wwPDB EM Validation Summary Report

Sep 8, 2026 – 06:15 am BST

PDB ID	:	8BQS / pdb_00008bqs
EMDB ID	:	EMD-16184
Title	:	Cryo-EM structure of the I-II-III2-IV2 respiratory supercomplex from Tetrahymena thermophila
Authors	:	Muhleip, A.; Kock Flygaard, R.; Baradaran, R.; Amunts, A.
Deposited on	:	2022-11-21
Resolution	:	2.90 Å(reported)

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

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

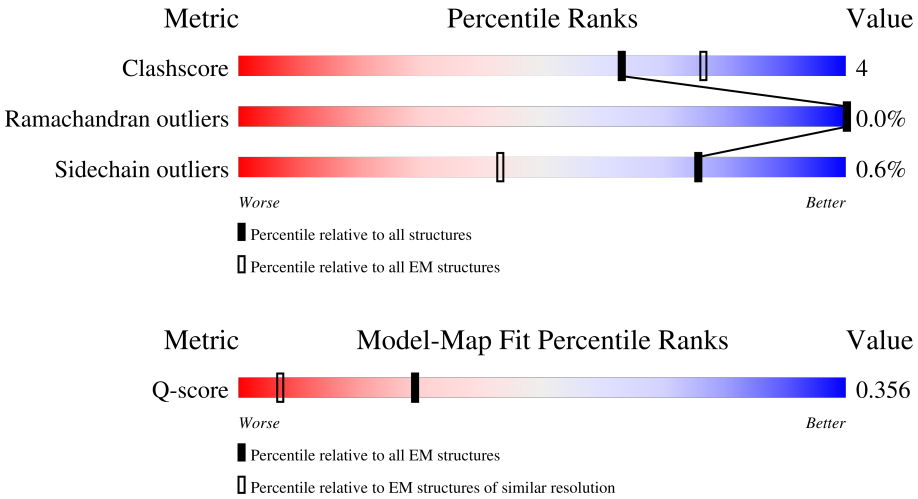
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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% 88% 9%
2	A1	362	88% 5% 7%
3	A2	317	6% 77% 8% 15%
4	A3	333	58% 77% 11% 13%

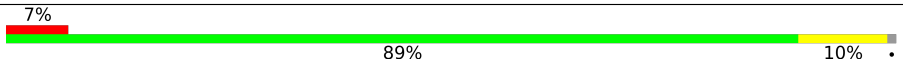
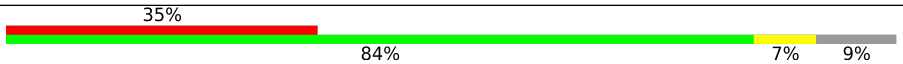
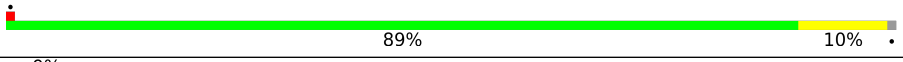
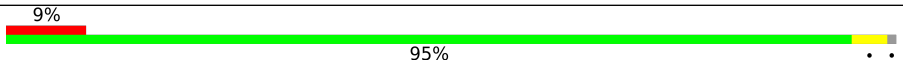
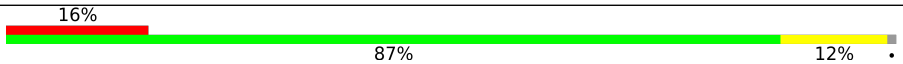
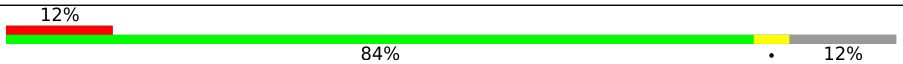
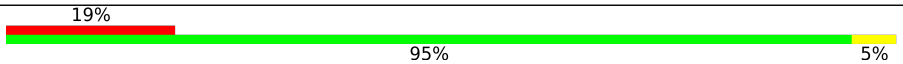
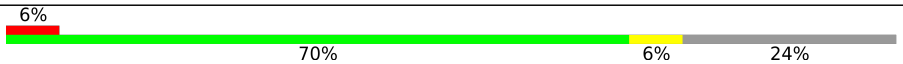
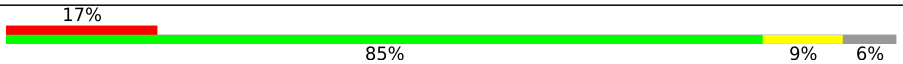
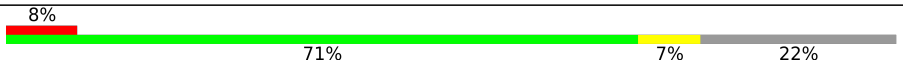
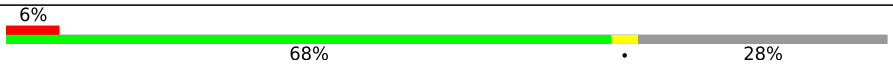
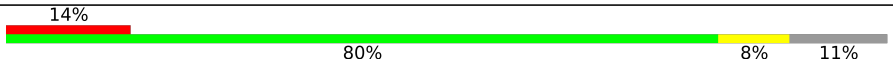
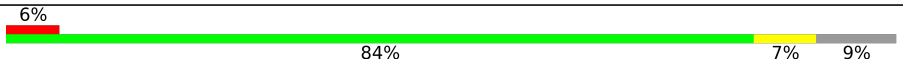
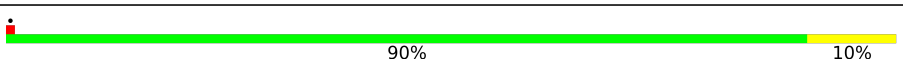
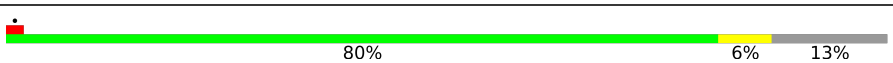
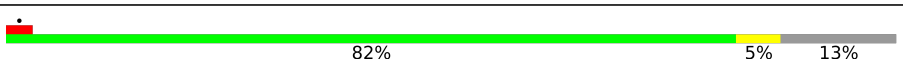
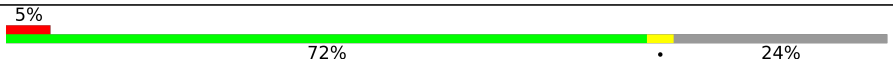
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Mol	Chain	Length	Quality of chain
5	A4	311	39% 93% 7%
6	A5	282	10% 88% 12%
7	A6	251	10% 78% 14% 8%
8	A7	238	6% 49% 7% 44%
9	A8	217	12% 89% 11%
10	A9	231	6% 93% 7%
11	AA	750	6% 81% 14% 5%
12	AB	718	25% 83% 13%
13	AC	505	86% 13%
14	AD	474	39% 80% 13% 7%
15	AE	442	86% 13%
16	AF	360	89% 11%
17	AG	346	95% 5%
18	AH	284	83% 17%
19	AI	274	36% 75% 9% 16%
20	AJ	255	92% 7%
21	AK	257	81% 9% 11%
22	AL	236	78% 14% 8%
23	AM	233	91% 8%
24	AN	206	9% 67% 9% 24%
25	AO	198	84% 15%
26	AP	194	11% 88% 10%
27	AQ	189	5% 92% 7%
28	AR	185	14% 88% 10%
29	AS	172	90% 9%

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Mol	Chain	Length	Quality of chain
30	AT	162	
31	AU	150	
32	AV	138	
33	AW	133	
34	AX	121	
35	AY	116	
36	AZ	103	
37	B0	94	
38	B1	93	
39	B2	94	
40	B3	83	
41	B4	73	
42	B5	71	
43	B6	59	
44	BA	212	
45	BB	214	
46	BC	207	
47	BD	205	
48	BE	189	
49	BF	188	
50	BG	175	
51	BH	178	
52	BI	172	
53	BJ	166	
54	BK	144	

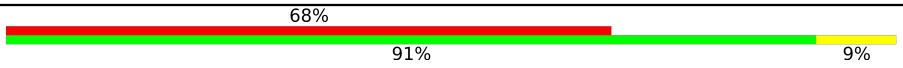
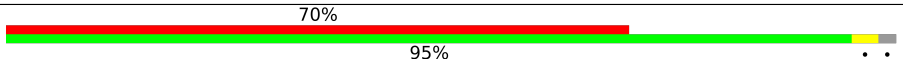
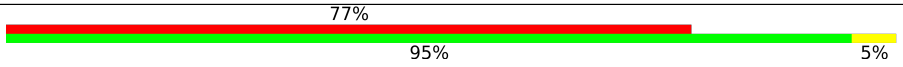
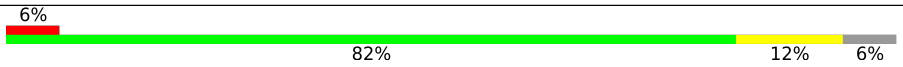
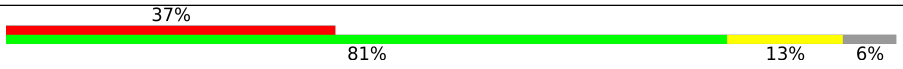
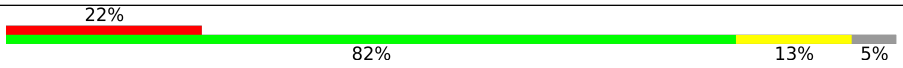
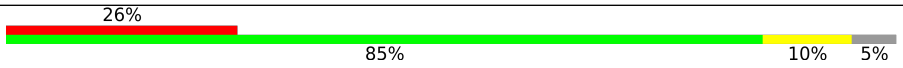
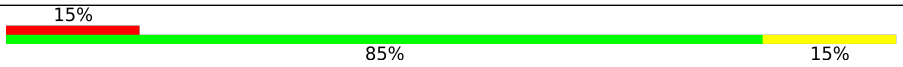
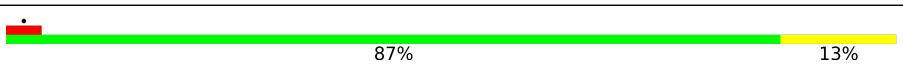
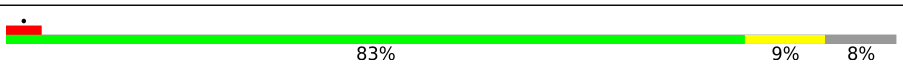
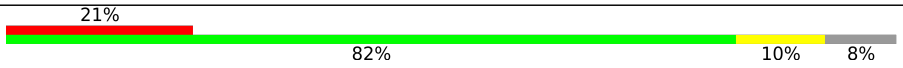
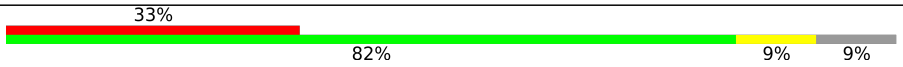
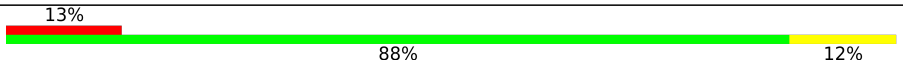
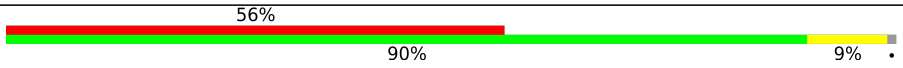
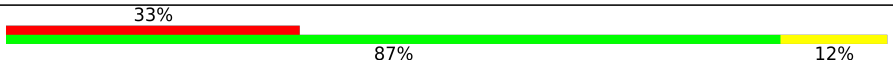
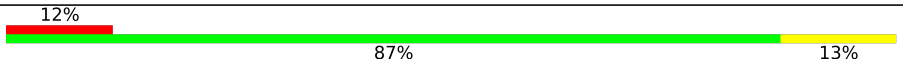
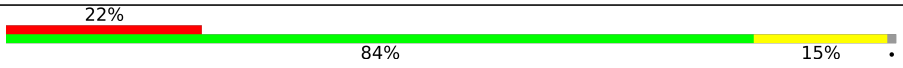
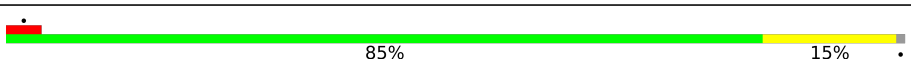
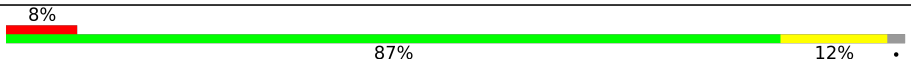
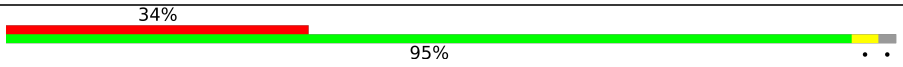
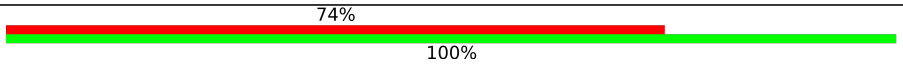
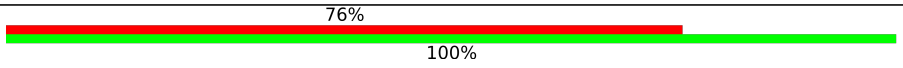
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Mol	Chain	Length	Quality of chain
55	BL	143	9% 89% 10%
56	BM	135	84% 11% 5%
57	BN	135	7% 87% 11%
58	BO	136	8% 96%
59	BP	129	51% 5% 44%
60	BQ	127	73% 6% 20%
61	BR	132	5% 64% 31%
62	BS	126	5% 89% 6% 5%
63	BT	125	84% 15%
64	BU	134	13% 86% 14%
65	BV	125	10% 98%
66	BW	120	7% 95%
67	BX	113	80% 5% 15%
68	BY	100	85% 15%
69	BZ	102	5% 93% 7%
70	CH	195	32% 52% 44%
71	CM	76	51% 92% 5%
72	CL	89	36% 89% 10%
73	CA	636	92% 83% 11% 6%
74	CI	114	39% 95% 5%
75	CB	312	76% 83% 8% 9%
76	CF	296	35% 69% 5% 26%
77	CG	198	82% 88% 11%
78	CK	93	59% 90% 9%
79	CE	322	92% 90% 9%

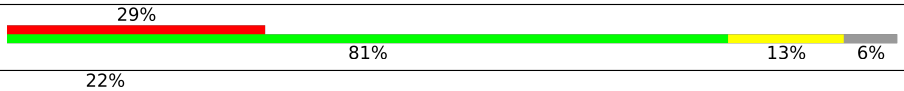
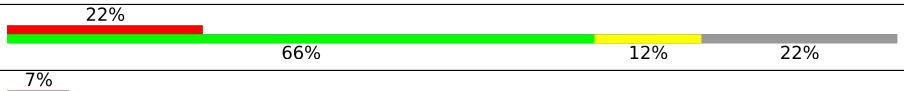
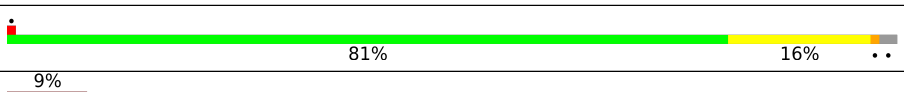
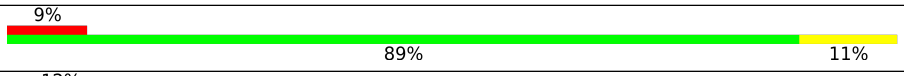
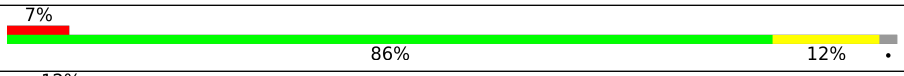
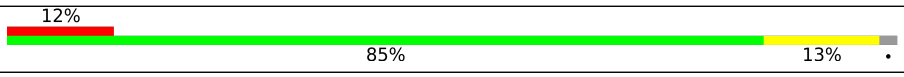
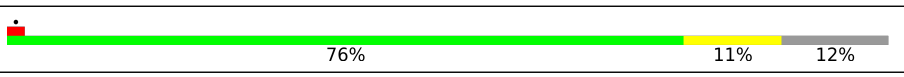
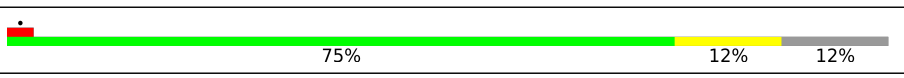
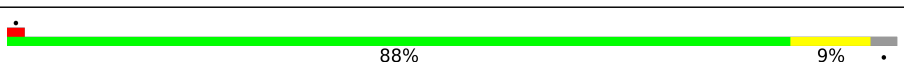
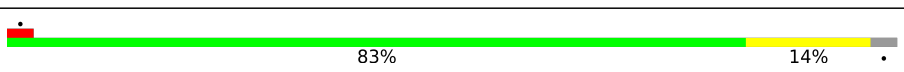
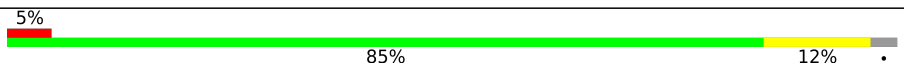
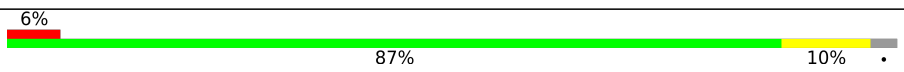
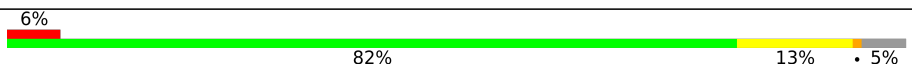
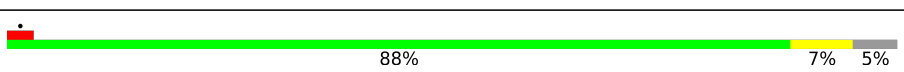
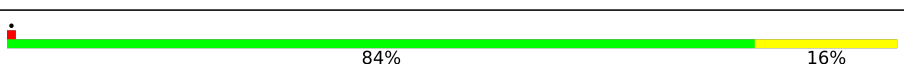
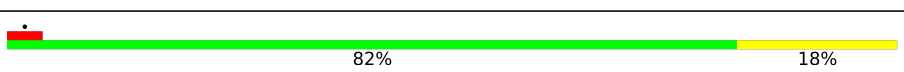
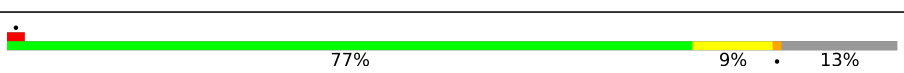
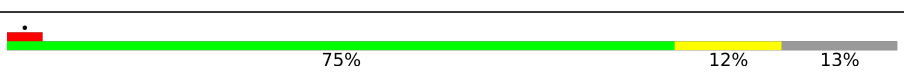
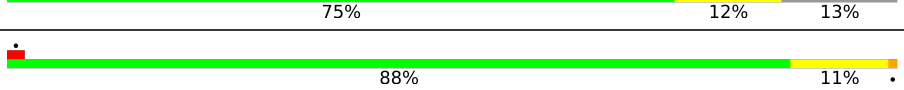
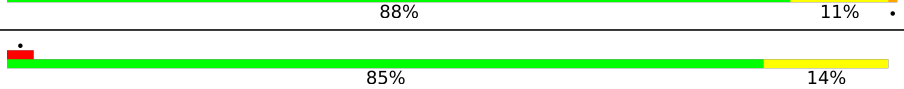
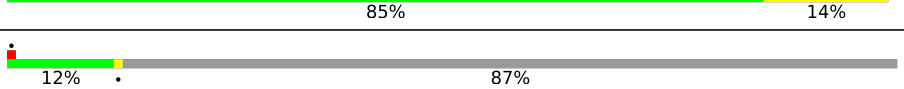
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Mol	Chain	Length	Quality of chain
80	CJ	103	
81	CN	62	
82	CC	60	
83	CO	46	
84	CD	44	
85	A	513	
85	a	513	
86	B	482	
86	b	482	
87	C	426	
87	c	426	
88	D	319	
88	d	319	
89	E	269	
89	e	269	
90	F	86	
90	f	86	
91	G	328	
91	g	328	
92	H	130	
92	h	130	
93	I	119	
93	i	119	
94	J	66	
94	j	66	

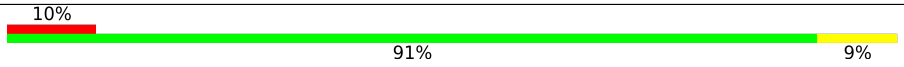
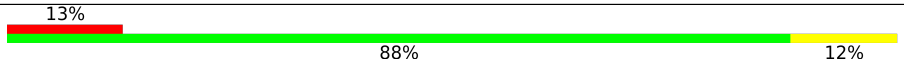
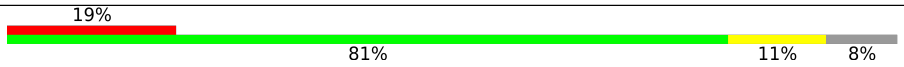
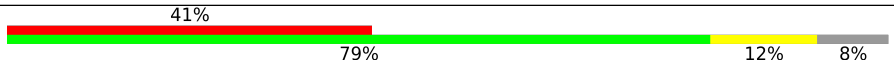
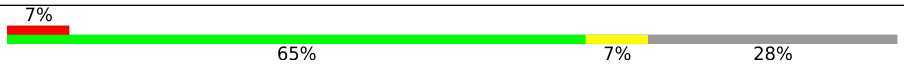
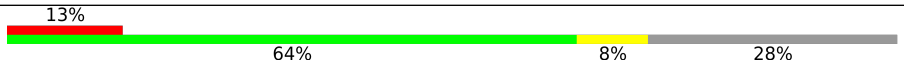
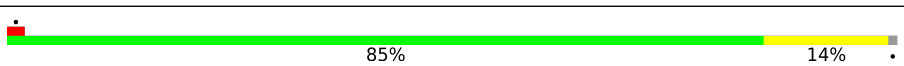
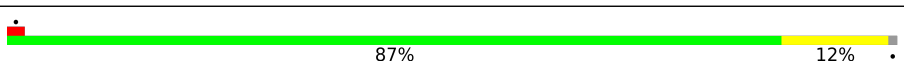
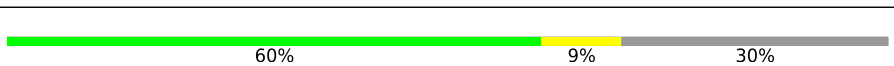
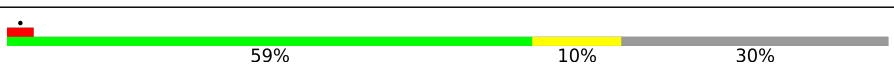
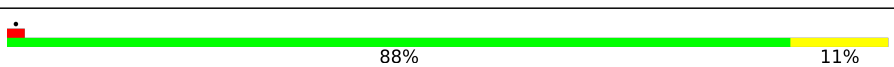
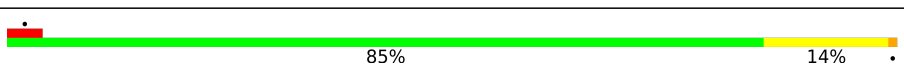
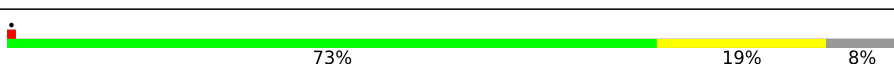
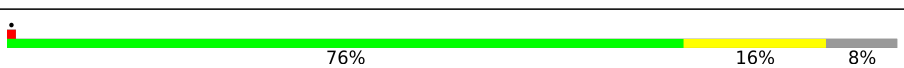
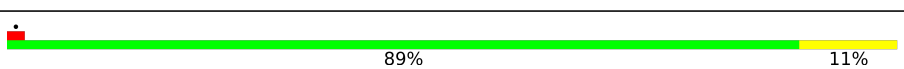
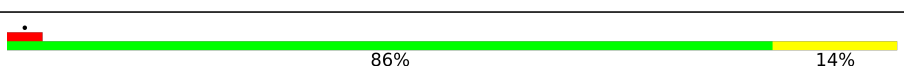
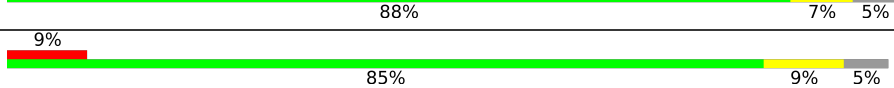
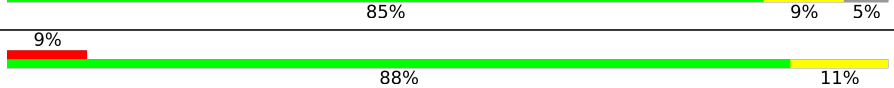
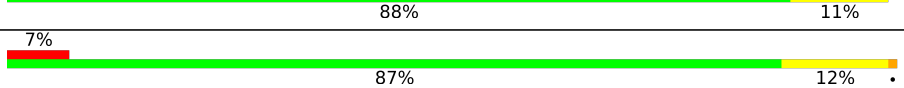
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Mol	Chain	Length	Quality of chain
95	K	62	
95	k	62	
96	L	41	
96	l	41	
97	DA	688	
97	Da	688	
98	DB	604	
98	Db	604	
99	DC	594	
99	Dc	594	
100	DD	637	
100	Dd	637	
101	DE	130	
101	De	130	
102	DF	230	
102	Df	230	
103	DG	103	
103	Dg	103	
104	DH	134	
104	Dh	134	
105	DI	236	
105	Di	236	
106	DJ	220	
106	Dj	220	
107	DK	990	

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Mol	Chain	Length	Quality of chain
107	Dk	990	
108	DM	490	
108	Dm	490	
109	DN	453	
109	Dn	453	
110	DO	473	
110	Do	473	
111	DP	402	
111	Dp	402	
112	DQ	386	
112	Dq	386	
113	DR	348	
113	Dr	348	
114	DS	347	
114	Ds	347	
115	DT	318	
115	Dt	318	
116	DU	330	
116	Du	330	
117	DV	319	
117	Dv	319	
118	DW	318	
118	Dw	318	
119	DX	252	
119	Dx	252	

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Mol	Chain	Length	Quality of chain
120	DY	234	69% 11% 20%
120	Dy	234	6% 70% 10% 20%
121	DZ	231	79% 10% 10%
121	Dz	231	6% 77% 13% 10%
122	EA	215	80% 9% 10%
122	Ea	215	6% 78% 12% 10%
123	EB	210	90% 10%
123	Eb	210	6% 86% 13%
124	EC	212	35% 84% 15%
124	Ec	212	50% 87% 12%
125	ED	190	10% 85% 14%
125	Ed	190	18% 87% 13%
126	EE	193	5% 59% 6% 35%
126	Ee	193	6% 59% 6% 35%
127	EF	188	89% 10%
127	Ef	188	87% 13%
128	EG	100	88% 10%
128	Eg	100	87% 11%
129	EH	174	86% 14%
129	Eh	174	79% 21%
130	EI	173	91% 9%
130	Ei	173	5% 87% 12%
131	EV	89	7% 78% 11% 11%
131	Ev	89	12% 82% 7% 11%
132	EK	170	6% 89% 11%

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Mol	Chain	Length	Quality of chain
132	Ek	170	86% 14%
133	EL	158	85% 11%
133	El	158	81% 16%
134	EM	154	88% 10%
134	Em	154	88% 11%
135	EN	149	5% 91% 5%
135	En	149	7% 91% 6%
136	EO	124	10% 85% 14%
136	Eo	124	7% 87% 12%
137	EP	127	68% 11% 21%
137	Ep	127	69% 10% 21%
138	EQ	123	85% 15%
138	Eq	123	86% 14%
139	ER	105	90% 9%
139	Er	105	87% 12%
140	ES	89	87% 13%
140	Es	89	78% 22%
141	ET	93	30% 80% 8% 12%
141	Et	93	38% 74% 13% 12%
142	EU	90	8% 93%
142	Eu	90	8% 88% 10%
143	EJ	175	8% 86% 14%
143	Ej	175	14% 81% 18%
144	EW	81	22% 74% 22%
144	Ew	81	35% 73% 5% 22%

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Mol	Chain	Length	Quality of chain
145	EX	72	19% 85% 11%
145	Ex	72	26% 83% 12%
146	EY	72	24% 88% 10%
146	Ey	72	19% 86% 11%
147	EZ	68	12% 76% 9% 15%
147	Ez	68	15% 72% 13% 15%
148	FA	72	15% 86% 11%
148	Fa	72	21% 88% 10%
149	DL	462	72% 11% 18%
149	Dl	462	7% 74% 8% 18%

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
158	FES	CB	1000	-	-	X	-
159	SF4	AL	302	-	-	X	-
166	HEC	CE	401	X	-	-	-
166	HEC	D	401	X	-	-	-
166	HEC	d	802	X	-	-	-

2 Entry composition (i)

There are 173 unique types of molecules in this entry. The entry contains 805862 atoms, of which 406234 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lipid-A-disaccharide synthase.

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

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

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

- Molecule 3 is a protein called DnaJ domain protein.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
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	conflict	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		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 44 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
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 chain 77.

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		

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Mol	Chain	Residues	Atoms						AltConf	Trace
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		
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		

- 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		

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms							AltConf	Trace
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		

- 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		
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	384	Total	C	H	N	O	S	0	0
			6271	2041	3102	546	575	7		
112	Dq	384	Total	C	H	N	O	S	0	0
			6271	2041	3102	546	575	7		

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 130 is a protein called Transmembrane protein.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
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		

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 139 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms						AltConf	Trace
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		
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		

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Mol	Chain	Residues	Atoms						AltConf	Trace
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		

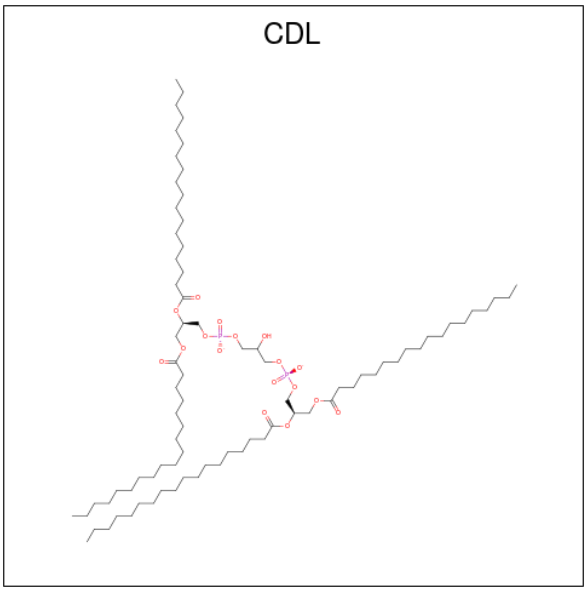
- Molecule 148 is a protein called Tim10/DDP family zinc finger protein.

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,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 (CCD ID: 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	

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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	

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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	

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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	

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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	

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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	

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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	

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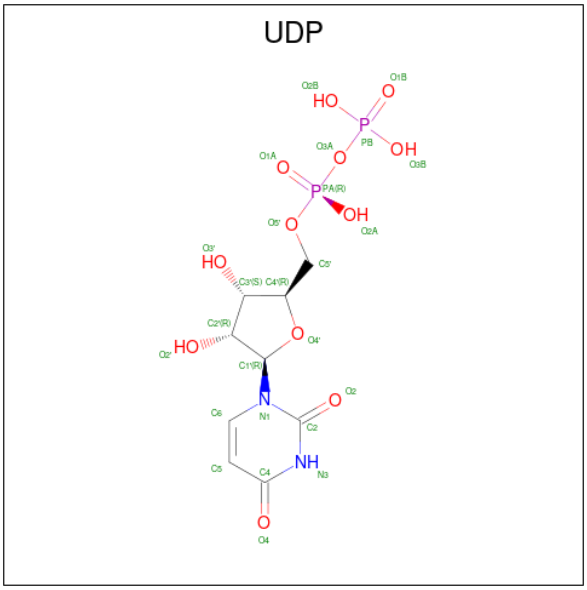
Mol	Chain	Residues	Atoms					AltConf
150	Du	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dv	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dv	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dv	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dx	1	Total	C	H	O	P	0
			256	81	156	17	2	
150	Dx	1	Total	C	H	O	P	0
			256	81	156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

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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 (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

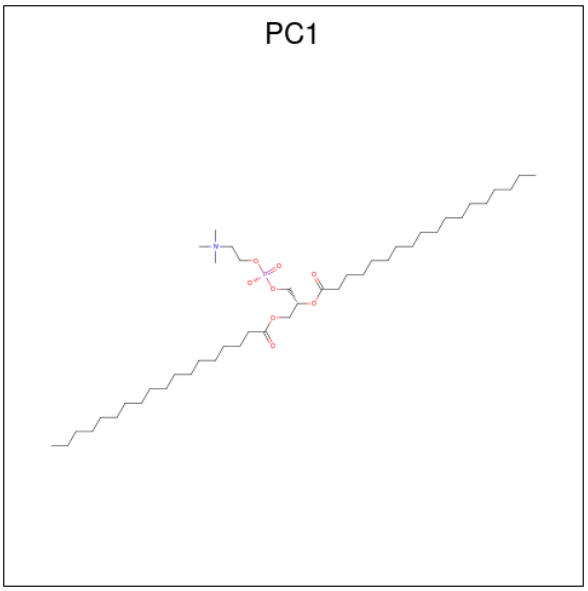


Mol	Chain	Residues	Atoms						AltConf
151	A0	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	

- Molecule 152 is MAGNESIUM ION (CCD ID: 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 (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
153	A0	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	A1	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	A2	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	A6	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	A6	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	A9	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	A9	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	AH	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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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	

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Mol	Chain	Residues	Atoms						AltConf
153	K	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	g	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	
153	DA	1	Total	C	H	N	O	P	0
			141	44	87	1	8	1	
153	DA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DB	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DC	1	Total	C	H	N	O	P	0
			141	44	87	1	8	1	
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	

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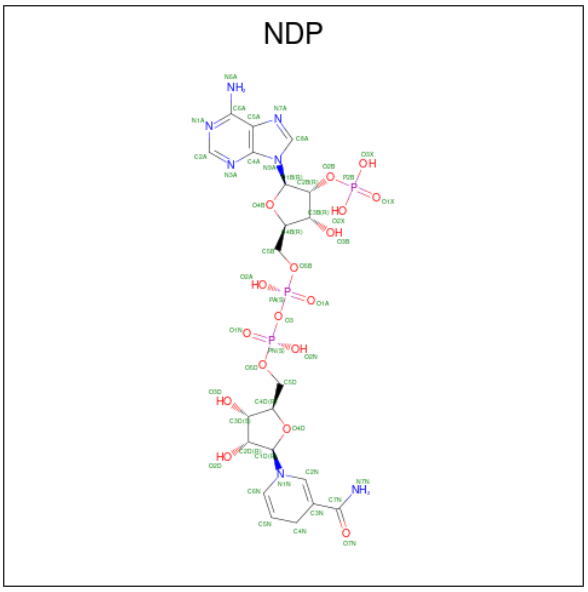
Mol	Chain	Residues	Atoms						AltConf
153	DV	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DV	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DV	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DX	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DX	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	DY	1	Total	C	H	N	O	P	0
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

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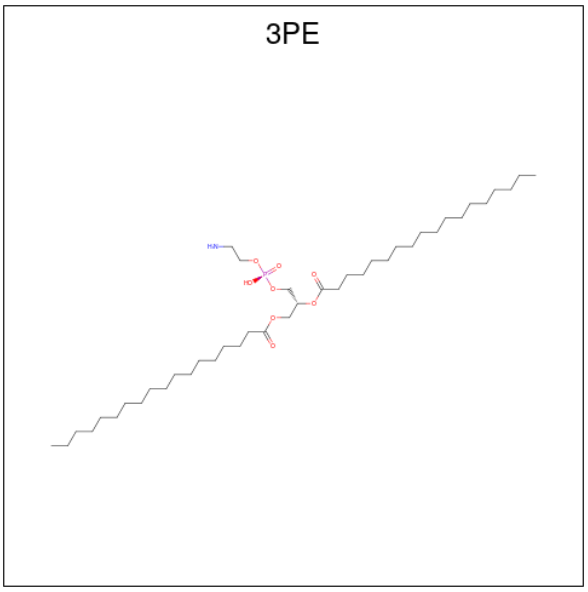
Mol	Chain	Residues	Atoms						AltConf
153	Dg	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Di	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Dj	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Dq	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Ds	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
153	Dv	1	Total	C	H	N	O	P	0
			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 (CCD ID: 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 (CCD ID: 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	

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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	

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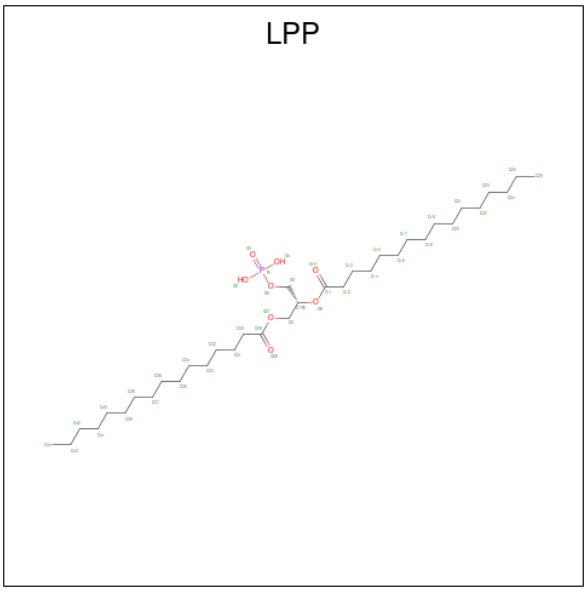
Mol	Chain	Residues	Atoms						AltConf
155	EL	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	EM	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	EN	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	EO	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	Da	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
155	Dc	1	Total	C	H	N	O	P	0
			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	

