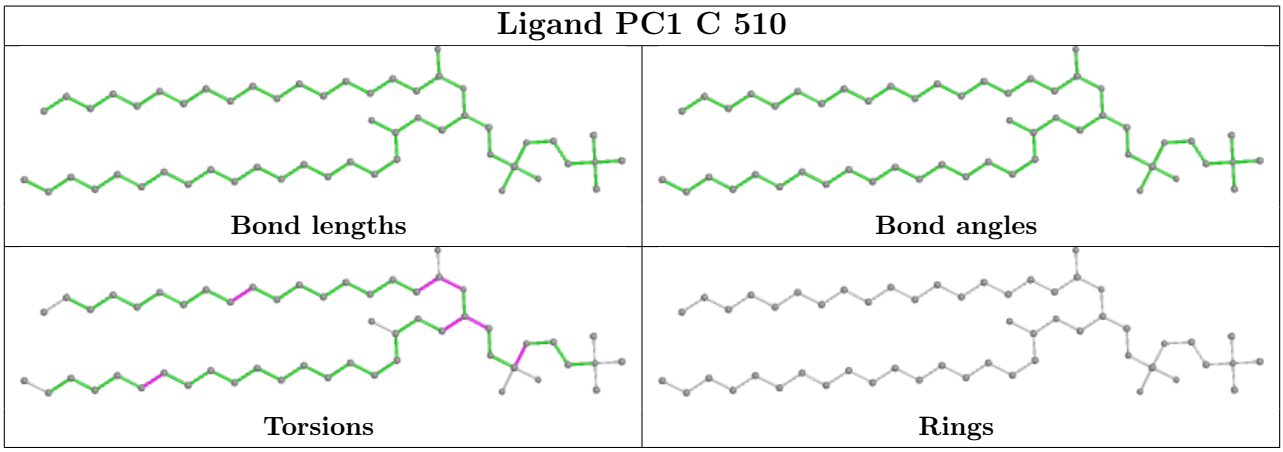
Ligand PC1 B1 403



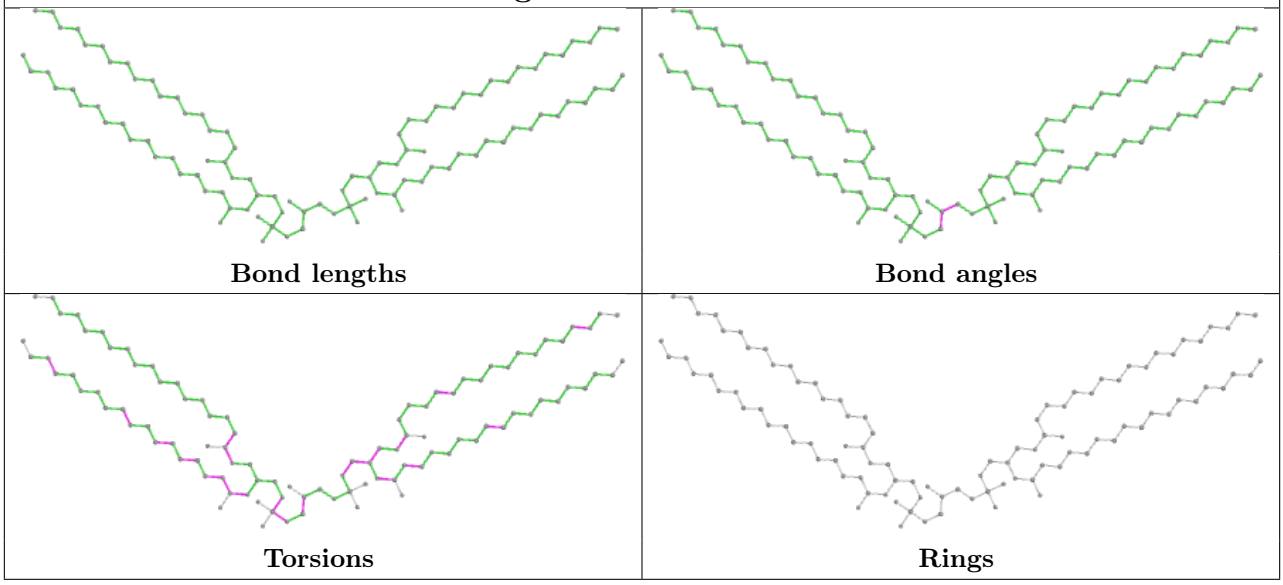
Ligand PC1 DY 302



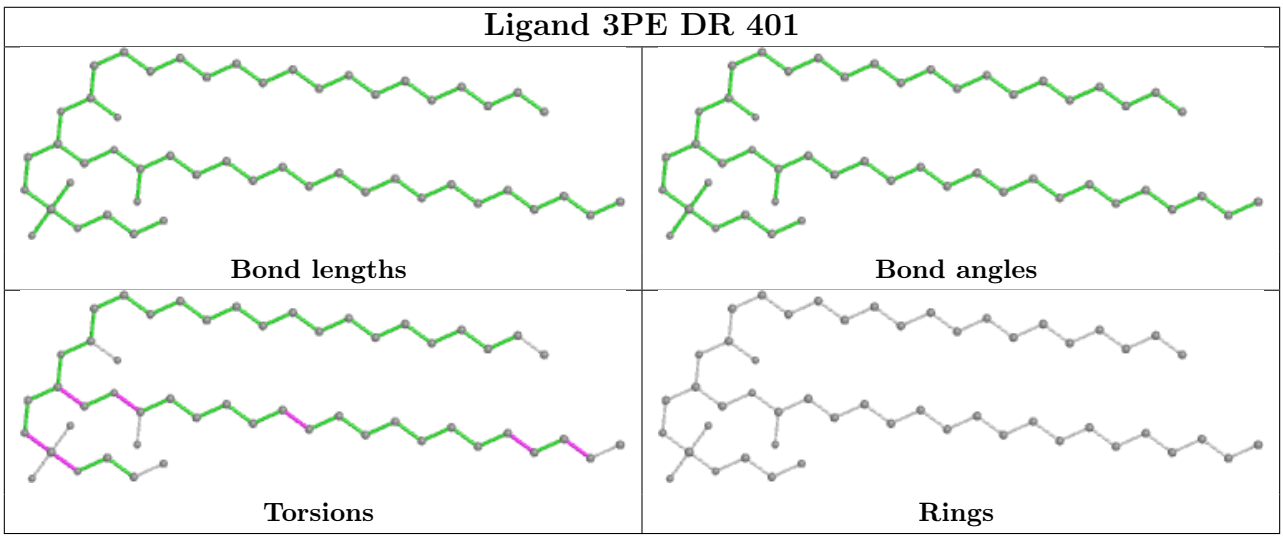
Ligand PC1 C 510



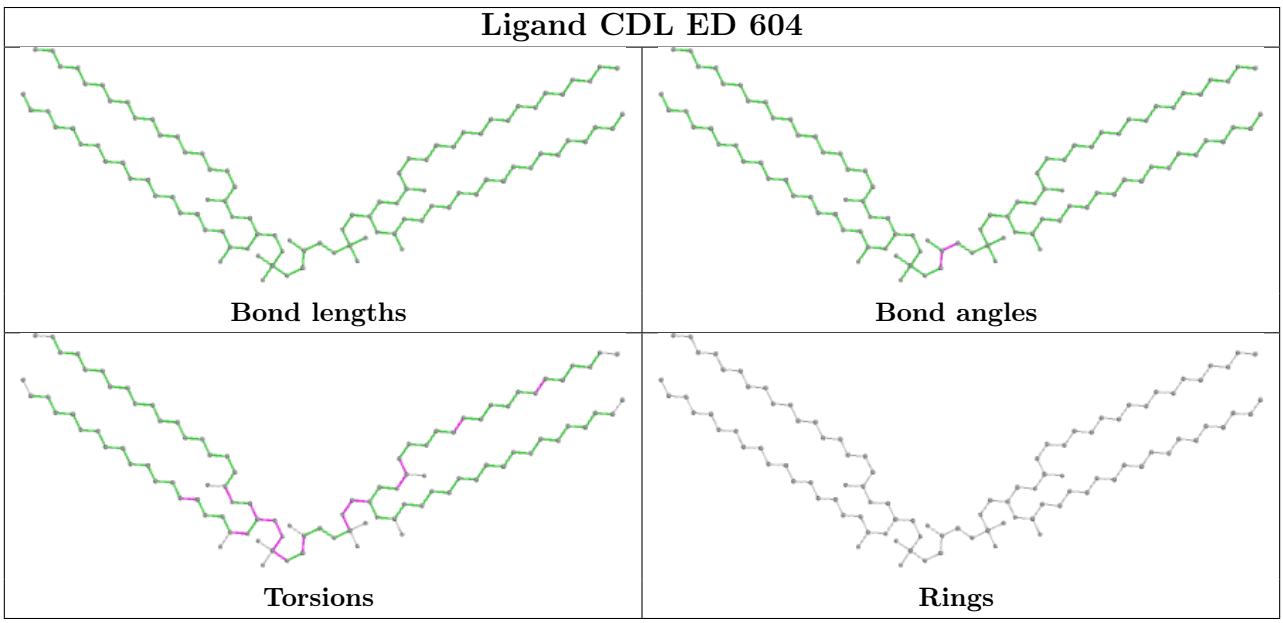
Ligand CDL Dn 503



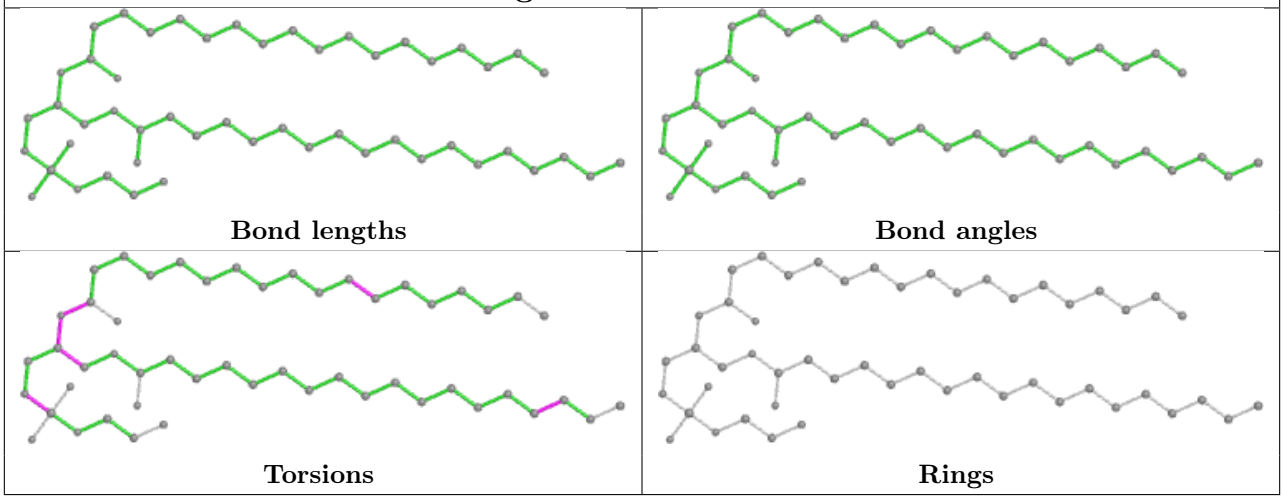
Ligand 3PE DR 401



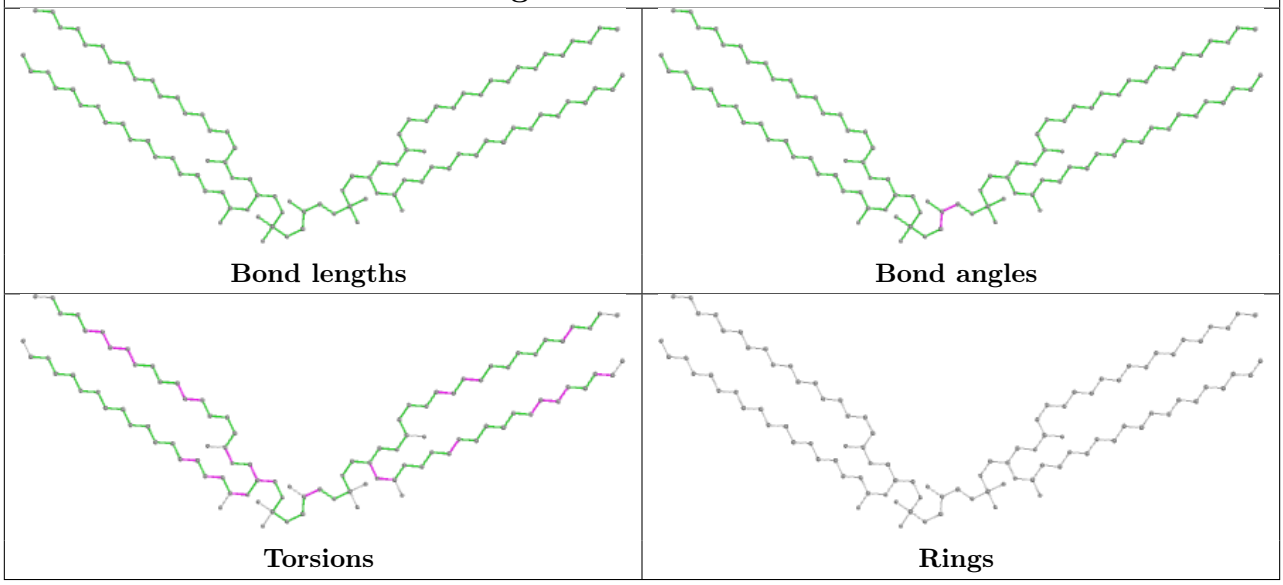
Ligand CDL ED 604



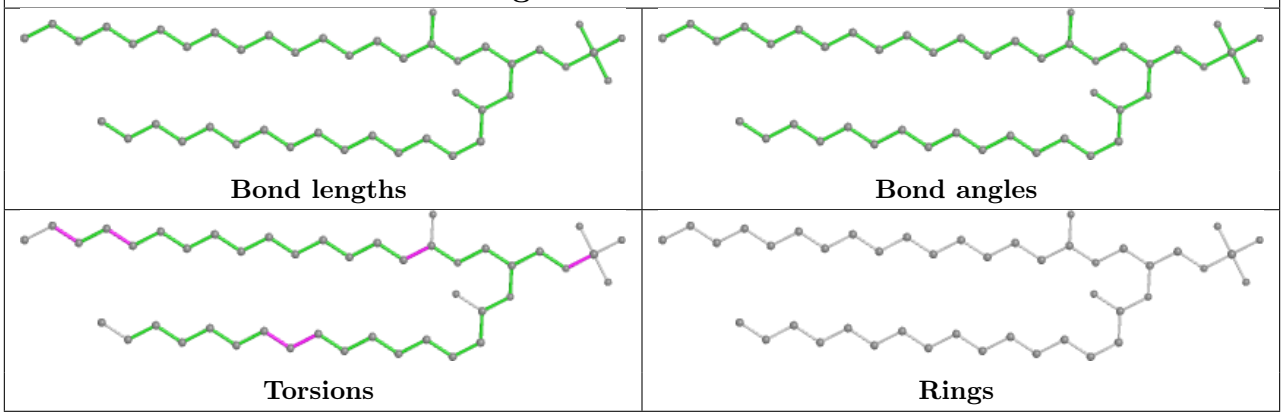
Ligand 3PE DC 606



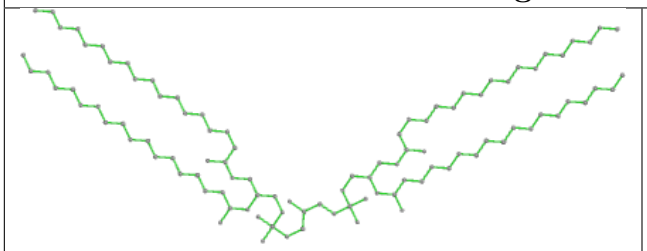
Ligand CDL AA 908



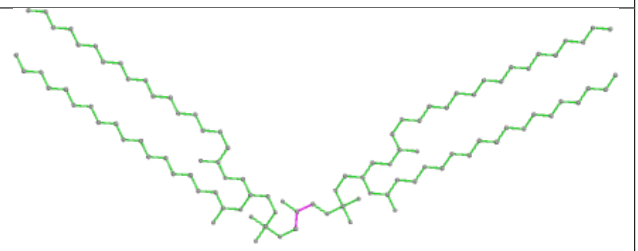
Ligand LPP Dl 1101



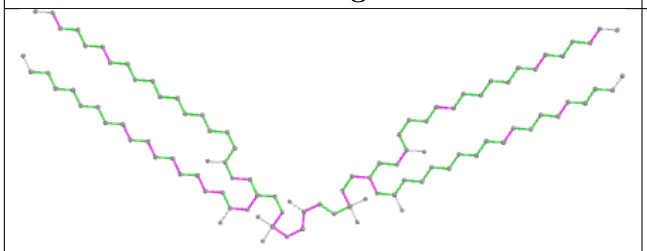
Ligand CDL Du 403



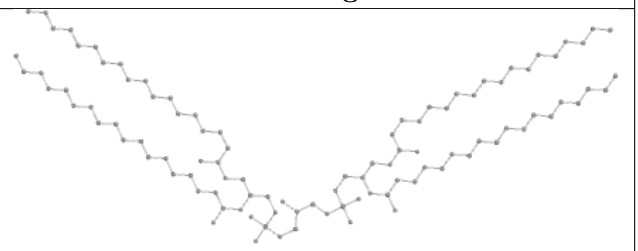
Bond lengths



Bond angles

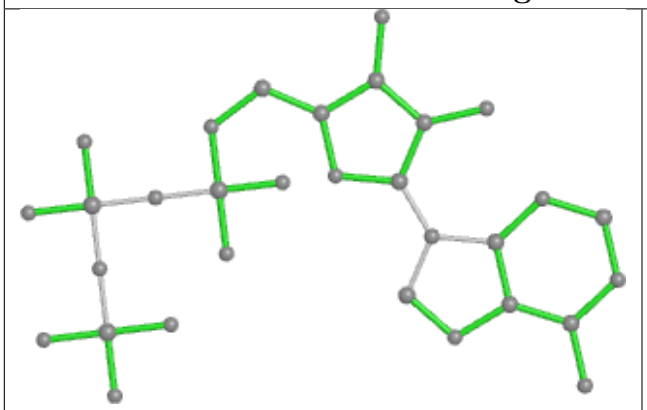


Torsions

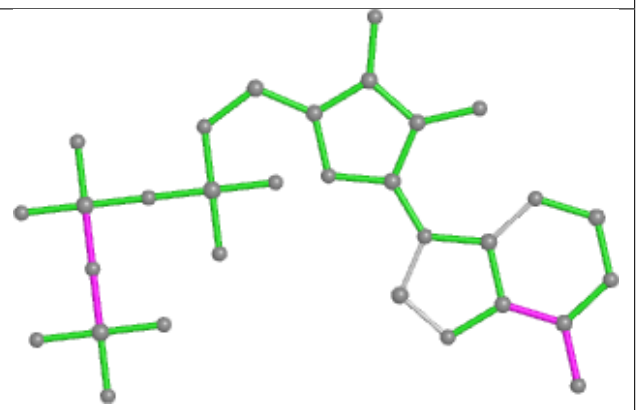


Rings

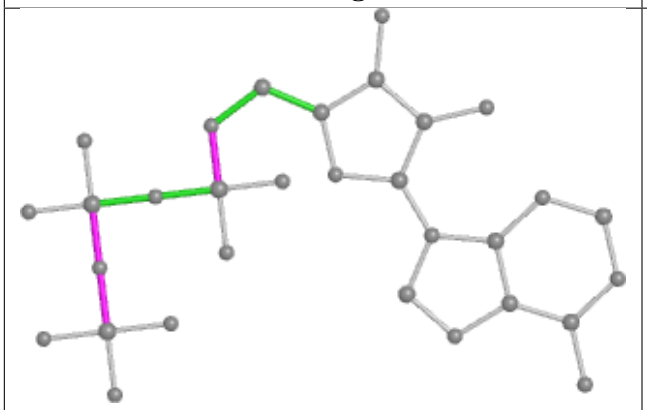
Ligand ATP ER 201



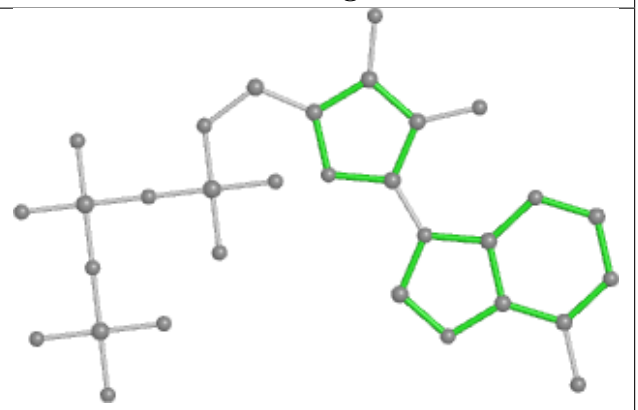
Bond lengths



Bond angles

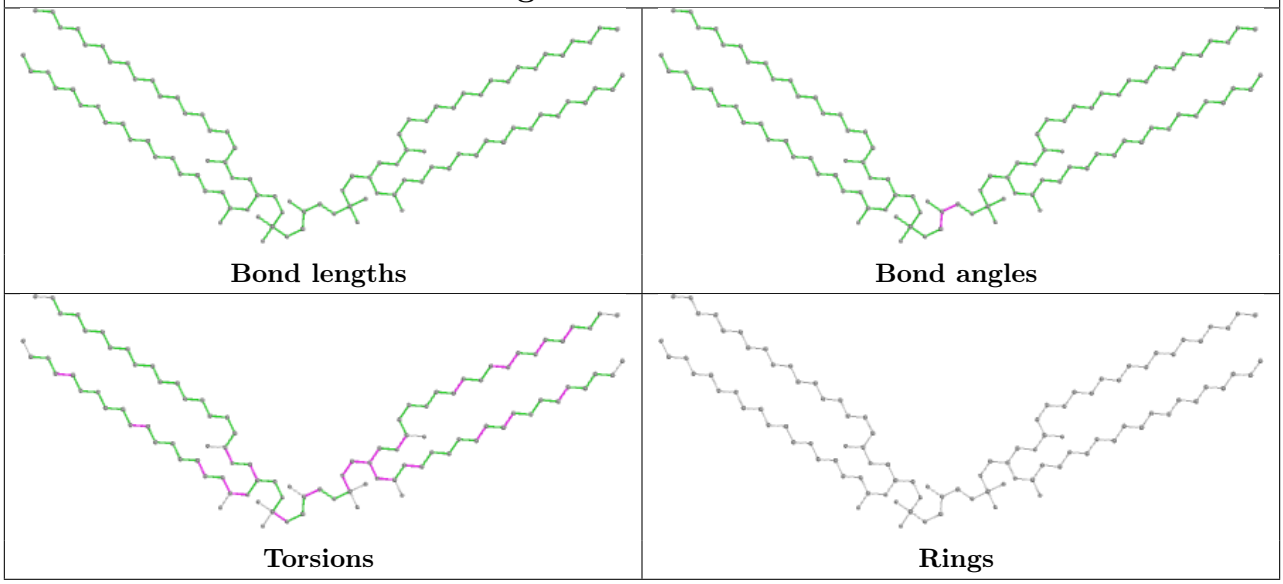


Torsions

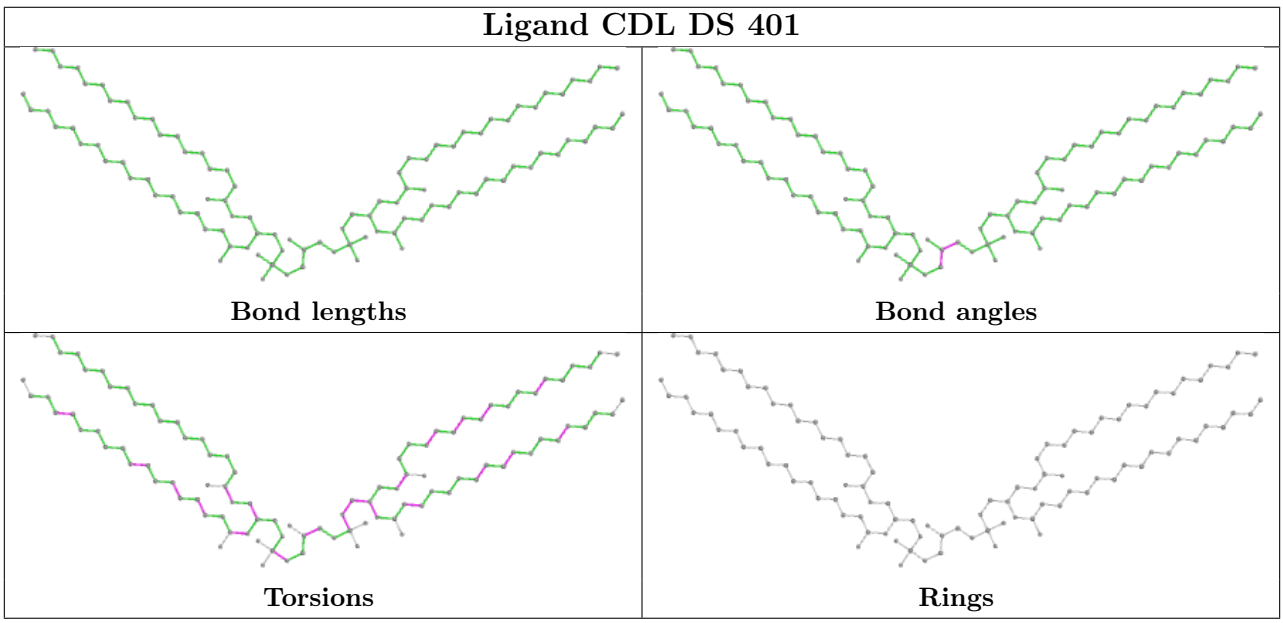


Rings

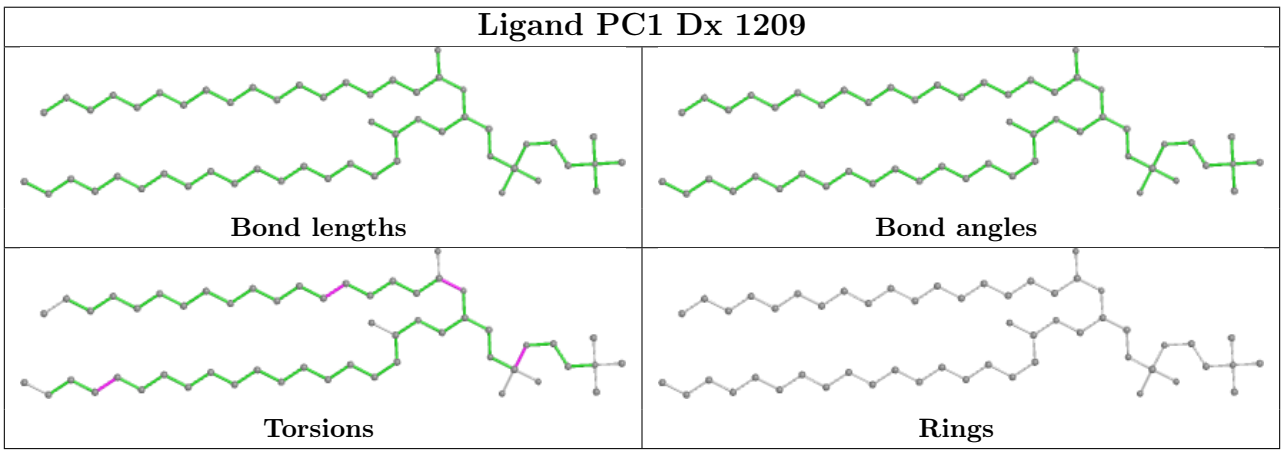
Ligand CDL Ds 402



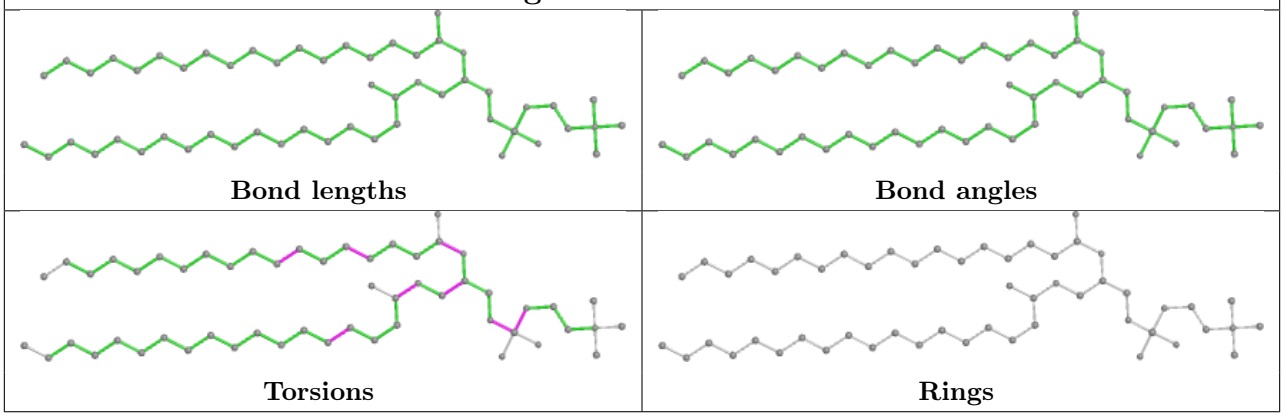
Ligand CDL DS 401



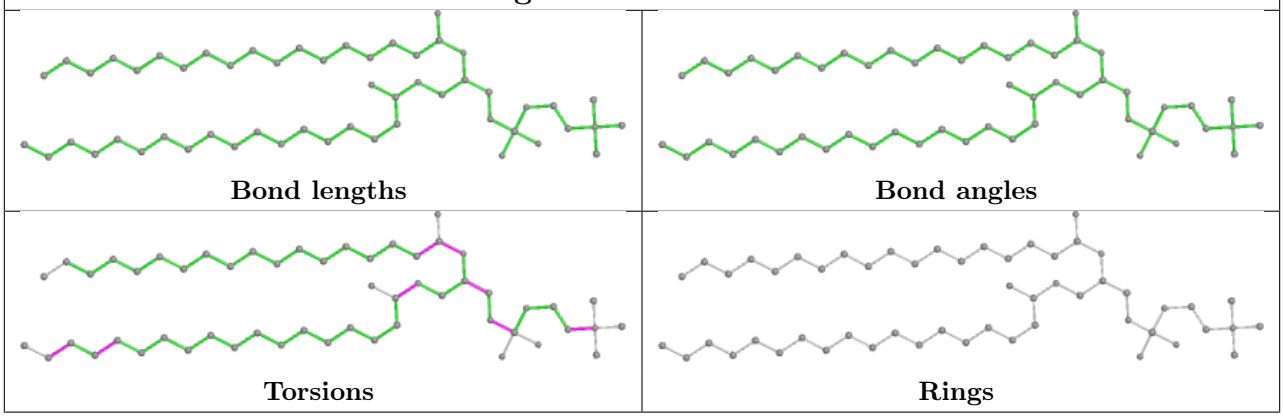
Ligand PC1 Dx 1209



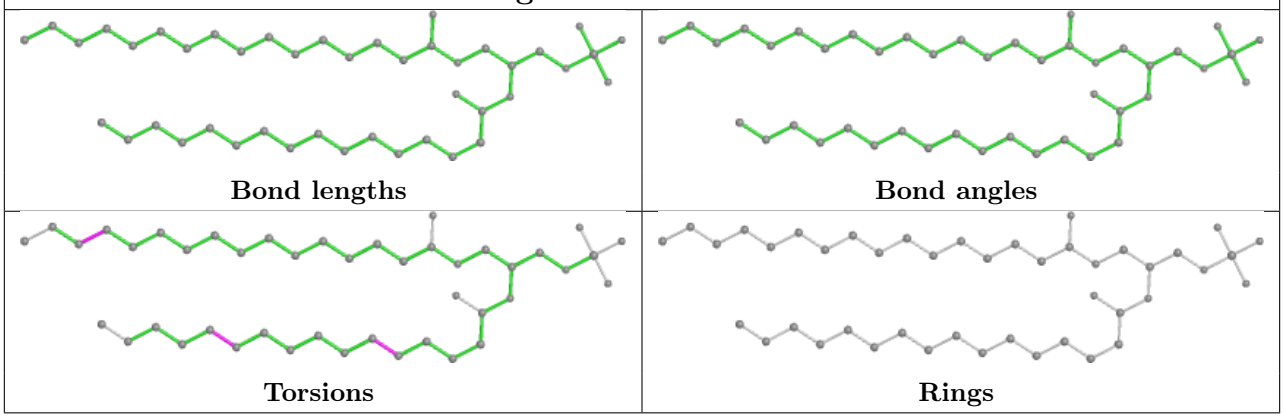
Ligand PC1 Ef 501



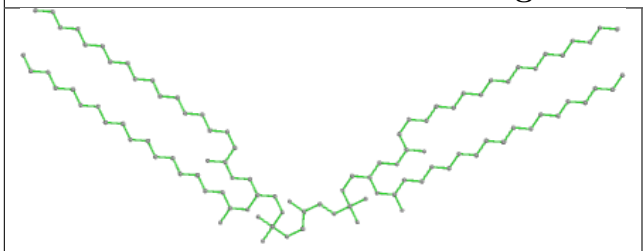
Ligand PC1 AA 904



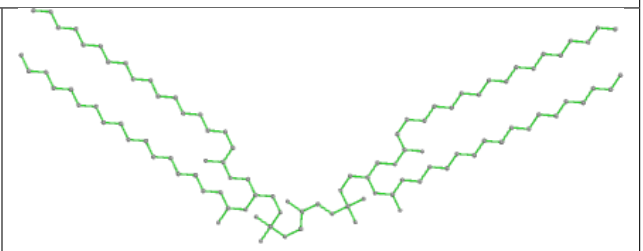
Ligand LPP AL 304



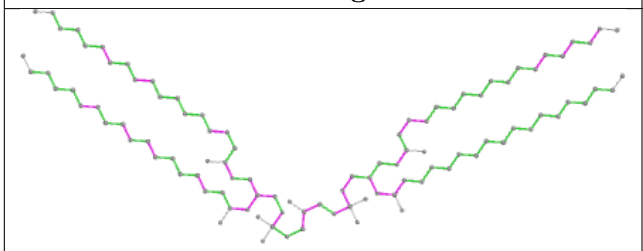
Ligand CDL A1 402



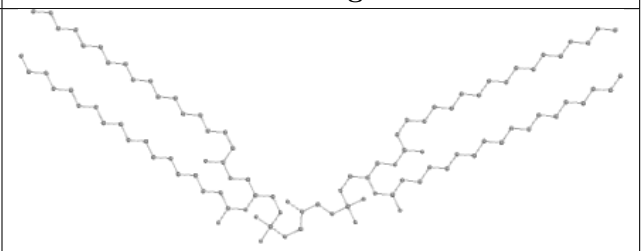
Bond lengths



Bond angles

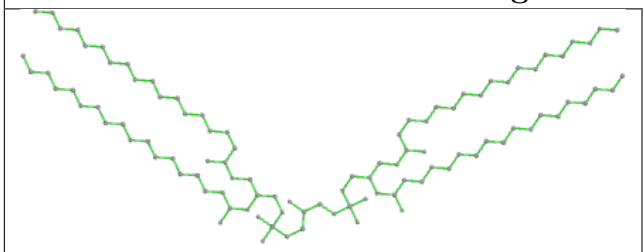


Torsions

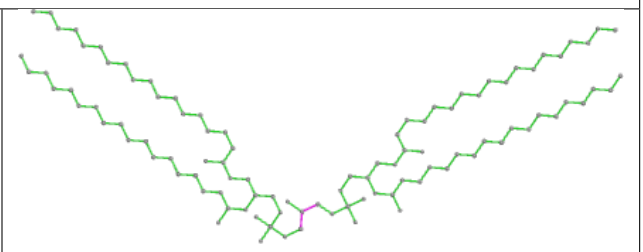


Rings

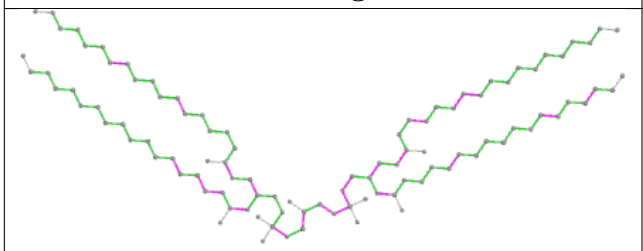
Ligand CDL BG 201



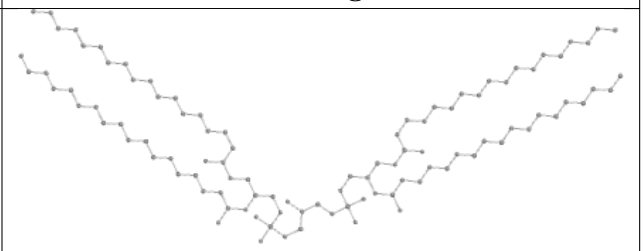
Bond lengths



Bond angles

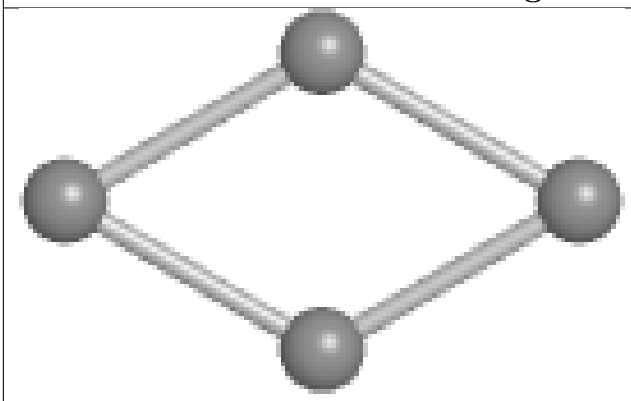


Torsions

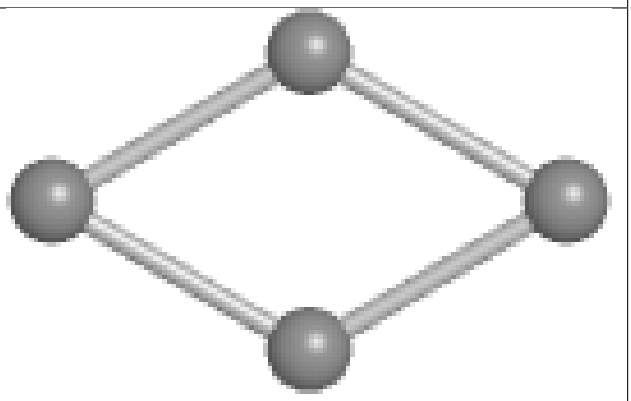


Rings

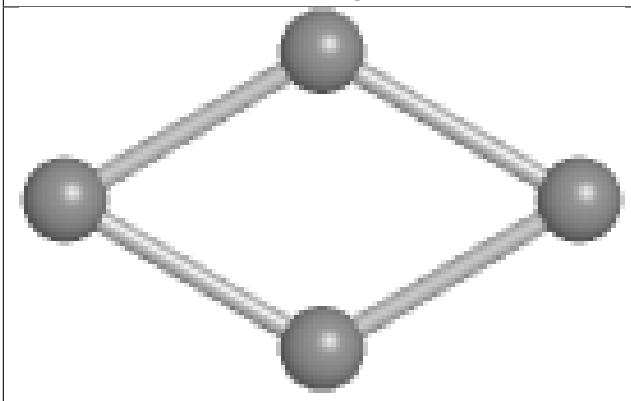
Ligand FES Ef 502



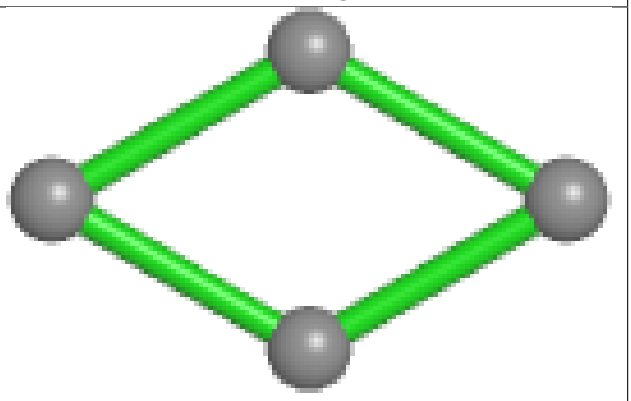
Bond lengths



Bond angles

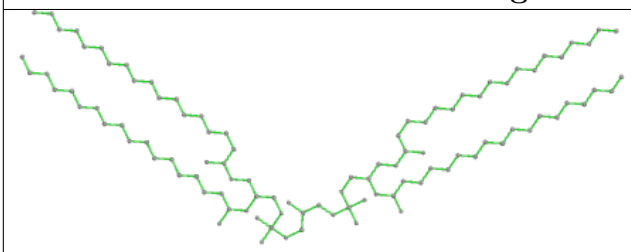


Torsions

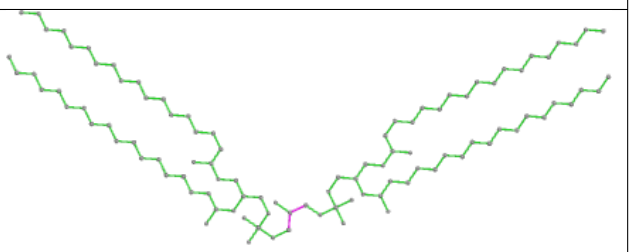


Rings

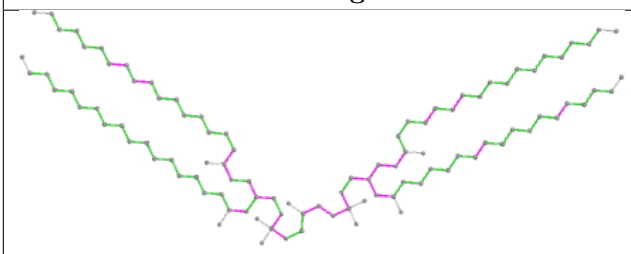
Ligand CDL CD 301



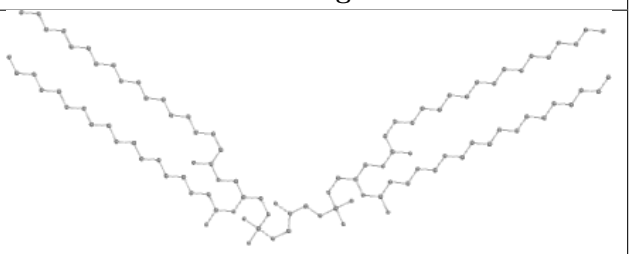
Bond lengths



Bond angles

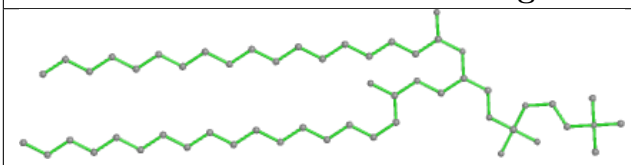
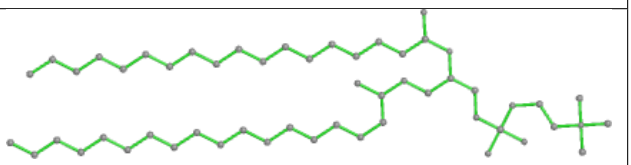
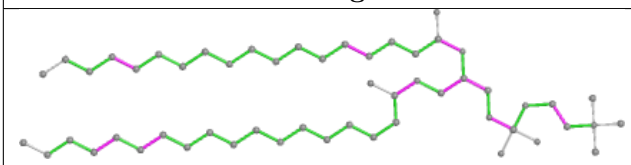
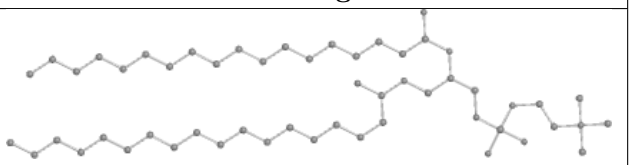


Torsions

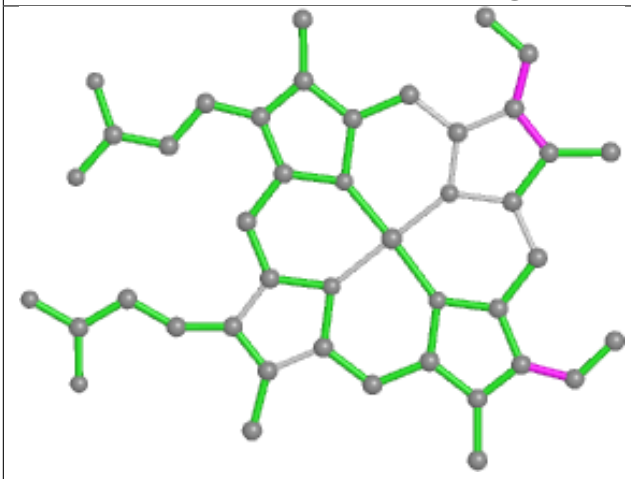


Rings

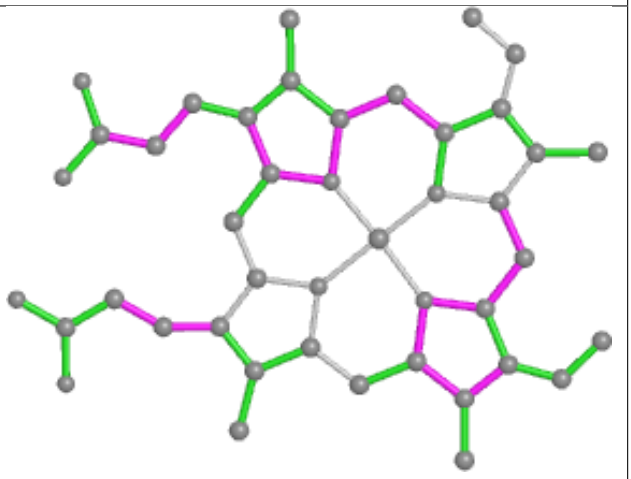
Ligand CUA DB 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 A9 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