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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 (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



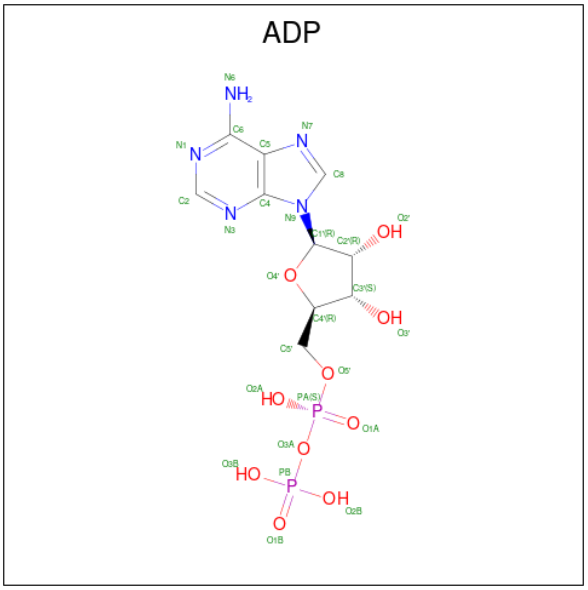
Mol	Chain	Residues	Atoms					AltConf
156	A6	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	AA	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	AC	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	AL	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	DA	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	DN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

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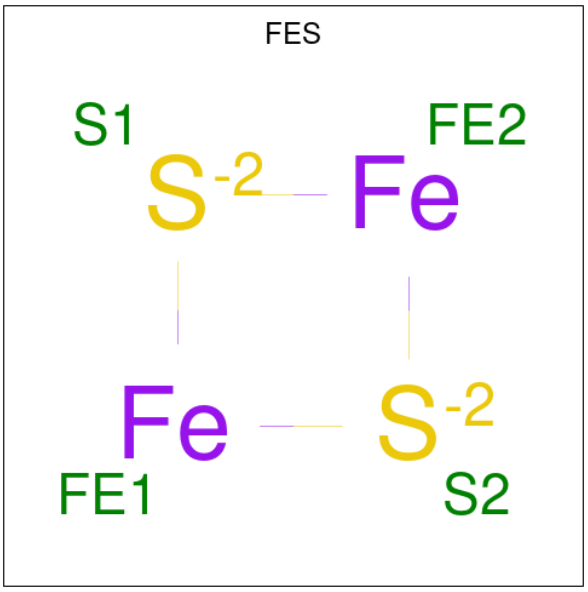
Mol	Chain	Residues	Atoms					AltConf
156	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	Ed	1	Total	C	H	O	P	0
			111	35	67	8	1	
156	Dl	1	Total	C	H	O	P	0
			111	35	67	8	1	

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



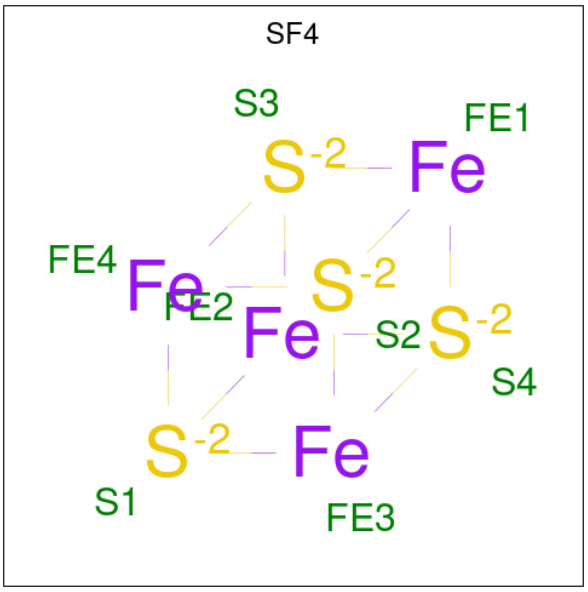
Mol	Chain	Residues	Atoms						AltConf
157	A8	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
157	AQ	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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



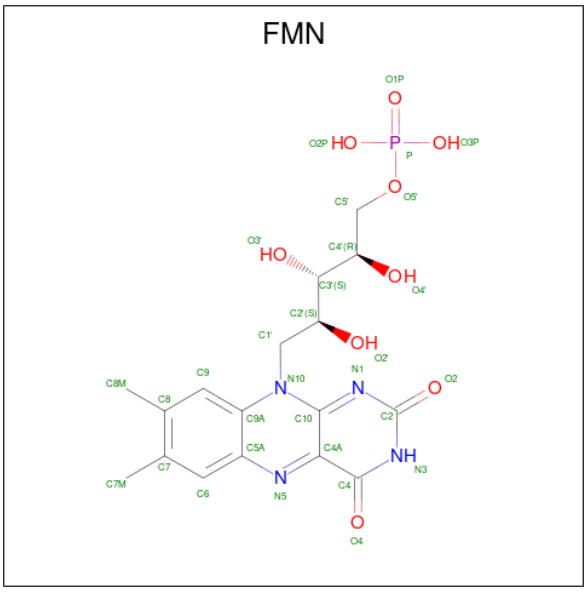
Mol	Chain	Residues	Atoms	AltConf
158	AB	1	Total Fe S 4 2 2	0
158	AI	1	Total Fe S 4 2 2	0
158	BI	1	Total Fe S 4 2 2	0
158	CB	1	Total Fe S 4 2 2	0
158	E	1	Total Fe S 4 2 2	0
158	e	1	Total Fe S 4 2 2	0
158	EF	1	Total Fe S 4 2 2	0
158	EF	1	Total Fe S 4 2 2	0
158	Ef	1	Total Fe S 4 2 2	0
158	Ef	1	Total Fe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

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



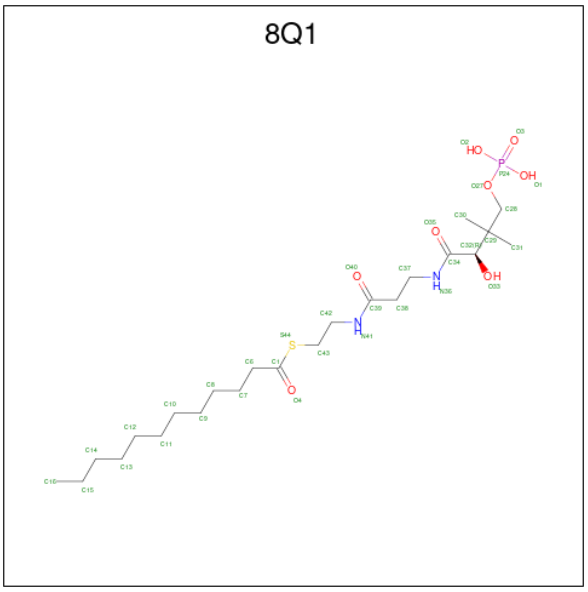
Mol	Chain	Residues	Atoms	AltConf
159	AB	1	Total Fe S 8 4 4	0
159	AB	1	Total Fe S 8 4 4	0
159	AD	1	Total Fe S 8 4 4	0
159	AL	1	Total Fe S 8 4 4	0
159	AL	1	Total Fe S 8 4 4	0
159	AT	1	Total Fe S 8 4 4	0
159	CB	1	Total Fe S 8 4 4	0

- Molecule 160 is FLAVIN MONONUCLEOTIDE (CCD ID: 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 (CCD ID: 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	

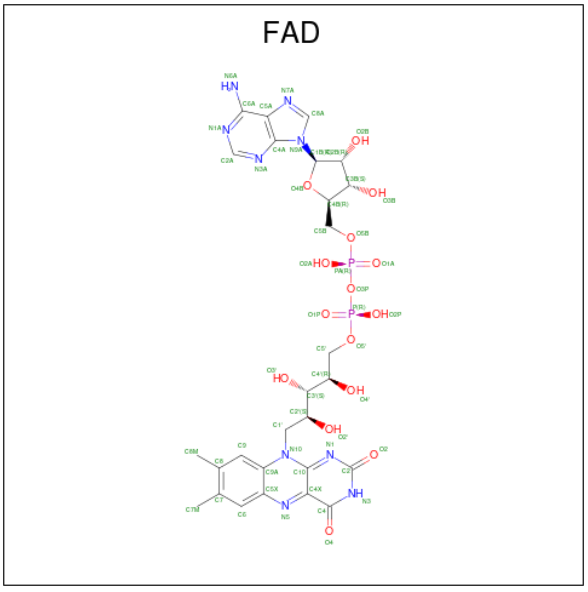
- Molecule 162 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: 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

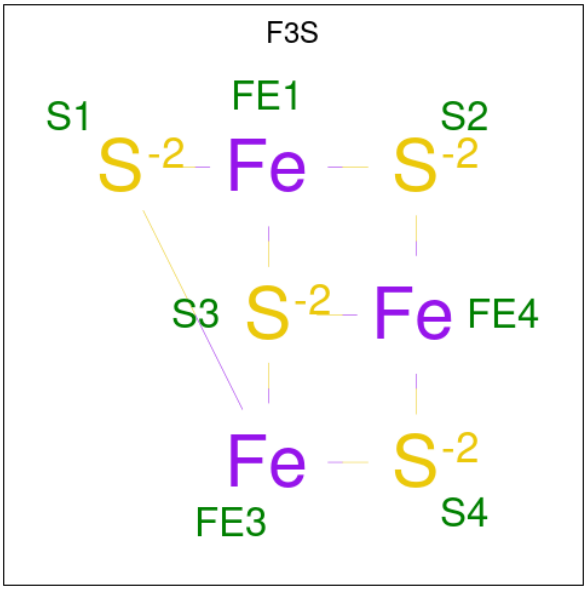
- Molecule 164 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

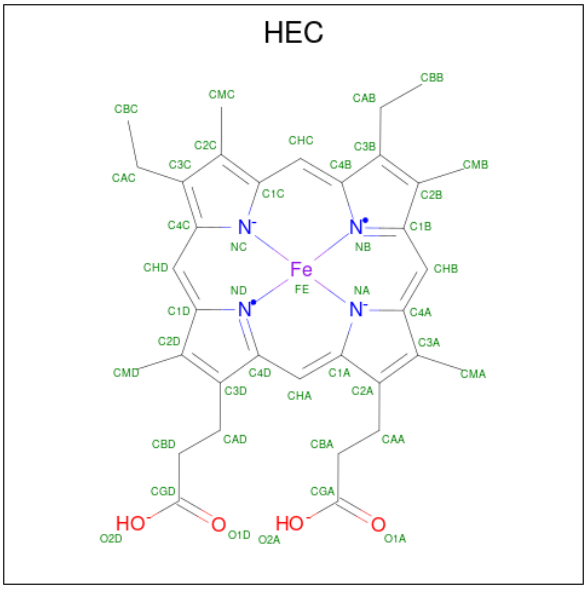
- Molecule 165 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of

Interest" by depositor).



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

- Molecule 166 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



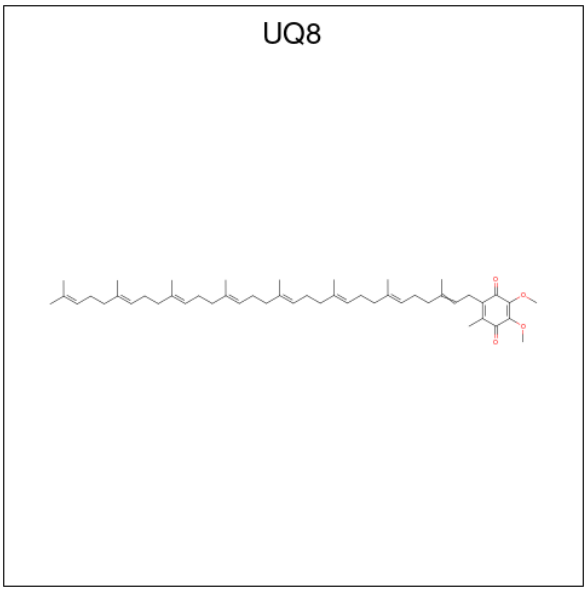
Mol	Chain	Residues	Atoms						AltConf
166	CE	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

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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 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



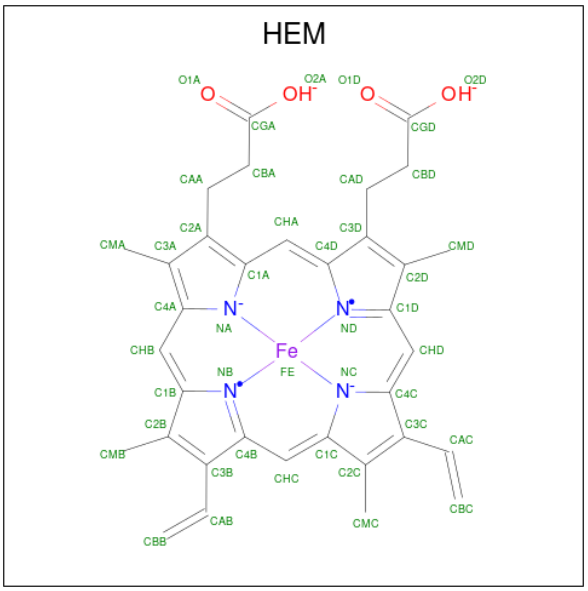
Mol	Chain	Residues	Atoms				AltConf
167	CC	1	Total	C	H	O	0
			127	49	74	4	
167	C	1	Total	C	O		0
			53	49	4		
167	C	1	Total	C	O		0
			53	49	4		
167	c	1	Total	C	O		0
			53	49	4		
167	DS	1	Total	C	H	O	0
			127	49	74	4	
167	ED	1	Total	C	H	O	0
			127	49	74	4	
167	EL	1	Total	C	H	O	0
			127	49	74	4	
167	EN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

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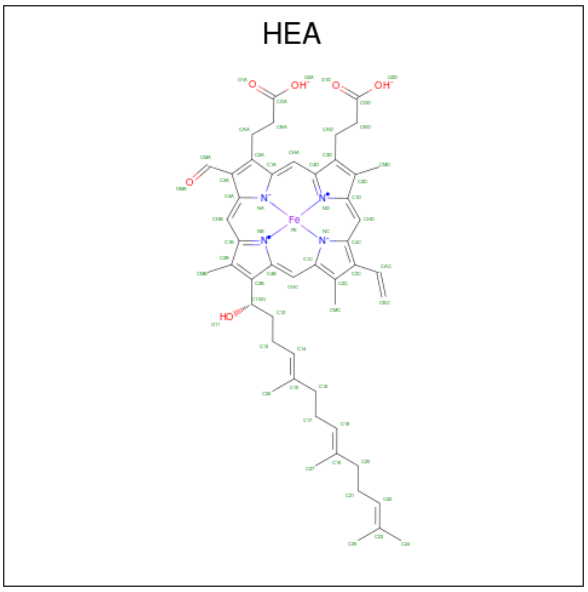
Mol	Chain	Residues	Atoms				AltConf
167	Ed	1	Total	C	H	O	0
			127	49	74	4	
167	El	1	Total	C	H	O	0
			127	49	74	4	
167	En	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 168 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

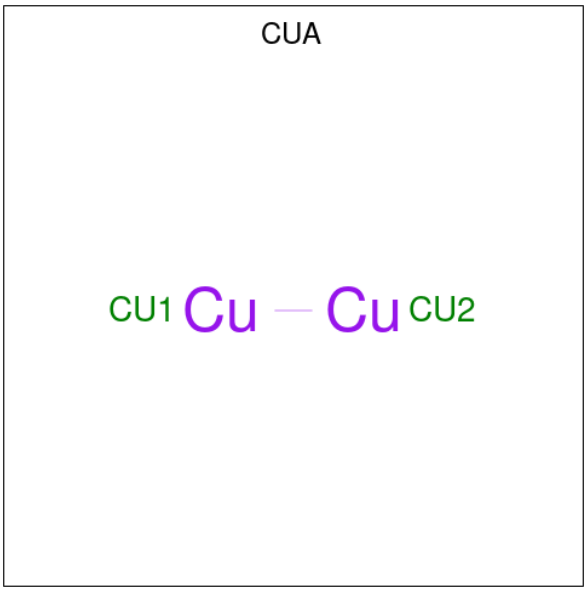


Mol	Chain	Residues	Atoms						AltConf
169	DA	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
169	DA	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
169	Da	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
169	Da	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 170 is COPPER (II) ION (CCD ID: 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 (CCD ID: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).

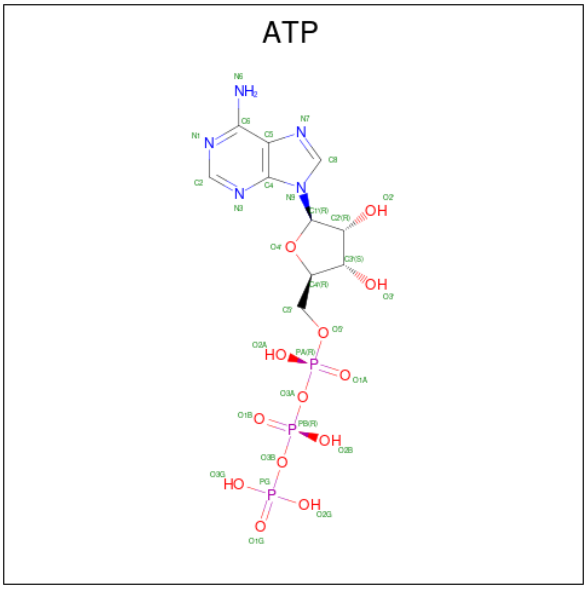


Mol	Chain	Residues	Atoms	AltConf
171	DB	1	Total Cu 2 2	0
171	Db	1	Total Cu 2 2	0

- Molecule 172 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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



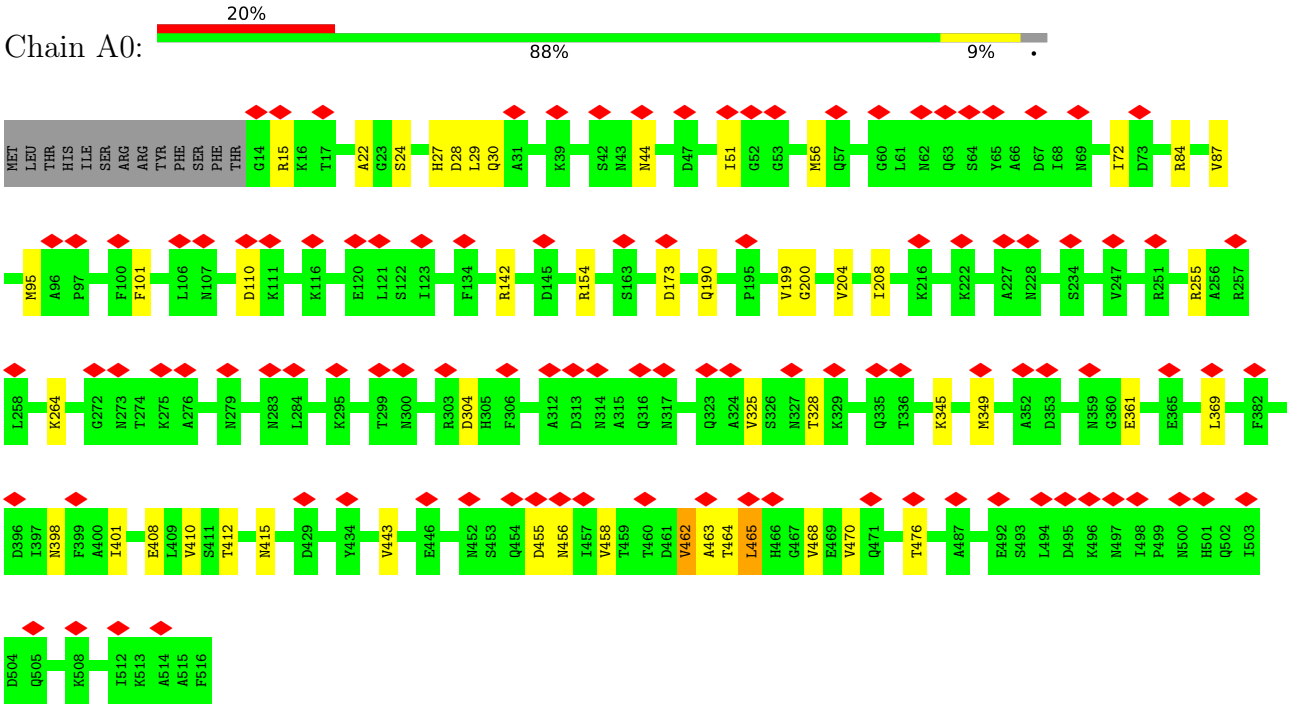
Mol	Chain	Residues	Atoms						AltConf
173	ER	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
173	Er	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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.

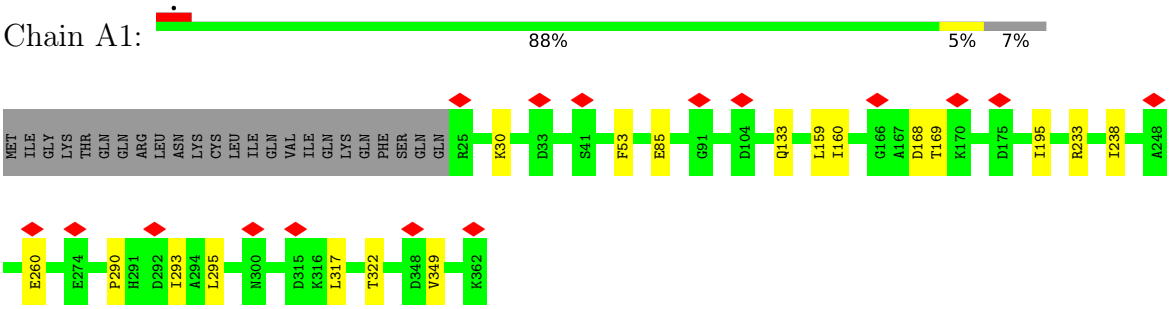
• Molecule 1: Lipid-A-disaccharide synthase

Chain A0:



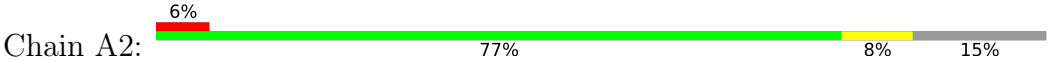
• Molecule 2: NAD-dependent epimerase/dehydratase family protein

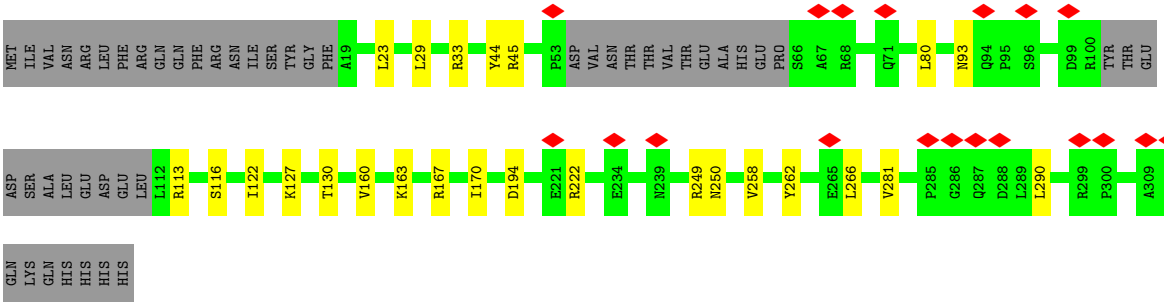
Chain A1:



• Molecule 3: DnaJ domain protein

Chain A2:

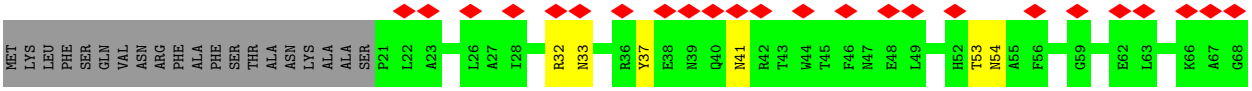




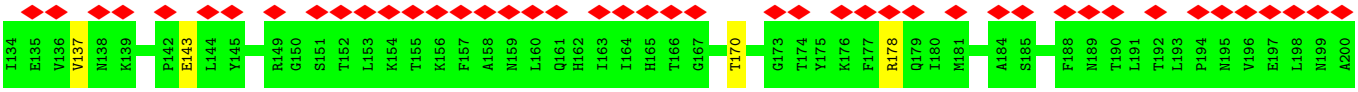
• Molecule 4: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

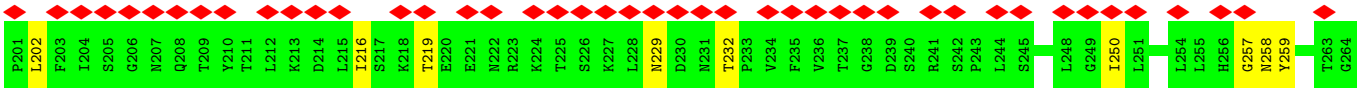
Chain A3:

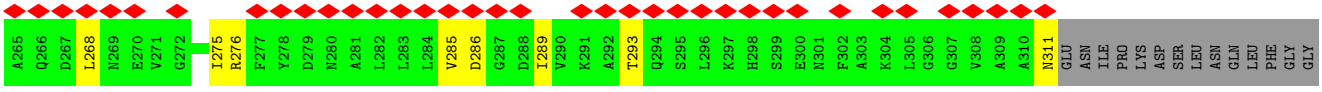








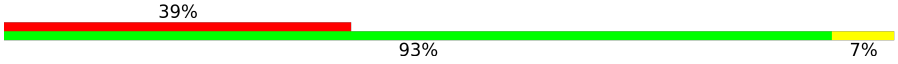


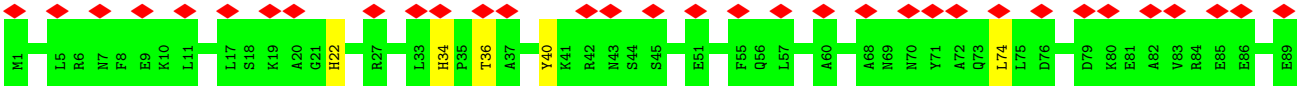


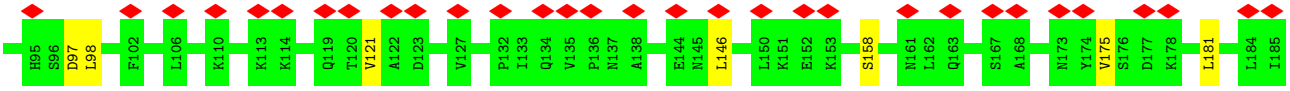


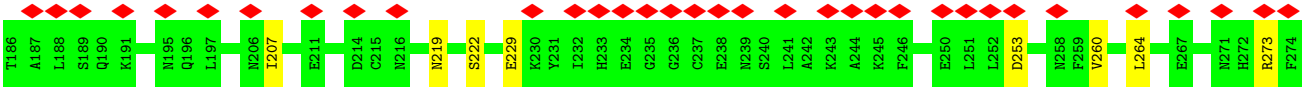
• Molecule 5: RNase III domain-containing protein

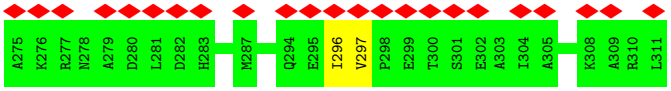
Chain A4:







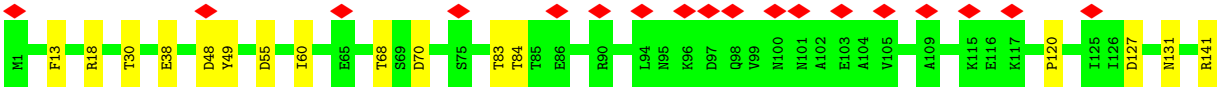




• Molecule 6: 37S ribosomal protein S25, mitochondrial

Chain A5:



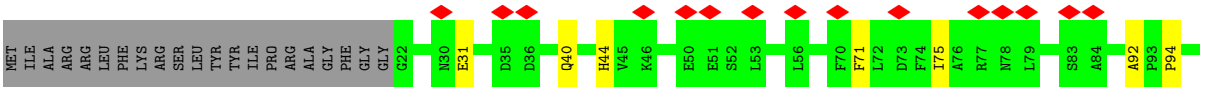


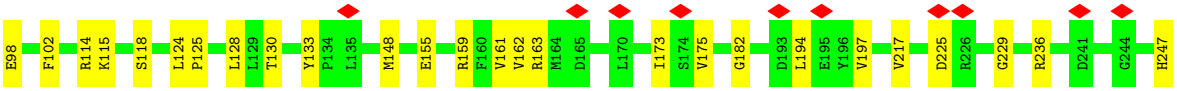


• Molecule 7: Transmembrane protein, putative

Chain A6:



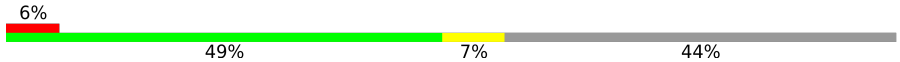


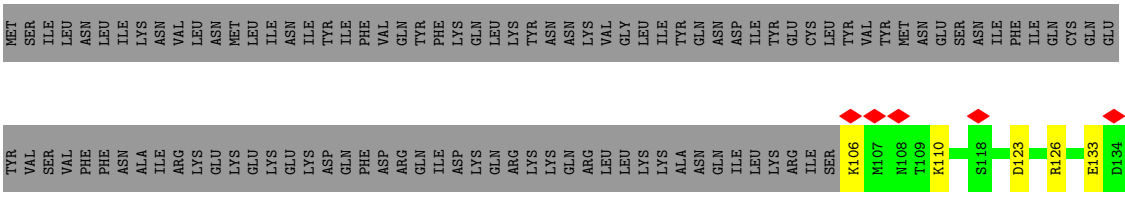


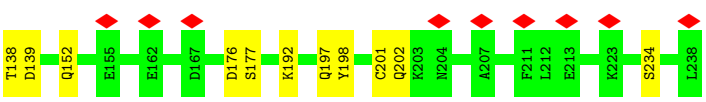


• Molecule 8: CX9C domain-containing protein

Chain A7:



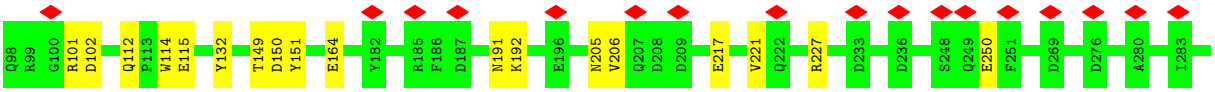


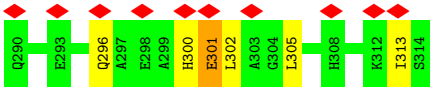


• Molecule 9: ND5a

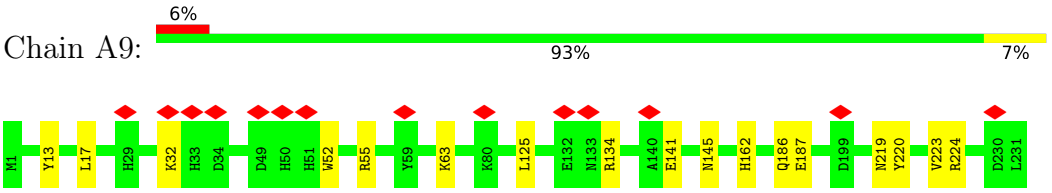
Chain A8:



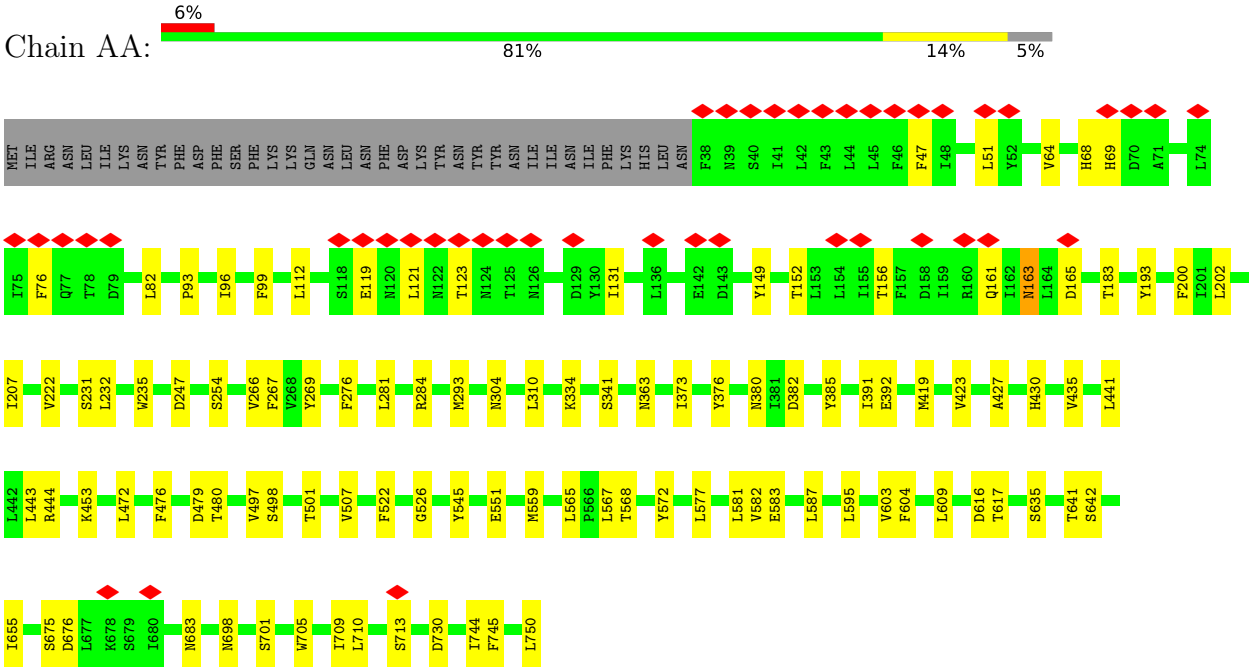




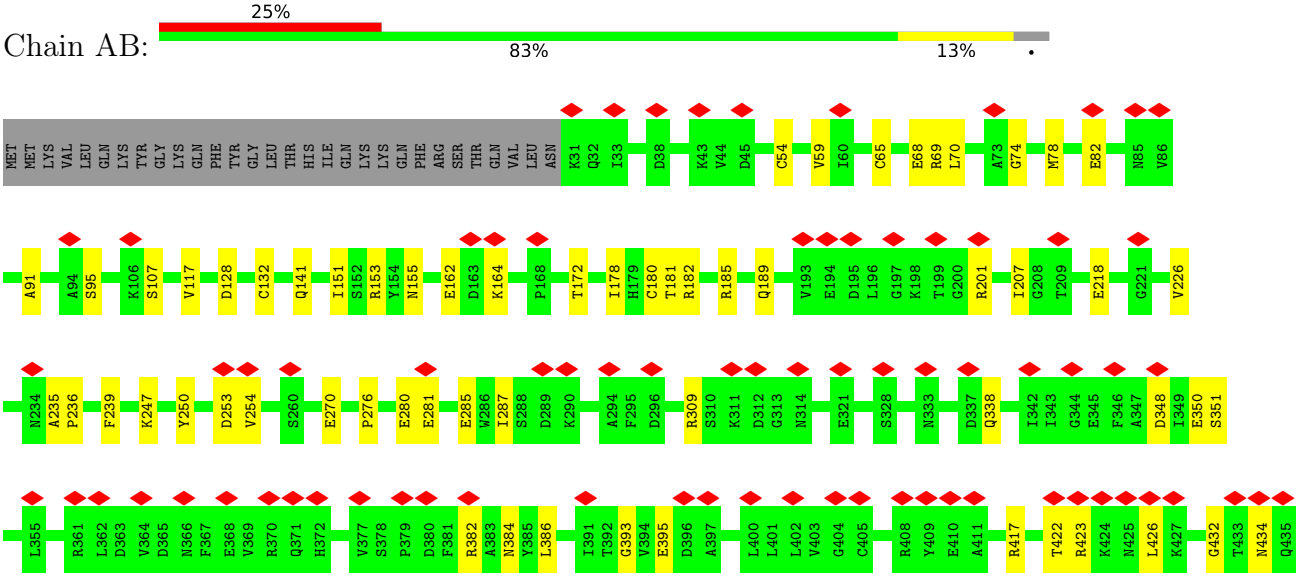
• Molecule 10: Transmembrane protein, putative