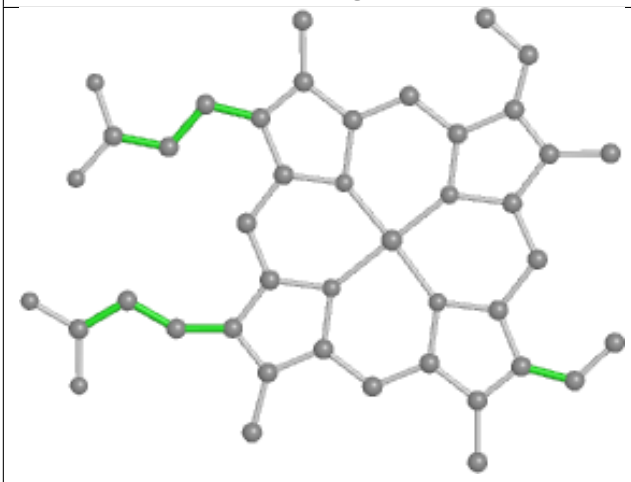
Ligand HEM ED 602



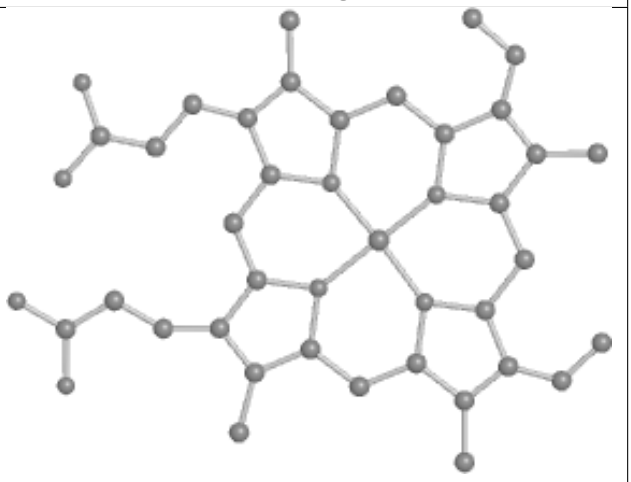
Bond lengths



Bond angles

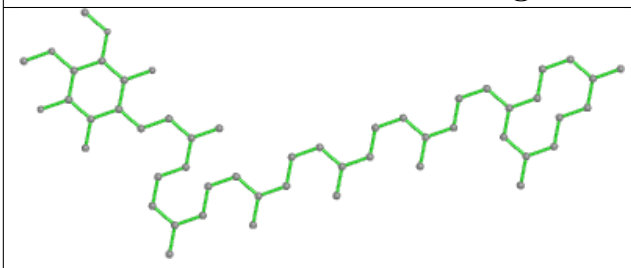


Torsions

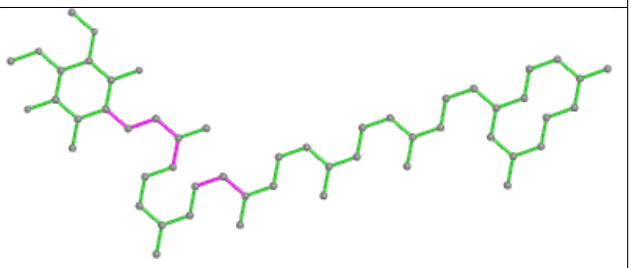


Rings

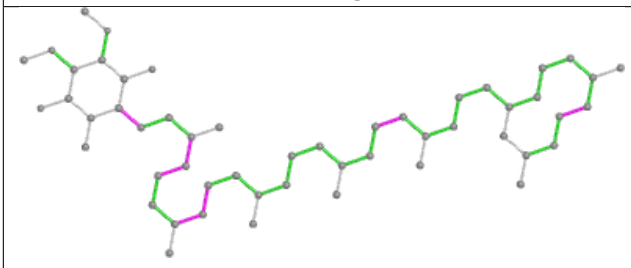
Ligand UQ8 CC 303



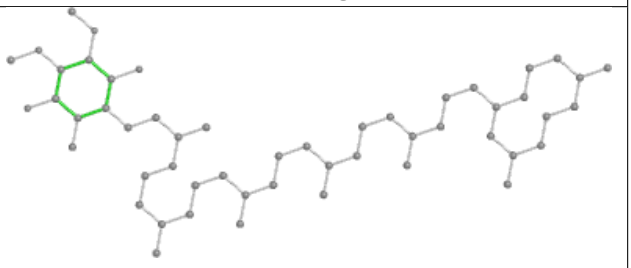
Bond lengths



Bond angles

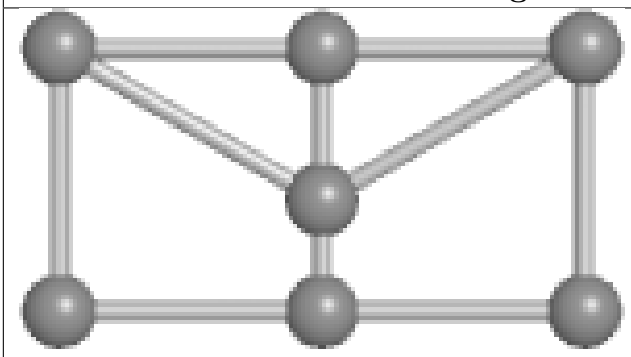


Torsions

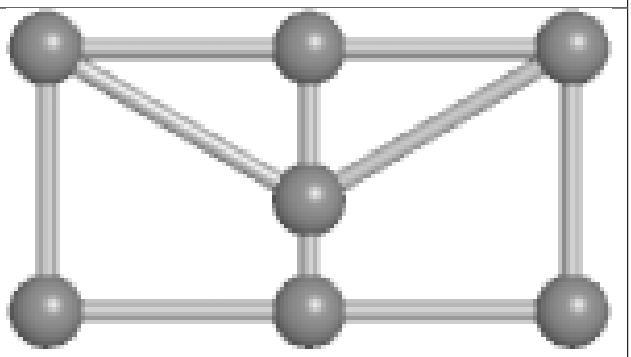


Rings

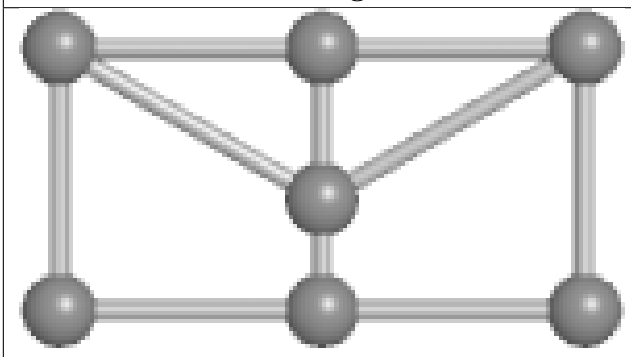
Ligand F3S CB 1002



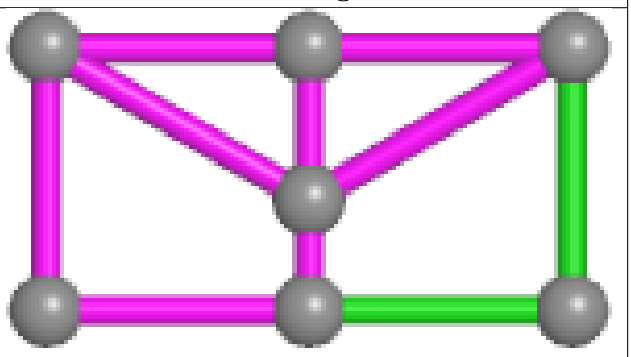
Bond lengths



Bond angles

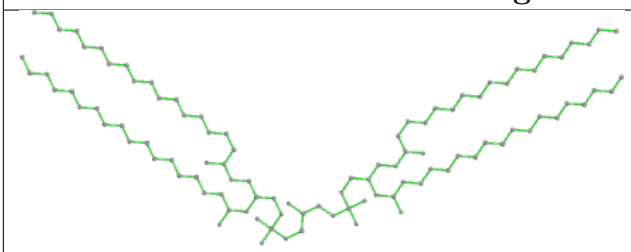


Torsions

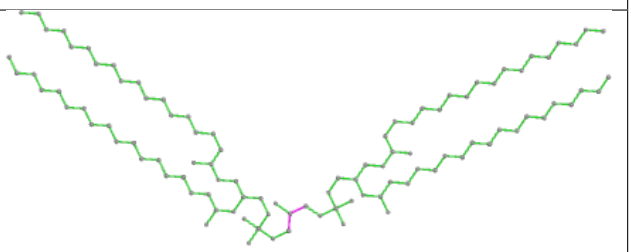


Rings

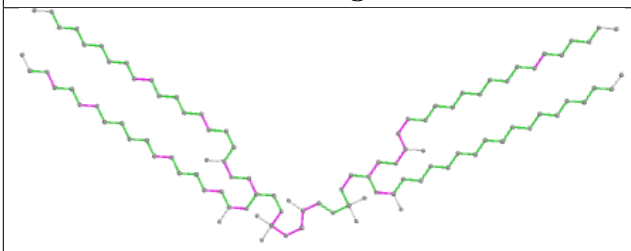
Ligand CDL Dd 702



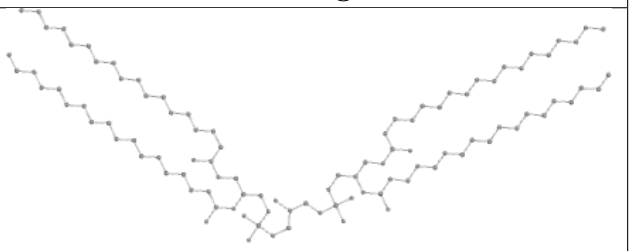
Bond lengths



Bond angles

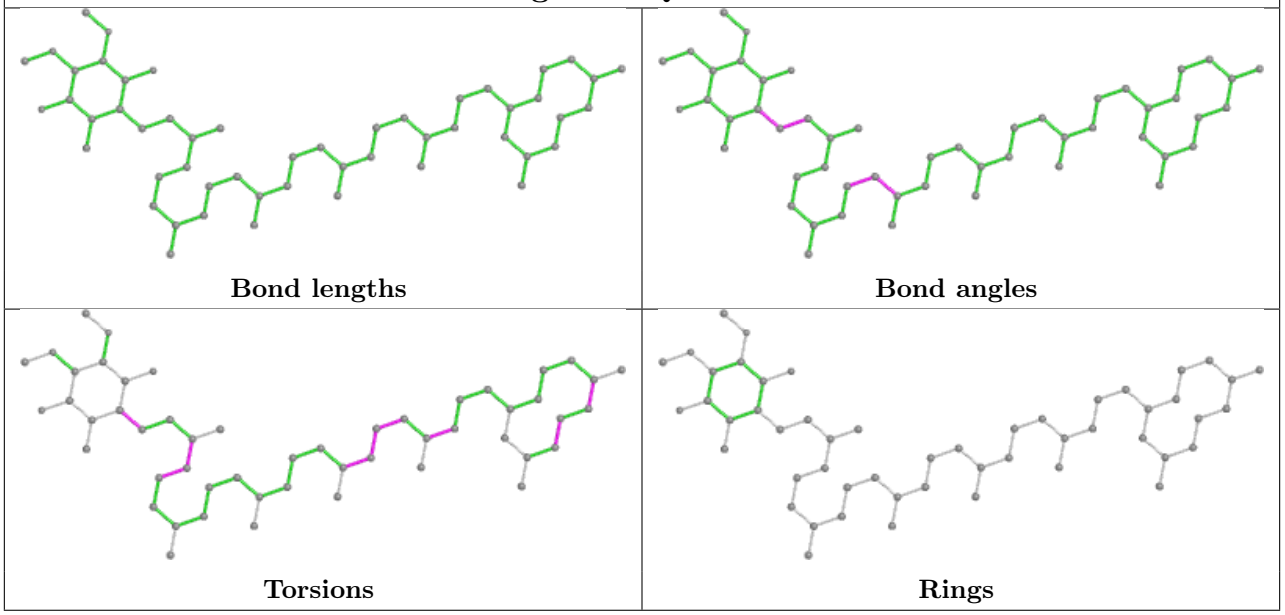


Torsions

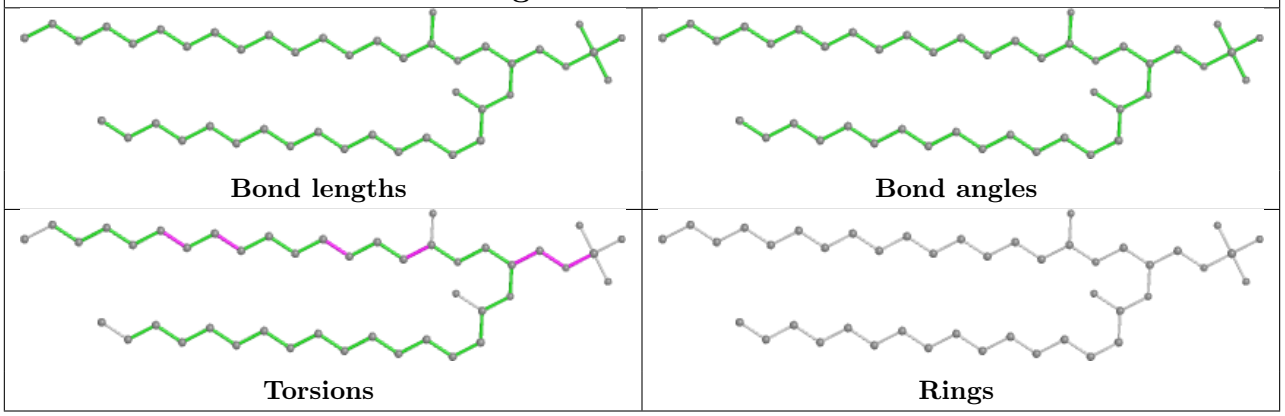


Rings

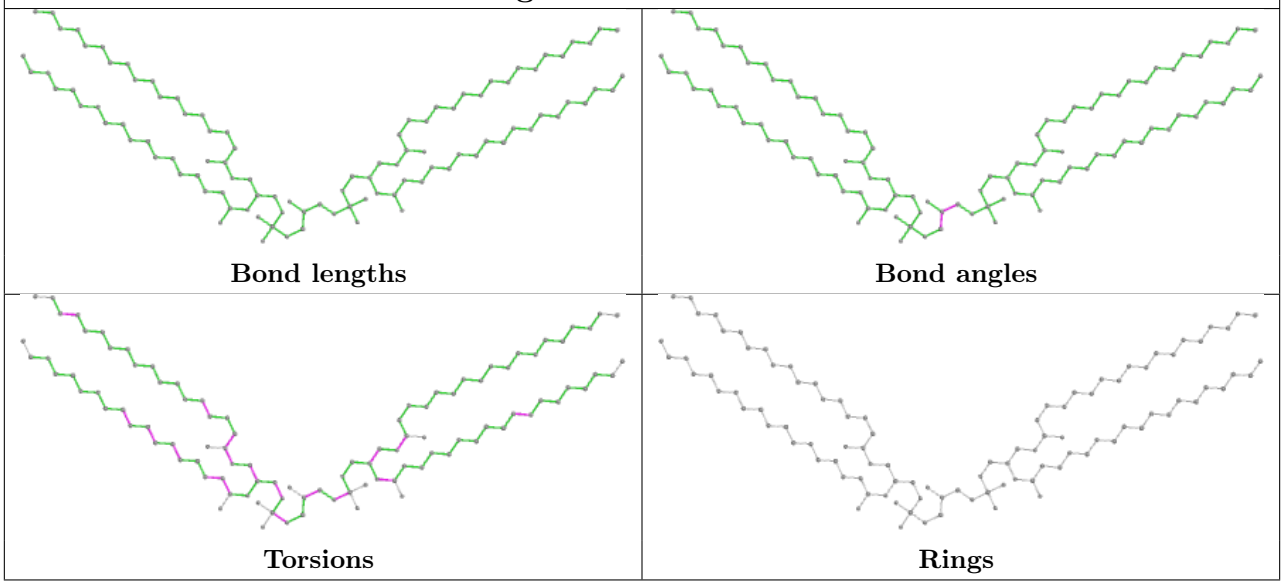
Ligand UQ8 c 510



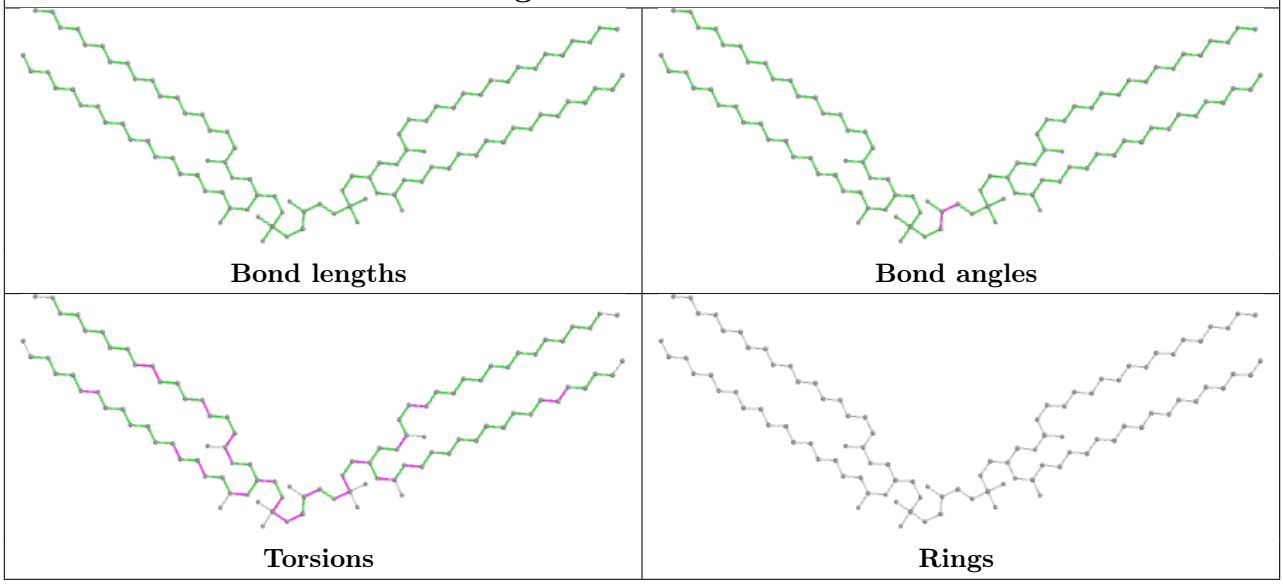
Ligand LPP DN 504



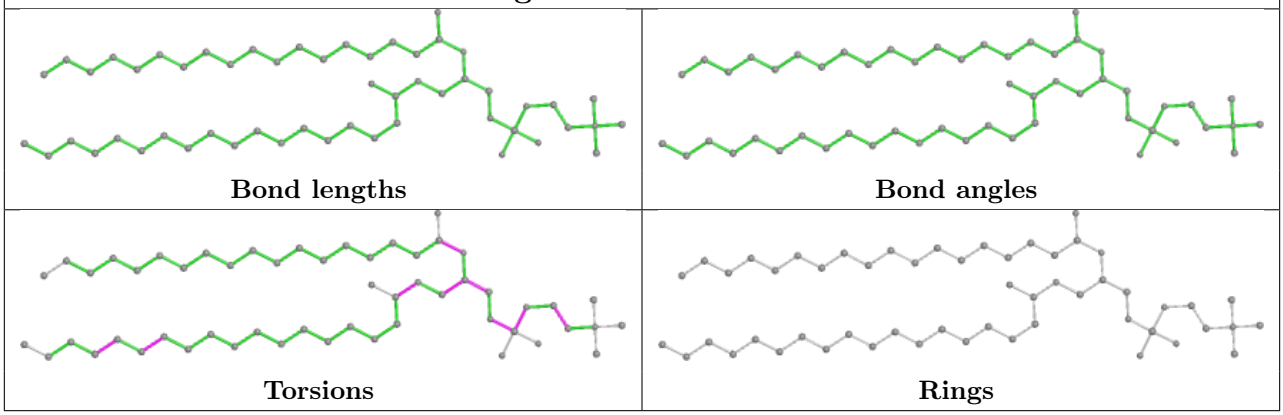
Ligand CDL B0 102



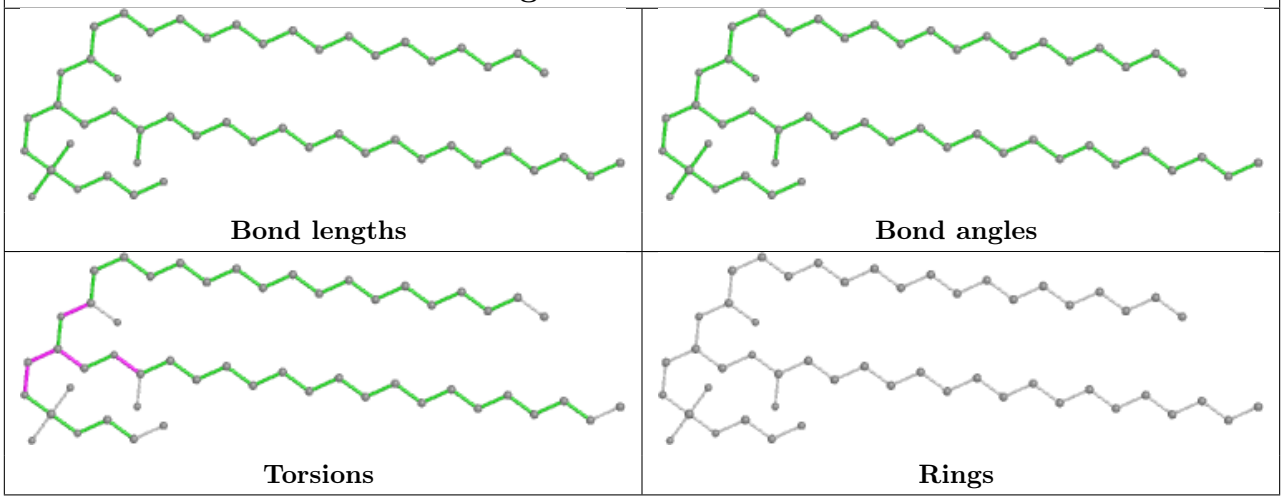
Ligand CDL Du 401



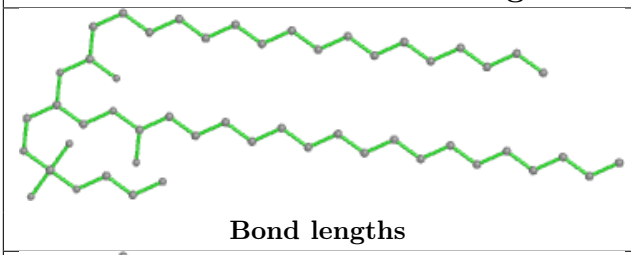
Ligand PC1 AA 905



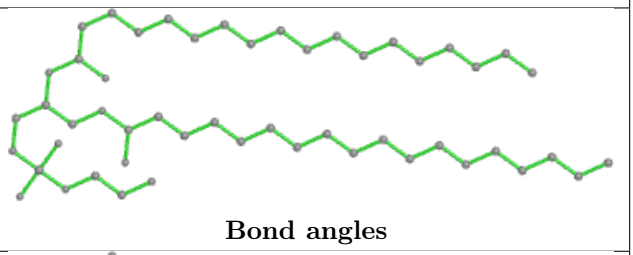
Ligand 3PE A2 401



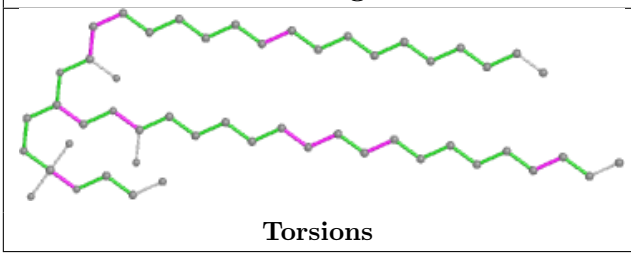
Ligand 3PE EN 1204



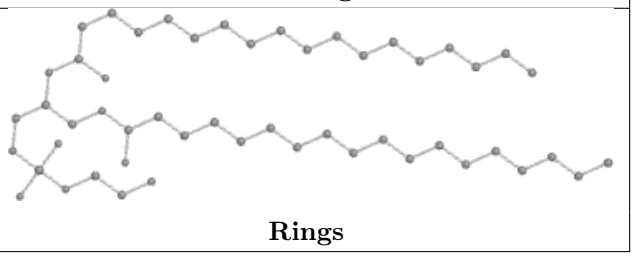
Bond lengths



Bond angles

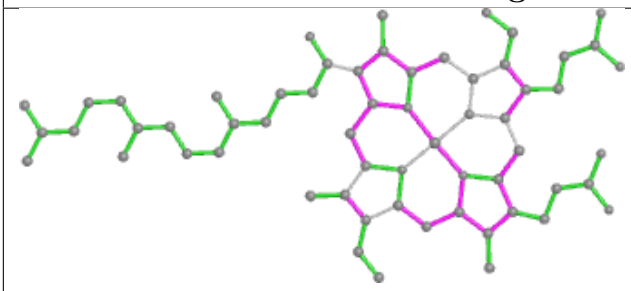


Torsions

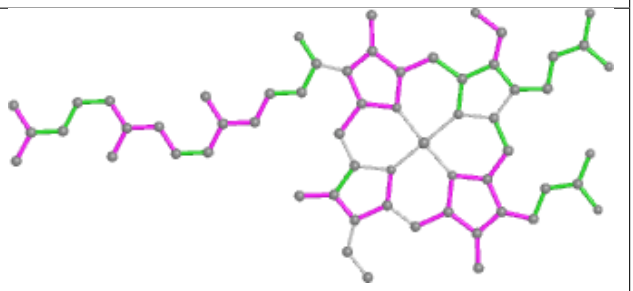


Rings

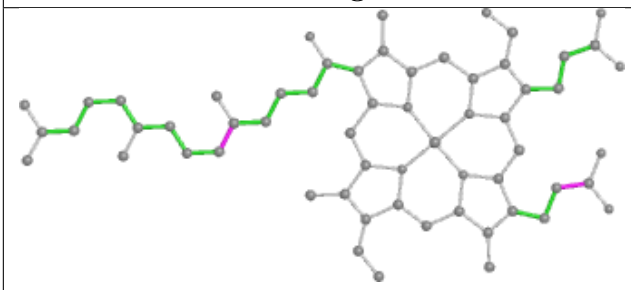
Ligand HEA DA 702



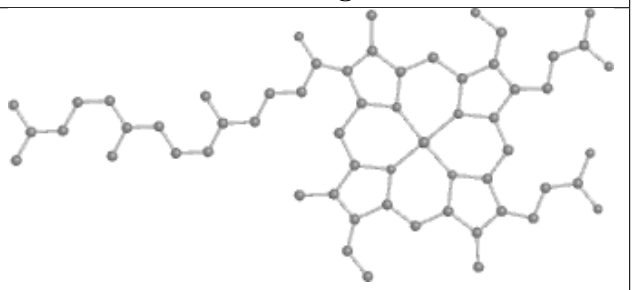
Bond lengths



Bond angles

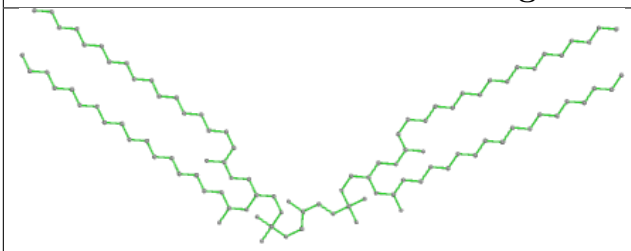


Torsions

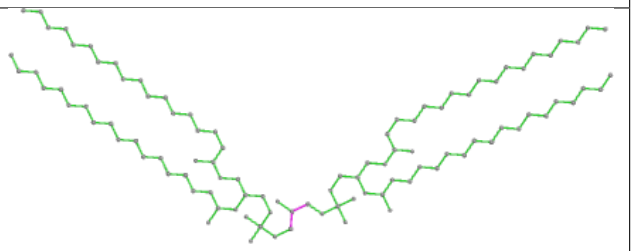


Rings

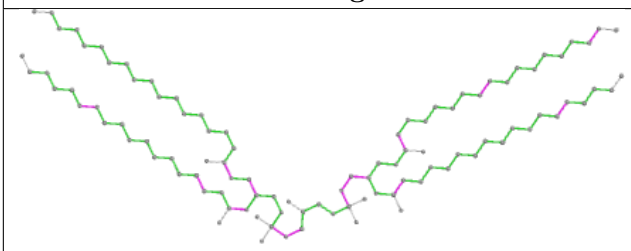
Ligand CDL EI 401



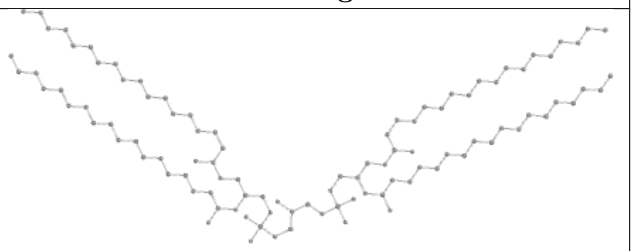
Bond lengths



Bond angles

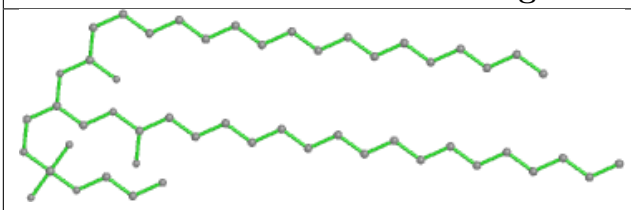


Torsions

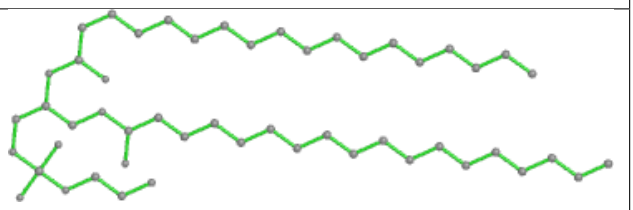


Rings

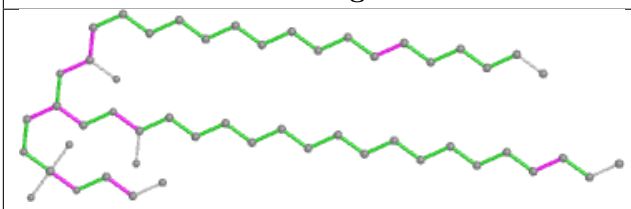
Ligand 3PE AJ 502



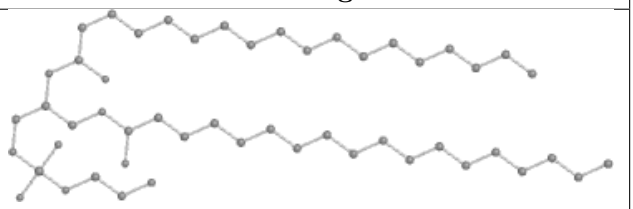
Bond lengths



Bond angles

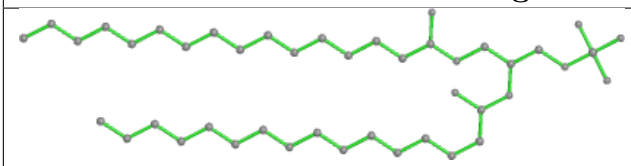


Torsions

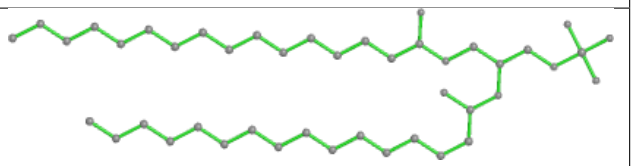


Rings

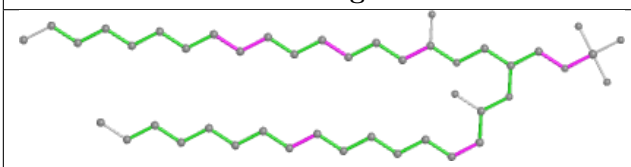
Ligand LPP AA 902



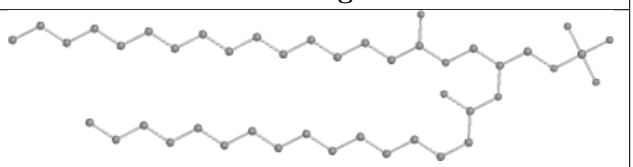
Bond lengths



Bond angles

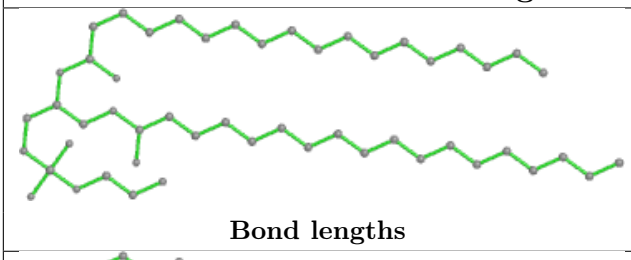


Torsions

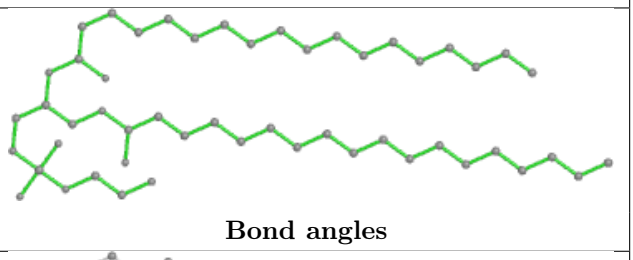


Rings

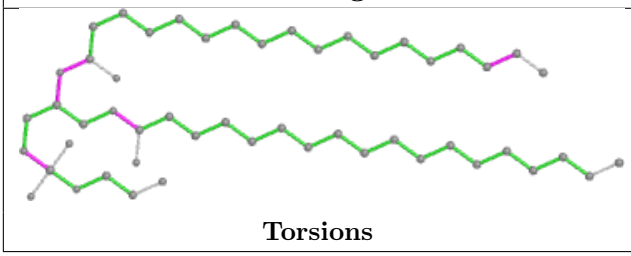
Ligand 3PE EO 203



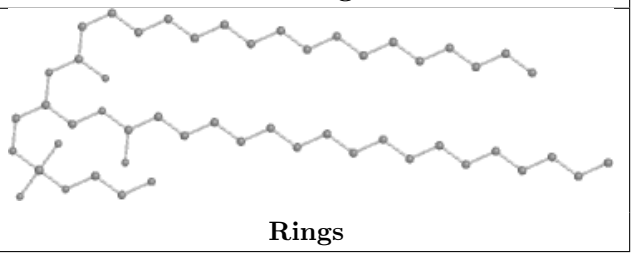
Bond lengths



Bond angles

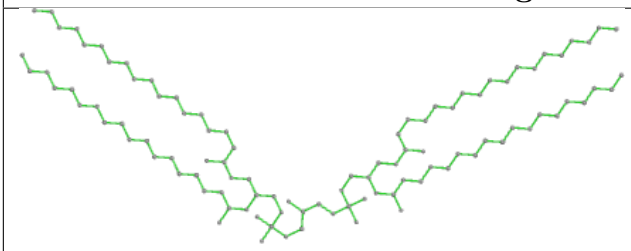


Torsions

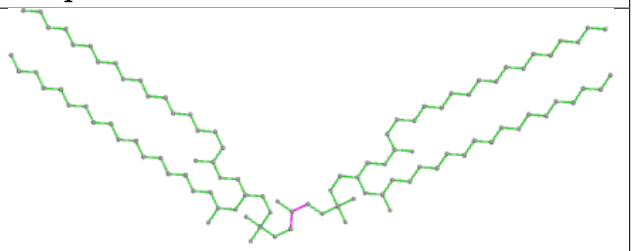


Rings

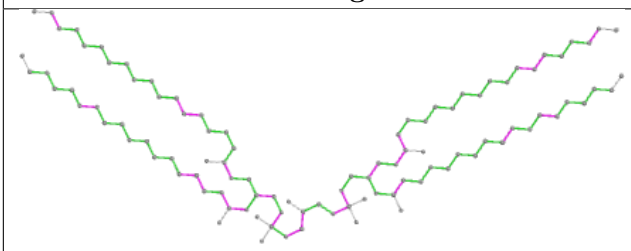
Ligand CDL Ep 701



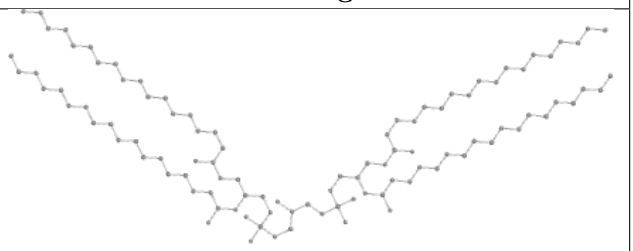
Bond lengths



Bond angles

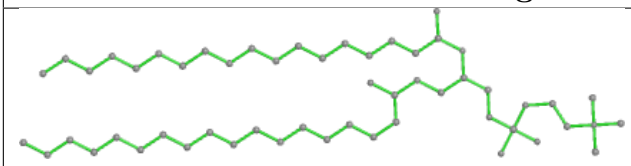


Torsions

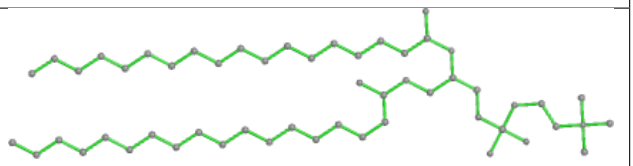


Rings

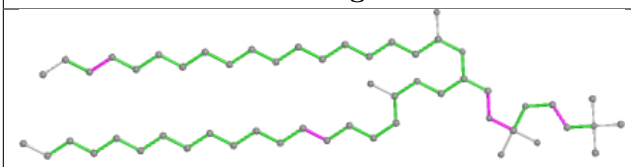
Ligand PC1 EB 303



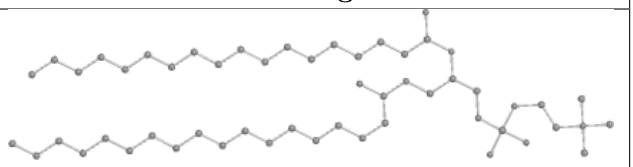
Bond lengths



Bond angles

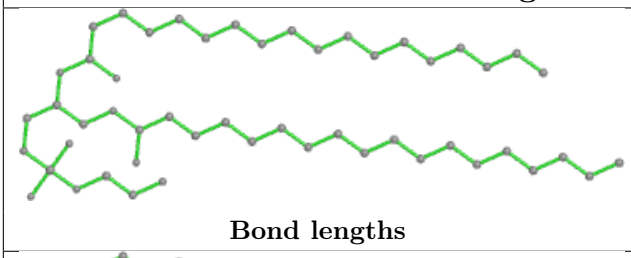


Torsions

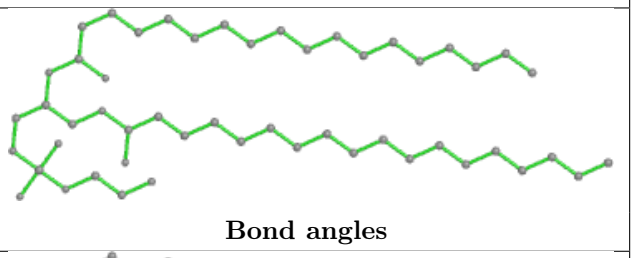


Rings

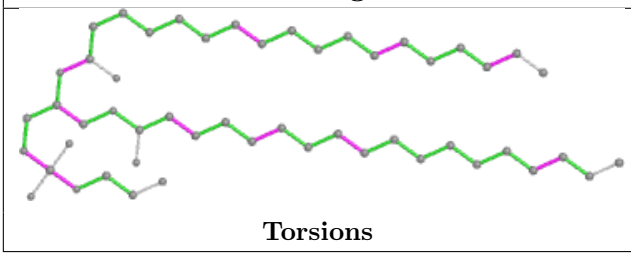
Ligand 3PE EL 904



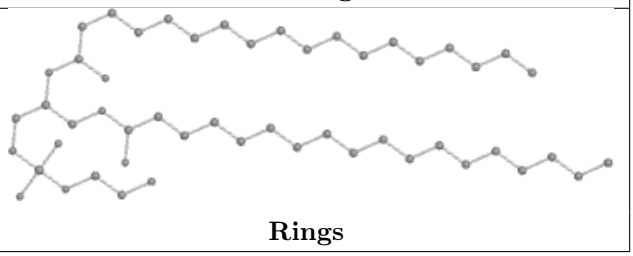
Bond lengths



Bond angles

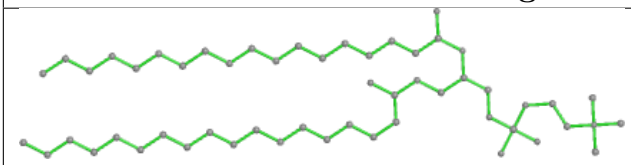


Torsions

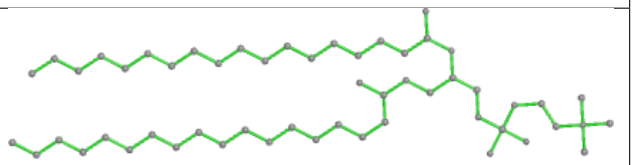


Rings

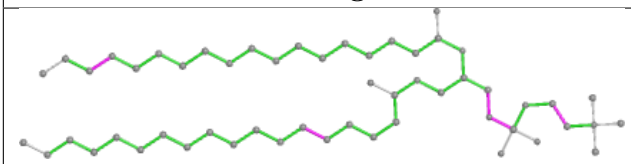
Ligand PC1 Eb 303



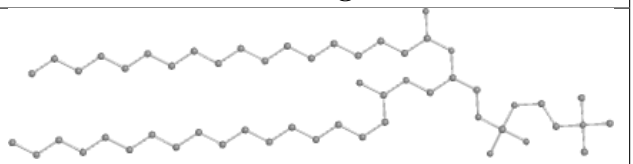
Bond lengths



Bond angles

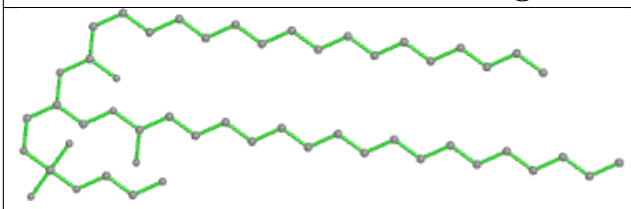


Torsions

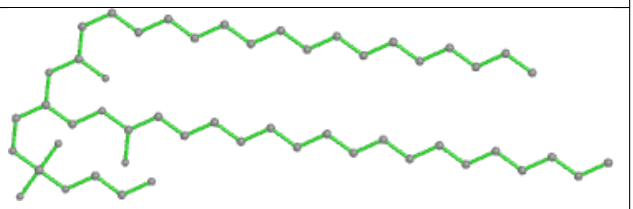


Rings

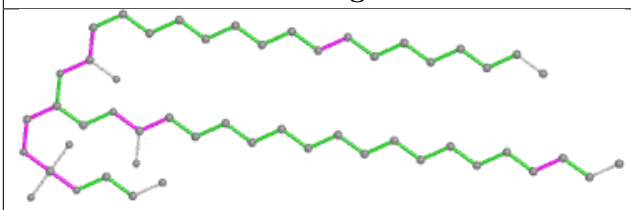
Ligand 3PE DG 205



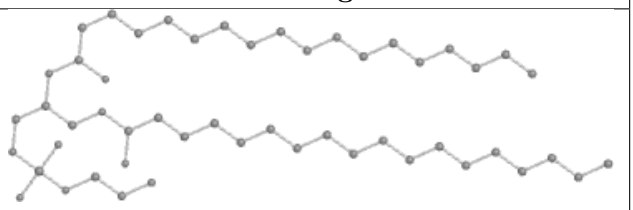
Bond lengths



Bond angles

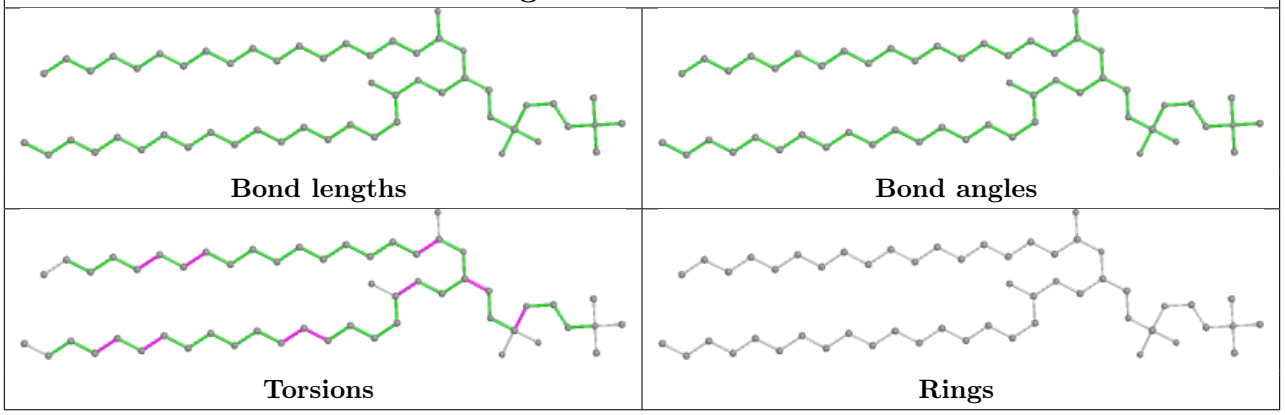


Torsions

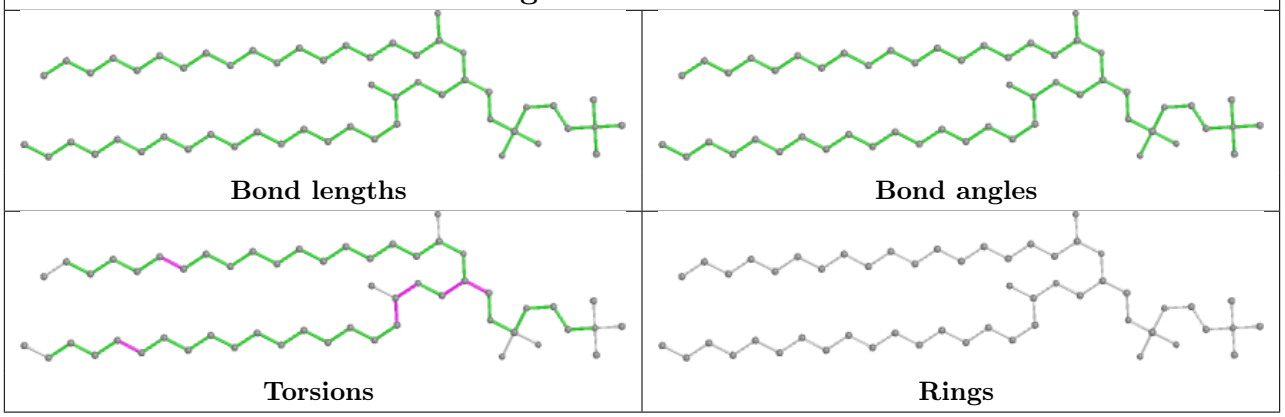


Rings

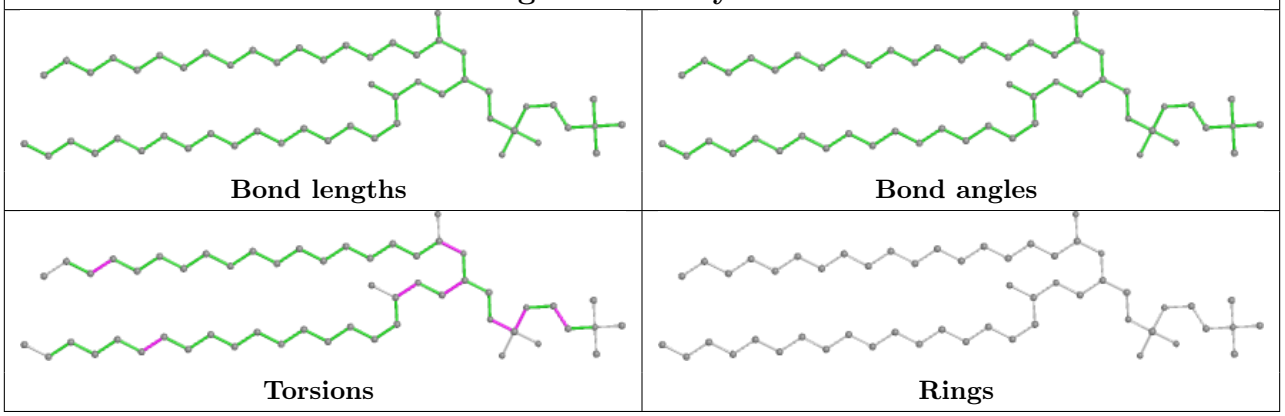
Ligand PC1 Dc 603



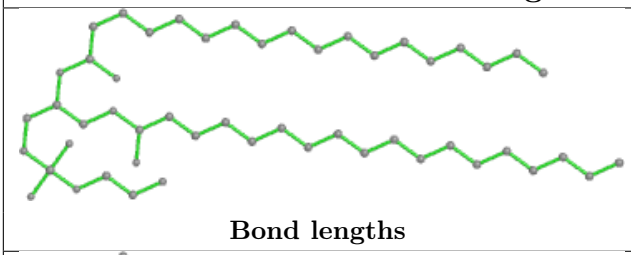
Ligand PC1 Ds 407



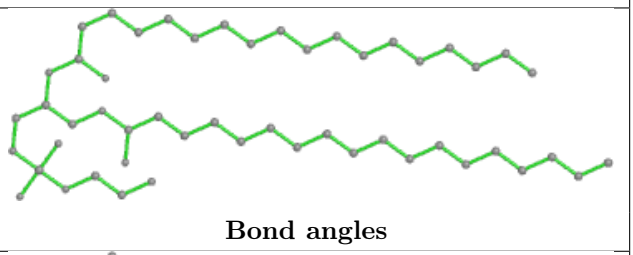
Ligand PC1 Dy 302



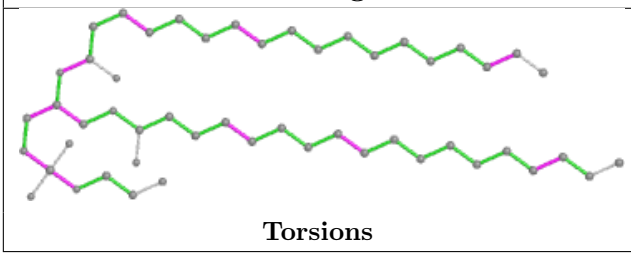
Ligand 3PE El 905



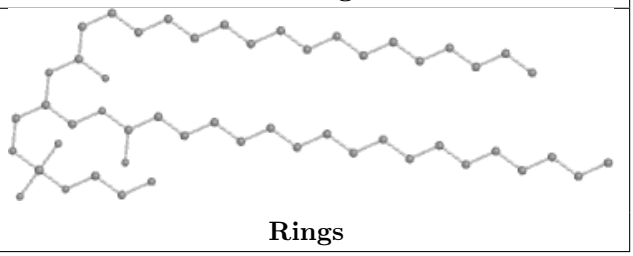
Bond lengths



Bond angles

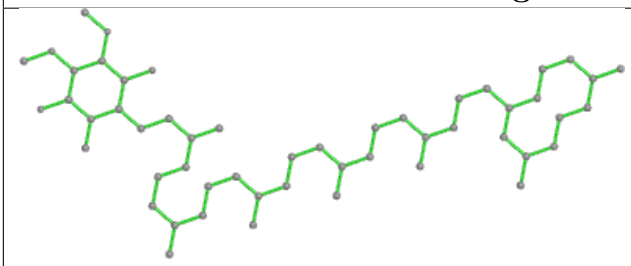


Torsions

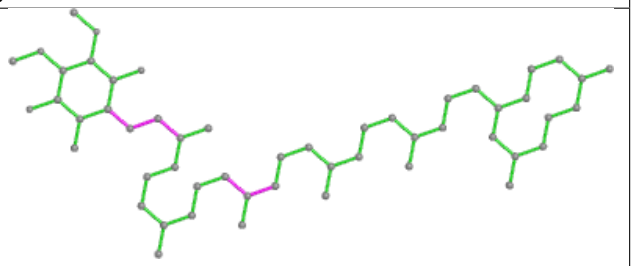


Rings

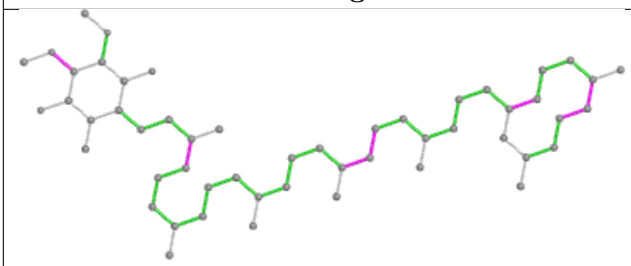
Ligand UQ8 ED 603



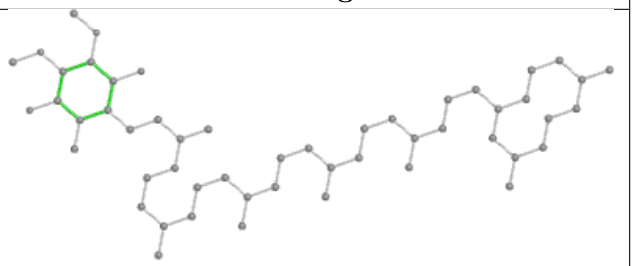
Bond lengths



Bond angles

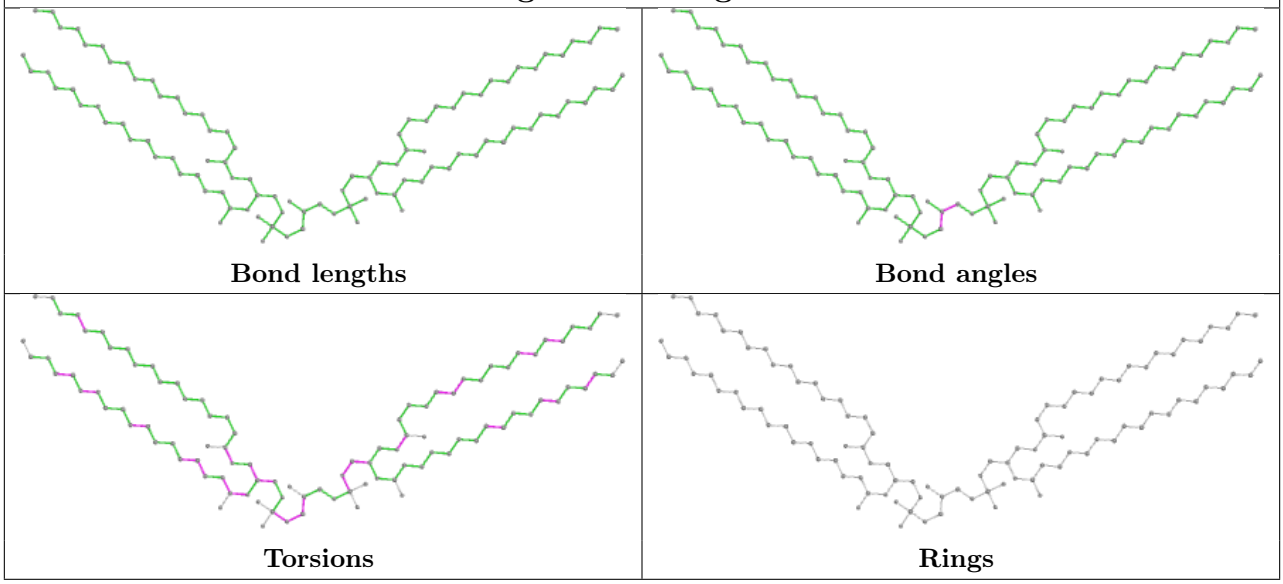


Torsions

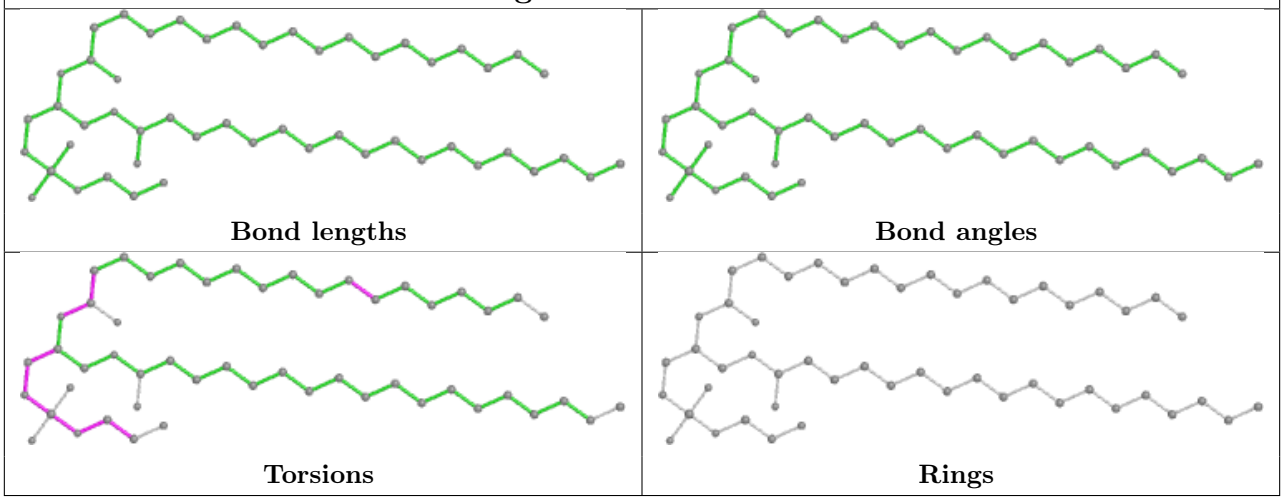


Rings

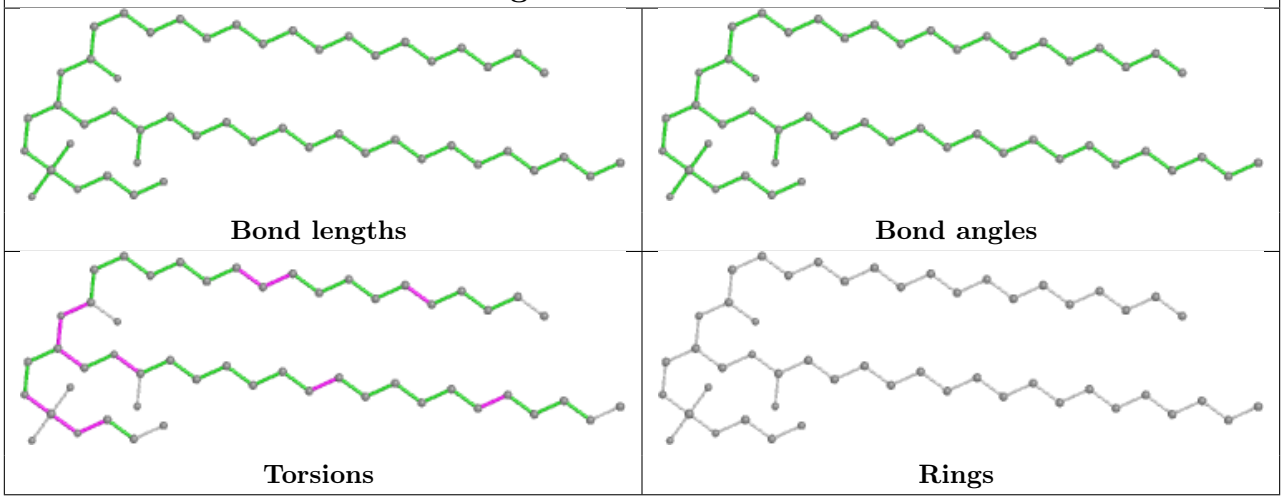
Ligand CDL Eg 101



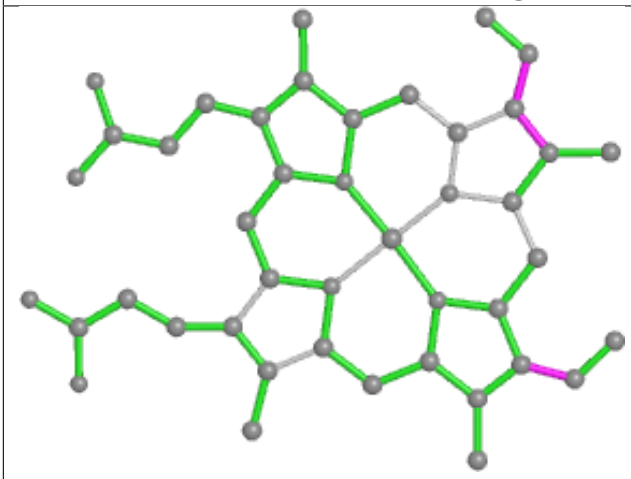
Ligand 3PE DG 204



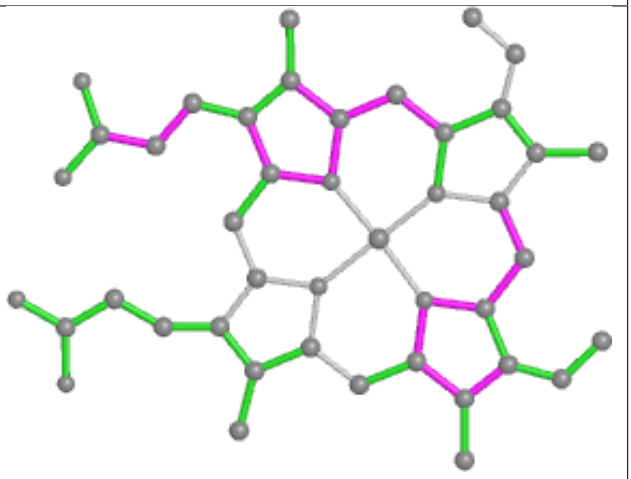
Ligand 3PE Dx 1202



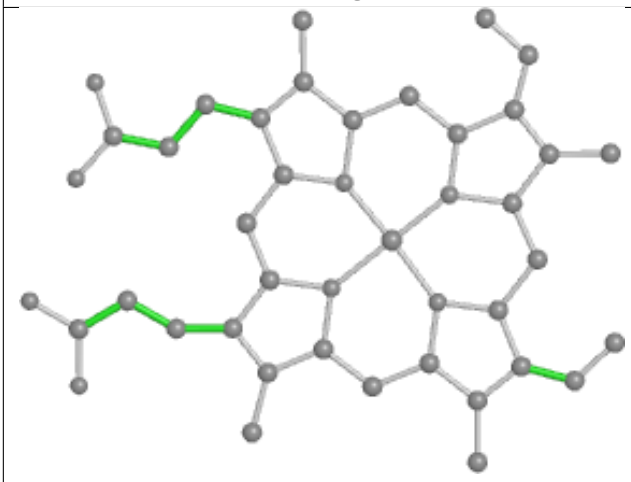
Ligand HEM Ed 201



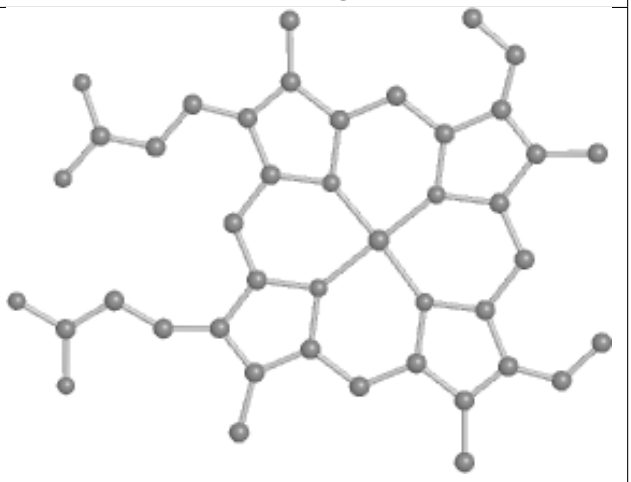
Bond lengths



Bond angles

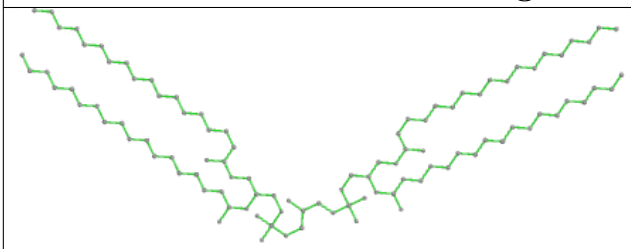


Torsions

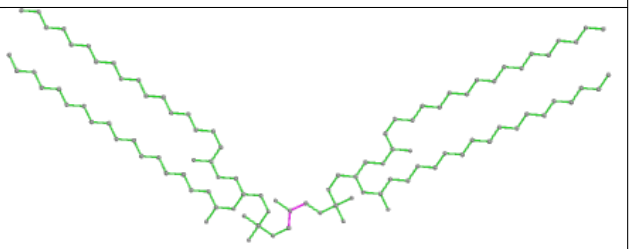


Rings

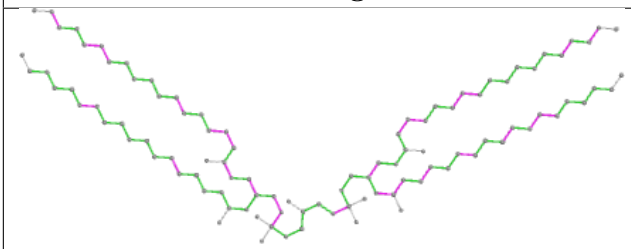
Ligand CDL Dr 402



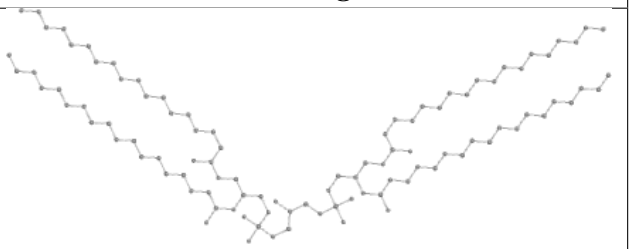
Bond lengths



Bond angles

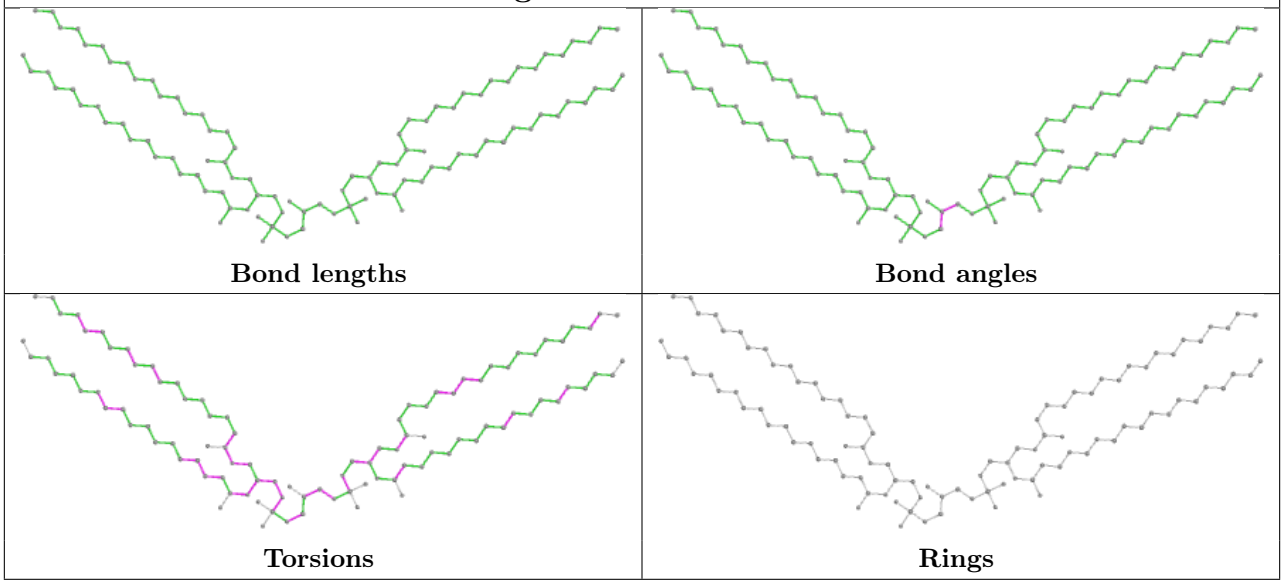


Torsions

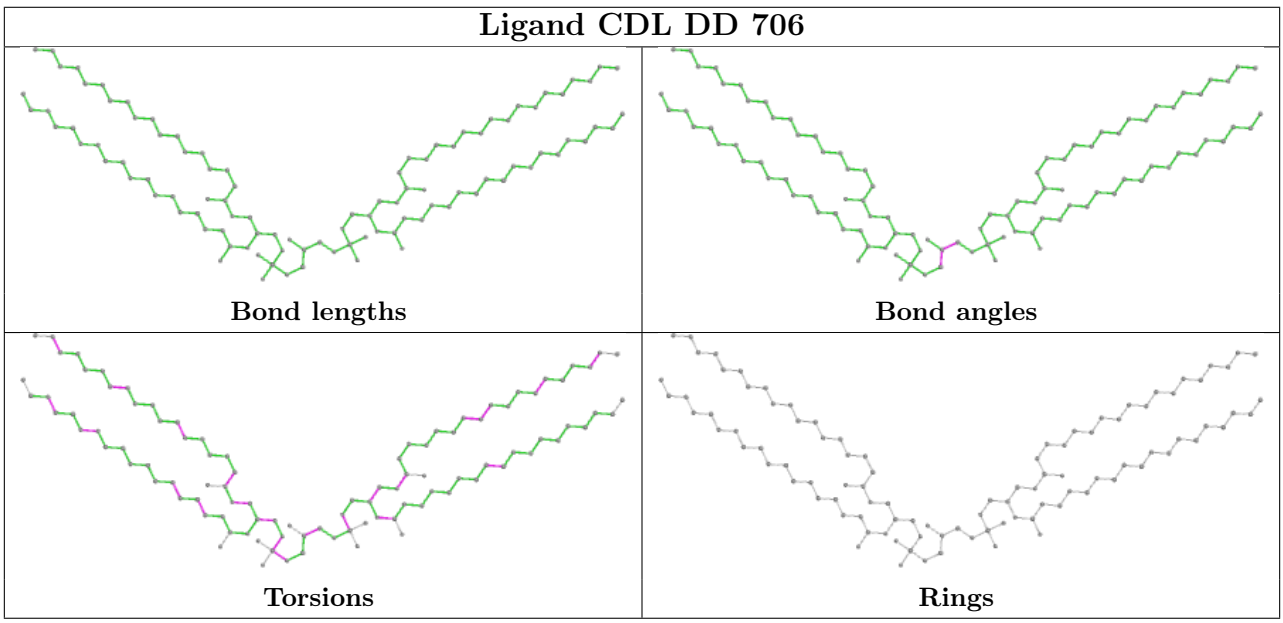


Rings

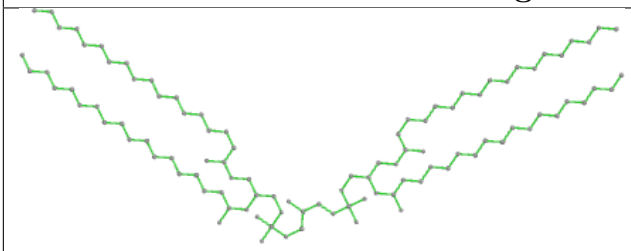
Ligand CDL Dn 502



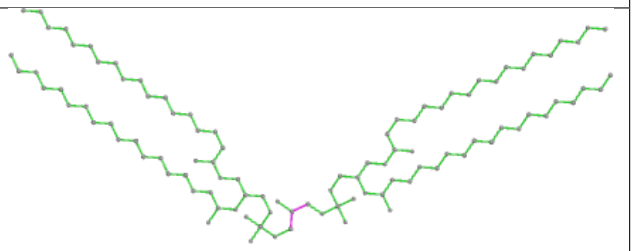
Ligand CDL DD 706



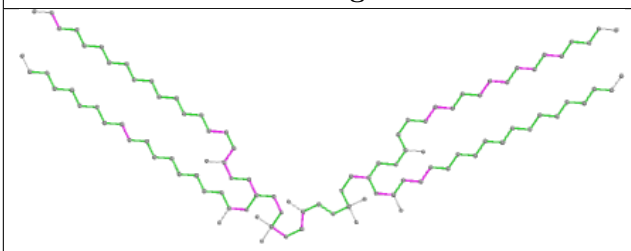
Ligand CDL CJ 201



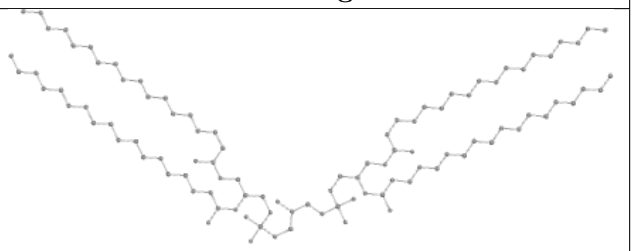
Bond lengths



Bond angles

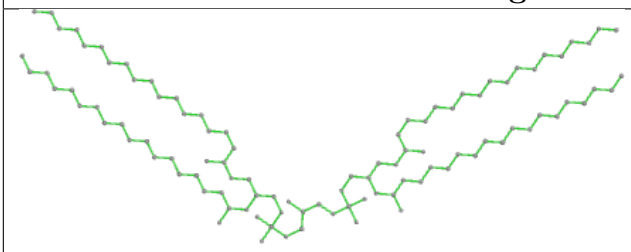


Torsions

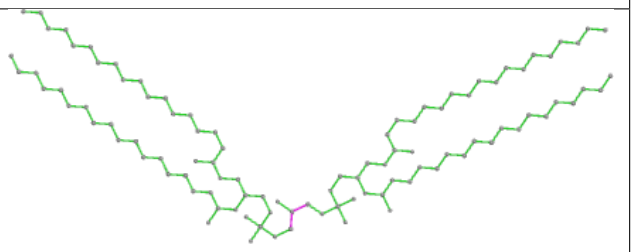


Rings

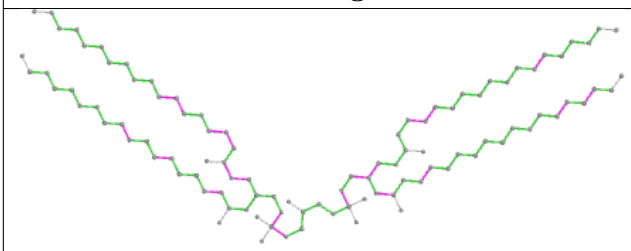
Ligand CDL DG 202



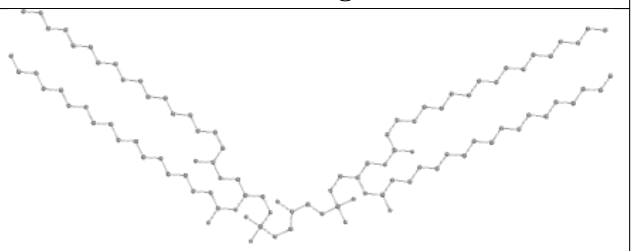
Bond lengths



Bond angles

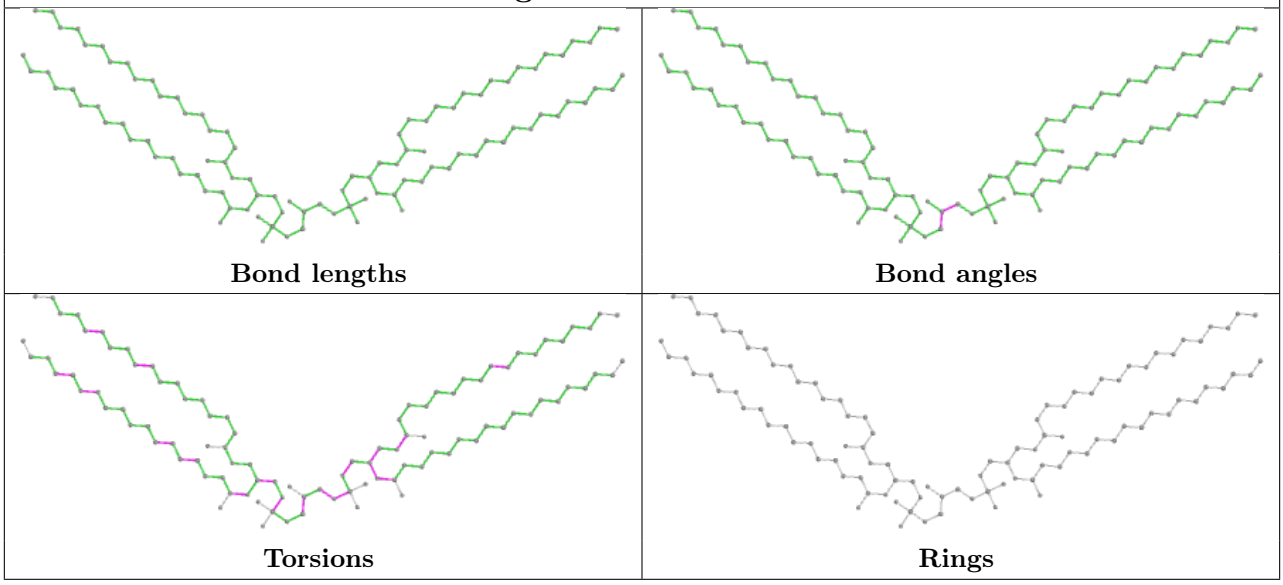


Torsions

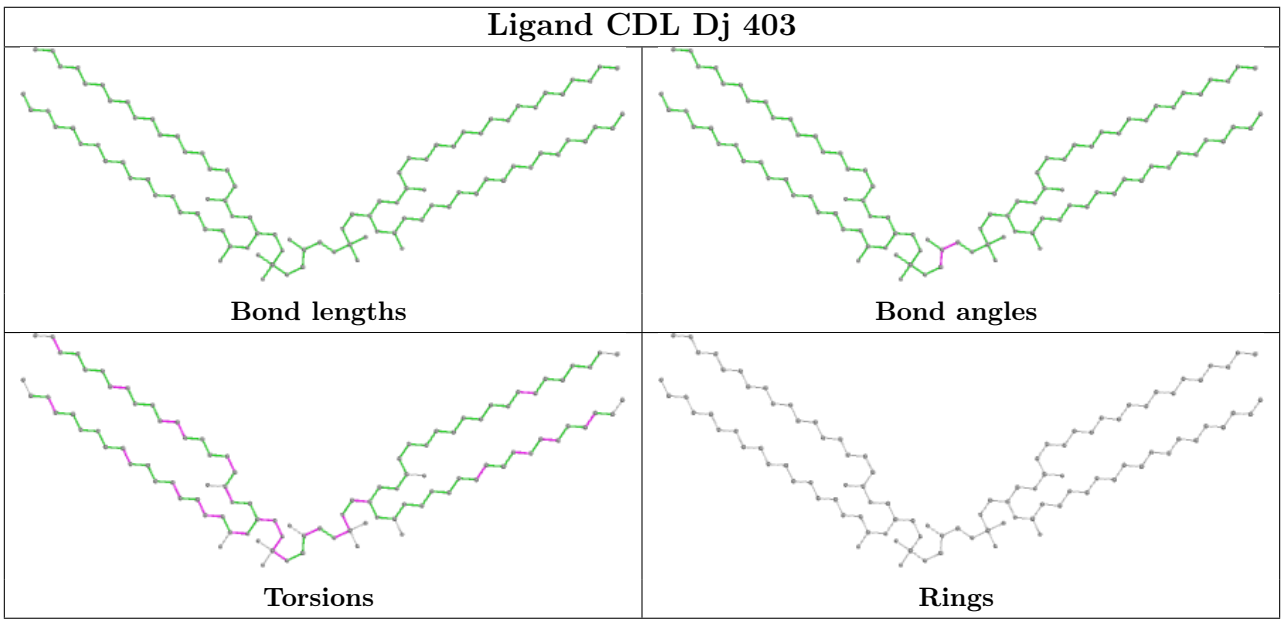


Rings

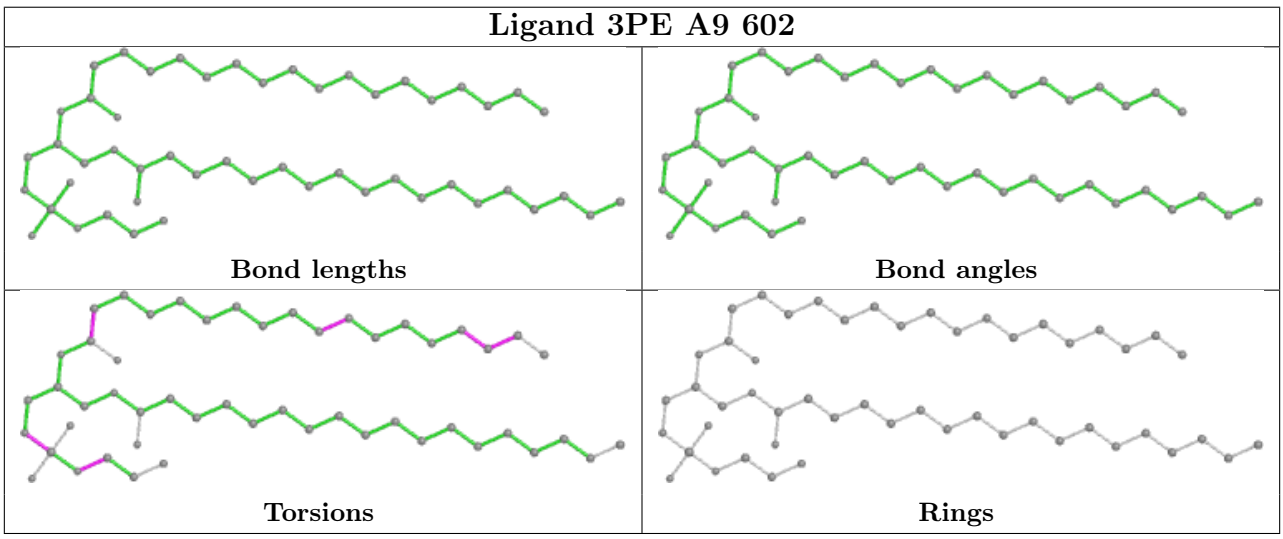
Ligand CDL DJ 305



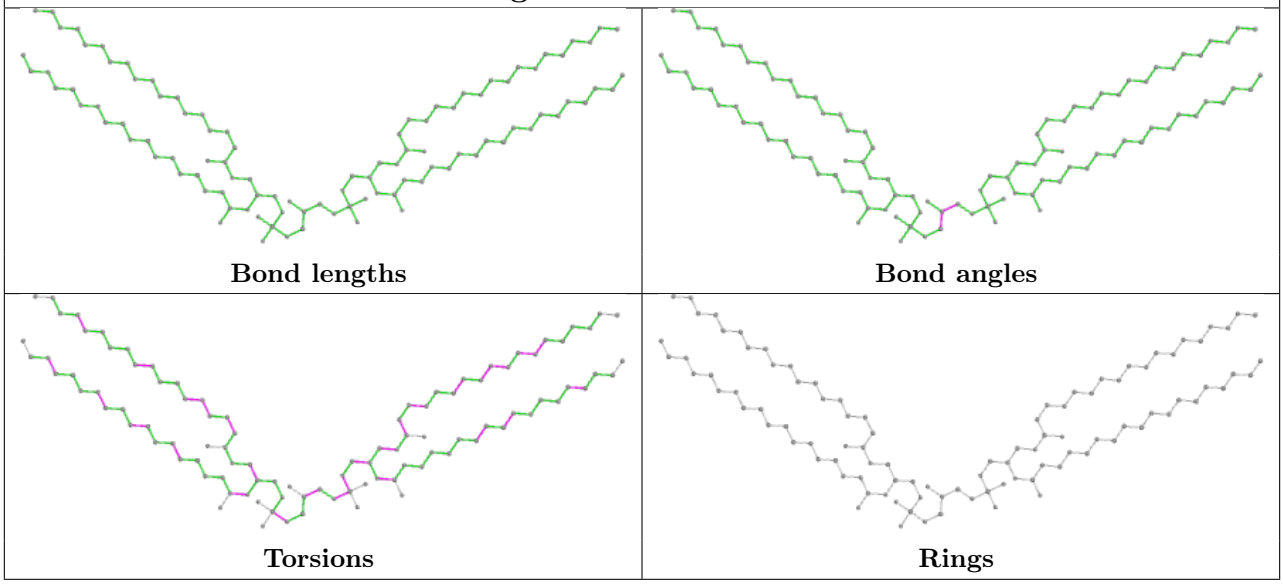
Ligand CDL Dj 403



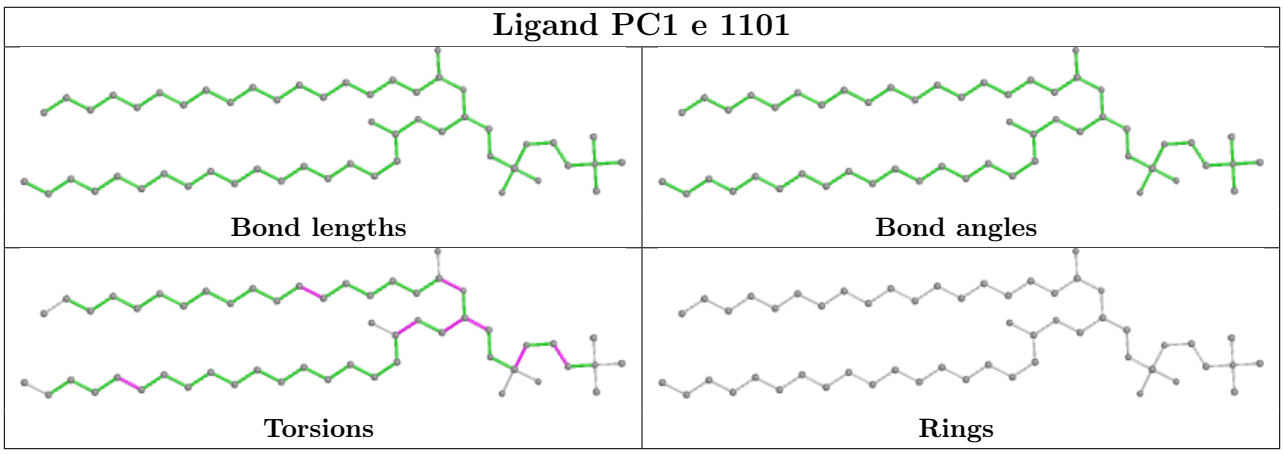
Ligand 3PE A9 602



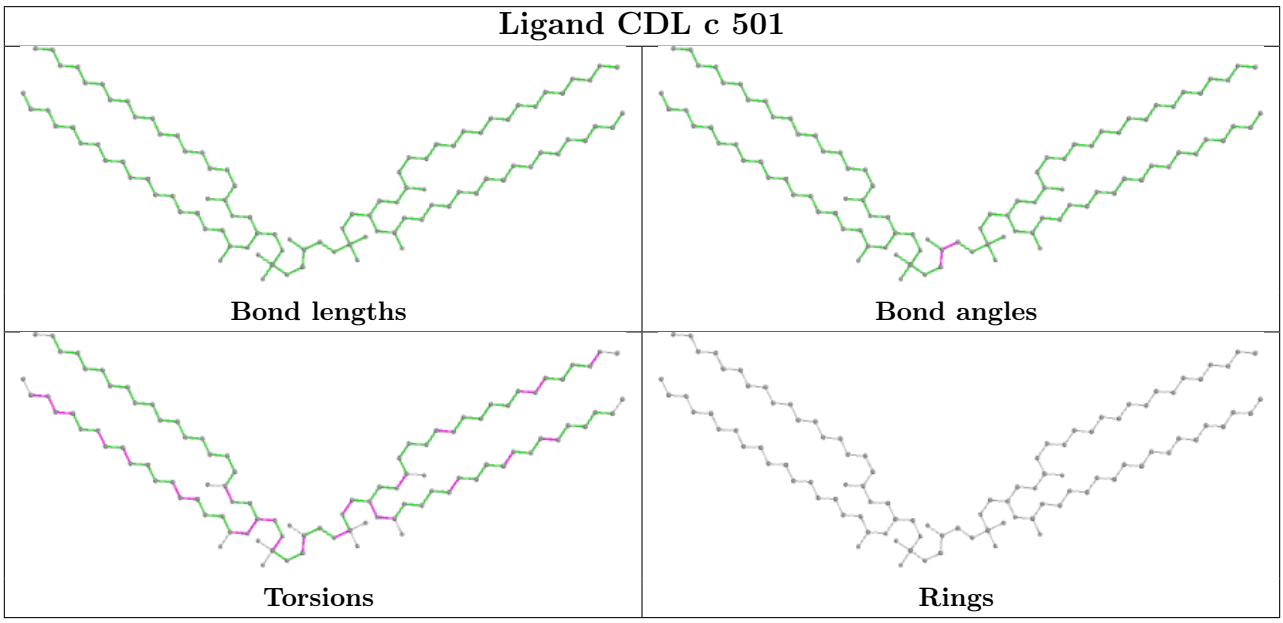
Ligand CDL Di 1103



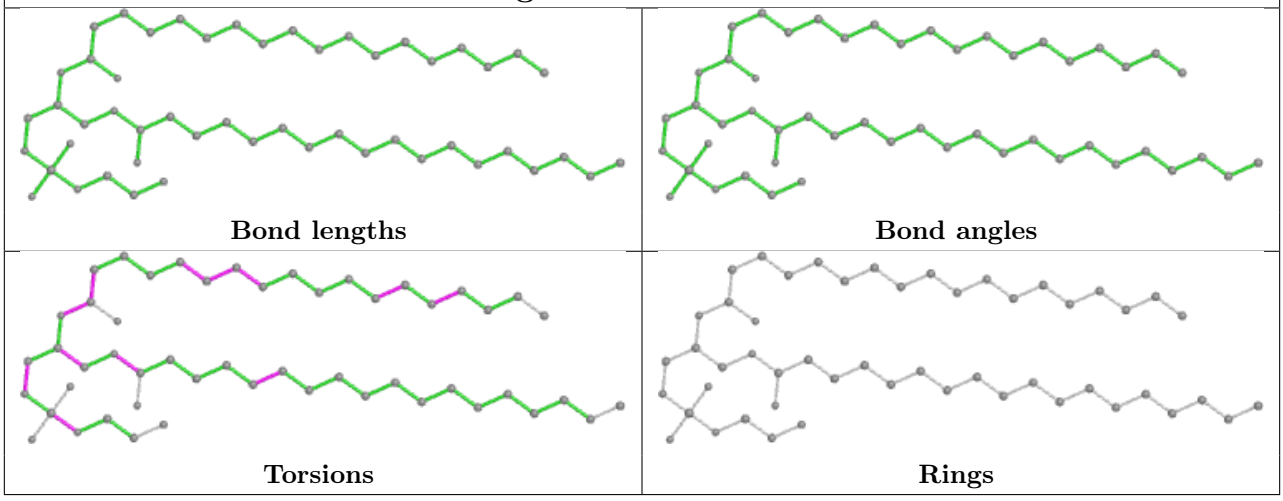
Ligand PC1 e 1101



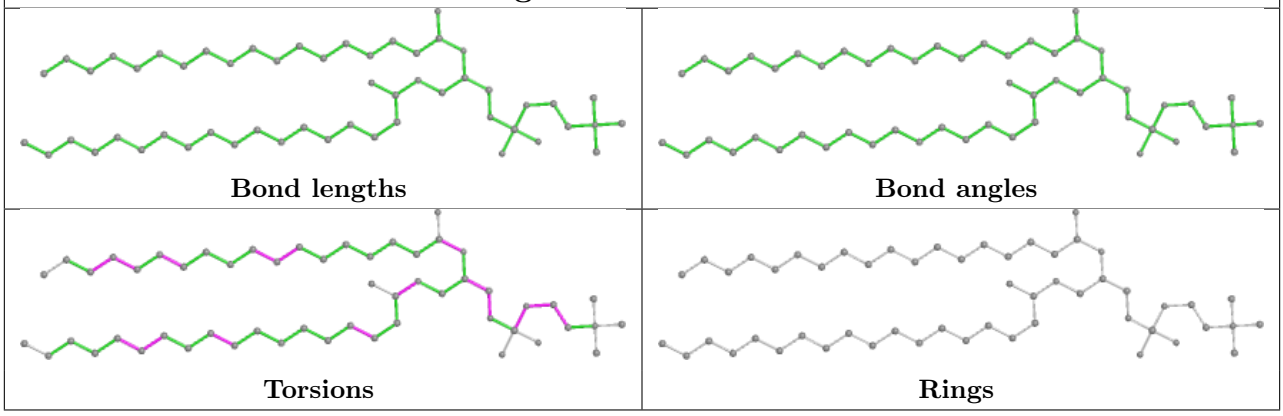
Ligand CDL c 501



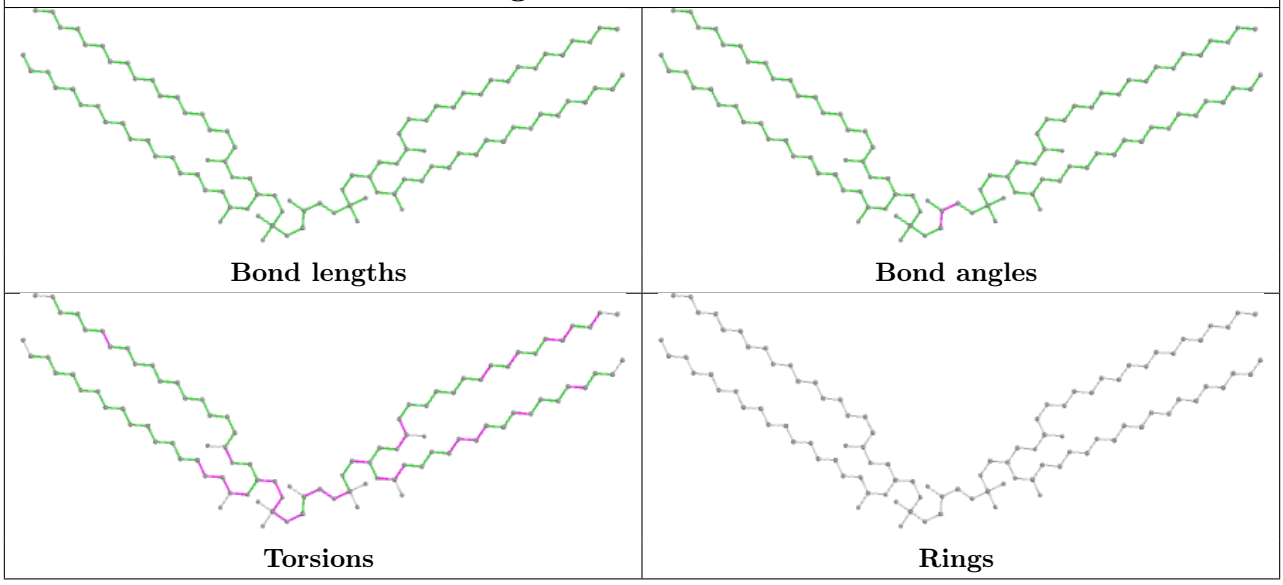
Ligand 3PE BA 301



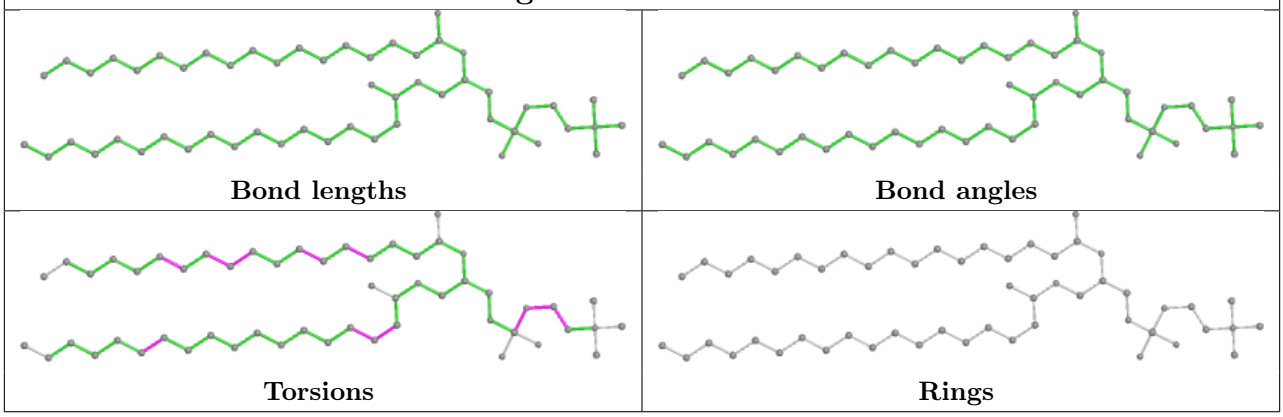
Ligand PC1 DB 702



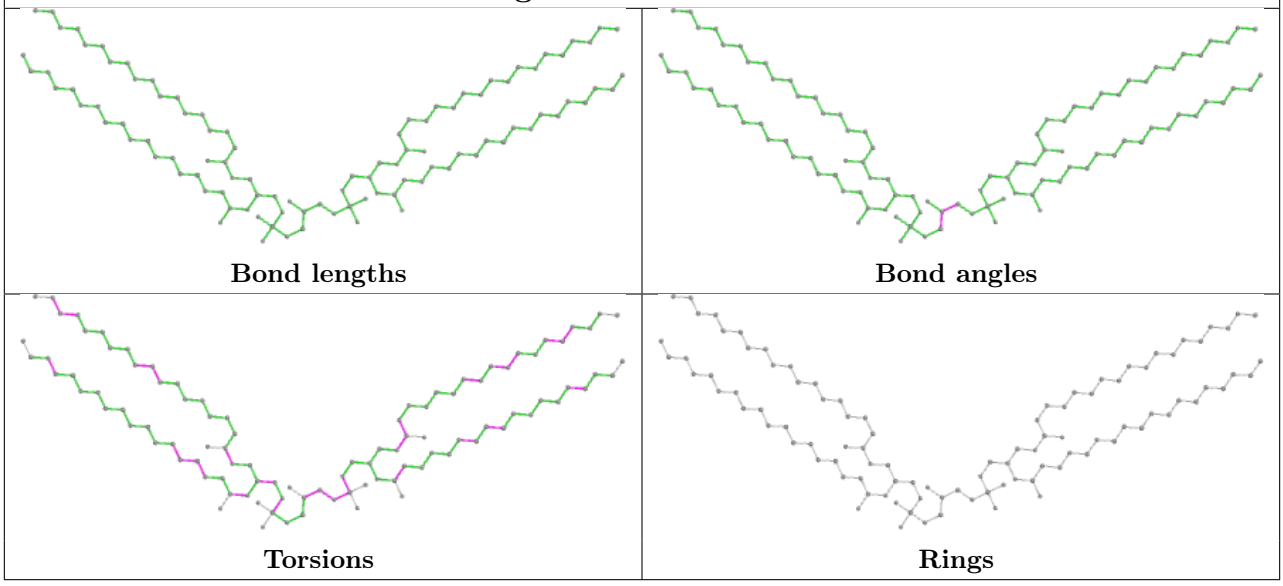
Ligand CDL Dm 501



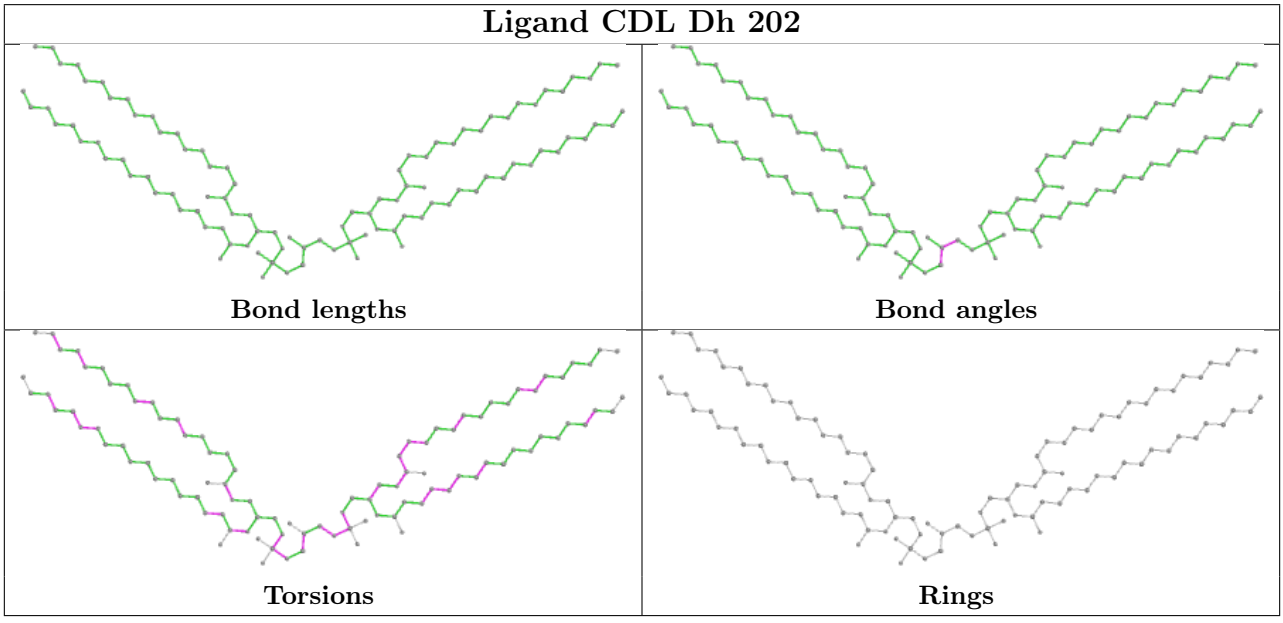
Ligand PC1 EO 201



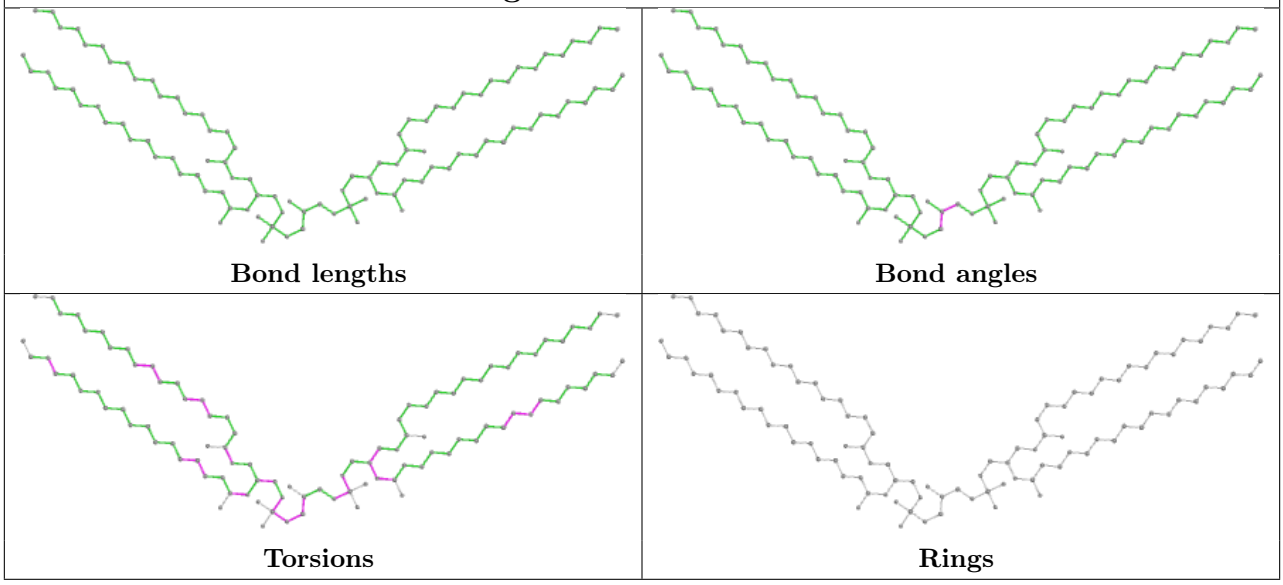
Ligand CDL Dv 402



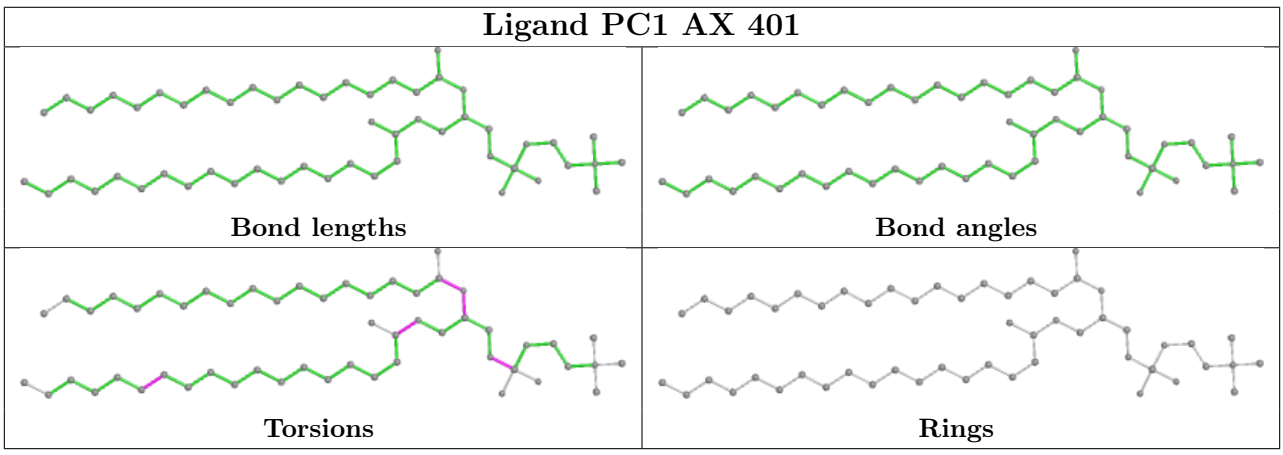
Ligand CDL Dh 202



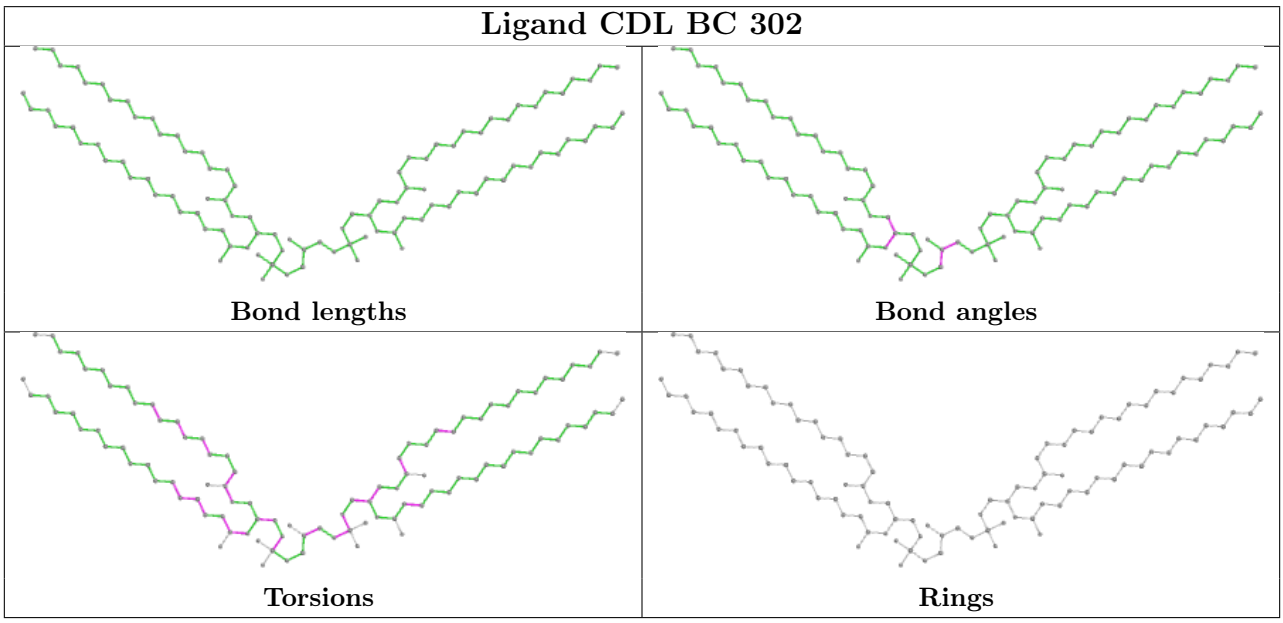
Ligand CDL EN 1202



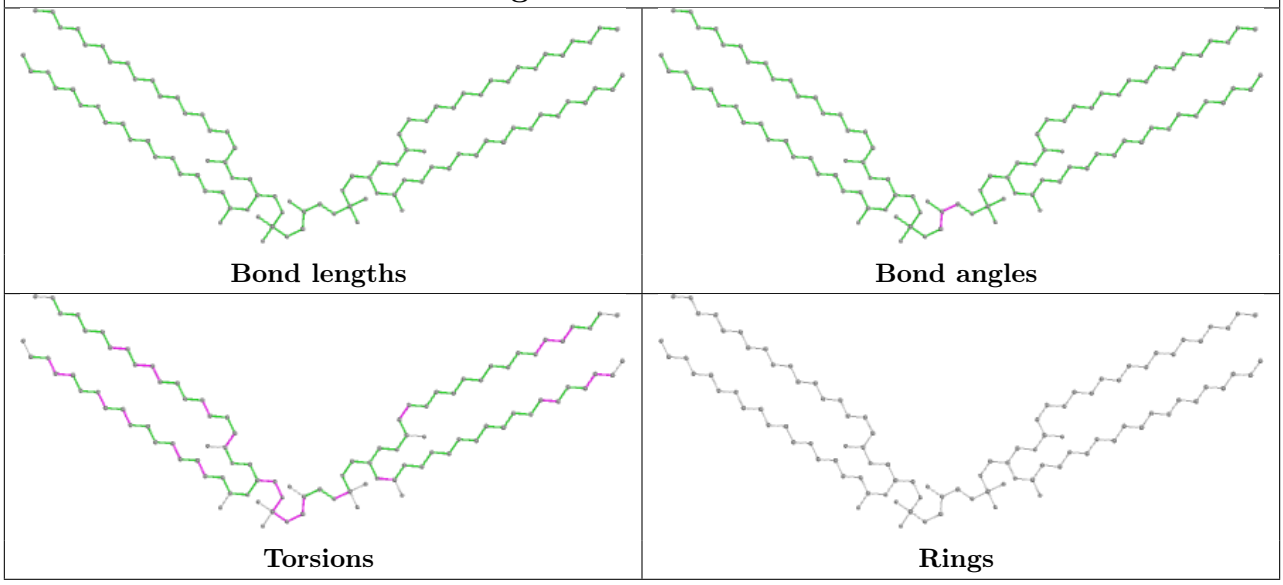
Ligand PC1 AX 401



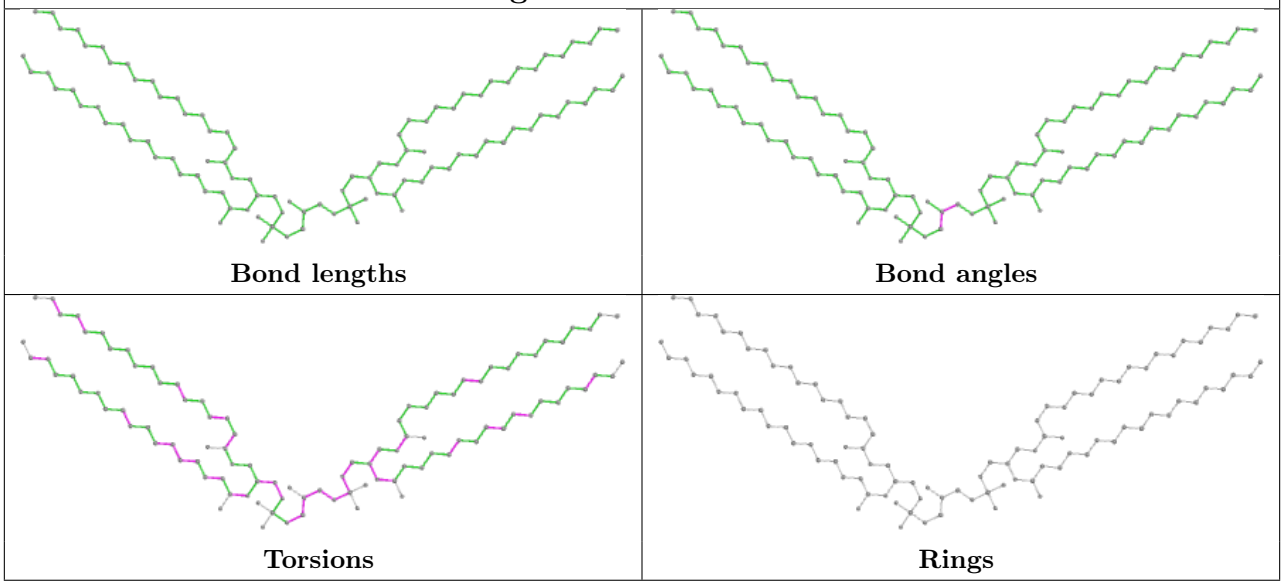
Ligand CDL BC 302



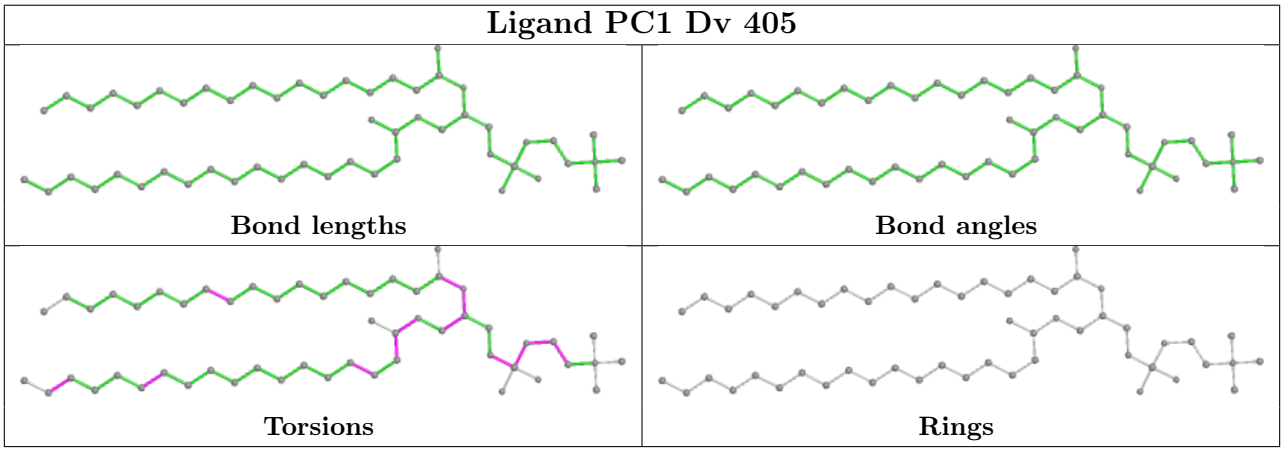
Ligand CDL AA 901



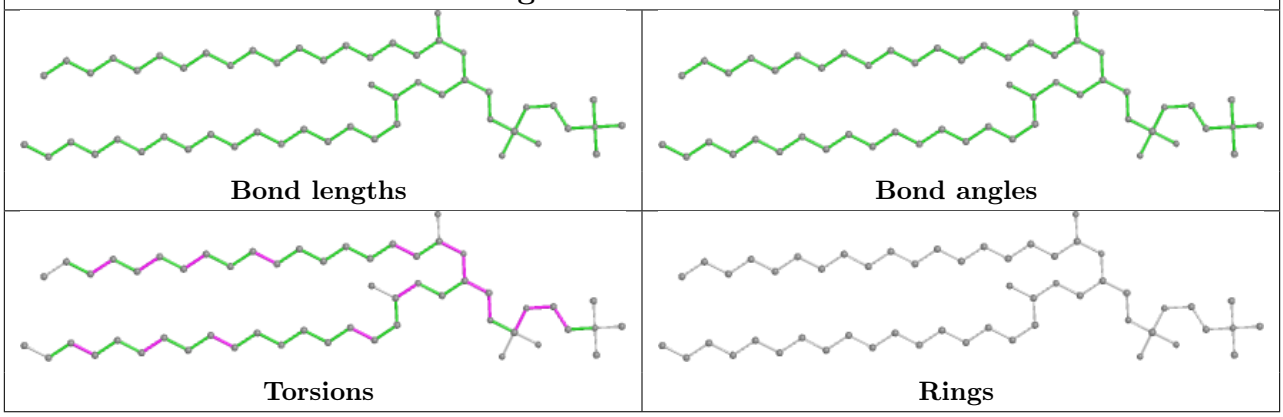
Ligand CDL DG 201



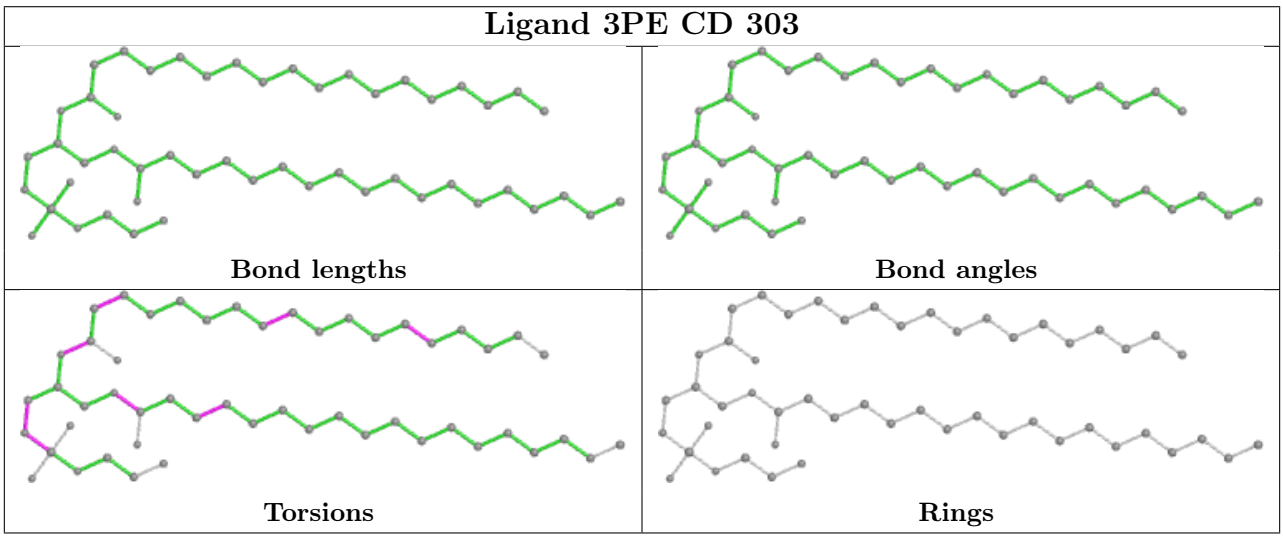
Ligand PC1 Dv 405



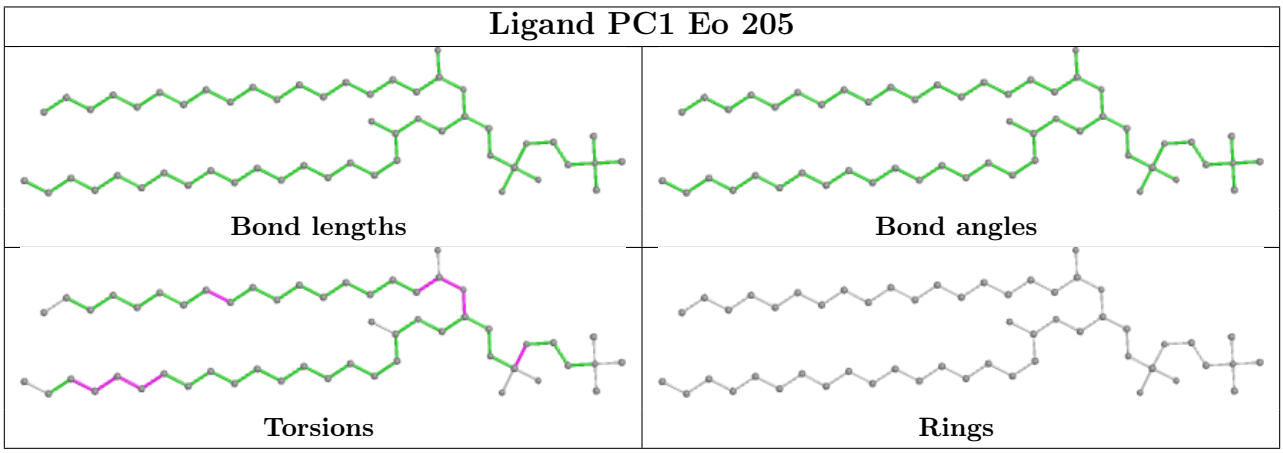
Ligand PC1 Db 702



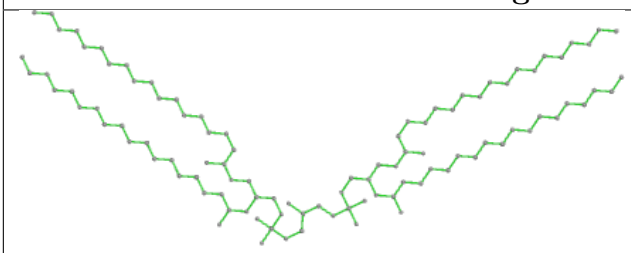
Ligand 3PE CD 303



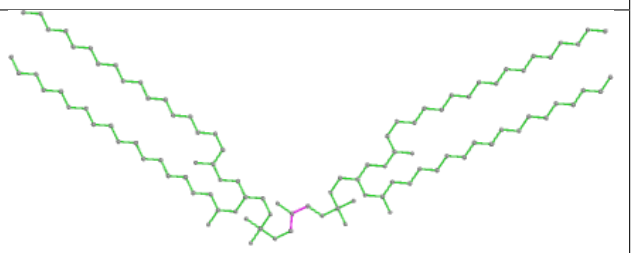
Ligand PC1 Eo 205



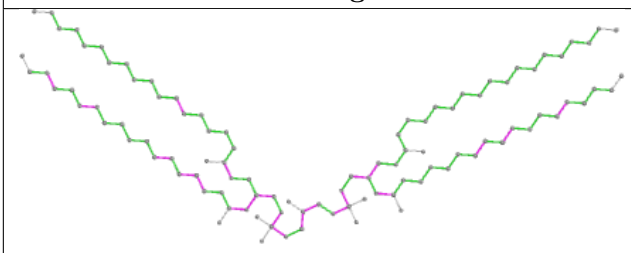
Ligand CDL EB 302



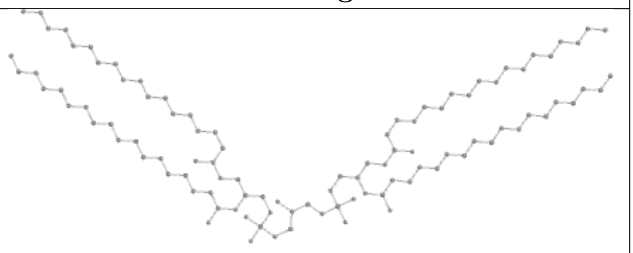
Bond lengths



Bond angles

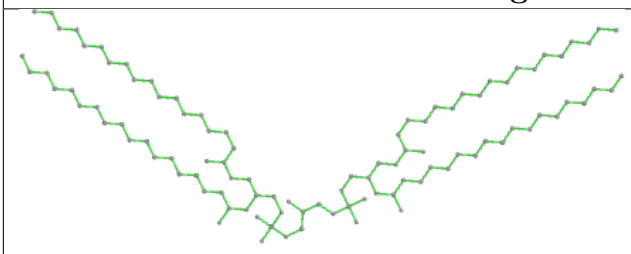


Torsions

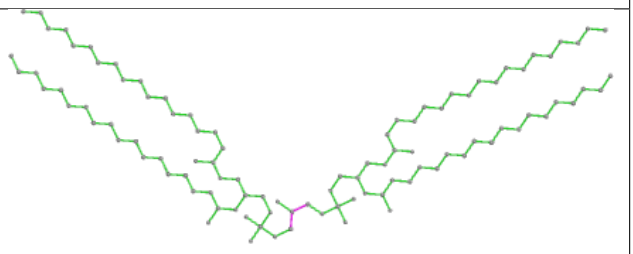


Rings

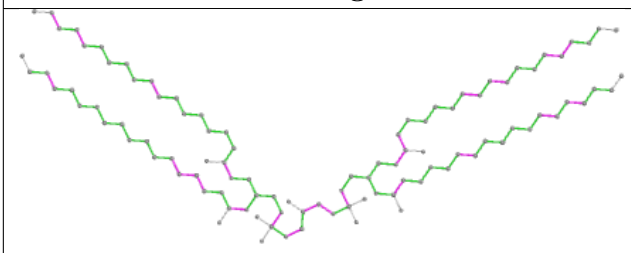
Ligand CDL DV 402



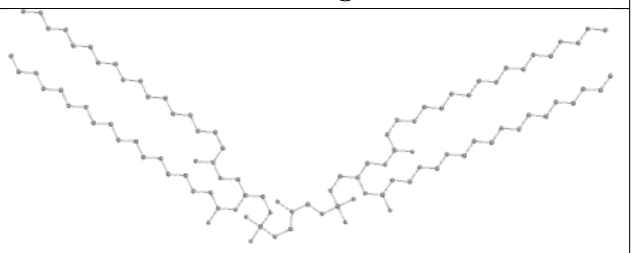
Bond lengths



Bond angles

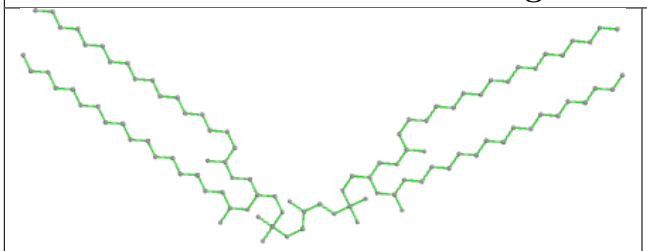


Torsions

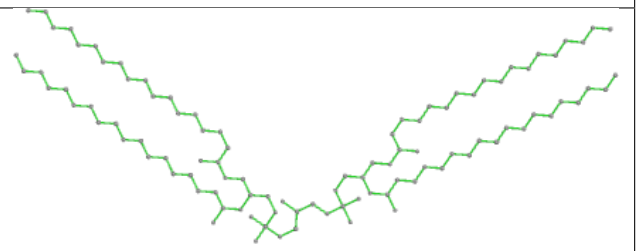


Rings

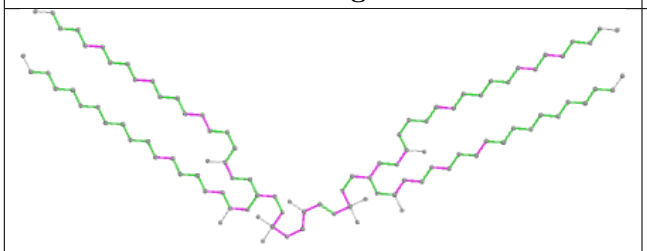
Ligand CDL C 503



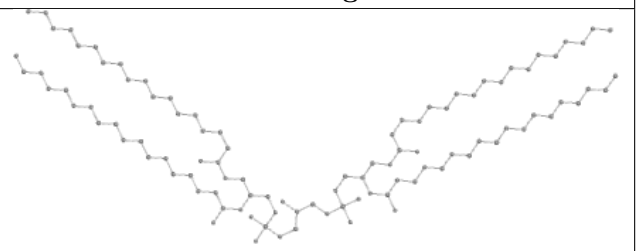
Bond lengths



Bond angles

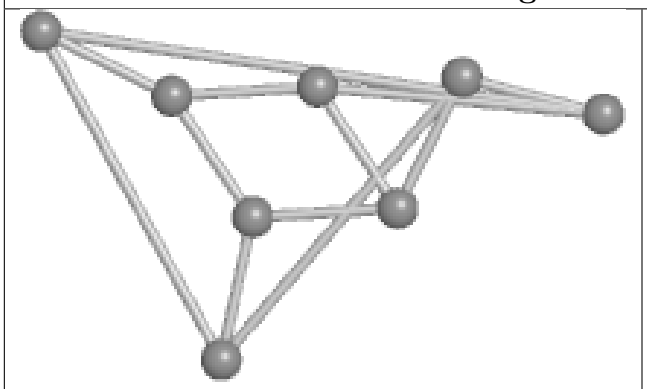


Torsions

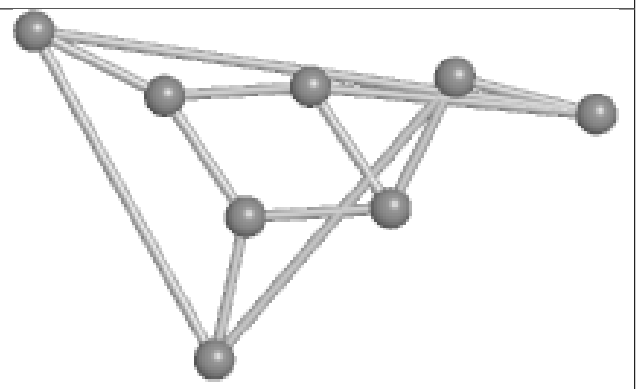


Rings

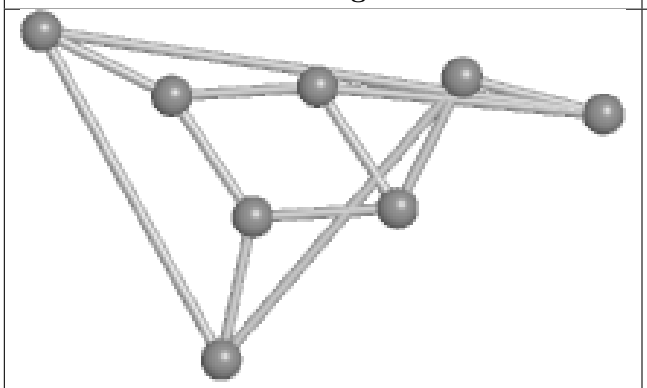
Ligand SF4 AB 802



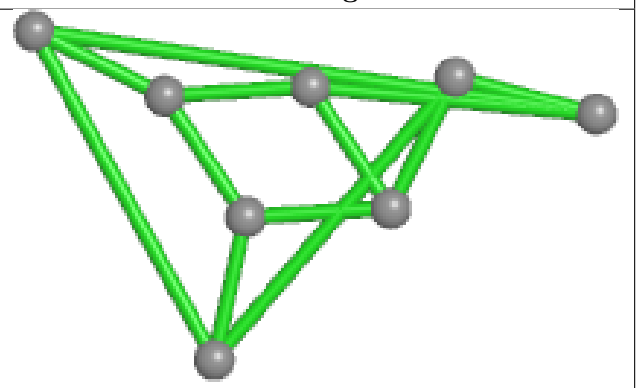
Bond lengths



Bond angles

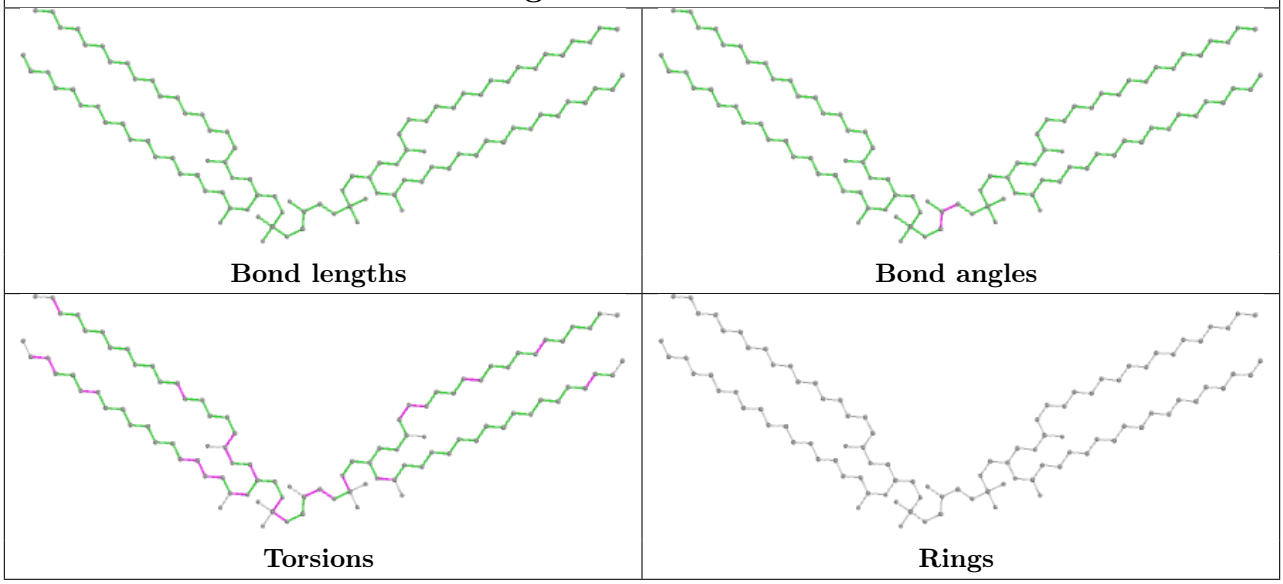


Torsions

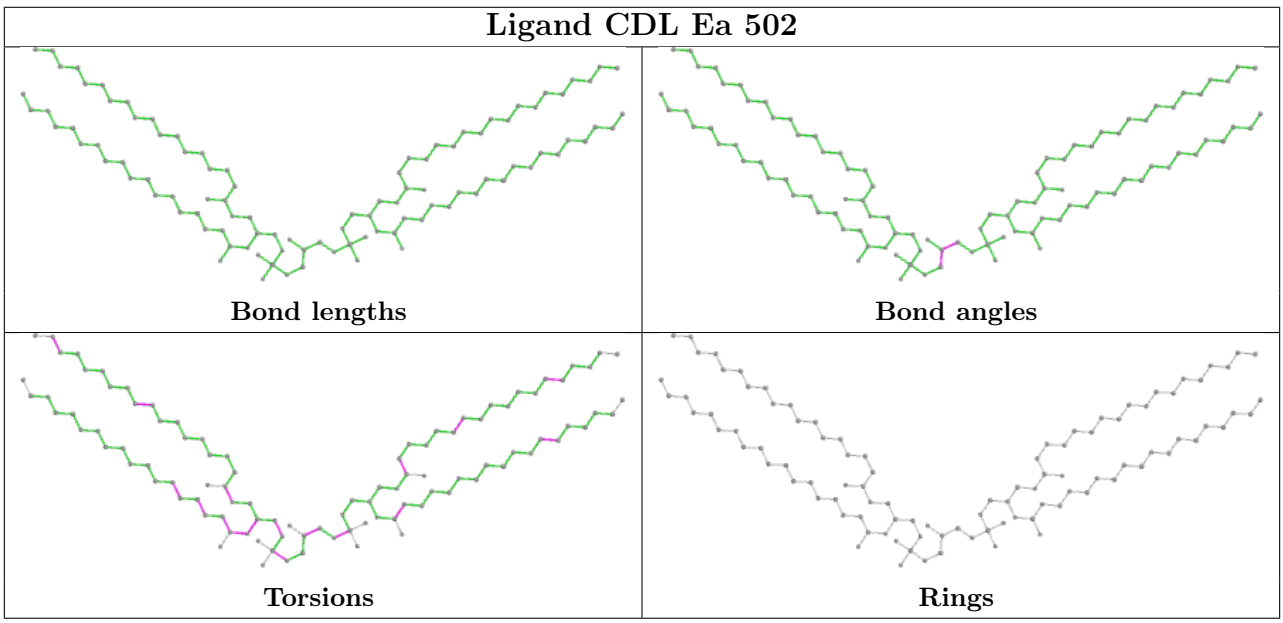


Rings

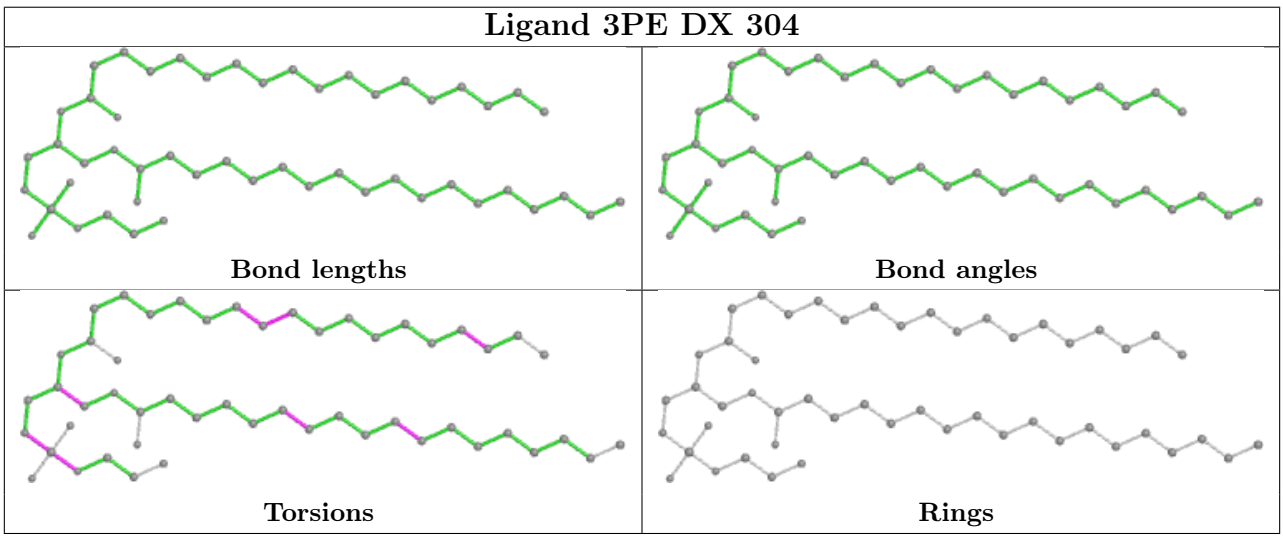
Ligand CDL C 506



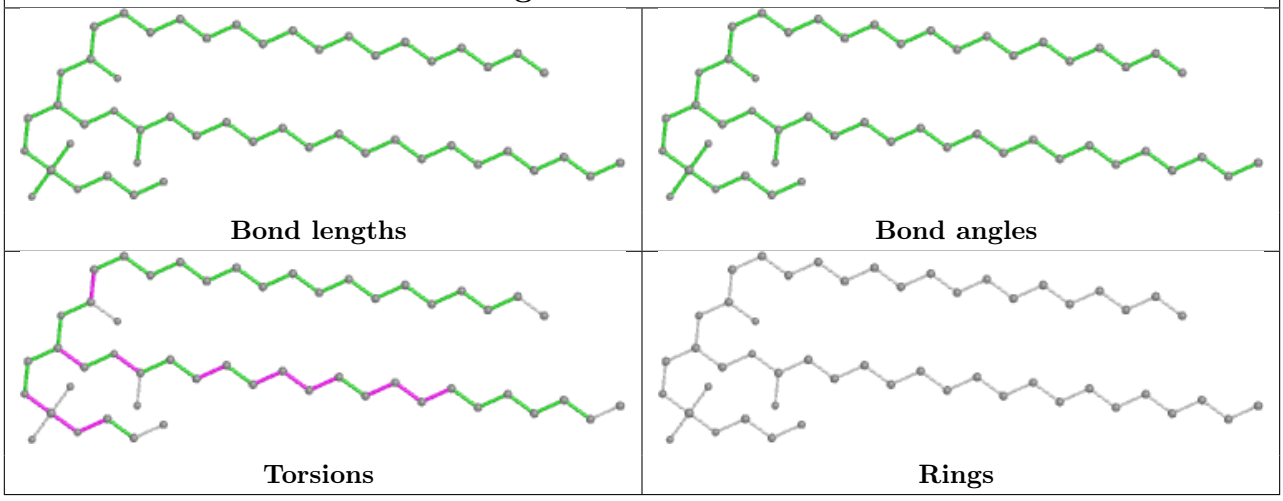
Ligand CDL Ea 502



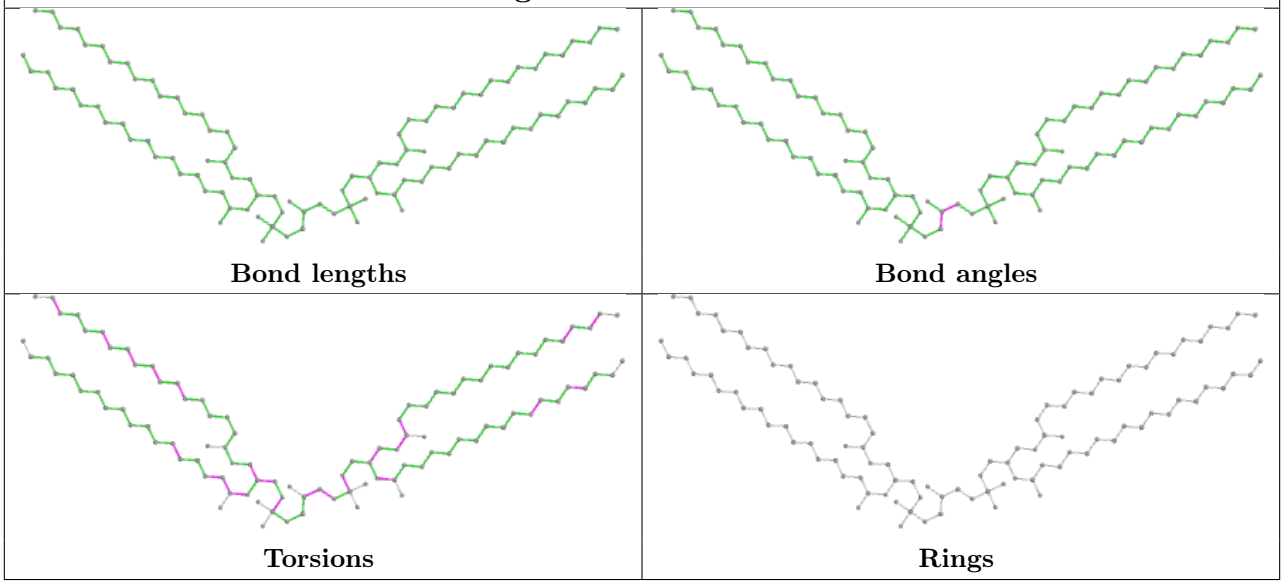
Ligand 3PE DX 304



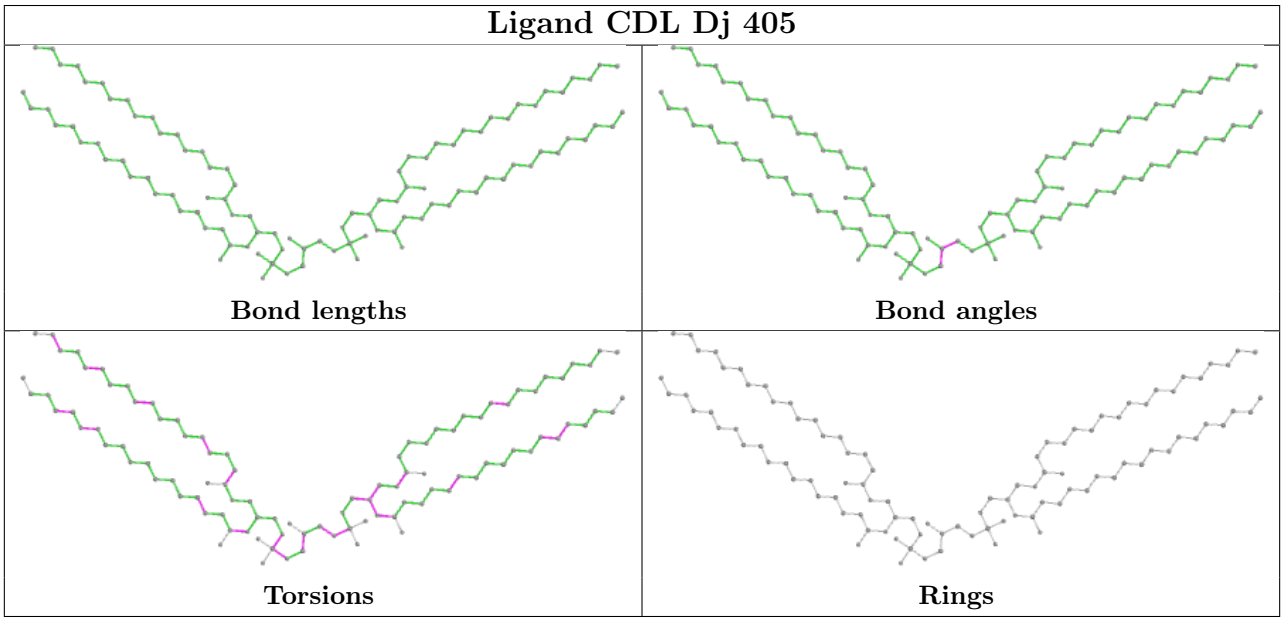
Ligand 3PE Di 1102



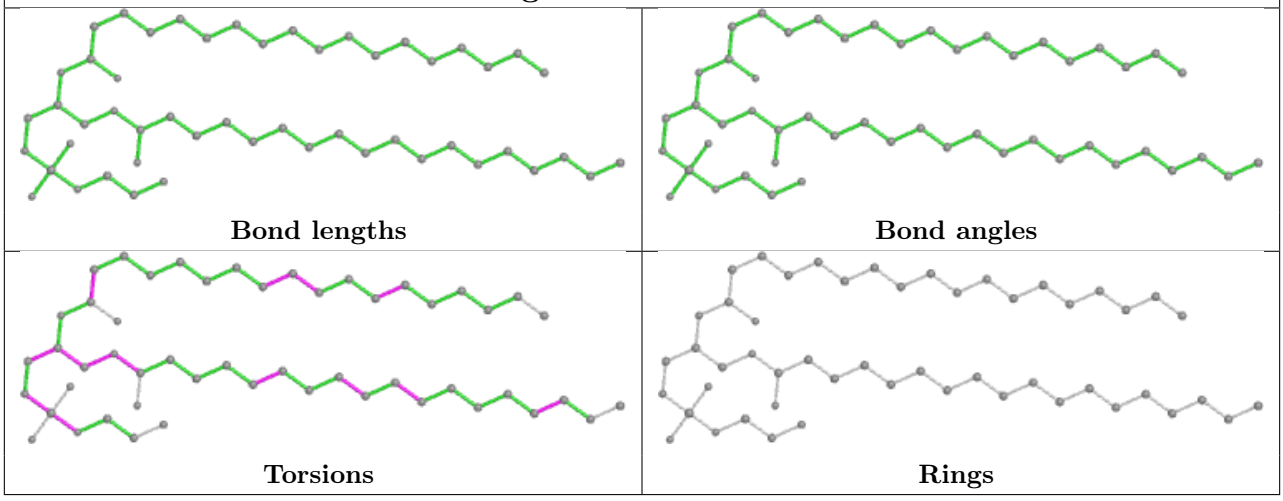
Ligand CDL Dd 705



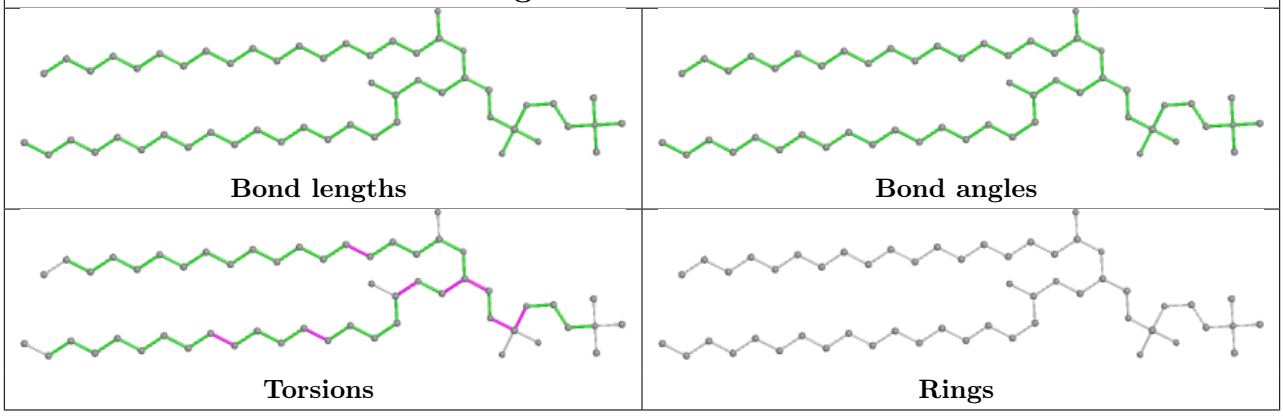
Ligand CDL Dj 405



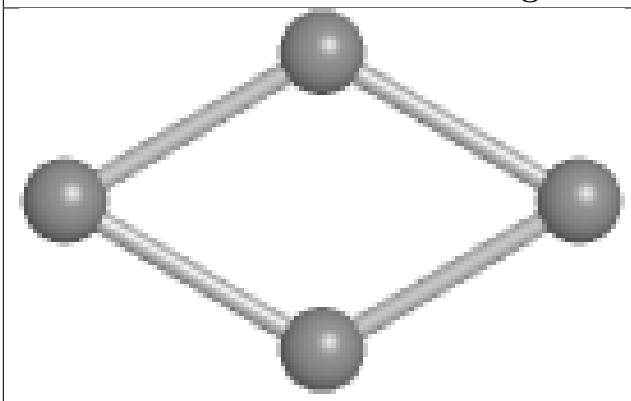
Ligand 3PE Ds 403



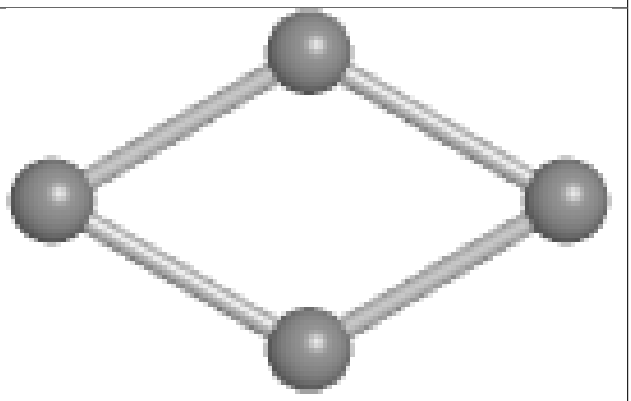
Ligand PC1 AA 903



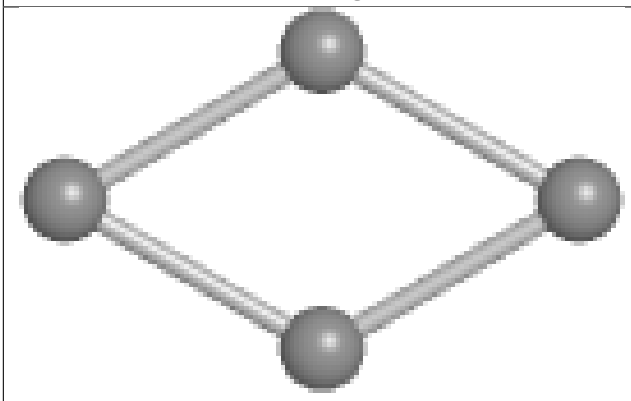
Ligand FES AI 301



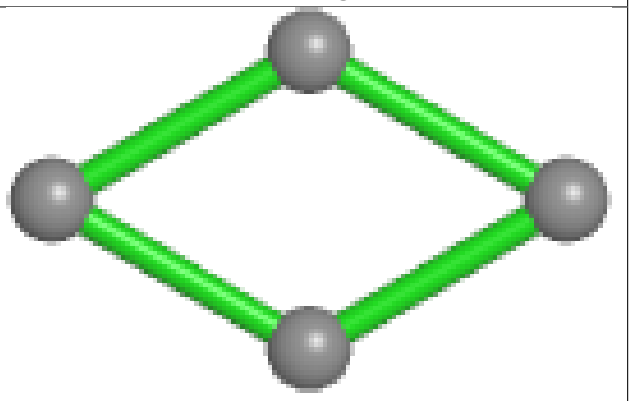
Bond lengths



Bond angles

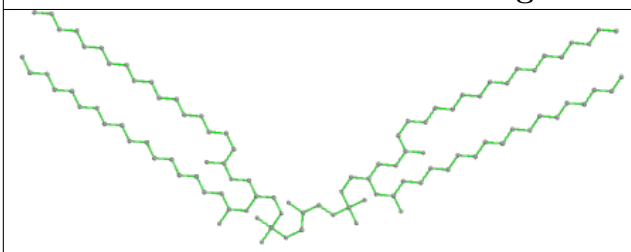


Torsions

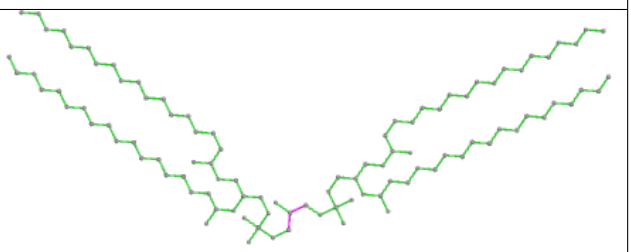


Rings

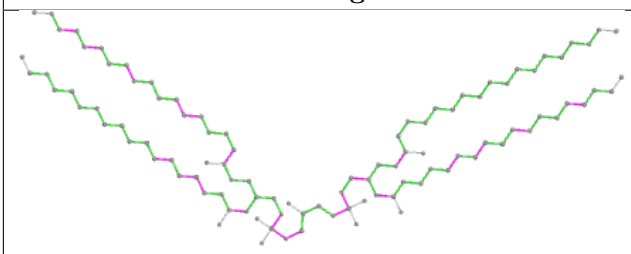
Ligand CDL Ds 406



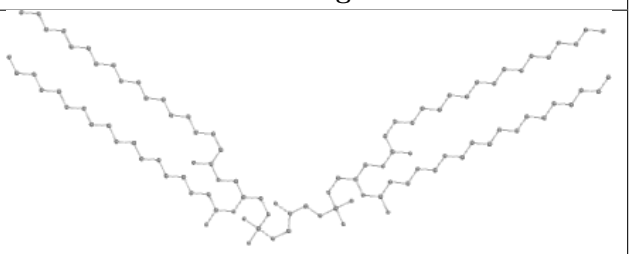
Bond lengths



Bond angles

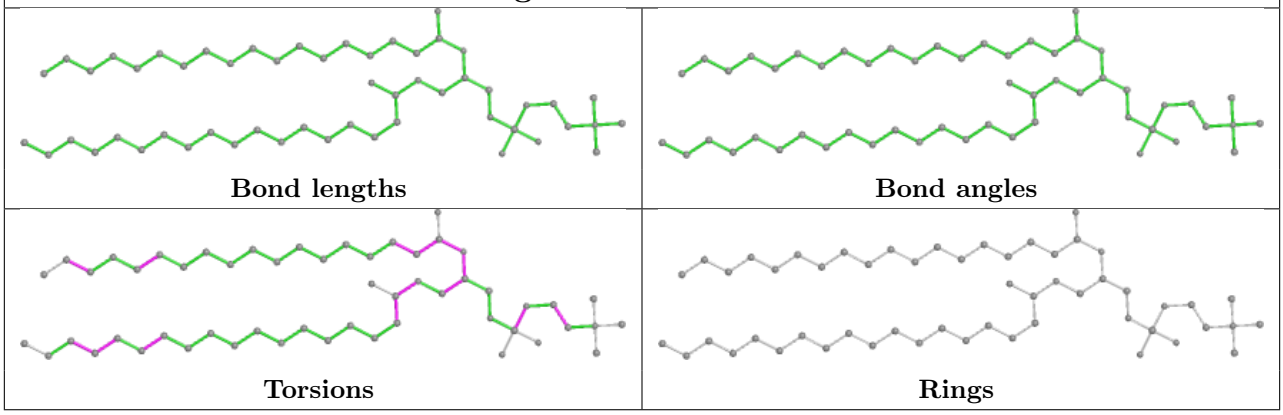


Torsions

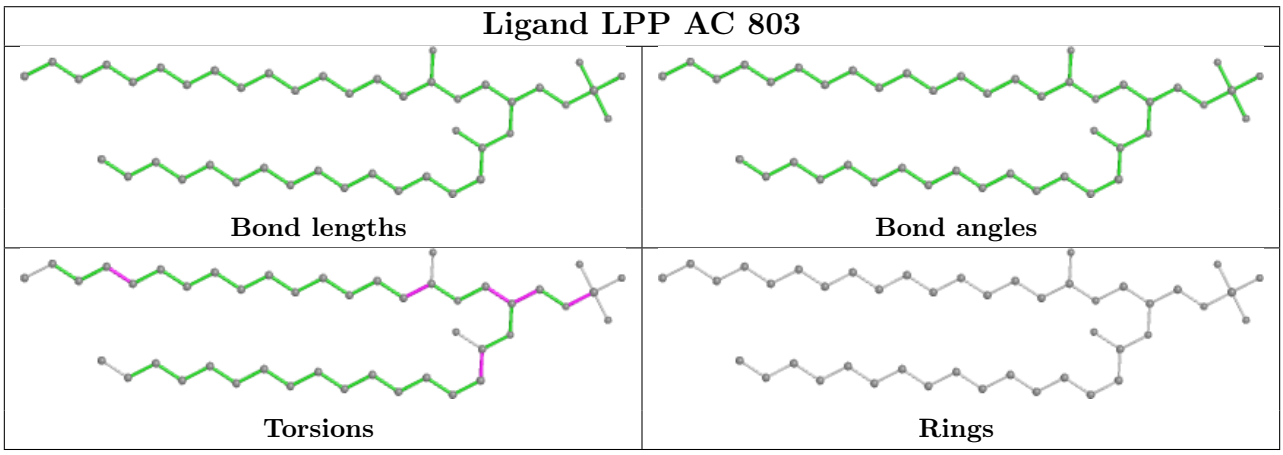


Rings

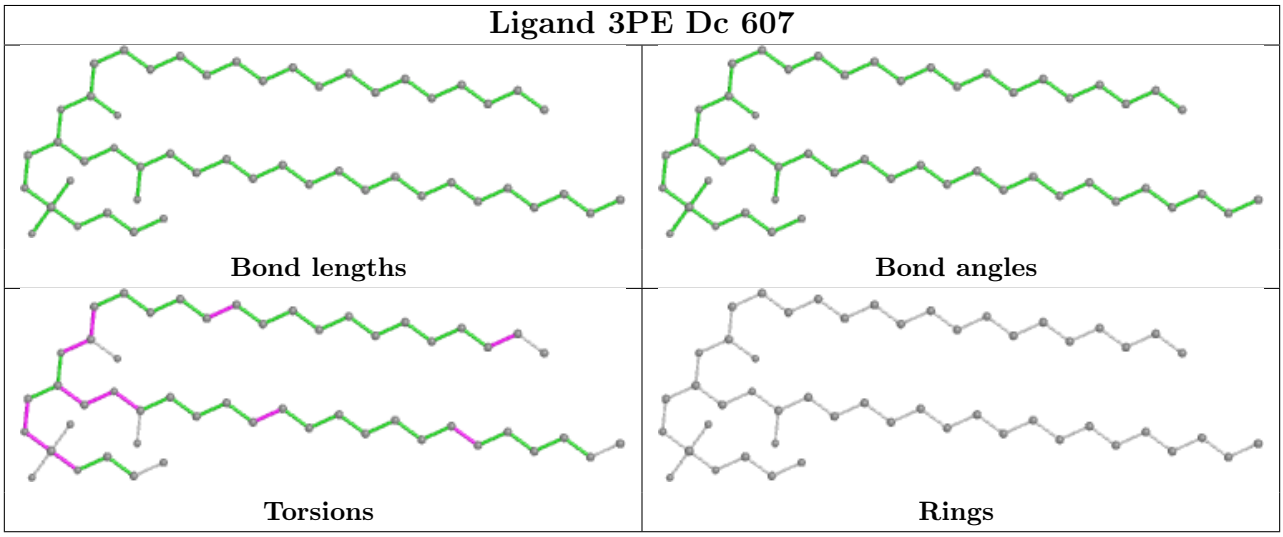
Ligand PC1 AA 906



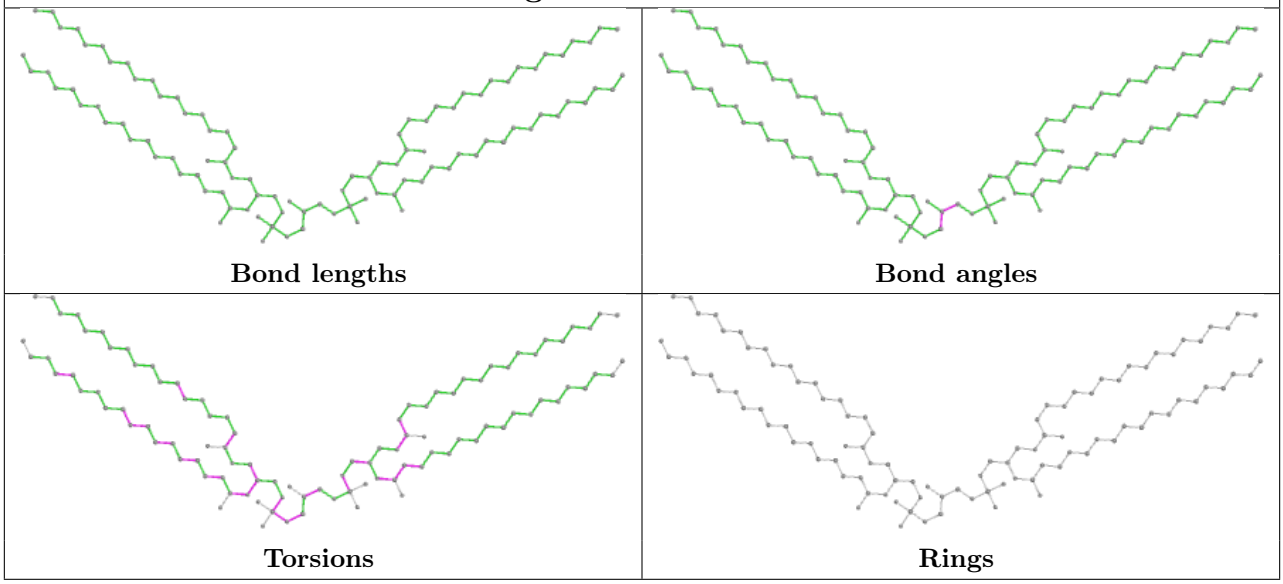
Ligand LPP AC 803



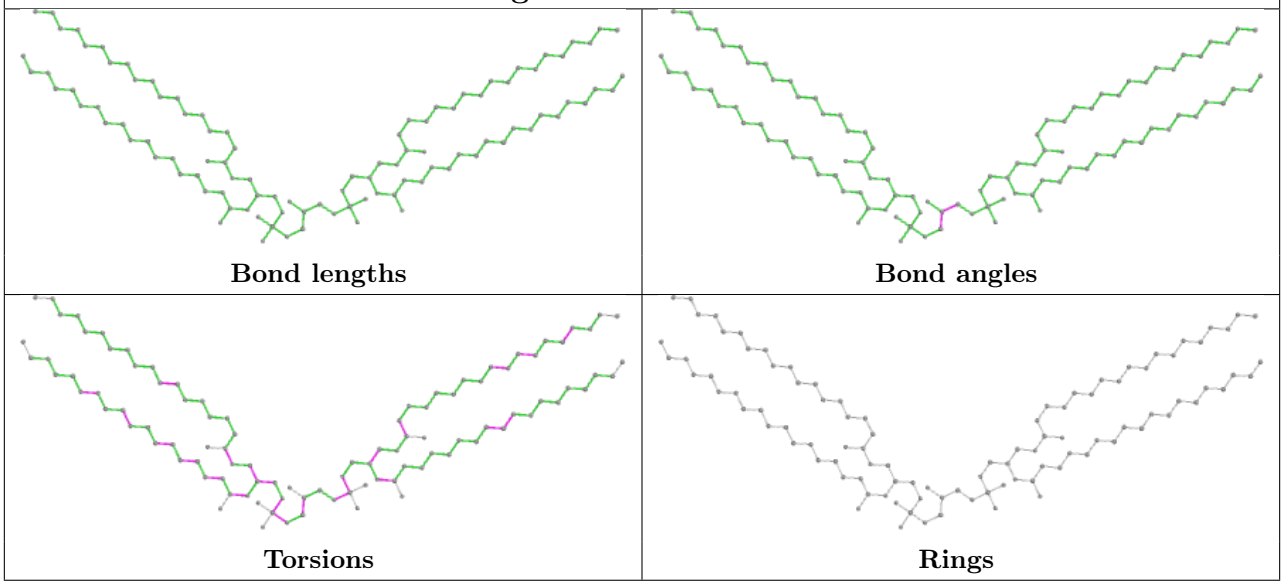
Ligand 3PE Dc 607



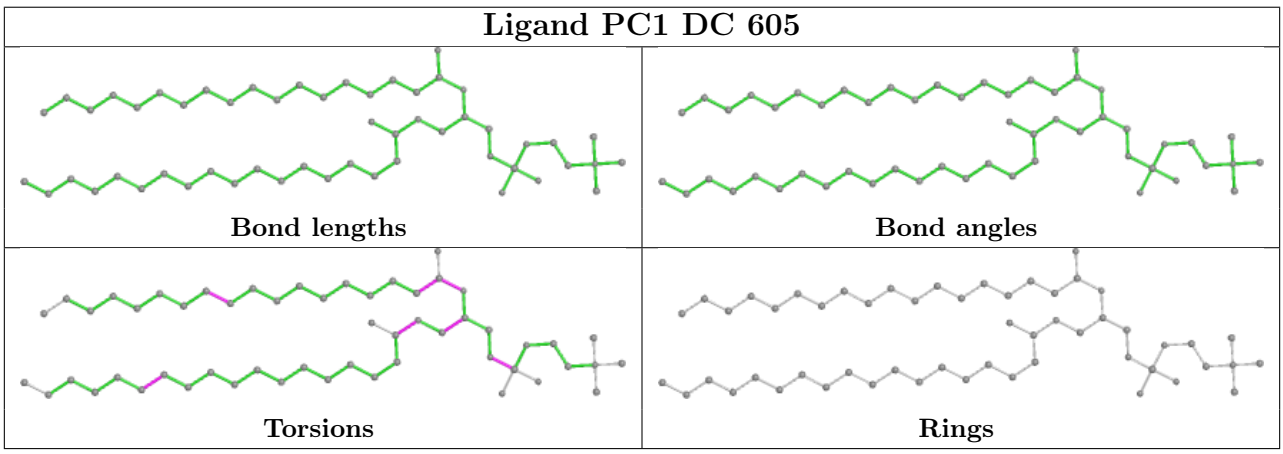
Ligand CDL C 507



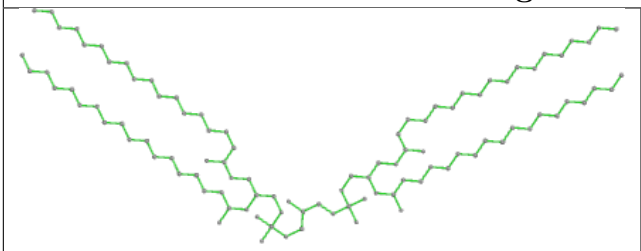
Ligand CDL DY 301



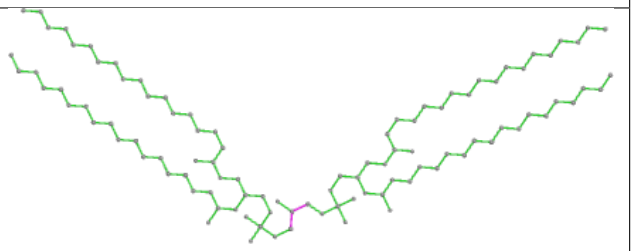
Ligand PC1 DC 605



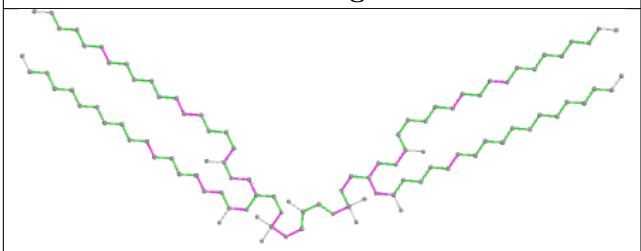