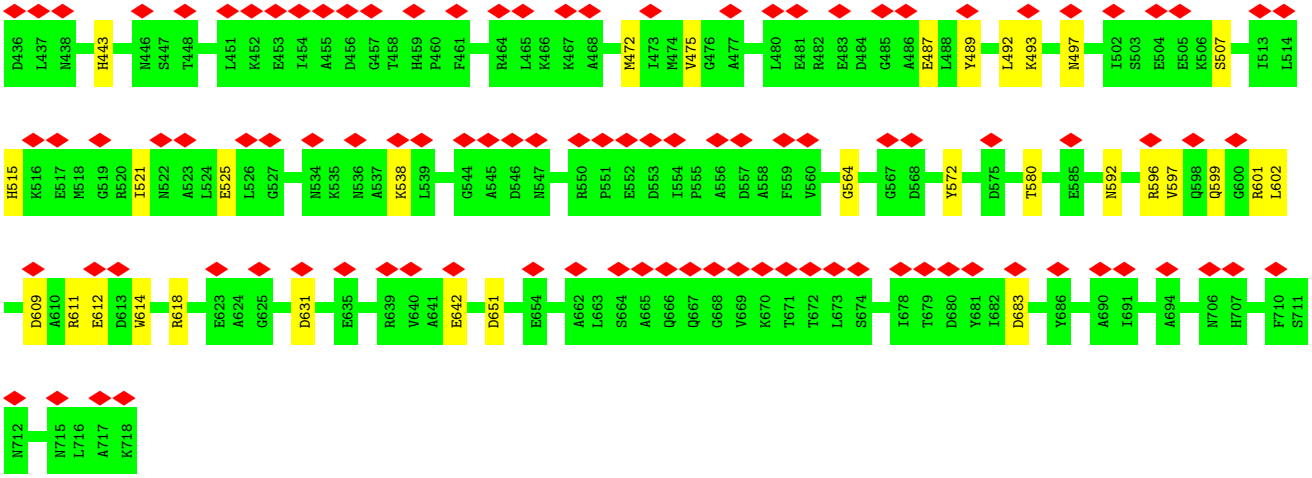


• Molecule 11: NADH dehydrogenase subunit 5



• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit

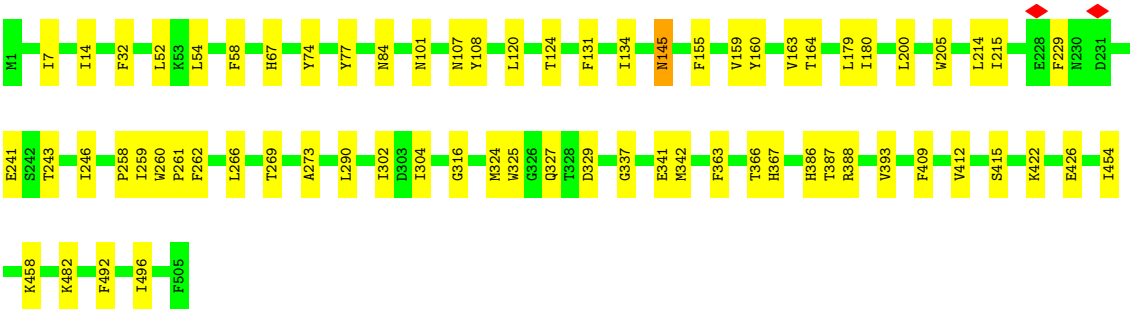




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain AC:

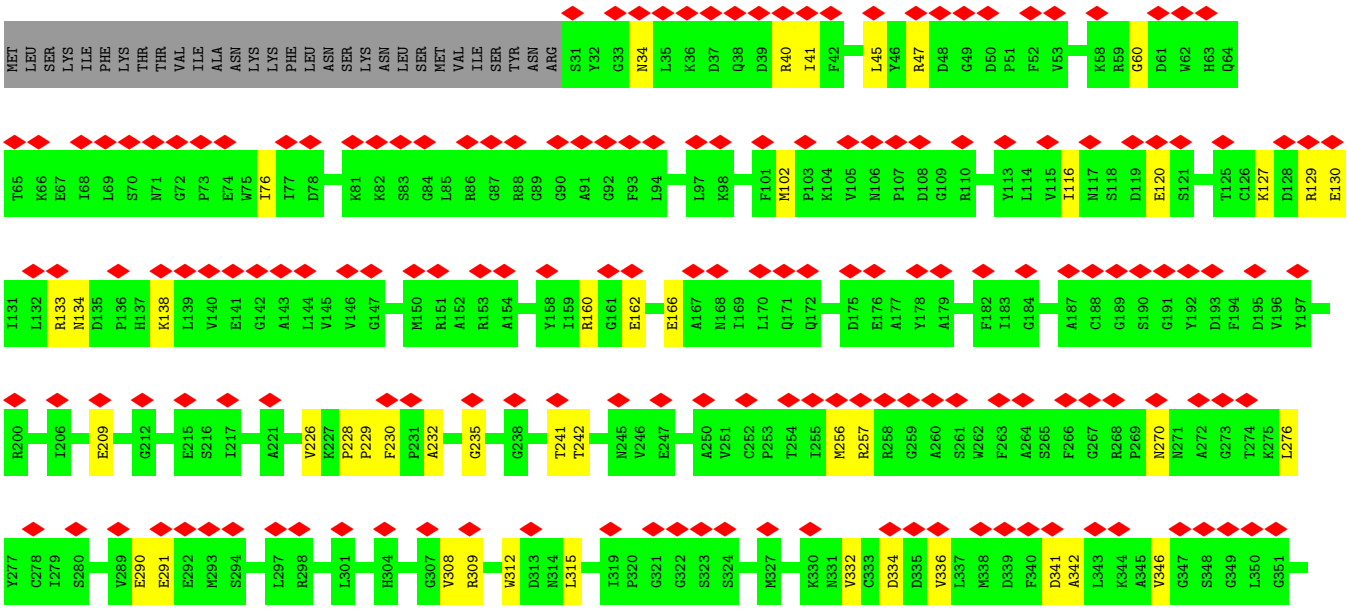


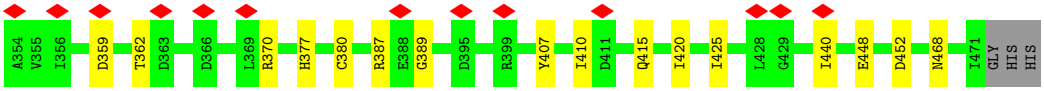


• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain AD:



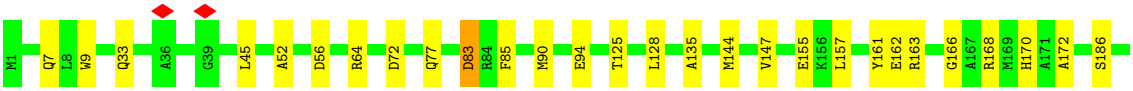


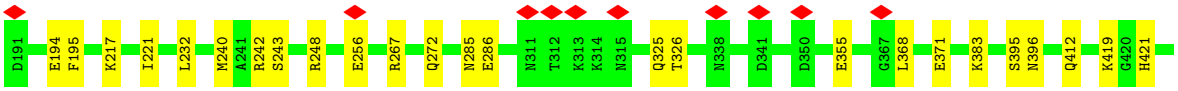


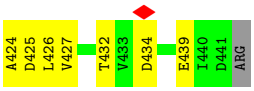
• Molecule 15: NADH dehydrogenase subunit 7

Chain AE:





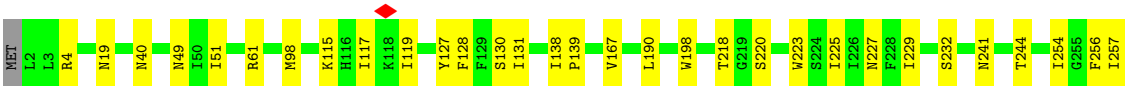


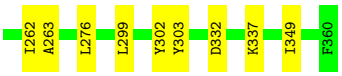


• Molecule 16: Ymf65

Chain AF:

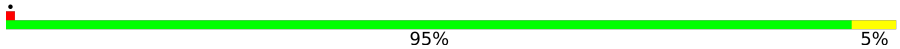


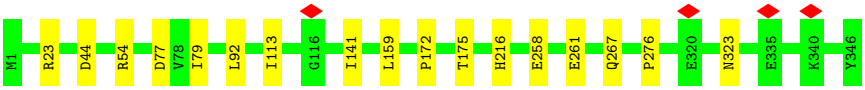




• Molecule 17: Transcription factor apfi protein, putative

Chain AG:





• Molecule 18: NADH-ubiquinone oxidoreductase chain 1

Chain AH:

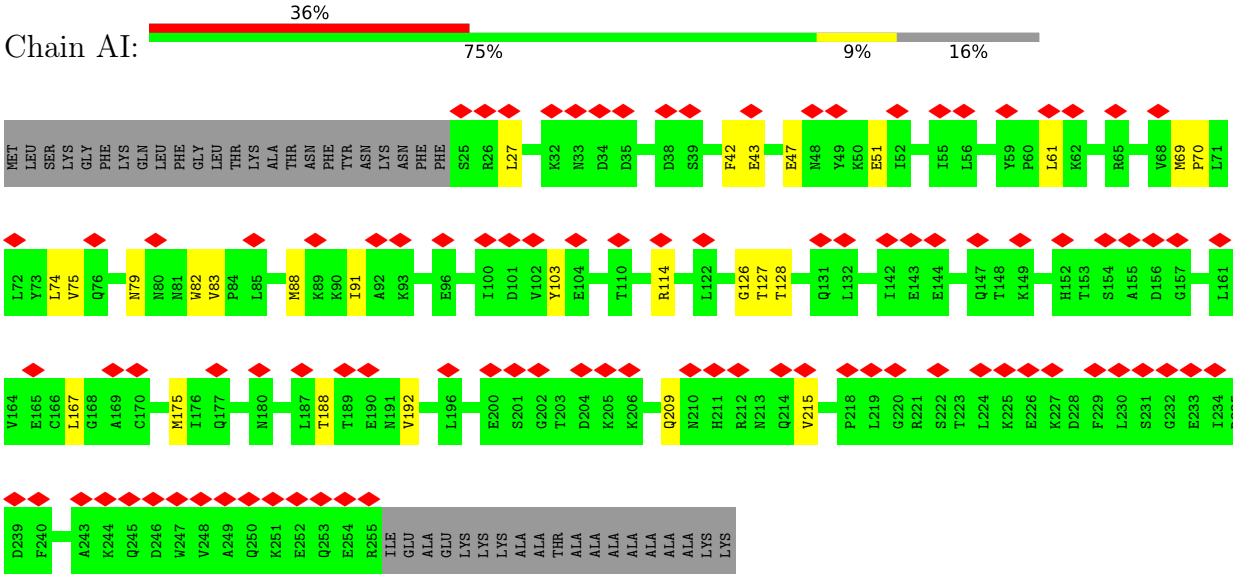






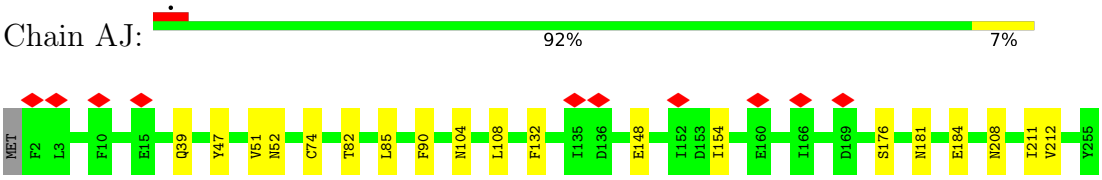
• Molecule 19: NADH-ubiquinone oxidoreductase 24 kDa subunit

Chain AI:



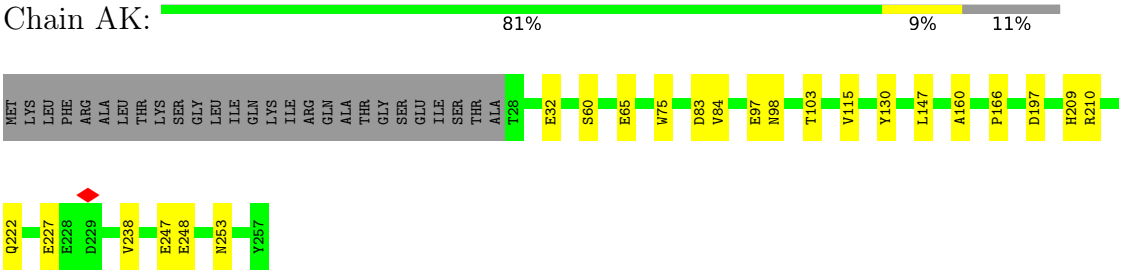
• Molecule 20: Ymf62

Chain AJ:



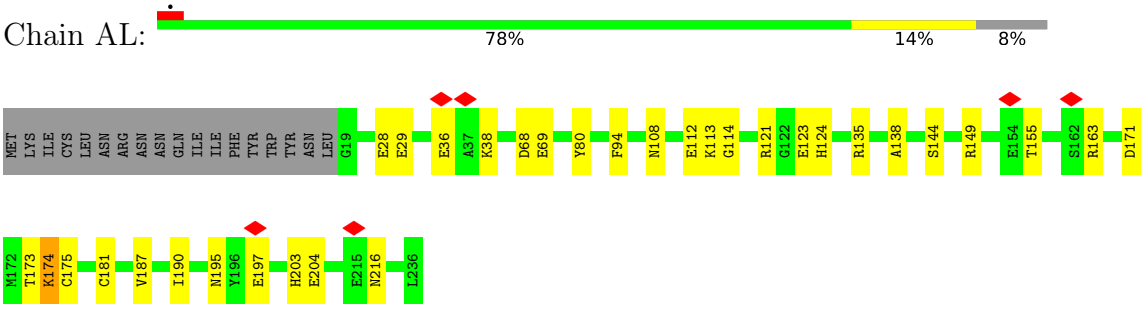
• Molecule 21: Gamma-carbonic anhydrase

Chain AK:



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

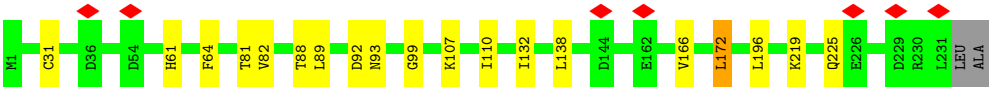
Chain AL:



• Molecule 23: Gamma-carbonic anhydrase

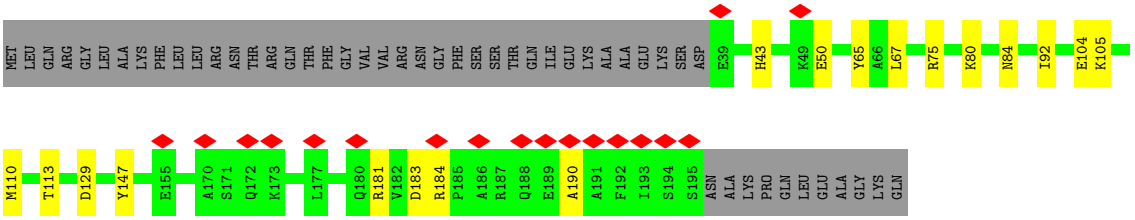
Chain AM:



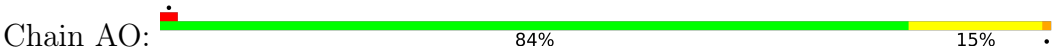


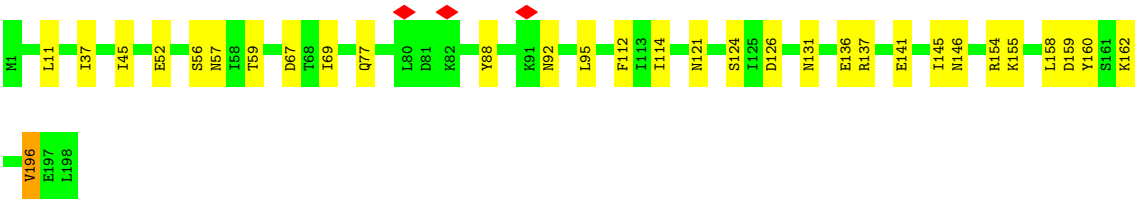
• Molecule 24: ETC complex I subunit motif protein



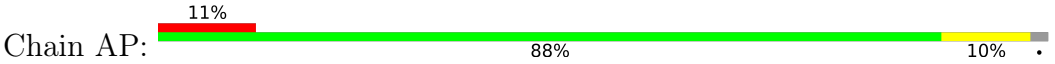


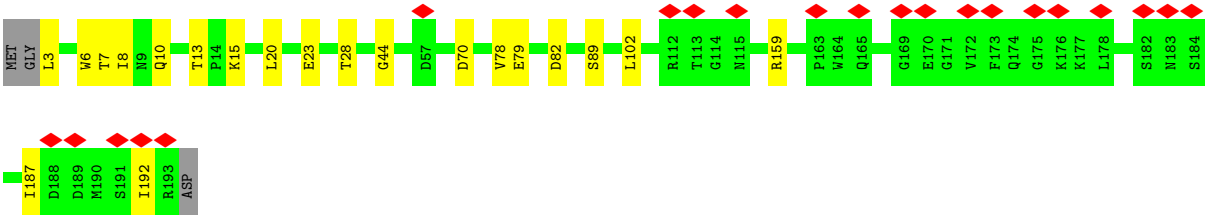
• Molecule 25: NADH dehydrogenase subunit 9



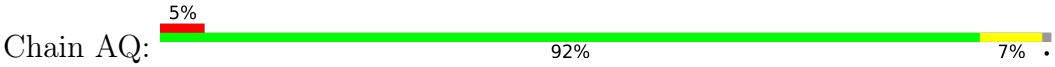


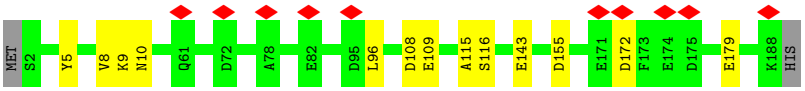
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



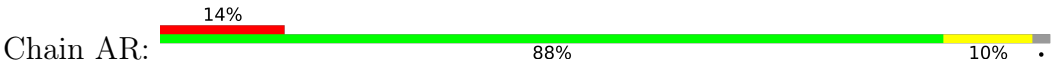


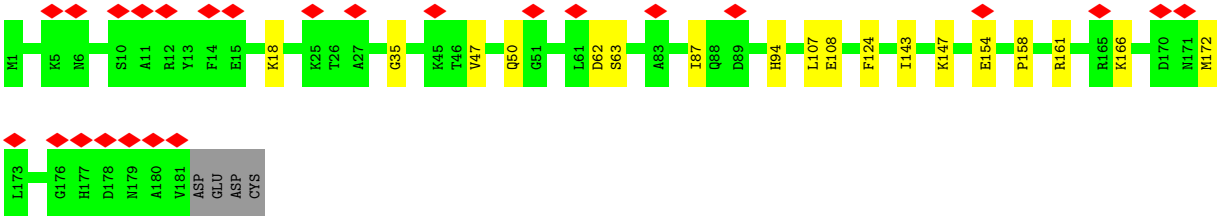
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





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

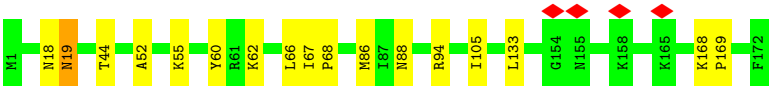




• Molecule 29: NADH dehydrogenase, putative

Chain AS:





• Molecule 30: NADH dehydrogenase subunit 10

Chain AT:

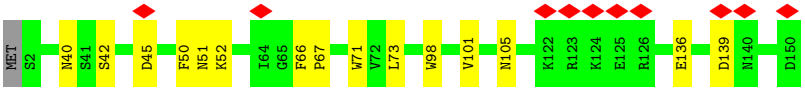




• Molecule 31: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

Chain AU:

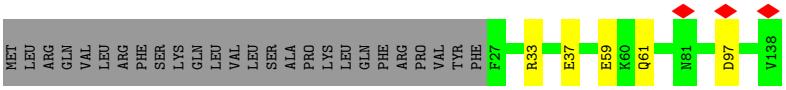




• Molecule 32: Acyl carrier protein

Chain AV:

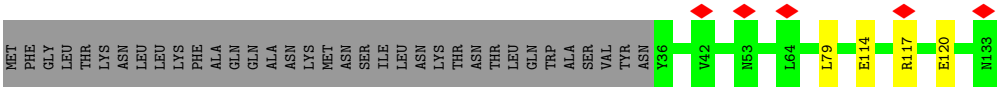




• Molecule 33: Acyl carrier protein

Chain AW:

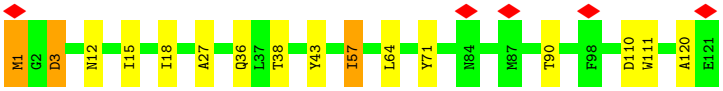




• Molecule 34: NADH-ubiquinone oxidoreductase chain 3

Chain AX:

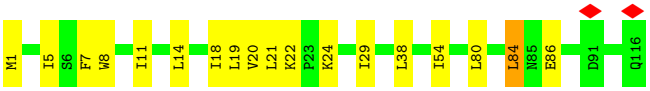




• Molecule 35: Ymf58

Chain AY:

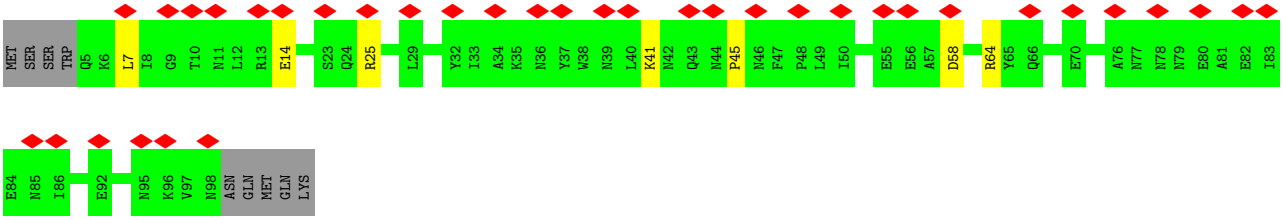




• Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein

Chain AZ:

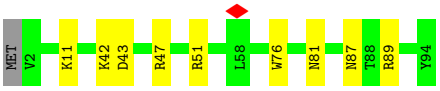




• Molecule 37: Transmembrane protein, putative

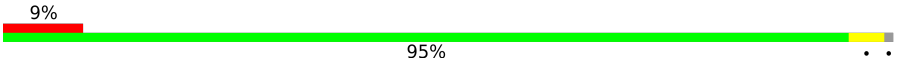
Chain B0:

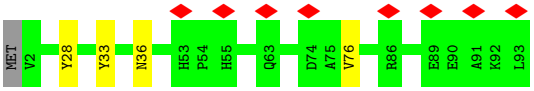




• Molecule 38: ATP synthase subunit e, mitochondrial

Chain B1:





• Molecule 39: GRAM domain protein

Chain B2:

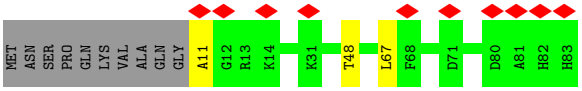




• Molecule 40: Transmembrane protein, putative

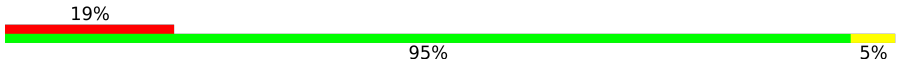
Chain B3:

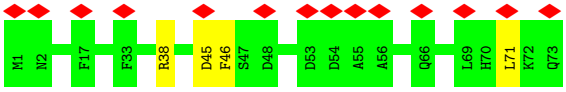




• Molecule 41: Transmembrane protein, putative

Chain B4:

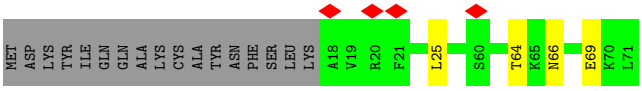




• Molecule 42: Transmembrane protein, putative

Chain B5:

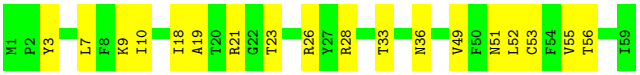




• Molecule 43: NADH dehydrogenase subunit 1

Chain B6:

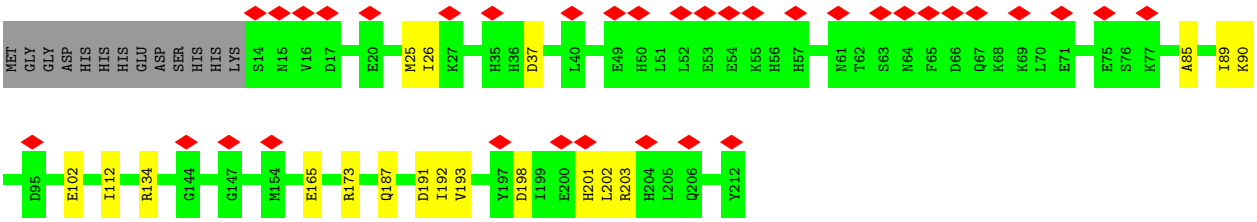




• Molecule 44: Transmembrane protein

Chain BA:

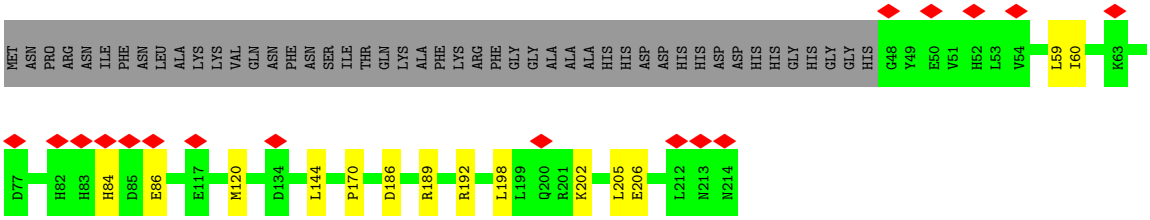




• Molecule 45: Transmembrane protein, putative

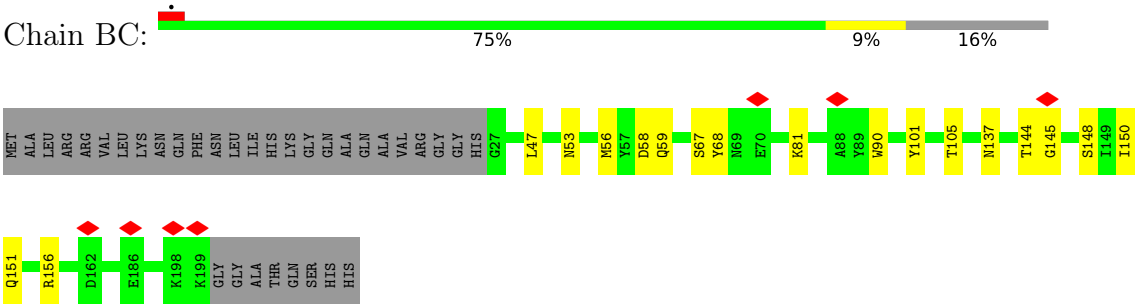
Chain BB:





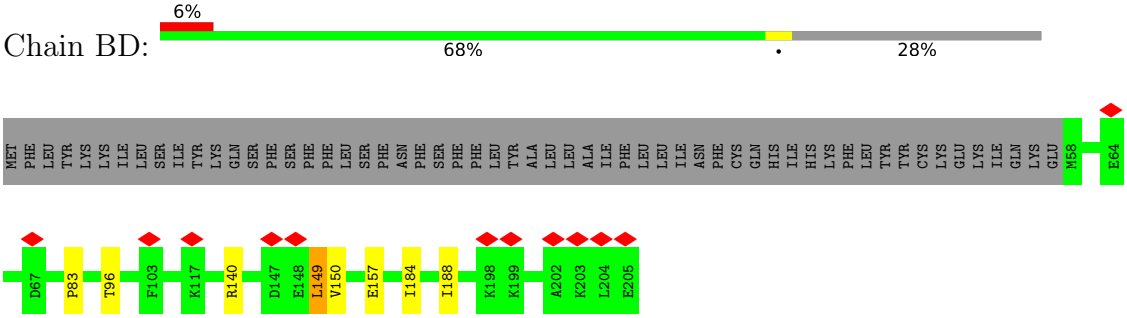
• Molecule 46: NDUB8

Chain BC:



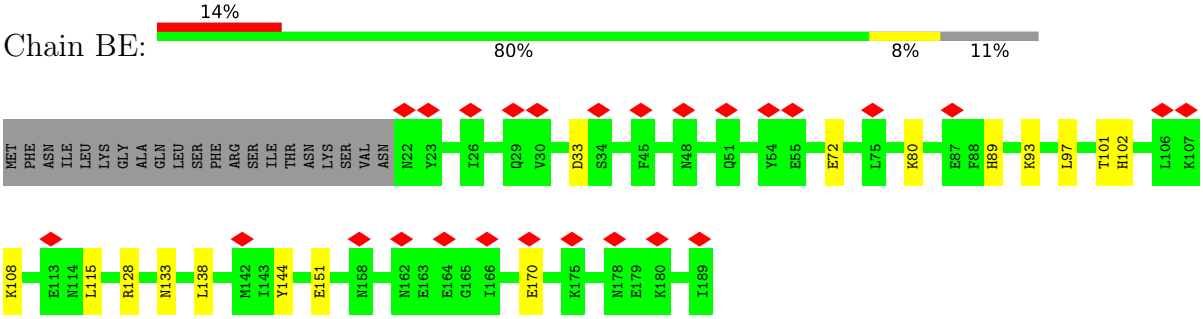
• Molecule 47: Transmembrane protein, putative

Chain BD:



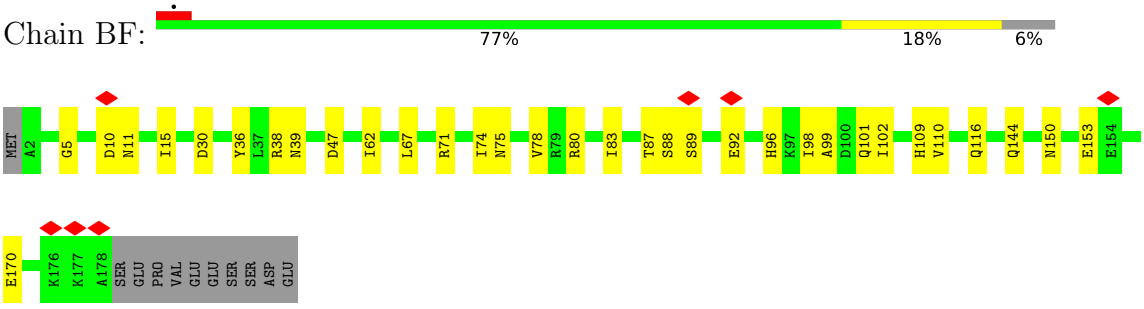
• Molecule 48: NDUPH2

Chain BE:



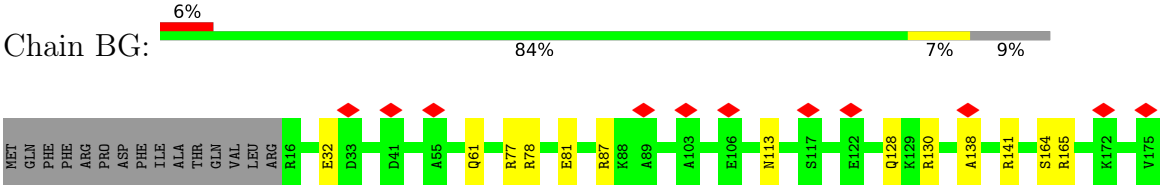
• Molecule 49: NDUB10

Chain BF:



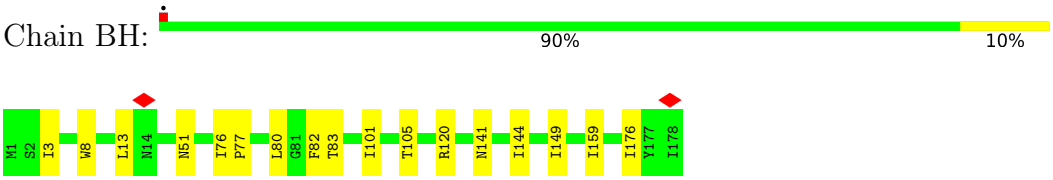
• Molecule 50: NDUA13

Chain BG:



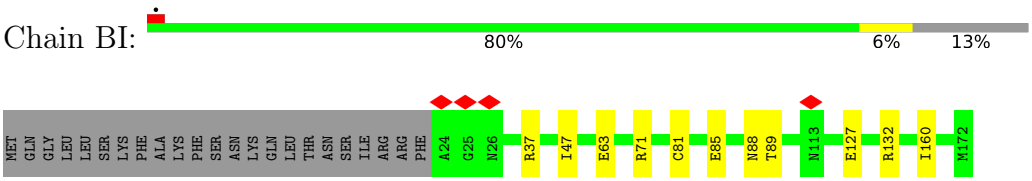
• Molecule 51: NADH dehydrogenase subunit 2

Chain BH:



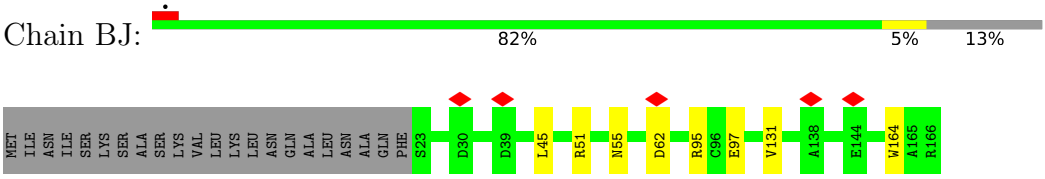
• Molecule 52: 2 iron, 2 sulfur cluster-binding protein

Chain BI:



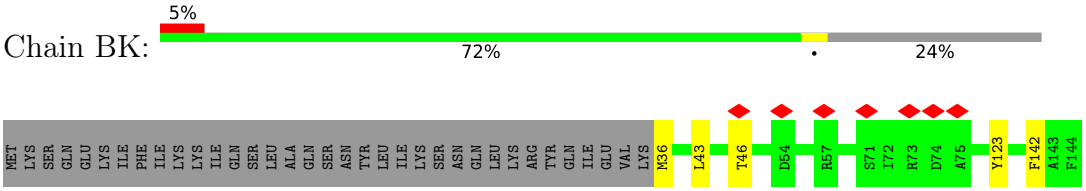
• Molecule 53: Thioredoxin

Chain BJ:



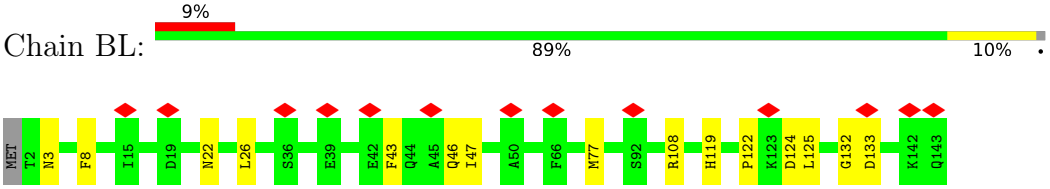
• Molecule 54: COX assembly mitochondrial protein

Chain BK:



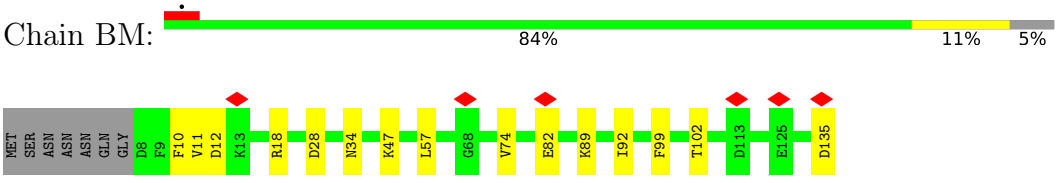
• Molecule 55: Transmembrane protein, putative

Chain BL:



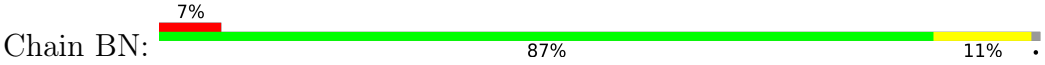
• Molecule 56: Transmembrane protein, putative

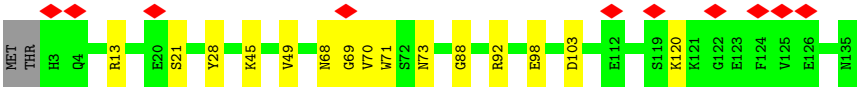
Chain BM:



• Molecule 57: PH domain-containing protein

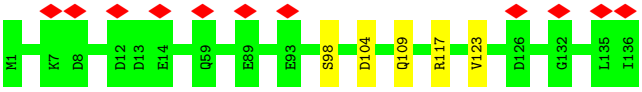
Chain BN:





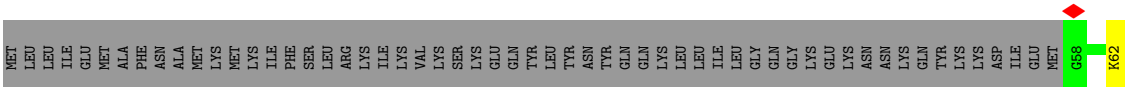
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