Ligand CDL Ek 201



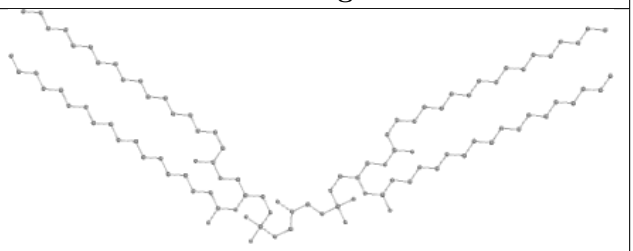
Bond lengths



Bond angles

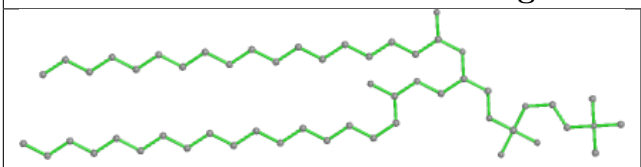


Torsions

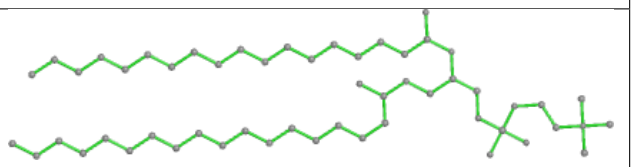


Rings

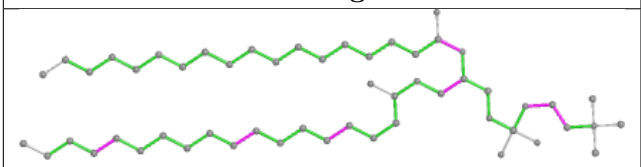
Ligand PC1 A2 402



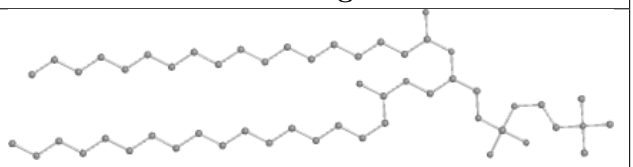
Bond lengths



Bond angles

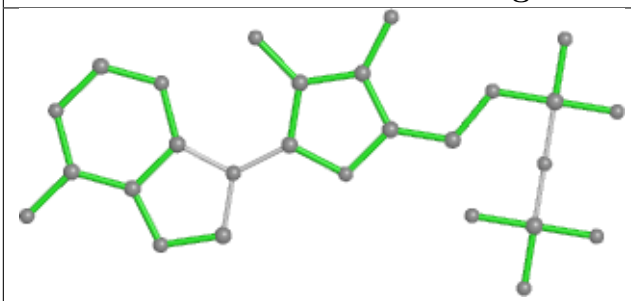


Torsions

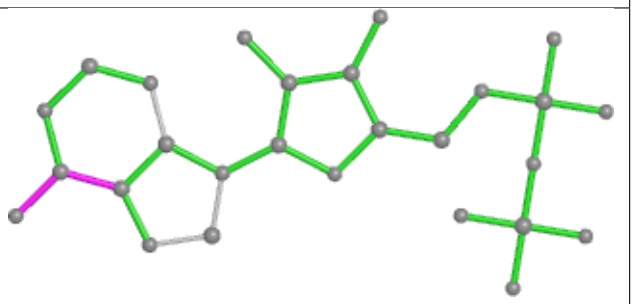


Rings

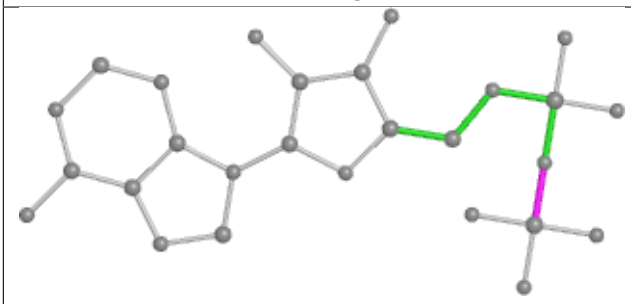
Ligand ADP A8 401



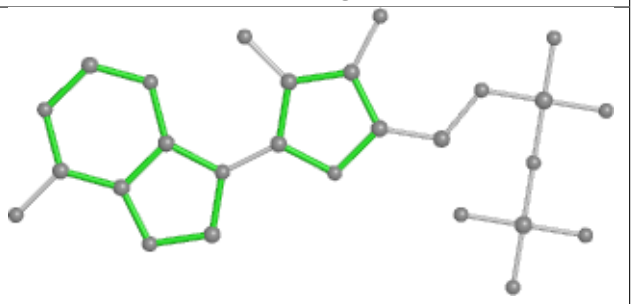
Bond lengths



Bond angles

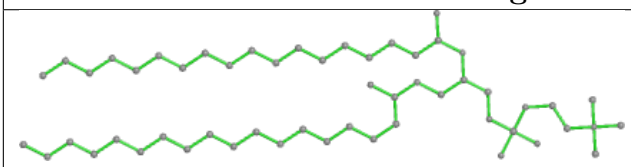


Torsions

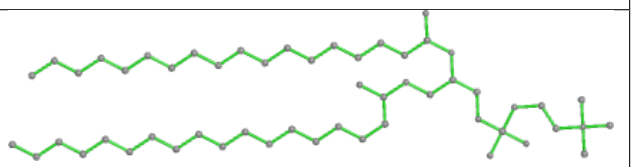


Rings

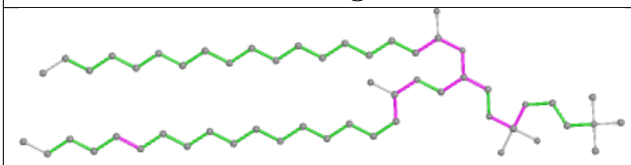
Ligand PC1 AM 302



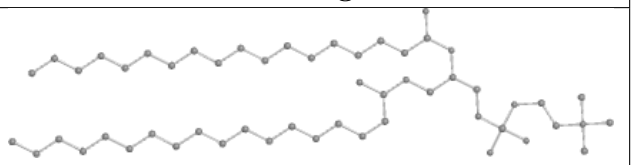
Bond lengths



Bond angles

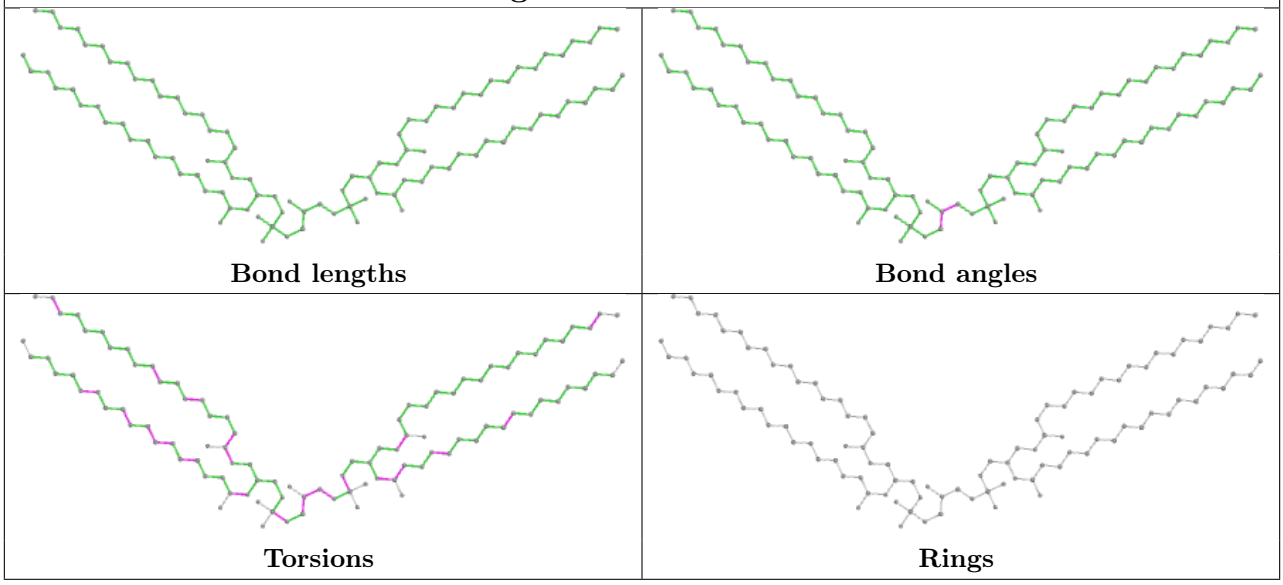


Torsions

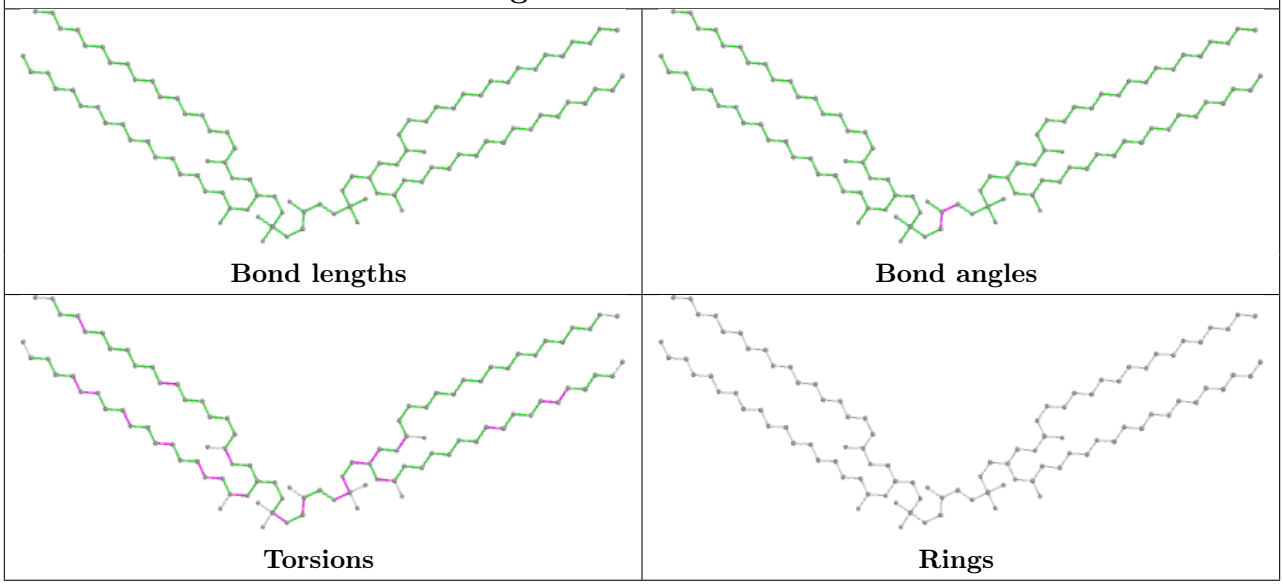


Rings

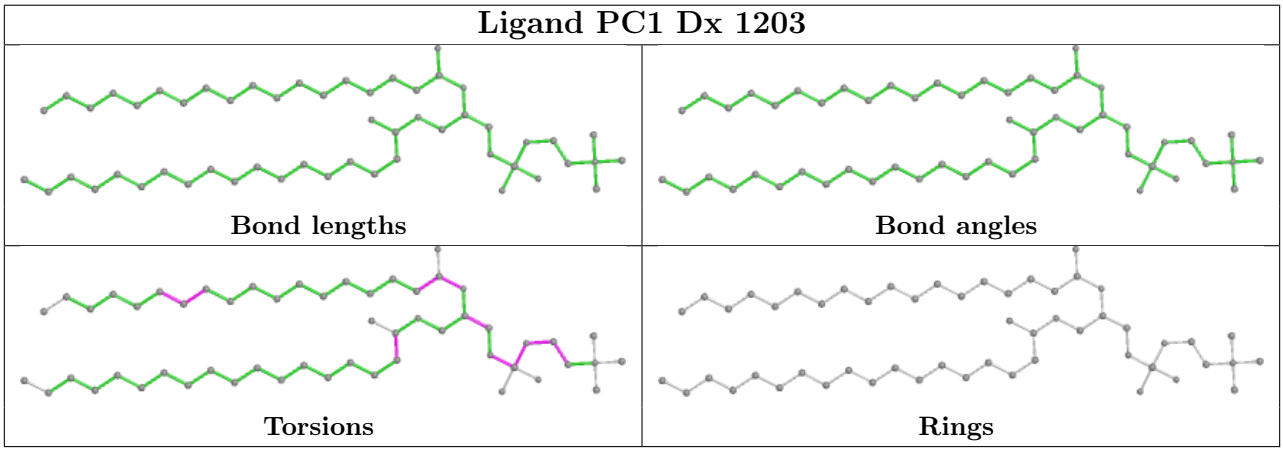
Ligand CDL DU 403



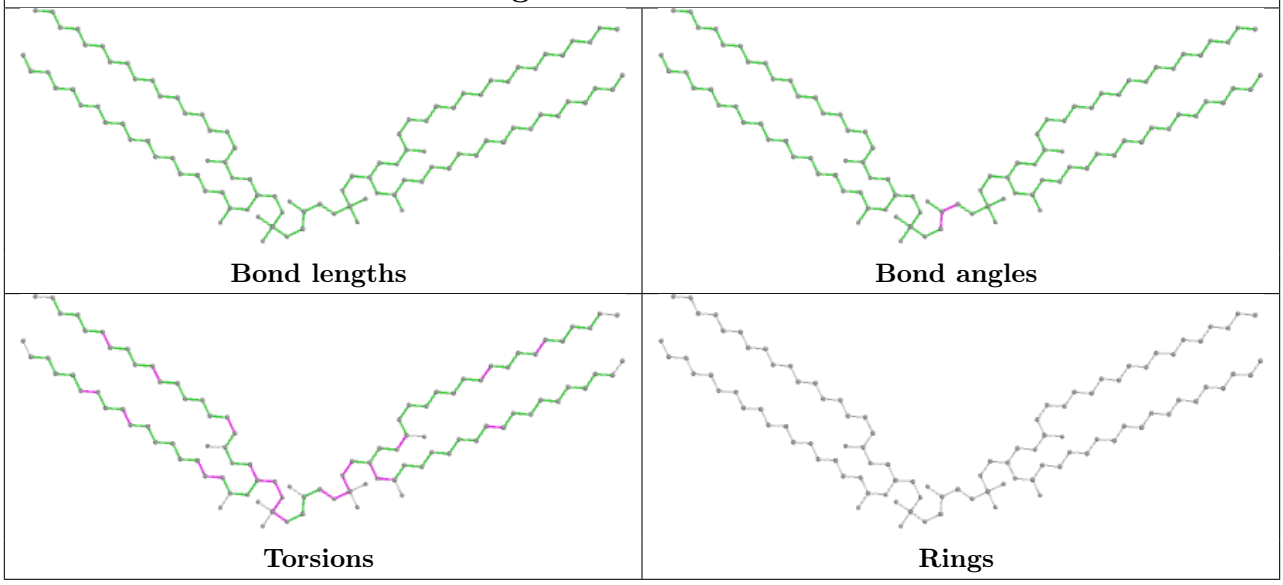
Ligand CDL DU 402



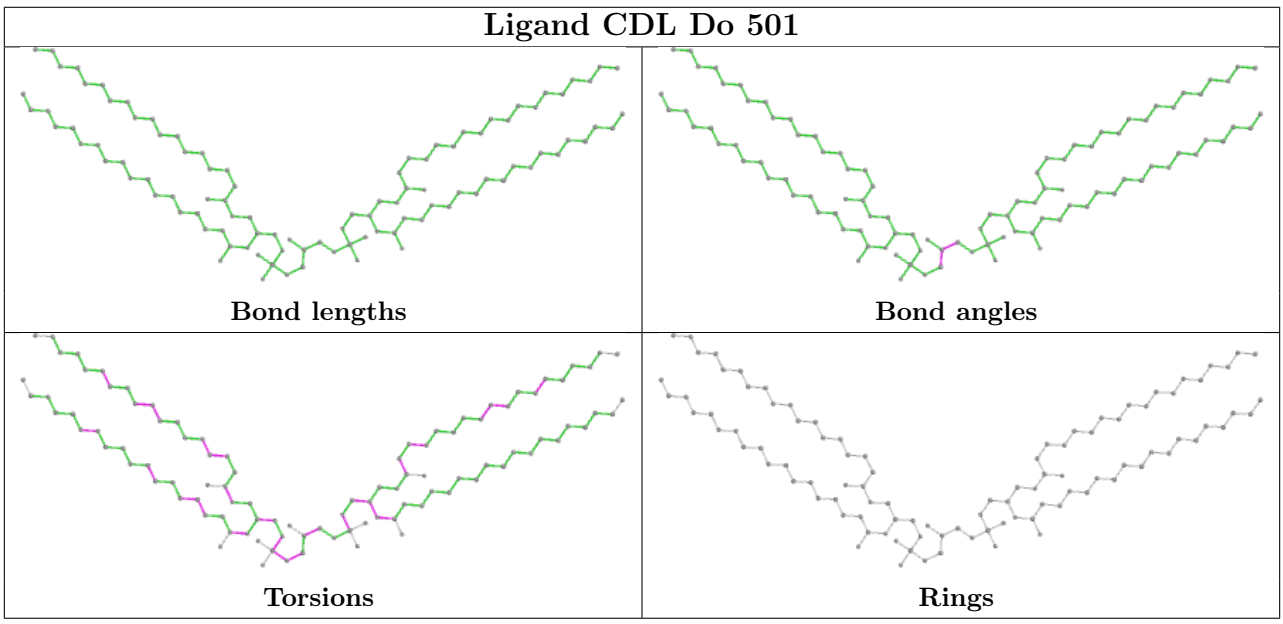
Ligand PC1 Dx 1203



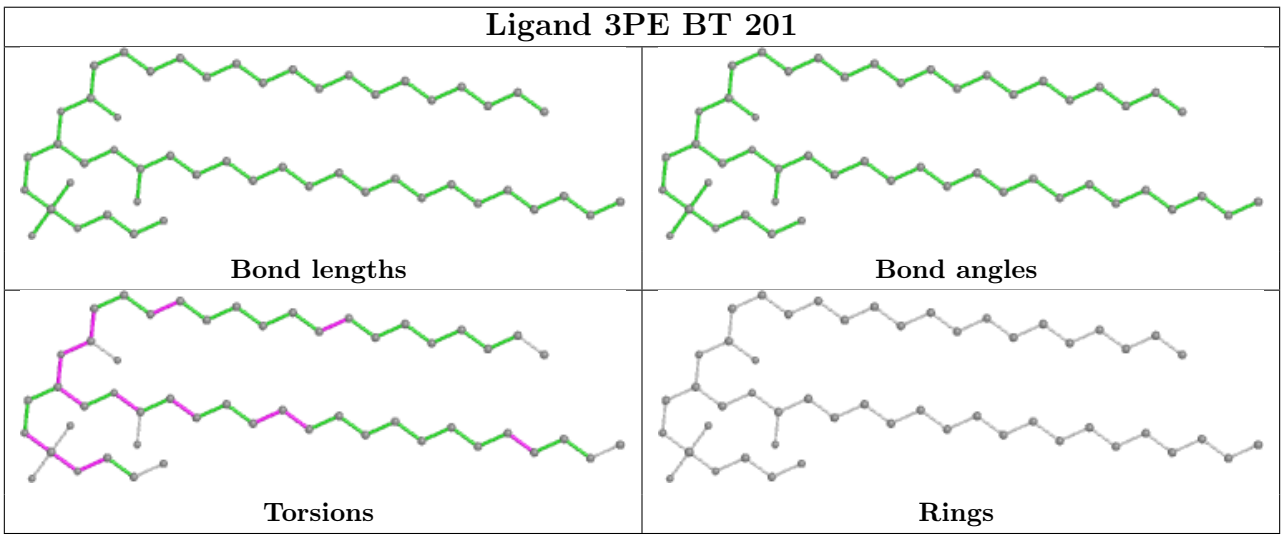
Ligand CDL BY 201



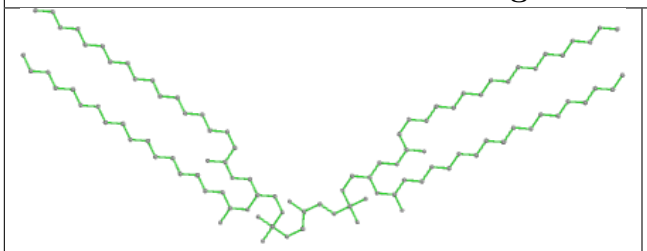
Ligand CDL Do 501



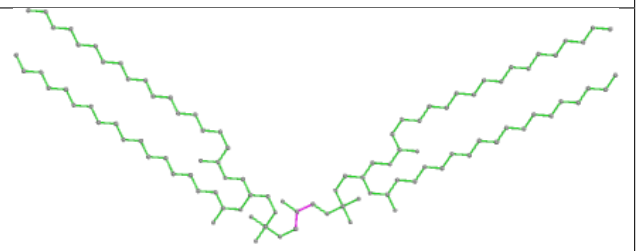
Ligand 3PE BT 201



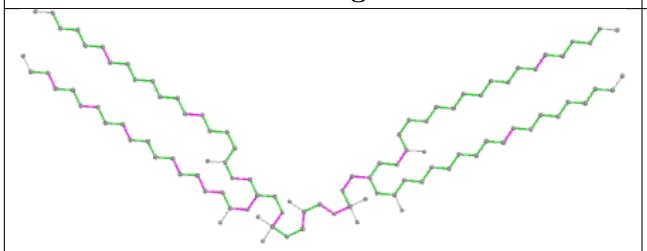
Ligand CDL DU 404



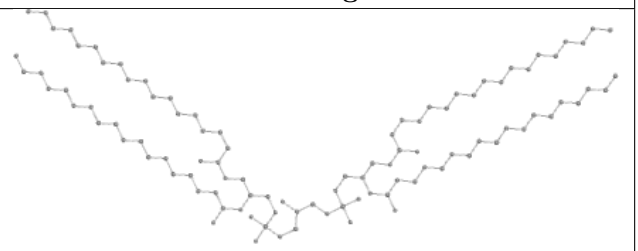
Bond lengths



Bond angles

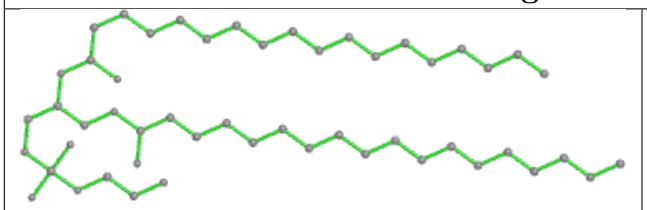


Torsions

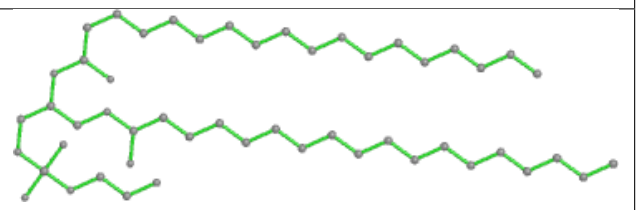


Rings

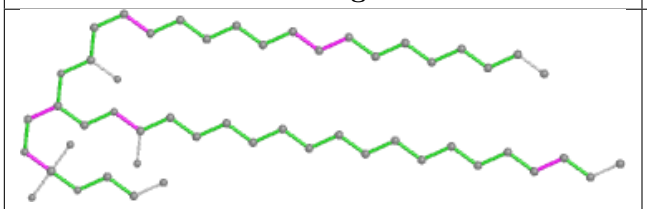
Ligand 3PE Dr 404



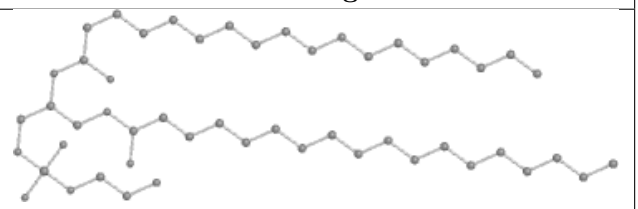
Bond lengths



Bond angles

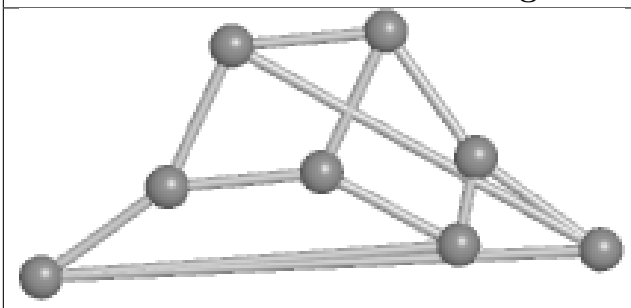


Torsions

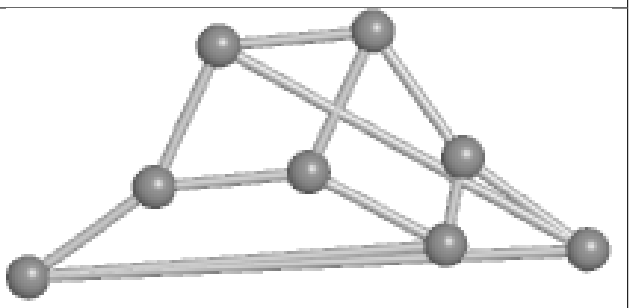


Rings

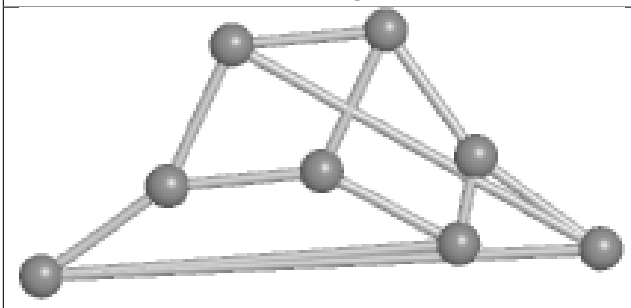
Ligand SF4 AT 201



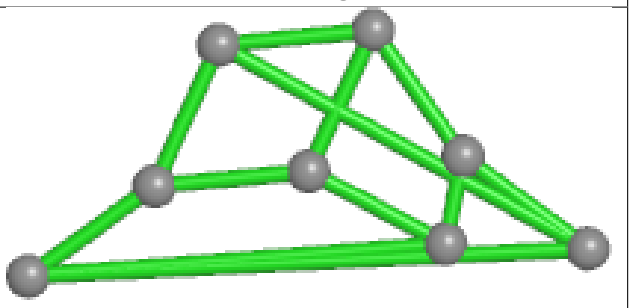
Bond lengths



Bond angles

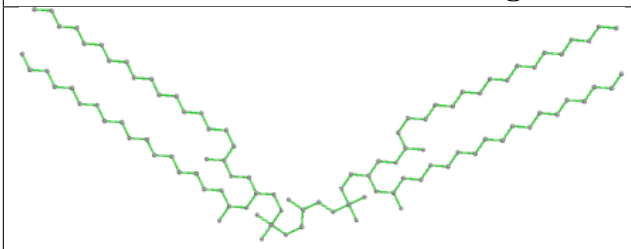


Torsions

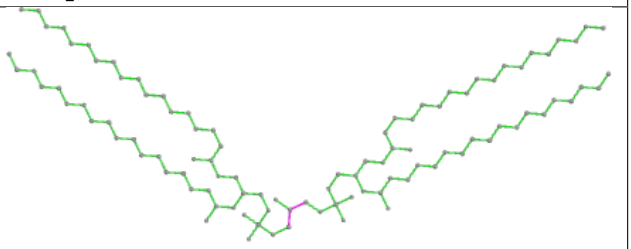


Rings

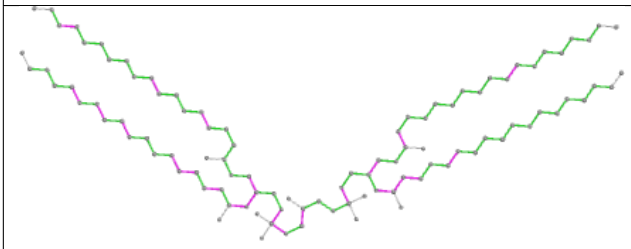
Ligand CDL Dq 1402



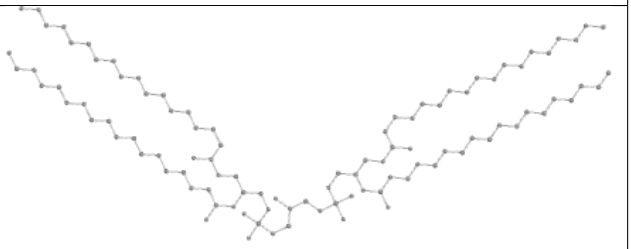
Bond lengths



Bond angles

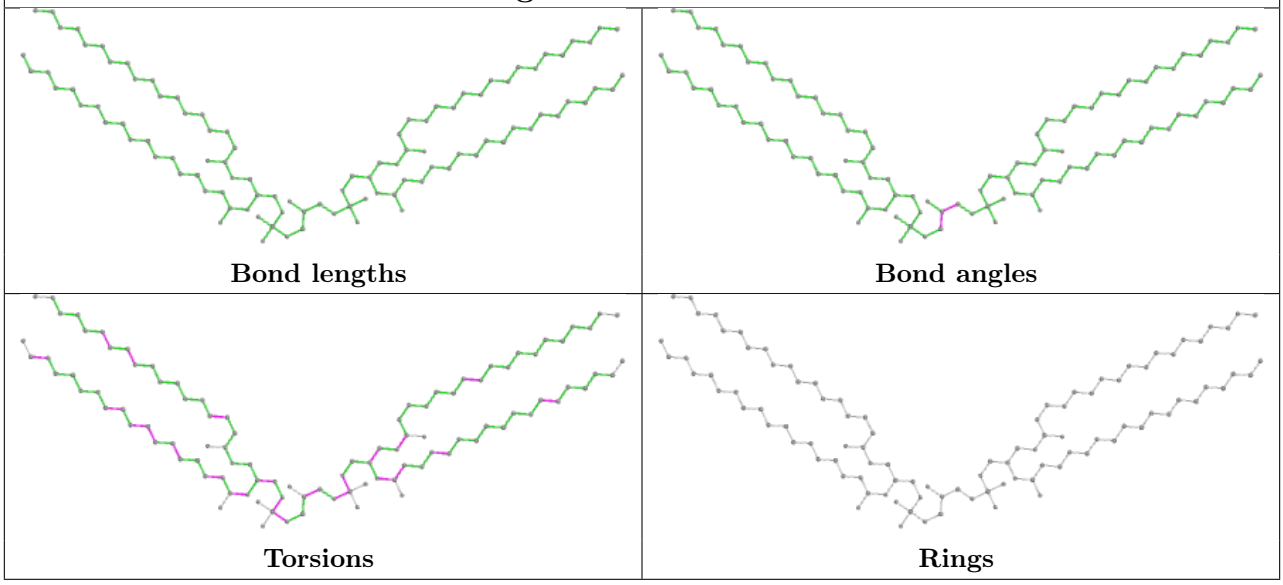


Torsions

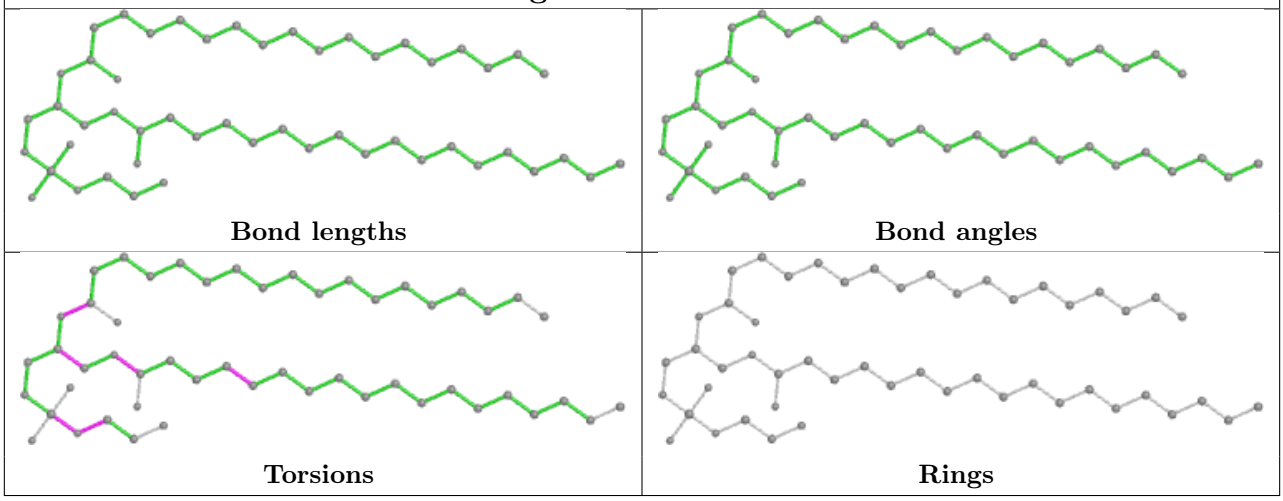


Rings

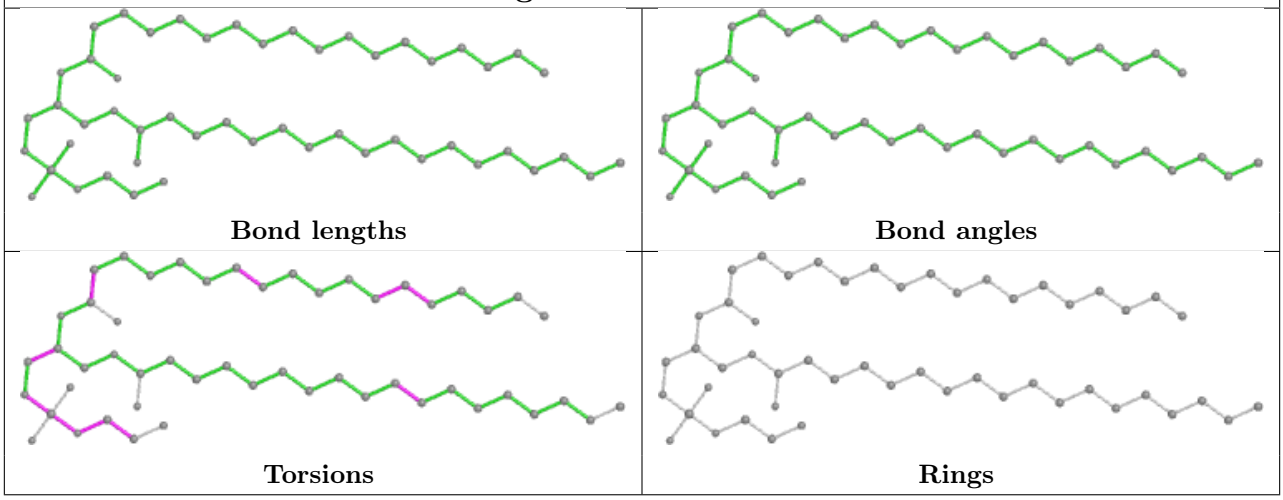
Ligand CDL B0 101



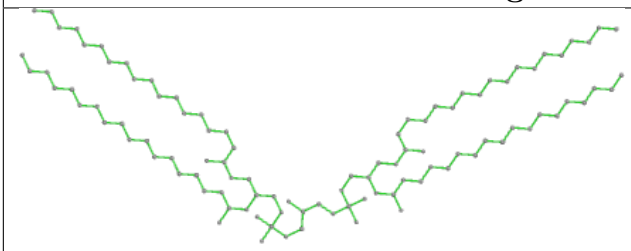
Ligand 3PE C 513



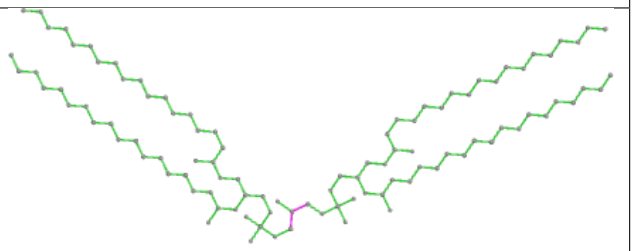
Ligand 3PE DX 302



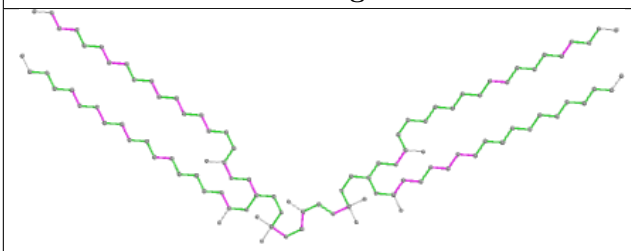
Ligand CDL En 1201



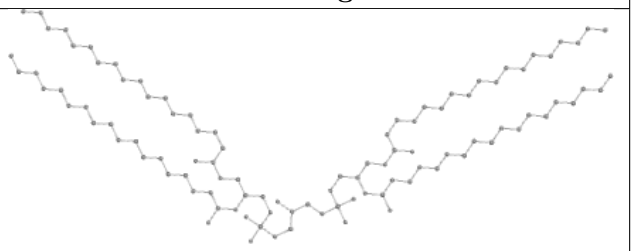
Bond lengths



Bond angles

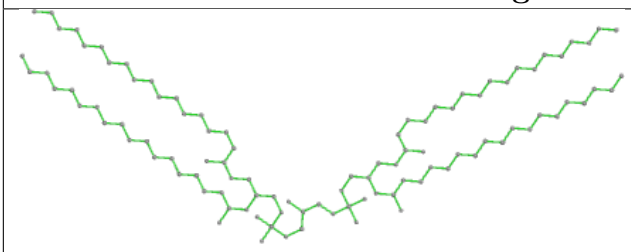


Torsions

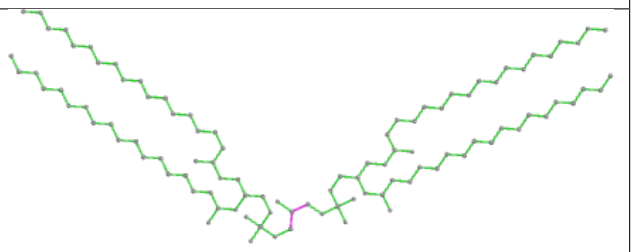


Rings

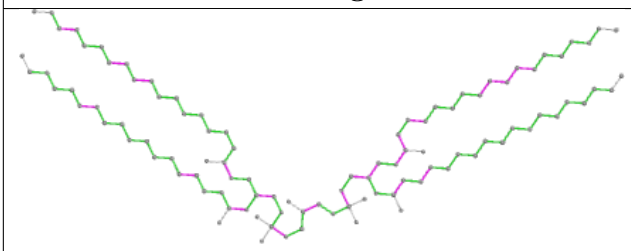
Ligand CDL AF 402



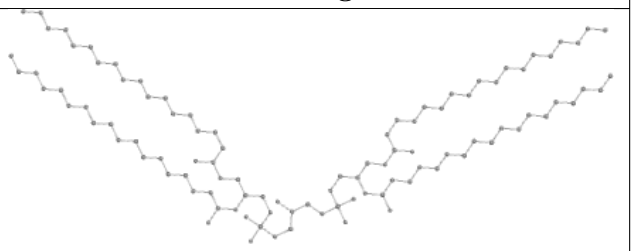
Bond lengths



Bond angles

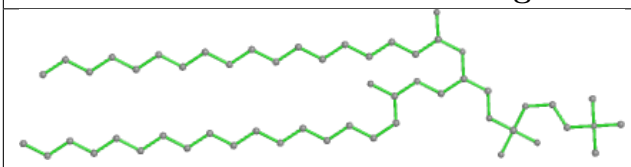


Torsions

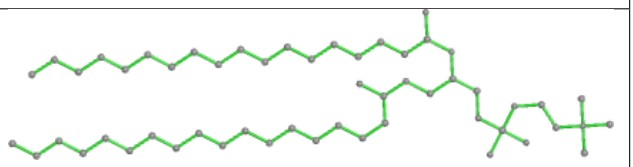


Rings

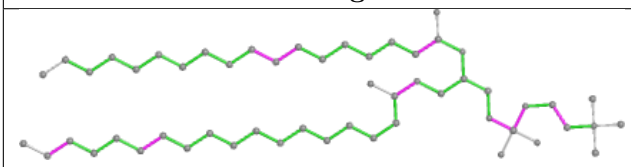
Ligand PC1 DC 604



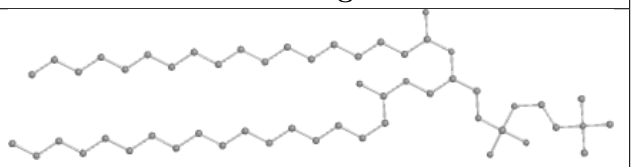
Bond lengths



Bond angles

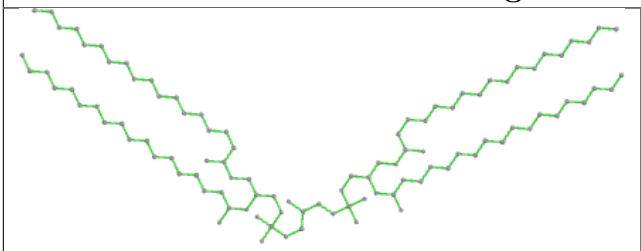


Torsions

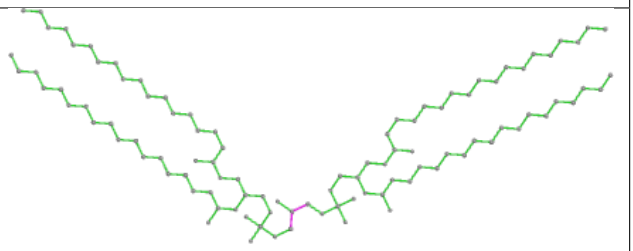


Rings

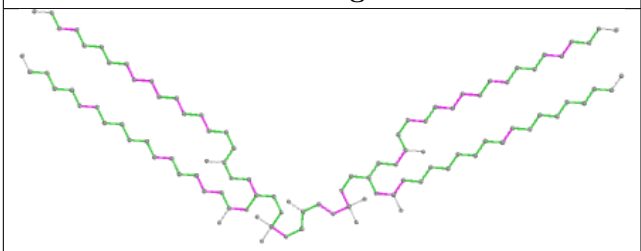
Ligand CDL Dx 1201



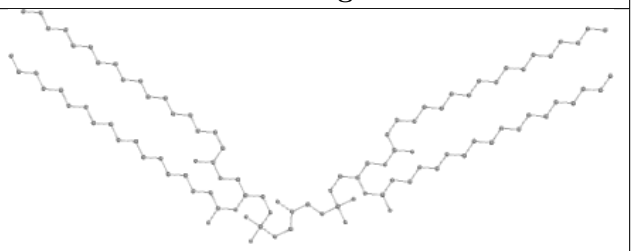
Bond lengths



Bond angles

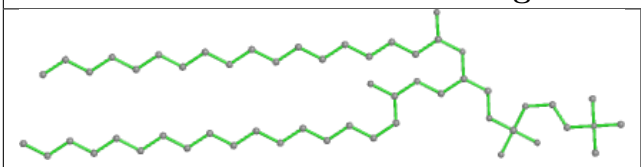


Torsions

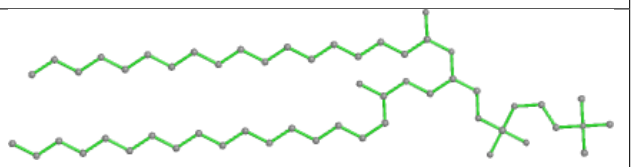


Rings

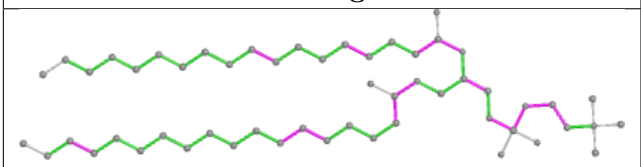
Ligand PC1 BG 202



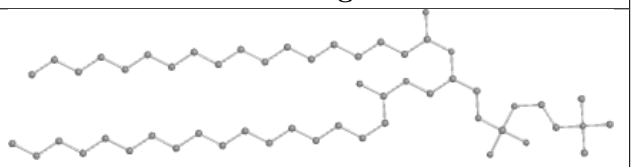
Bond lengths



Bond angles

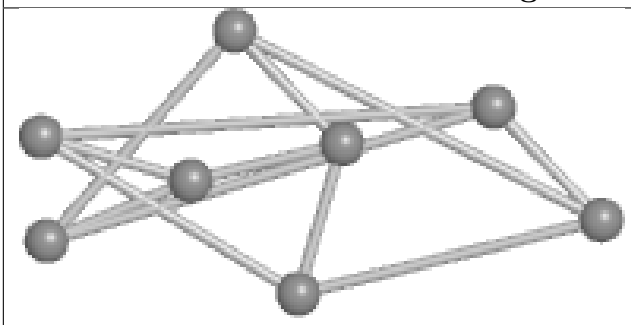


Torsions

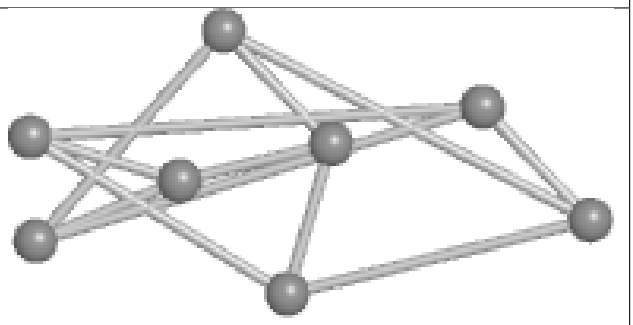


Rings

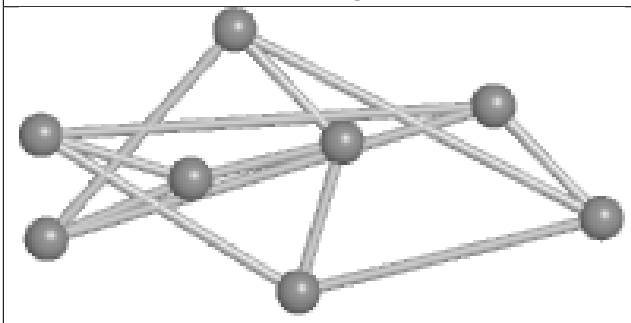
Ligand SF4 AL 301



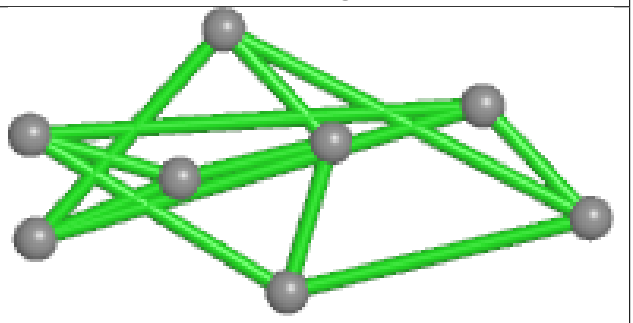
Bond lengths



Bond angles

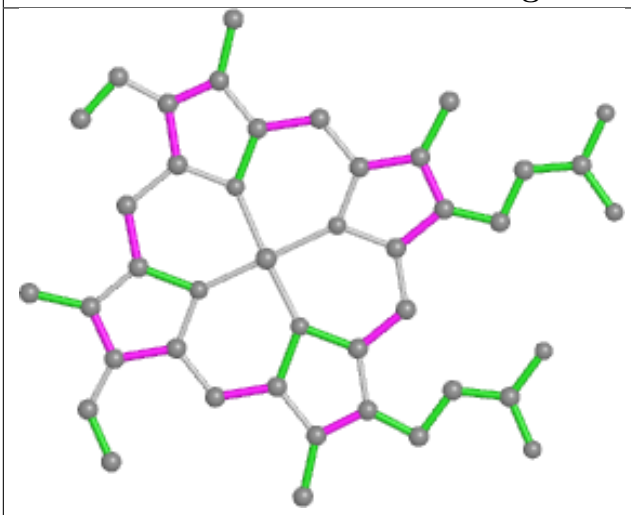


Torsions

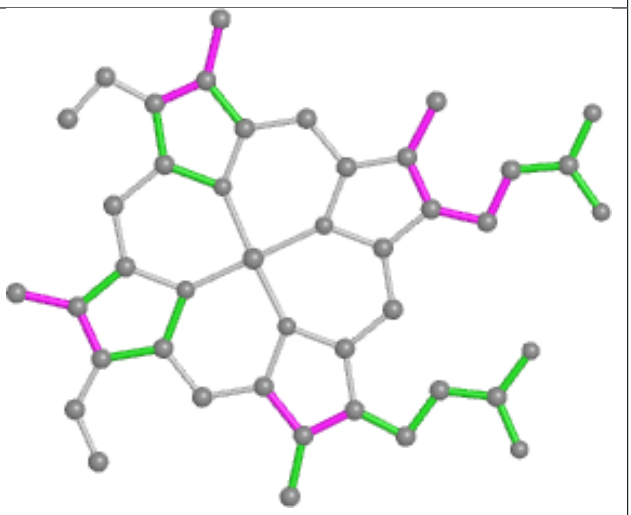


Rings

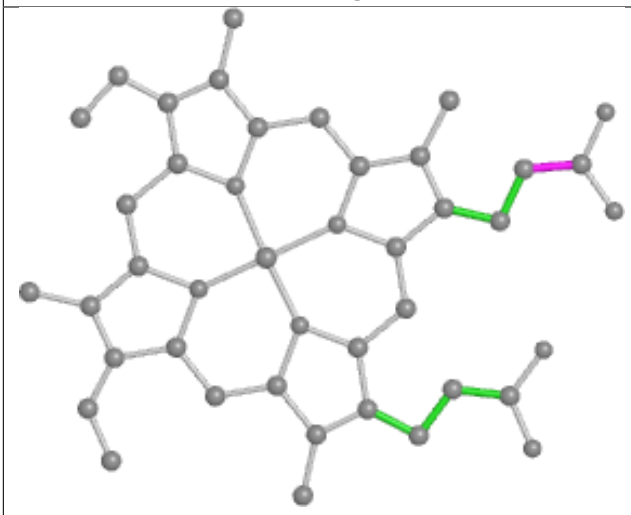
Ligand HEC D 401



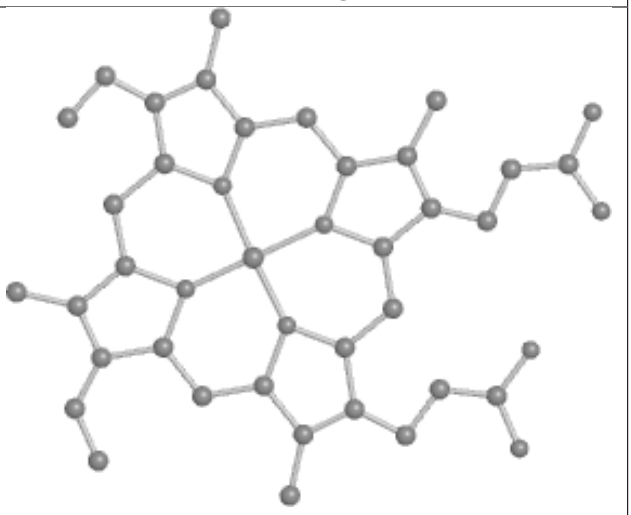
Bond lengths



Bond angles

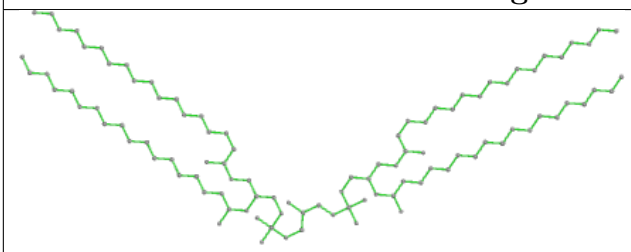


Torsions

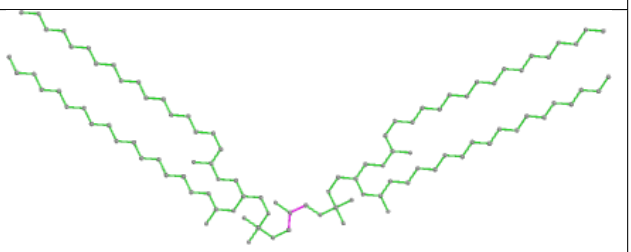


Rings

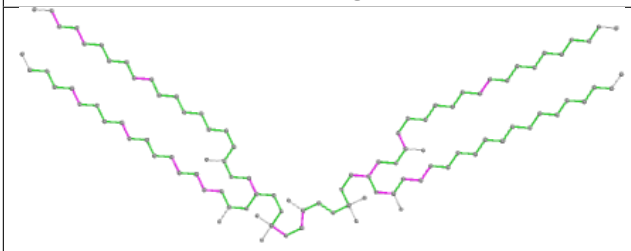
Ligand CDL BV 201



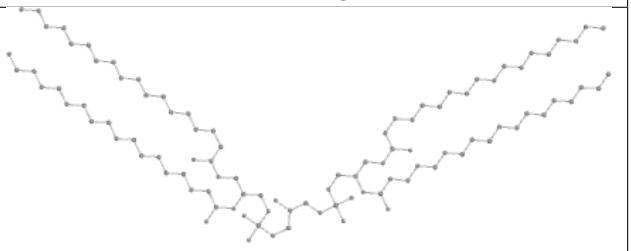
Bond lengths



Bond angles

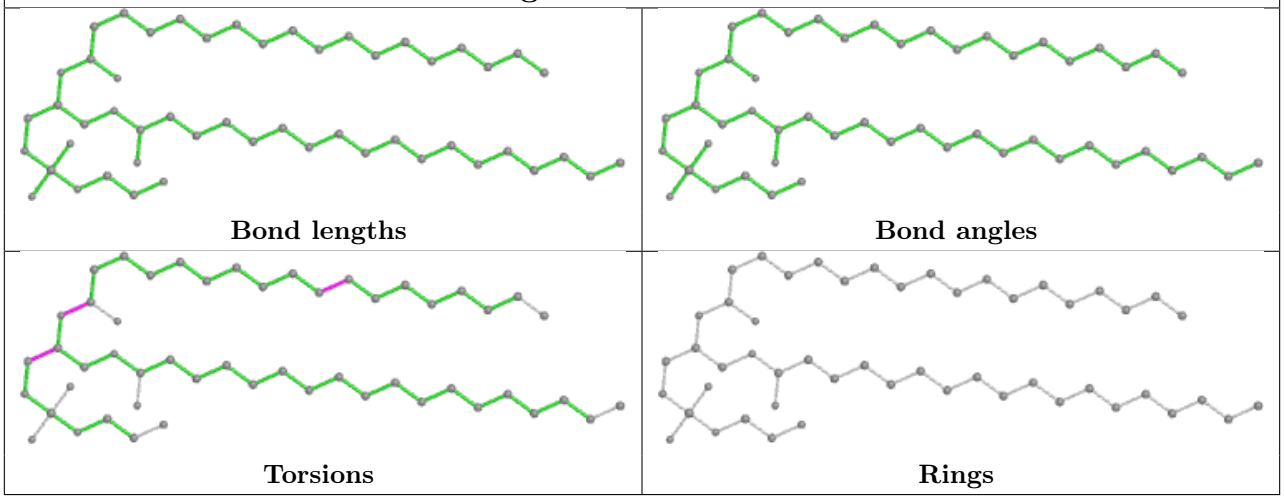


Torsions

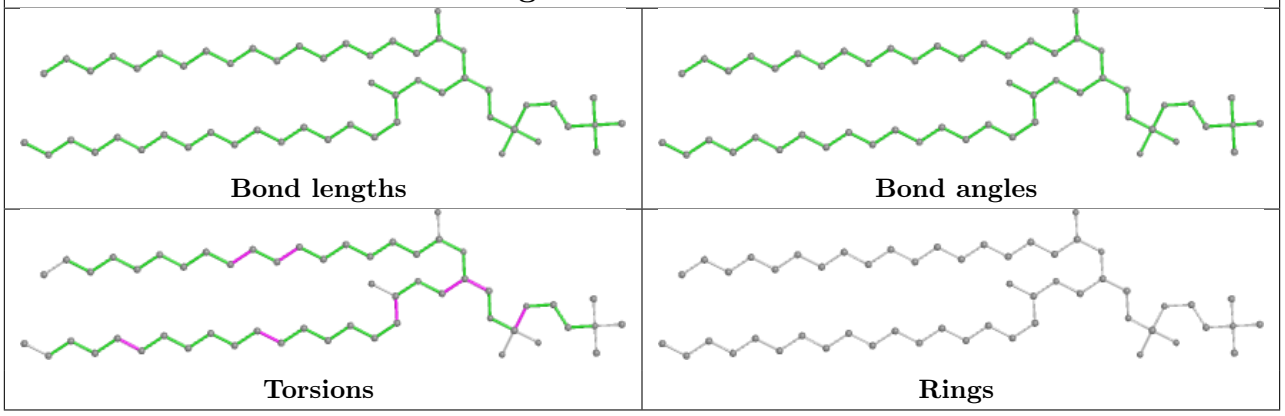


Rings

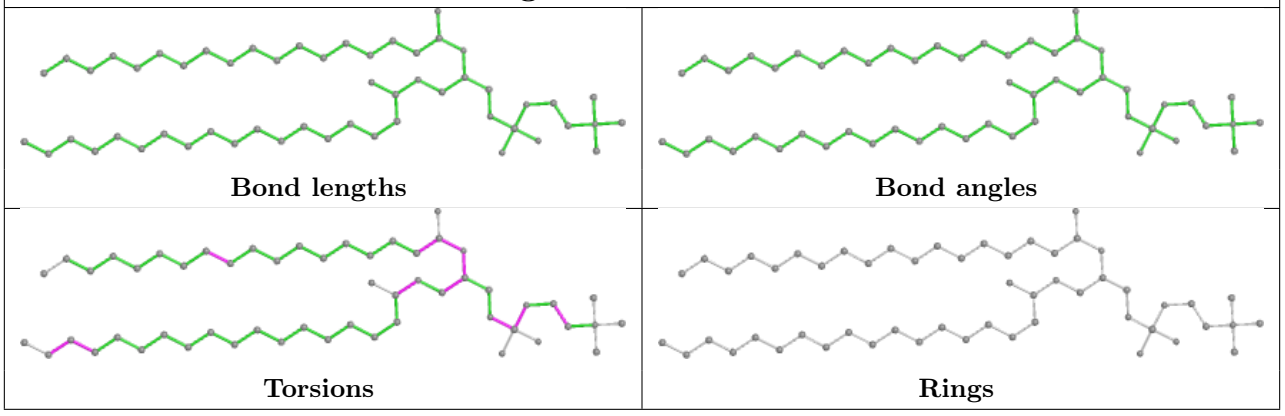
Ligand 3PE Dc 606



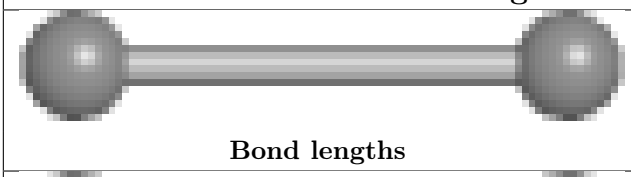
Ligand PC1 A6 302



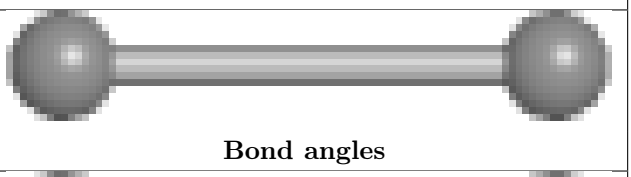
Ligand PC1 Dc 605



Ligand CUA Db 701



Bond lengths

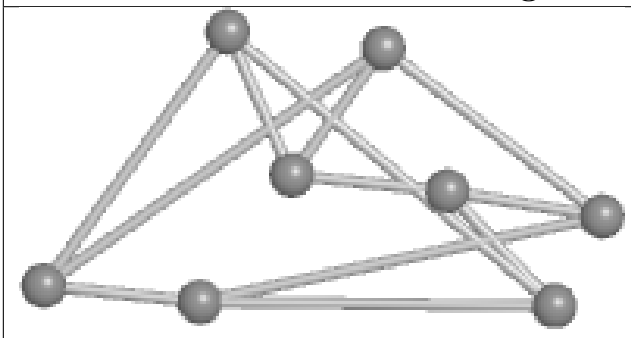


Bond angles

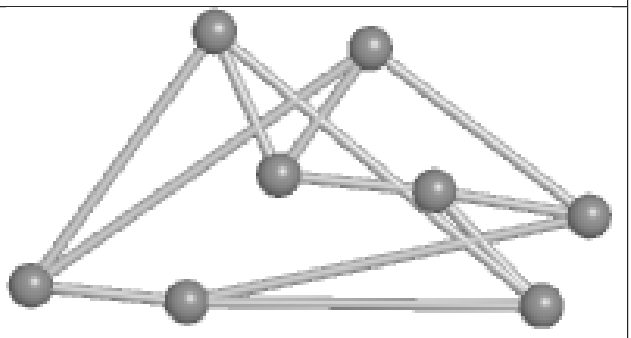
Torsions

Rings

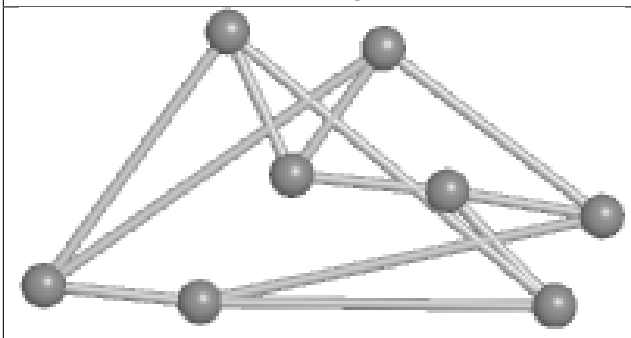
Ligand SF4 AL 302



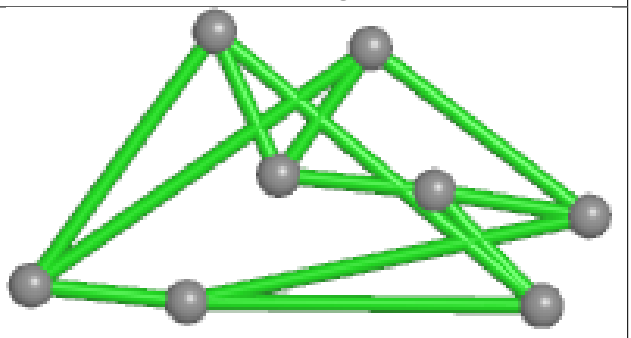
Bond lengths



Bond angles

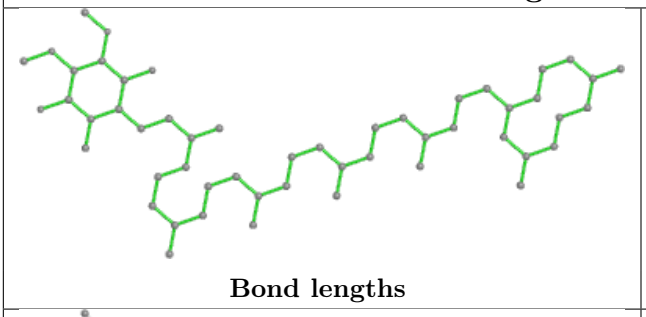


Torsions

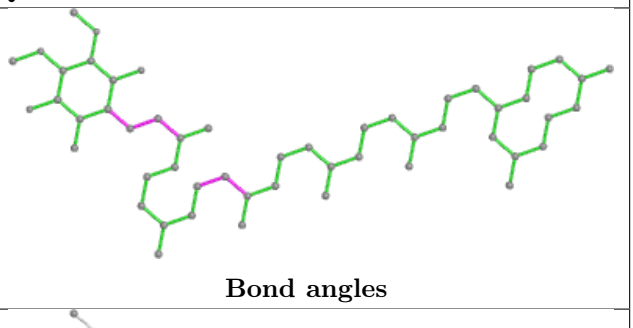


Rings

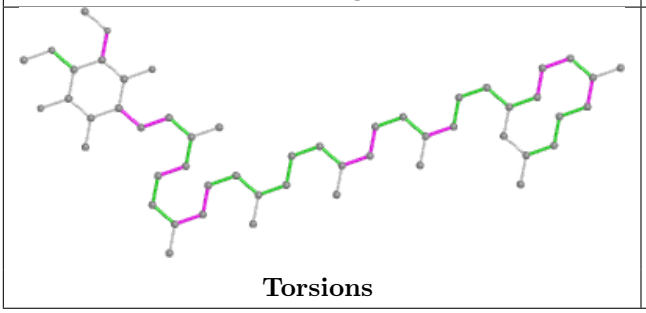
Ligand UQ8 C 511



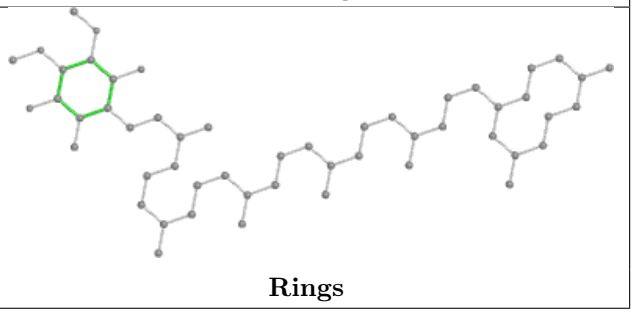
Bond lengths



Bond angles

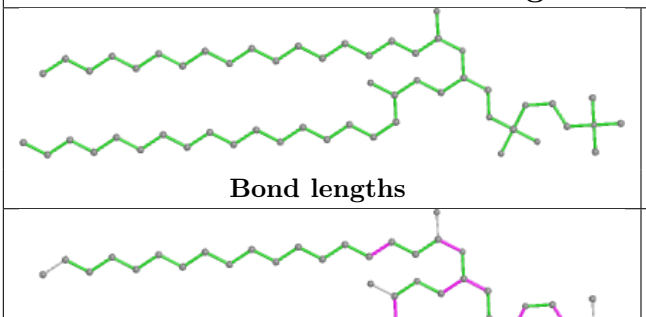


Torsions

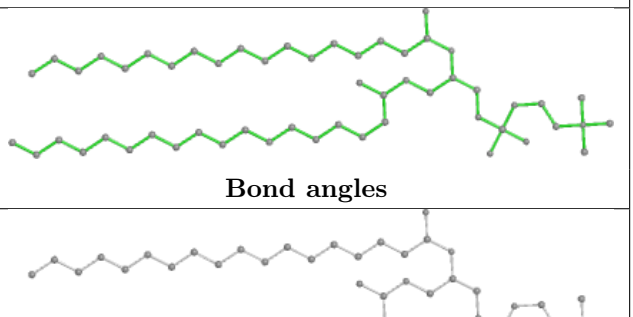


Rings

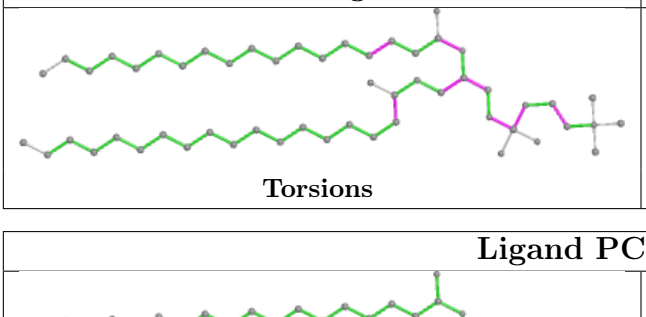
Ligand PC1 K 501



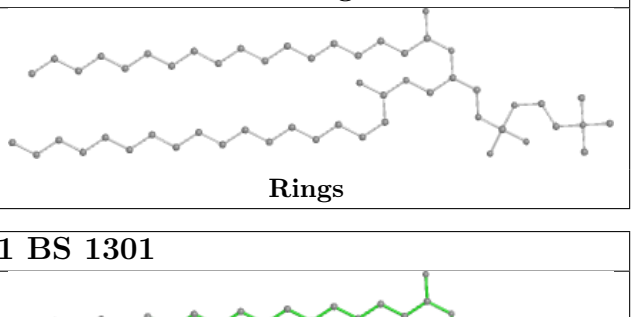
Bond lengths



Bond angles

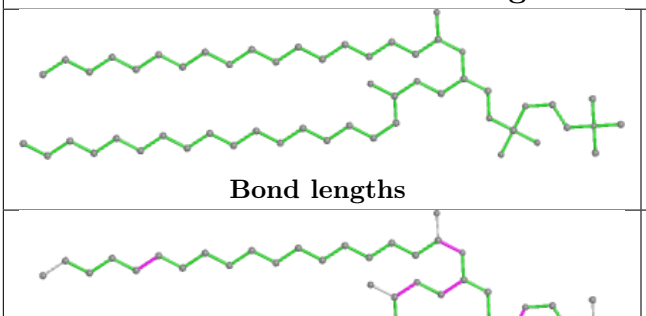


Torsions

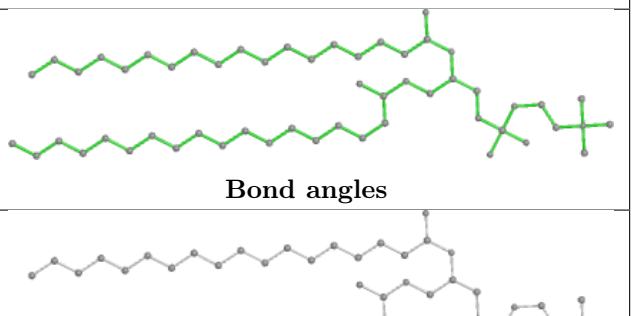


Rings

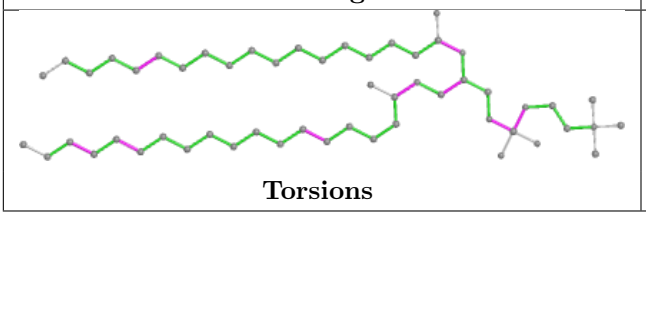
Ligand PC1 BS 1301



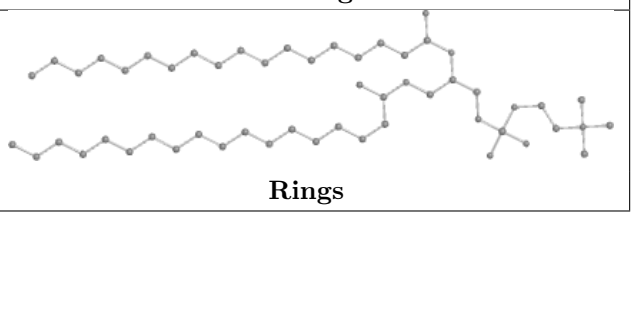
Bond lengths



Bond angles

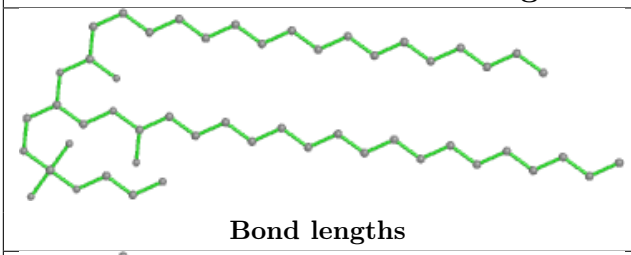


Torsions

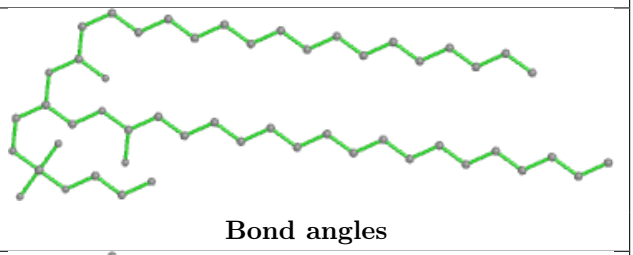


Rings

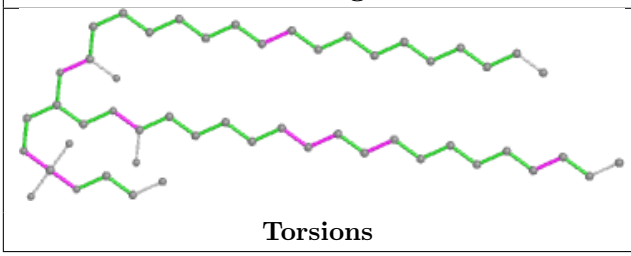
Ligand 3PE Ds 408



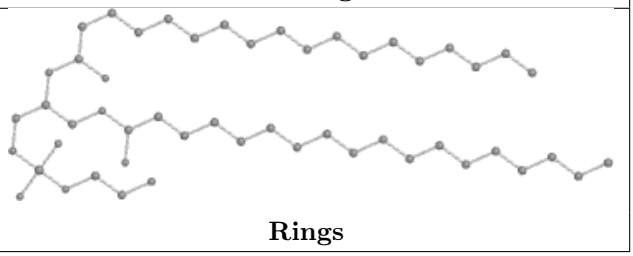
Bond lengths



Bond angles

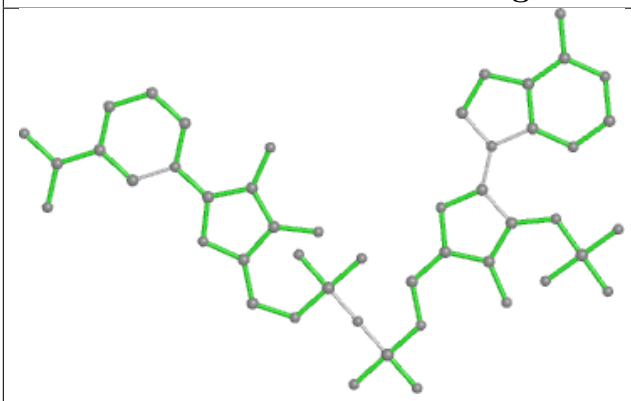


Torsions

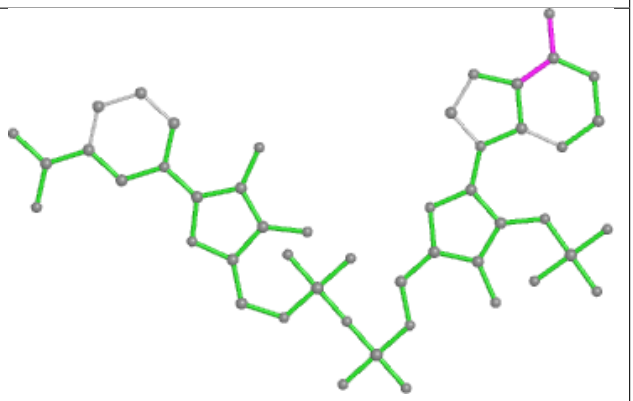


Rings

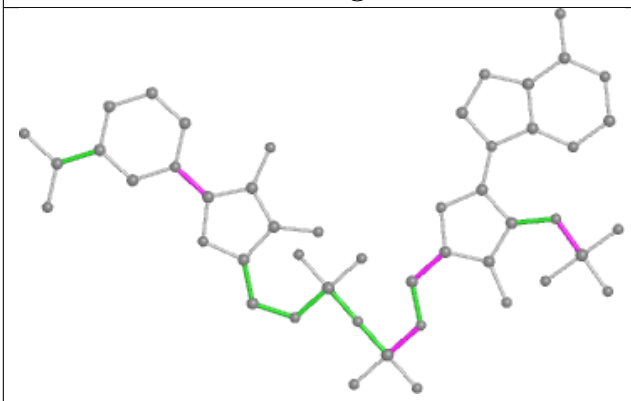
Ligand NDP A1 401



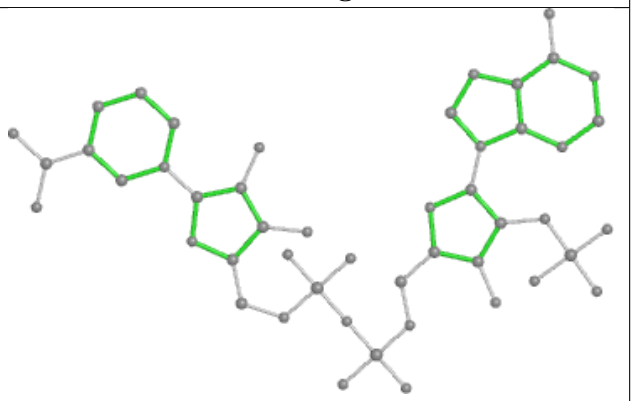
Bond lengths



Bond angles

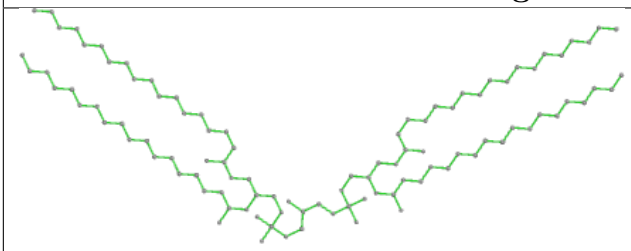


Torsions

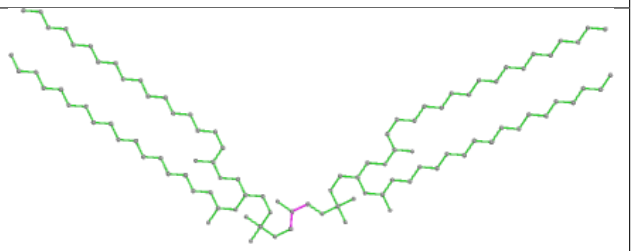


Rings

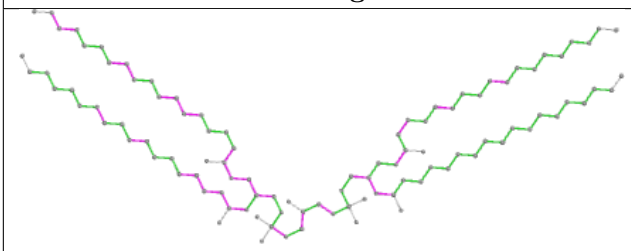
Ligand CDL DZ 501



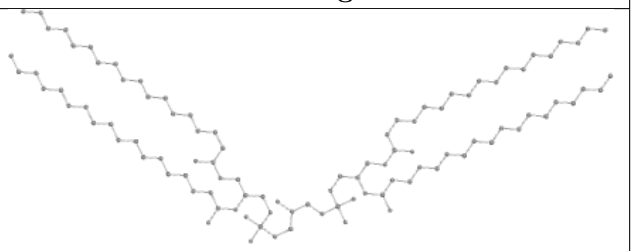
Bond lengths



Bond angles

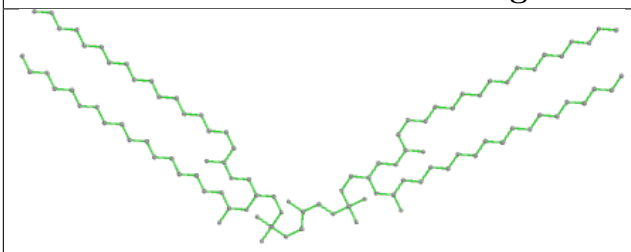


Torsions

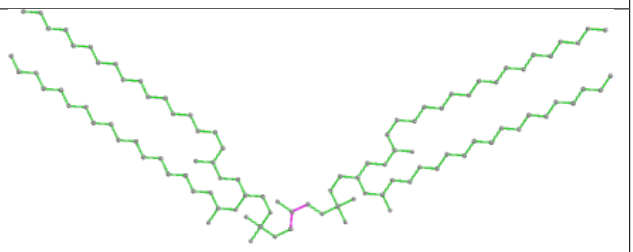


Rings

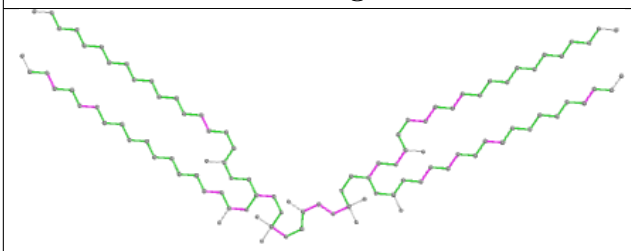
Ligand CDL CG 301



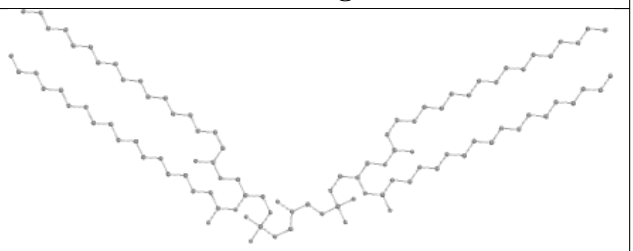
Bond lengths



Bond angles

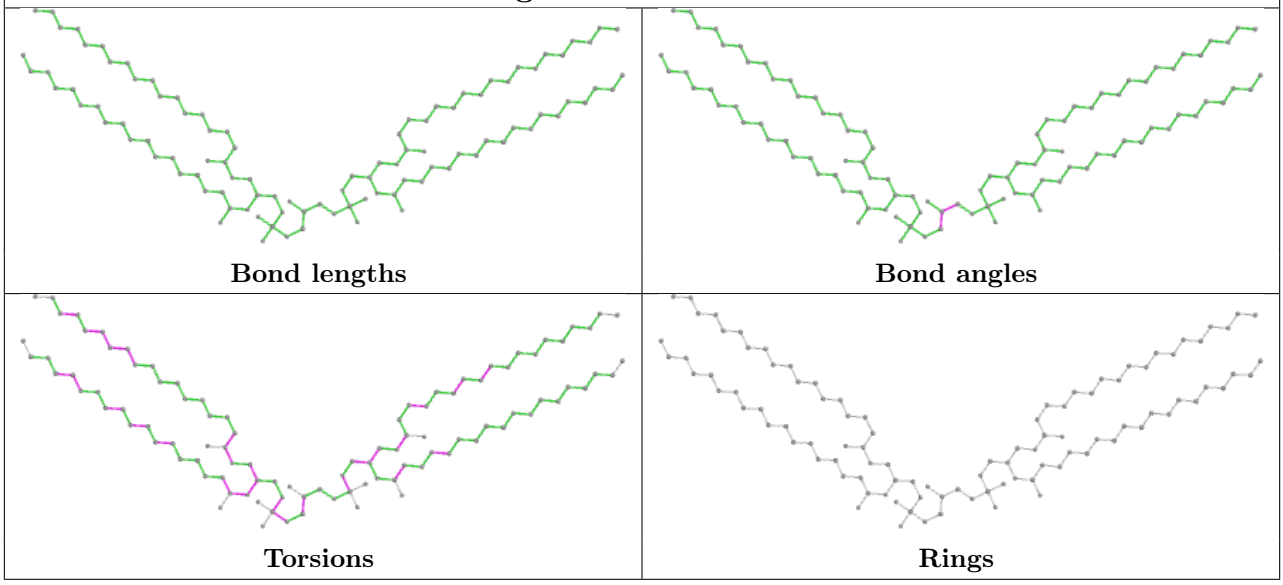


Torsions

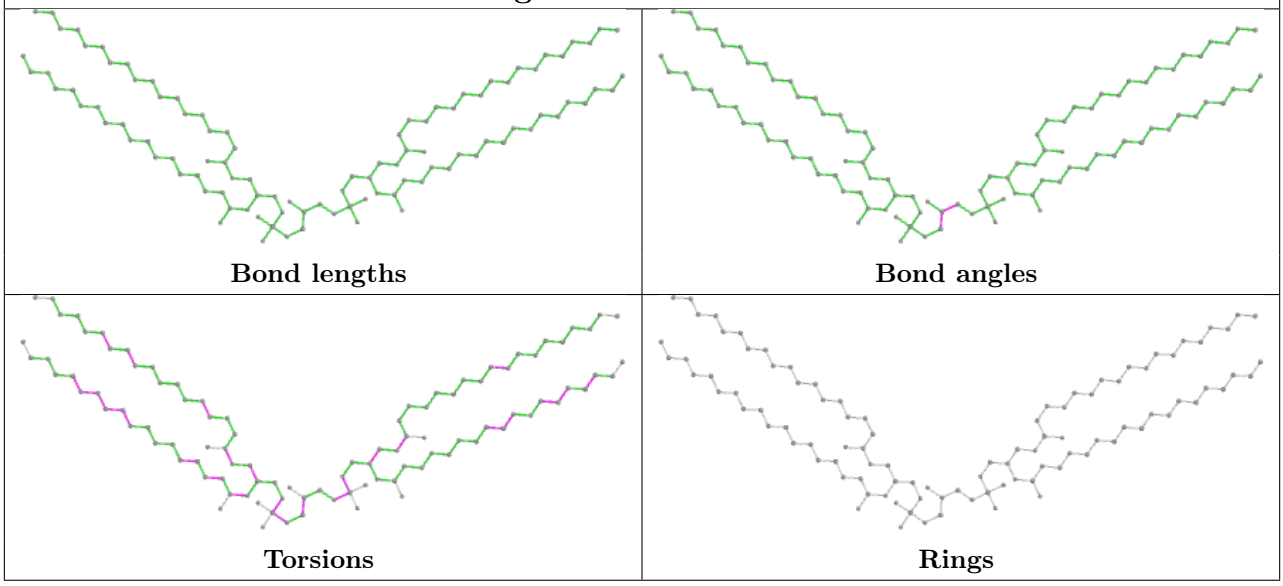


Rings

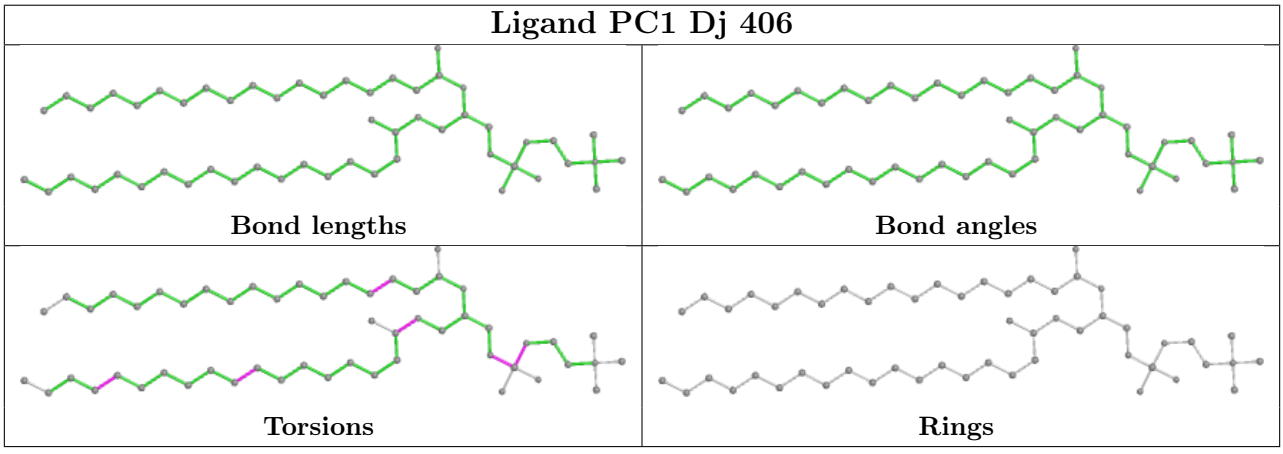
Ligand CDL Da 709



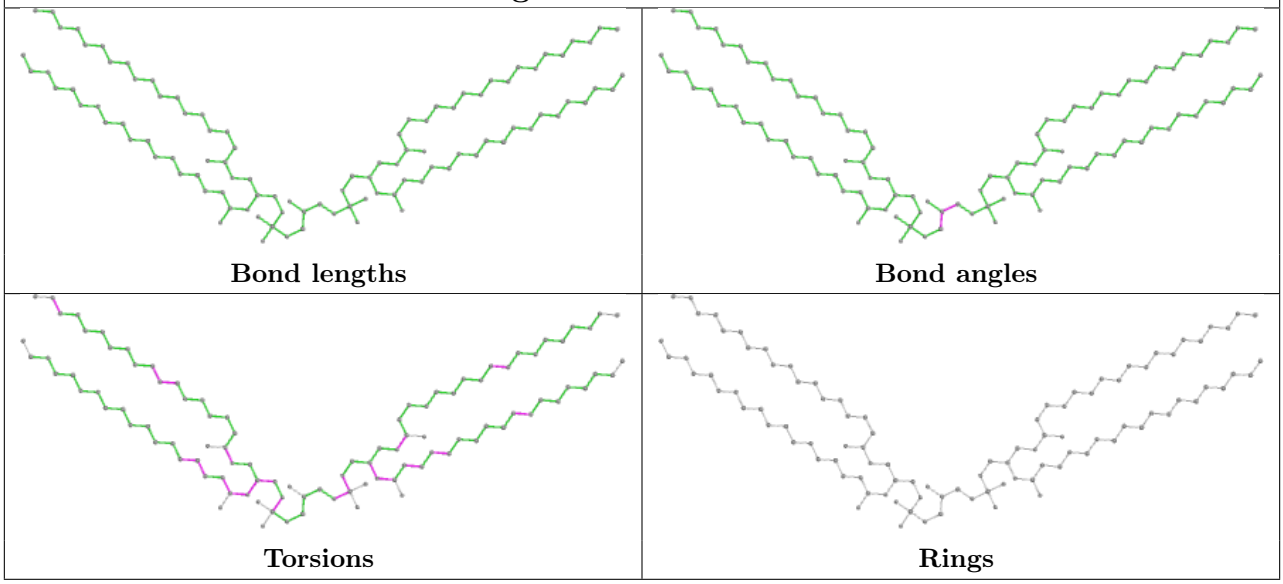
Ligand CDL Dh 201



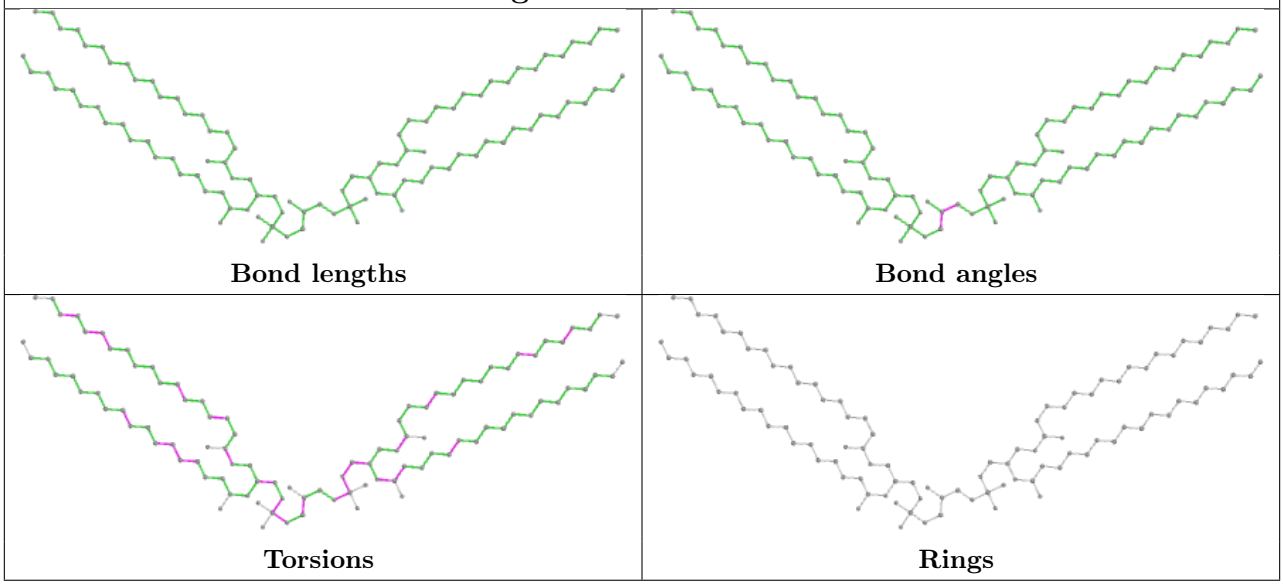
Ligand PC1 Dj 406



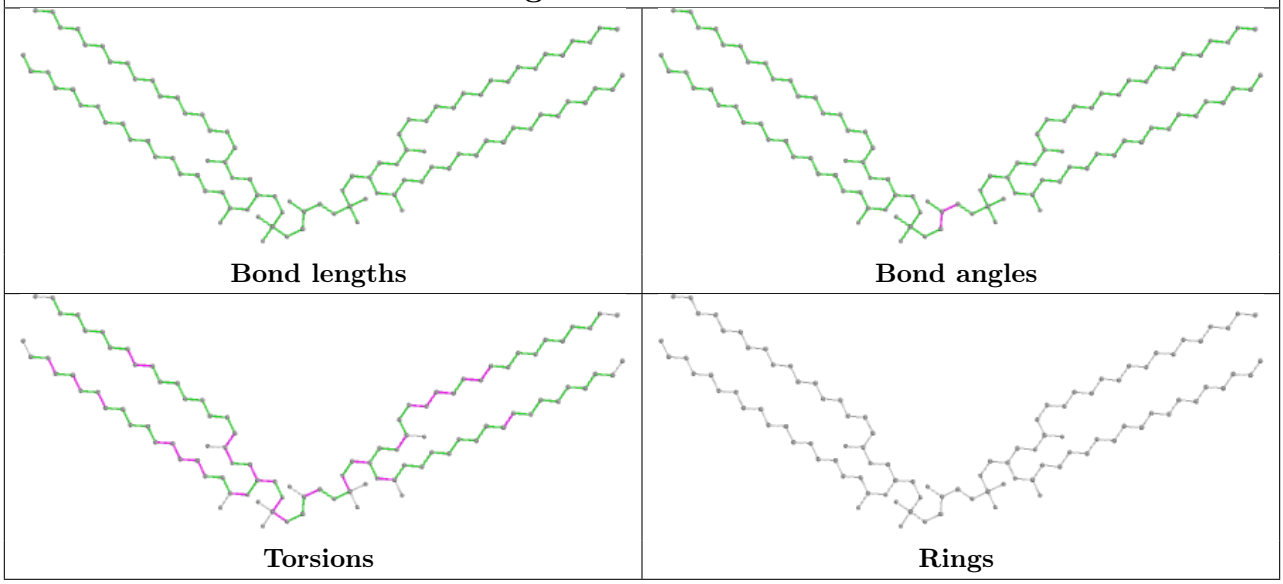
Ligand CDL CC 305



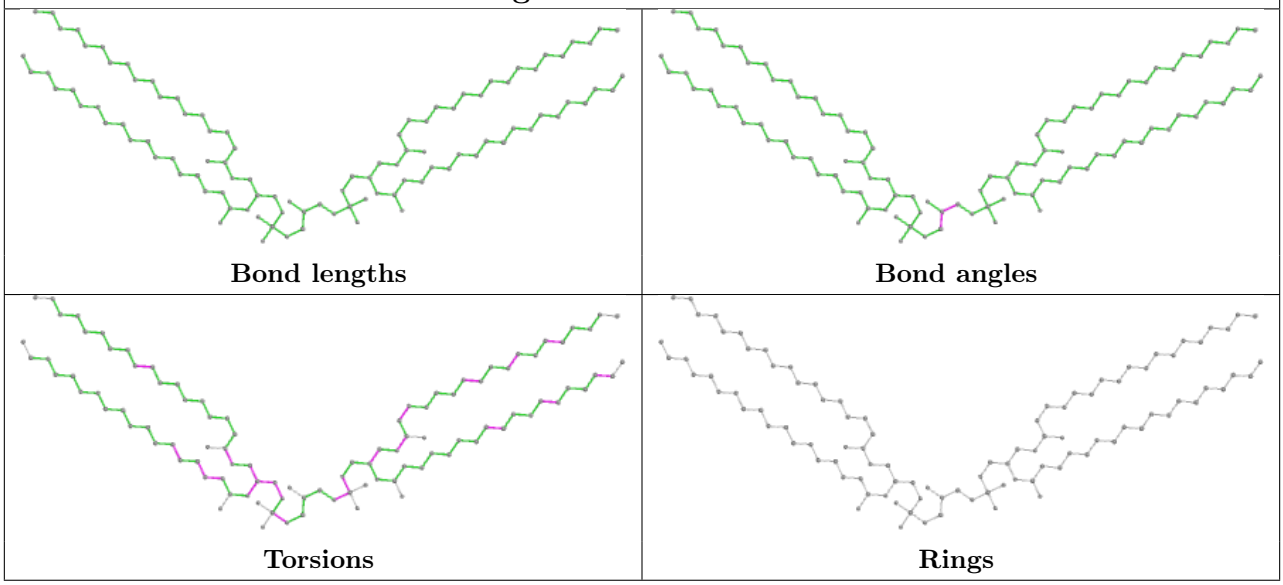
Ligand CDL DV 403



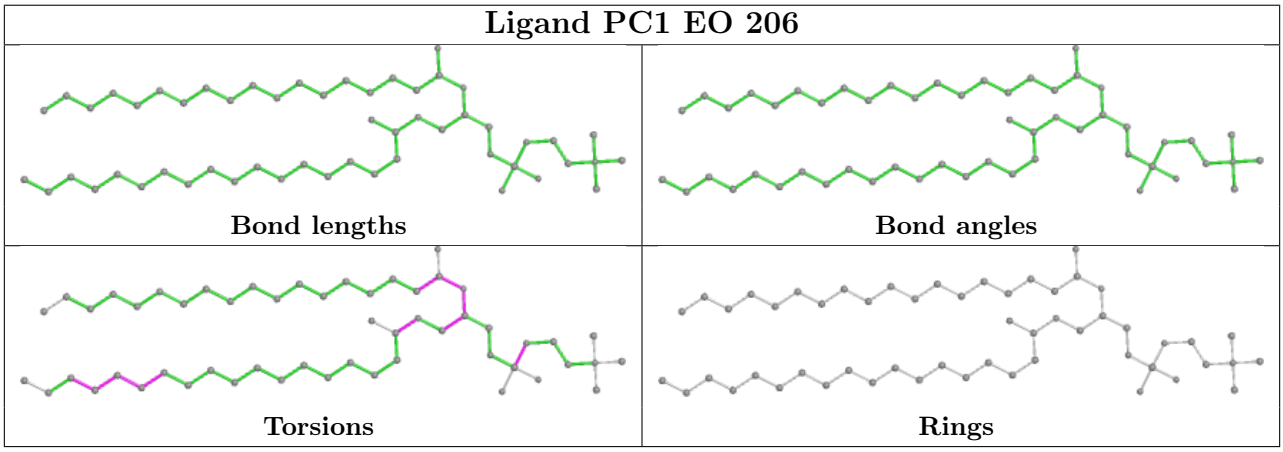
Ligand CDL C 505



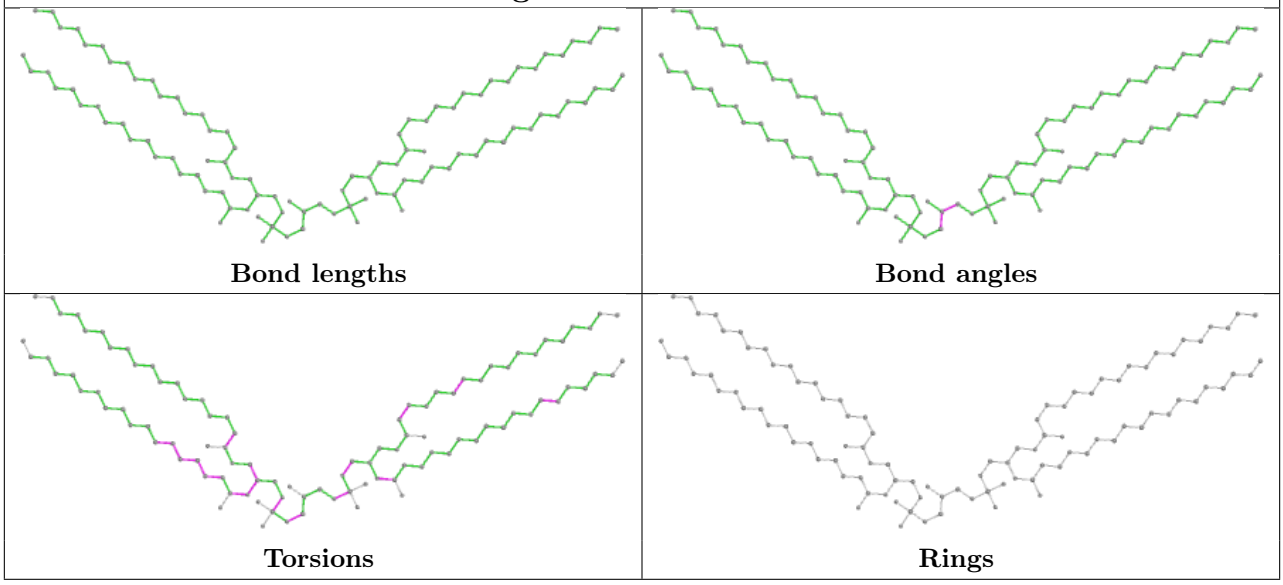
Ligand CDL EA 301



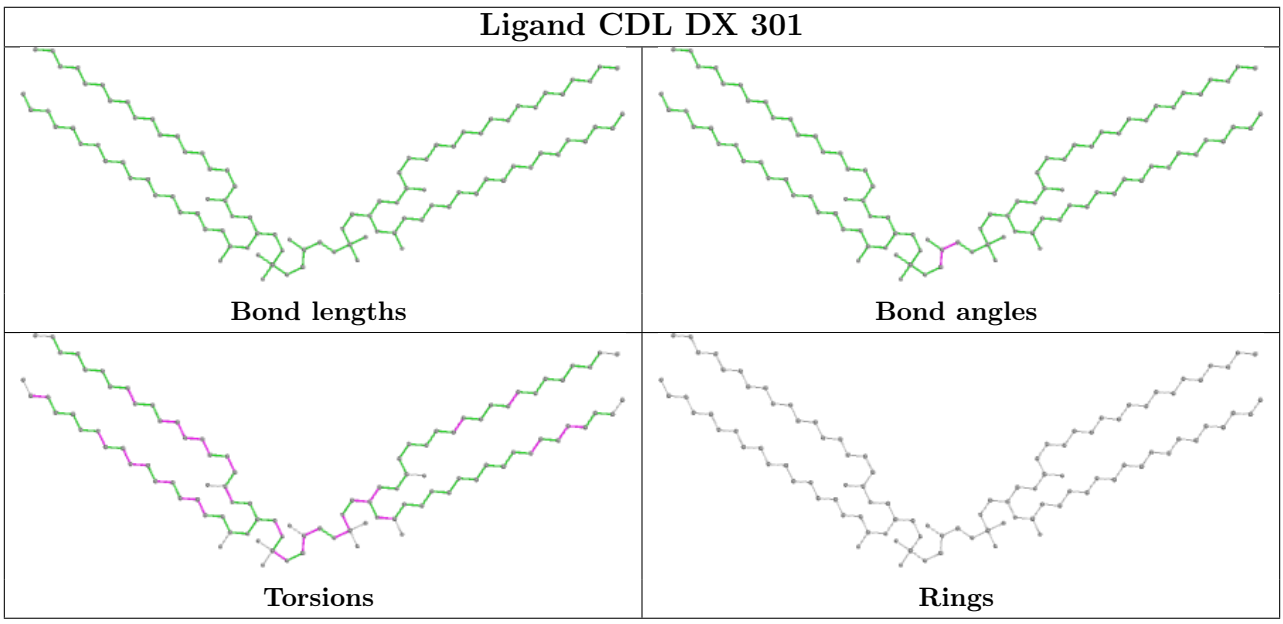
Ligand PC1 EO 206



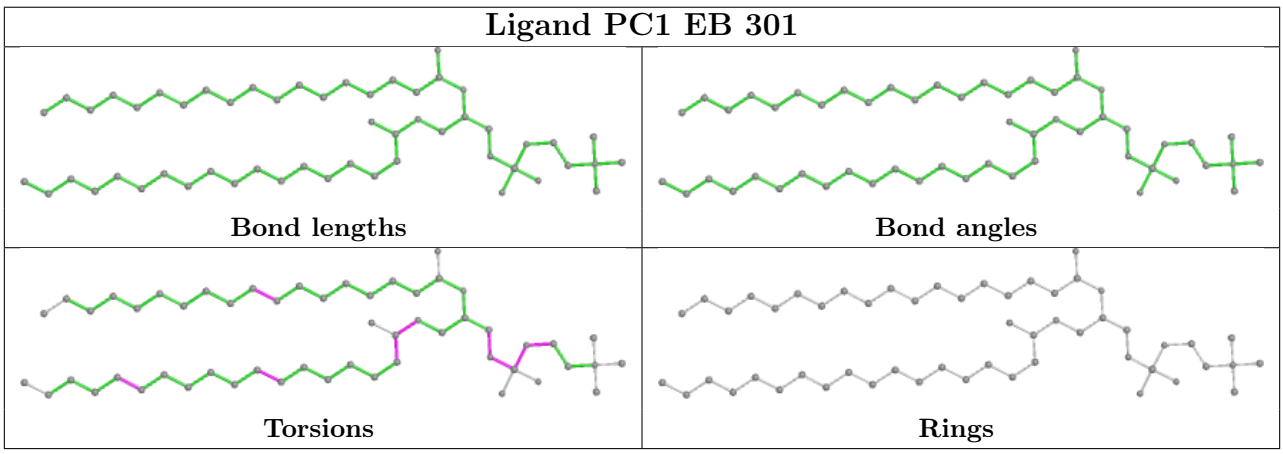
Ligand CDL AP 301



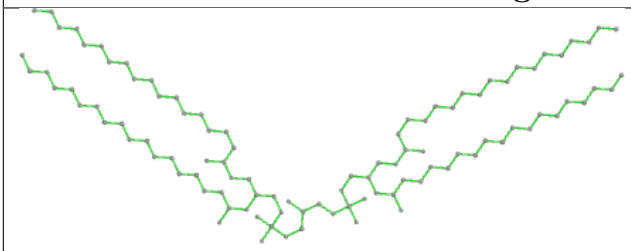
Ligand CDL DX 301



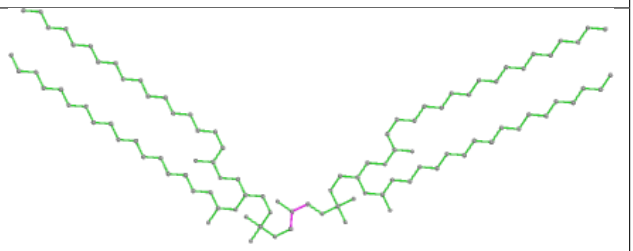
Ligand PC1 EB 301



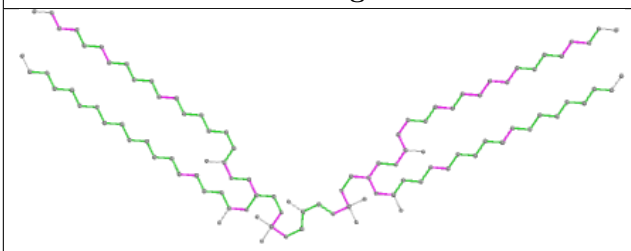
Ligand CDL Dn 501



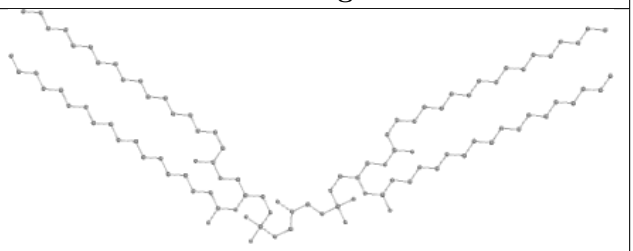
Bond lengths



Bond angles

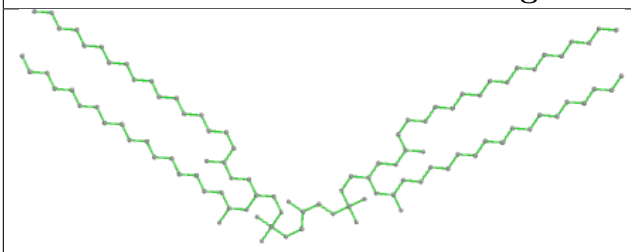


Torsions

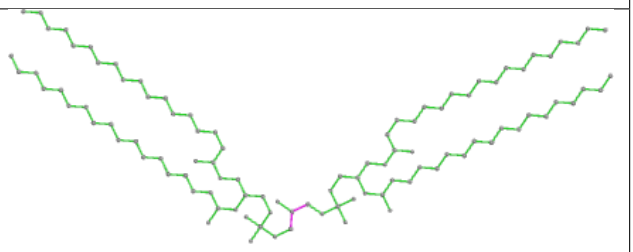


Rings

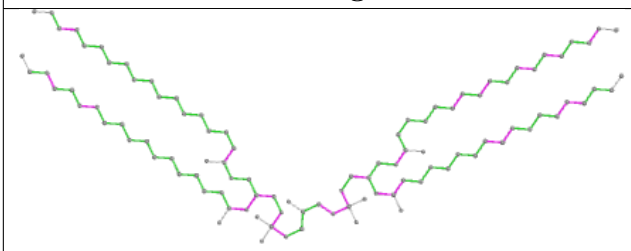
Ligand CDL El 903



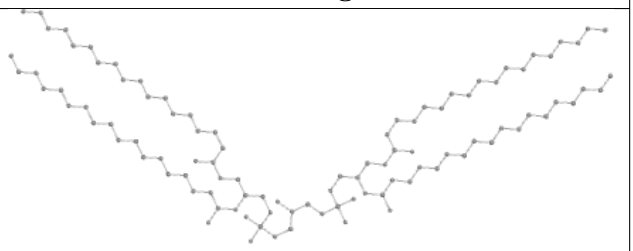
Bond lengths



Bond angles

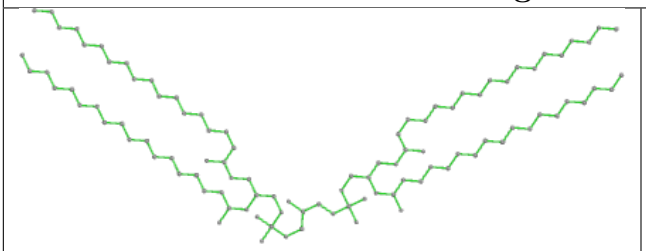


Torsions

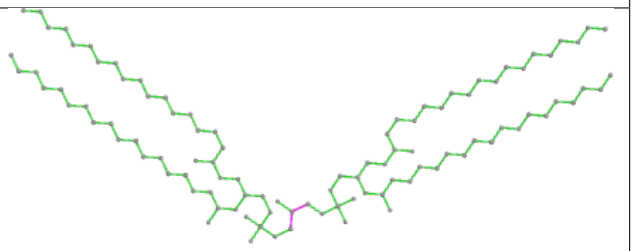


Rings

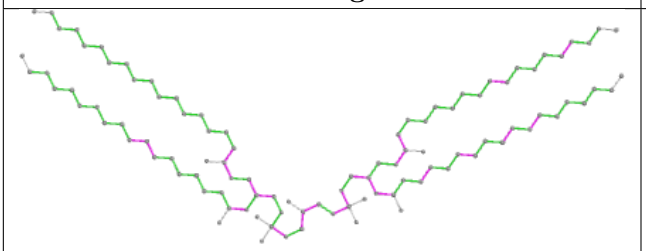
Ligand CDL DJ 307



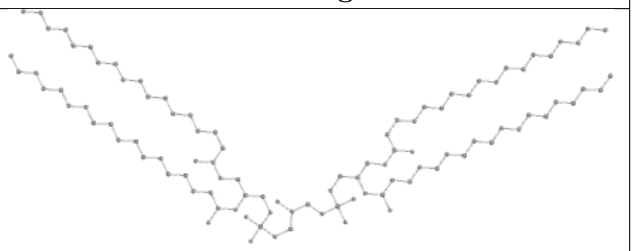
Bond lengths



Bond angles

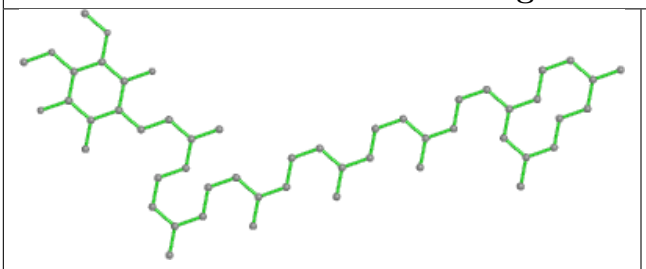


Torsions

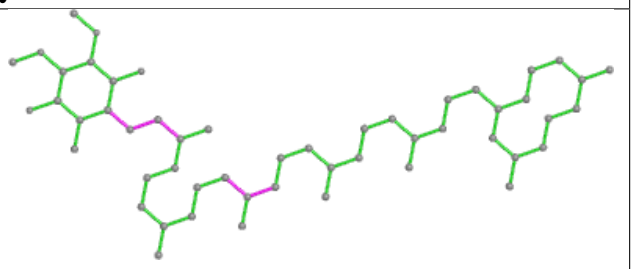


Rings

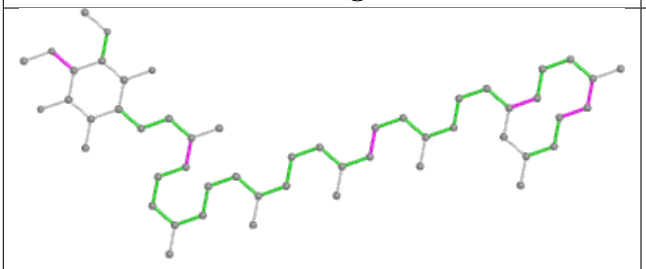
Ligand UQ8 Ed 202



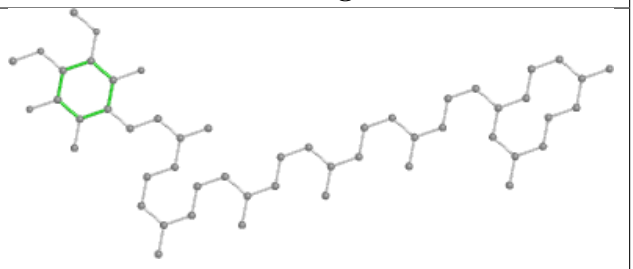
Bond lengths



Bond angles

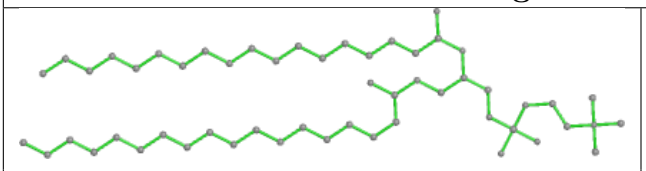


Torsions

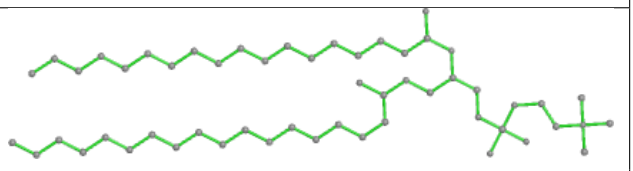


Rings

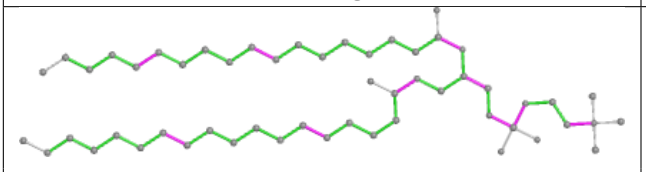
Ligand PC1 Di 1104



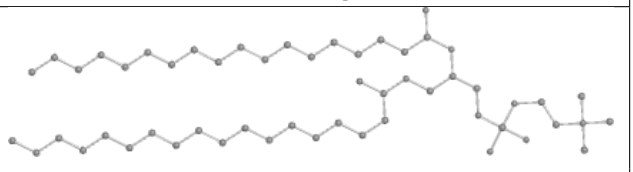
Bond lengths



Bond angles

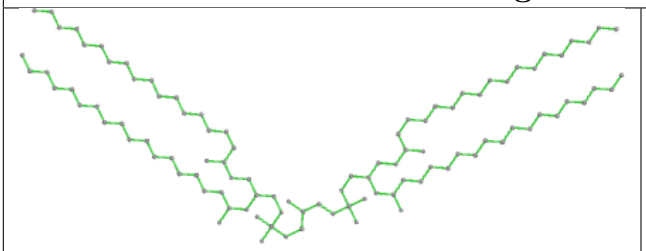


Torsions

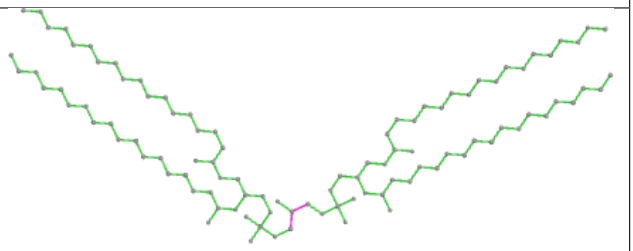


Rings

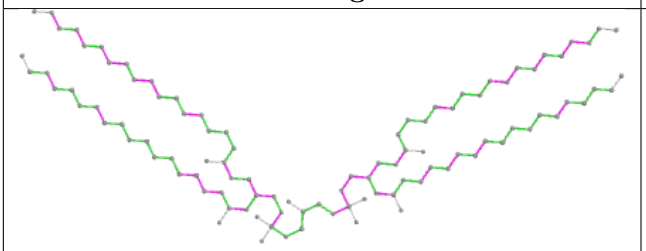
Ligand CDL EL 901



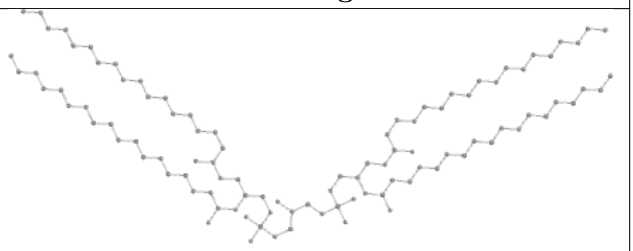
Bond lengths



Bond angles

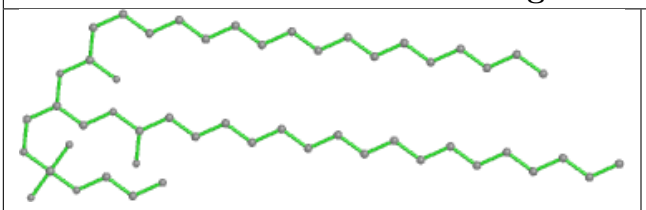


Torsions

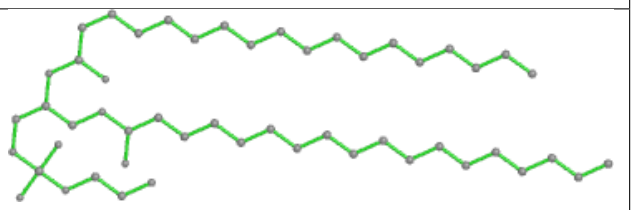


Rings

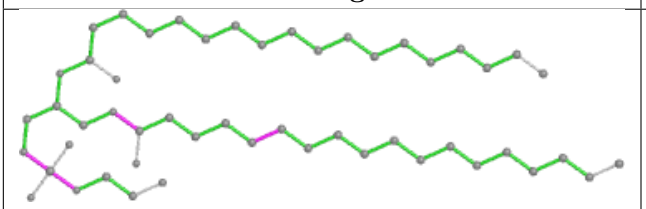
Ligand 3PE G 401



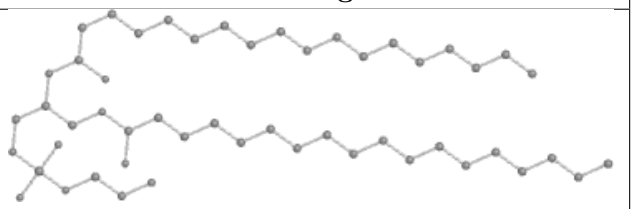
Bond lengths



Bond angles

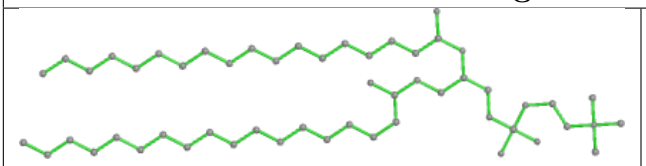


Torsions

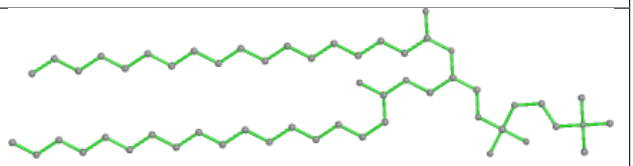


Rings

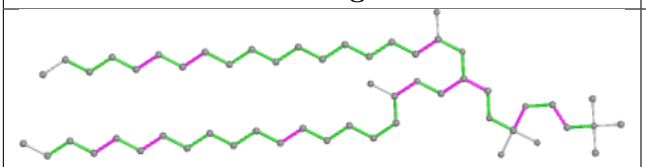
Ligand PC1 DC 603



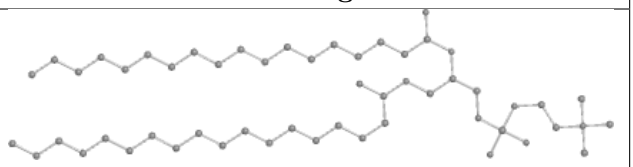
Bond lengths



Bond angles

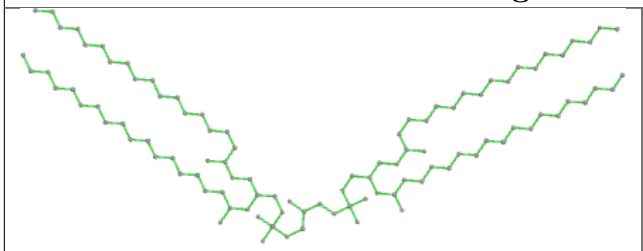


Torsions

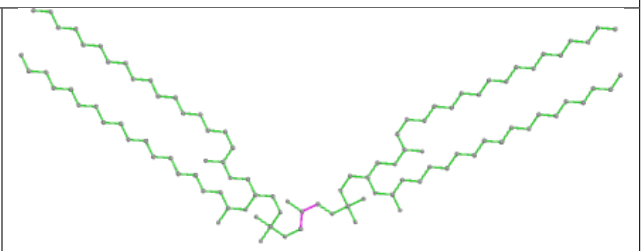


Rings

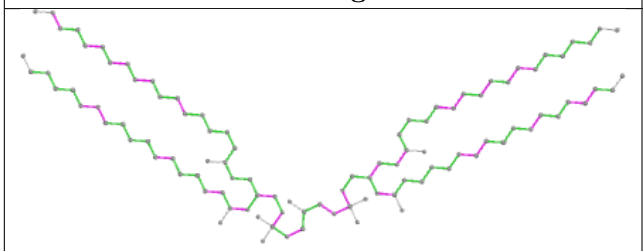
Ligand CDL AC 801



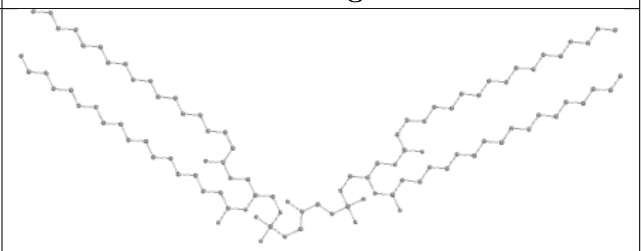
Bond lengths



Bond angles

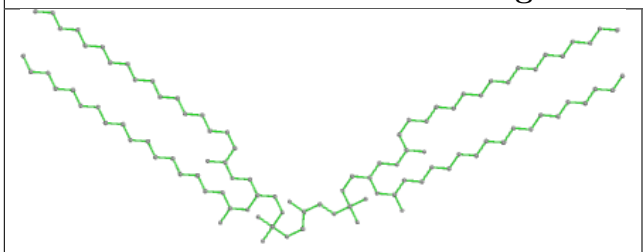


Torsions

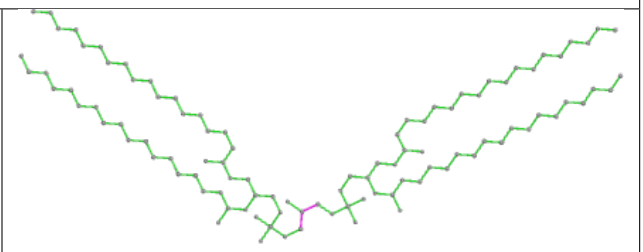


Rings

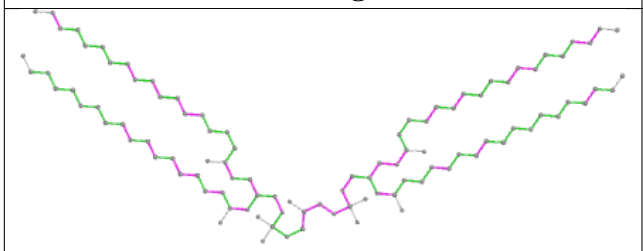
Ligand CDL EL 902



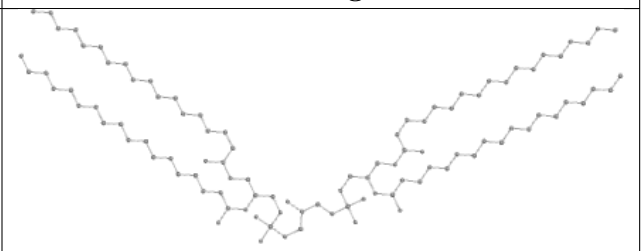