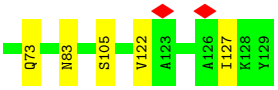




• Molecule 59: NDUB6

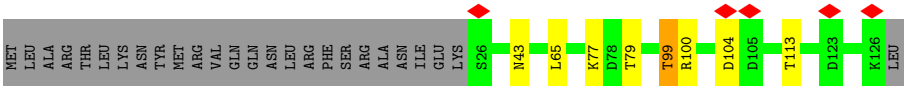






• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



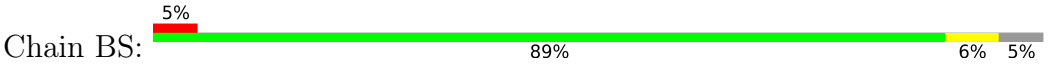


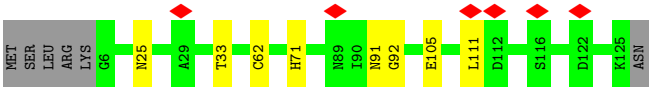
• Molecule 61: Zinc-finger protein



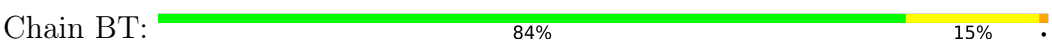


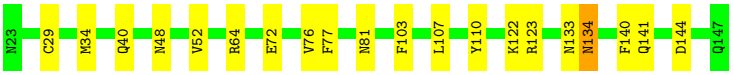
• Molecule 62: NDUB4





• Molecule 63: NDUTT10

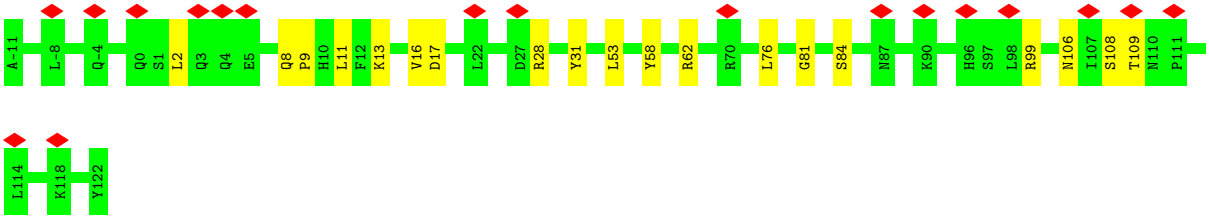




• Molecule 64: NDUTT11

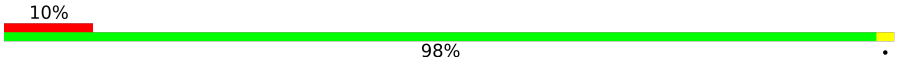
Chain BU:

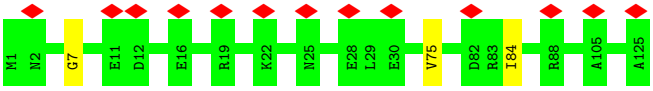




• Molecule 65: NDUTT12

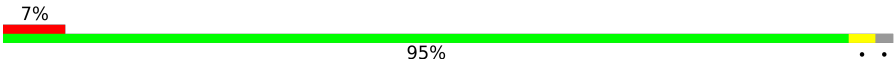
Chain BV:

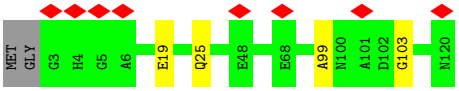




• Molecule 66: CHCH domain-containing protein

Chain BW:

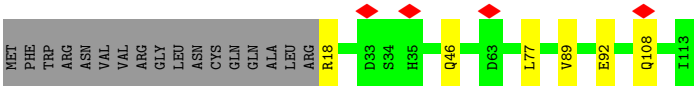




• Molecule 67: Transmembrane protein, putative

Chain BX:

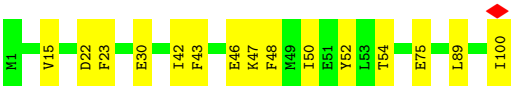




• Molecule 68: Ymf57

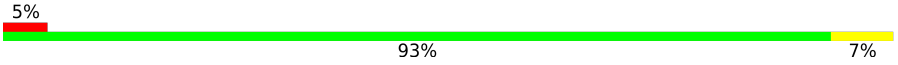
Chain BY:





• Molecule 69: Complex I-MNLL

Chain BZ:





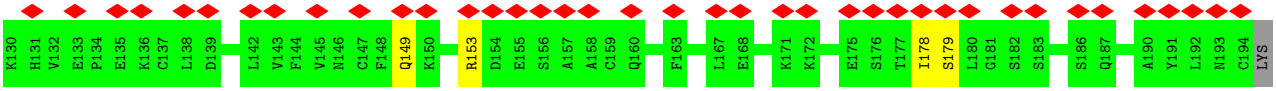
• Molecule 70: Diphthamide synthesis protein

Chain CH:



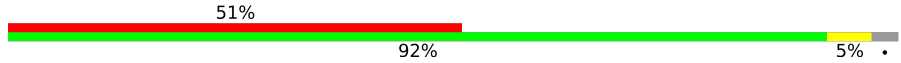


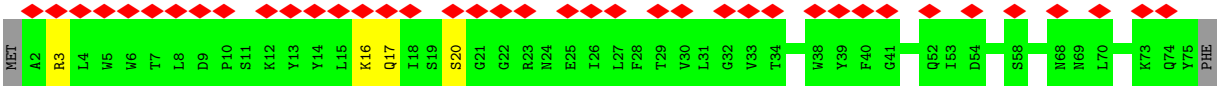




• Molecule 71: Transmembrane protein, putative

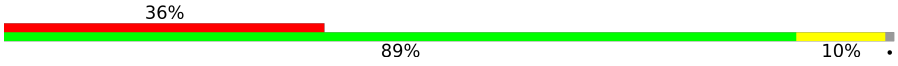
Chain CM:





• Molecule 72: Transposase

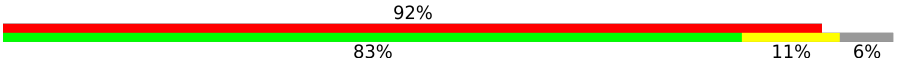
Chain CL:

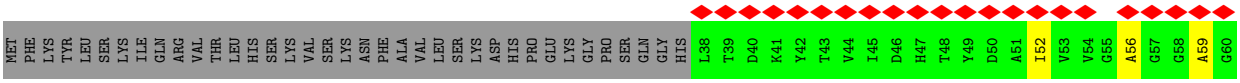


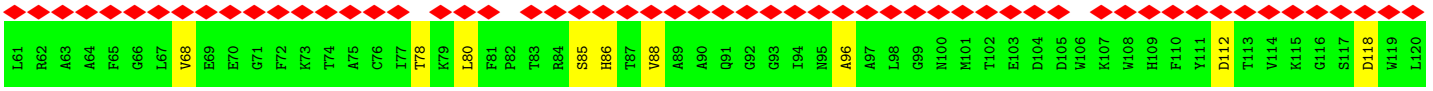


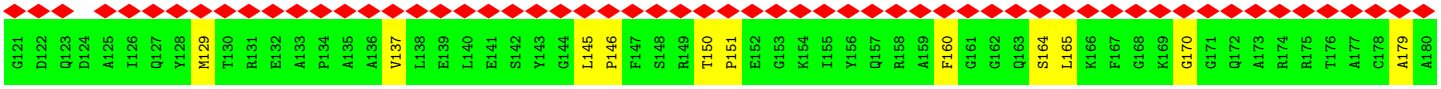
• Molecule 73: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain CA:

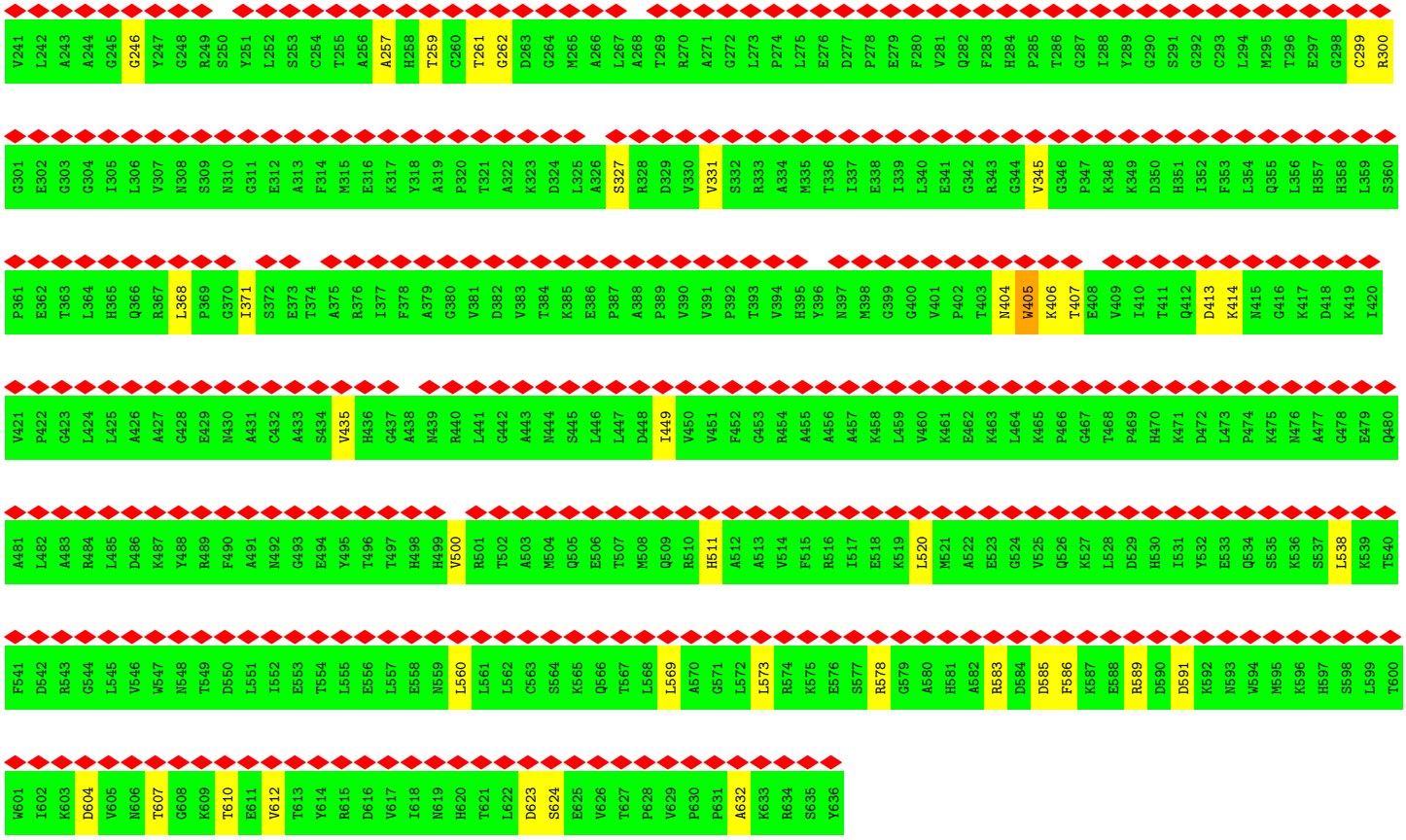






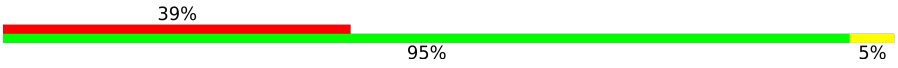


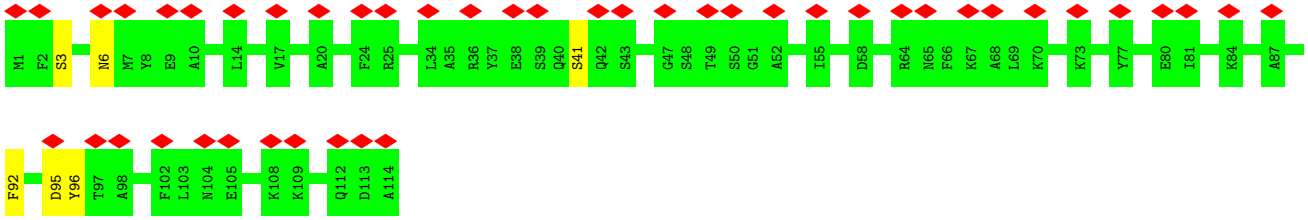




• Molecule 74: DUF4885 domain-containing protein

Chain CI:

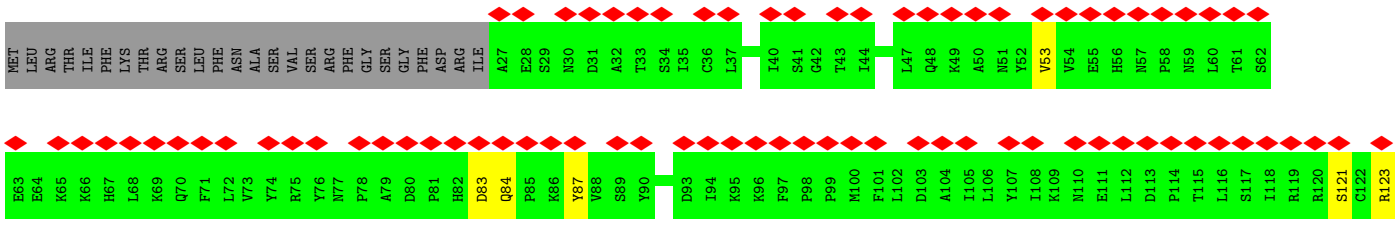




• Molecule 75: succinate dehydrogenase

Chain CB:



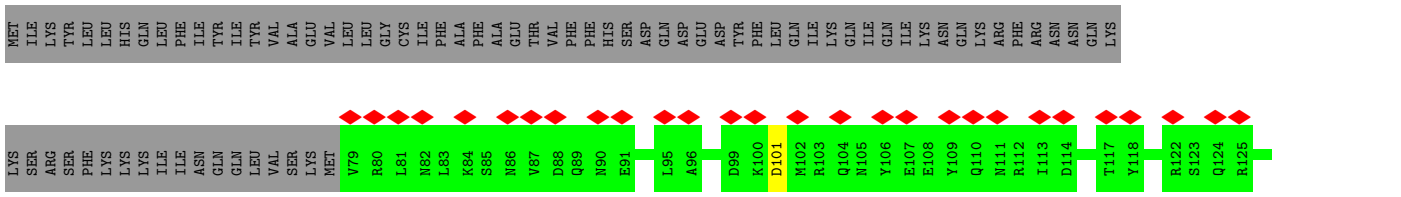




• Molecule 76: Transmembrane protein, putative

Chain CF:

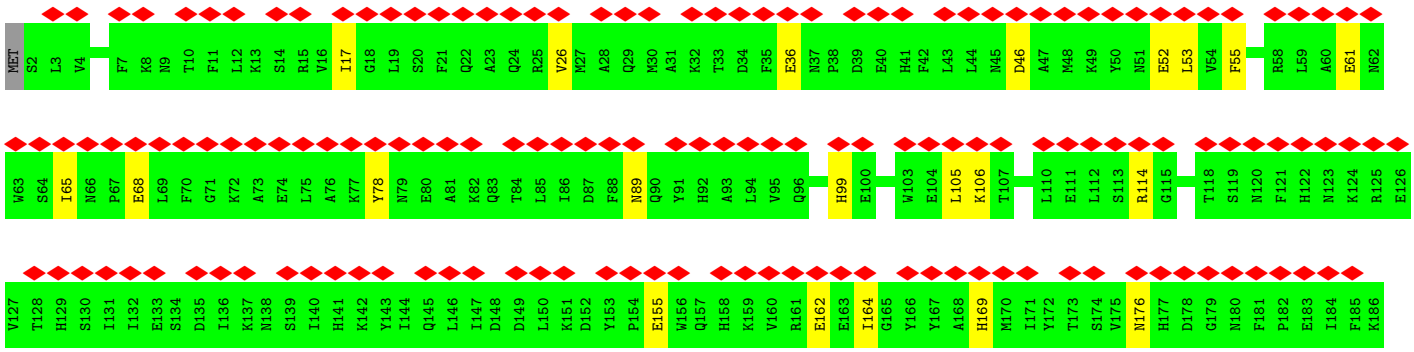


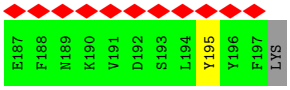


• Molecule 77: chain 77

Chain CG:

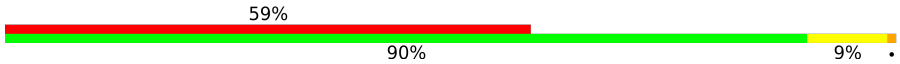


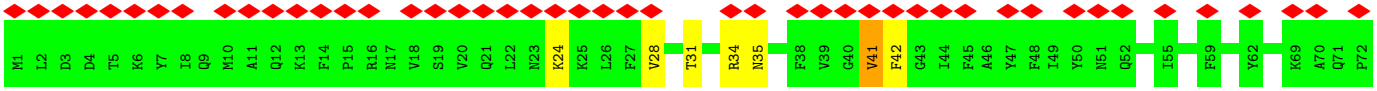


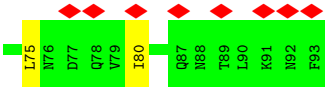


• Molecule 78: Transmembrane protein, putative

Chain CK:

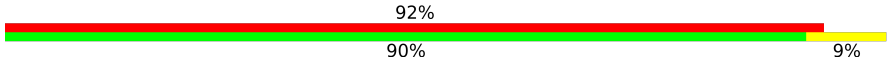


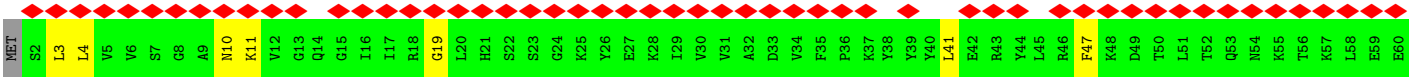


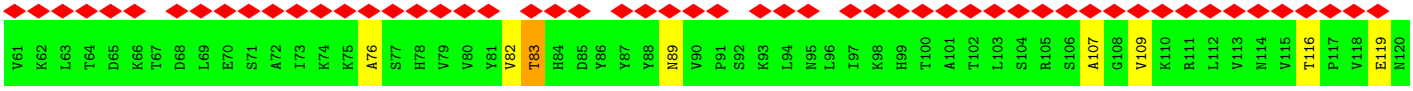


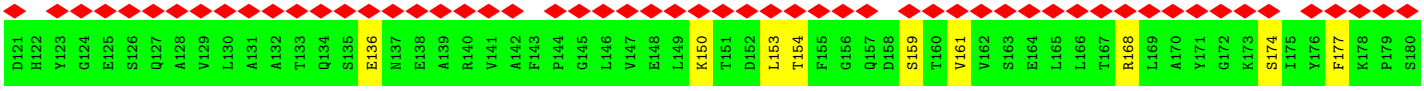
• Molecule 79: NmrA domain-containing protein

Chain CE:

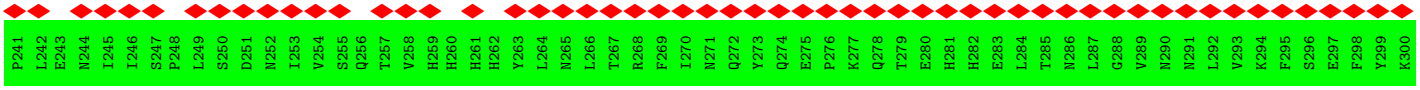


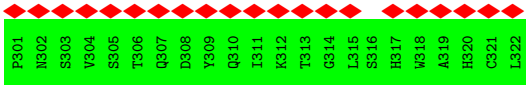






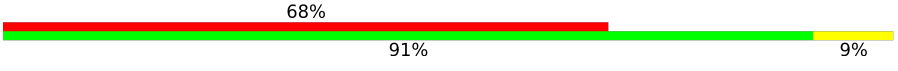


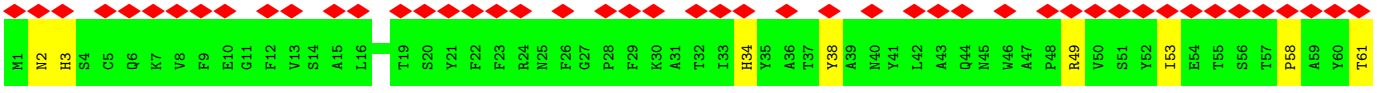


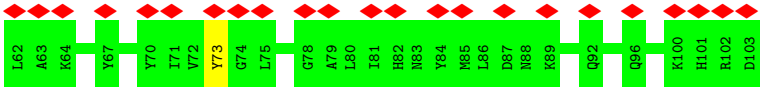


• Molecule 80: Transmembrane protein, putative

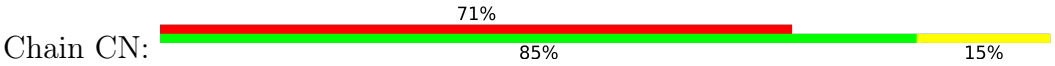
Chain CJ:

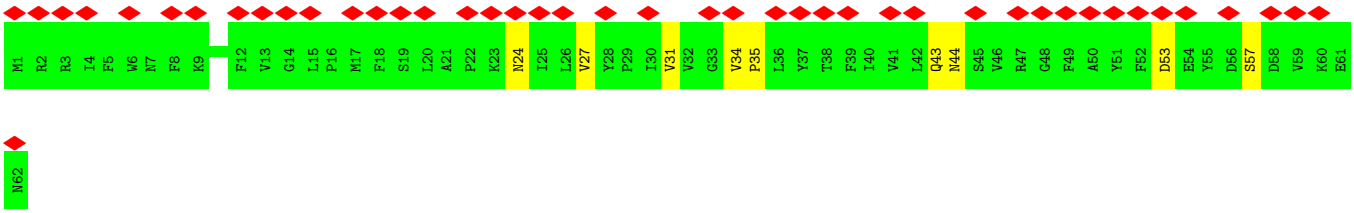






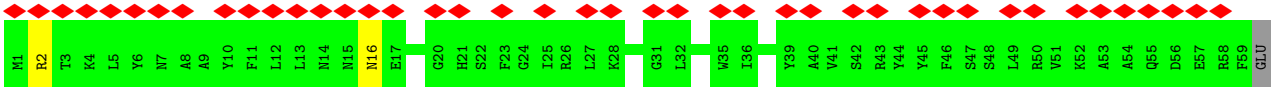
• Molecule 81: Transmembrane protein, putative



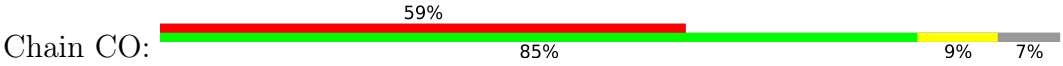


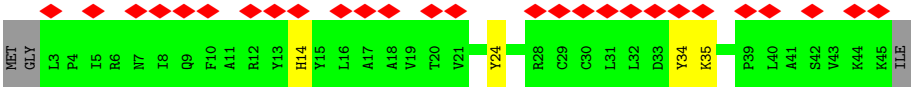
• Molecule 82: Transmembrane protein



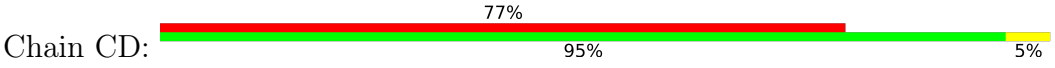


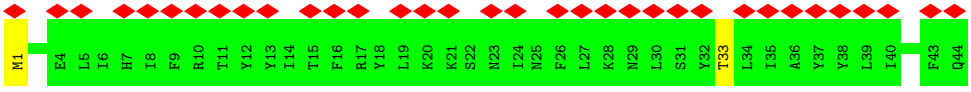
• Molecule 83: SDHTT11



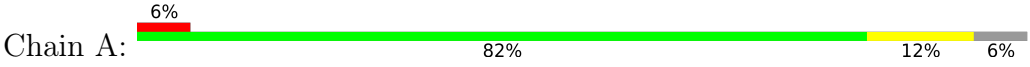


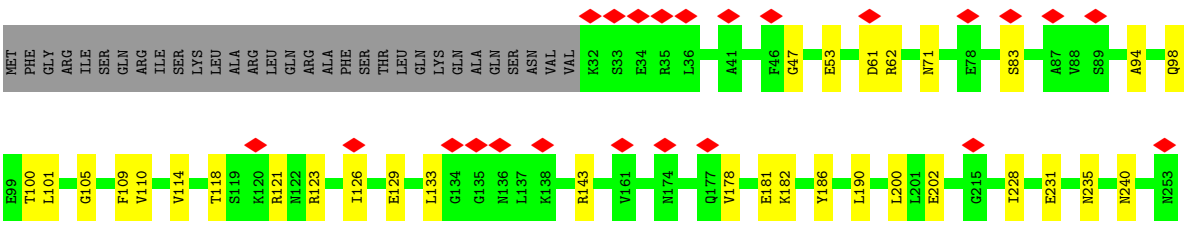
• Molecule 84: succinate dehydrogenase complex iron-sulfur subunit D

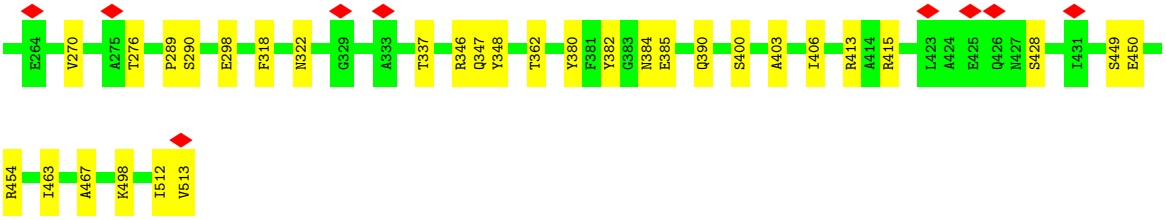




• Molecule 85: Peptidase M16 inactive domain protein



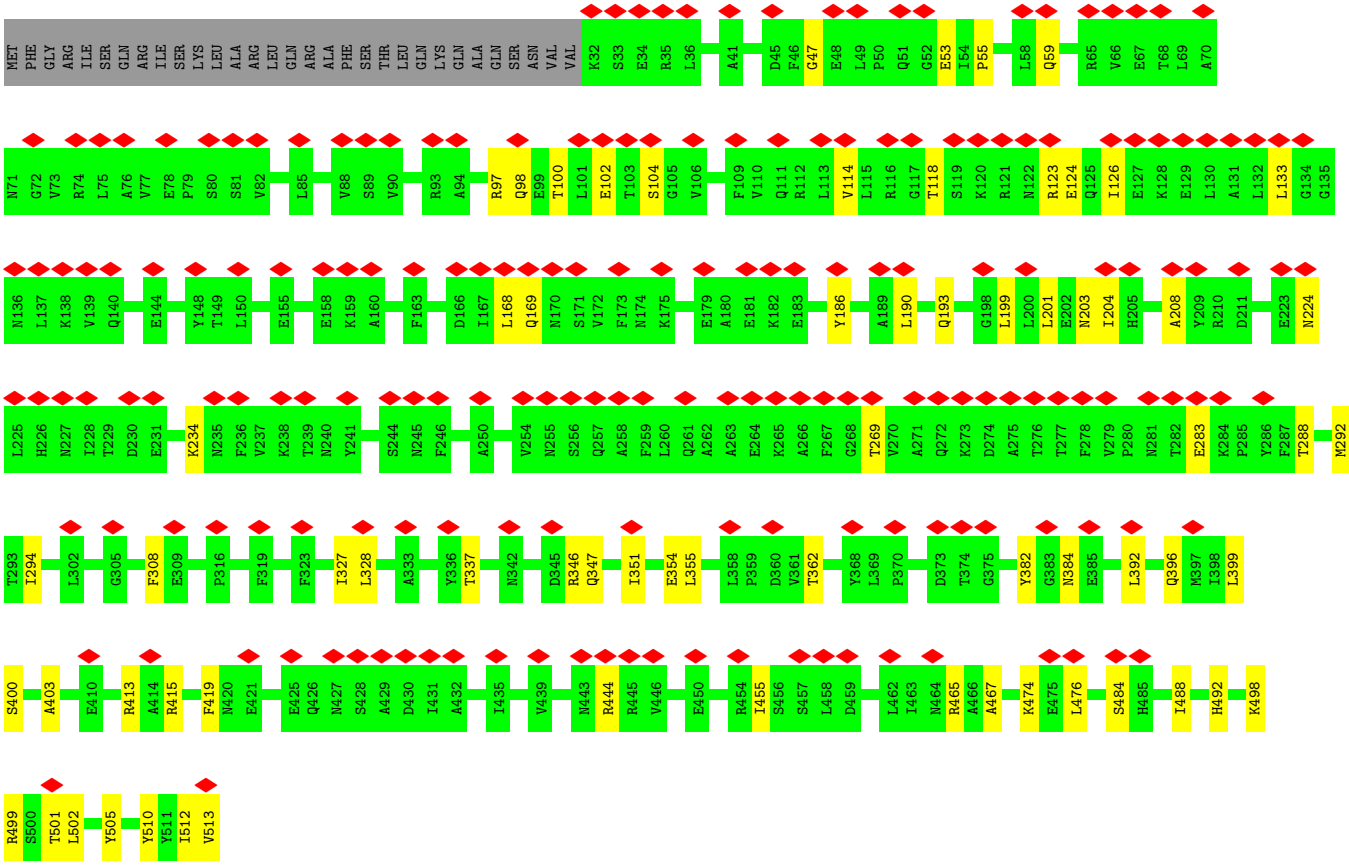




• Molecule 85: Peptidase M16 inactive domain protein

Chain a:

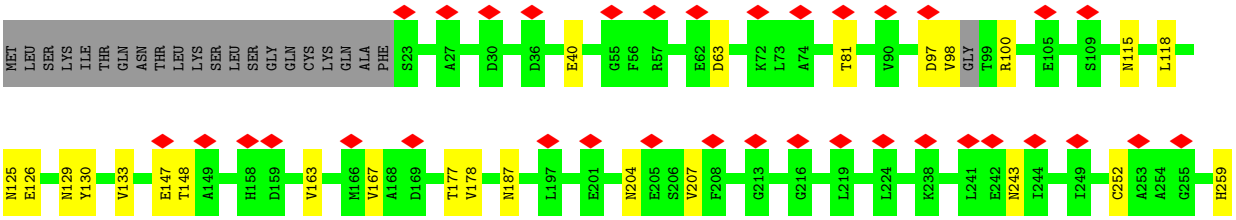


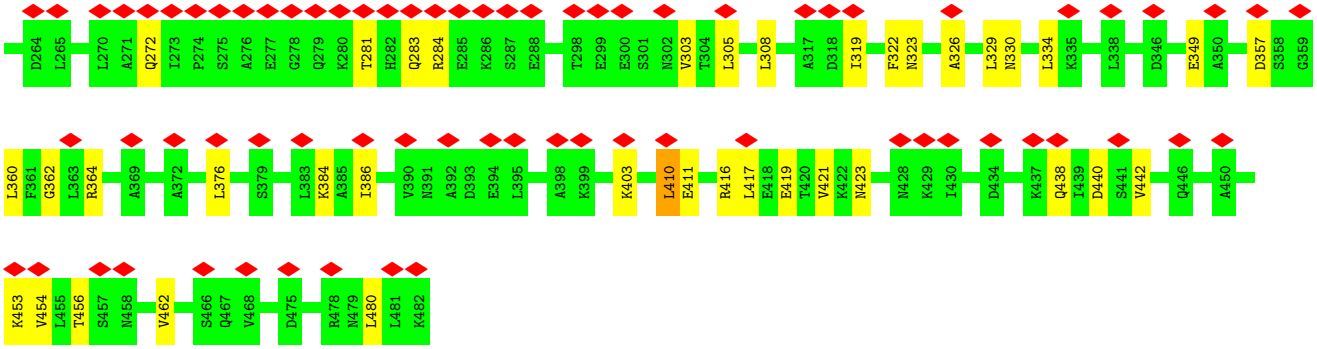


• Molecule 86: M16 family peptidase, putative

Chain B:



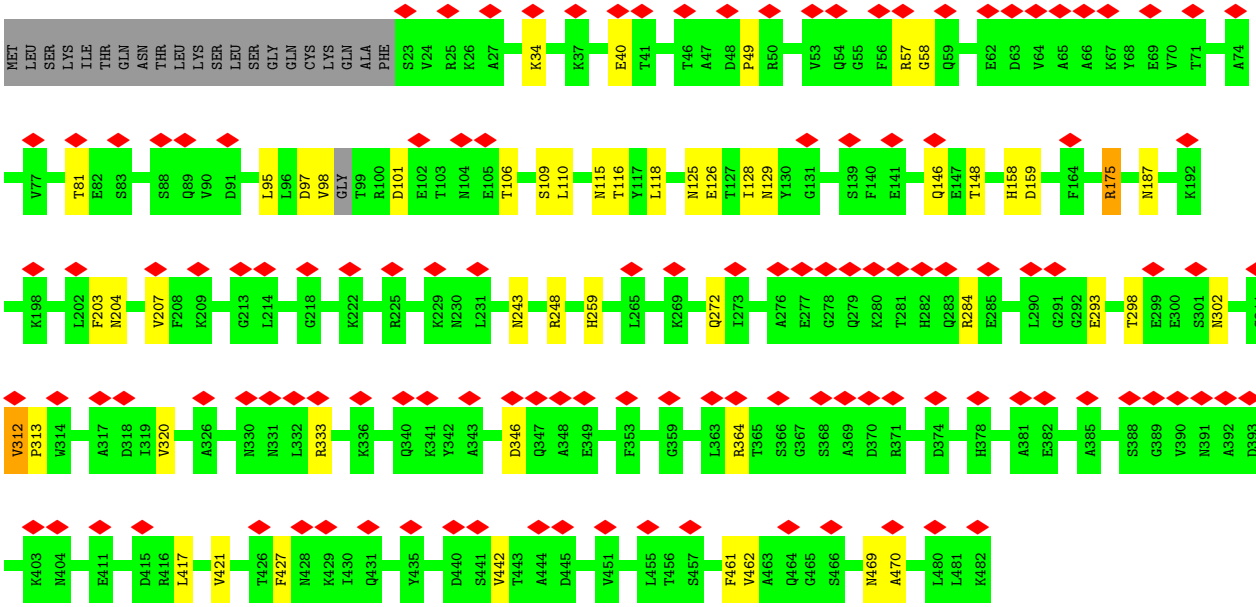




• Molecule 86: M16 family peptidase, putative

Chain b:

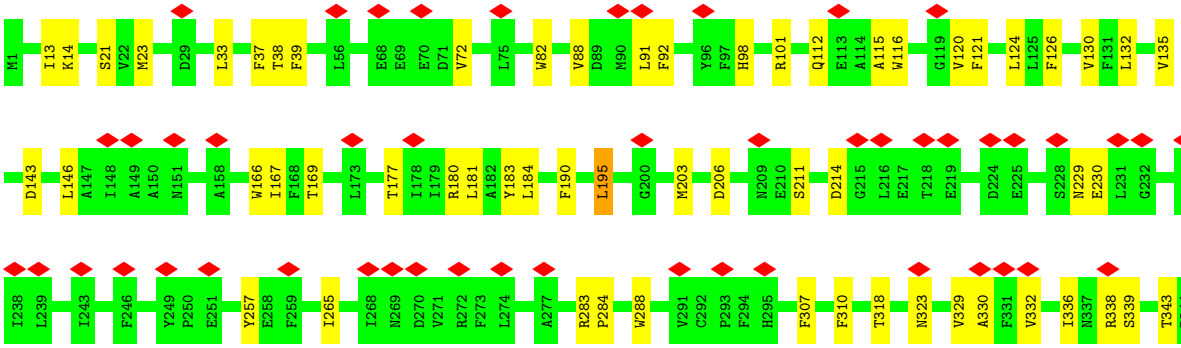


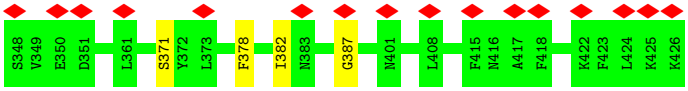


• Molecule 87: Apocytochrome b

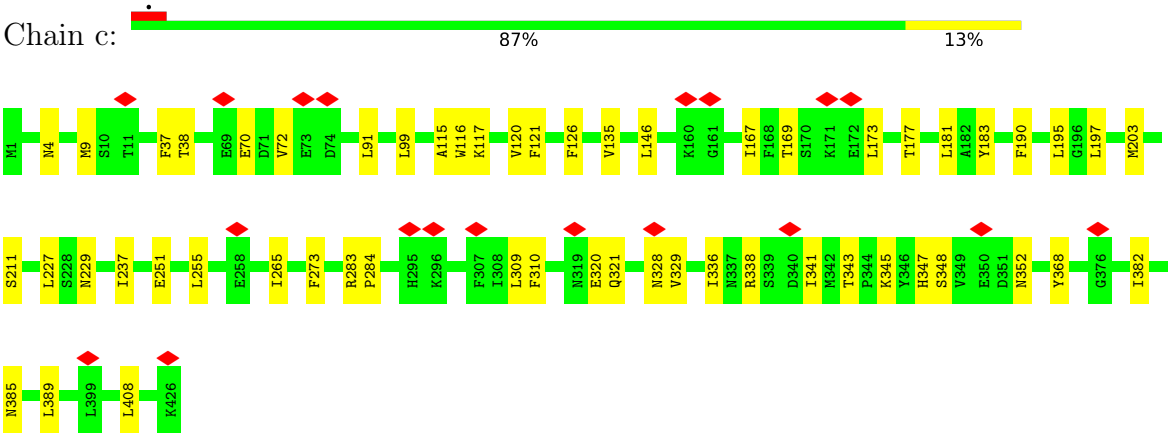
Chain C:



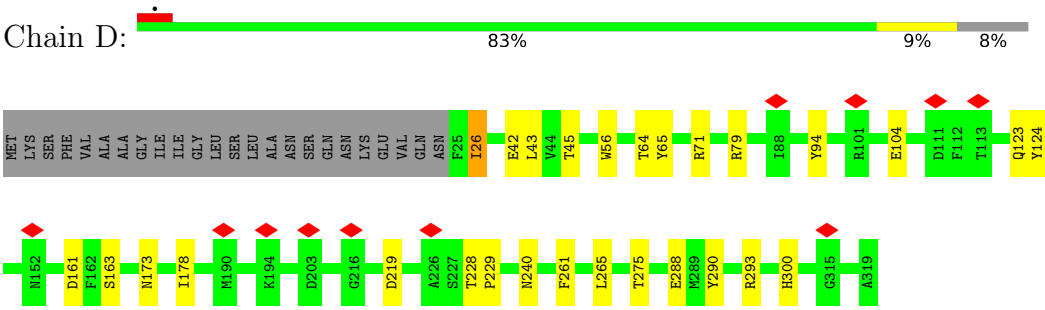




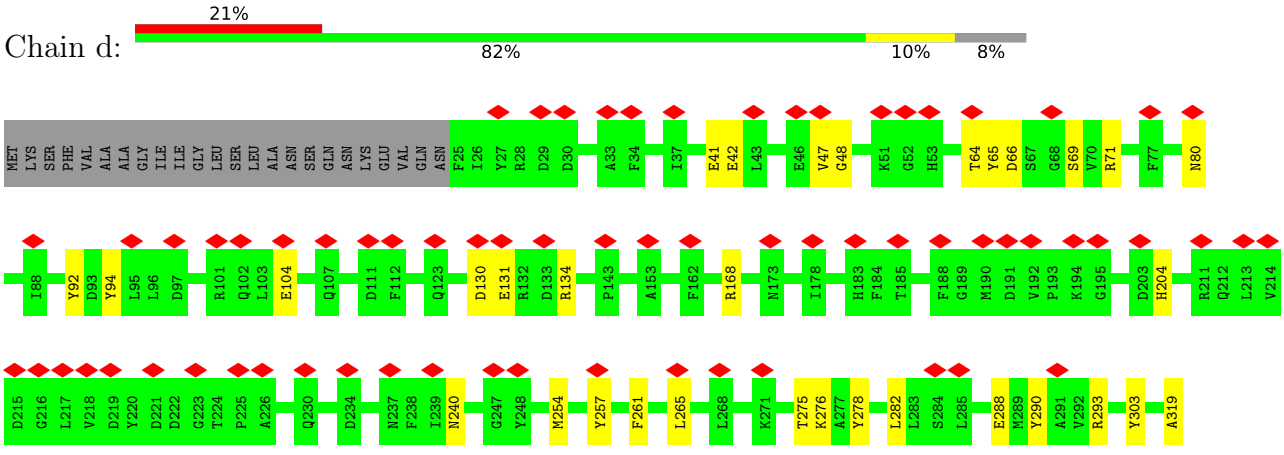
• Molecule 87: Apocytochrome b



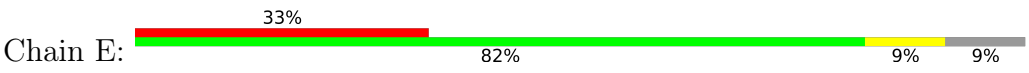
• Molecule 88: Cytochrome protein c1

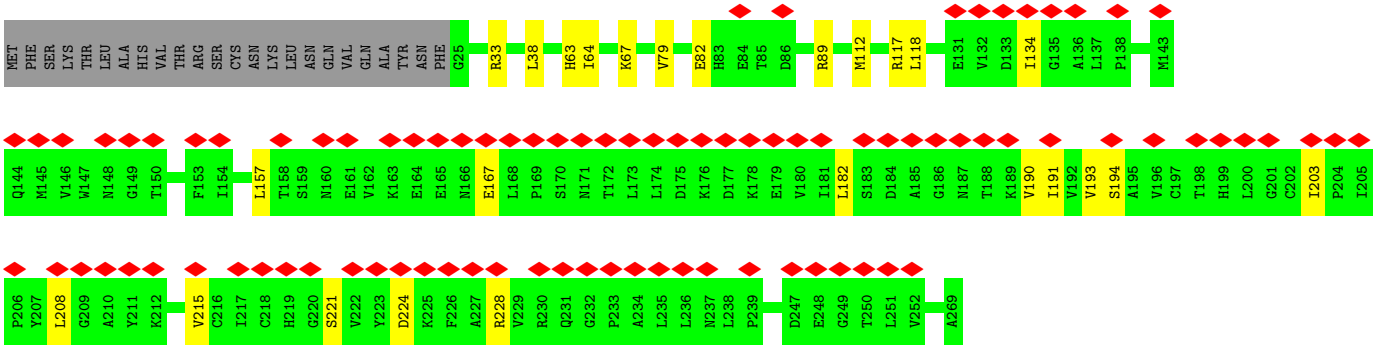


• Molecule 88: Cytochrome protein c1



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

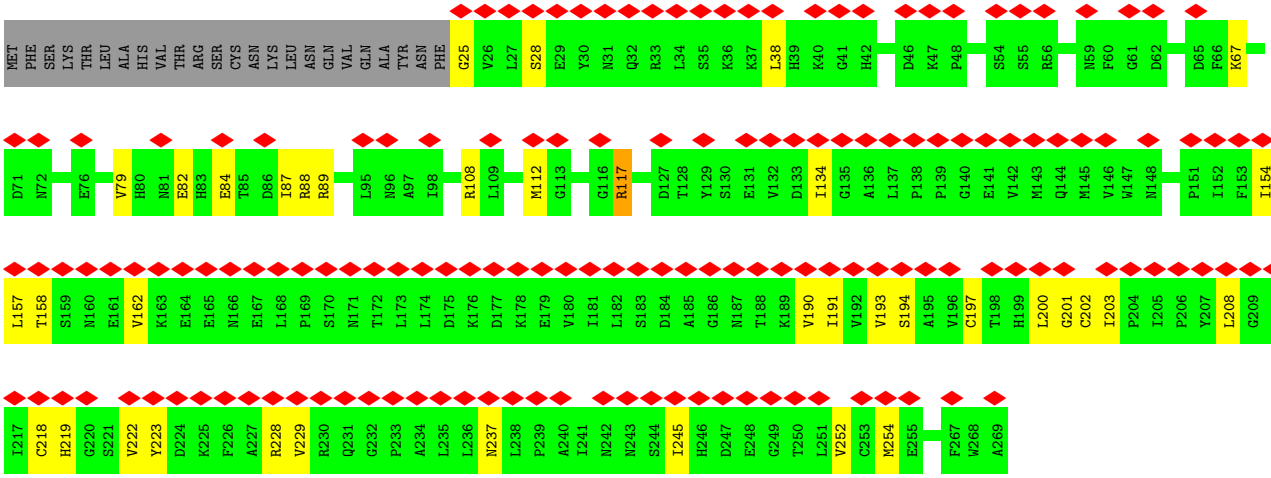




• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain e:

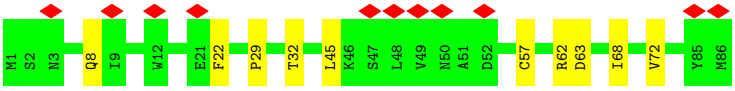




• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

Chain F:

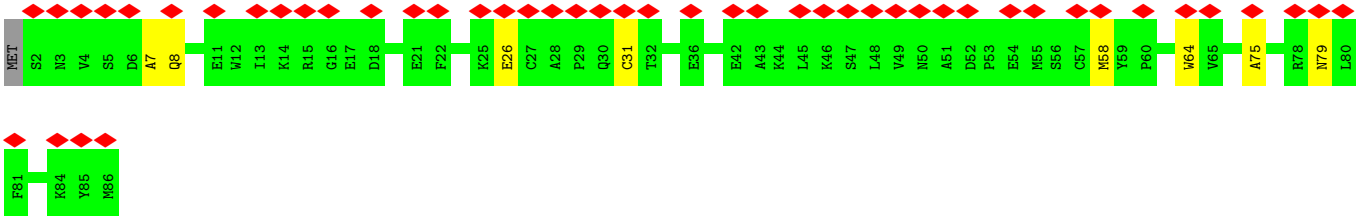




• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

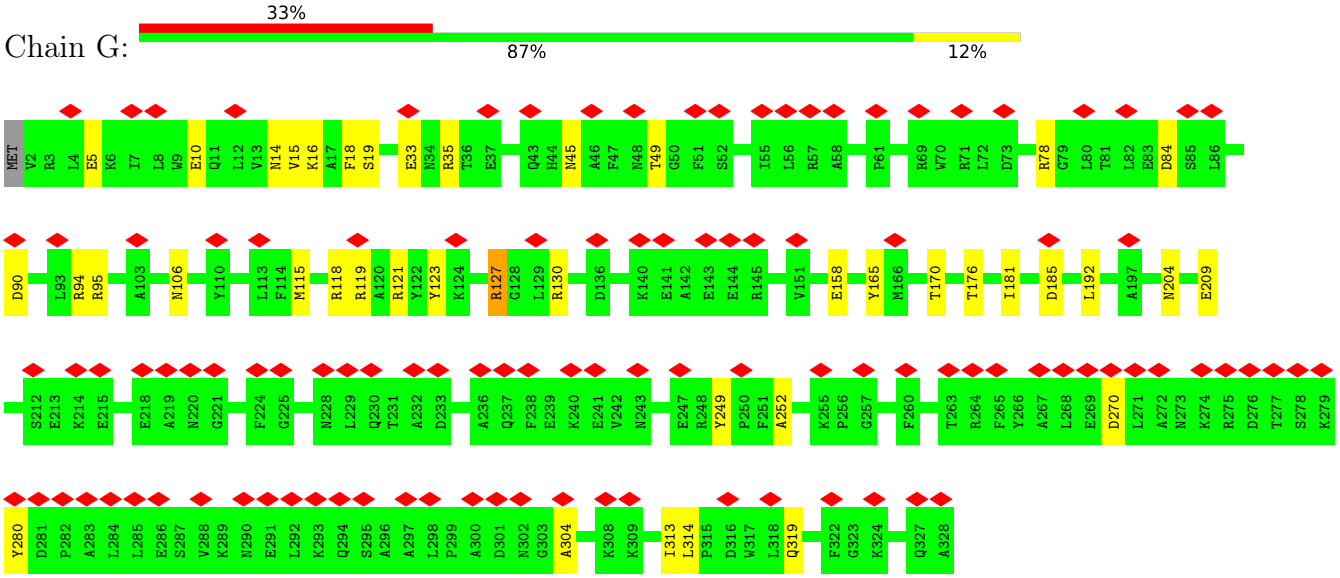
Chain f:





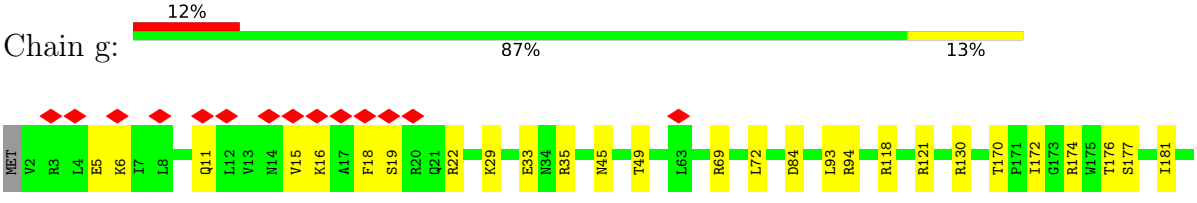
• Molecule 91: UQCRTT1

Chain G:



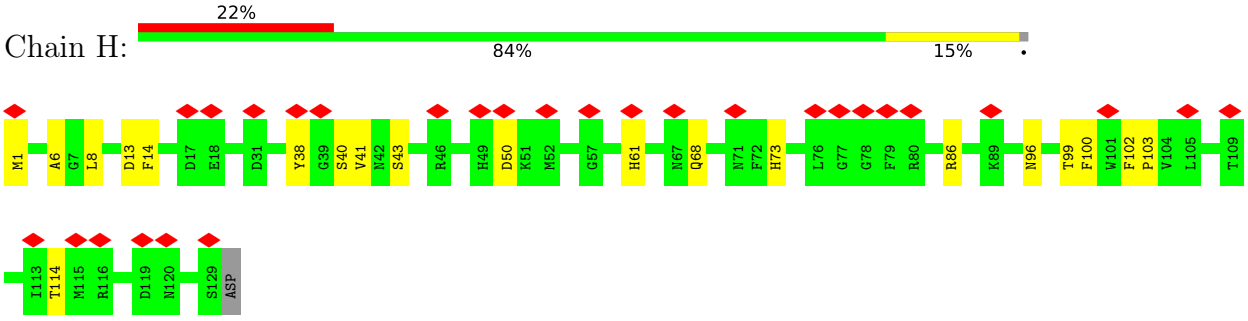
• Molecule 91: UQCRTT1

Chain g:



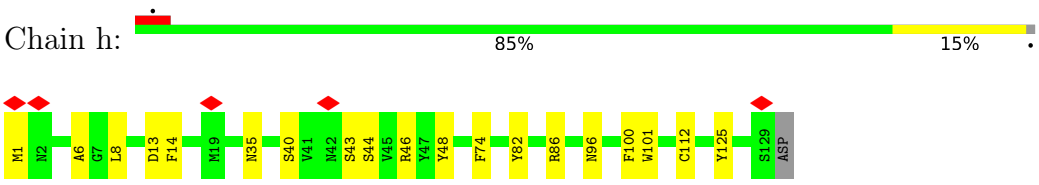
• Molecule 92: Transmembrane protein, putative

Chain H:



• Molecule 92: Transmembrane protein, putative

Chain h:



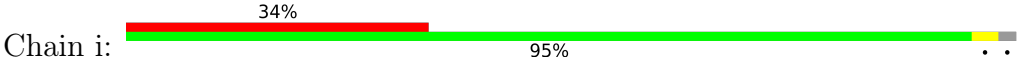
• Molecule 93: Transmembrane protein, putative

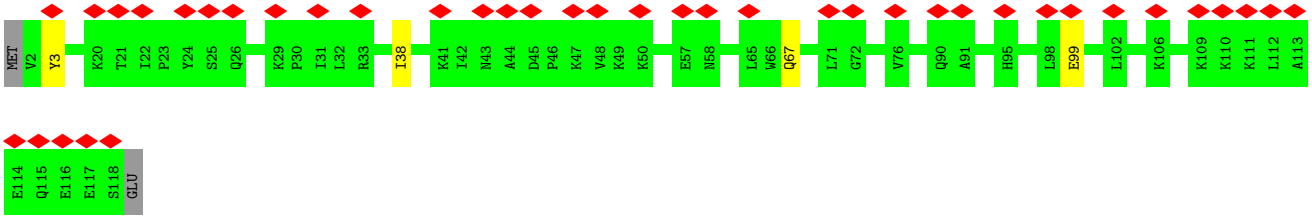
Chain I:





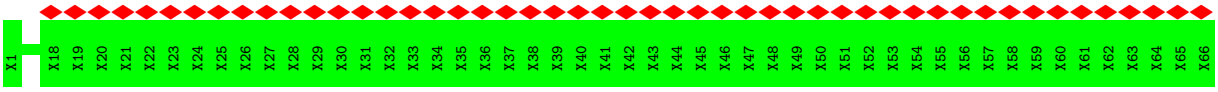
• Molecule 93: Transmembrane protein, putative



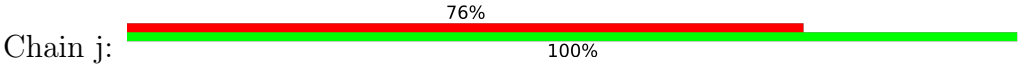


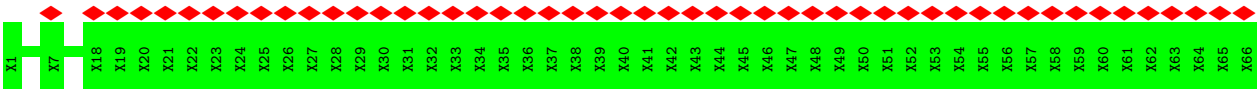
• Molecule 94: UQCRTT3



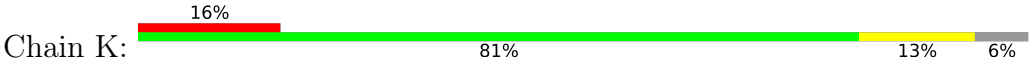


• Molecule 94: UQCRTT3



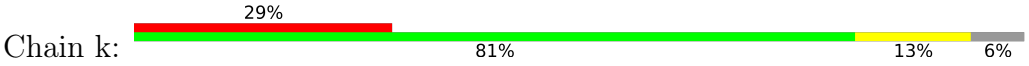


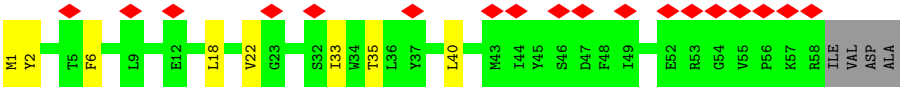
• Molecule 95: Transmembrane protein, putative





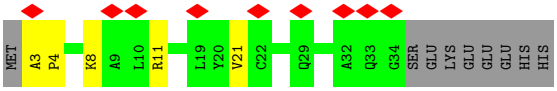
• Molecule 95: Transmembrane protein, putative





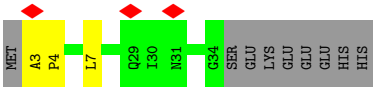
• Molecule 96: UQCRTT2



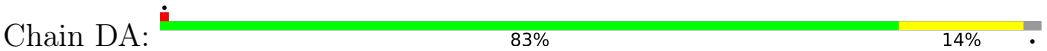


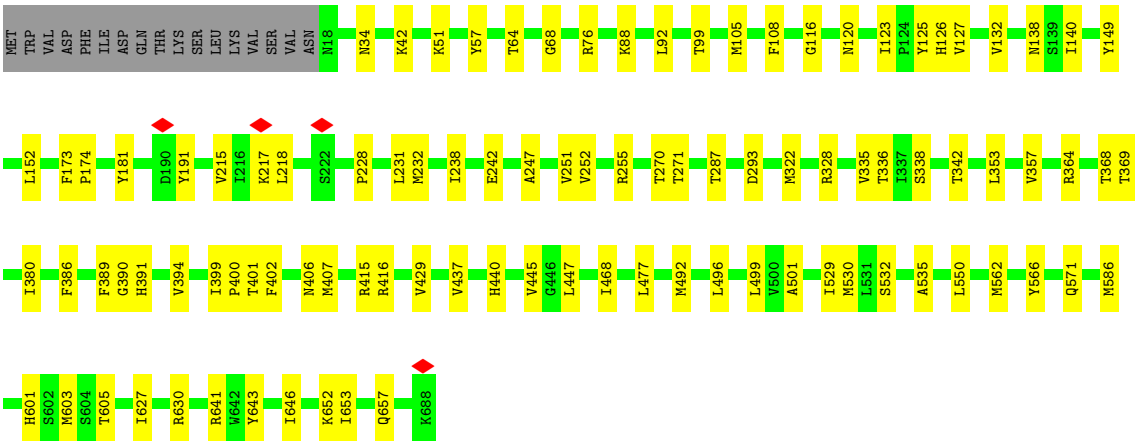
• Molecule 96: UQCRTT2



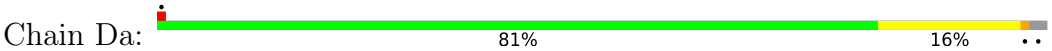


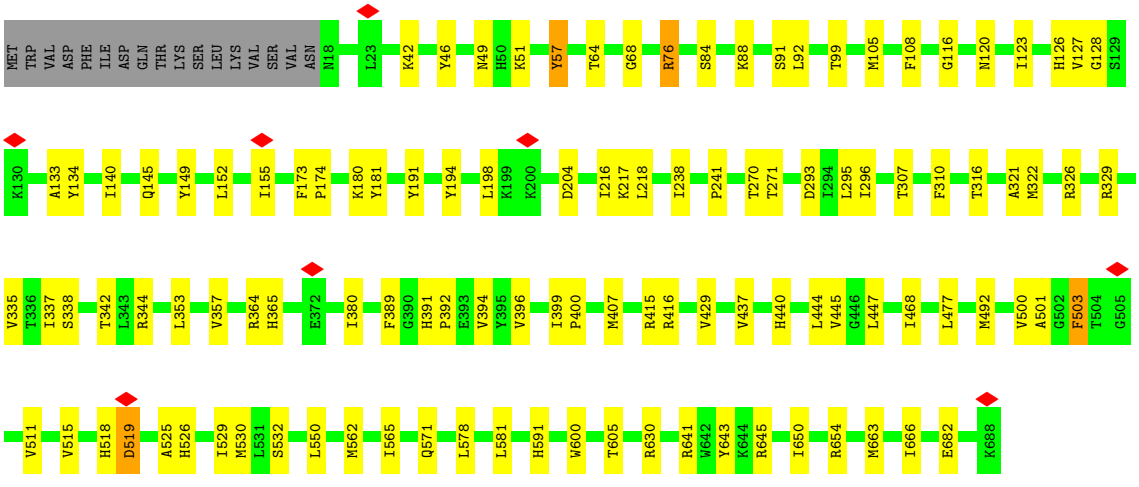
• Molecule 97: Cytochrome c oxidase subunit 1





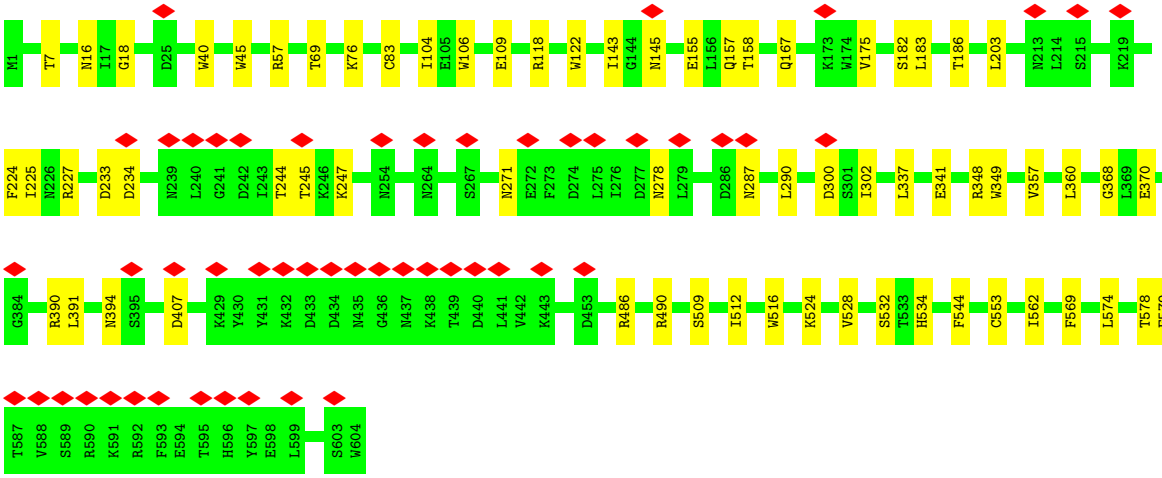
• Molecule 97: Cytochrome c oxidase subunit 1





• Molecule 98: Cytochrome c oxidase subunit 2

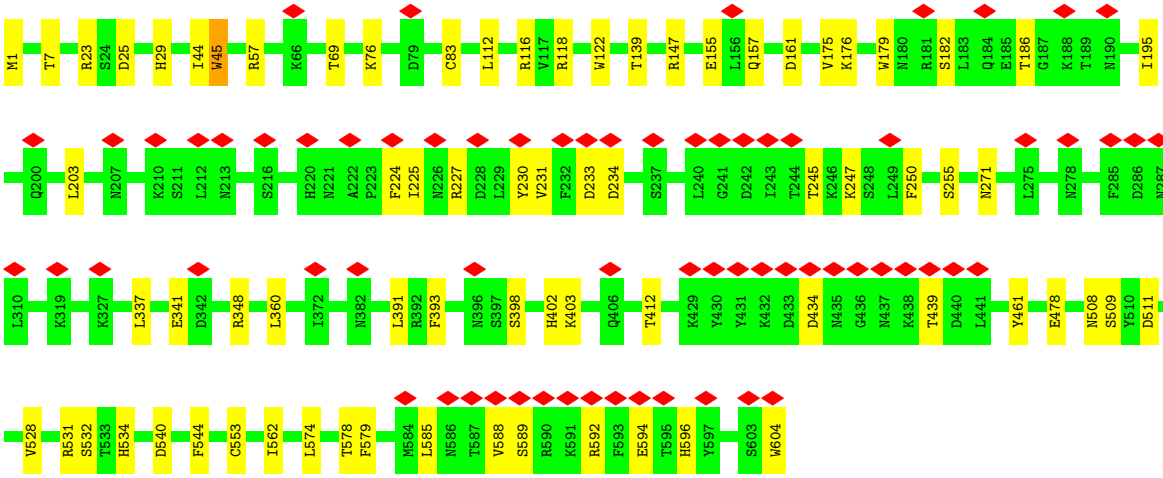




• Molecule 98: Cytochrome c oxidase subunit 2

Chain Db:

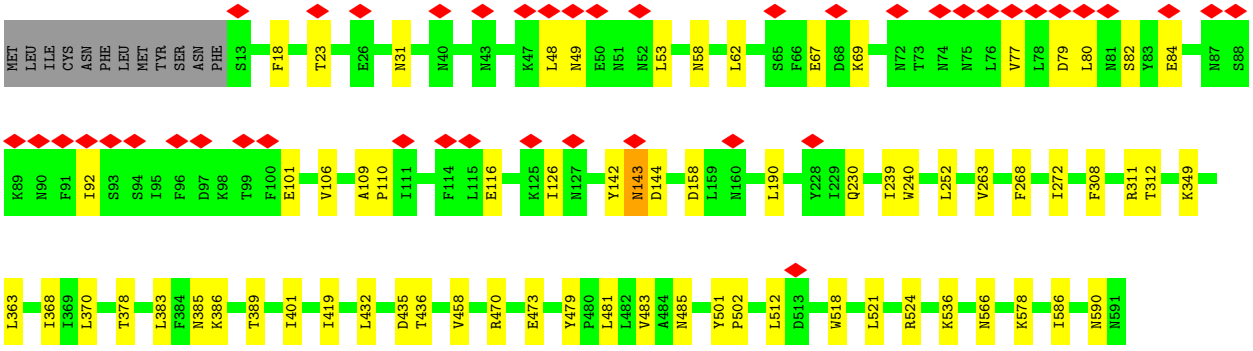




• Molecule 99: Ymf68

Chain DC:

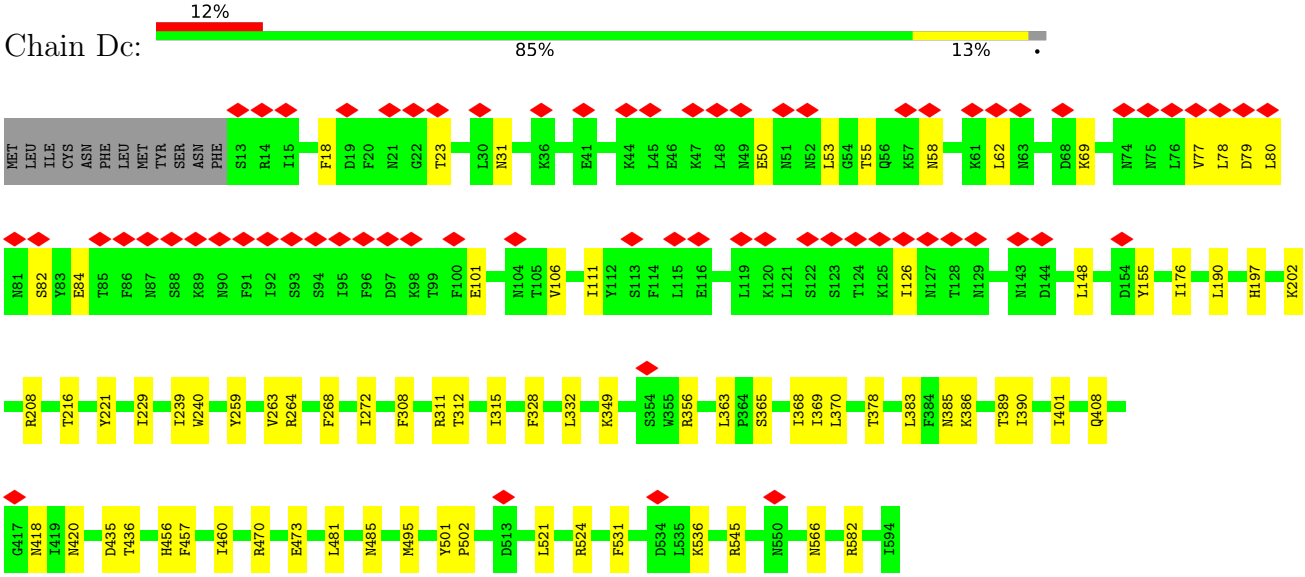






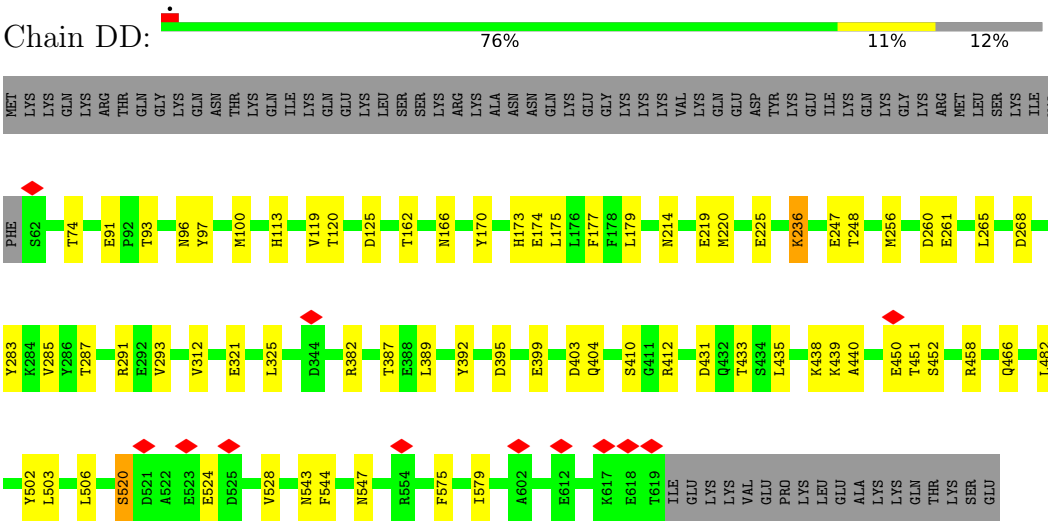
• Molecule 99: Ymf68

Chain Dc:



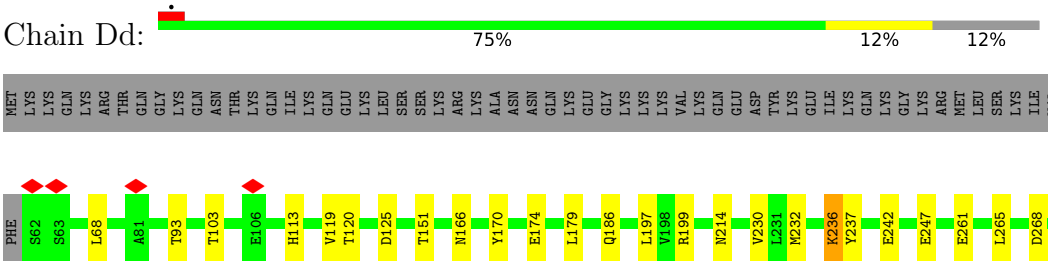
• Molecule 100: Cytochrome C oxidase subunit Vb protein

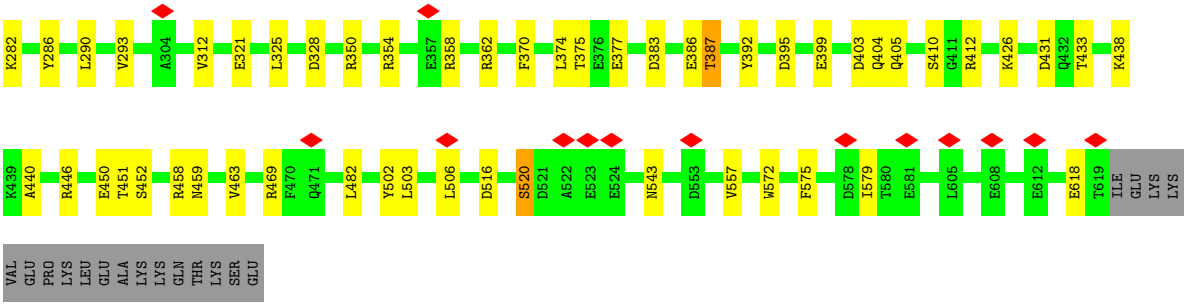
Chain DD:



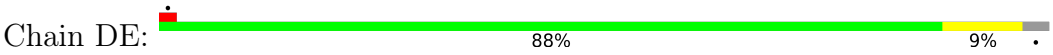
• Molecule 100: Cytochrome C oxidase subunit Vb protein

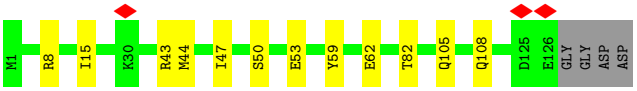
Chain Dd:



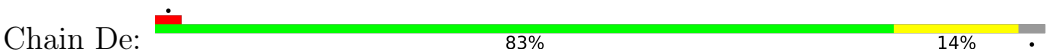


• Molecule 101: Transmembrane protein, putative



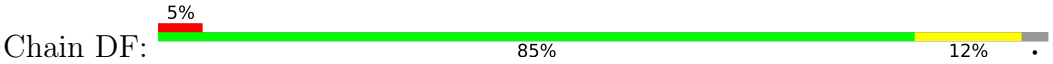


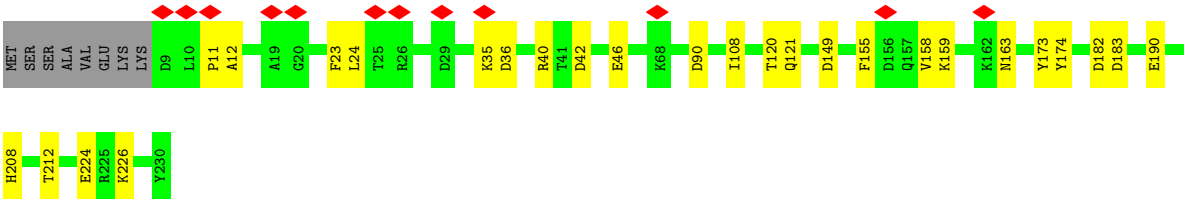
• Molecule 101: Transmembrane protein, putative



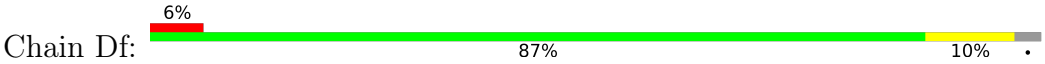


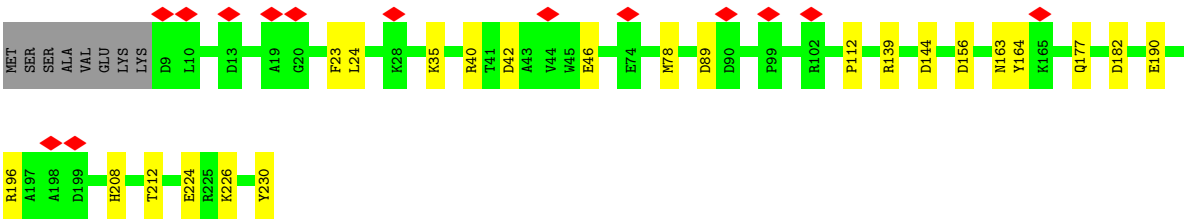
• Molecule 102: Structural protein



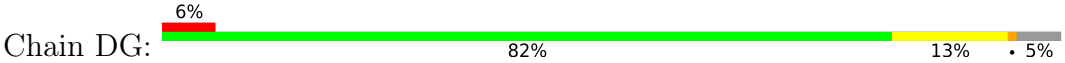


• Molecule 102: Structural protein





• Molecule 103: Transmembrane protein, putative





• Molecule 103: Transmembrane protein, putative

Chain Dg:

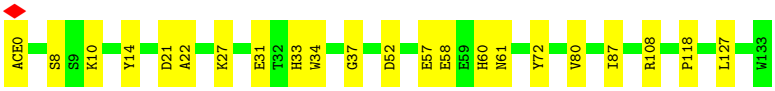




• Molecule 104: Transmembrane protein, putative

Chain DH:

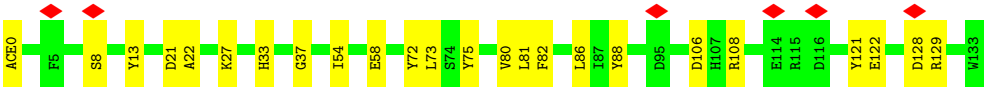




• Molecule 104: Transmembrane protein, putative

Chain Dh:

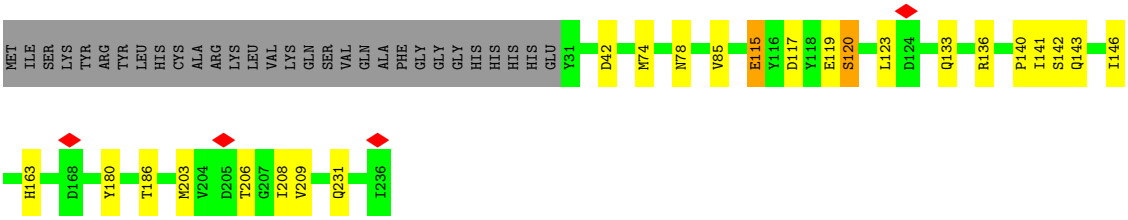




• Molecule 105: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain DI:

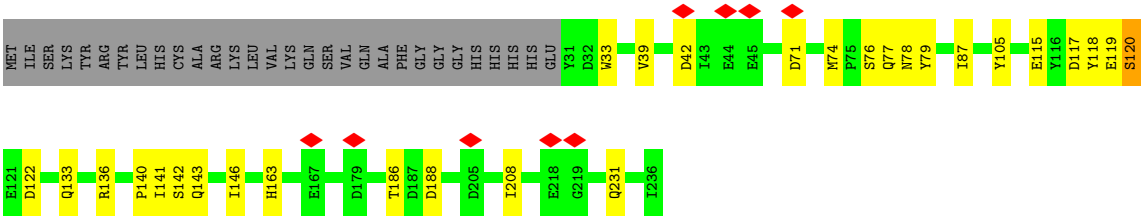




• Molecule 105: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

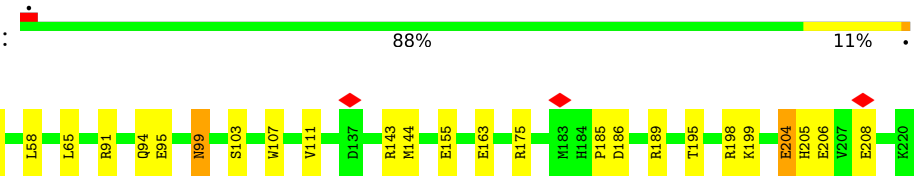
Chain Di:





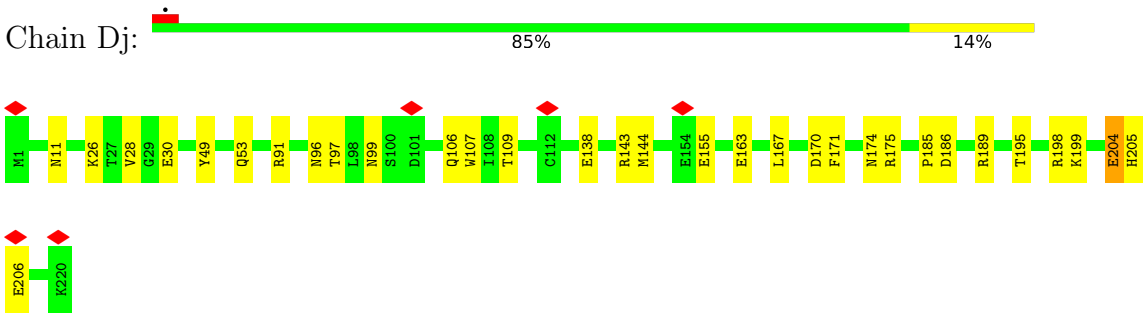
• Molecule 106: Transmembrane protein, putative

Chain DJ:



• Molecule 106: Transmembrane protein, putative

Chain Dj:



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

Chain DK:



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

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

THR LEU ILE TYR LYS GLN PHE ASN ILE GLN LYS LYS ASN ASN ASN ASN ILE ASN ASN ASN THR GLY GLN PHE PHE ILE GLU LYS ASP LYS GLN ASN ASN LEU ASN LEU SER GLN PRO HIS GLN ILE ILE LYS SER LYS GLN GLY HIS LYS ARG SER PHE THR ASN THR LEU TYR CYS SER SER ASN

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

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

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

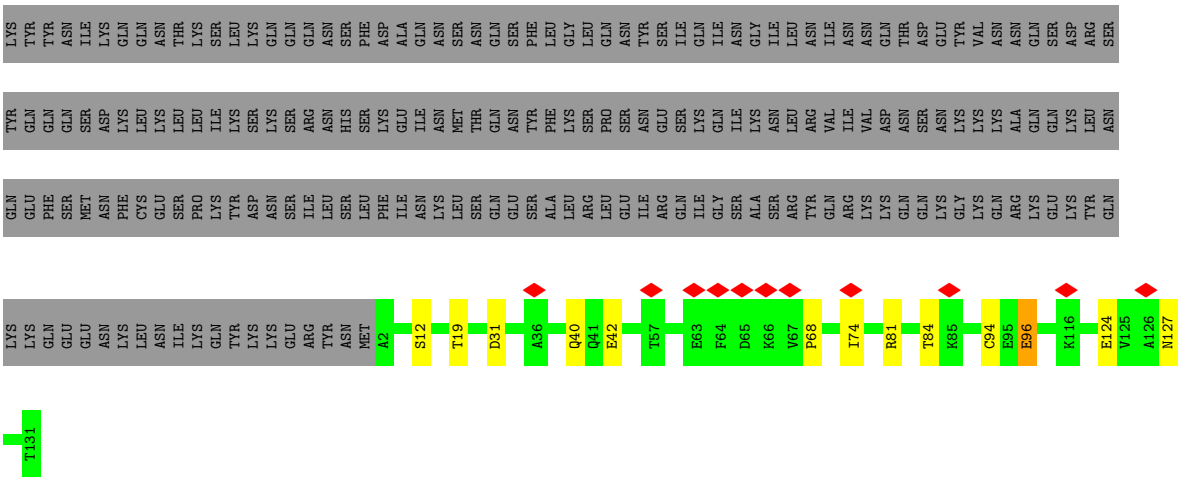
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MET ILE ASP GLY ILE LYS ALA ASP GLU GLU VAL LYS LYS ILE SER ASN ILE MET LEU LYS ASN ARG LYS TYR SER ASN TYR PRO THR LEU GLN ASN ILE ARG ILE ILE GLN GLU THR SER ASP GLY GLN PRO LEU GLN LYS THR ILE ARG LYS SER LYS ILE ILE ASN PRO GLN PHE GLN

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

LEU ASN TYR ASN LYS PHE PRO ILE GLY LEU VAL PHE LYS ASN GLN SER VAL LEU ASN PHE PRO ASN SER SER ASN GLN PRO GLN LEU VAL VAL GLY PRO TYR ALA ASN LYS ILE TYR ASN GLN GLU LEU SER SER THR TYR SER SER ARG GLN ARG ILE SER HIS GLN THR PRO ASN ARG

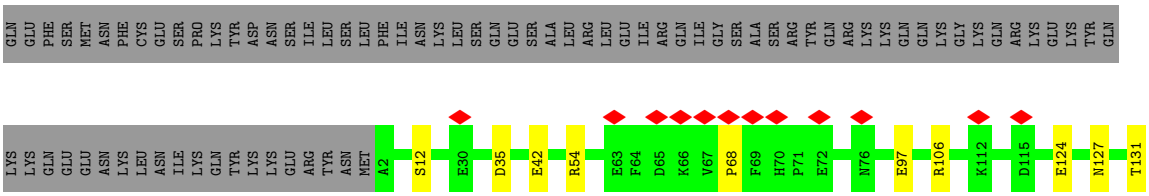
GLU PHE PHE ASN TYR HIS SER GLN LEU GLN GLN VAL LYS GLU GLN THR GLN LEU ASN GLN MET LYS GLN GLN TYR ASN GLN ILE VAL ASP SER ILE GLU LEU ALA ASN HIS LEU ILE VAL LEU LYS ASN LEU LYS LYS VAL LYS ASP LEU PHE GLN ASN LEU ILE PRO TYR LEU ASN GLU



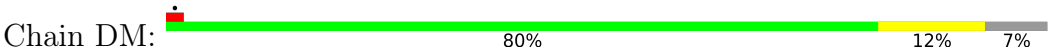
• Molecule 107: CTF/NF-I domain-containing protein

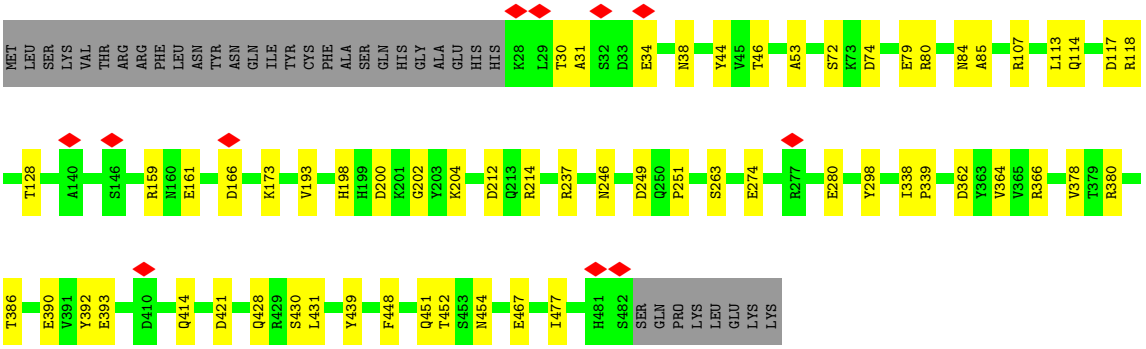
Chain Dk:



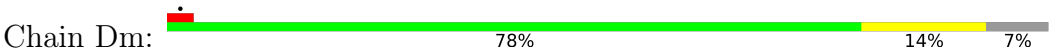


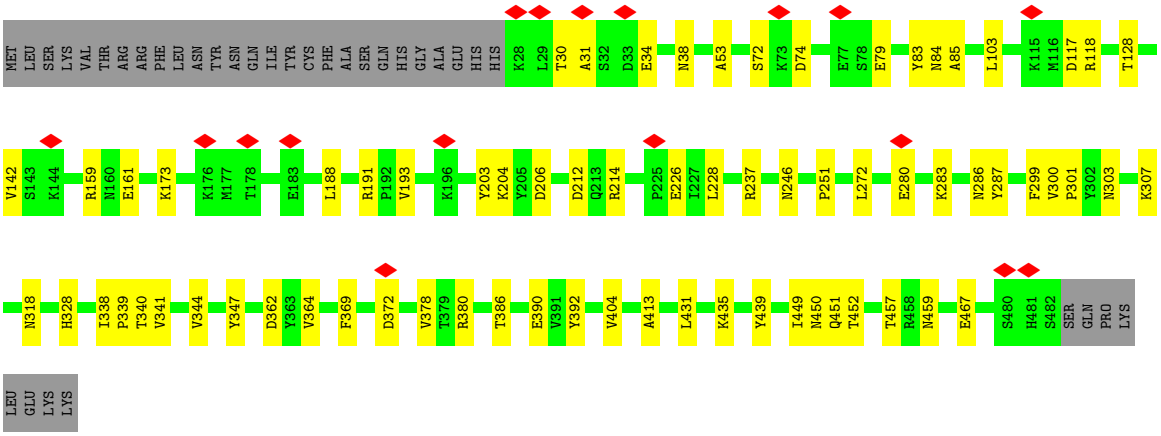
• Molecule 108: Transmembrane protein, putative



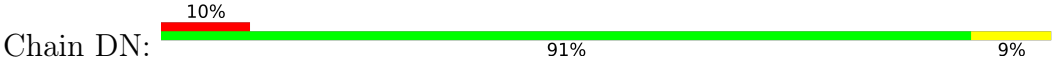


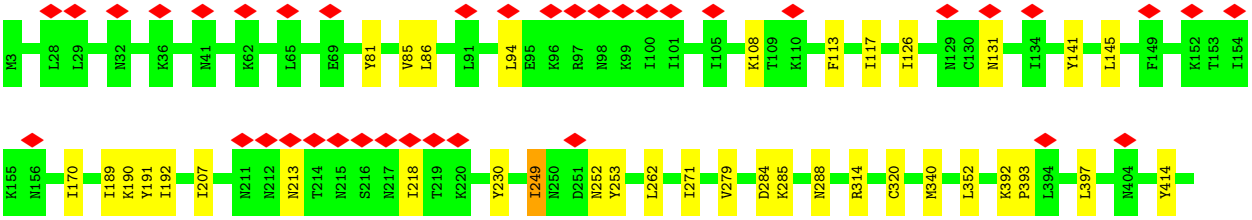
• Molecule 108: Transmembrane protein, putative

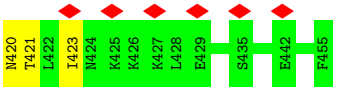




• Molecule 109: Ymf67

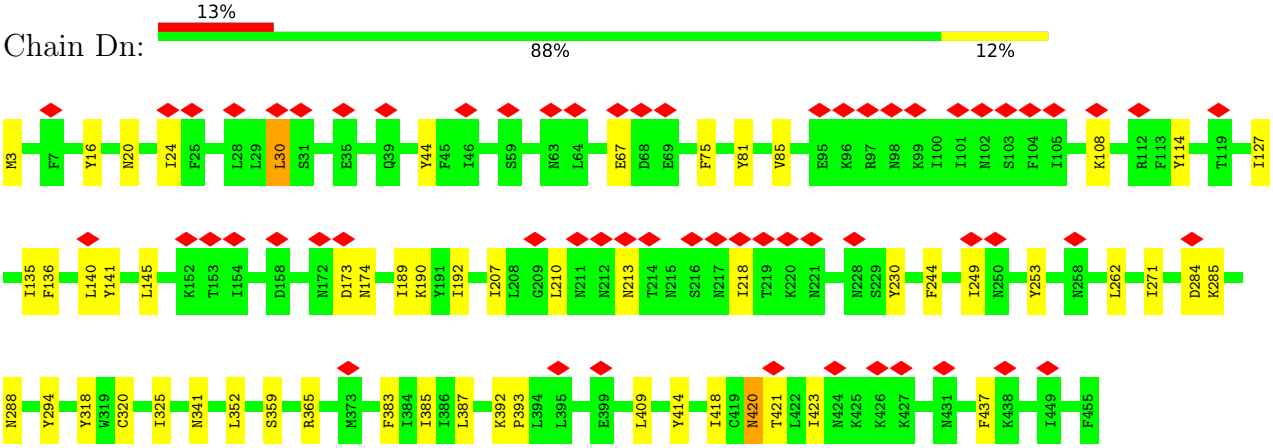






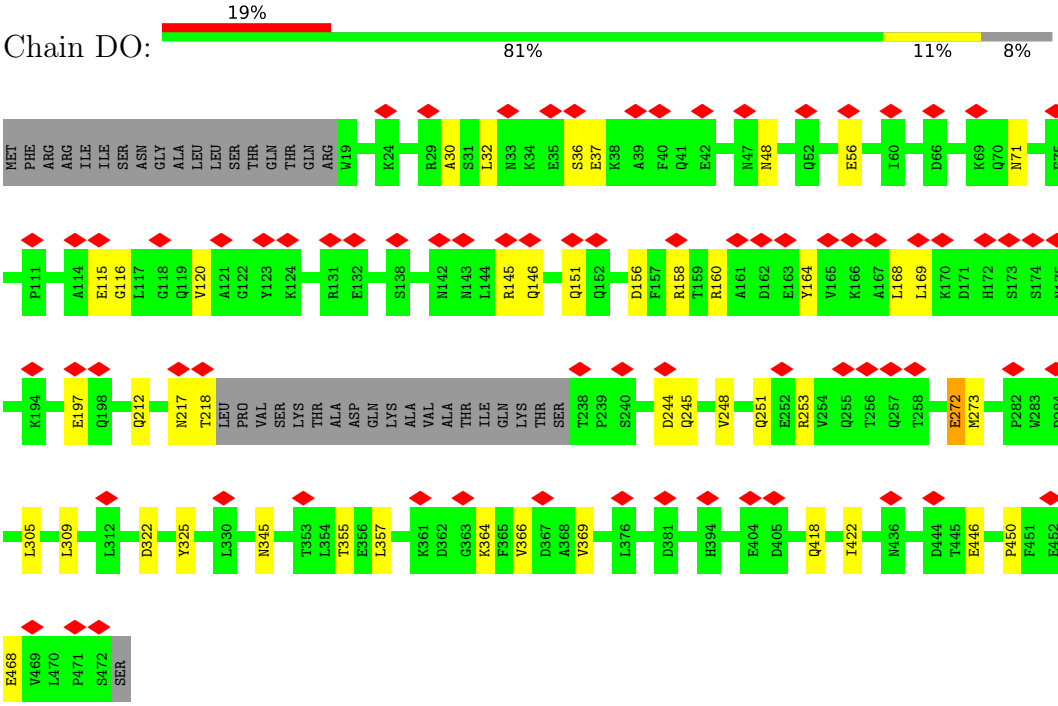
• Molecule 109: Ymf67

Chain Dn:



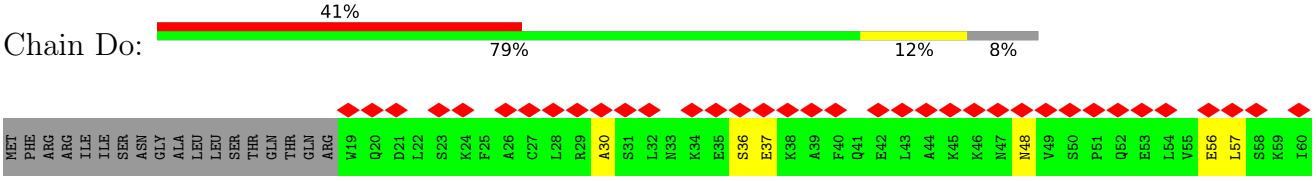
• Molecule 110: Protein phosphatase 2C, putative

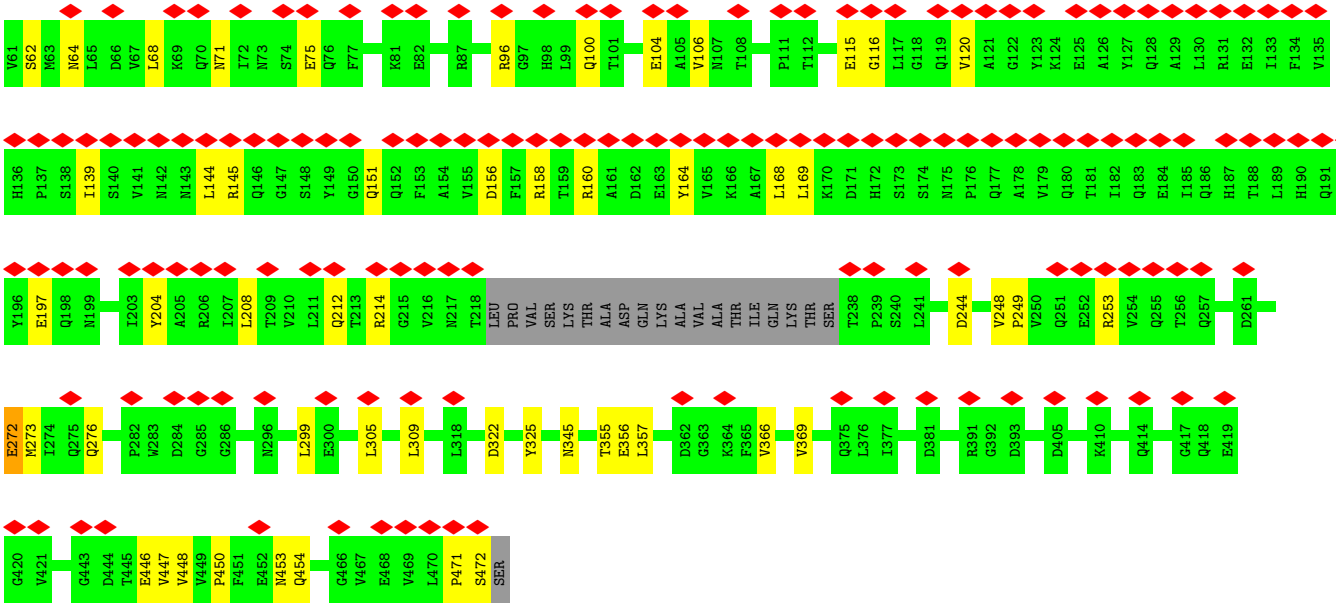
Chain DO:



• Molecule 110: Protein phosphatase 2C, putative

Chain Do:

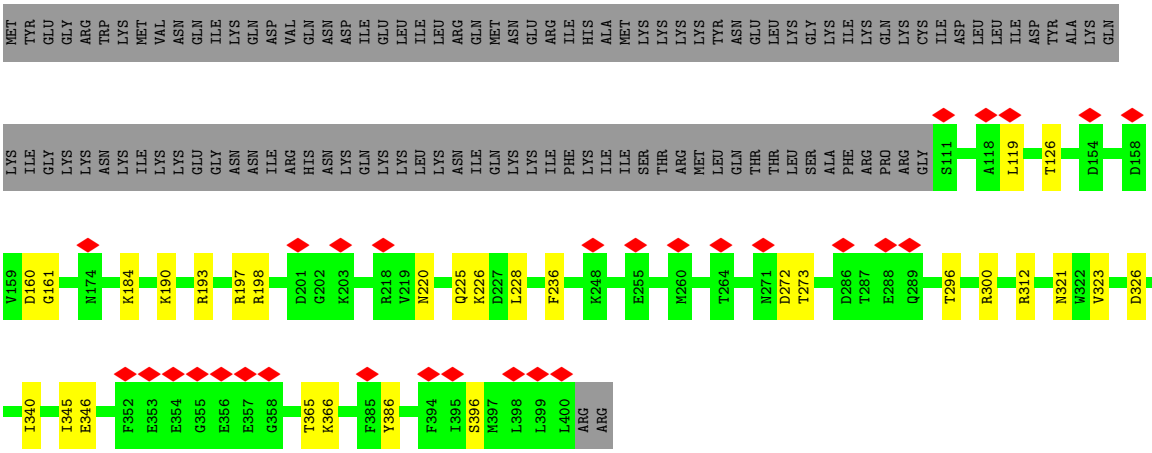




• Molecule 111: SURF1-like protein

Chain DP:

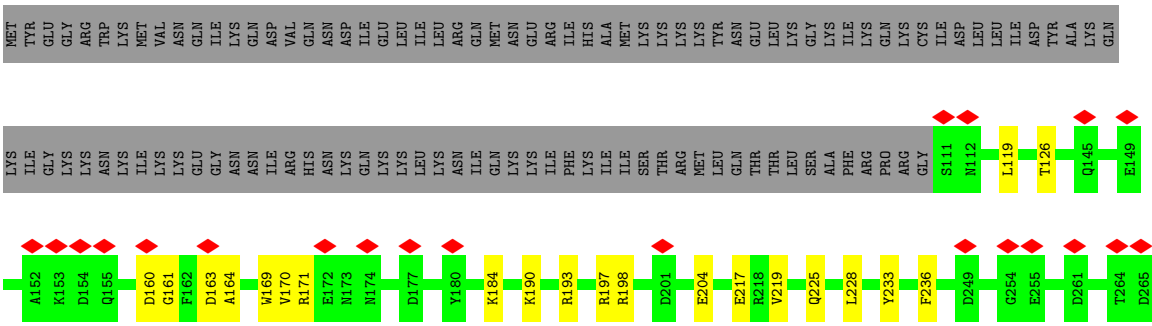


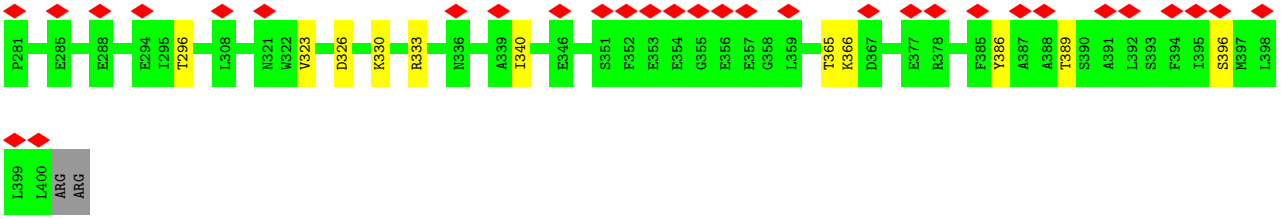


• Molecule 111: SURF1-like protein

Chain Dp:



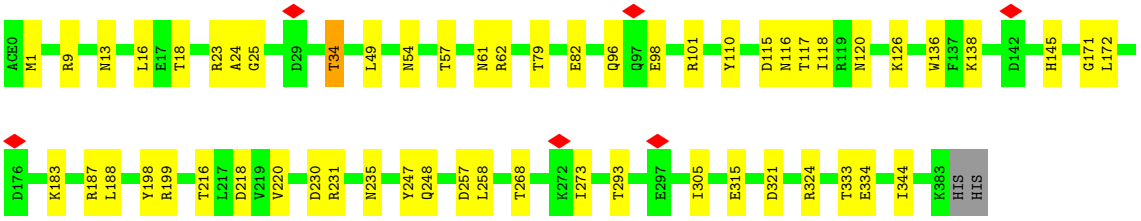




• Molecule 112: TraB family protein

Chain DQ:

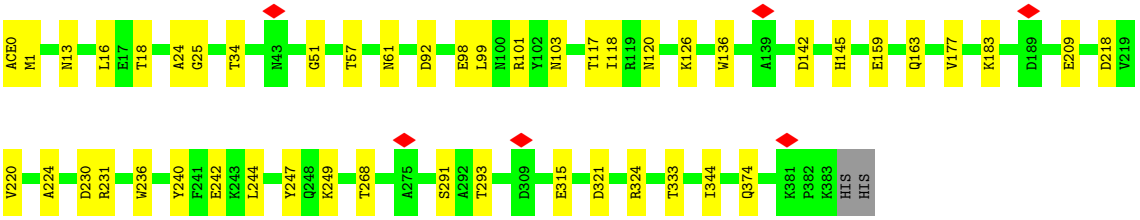




• Molecule 112: TraB family protein

Chain Dq:

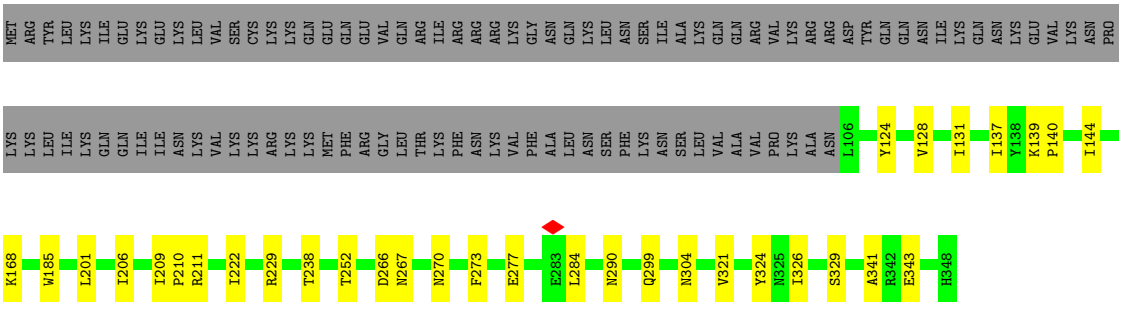




• Molecule 113: Transmembrane protein, putative

Chain DR:



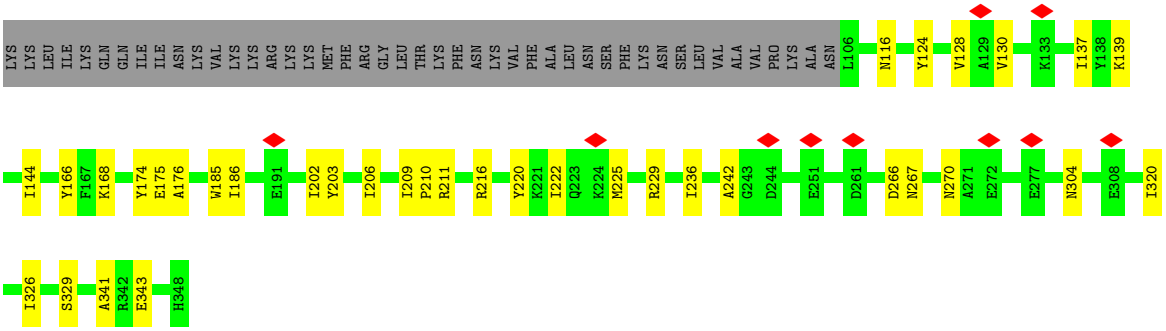


• Molecule 113: Transmembrane protein, putative

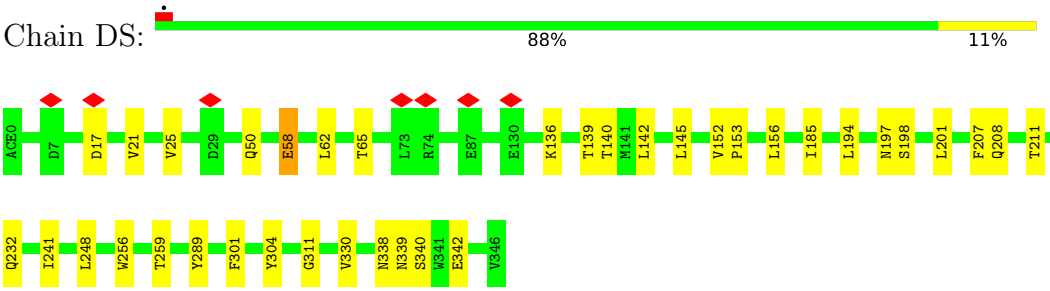
Chain Dr:



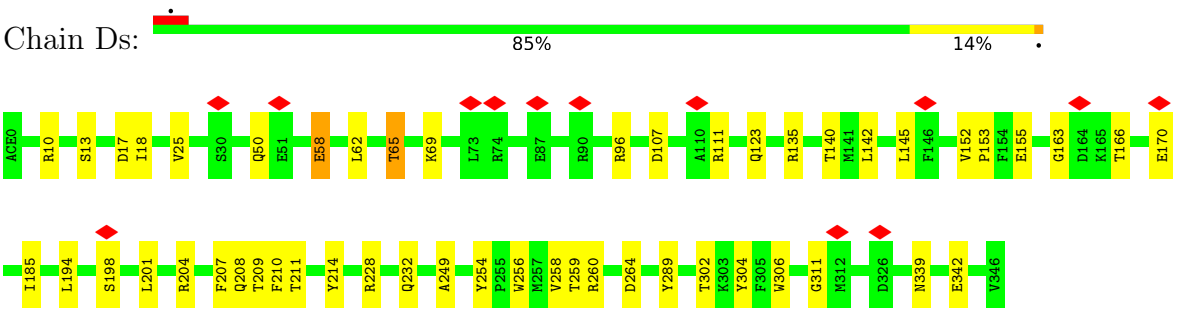




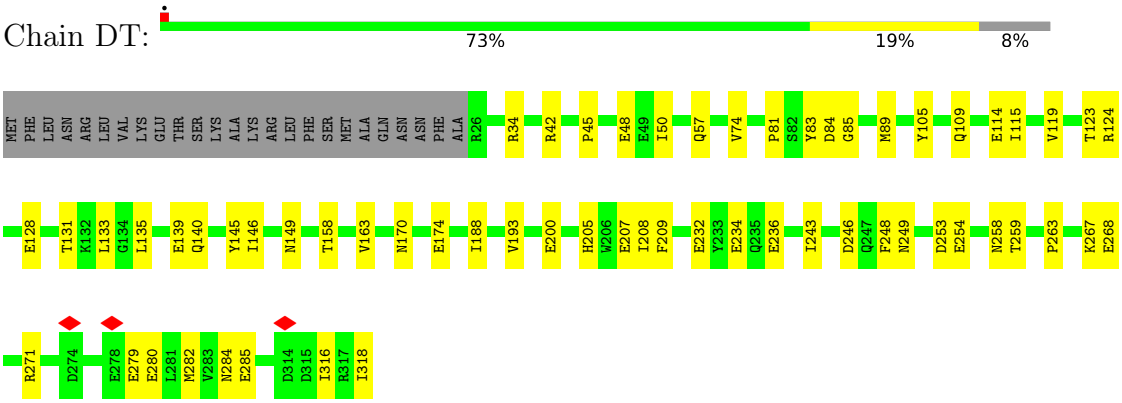
• Molecule 114: Oxoglutarate/malate translocator protein, putative



• Molecule 114: Oxoglutarate/malate translocator protein, putative

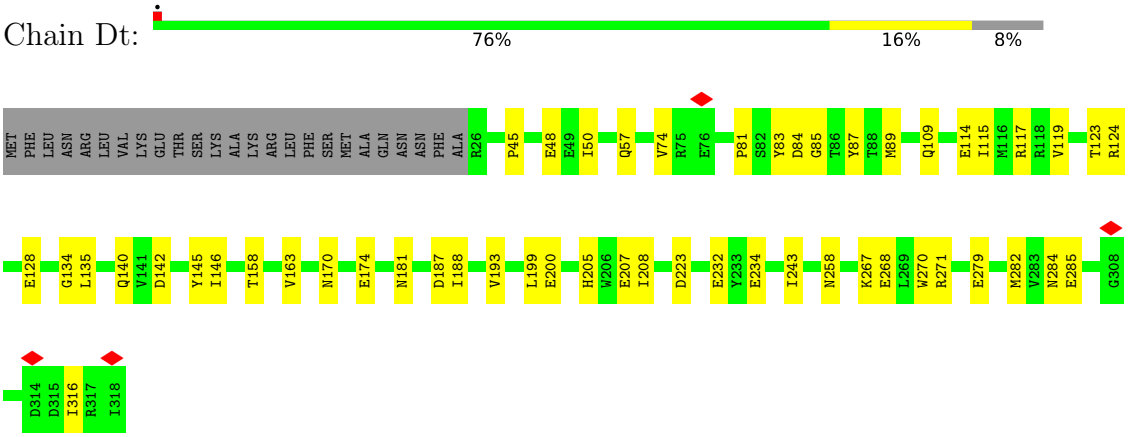


• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial



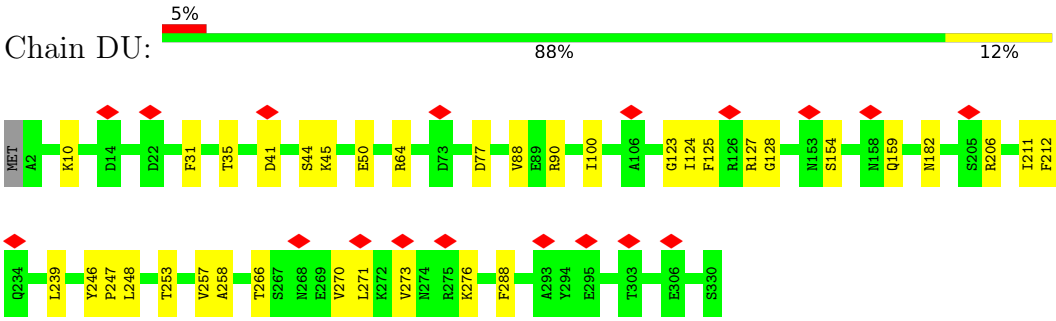
• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt:



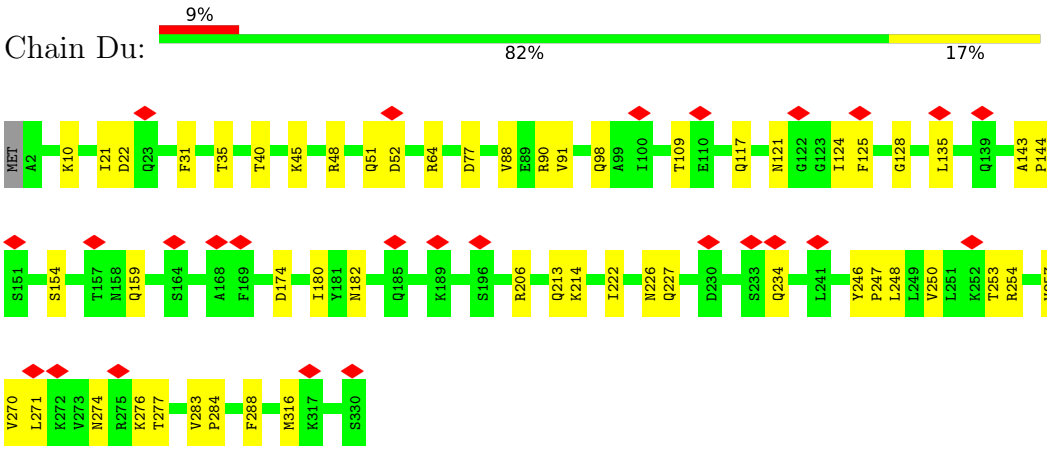
• Molecule 116: Carrier protein

Chain DU:



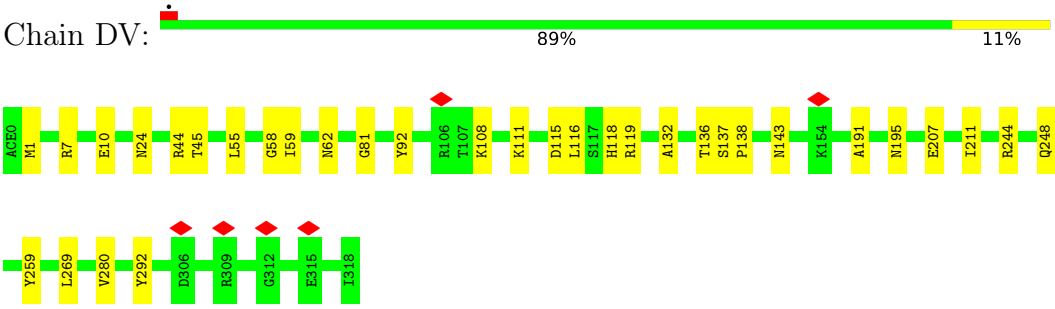
• Molecule 116: Carrier protein

Chain Du:



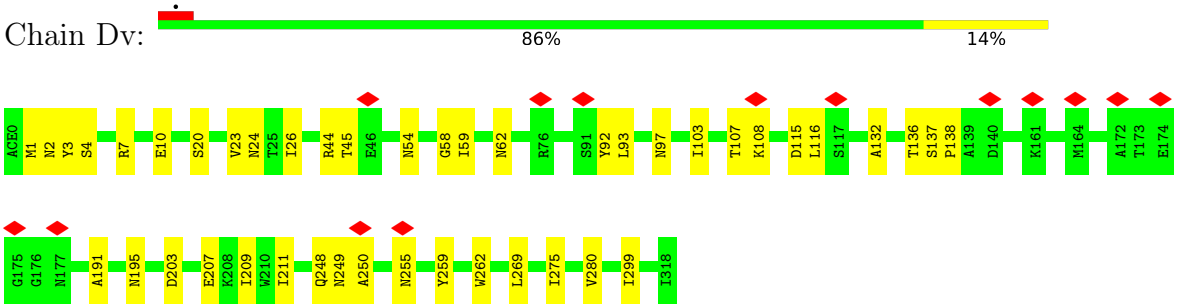
• Molecule 117: 2-oxoglutarate/malate carrier protein