Bond lengths



Bond angles

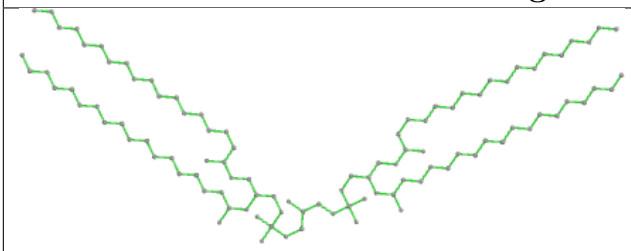


Torsions

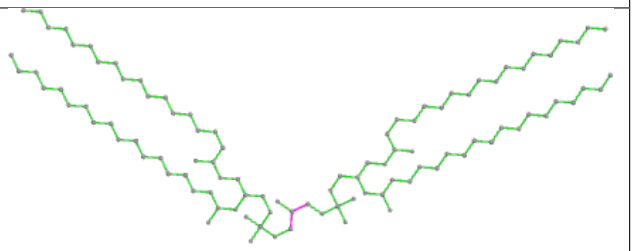


Rings

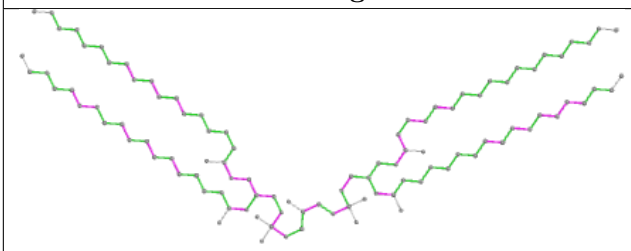
Ligand CDL c 506



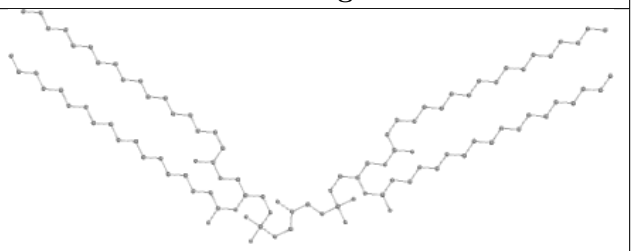
Bond lengths



Bond angles

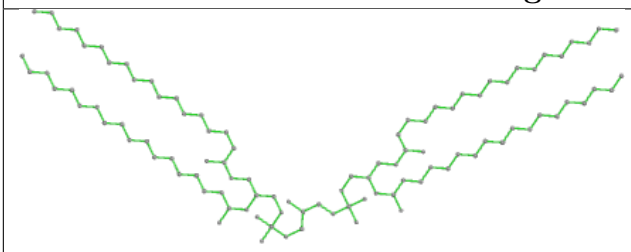


Torsions

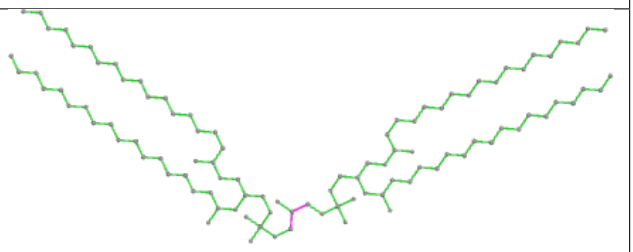


Rings

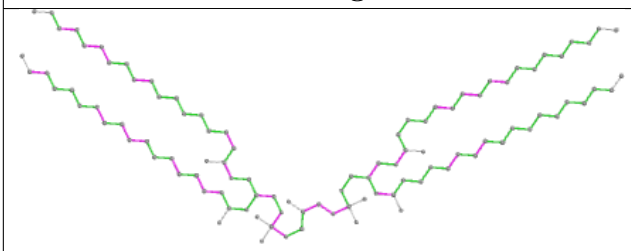
Ligand CDL C 504



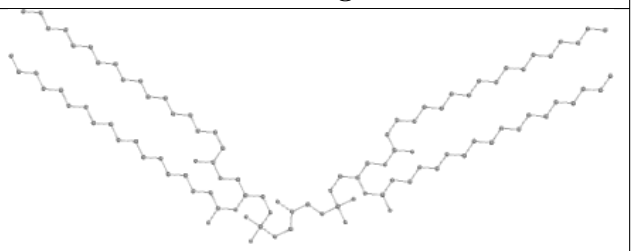
Bond lengths



Bond angles

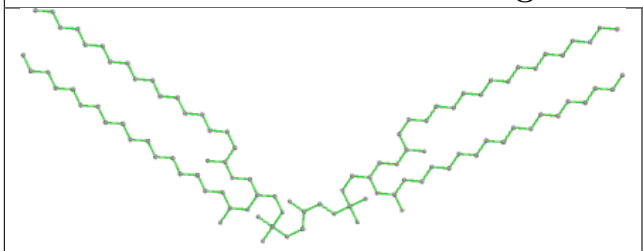


Torsions

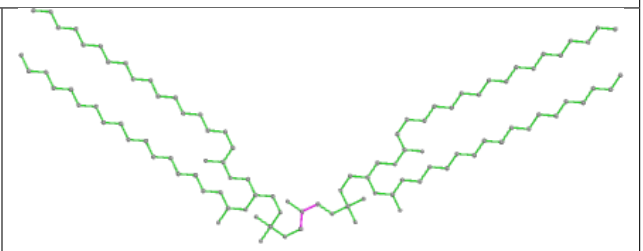


Rings

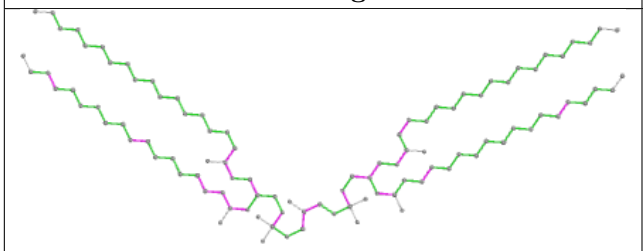
Ligand CDL Ed 205



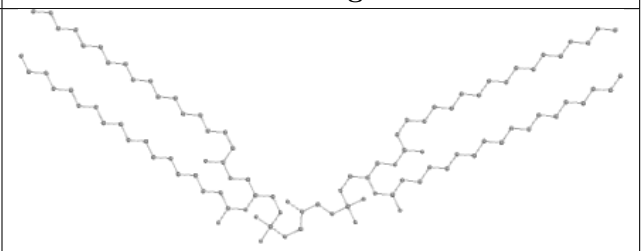
Bond lengths



Bond angles

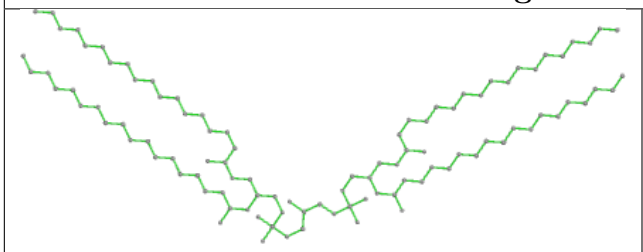


Torsions

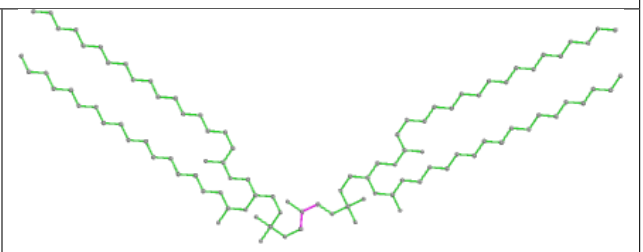


Rings

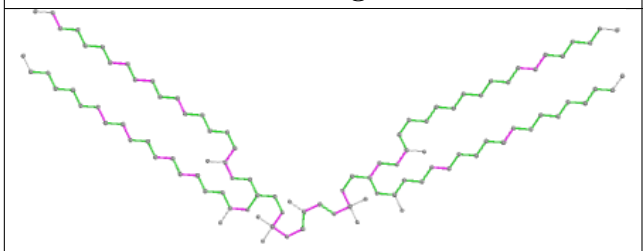
Ligand CDL Du 402



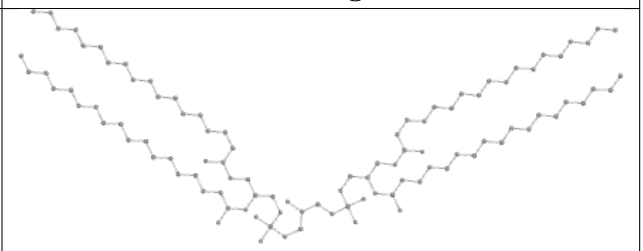
Bond lengths



Bond angles

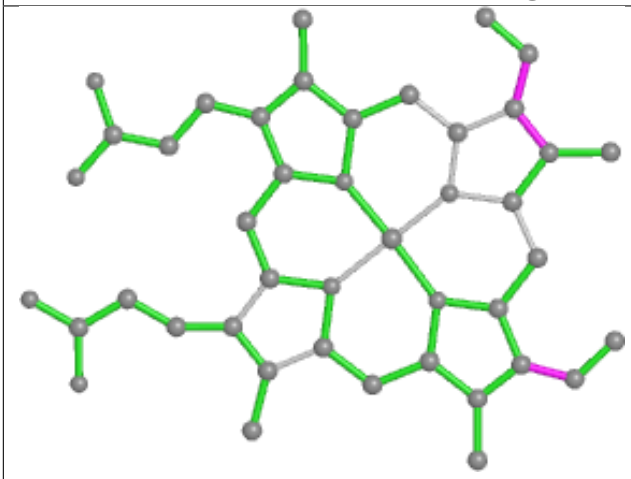


Torsions

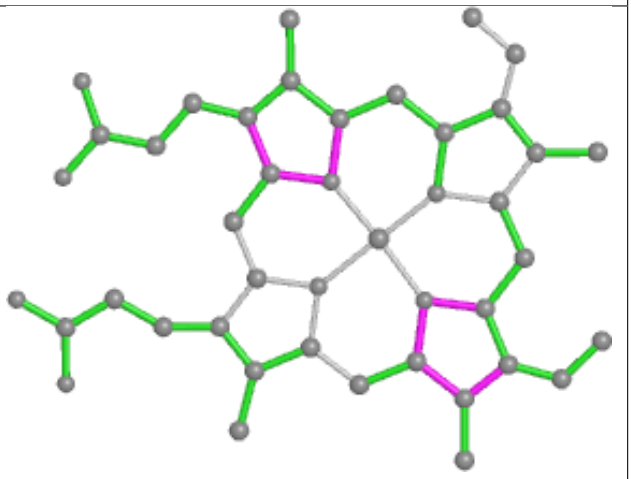


Rings

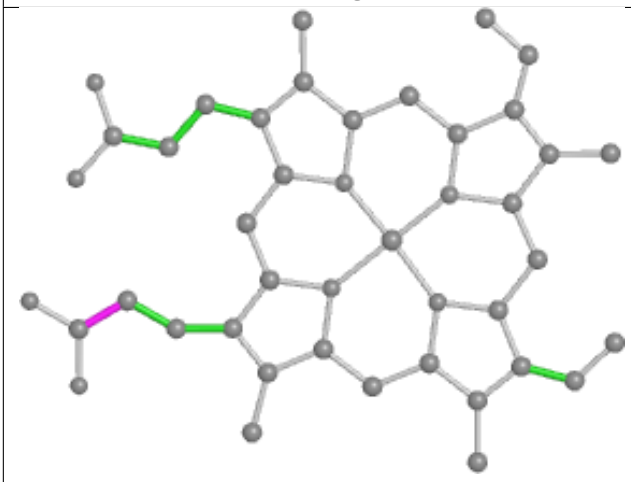
Ligand HEM c 505



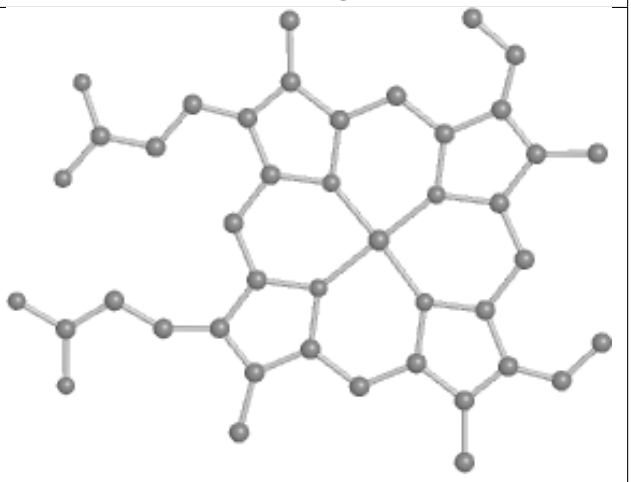
Bond lengths



Bond angles

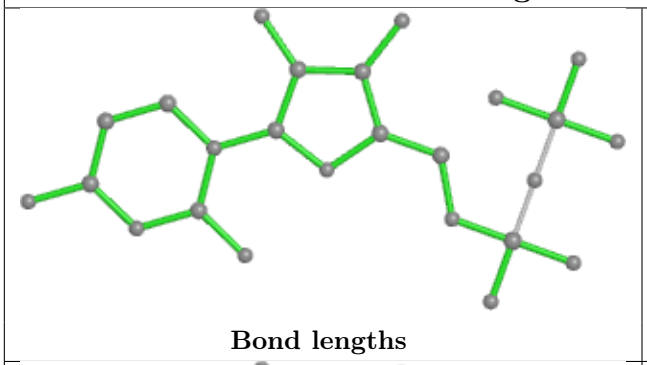


Torsions

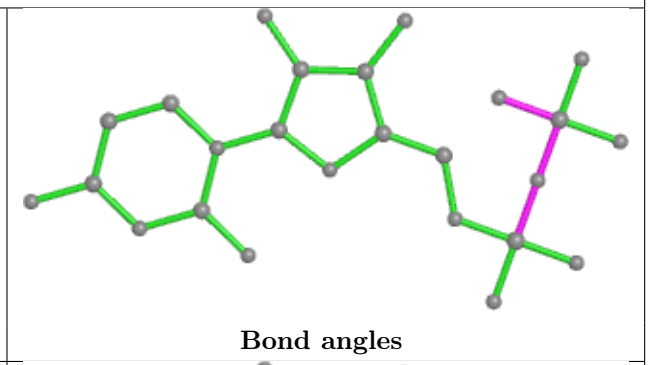


Rings

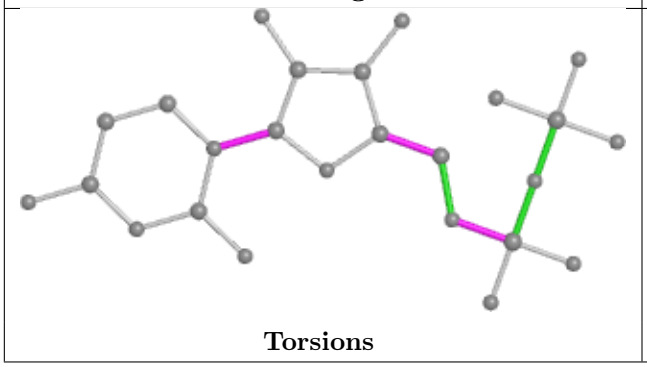
Ligand UDP A0 603



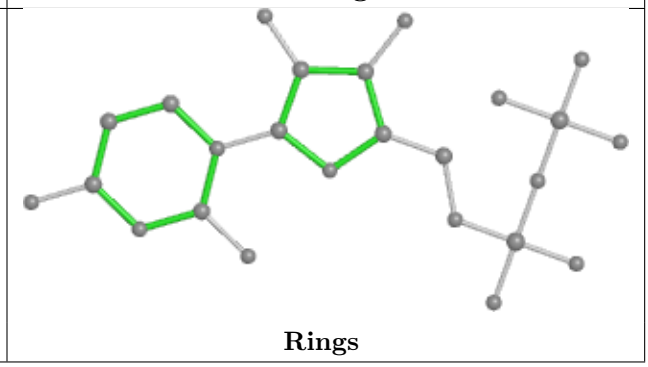
Bond lengths



Bond angles

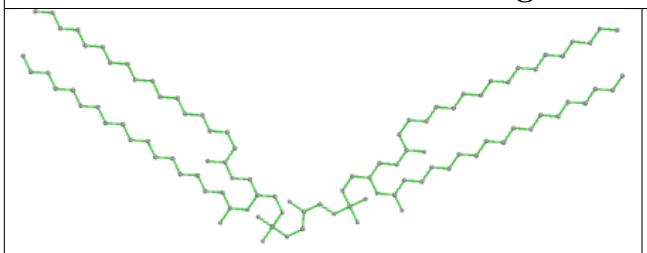


Torsions

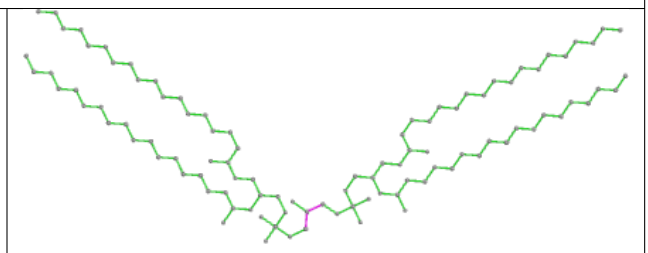


Rings

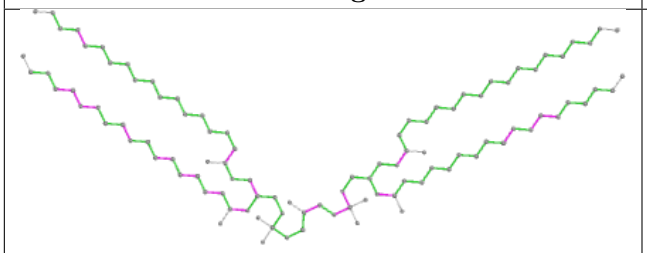
Ligand CDL Dc 608



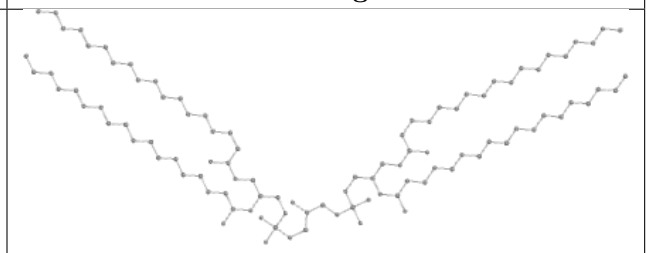
Bond lengths



Bond angles

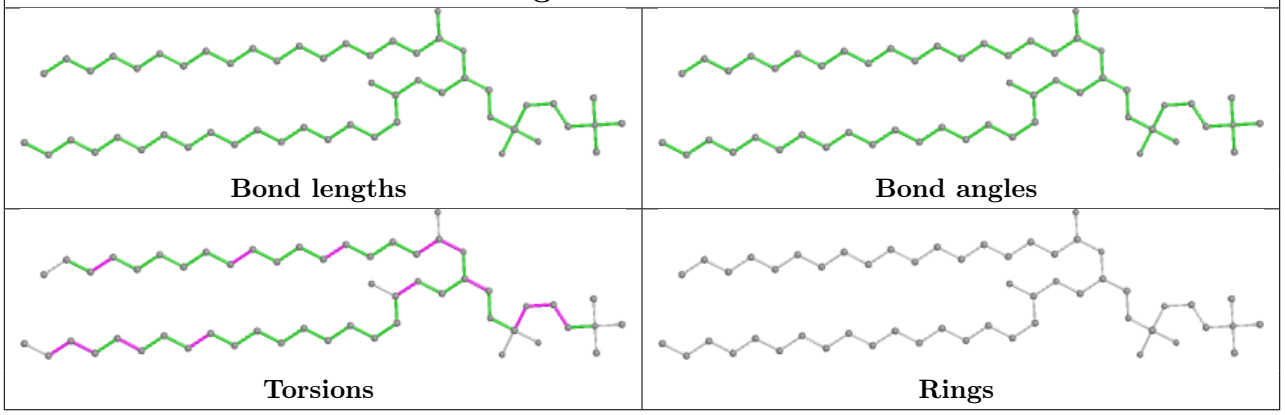


Torsions

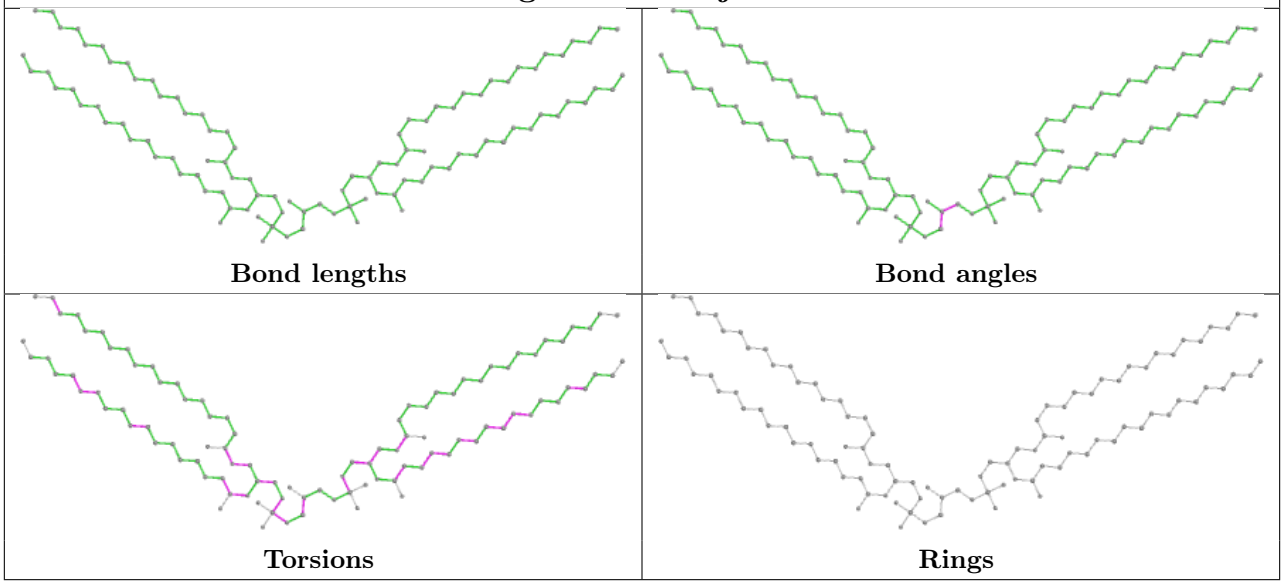


Rings

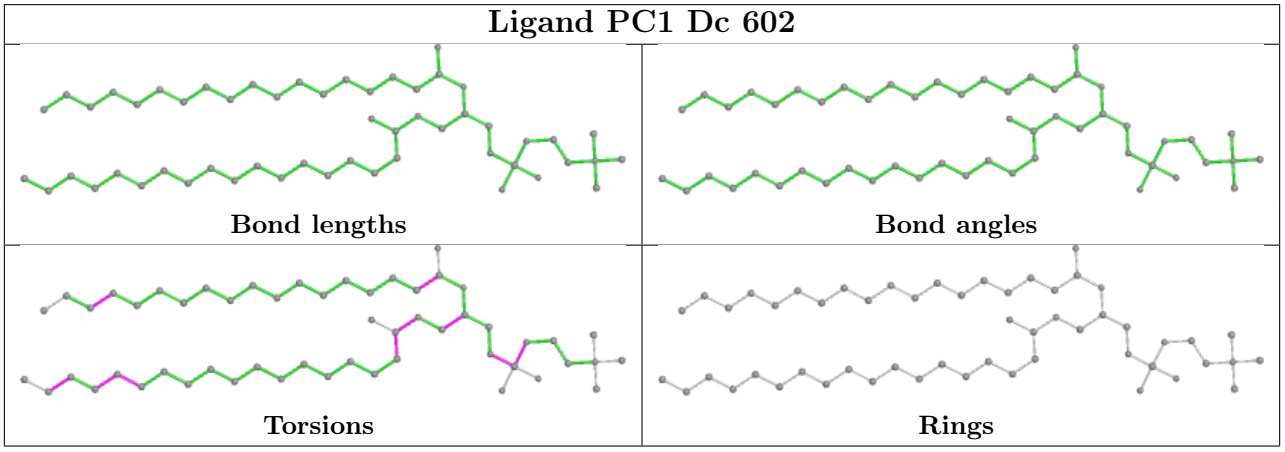
Ligand PC1 c 507



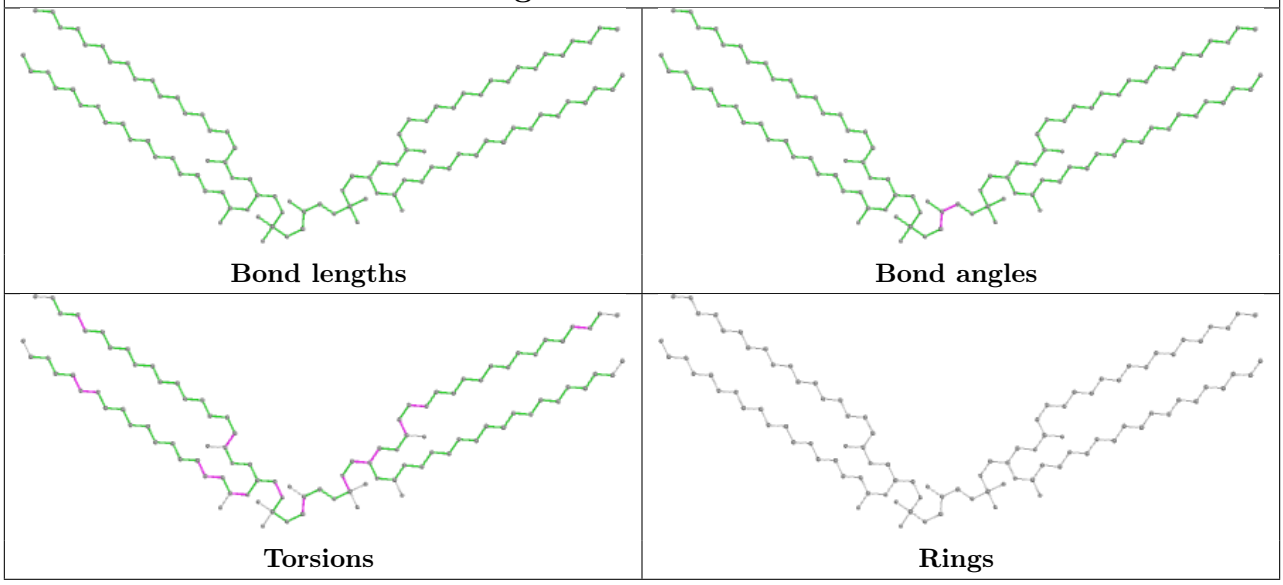
Ligand CDL Dj 402



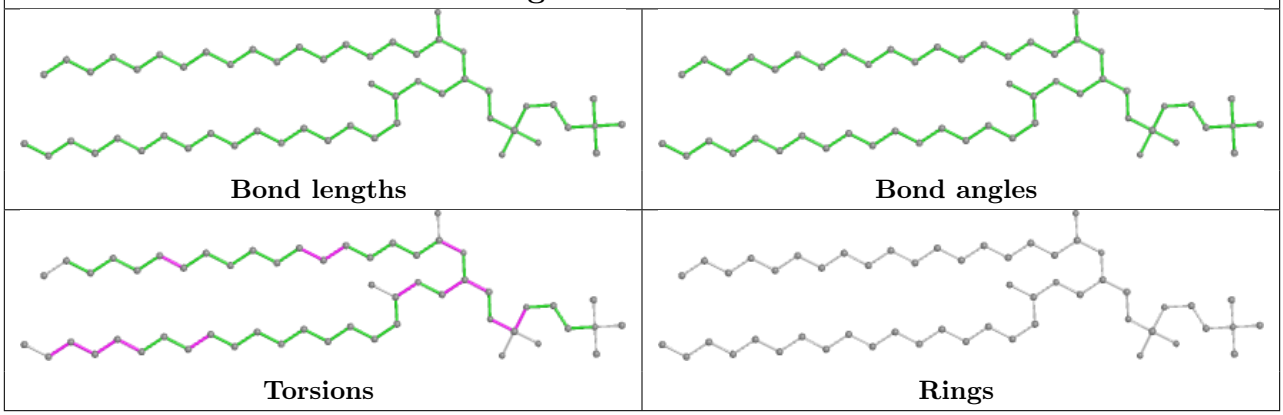
Ligand PC1 Dc 602



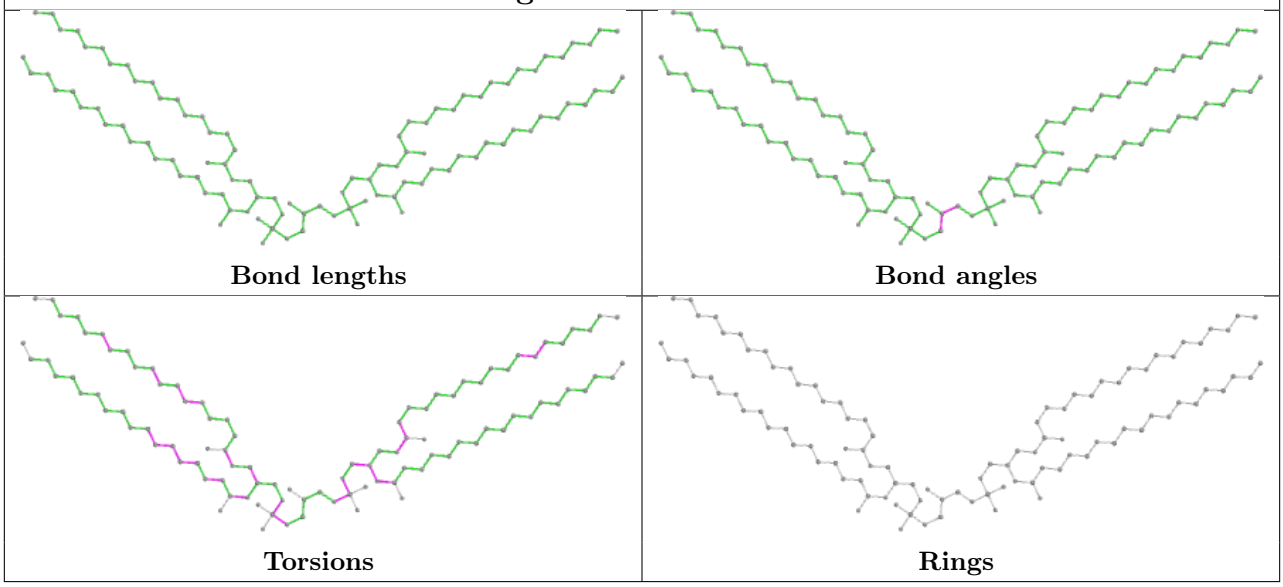
Ligand CDL BL 301



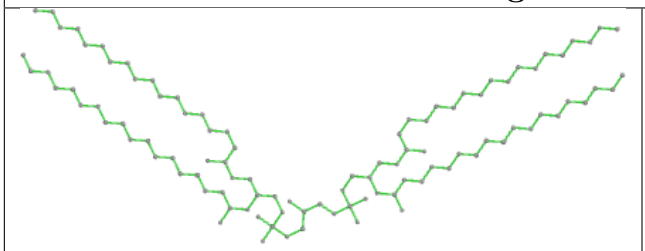
Ligand PC1 D 402



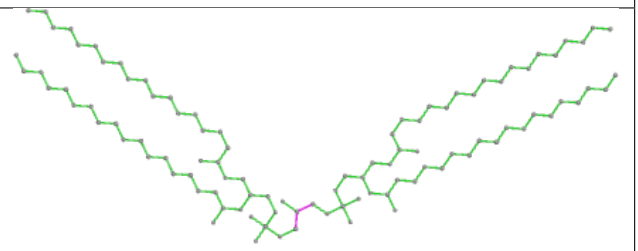
Ligand CDL Dc 601



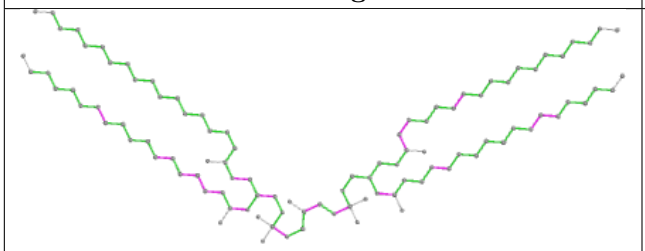
Ligand CDL DM 502



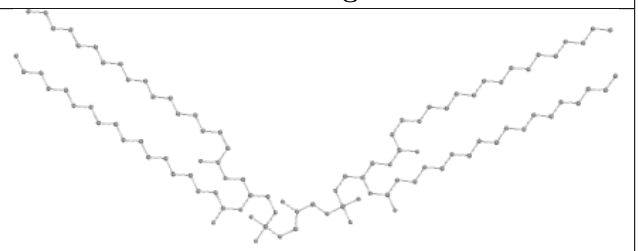
Bond lengths



Bond angles

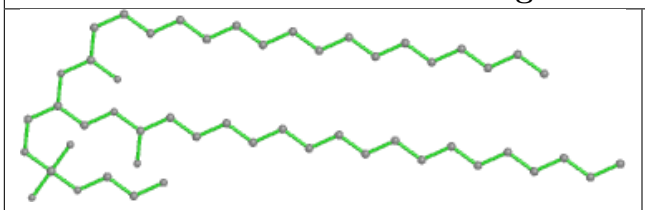


Torsions

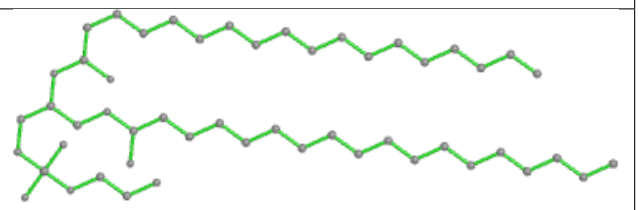


Rings

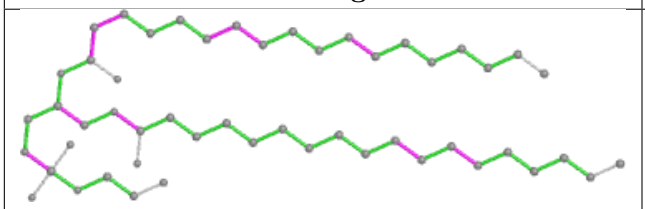
Ligand 3PE Em 901



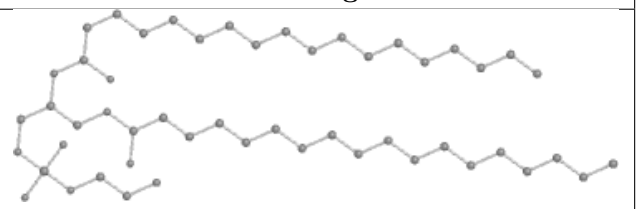
Bond lengths



Bond angles

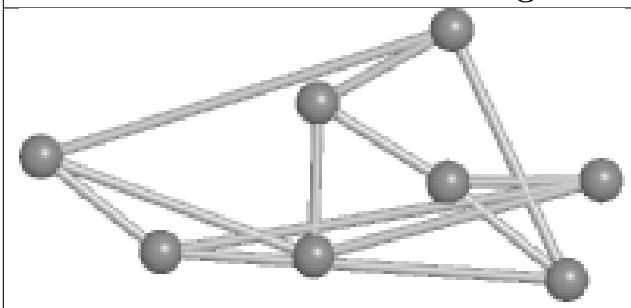


Torsions

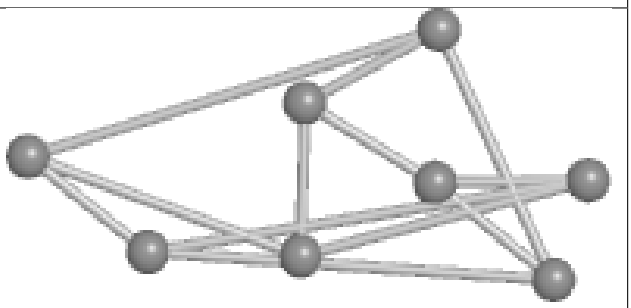


Rings

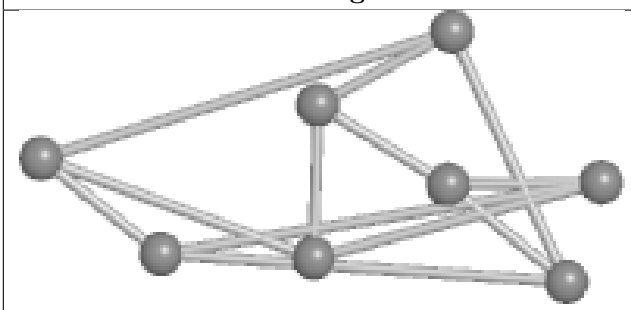
Ligand SF4 AD 501



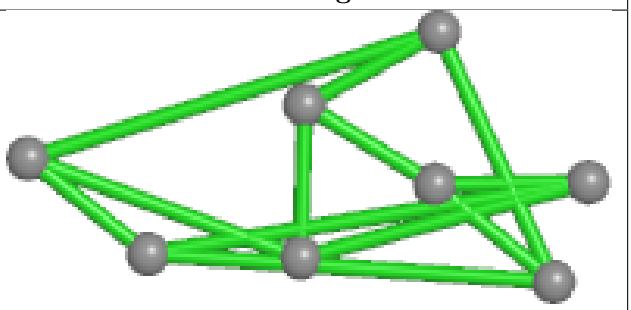
Bond lengths



Bond angles

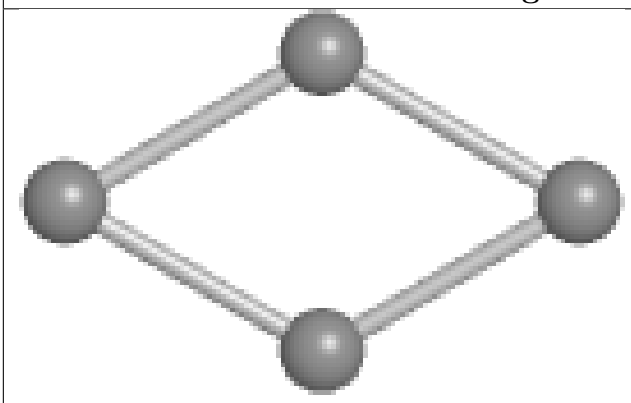


Torsions

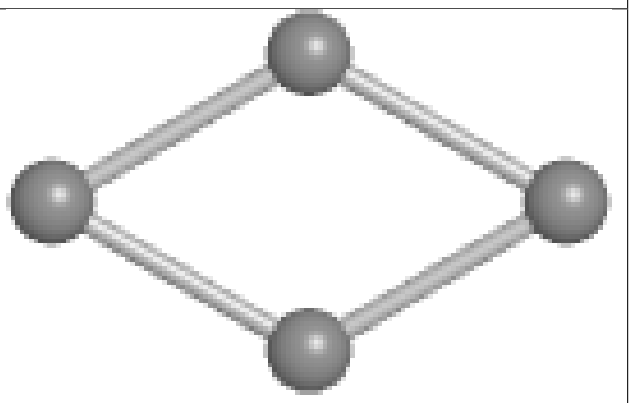


Rings

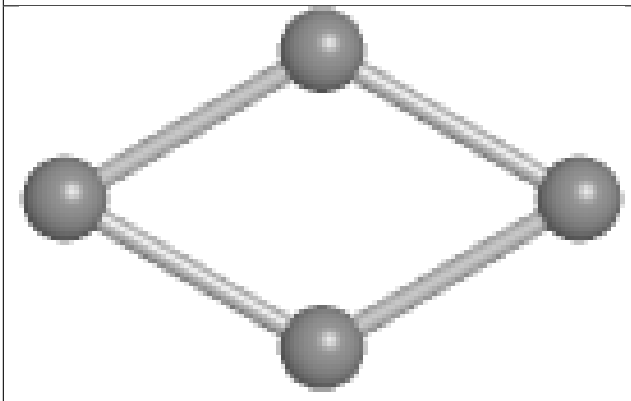
Ligand FES BI 201



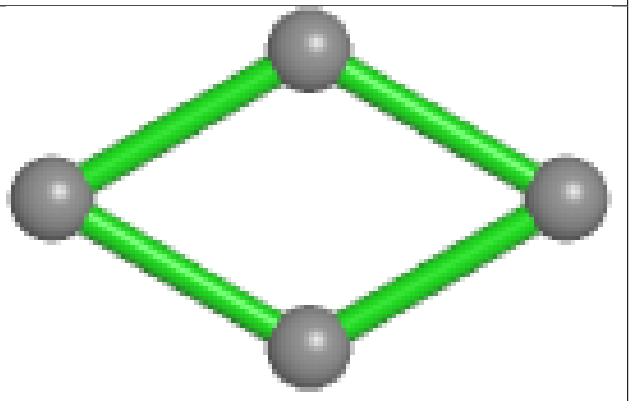
Bond lengths



Bond angles

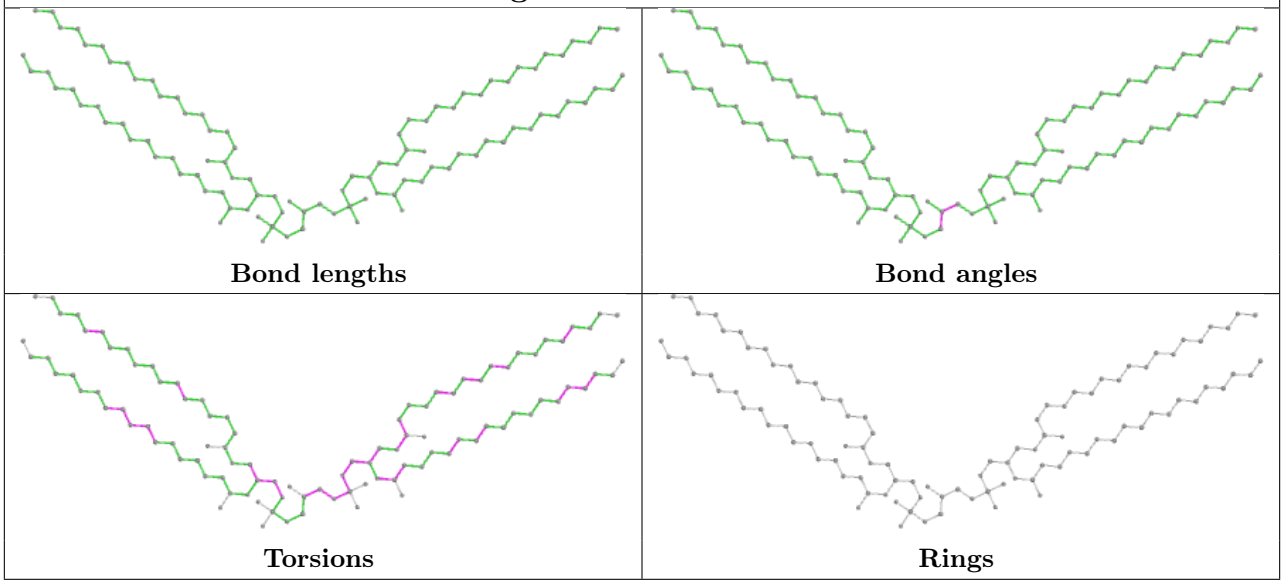


Torsions

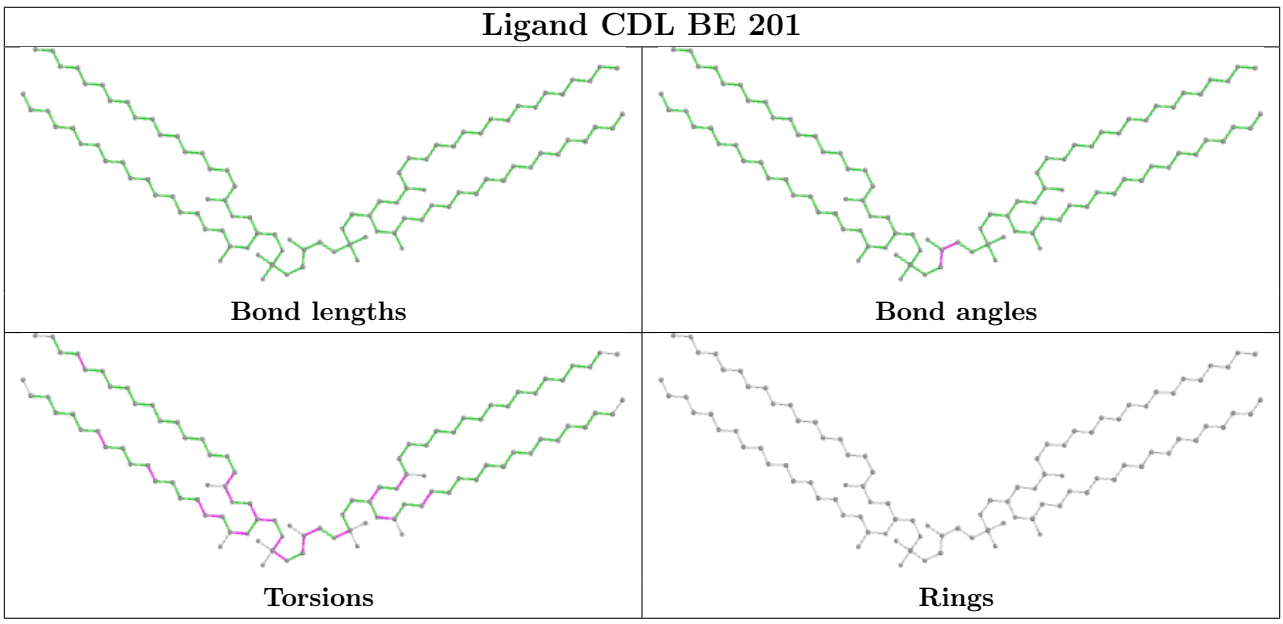


Rings

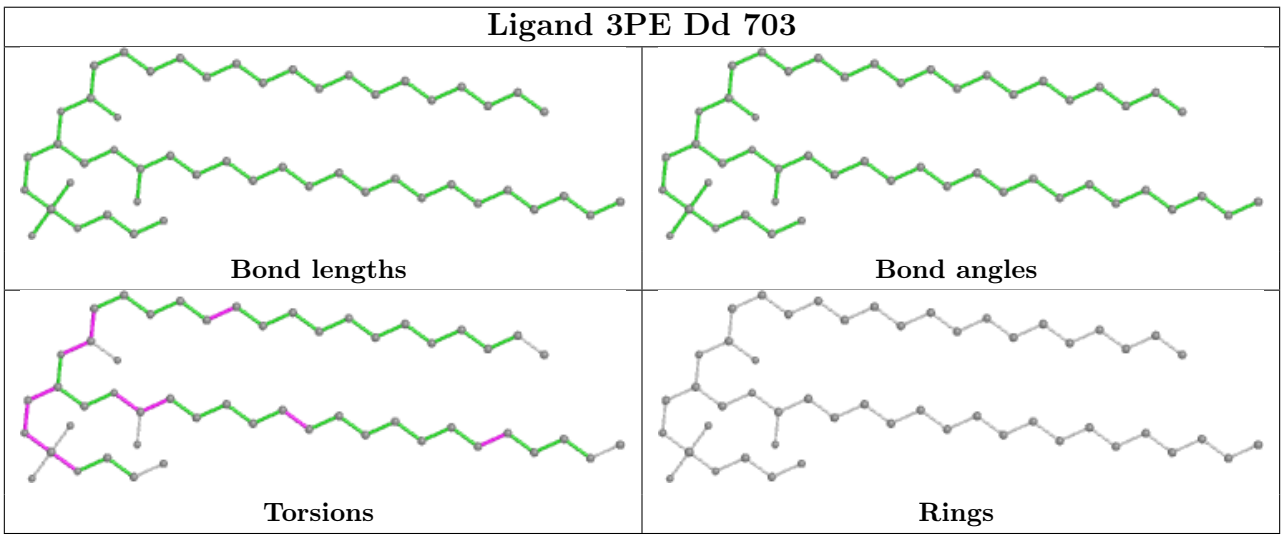
Ligand CDL Di 1101



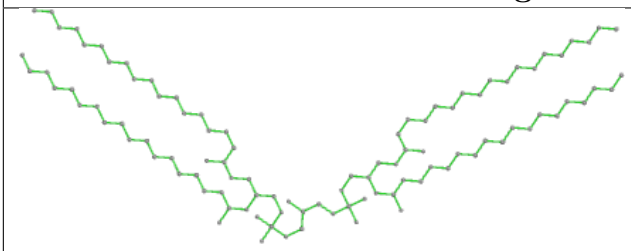
Ligand CDL BE 201



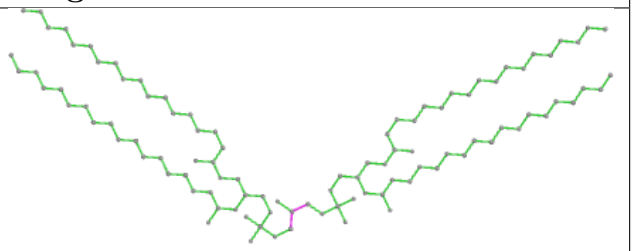
Ligand 3PE Dd 703



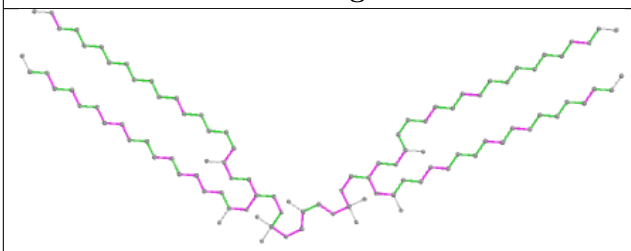
Ligand CDL Dg 201



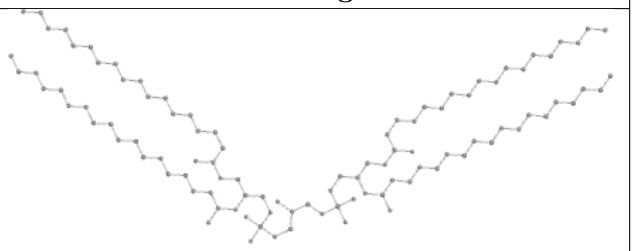
Bond lengths



Bond angles

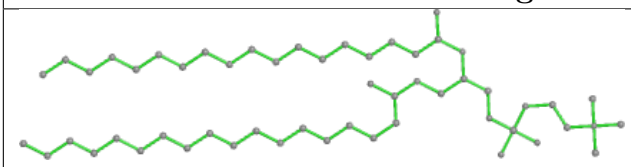


Torsions

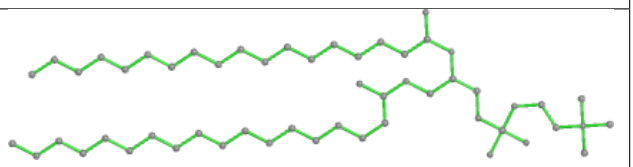


Rings

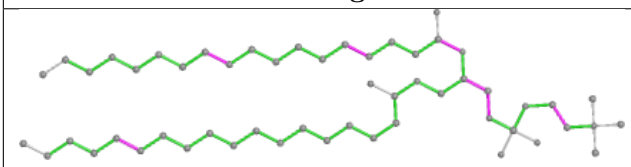
Ligand PC1 AL 303



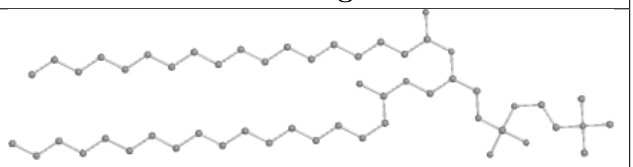
Bond lengths



Bond angles

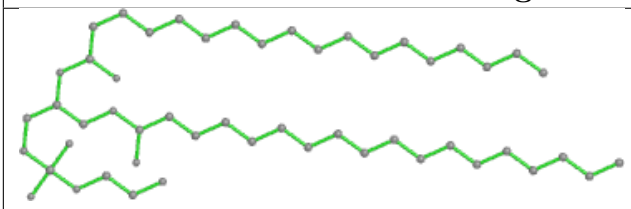


Torsions

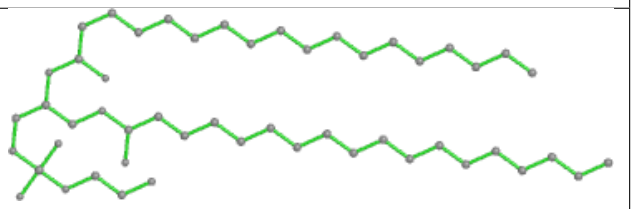


Rings

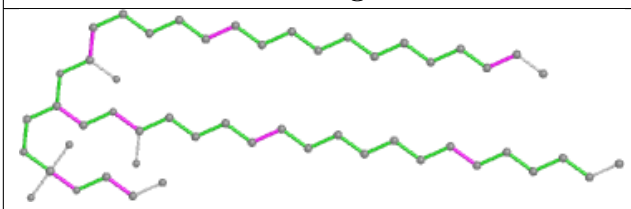
Ligand 3PE DC 607



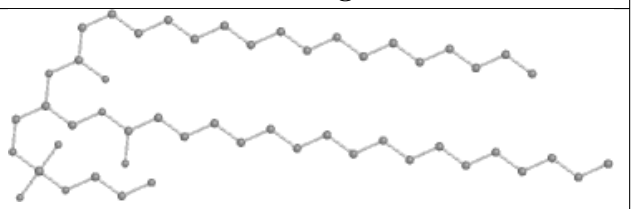
Bond lengths



Bond angles

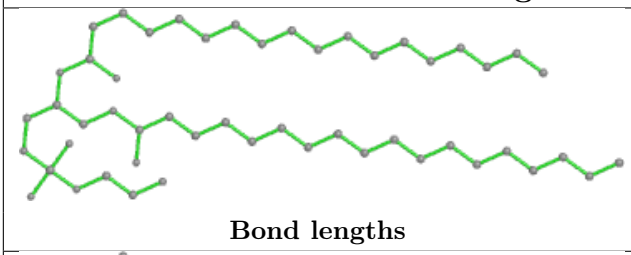


Torsions

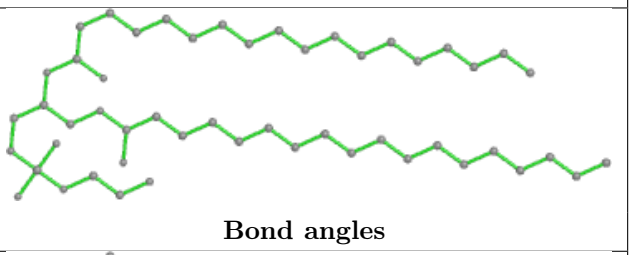


Rings

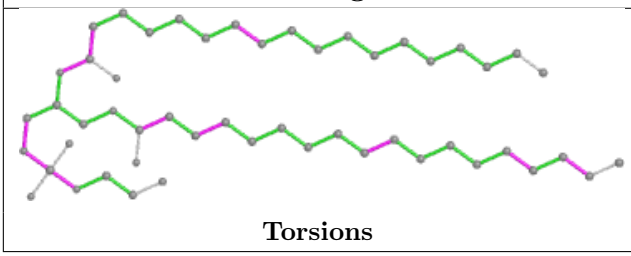
Ligand 3PE DX 303



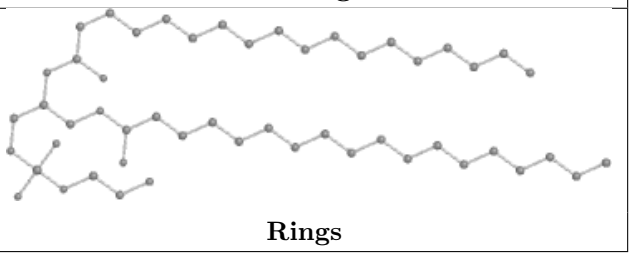
Bond lengths



Bond angles

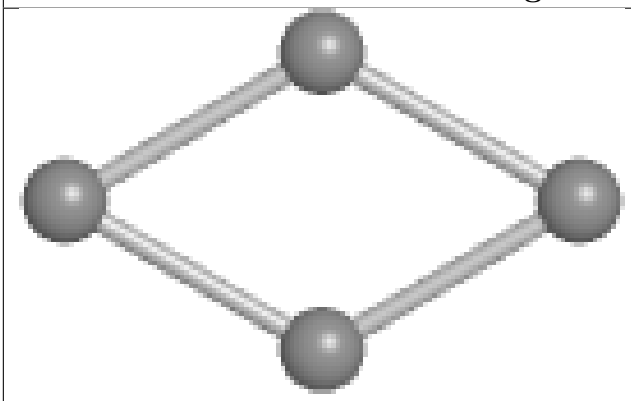


Torsions

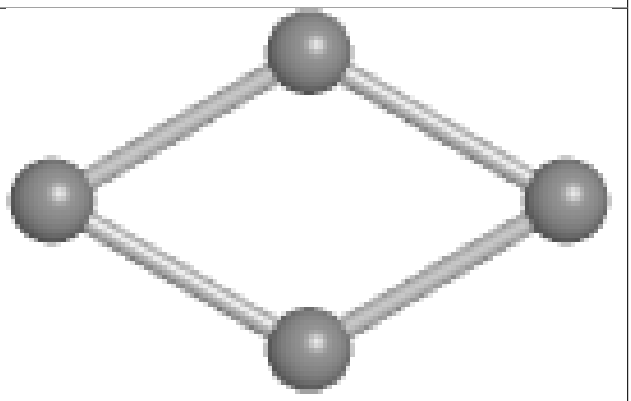


Rings

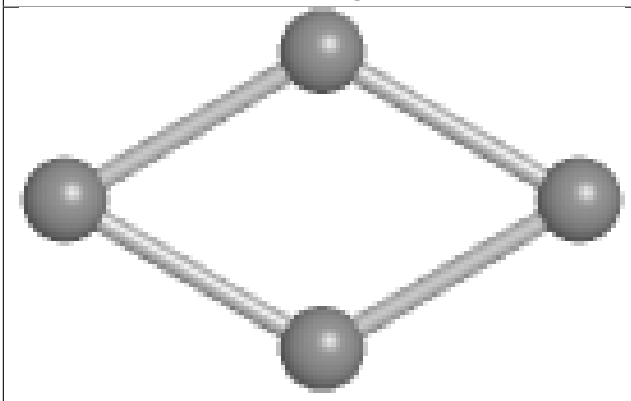
Ligand FES Ef 503



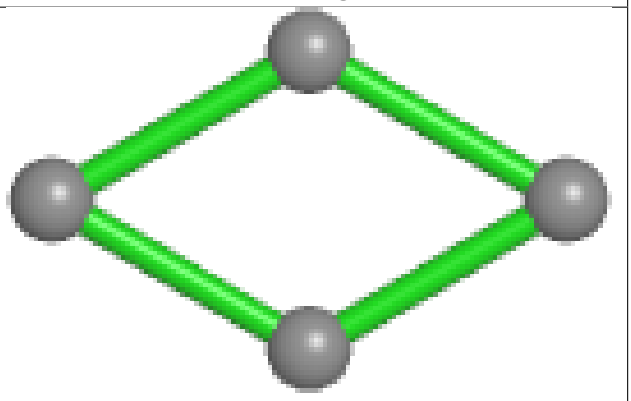
Bond lengths



Bond angles

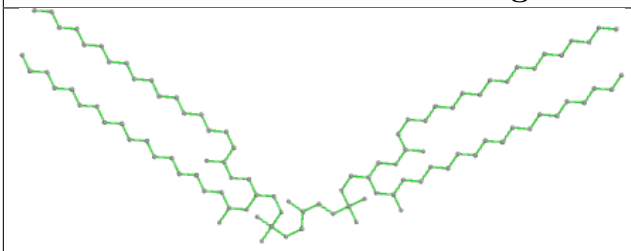


Torsions

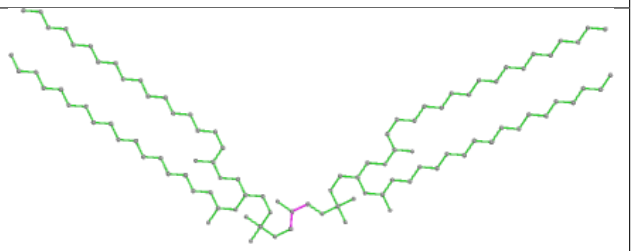


Rings

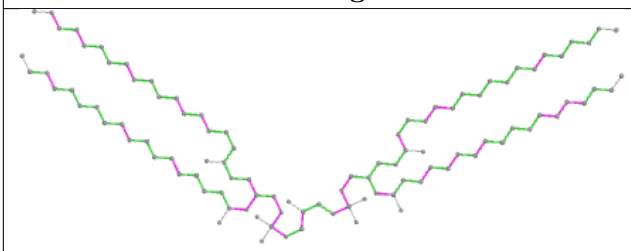
Ligand CDL AC 802



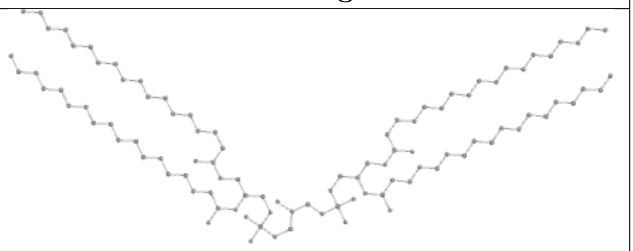
Bond lengths



Bond angles

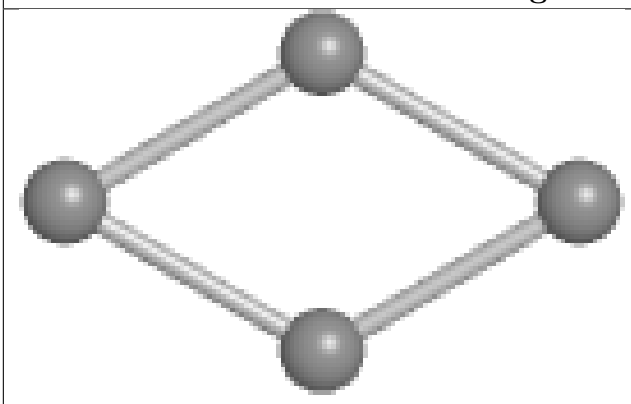


Torsions

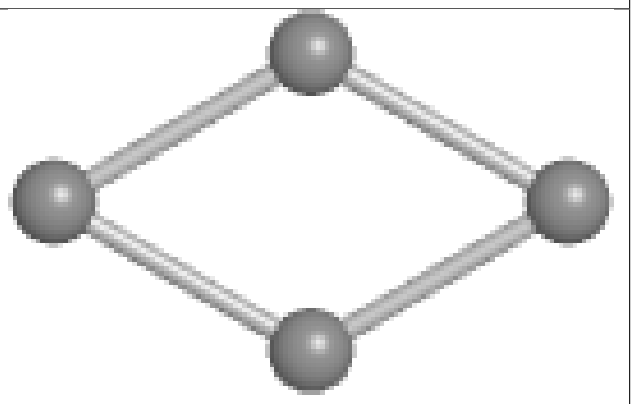


Rings

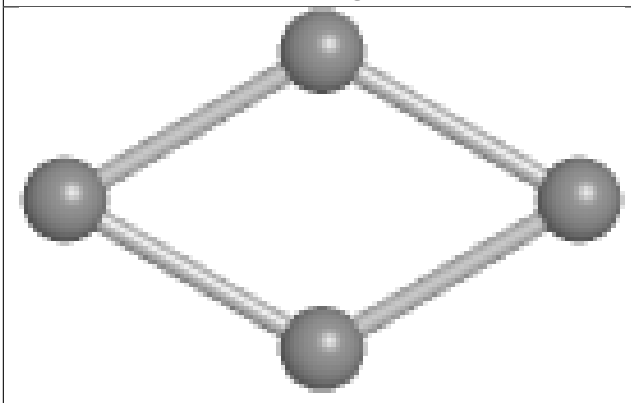
Ligand FES E 302



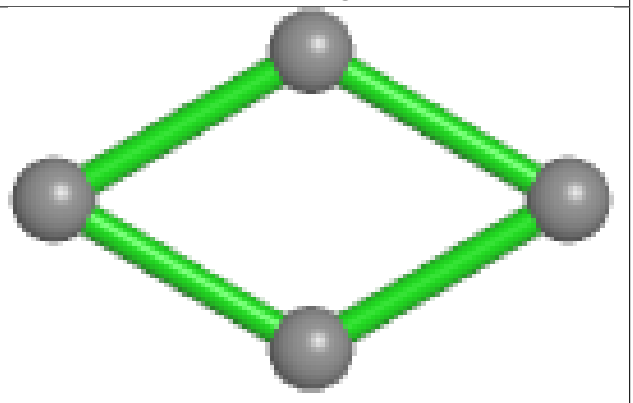
Bond lengths



Bond angles

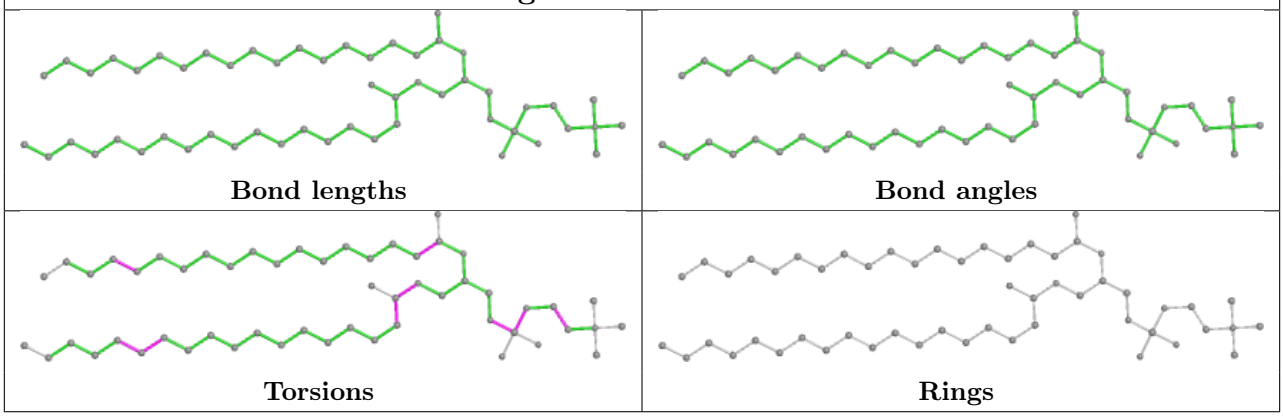


Torsions

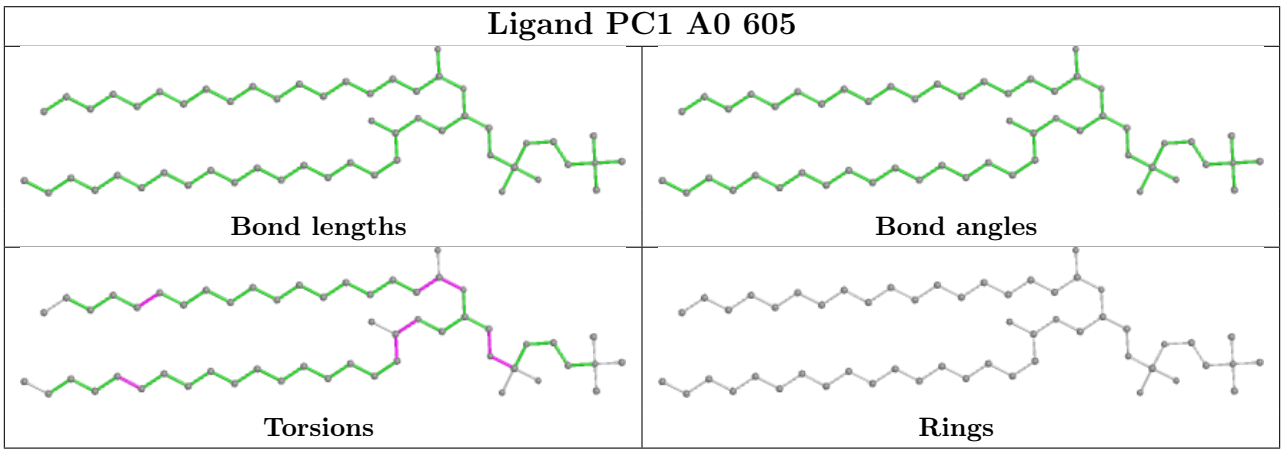


Rings

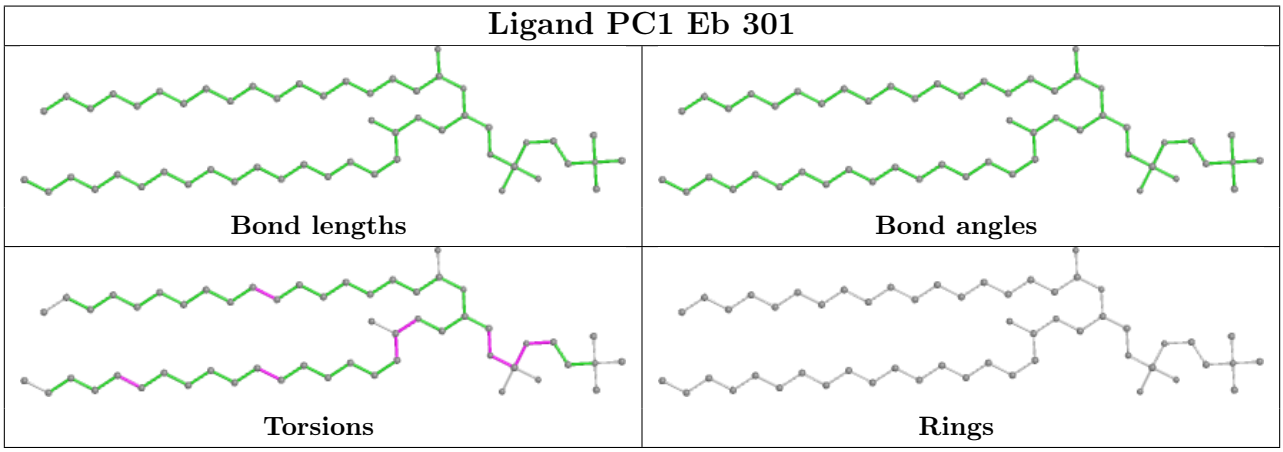
Ligand PC1 Dv 406



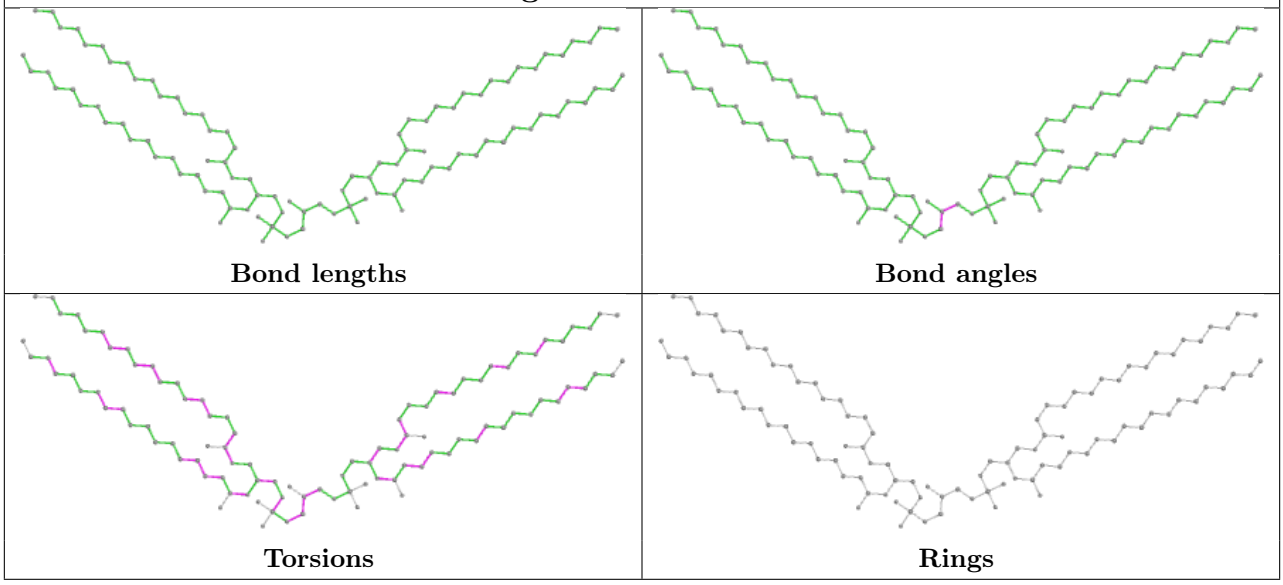
Ligand PC1 A0 605



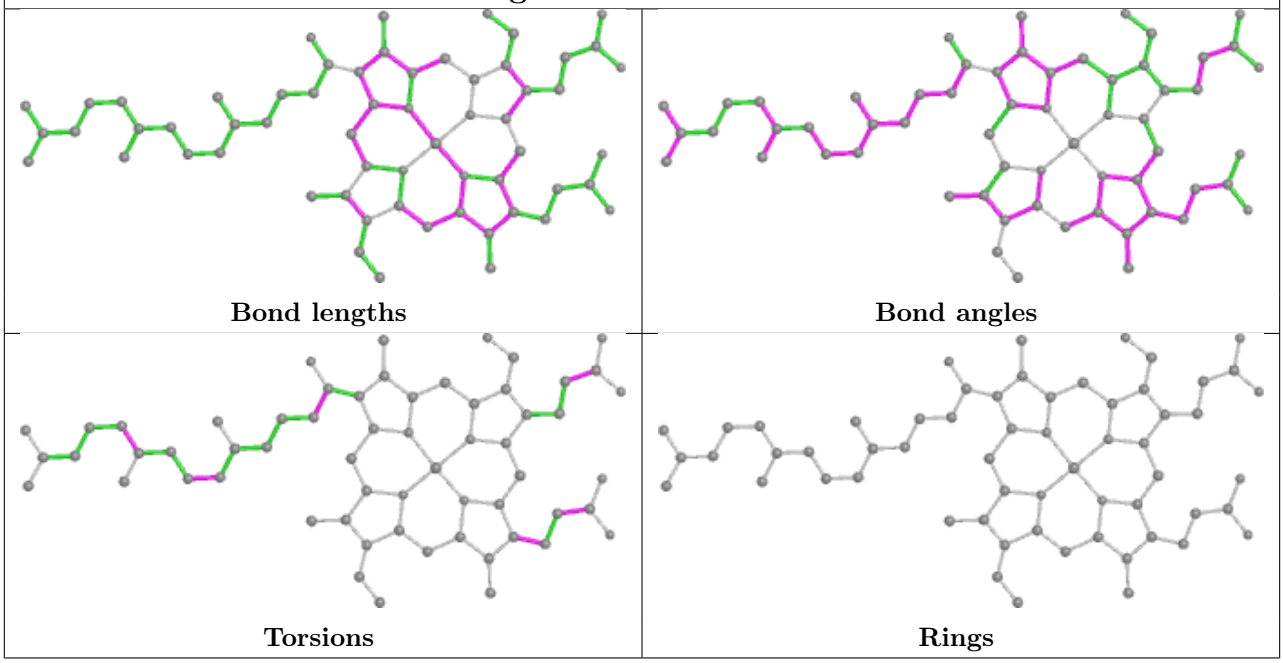
Ligand PC1 Eb 301



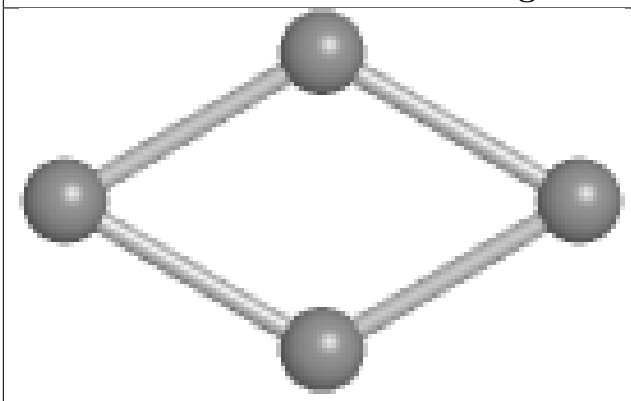
Ligand CDL El 901



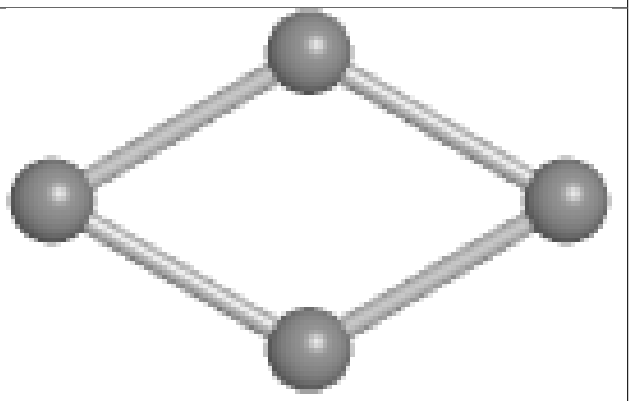
Ligand HEA DA 703



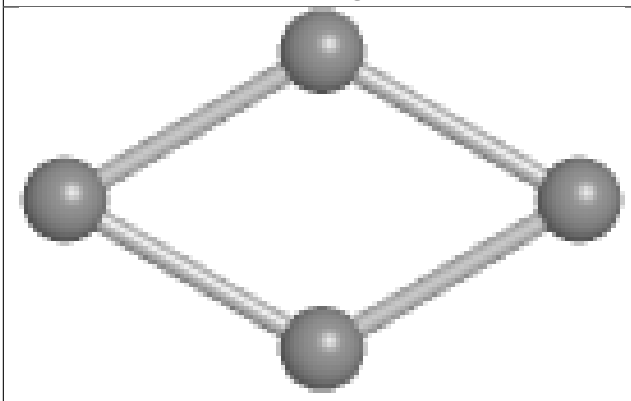
Ligand FES EF 201



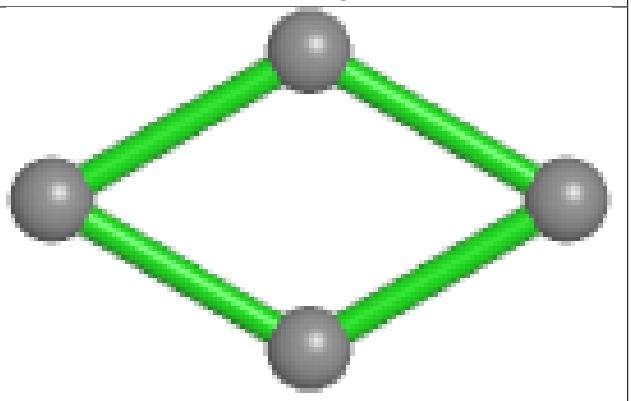
Bond lengths



Bond angles

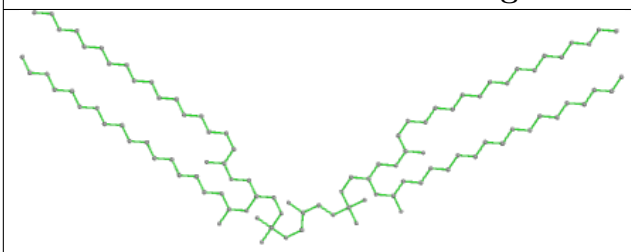


Torsions

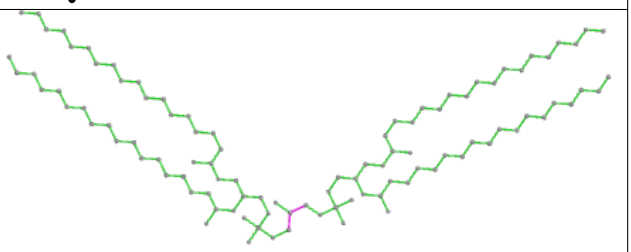


Rings

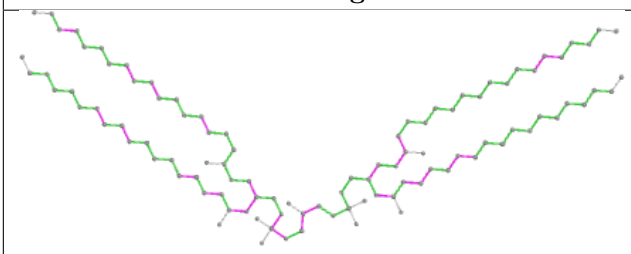
Ligand CDL DQ 1501



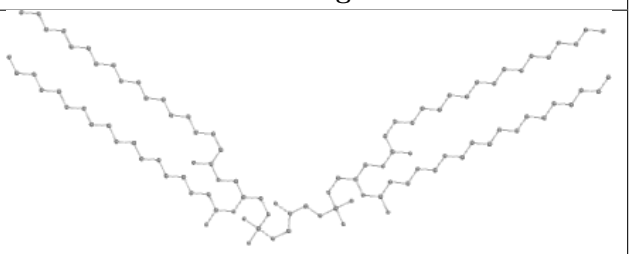
Bond lengths



Bond angles

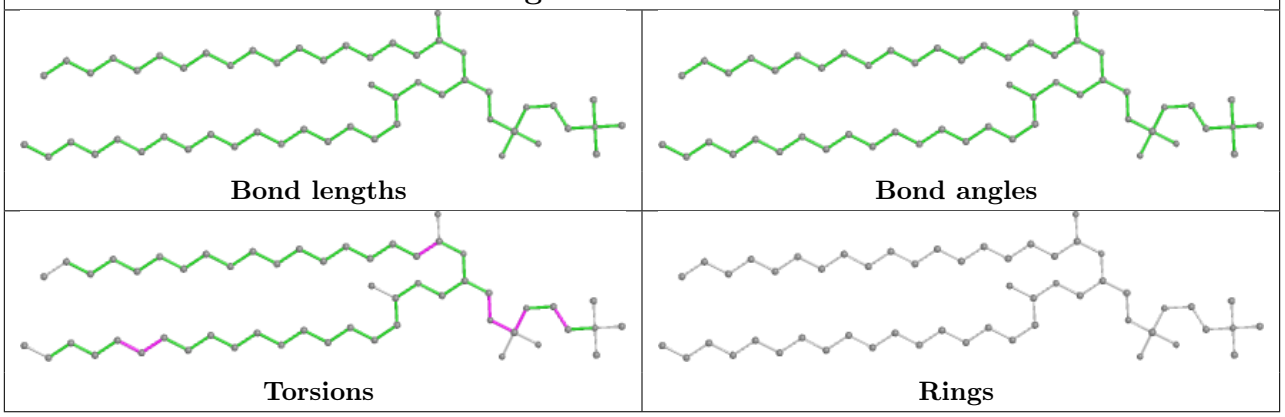


Torsions

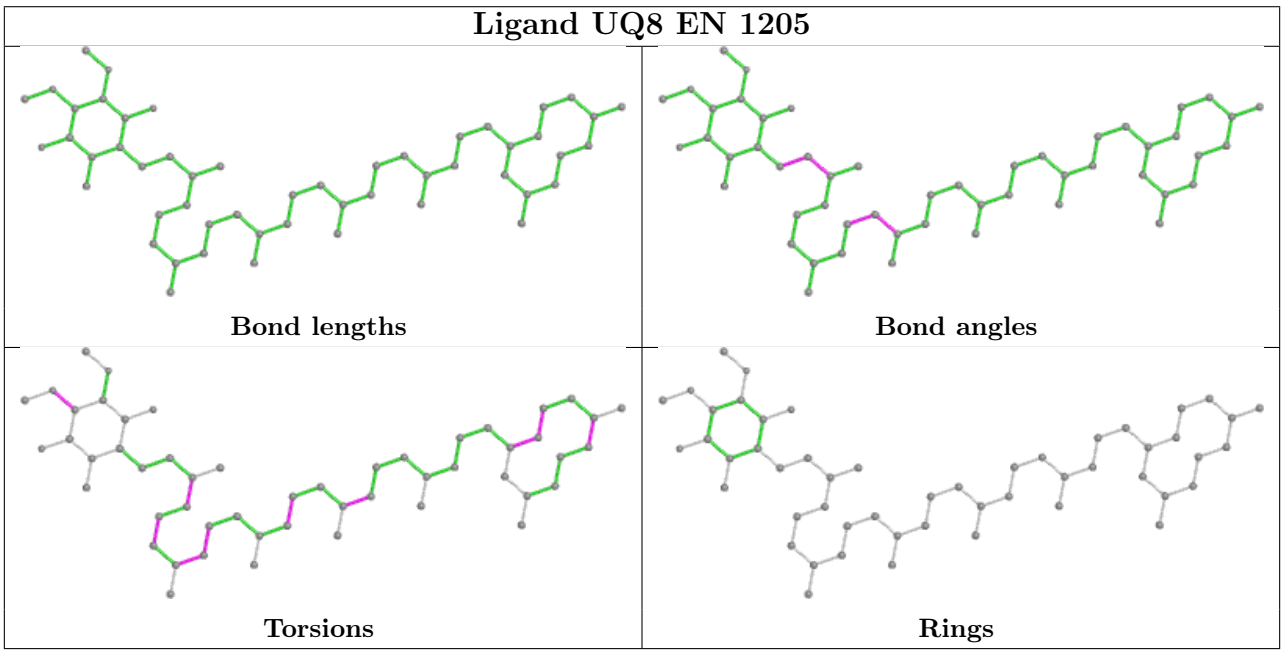


Rings

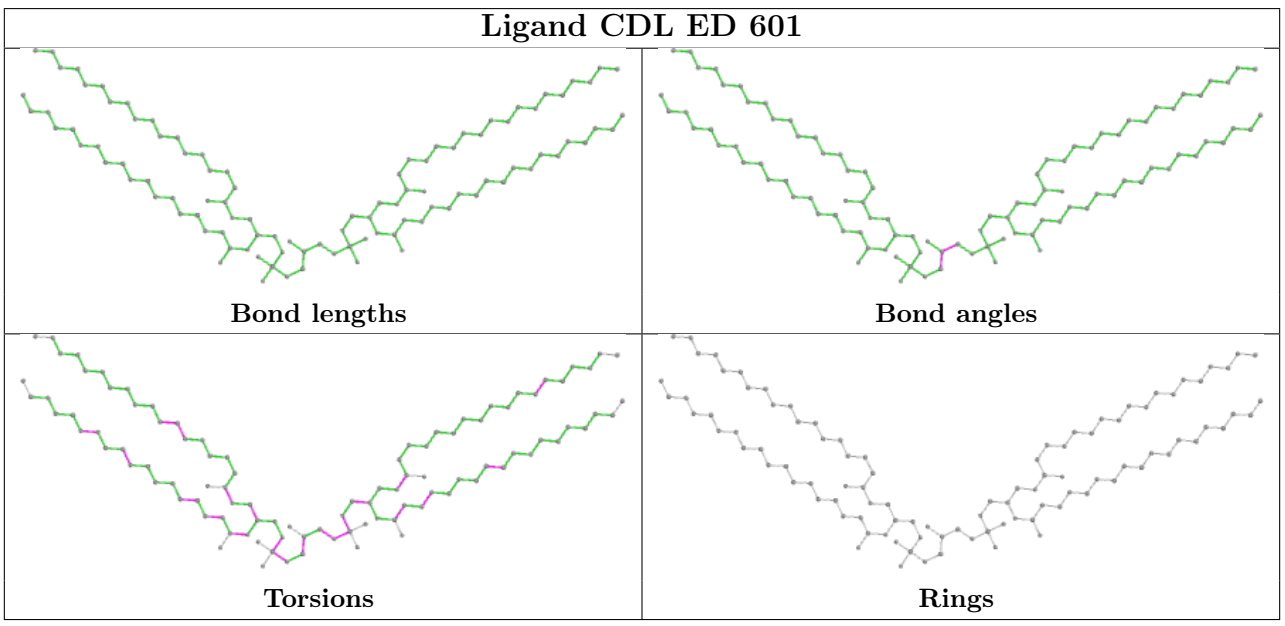
Ligand PC1 El 904



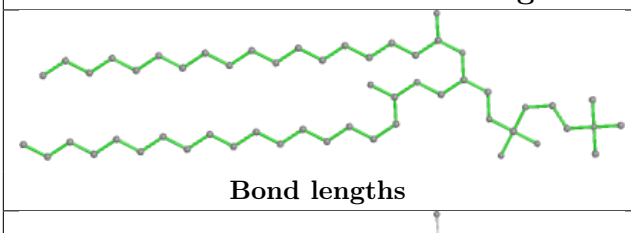
Ligand UQ8 EN 1205



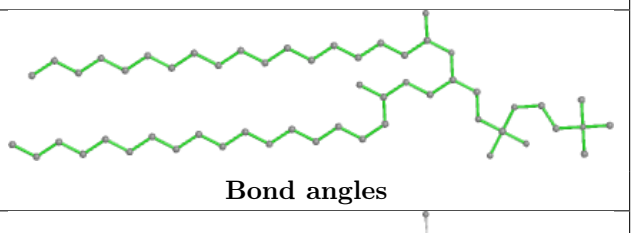
Ligand CDL ED 601



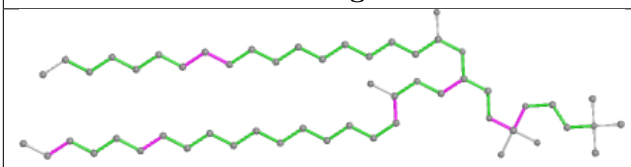
Ligand PC1 Dv 404



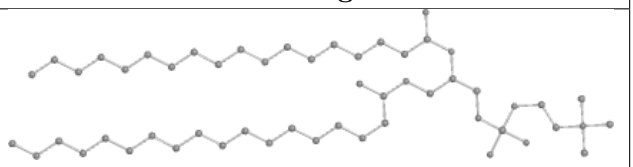
Bond lengths



Bond angles

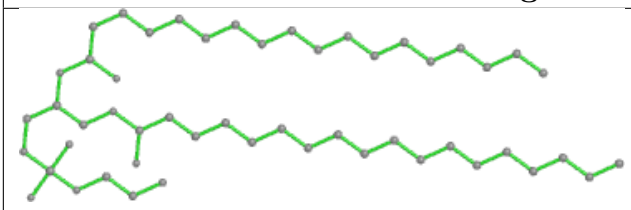


Torsions

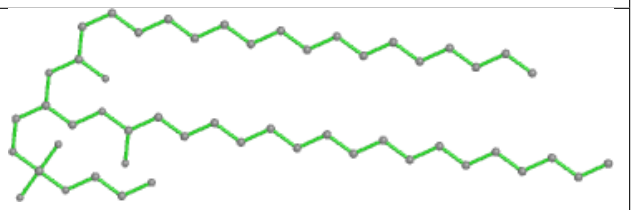


Rings

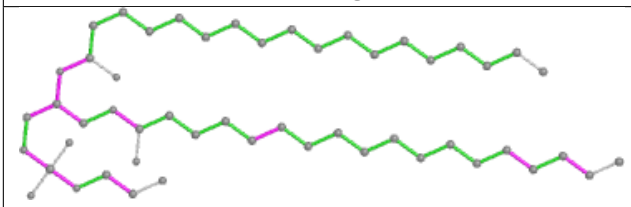
Ligand 3PE Dr 401



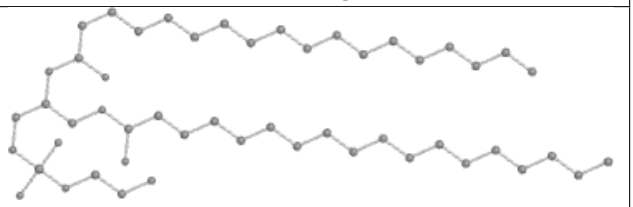
Bond lengths



Bond angles

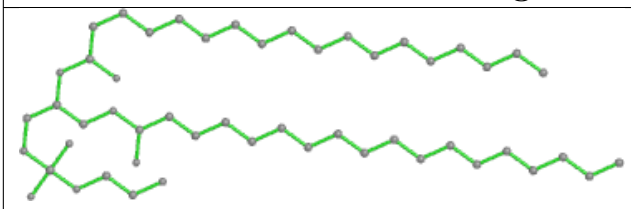


Torsions

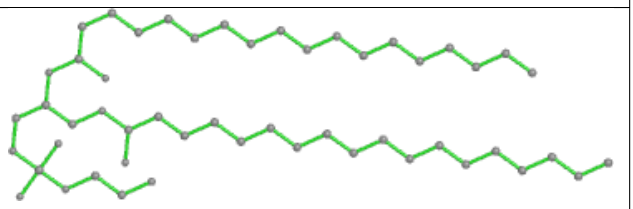


Rings

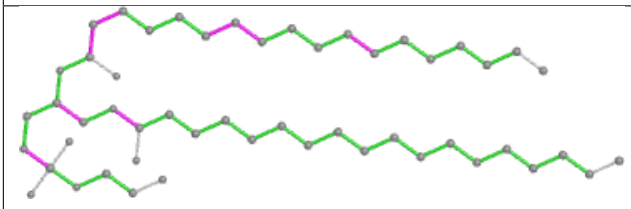
Ligand 3PE EM 901



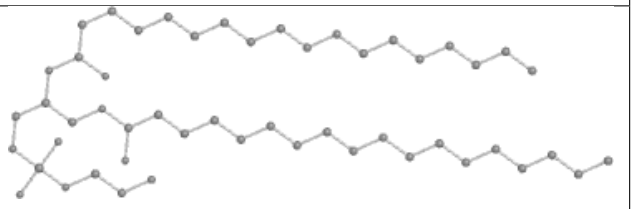
Bond lengths



Bond angles

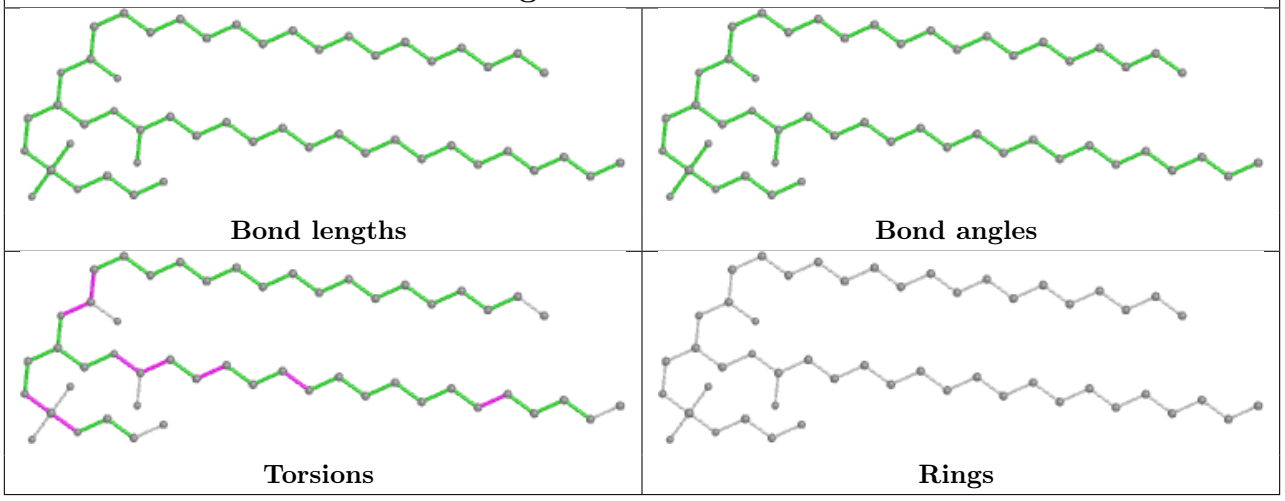


Torsions

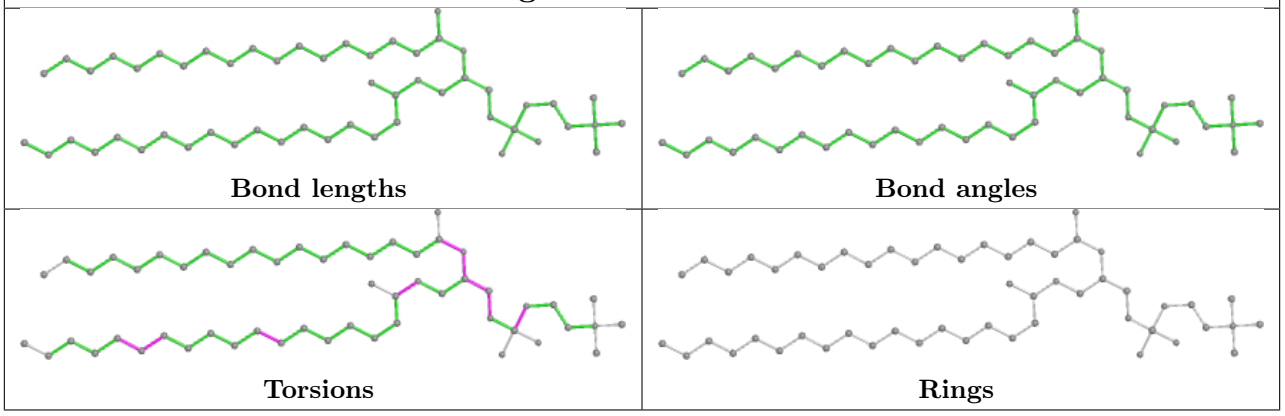


Rings

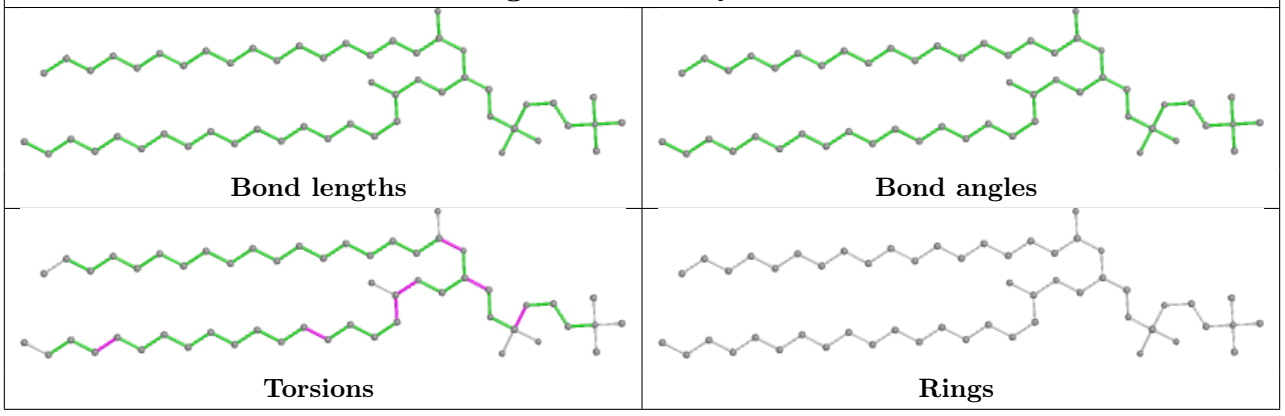
Ligand 3PE DJ 301



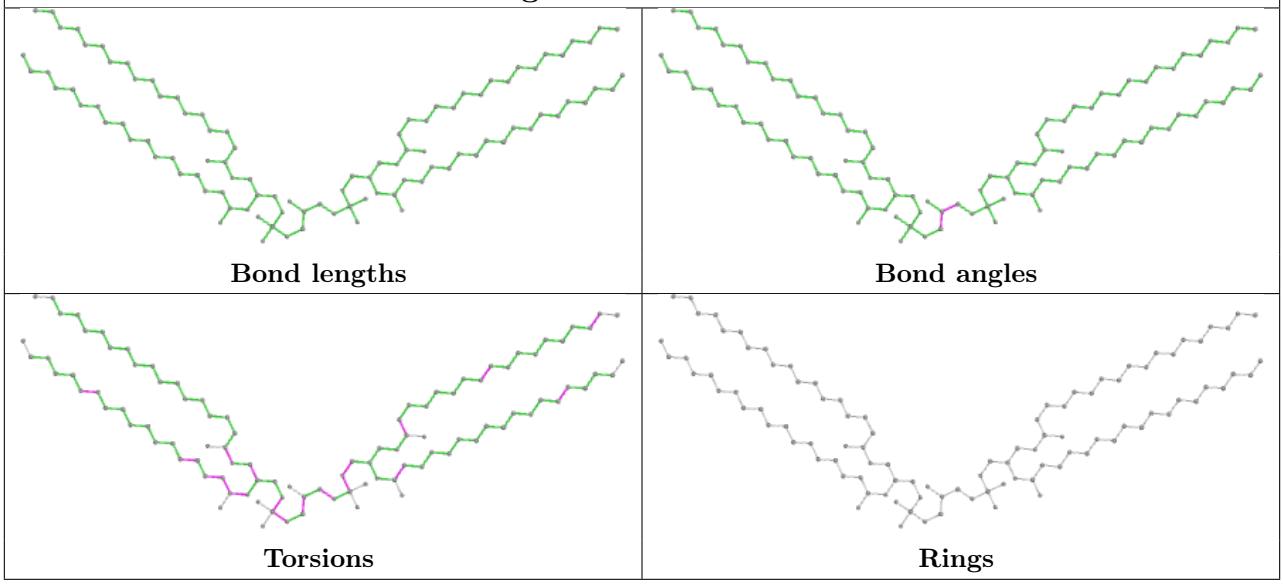
Ligand PC1 A 1201



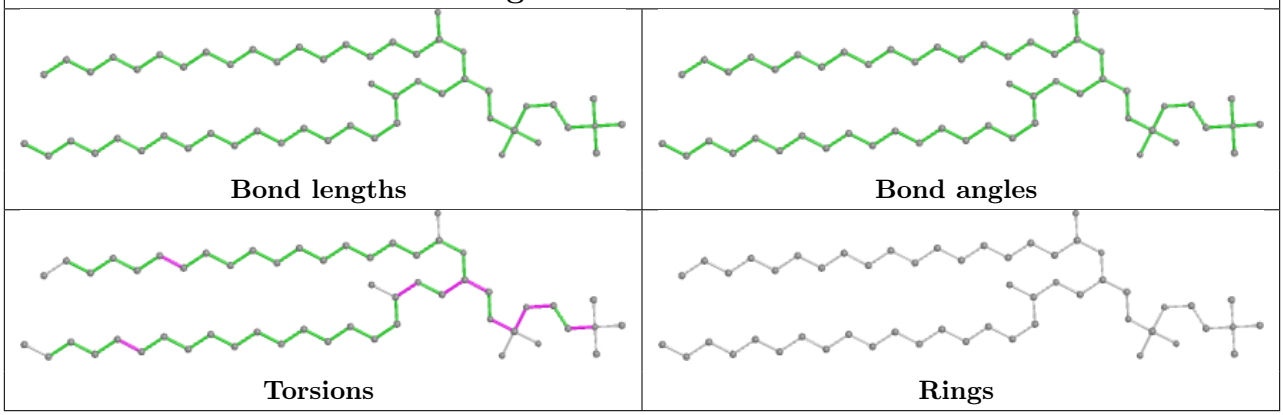
Ligand PC1 DQ 1503



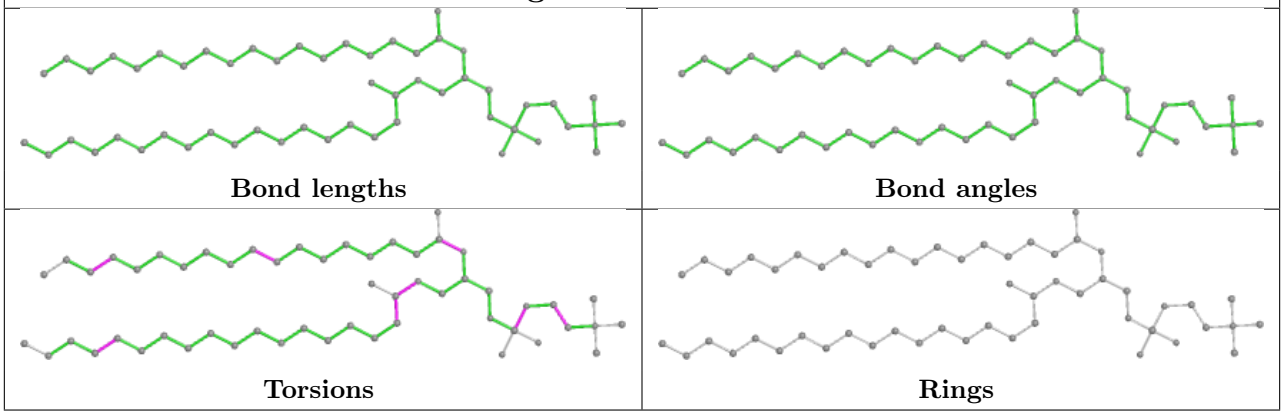
Ligand CDL Ei 401



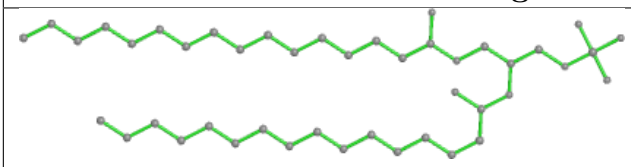
Ligand PC1 EN 1203



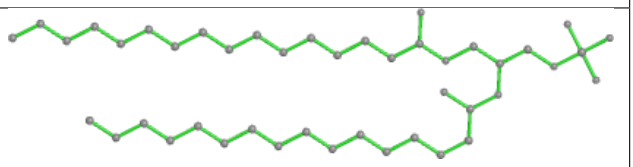
Ligand PC1 K 502



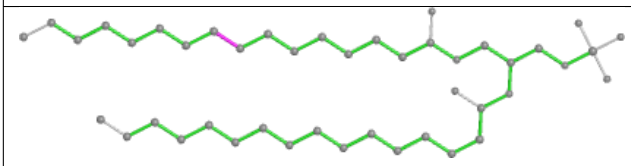
Ligand LPP DN 505



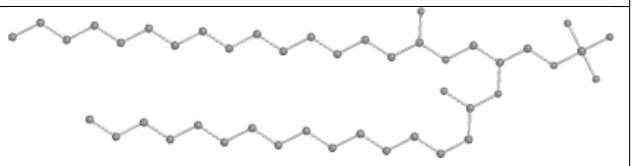
Bond lengths



Bond angles

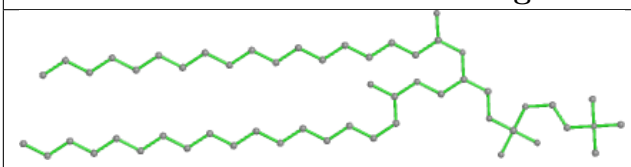


Torsions

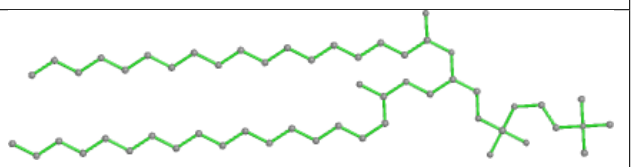


Rings

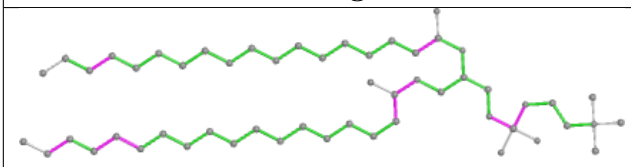
Ligand PC1 DC 602



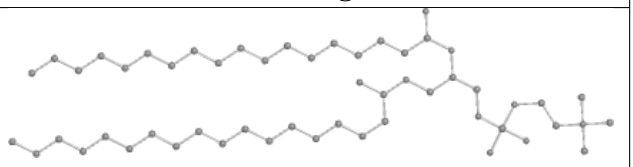
Bond lengths



Bond angles

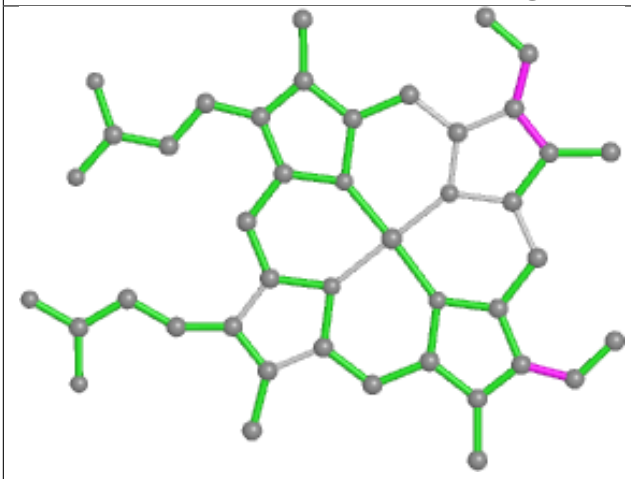


Torsions

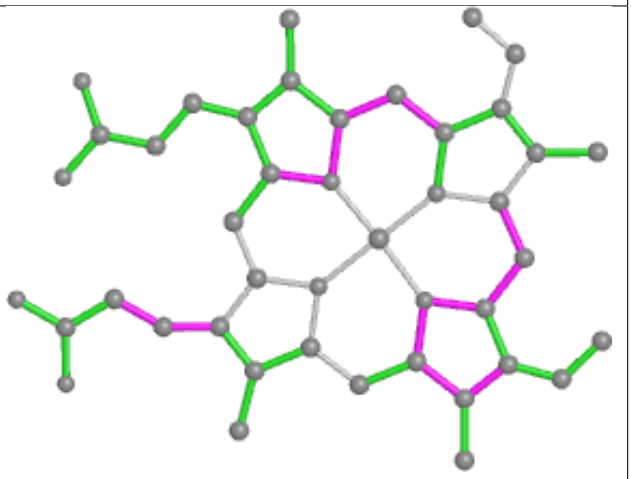


Rings

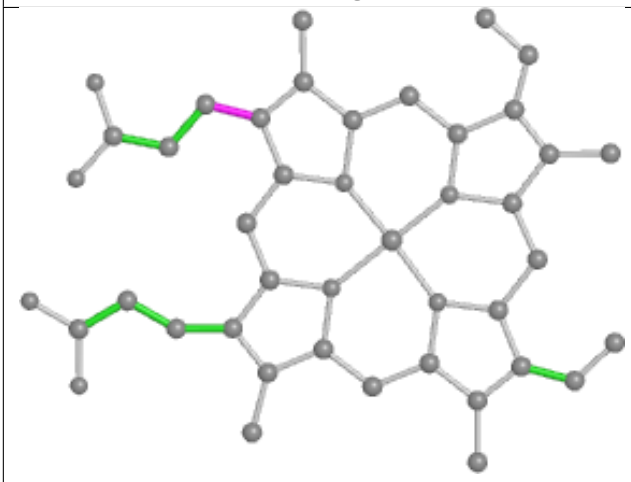
Ligand HEM c 504



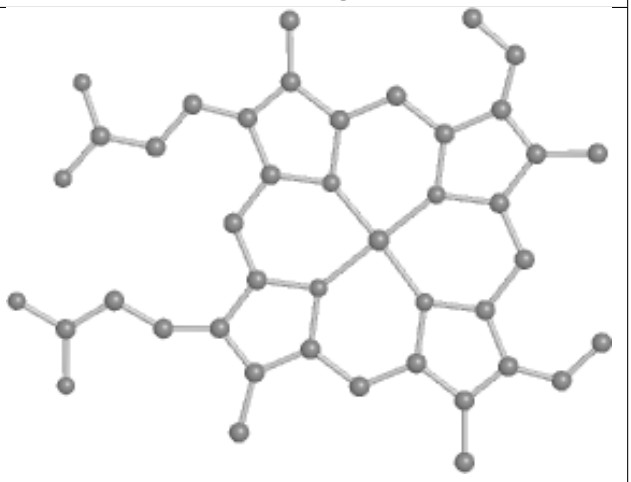
Bond lengths



Bond angles

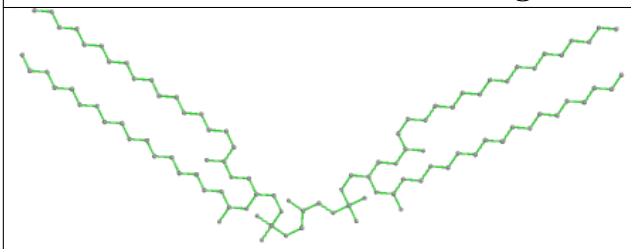


Torsions

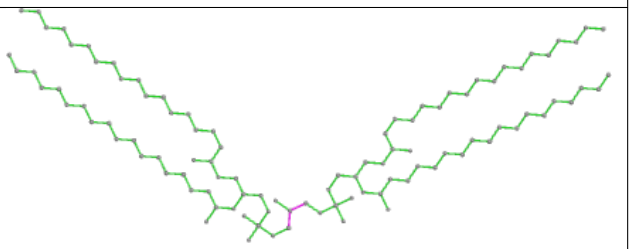


Rings

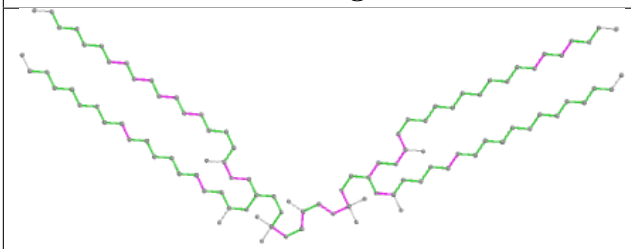
Ligand CDL DJ 302



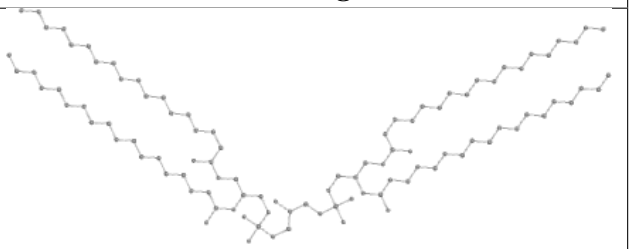
Bond lengths



Bond angles

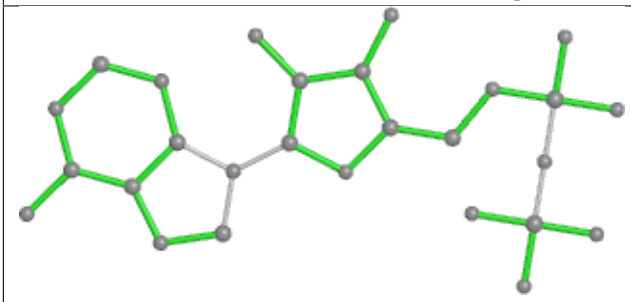


Torsions

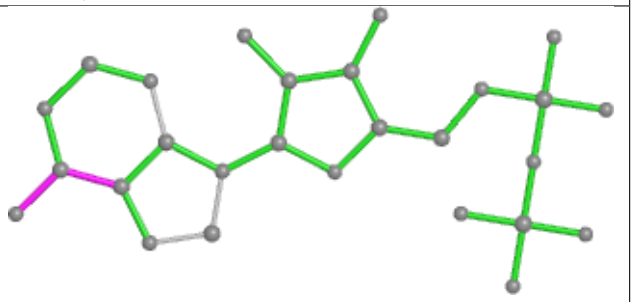


Rings

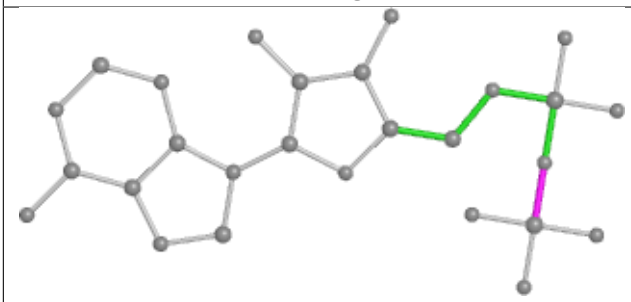
Ligand ADP AQ 201



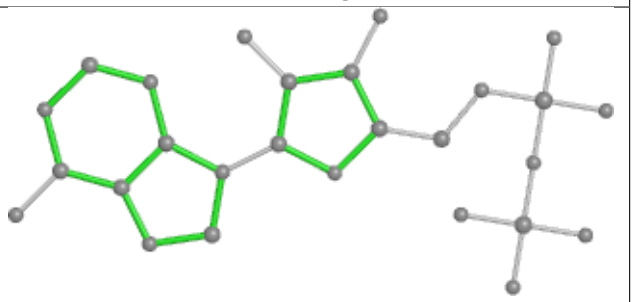
Bond lengths



Bond angles

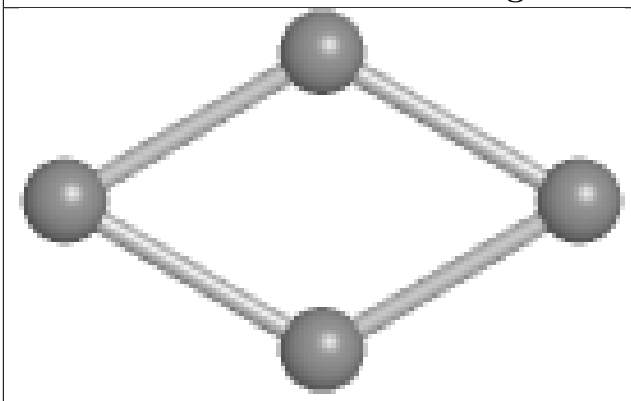


Torsions

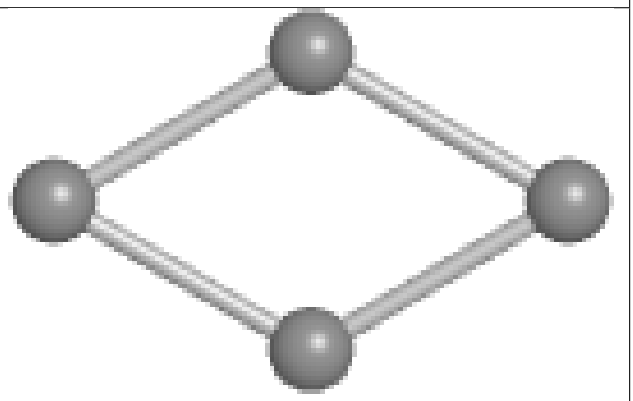


Rings

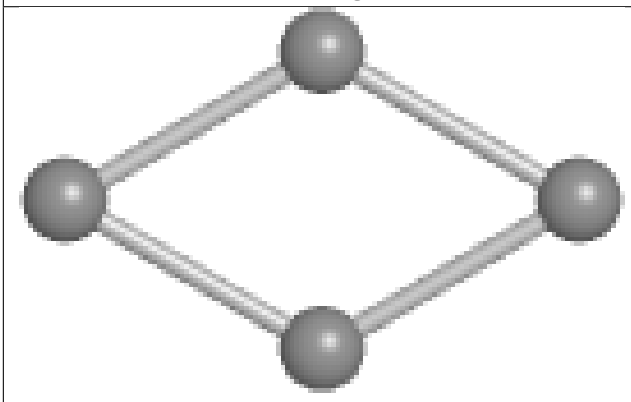
Ligand FES CB 1000



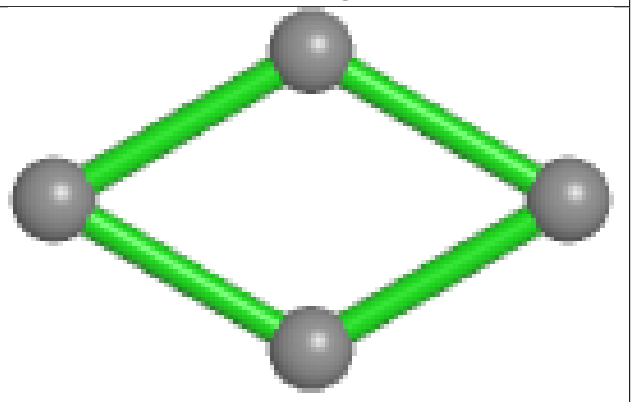
Bond lengths



Bond angles

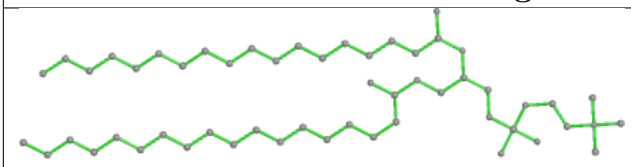


Torsions

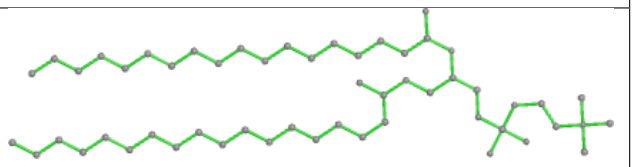


Rings

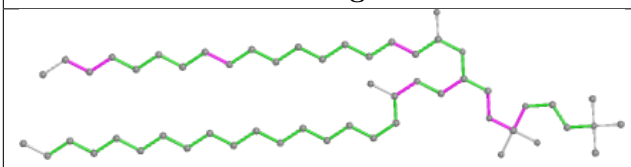
Ligand PC1 AC 804



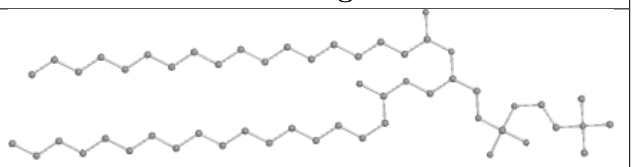
Bond lengths



Bond angles

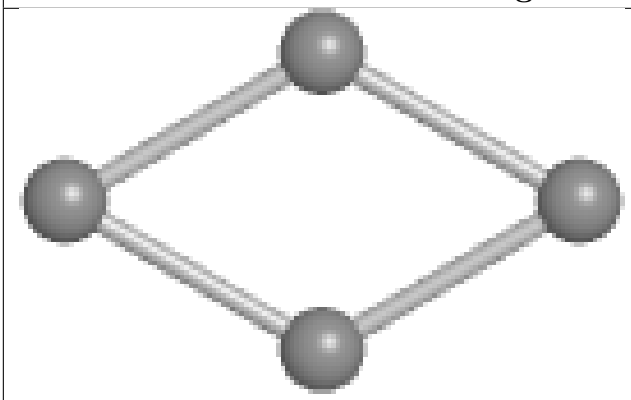


Torsions

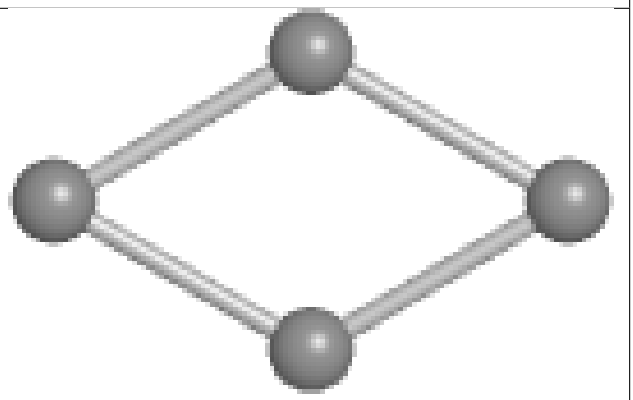


Rings

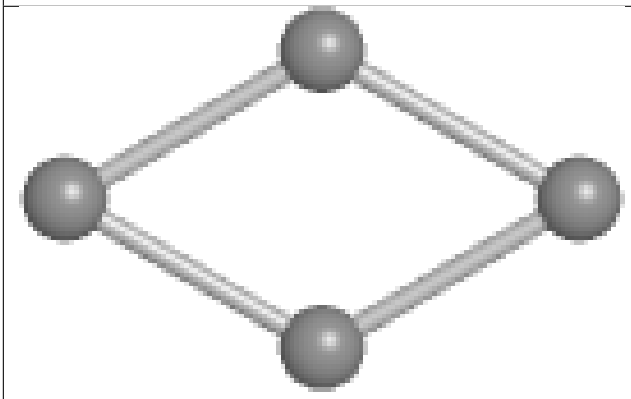
Ligand FES AB 801



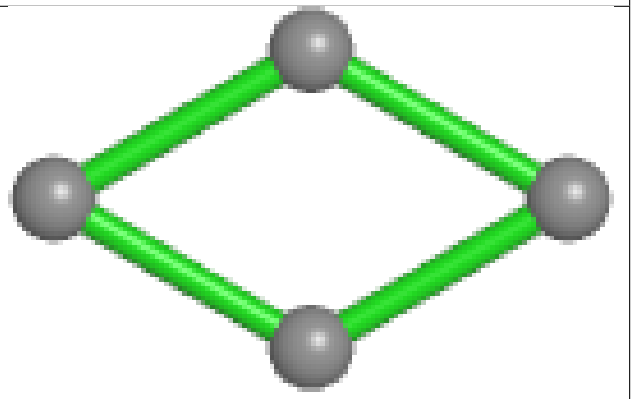
Bond lengths



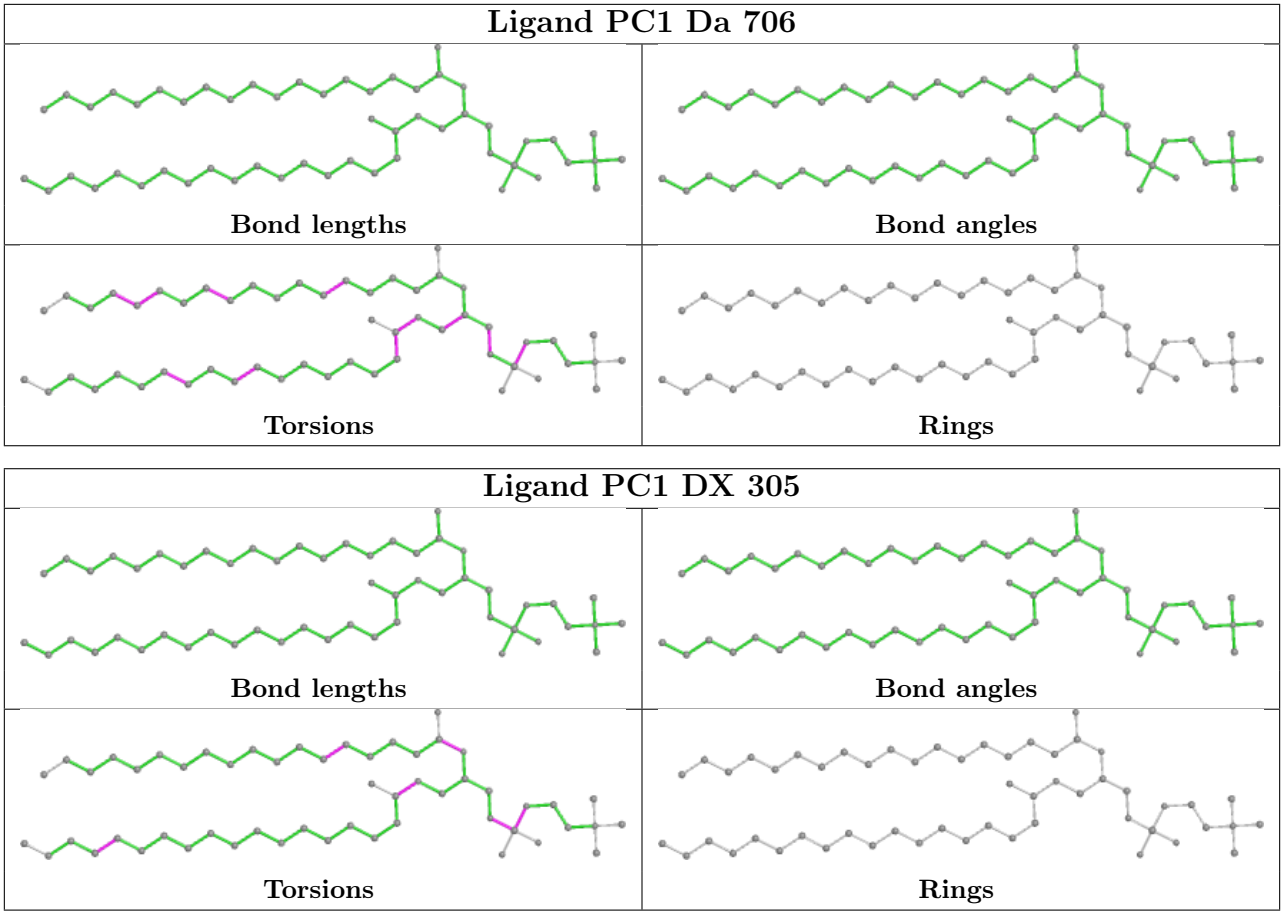
Bond angles



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.

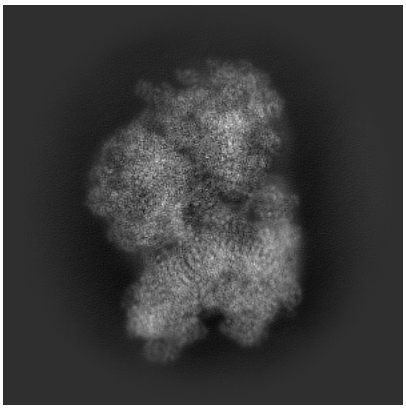
6 Map visualisation

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.

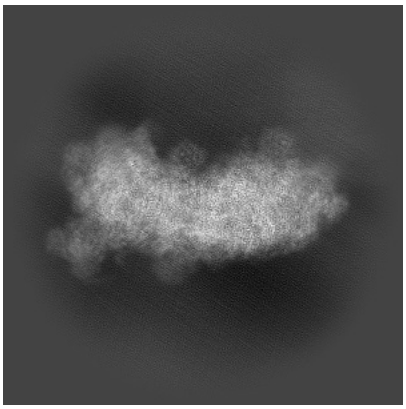
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

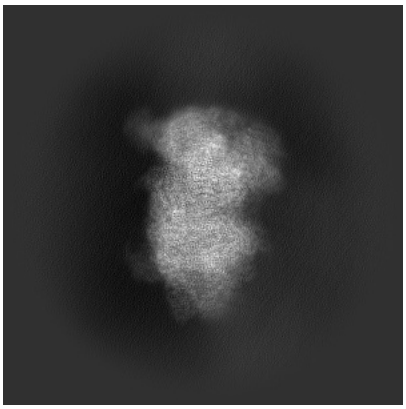
6.1.1 Primary map



X

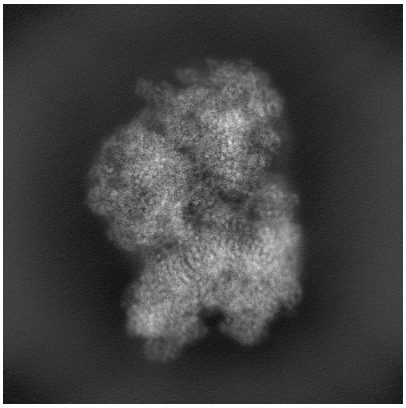


Y

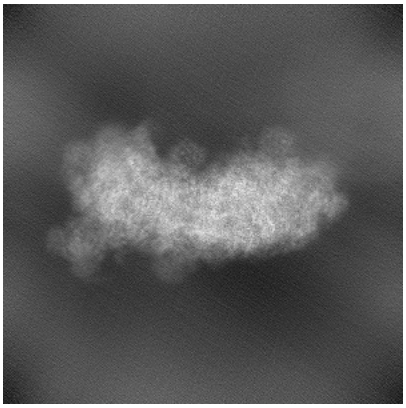


Z

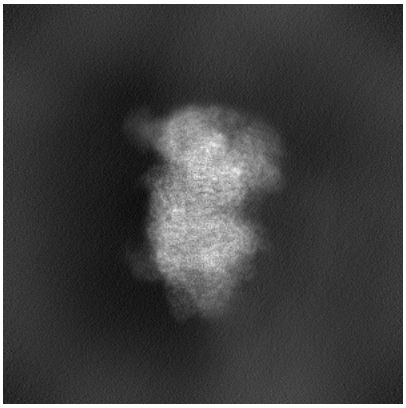
6.1.2 Raw map



X



Y

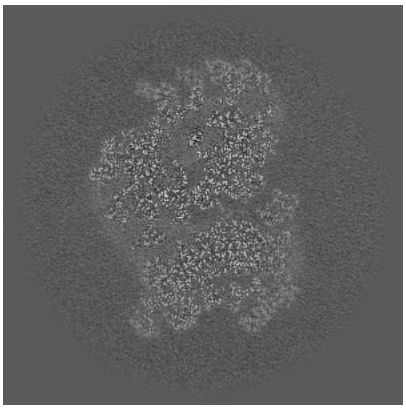


Z

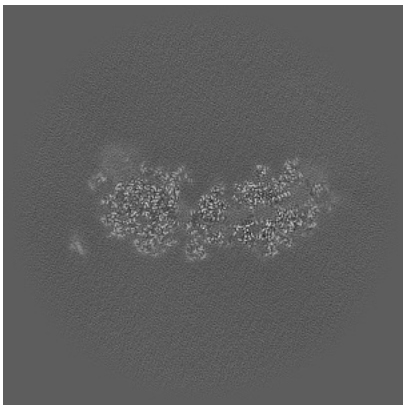
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



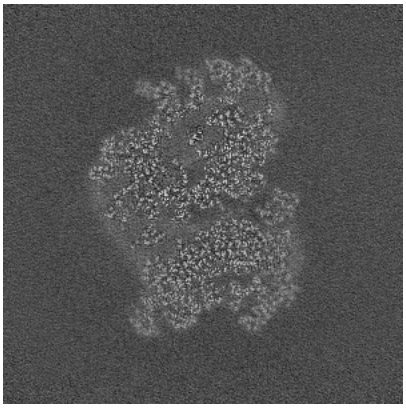
X Index: 240



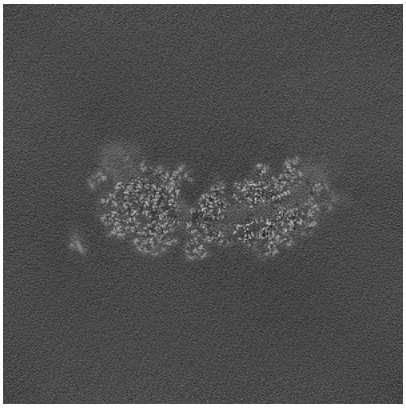
Y Index: 240

Z Index: 240

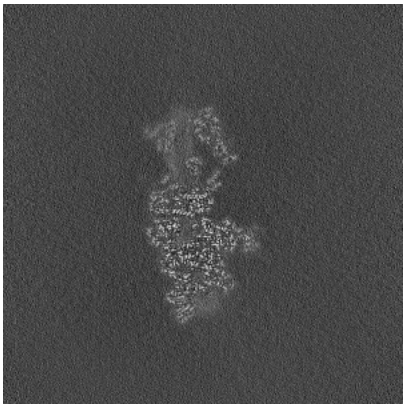
6.2.2 Raw map



X Index: 240



Y Index: 240

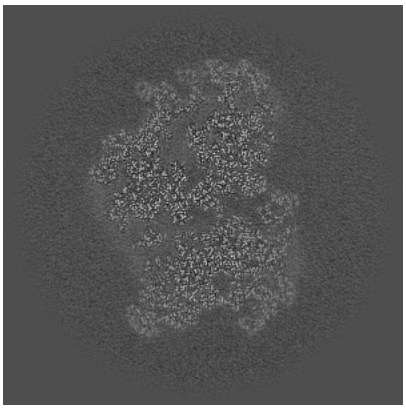


Z Index: 240

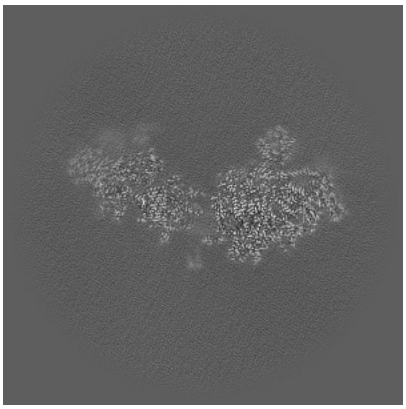
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

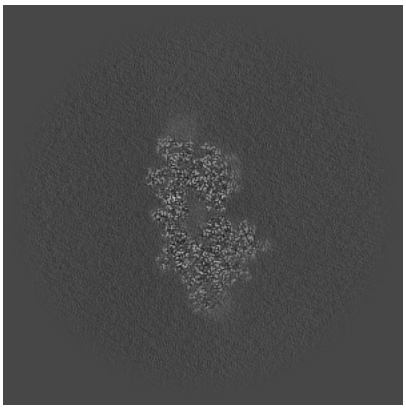
6.3.1 Primary map



X Index: 243

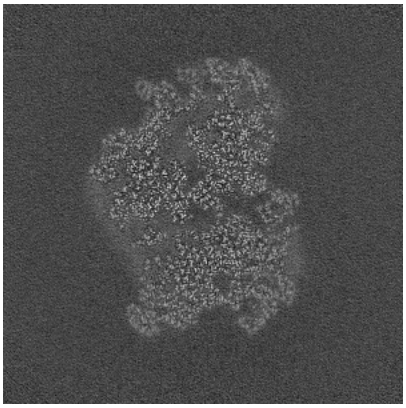


Y Index: 272

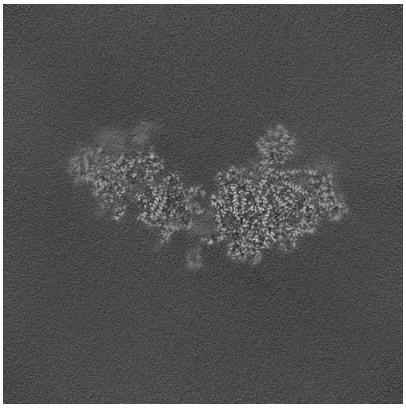


Z Index: 287

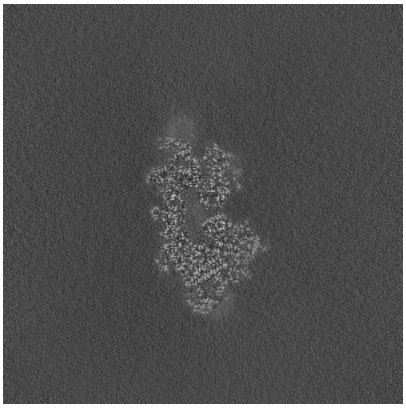
6.3.2 Raw map



X Index: 243



Y Index: 271

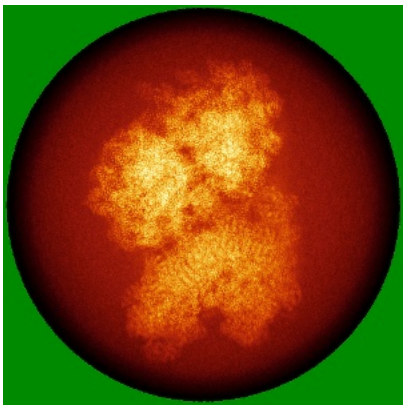


Z Index: 284

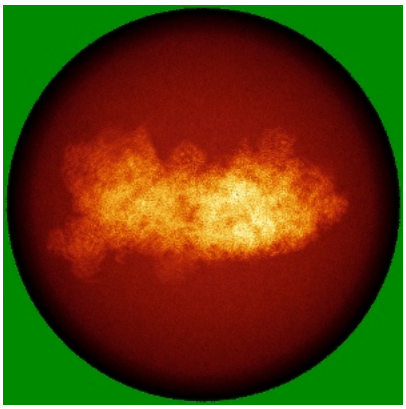
The images above show the largest variance slices of the map in three orthogonal directions.

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

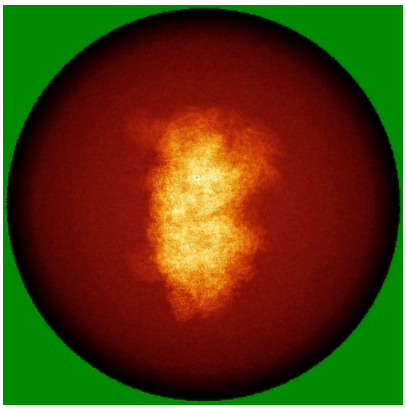
6.4.1 Primary map



X

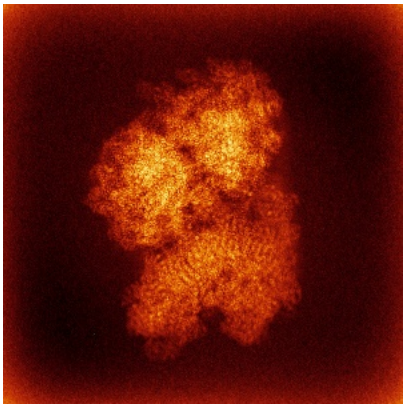


Y

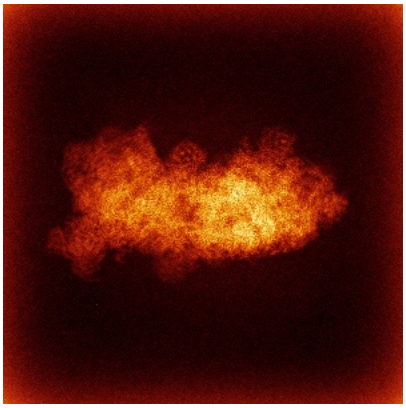


Z

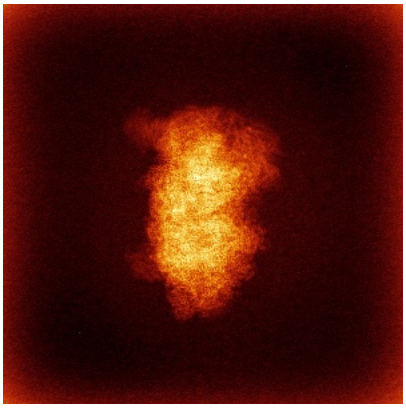
6.4.2 Raw map



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.

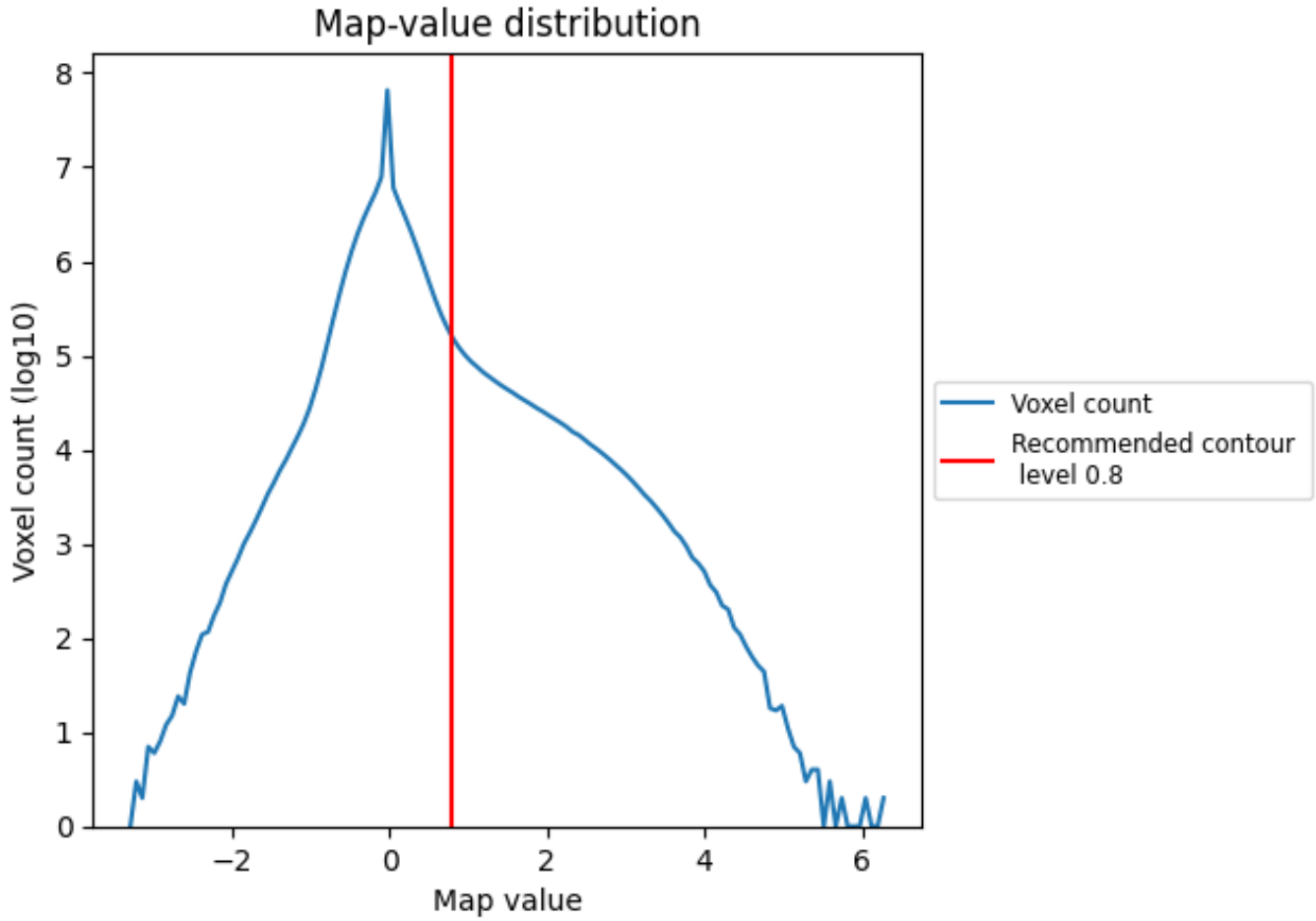
6.6 Mask visualisation (i)

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

7 Map analysis

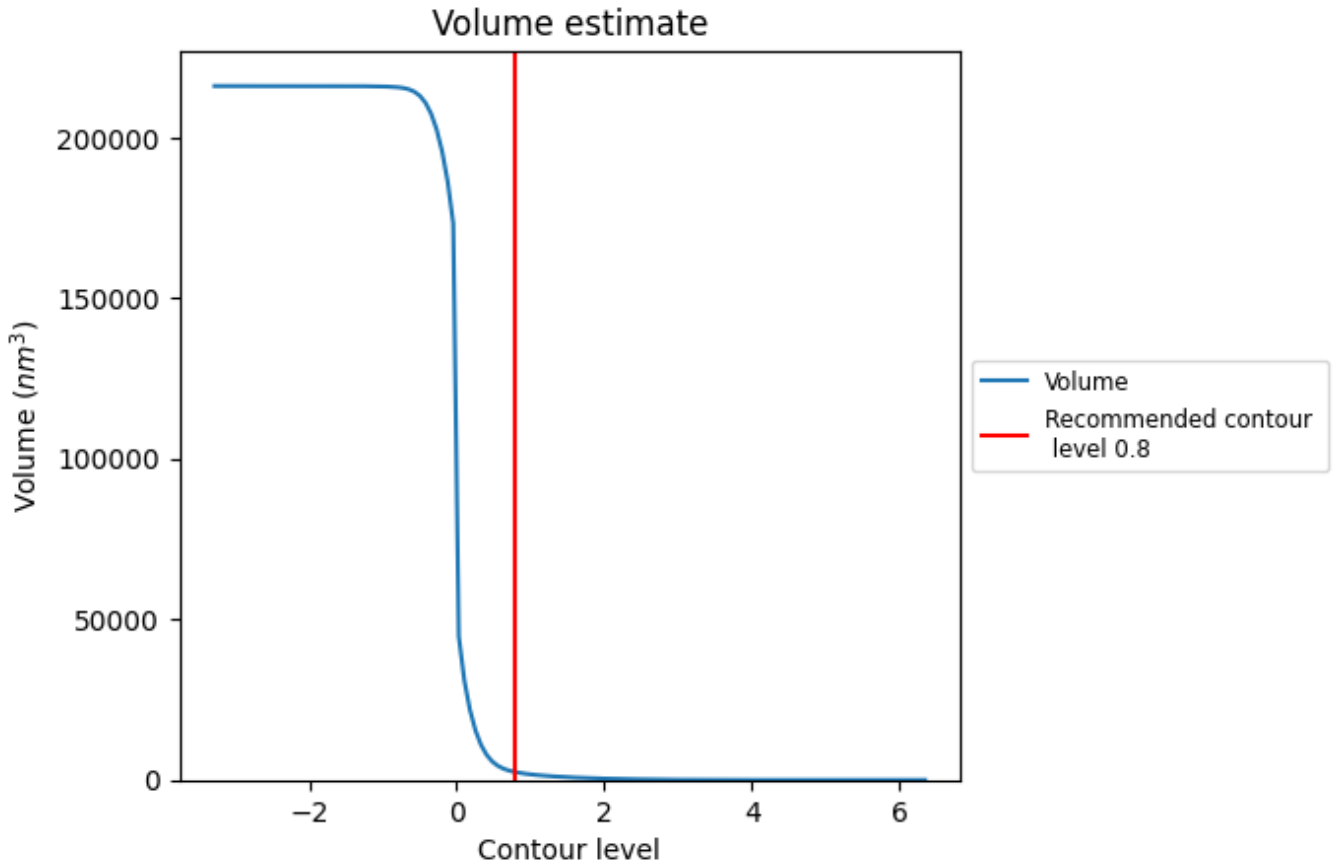
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

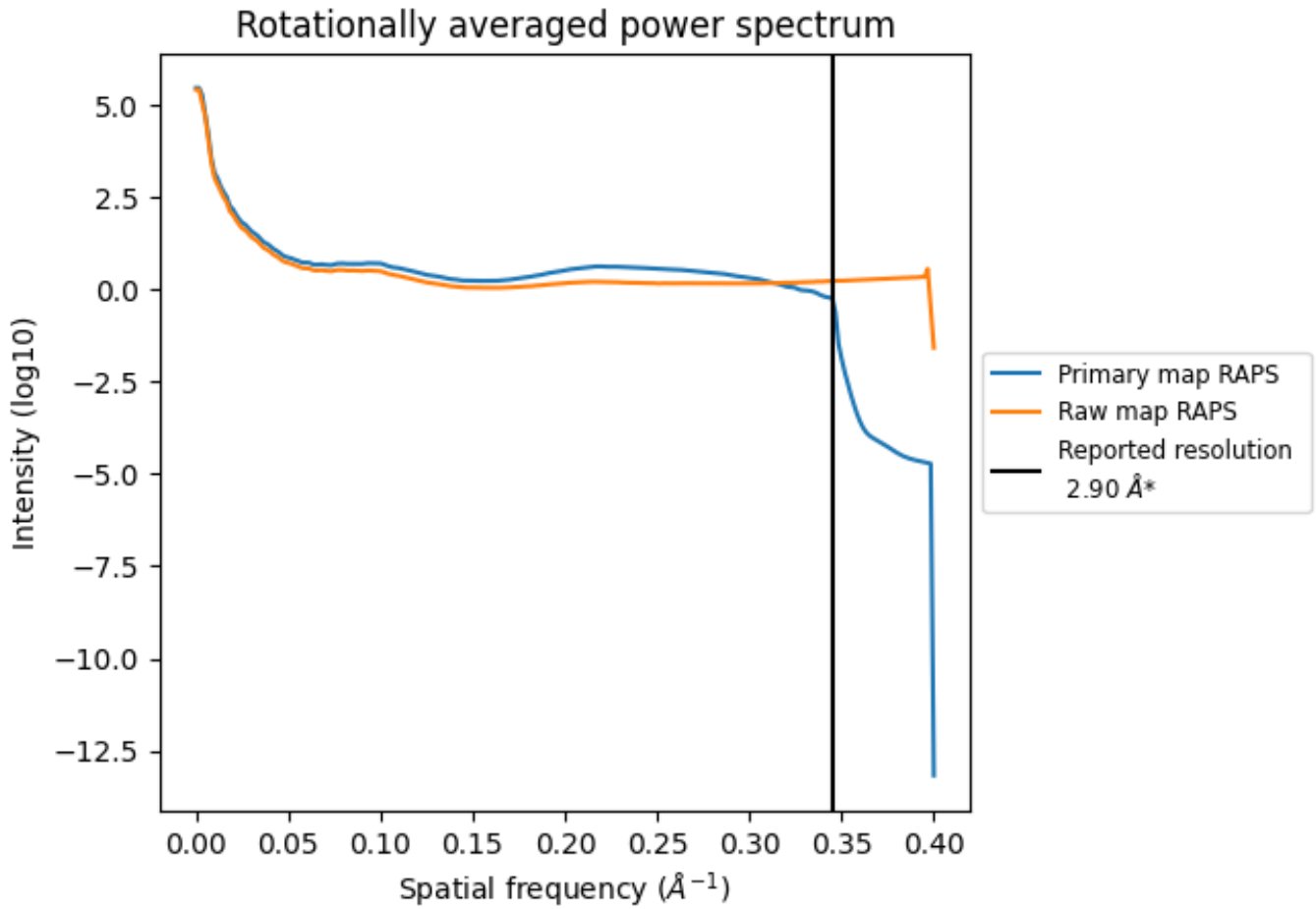
7.2 Volume estimate



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)

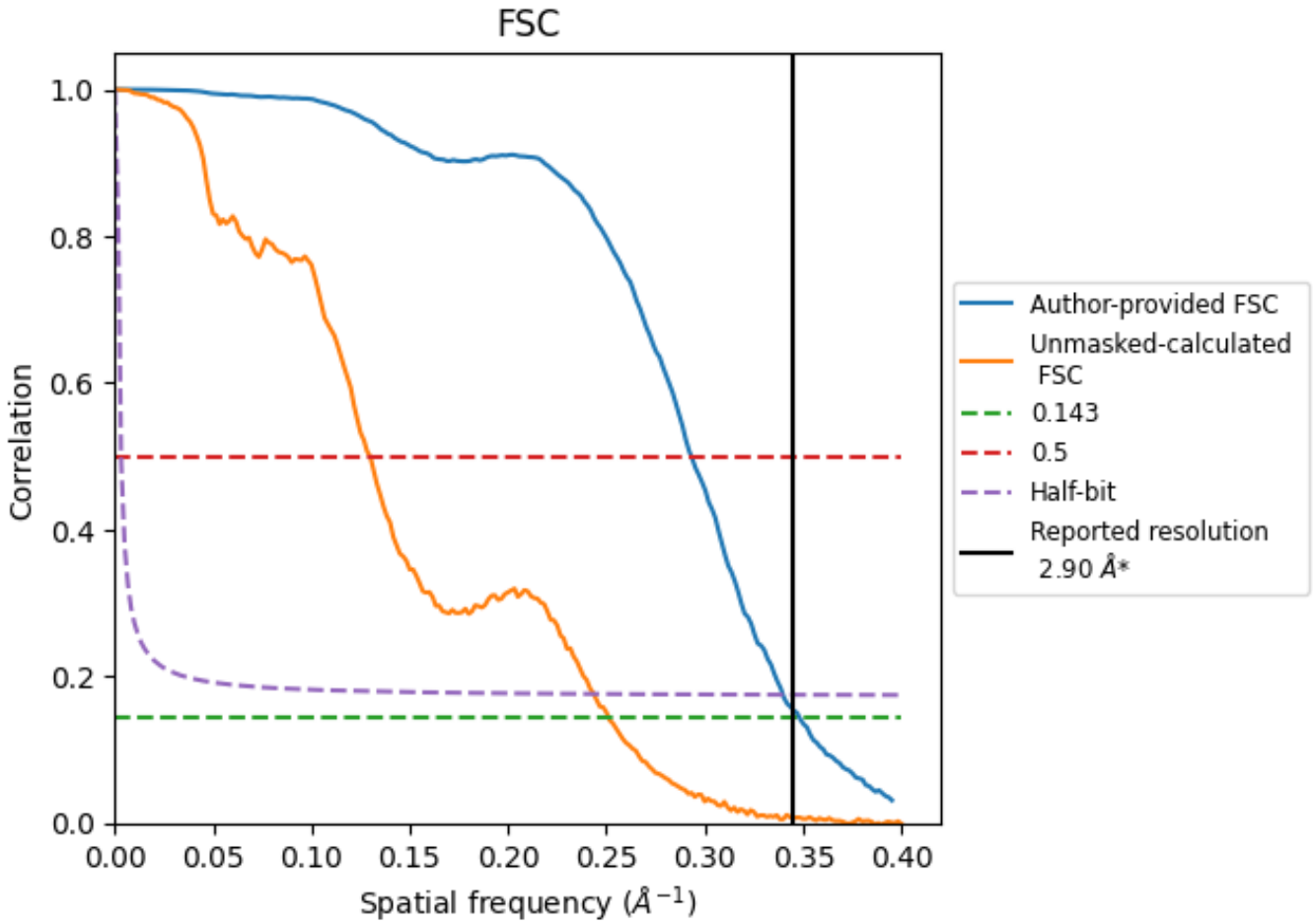


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

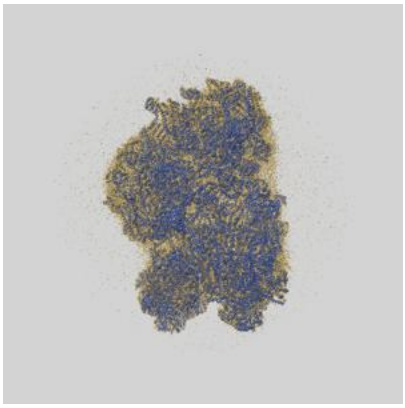
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.41	2.94
Unmasked-calculated*	3.98	7.70	4.11

*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 %

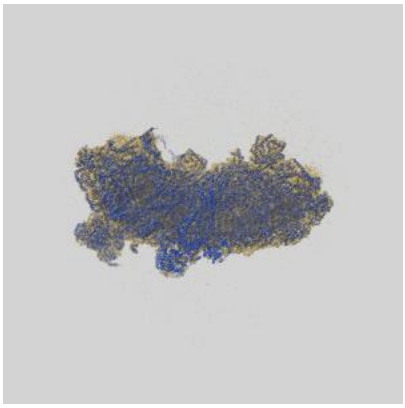
9 Map-model fit

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 66.

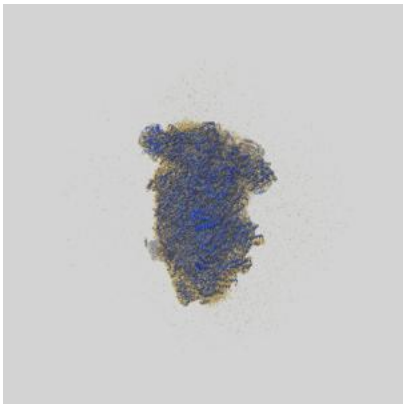
9.1 Map-model overlay



X



Y



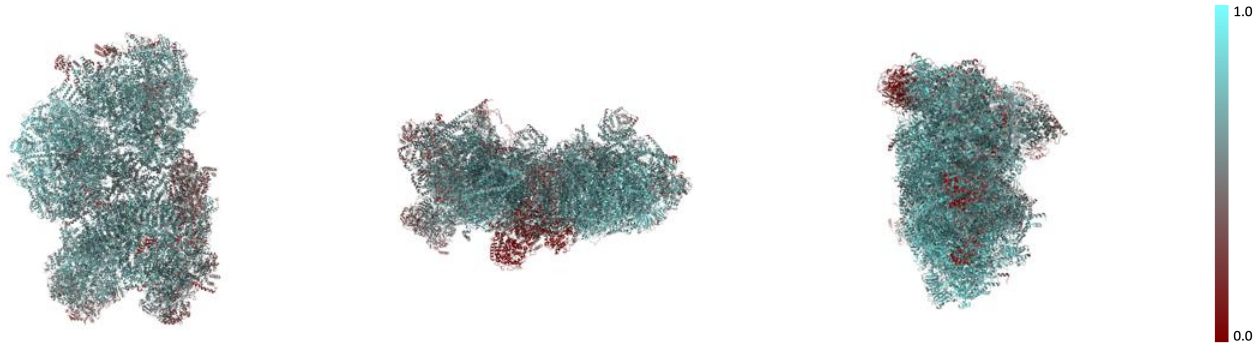
Z

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

This section was not generated.

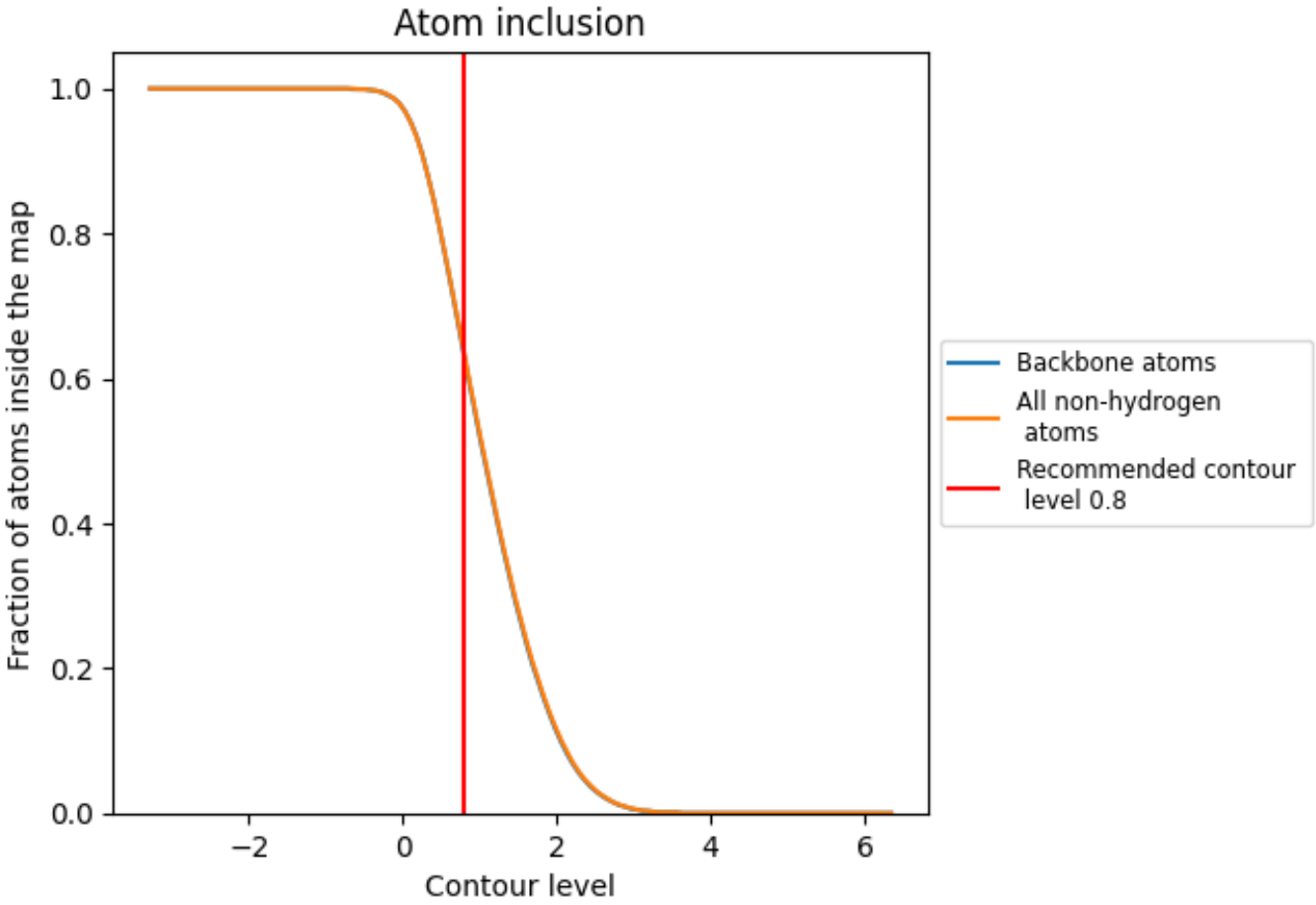
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

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
All	0.6340
A	0.6900
A0	0.5580
A1	0.7020
A2	0.6870
A3	0.3210
A4	0.4820
A5	0.6710
A6	0.6190
A7	0.6260
A8	0.6270
A9	0.6910
AA	0.6900
AB	0.5450
AC	0.7630
AD	0.4530
AE	0.7470
AF	0.7650
AG	0.7390
AH	0.7210
AI	0.4290
AJ	0.7330
AK	0.7970
AL	0.7440
AM	0.7170
AN	0.6640
AO	0.7280
AP	0.6560
AQ	0.7170
AR	0.6200
AS	0.7760
AT	0.7660
AU	0.6920
AV	0.7320
AW	0.7000

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
AX	0.7350
AY	0.7720
AZ	0.4770
B	0.5680
B0	0.6460
B1	0.6240
B2	0.6540
B3	0.6780
B4	0.5530
B5	0.6580
B6	0.8040
BA	0.5800
BB	0.6660
BC	0.6700
BD	0.6770
BE	0.5990
BF	0.7270
BG	0.6600
BH	0.7940
BI	0.7970
BJ	0.7320
BK	0.6760
BL	0.6280
BM	0.7640
BN	0.7100
BO	0.6560
BP	0.7250
BQ	0.6750
BR	0.6530
BS	0.6550
BT	0.6870
BU	0.6240
BV	0.6690
BW	0.6940
BX	0.7270
BY	0.7240
BZ	0.7560
C	0.5340
CA	0.0900
CB	0.2010
CC	0.2300
CD	0.2130

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
CE	0.1450
CF	0.4250
CG	0.2040
CH	0.3990
CI	0.4700
CJ	0.2820
CK	0.3240
CL	0.4740
CM	0.4110
CN	0.2580
CO	0.3660
D	0.7510
DA	0.7960
DB	0.7030
DC	0.7190
DD	0.7360
DE	0.7810
DF	0.7410
DG	0.6970
DH	0.7450
DI	0.7430
DJ	0.6900
DK	0.6650
DL	0.7430
DM	0.7690
DN	0.6450
DO	0.5870
DP	0.6520
DQ	0.7510
DR	0.7590
DS	0.7360
DT	0.8250
DU	0.6570
DV	0.7340
DW	0.6420
DX	0.6340
DY	0.7110
DZ	0.7190
Da	0.7620
Db	0.6650
Dc	0.6630
Dd	0.7010

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
De	0.7560
Df	0.7050
Dg	0.6730
Dh	0.7200
Di	0.6850
Dj	0.6590
Dk	0.6730
Dl	0.6650
Dm	0.7170
Dn	0.5970
Do	0.4320
Dp	0.5860
Dq	0.7400
Dr	0.6920
Ds	0.6680
Dt	0.7780
Du	0.6080
Dv	0.6530
Dw	0.6450
Dx	0.6430
Dy	0.6540
Dz	0.6690
E	0.5140
EA	0.6640
EB	0.7100
EC	0.4860
ED	0.6160
EE	0.7020
EF	0.8180
EG	0.7370
EH	0.7540
EI	0.6930
EJ	0.6870
EK	0.6680
EL	0.6940
EM	0.7180
EN	0.7070
EO	0.6360
EP	0.8090
EQ	0.7660
ER	0.7790
ES	0.7710

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
ET	0.5080
EU	0.6900
EV	0.6310
EW	0.5360
EX	0.5960
EY	0.5790
EZ	0.6110
Ea	0.6200
Eb	0.6740
Ec	0.4020
Ed	0.5810
Ee	0.6410
Ef	0.7580
Eg	0.6830
Eh	0.7250
Ei	0.6840
Ej	0.6250
Ek	0.6970
El	0.6710
Em	0.7140
En	0.6810
Eo	0.6640
Ep	0.7390
Eq	0.7470
Er	0.7920
Es	0.8220
Et	0.4450
Eu	0.6080
Ev	0.6280
Ew	0.4570
Ex	0.5400
Ey	0.5610
Ez	0.5880
F	0.6180
FA	0.6260
Fa	0.6000
G	0.5030
H	0.5110
I	0.7290
J	0.2640
K	0.6340
L	0.5490

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
a	0.4730
b	0.5200
c	0.6660
d	0.5600
e	0.3240
f	0.3590
g	0.6290
h	0.7170
i	0.4860
j	0.2180
k	0.5070
l	0.6160