Chain DV:



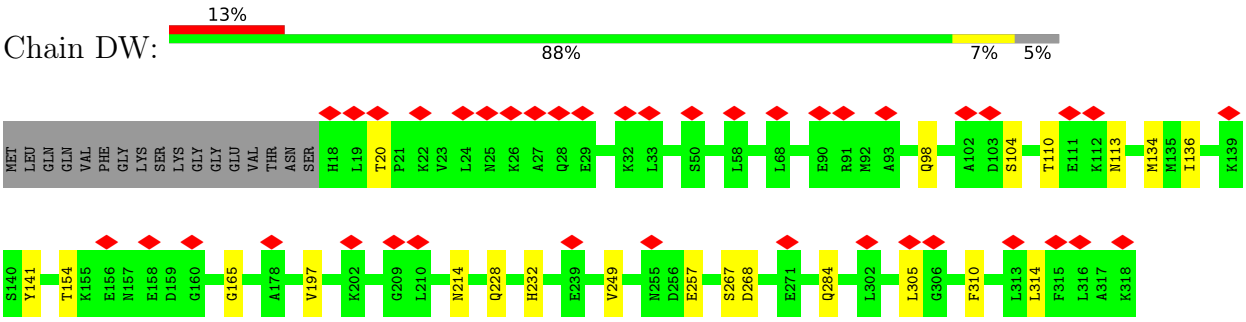
• Molecule 117: 2-oxoglutarate/malate carrier protein

Chain Dv:



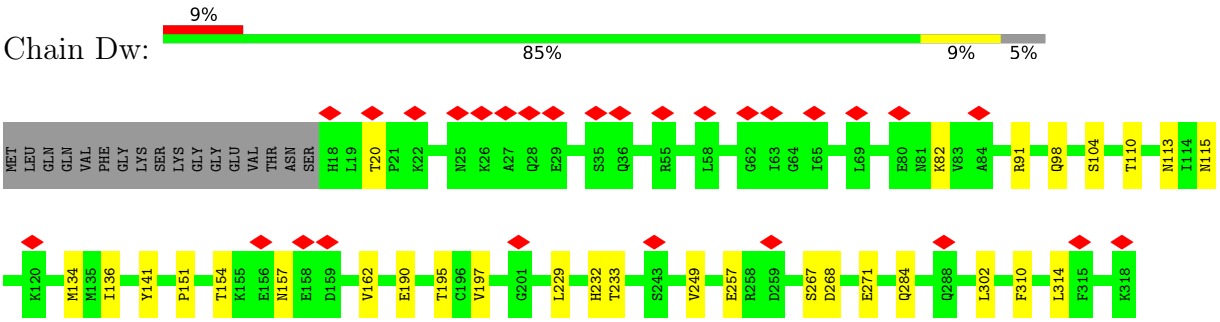
• Molecule 118: SURF1-like protein

Chain DW:



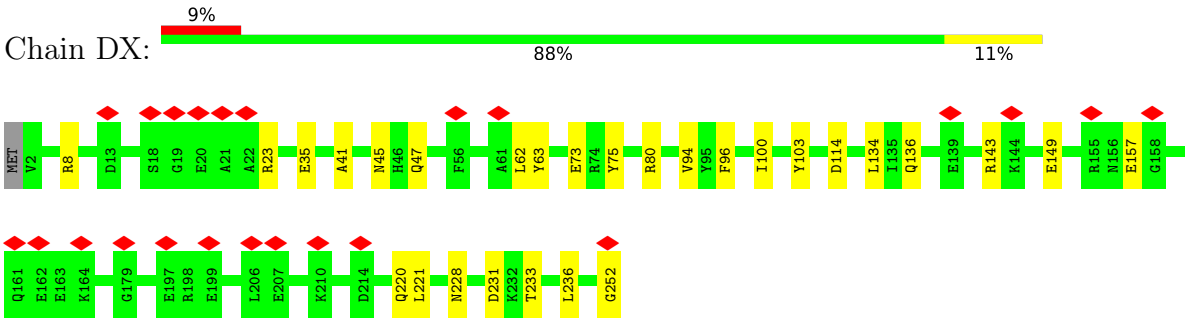
• Molecule 118: SURF1-like protein

Chain Dw:



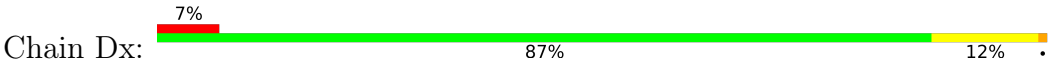
• Molecule 119: COXTT9

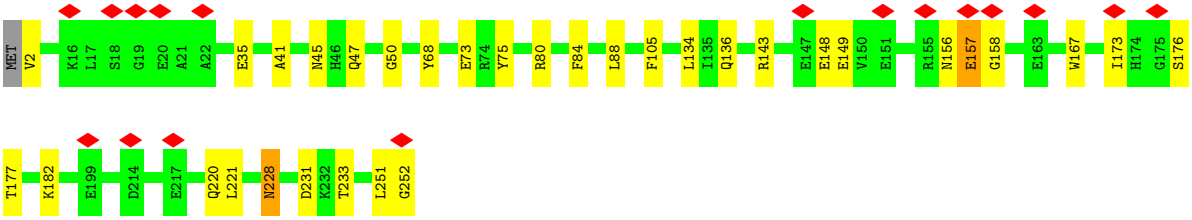
Chain DX:



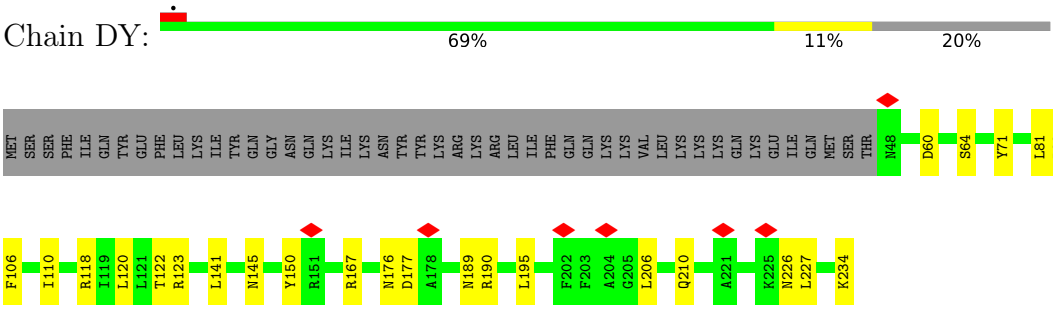
• Molecule 119: COXTT9

Chain Dx:

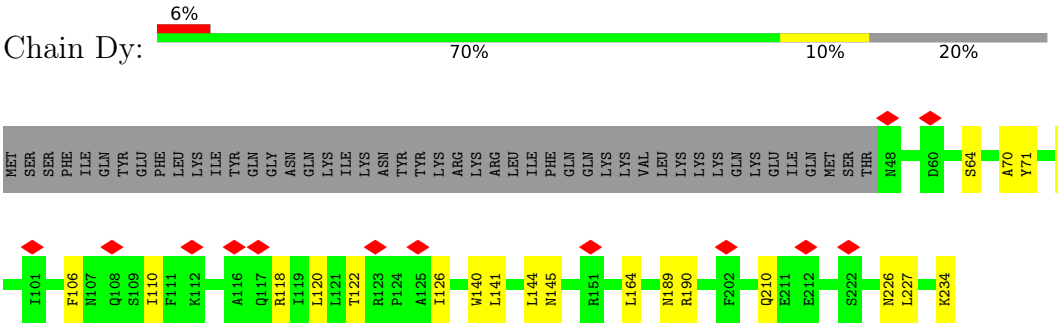




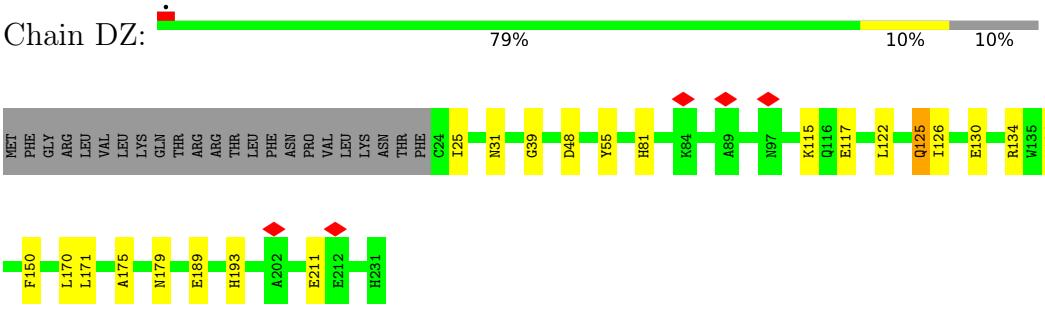
• Molecule 120: COXTT10



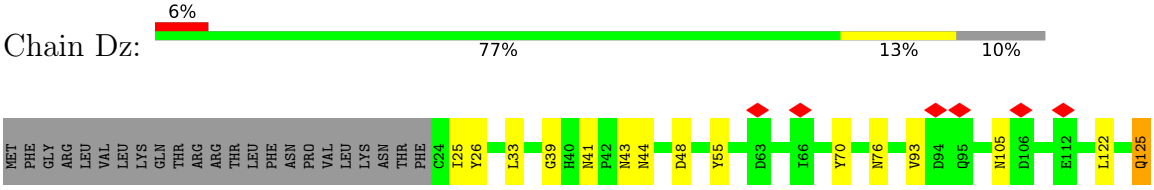
• Molecule 120: COXTT10



• Molecule 121: 39S ribosomal protein L9, mitochondrial



• Molecule 121: 39S ribosomal protein L9, mitochondrial

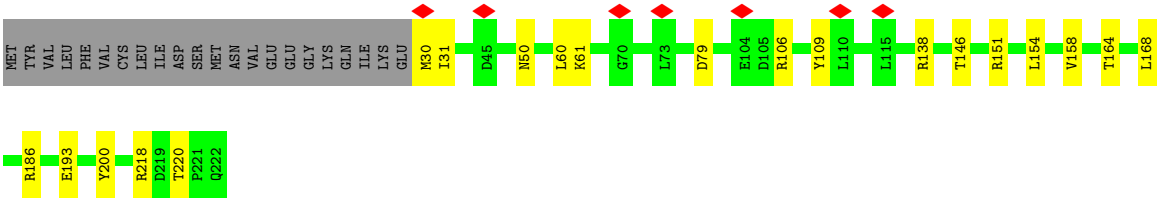




• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein,Transmembrane protein

Chain EA:

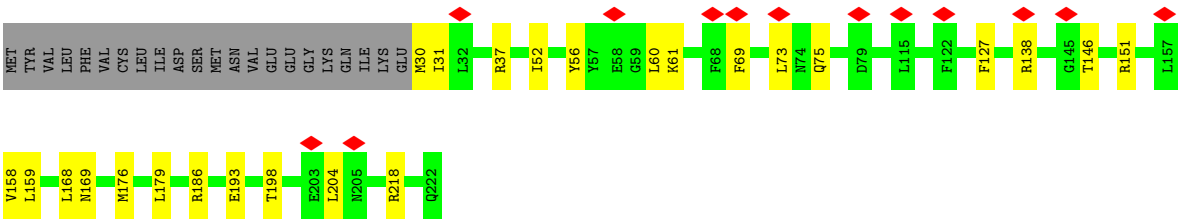




• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein,Transmembrane protein

Chain Ea:





• Molecule 123: Transmembrane protein, putative

Chain EB:

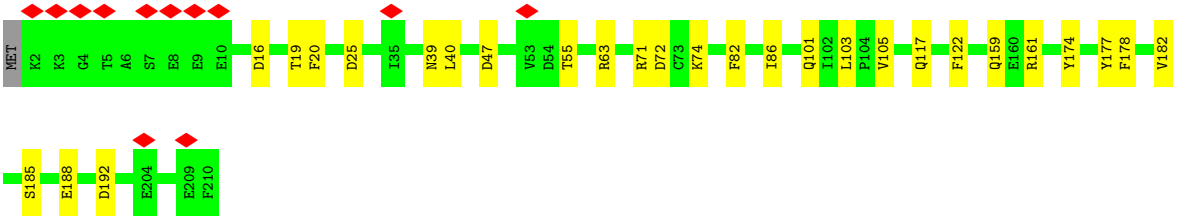




• Molecule 123: Transmembrane protein, putative

Chain Eb:

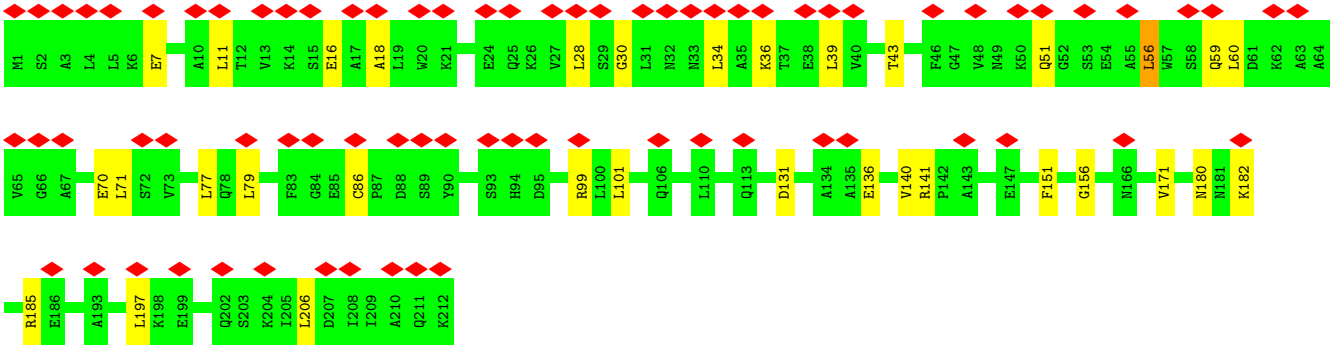




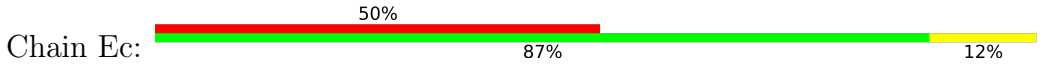
• Molecule 124: COXTT27

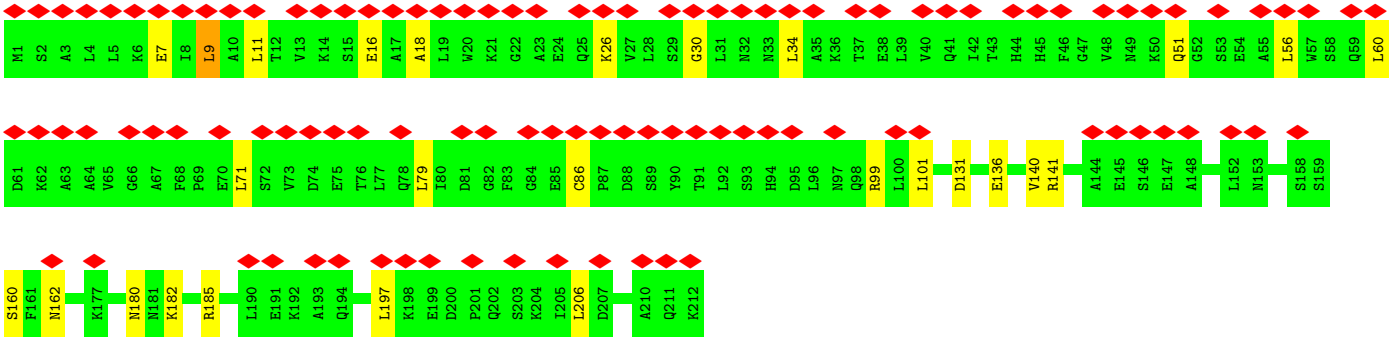
Chain EC:



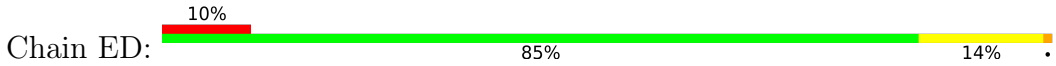


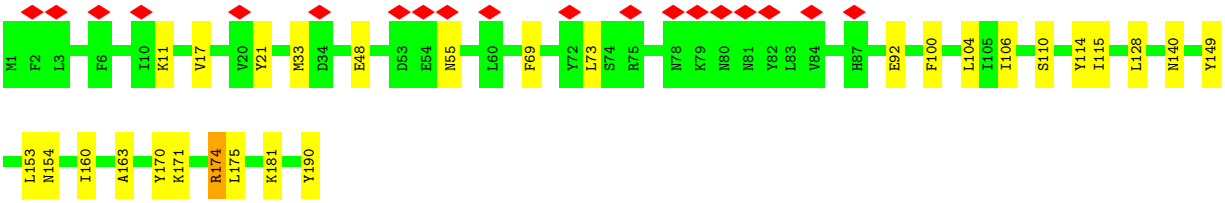
• Molecule 124: COXTT27



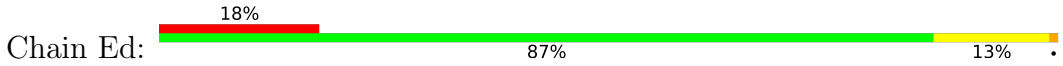


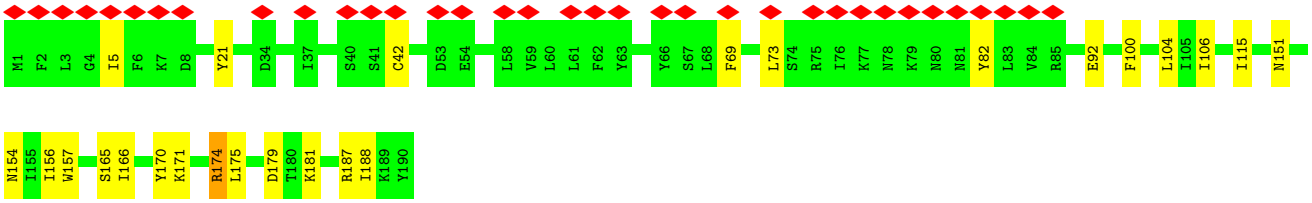
• Molecule 125: Ymf75





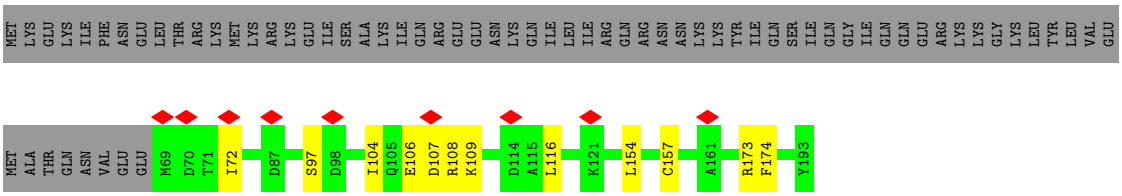
• Molecule 125: Ymf75





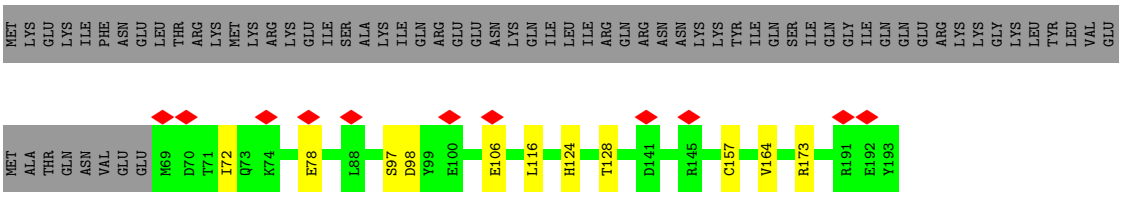
• Molecule 126: Mobilization protein



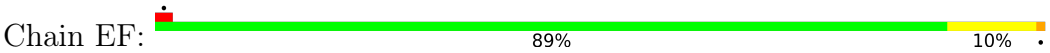


• Molecule 126: Mobilization protein



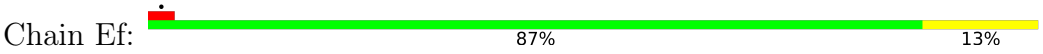


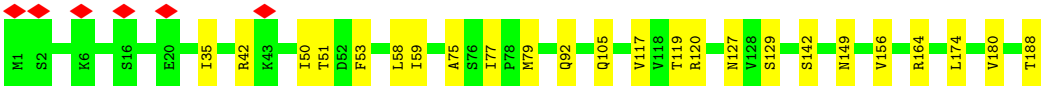
• Molecule 127: Iron-binding zinc finger CDGSH type protein



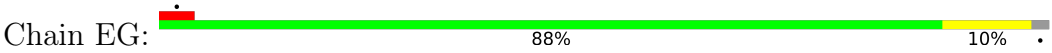


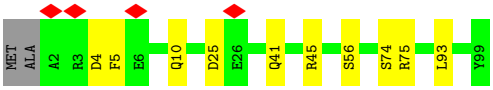
• Molecule 127: Iron-binding zinc finger CDGSH type protein



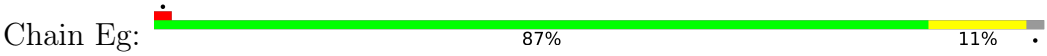


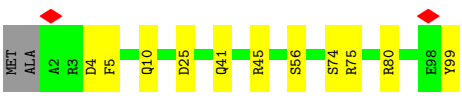
• Molecule 128: COXTT28



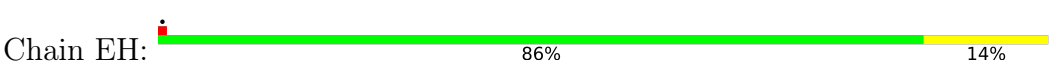


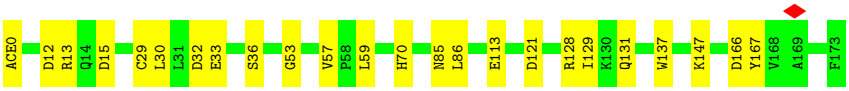
• Molecule 128: COXTT28





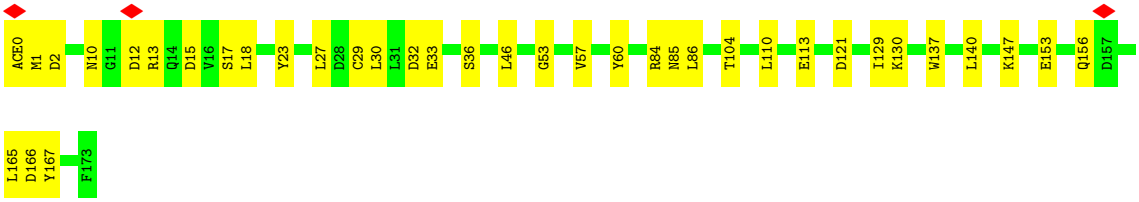
• Molecule 129: Transmembrane protein, putative



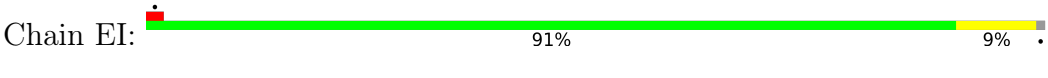


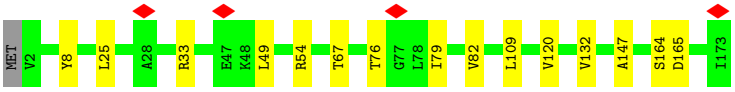
• Molecule 129: Transmembrane protein, putative



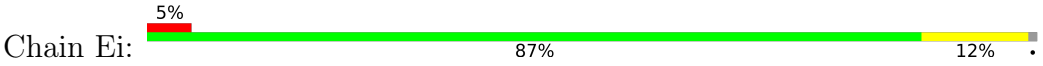


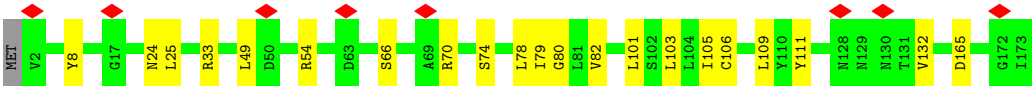
• Molecule 130: Transmembrane protein



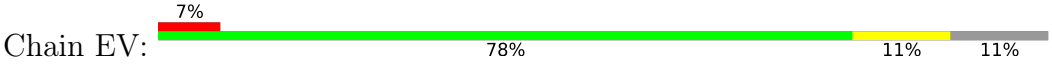


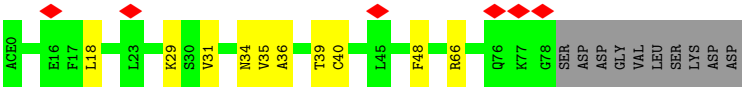
• Molecule 130: Transmembrane protein



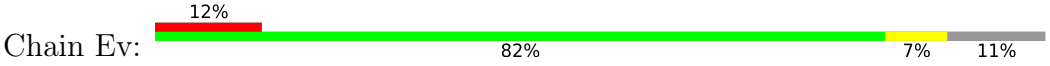


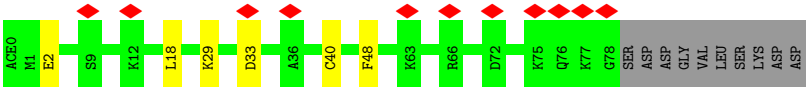
• Molecule 131: Decapping nuclease



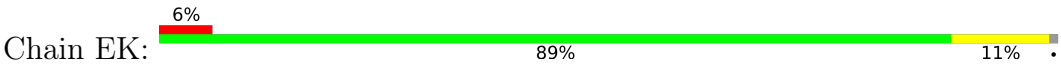


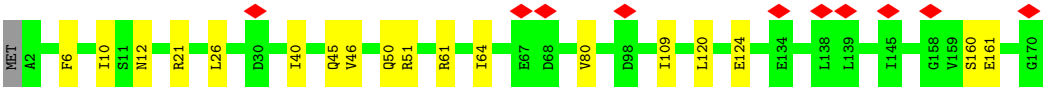
• Molecule 131: Decapping nuclease





• Molecule 132: Complex III subunit VII

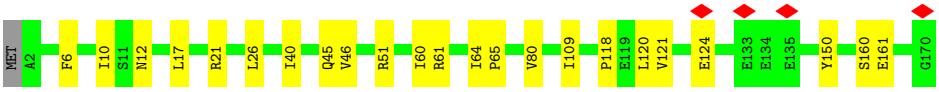




• Molecule 132: Complex III subunit VII

Chain Ek:





• Molecule 133: Transmembrane protein, putative

Chain EL:

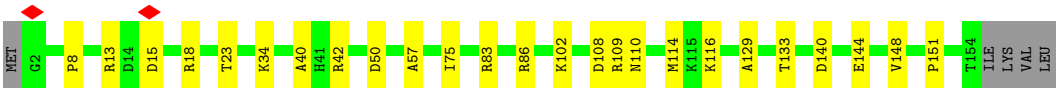




• Molecule 133: Transmembrane protein, putative

Chain El:

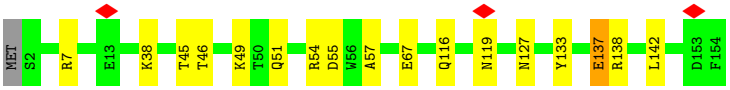




• Molecule 134: Transmembrane protein, putative

Chain EM:

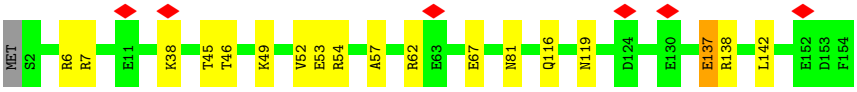




• Molecule 134: Transmembrane protein, putative

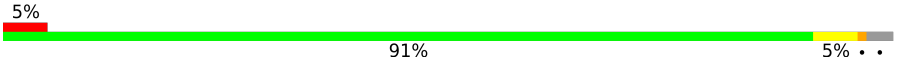
Chain Em:

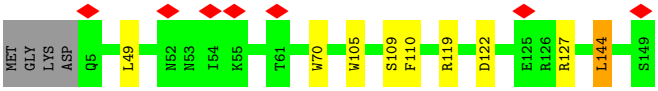




• Molecule 135: COXTT22

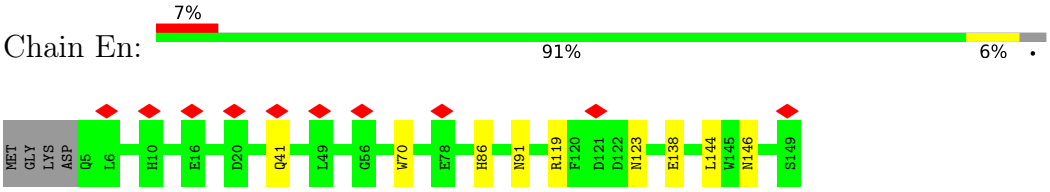
Chain EN:





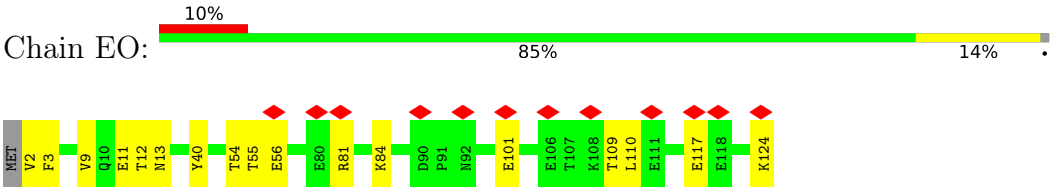
• Molecule 135: COXTT22

Chain En:



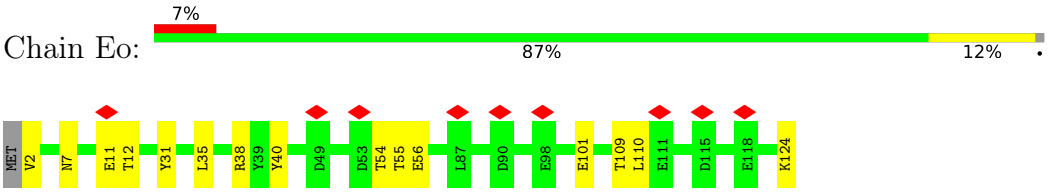
• Molecule 136: Transmembrane protein, putative

Chain EO:



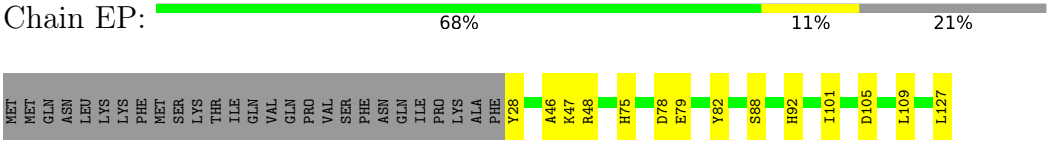
• Molecule 136: Transmembrane protein, putative

Chain Eo:



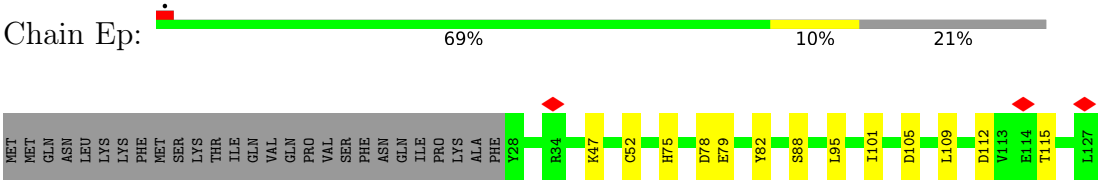
• Molecule 137: Phage protein

Chain EP:



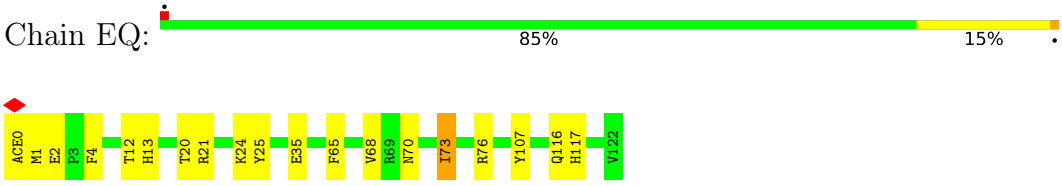
• Molecule 137: Phage protein

Chain Ep:



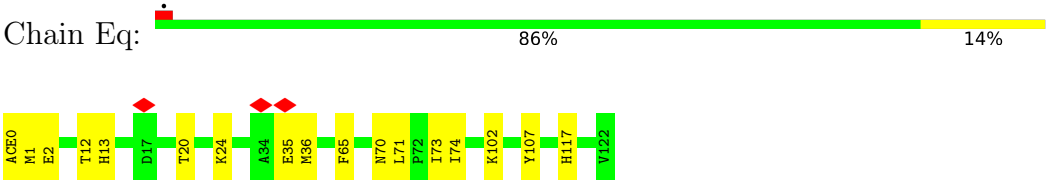
• Molecule 138: Transmembrane protein, putative

Chain EQ:



• Molecule 138: Transmembrane protein, putative

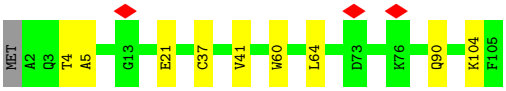
Chain Eq:



• Molecule 139: Lysozyme

Chain ER:

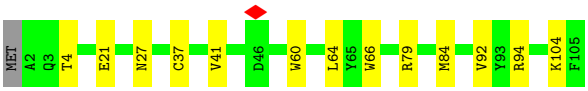




• Molecule 139: Lysozyme

Chain Er:





• Molecule 140: Ymf70

Chain ES:

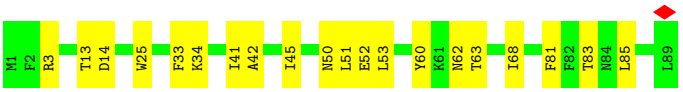




• Molecule 140: Ymf70

Chain Es:

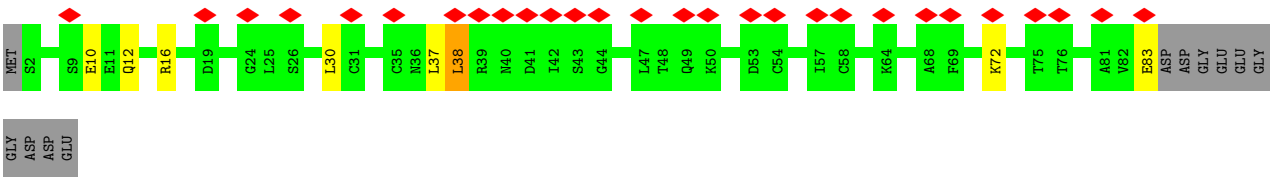




• Molecule 141: Zf-Tim10_DDP domain-containing protein

Chain ET:

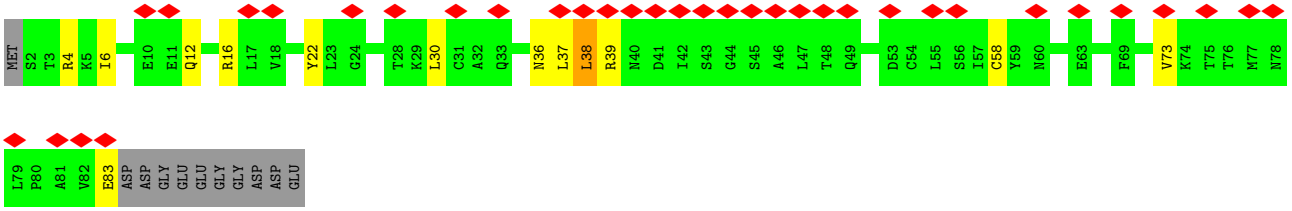




• Molecule 141: Zf-Tim10_DDP domain-containing protein

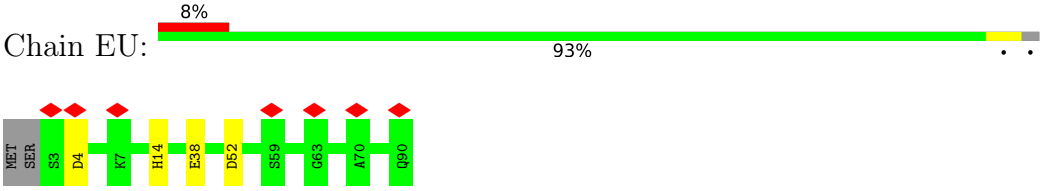
Chain Et:





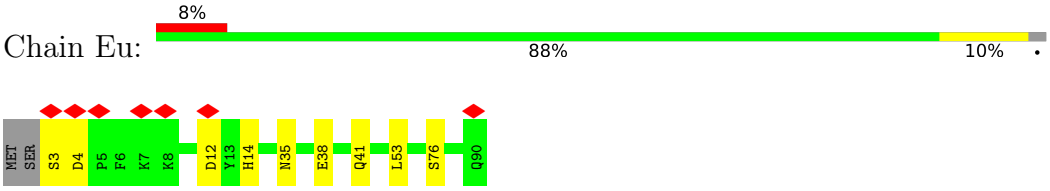
• Molecule 142: ABC transporter

Chain EU:



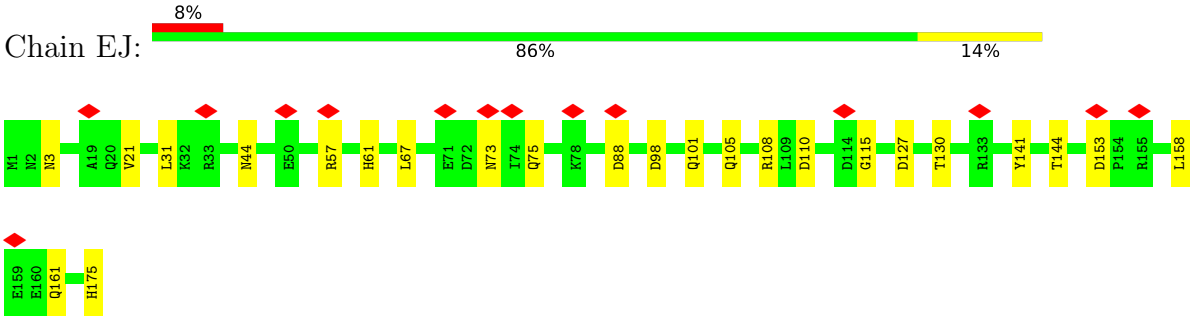
• Molecule 142: ABC transporter

Chain Eu:



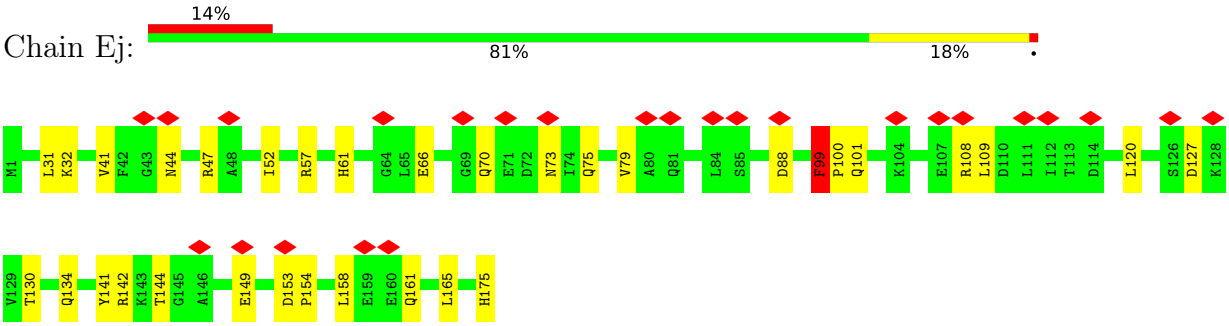
• Molecule 143: YflT domain-containing protein

Chain EJ:



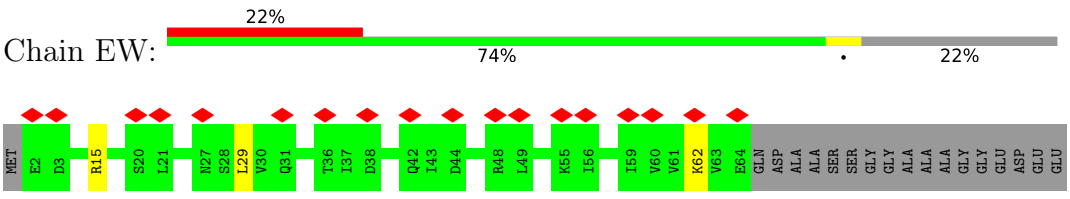
• Molecule 143: YflT domain-containing protein

Chain Ej:



• Molecule 144: Cullin domain-containing protein

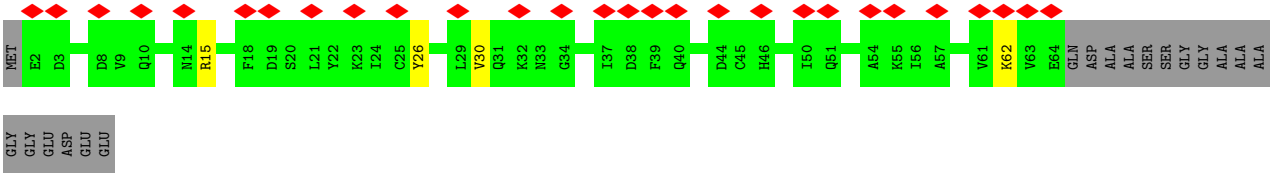
Chain EW:



• Molecule 144: Cullin domain-containing protein

Chain Ew:

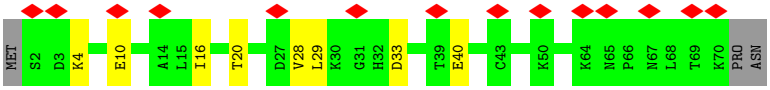




• Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain EX:

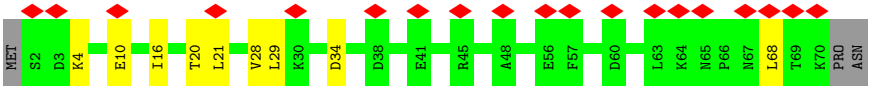




• Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain Ex:

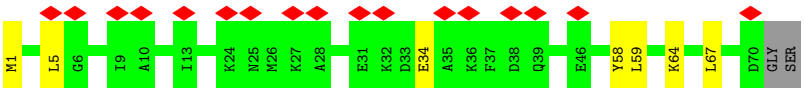




• Molecule 146: Annexin

Chain EY:

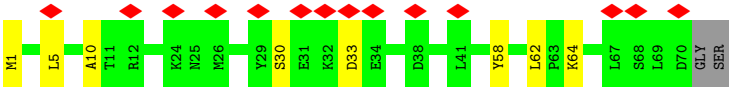




• Molecule 146: Annexin

Chain Ey:

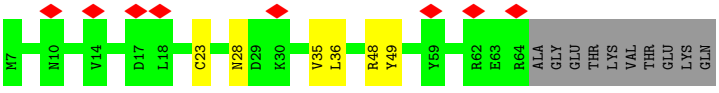




• Molecule 147: Transposase

Chain EZ:

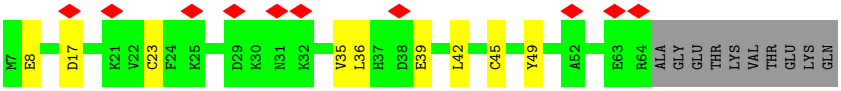




• Molecule 147: Transposase

Chain Ez:

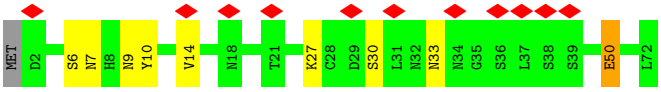




• Molecule 148: Tim10/DDP family zinc finger protein

Chain FA:

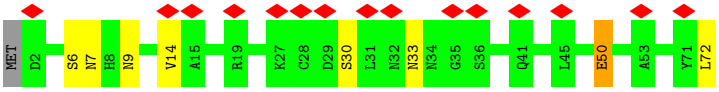




• Molecule 148: Tim10/DDP family zinc finger protein

Chain Fa:

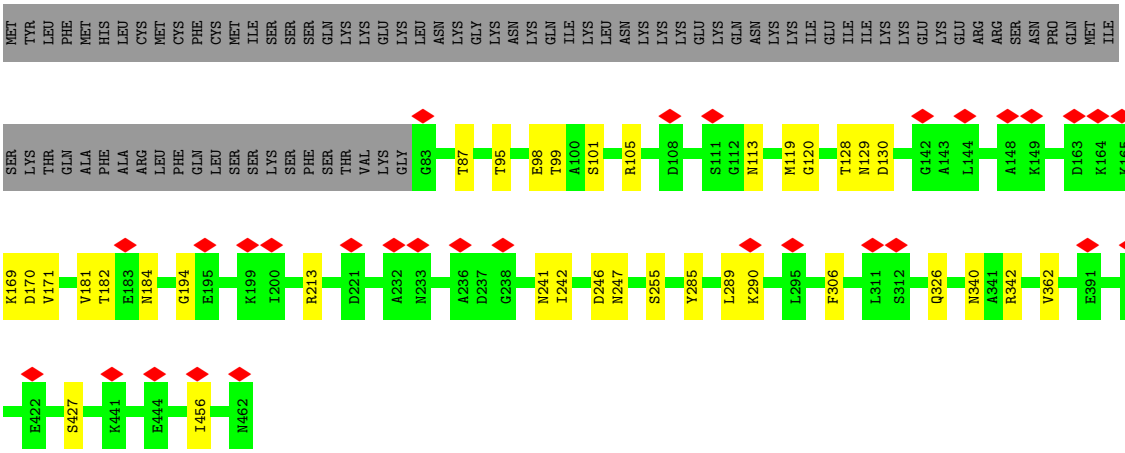




• Molecule 149: Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150

Chain Dl:

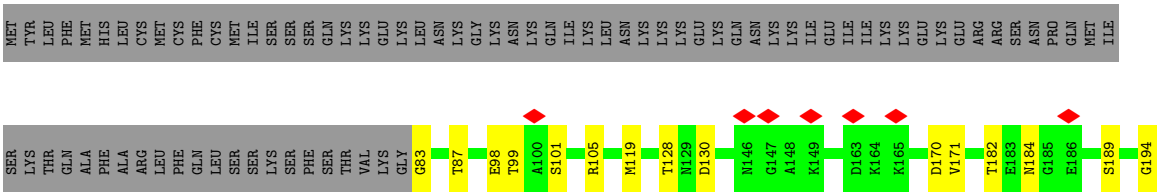


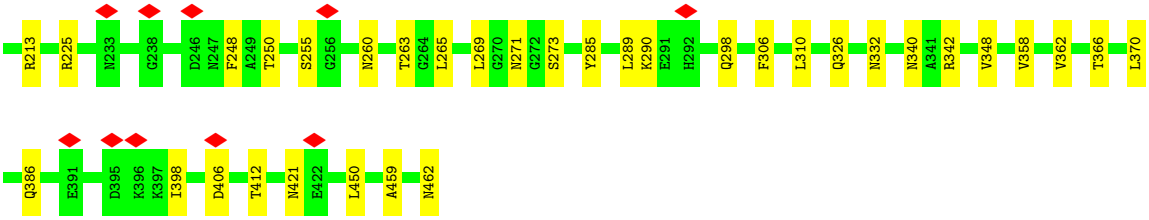


• Molecule 149: Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150

Chain DL:






R213
R225
N233
G238
D246
N247
F248
A249
T250
S255
G256
N260
T263
G264
L265
L269
G270
N271
G272
S273
Y285
L289
K290
E291
H292
Q298
F306
L310
Q326
N332
N340
A341
R342
V348
V358
V362
T366
L370

Q386
E391
D395
K396
K397
T398
D406
T412
N421
E422
L450
A459
N462

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	6.348	Depositor
Minimum map value	-3.280	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.240	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.09	0/4166	0.23	0/5634
2	A1	0.08	0/2789	0.24	0/3777
3	A2	0.09	0/2248	0.20	0/3027
4	A3	0.07	0/2308	0.19	0/3134
5	A4	0.07	0/2542	0.20	0/3441
6	A5	0.07	0/2408	0.20	0/3269
7	A6	0.09	0/1963	0.21	0/2658
8	A7	0.09	0/1108	0.22	0/1488
9	A8	0.07	0/1833	0.20	0/2479
10	A9	0.09	0/1935	0.22	0/2616
11	AA	0.10	0/6132	0.23	0/8343
12	AB	0.08	0/5511	0.21	0/7465
13	AC	0.12	0/4303	0.26	0/5844
14	AD	0.10	0/3474	0.24	0/4699
15	AE	0.09	0/3669	0.23	0/4955
16	AF	0.11	0/3168	0.24	0/4307
17	AG	0.08	0/2865	0.21	0/3877
18	AH	0.11	0/2377	0.23	0/3234
19	AI	0.08	0/1899	0.19	0/2563
20	AJ	0.11	0/2224	0.23	0/3025
21	AK	0.10	0/1816	0.24	0/2475
22	AL	0.10	0/1867	0.23	0/2538
23	AM	0.08	0/1801	0.22	0/2449
24	AN	0.10	0/1351	0.22	0/1817
25	AO	0.07	0/1720	0.23	0/2322
26	AP	0.08	0/1654	0.20	0/2240
27	AQ	0.09	0/1636	0.21	0/2214
28	AR	0.07	0/1535	0.22	0/2077
29	AS	0.08	0/1458	0.22	0/1965
30	AT	0.10	0/1310	0.25	0/1779
31	AU	0.11	0/1261	0.20	0/1698

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	AV	0.09	0/941	0.18	0/1272
33	AW	0.10	0/819	0.21	0/1110
34	AX	0.10	0/1061	0.24	0/1441
35	AY	0.10	0/982	0.24	0/1335
36	AZ	0.10	0/790	0.23	0/1066
37	B0	0.10	0/833	0.22	0/1132
38	B1	0.09	0/812	0.19	0/1093
39	B2	0.10	0/776	0.20	0/1048
40	B3	0.10	0/654	0.21	0/884
41	B4	0.07	0/642	0.18	0/865
42	B5	0.10	0/466	0.19	0/630
43	B6	0.10	0/535	0.22	0/727
44	BA	0.10	0/1696	0.22	0/2292
45	BB	0.11	0/1376	0.20	0/1862
46	BC	0.10	0/1479	0.20	0/1996
47	BD	0.11	0/1216	0.21	0/1643
48	BE	0.10	0/1462	0.22	0/1981
49	BF	0.10	0/1503	0.22	0/2018
50	BG	0.10	0/1379	0.21	0/1841
51	BH	0.11	0/1519	0.24	0/2058
52	BI	0.09	0/1203	0.21	0/1630
53	BJ	0.10	0/1234	0.20	0/1662
54	BK	0.10	0/923	0.21	0/1239
55	BL	0.11	0/1223	0.21	0/1648
56	BM	0.11	0/1110	0.22	0/1502
57	BN	0.10	0/1132	0.23	0/1534
58	BO	0.09	0/1120	0.22	0/1500
59	BP	0.13	0/631	0.22	0/860
60	BQ	0.11	0/868	0.21	0/1170
61	BR	0.09	0/747	0.21	0/1011
62	BS	0.12	0/991	0.19	0/1333
63	BT	0.09	0/1106	0.23	0/1504
64	BU	0.10	0/1102	0.23	0/1486
65	BV	0.09	0/1003	0.20	0/1353
66	BW	0.11	0/983	0.21	0/1327
67	BX	0.09	0/821	0.20	0/1111
68	BY	0.10	0/916	0.29	0/1224
69	BZ	0.10	0/873	0.22	0/1175
70	CH	0.11	0/867	0.21	0/1166
71	CM	0.10	0/648	0.18	0/879
72	CL	0.09	0/788	0.20	0/1058
73	CA	0.09	0/4722	0.23	0/6385
74	CI	0.09	0/930	0.19	0/1244

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	CB	0.10	0/2355	0.25	0/3191
76	CF	0.12	0/1857	0.26	0/2512
77	CG	0.10	0/1699	0.22	0/2296
78	CK	0.09	0/821	0.23	0/1112
79	CE	0.09	0/2615	0.23	0/3553
80	CJ	0.10	0/875	0.23	0/1186
81	CN	0.08	0/530	0.23	0/719
82	CC	0.11	0/501	0.21	0/674
83	CO	0.12	0/375	0.21	0/508
84	CD	0.07	0/406	0.21	0/546
85	A	0.10	0/3933	0.26	0/5338
85	a	0.09	0/3933	0.23	0/5338
86	B	0.10	0/3616	0.24	0/4897
86	b	0.09	0/3616	0.23	0/4897
87	C	0.09	0/3716	0.23	0/5046
87	c	0.10	0/3716	0.24	0/5046
88	D	0.11	0/2580	0.25	0/3491
88	d	0.10	0/2580	0.24	0/3491
89	E	0.09	0/2015	0.22	0/2732
89	e	0.09	0/2015	0.24	0/2732
90	F	0.09	0/700	0.23	0/942
90	f	0.08	0/692	0.21	0/932
91	G	0.08	0/2846	0.24	0/3839
91	g	0.08	0/2846	0.23	0/3839
92	H	0.07	0/1133	0.21	0/1524
92	h	0.10	0/1133	0.28	0/1524
93	I	0.10	0/1029	0.23	0/1397
93	i	0.09	0/1029	0.22	0/1397
95	K	0.09	0/522	0.22	0/712
95	k	0.07	0/522	0.20	0/712
96	L	0.13	0/269	0.28	0/366
96	l	0.14	0/269	0.29	0/366
97	DA	0.08	0/5748	0.21	0/7793
97	Da	0.11	0/5748	0.25	0/7793
98	DB	0.07	0/5282	0.21	0/7159
98	Db	0.08	0/5282	0.23	0/7159
99	DC	0.08	0/5256	0.20	0/7142
99	Dc	0.09	0/5256	0.23	0/7142
100	DD	0.07	0/4734	0.19	0/6387
100	Dd	0.08	0/4734	0.21	0/6387
101	DE	0.08	0/1116	0.18	0/1512
101	De	0.10	0/1116	0.20	0/1512
102	DF	0.08	0/1977	0.23	0/2673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
102	Df	0.09	0/1977	0.23	0/2673
103	DG	0.07	0/906	0.17	0/1230
103	Dg	0.10	0/906	0.21	0/1230
104	DH	0.08	0/1208	0.20	0/1633
104	Dh	0.08	0/1208	0.22	0/1633
105	DI	0.07	0/1829	0.18	0/2486
105	Di	0.08	0/1829	0.20	0/2486
106	DJ	0.07	0/1950	0.19	0/2647
106	Dj	0.09	0/1950	0.21	0/2647
107	DK	0.08	0/1100	0.24	0/1495
107	Dk	0.09	0/1100	0.25	0/1495
108	DM	0.07	0/3910	0.19	0/5320
108	Dm	0.08	0/3910	0.21	0/5320
109	DN	0.07	0/3963	0.18	0/5359
109	Dn	0.08	0/3963	0.22	0/5359
110	DO	0.06	0/3505	0.16	0/4745
110	Do	0.07	0/3505	0.18	0/4745
111	DP	0.07	0/2433	0.19	0/3307
111	Dp	0.08	0/2433	0.20	0/3307
112	DQ	0.08	0/3256	0.20	0/4422
112	Dq	0.09	0/3256	0.22	0/4422
113	DR	0.07	0/2077	0.21	0/2824
113	Dr	0.08	0/2077	0.23	0/2824
114	DS	0.07	0/2959	0.19	0/4015
114	Ds	0.10	0/2959	0.23	0/4015
115	DT	0.08	0/2518	0.21	0/3433
115	Dt	0.08	0/2518	0.21	0/3433
116	DU	0.07	0/2689	0.19	0/3657
116	Du	0.09	0/2689	0.22	0/3657
117	DV	0.08	0/2631	0.20	0/3566
117	Dv	0.10	0/2631	0.23	1/3566 (0.0%)
118	DW	0.06	0/2449	0.18	0/3312
118	Dw	0.08	0/2449	0.21	0/3312
119	DX	0.07	0/2171	0.18	0/2930
119	Dx	0.08	0/2171	0.19	0/2930
120	DY	0.07	0/1619	0.19	0/2198
120	Dy	0.08	0/1619	0.21	0/2198
121	DZ	0.06	0/1752	0.17	0/2372
121	Dz	0.07	0/1752	0.19	0/2372
122	EA	0.07	0/1709	0.17	0/2321
122	Ea	0.07	0/1709	0.18	0/2321
123	EB	0.07	0/1793	0.19	0/2418
123	Eb	0.07	0/1793	0.20	0/2418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
124	EC	0.07	0/1673	0.22	0/2258
124	Ec	0.08	0/1673	0.23	0/2258
125	ED	0.07	0/1708	0.16	0/2306
125	Ed	0.08	0/1708	0.19	0/2306
126	EE	0.06	0/1066	0.15	0/1432
126	Ee	0.10	0/1066	0.21	0/1432
127	EF	0.09	0/1562	0.22	0/2123
127	Ef	0.10	0/1562	0.24	0/2123
128	EG	0.07	0/786	0.14	0/1060
128	Eg	0.10	0/786	0.19	0/1060
129	EH	0.08	0/1480	0.19	0/2007
129	Eh	0.09	0/1480	0.22	0/2007
130	EI	0.09	0/1442	0.25	0/1952
130	Ei	0.10	0/1442	0.27	0/1952
131	EV	0.08	0/654	0.21	0/878
131	Ev	0.09	0/654	0.21	0/878
132	EK	0.07	0/1410	0.18	0/1900
132	Ek	0.10	0/1410	0.22	0/1900
133	EL	0.08	0/1335	0.19	0/1810
133	El	0.10	0/1335	0.22	0/1810
134	EM	0.07	0/1335	0.20	0/1794
134	Em	0.10	0/1335	0.23	0/1794
135	EN	0.08	0/1270	0.24	0/1724
135	En	0.09	0/1270	0.26	0/1724
136	EO	0.07	0/1137	0.23	0/1545
136	Eo	0.08	0/1137	0.20	0/1545
137	EP	0.08	0/837	0.20	0/1133
137	Ep	0.09	0/837	0.21	0/1133
138	EQ	0.09	0/1044	0.19	0/1415
138	Eq	0.11	0/1044	0.22	0/1415
139	ER	0.08	0/874	0.17	0/1182
139	Er	0.09	0/874	0.20	0/1182
140	ES	0.08	0/802	0.19	0/1087
140	Es	0.09	0/802	0.21	0/1087
141	ET	0.05	0/654	0.16	0/878
141	Et	0.07	0/654	0.17	0/878
142	EU	0.07	0/744	0.17	0/1003
142	Eu	0.07	0/744	0.18	0/1003
143	EJ	0.06	0/1437	0.18	0/1941
143	Ej	0.09	0/1437	0.22	0/1941
144	EW	0.06	0/523	0.17	0/705
144	Ew	0.09	0/523	0.19	0/705
145	EX	0.06	0/564	0.16	0/757

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
145	Ex	0.07	0/564	0.18	0/757
146	EY	0.08	0/573	0.26	0/770
146	Ey	0.10	0/573	0.29	0/770
147	EZ	0.07	0/502	0.18	0/676
147	Ez	0.09	0/502	0.20	0/676
148	FA	0.05	0/554	0.15	0/746
148	Fa	0.08	0/554	0.19	0/746
149	DL	0.08	0/2984	0.24	0/4047
149	Dl	0.06	0/2984	0.19	0/4047
All	All	0.09	0/382937	0.22	1/518529 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
117	Dv	54	ASN	CB-CA-C	-6.03	109.63	116.63

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)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	4071	4019	4018	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A1	2718	2650	2649	11	0
3	A2	2199	2163	2160	22	0
4	A3	2263	2260	2260	22	0
5	A4	2494	2491	2491	15	0
6	A5	2347	2249	2249	23	0
7	A6	1908	1862	1861	24	0
8	A7	1084	1040	1039	15	0
9	A8	1794	1803	1800	17	0
10	A9	1879	1818	1818	12	0
11	AA	5941	5978	5977	71	0
12	AB	5403	5359	5358	62	0
13	AC	4170	4223	4223	48	0
14	AD	3399	3345	3344	39	0
15	AE	3587	3539	3539	43	0
16	AF	3068	3148	3147	38	0
17	AG	2804	2727	2727	14	0
18	AH	2306	2350	2349	35	0
19	AI	1862	1848	1847	17	0
20	AJ	2160	2156	2155	15	0
21	AK	1779	1740	1739	19	0
22	AL	1812	1689	1688	24	0
23	AM	1770	1788	1788	13	0
24	AN	1322	1329	1328	13	0
25	AO	1683	1680	1680	22	0
26	AP	1599	1505	1504	15	0
27	AQ	1588	1496	1495	8	0
28	AR	1492	1445	1445	14	0
29	AS	1420	1382	1382	9	0
30	AT	1277	1272	1271	19	0
31	AU	1227	1209	1208	10	0
32	AV	925	904	903	4	0
33	AW	803	781	780	2	0
34	AX	1027	1020	1020	16	0
35	AY	957	987	987	18	0
36	AZ	777	775	774	4	0
37	B0	805	802	801	6	0
38	B1	790	746	745	4	0
39	B2	757	728	727	12	0
40	B3	633	618	617	4	0
41	B4	624	623	623	4	0
42	B5	453	464	463	3	0
43	B6	515	528	528	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BA	1651	1638	1637	15	0
45	BB	1346	1280	1279	10	0
46	BC	1442	1406	1405	15	0
47	BD	1191	1223	1222	8	0
48	BE	1422	1385	1384	9	0
49	BF	1475	1486	1485	30	0
50	BG	1349	1376	1375	11	0
51	BH	1482	1554	1554	19	0
52	BI	1179	1139	1134	9	0
53	BJ	1205	1156	1155	5	0
54	BK	903	854	853	4	0
55	BL	1187	1138	1137	11	0
56	BM	1072	1002	1001	15	0
57	BN	1103	1126	1125	11	0
58	BO	1098	1058	1058	3	0
59	BP	604	590	589	6	0
60	BQ	845	829	828	8	0
61	BR	730	719	718	5	0
62	BS	966	941	940	8	0
63	BT	1063	953	950	13	0
64	BU	1082	1094	1094	13	0
65	BV	987	1014	1014	2	0
66	BW	955	893	892	3	0
67	BX	797	755	754	6	0
68	BY	889	917	917	12	0
69	BZ	850	840	840	5	0
70	CH	855	845	844	6	0
71	CM	629	603	602	4	0
72	CL	770	752	752	7	0
73	CA	4624	4574	4573	44	0
74	CI	915	890	890	4	0
75	CB	2300	2261	2259	19	0
76	CF	1812	1786	1785	11	0
77	CG	1654	1593	1592	16	0
78	CK	795	782	782	7	0
79	CE	2561	2554	2553	16	0
80	CJ	848	815	815	7	0
81	CN	514	515	515	6	0
82	CC	489	487	487	2	0
83	CO	364	376	375	4	0
84	CD	395	412	412	2	0
85	A	3847	3740	3740	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	a	3847	3740	3740	44	0
86	B	3563	3555	3554	38	0
86	b	3563	3555	3554	30	0
87	C	3590	3485	3483	63	0
87	c	3590	3484	3483	49	0
88	D	2489	2343	2343	21	0
88	d	2489	2343	2343	22	0
89	E	1966	1927	1927	21	0
89	e	1966	1925	1925	34	0
90	F	686	686	686	7	0
90	f	678	674	674	4	0
91	G	2768	2706	2706	30	0
91	g	2768	2706	2706	29	0
92	H	1098	1040	1040	17	0
92	h	1098	1040	1040	17	0
93	I	995	1003	1003	9	0
93	i	995	1003	1003	3	0
94	J	330	266	70	0	0
94	j	330	266	73	0	0
95	K	501	503	503	7	0
95	k	501	503	503	7	0
96	L	262	273	273	3	0
96	l	262	273	273	2	0
97	DA	5559	5609	5607	70	0
97	Da	5559	5608	5607	85	0
98	DB	5131	5101	5104	50	0
98	Db	5131	5102	5104	56	0
99	DC	5084	5067	5067	61	0
99	Dc	5084	5067	5067	71	0
100	DD	4652	4424	4424	61	0
100	Dd	4652	4424	4424	62	0
101	DE	1083	1021	1020	13	0
101	De	1083	1020	1020	18	0
102	DF	1913	1768	1768	21	0
102	Df	1913	1768	1768	18	0
103	DG	871	788	788	13	0
103	Dg	871	788	788	5	0
104	DH	1170	1129	1130	19	0
104	Dh	1170	1129	1130	18	0
105	DI	1777	1604	1603	19	0
105	Di	1777	1604	1603	20	0
106	DJ	1881	1772	1772	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
106	Dj	1881	1772	1772	26	0
107	DK	1071	1062	1062	12	0
107	Dk	1071	1062	1062	10	0
108	DM	3793	3592	3592	41	0
108	Dm	3793	3592	3592	48	0
109	DN	3869	3980	3980	39	0
109	Dn	3869	3980	3980	45	0
110	DO	3448	3508	3508	38	0
110	Do	3448	3508	3508	39	0
111	DP	2369	2291	2291	17	0
111	Dp	2369	2291	2291	21	0
112	DQ	3169	3102	3102	41	0
112	Dq	3169	3102	3102	41	0
113	DR	2024	1958	1958	25	0
113	Dr	2024	1958	1958	30	0
114	DS	2866	2770	2782	28	0
114	Ds	2866	2770	2782	36	0
115	DT	2443	2290	2290	51	0
115	Dt	2443	2290	2290	44	0
116	DU	2620	2584	2584	30	0
116	Du	2620	2584	2584	34	0
117	DV	2562	2552	2553	25	0
117	Dv	2562	2552	2553	28	0
118	DW	2394	2344	2344	16	0
118	Dw	2394	2344	2344	23	0
119	DX	2108	2018	2018	22	0
119	Dx	2108	2018	2018	22	0
120	DY	1573	1562	1562	17	0
120	Dy	1573	1562	1562	17	0
121	DZ	1711	1671	1670	19	0
121	Dz	1711	1672	1670	25	0
122	EA	1659	1637	1637	15	0
122	Ea	1659	1637	1637	15	0
123	EB	1739	1678	1677	14	0
123	Eb	1739	1678	1677	21	0
124	EC	1647	1660	1660	21	0
124	Ec	1647	1660	1660	18	0
125	ED	1659	1725	1725	23	0
125	Ed	1659	1725	1725	19	0
126	EE	1049	1024	1026	10	0
126	Ee	1049	1024	1026	12	0
127	EF	1509	1477	1477	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
127	Ef	1509	1477	1477	20	0
128	EG	771	752	752	7	0
128	Eg	771	752	752	9	0
129	EH	1438	1382	1394	13	0
129	Eh	1438	1382	1394	25	0
130	EI	1408	1419	1419	11	0
130	Ei	1408	1419	1419	12	0
131	EV	643	633	645	6	0
131	Ev	643	633	645	4	0
132	EK	1389	1407	1406	15	0
132	Ek	1389	1407	1407	20	0
133	EL	1291	1253	1253	14	0
133	El	1291	1253	1253	19	0
134	EM	1304	1299	1299	13	0
134	Em	1304	1299	1299	13	0
135	EN	1227	1190	1190	6	0
135	En	1227	1190	1190	7	0
136	EO	1097	1031	1031	12	0
136	Eo	1097	1031	1031	14	0
137	EP	817	795	795	14	0
137	Ep	817	795	795	10	0
138	EQ	1015	989	1001	15	0
138	Eq	1015	989	1001	10	0
139	ER	851	800	800	9	0
139	Er	851	800	800	11	0
140	ES	776	798	798	11	0
140	Es	776	798	798	16	0
141	ET	647	655	655	8	0
141	Et	647	655	655	10	0
142	EU	724	699	699	4	0
142	Eu	724	699	699	7	0
143	EJ	1411	1391	1391	15	0
143	Ej	1411	1391	1391	24	0
144	EW	515	510	510	2	0
144	Ew	515	510	510	2	0
145	EX	558	559	559	7	0
145	Ex	558	559	559	10	0
146	EY	561	562	562	6	0
146	Ey	561	562	562	8	0
147	EZ	492	474	473	7	0
147	Ez	492	474	473	8	0
148	FA	548	536	536	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
148	Fa	548	536	536	6	0
149	DL	2916	2814	2814	27	0
149	Dl	2916	2814	2814	20	0
150	A0	200	312	312	0	0
150	A1	100	156	156	0	0
150	AA	200	312	312	1	0
150	AC	200	312	312	4	0
150	AF	200	312	312	2	0
150	AM	100	156	156	0	0
150	AP	100	156	156	3	0
150	B0	200	312	312	1	0
150	B1	100	156	156	1	0
150	BC	200	312	312	2	0
150	BE	100	156	156	0	0
150	BG	100	156	156	0	0
150	BL	100	156	156	0	0
150	BT	200	312	312	3	0
150	BV	100	156	156	0	0
150	BY	100	156	156	0	0
150	C	500	780	780	8	0
150	CC	200	312	312	0	0
150	CD	200	312	312	1	0
150	CG	200	312	312	1	0
150	CJ	100	156	156	2	0
150	DA	200	312	312	0	0
150	DC	100	156	156	1	0
150	DD	400	624	624	5	0
150	DG	200	312	312	1	0
150	DH	200	312	312	4	0
150	DI	100	156	156	2	0
150	DJ	500	780	780	3	0
150	DM	200	312	312	0	0
150	DN	400	624	624	6	0
150	DO	100	156	156	2	0
150	DQ	300	468	468	3	0
150	DR	200	312	312	1	0
150	DS	300	468	468	6	0
150	DU	400	624	624	0	0
150	DV	300	468	468	0	0
150	DX	300	468	468	3	0
150	DY	100	156	156	0	0
150	DZ	100	156	156	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
150	Da	100	156	156	5	0
150	Dc	200	312	312	3	0
150	Dd	400	624	624	7	0
150	Dg	200	312	312	6	0
150	Dh	200	312	312	4	0
150	Di	200	312	312	3	0
150	Dj	600	936	936	5	0
150	Dm	200	312	312	2	0
150	Dn	400	624	624	5	0
150	Do	100	156	156	1	0
150	Dq	300	468	468	0	0
150	Dr	200	312	312	4	0
150	Ds	400	624	624	6	0
150	Du	300	468	468	1	0
150	Dv	300	468	468	1	0
150	Dx	200	312	312	6	0
150	Dy	100	156	156	0	0
150	E	100	156	156	0	0
150	EA	100	156	156	1	0
150	EB	100	156	156	2	0
150	ED	300	467	468	0	0
150	EH	100	156	156	5	0
150	EI	100	156	156	1	0
150	EK	100	156	156	0	0
150	EL	300	468	468	3	0
150	EN	200	312	312	3	0
150	EO	100	156	156	0	0
150	ES	100	156	156	1	0
150	Ea	200	312	312	1	0
150	Eb	100	156	156	0	0
150	Ed	200	311	312	0	0
150	Eg	100	156	156	3	0
150	Eh	100	156	156	2	0
150	Ei	100	156	156	0	0
150	Ek	100	156	156	1	0
150	El	300	468	468	2	0
150	En	100	156	156	2	0
150	Ep	100	156	156	0	0
150	Eu	100	156	156	0	0
150	H	200	312	312	2	0
150	c	400	624	624	5	0
150	g	100	156	156	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
150	h	100	156	156	1	0
151	A0	25	11	11	1	0
152	A0	1	0	0	0	0
152	A8	1	0	0	0	0
152	DA	1	0	0	0	0
152	Da	1	0	0	0	0
153	A	54	88	88	0	0
153	A0	54	88	88	0	0
153	A1	54	88	88	0	0
153	A2	54	88	88	0	0
153	A6	108	176	176	3	0
153	A9	108	176	176	0	0
153	AA	270	440	440	1	0
153	AC	54	88	88	1	0
153	AH	54	88	88	0	0
153	AJ	54	88	88	0	0
153	AL	54	88	88	1	0
153	AM	54	88	88	0	0
153	AQ	54	88	88	0	0
153	AU	108	176	176	0	0
153	AX	54	88	88	0	0
153	B1	108	176	176	0	0
153	BG	54	88	88	0	0
153	BS	108	176	176	1	0
153	BT	54	88	88	1	0
153	C	162	264	264	3	0
153	CC	54	88	88	0	0
153	D	54	88	88	0	0
153	DA	108	175	176	1	0
153	DB	54	88	88	0	0
153	DC	270	439	440	6	0
153	DG	54	88	88	2	0
153	DI	54	88	88	1	0
153	DJ	54	88	88	0	0
153	DQ	54	88	88	1	0
153	DS	54	88	88	0	0
153	DV	162	264	264	1	0
153	DX	108	176	176	2	0
153	DY	54	88	88	0	0
153	Da	108	175	176	1	0
153	Db	54	88	88	0	0
153	Dc	270	439	440	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	Dg	54	88	88	0	0
153	Di	54	88	88	2	0
153	Dj	54	88	88	0	0
153	Dq	54	88	88	0	0
153	Ds	54	88	88	0	0
153	Dv	216	352	352	1	0
153	Dx	162	264	264	3	0
153	Dy	54	88	88	0	0
153	E	54	88	88	1	0
153	EB	108	176	176	1	0
153	EN	54	88	88	0	0
153	EO	216	352	352	4	0
153	Eb	108	176	176	1	0
153	Ef	54	88	88	2	0
153	El	54	88	88	0	0
153	Eo	162	264	264	4	0
153	K	108	176	176	1	0
153	c	162	264	264	1	0
153	d	54	88	88	0	0
153	e	54	88	88	0	0
153	g	54	88	88	0	0
153	k	54	88	88	0	0
154	A1	48	26	26	0	0
155	A2	51	82	82	1	0
155	A9	51	82	82	0	0
155	AJ	51	82	82	0	0
155	BA	51	82	82	1	0
155	BP	51	82	82	0	0
155	BT	51	82	82	1	0
155	C	51	82	82	3	0
155	CC	51	82	82	0	0
155	CD	51	82	82	1	0
155	CK	51	82	82	0	0
155	DC	102	164	164	2	0
155	DG	102	164	164	1	0
155	DI	51	82	82	0	0
155	DJ	51	82	82	0	0
155	DN	51	82	82	0	0
155	DR	51	82	82	1	0
155	DS	51	82	82	1	0
155	DX	153	246	246	2	0
155	Da	51	82	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
155	Dc	102	164	164	2	0
155	Dd	51	82	82	1	0
155	Dg	51	82	82	1	0
155	Di	51	82	82	0	0
155	Dr	102	164	164	2	0
155	Ds	102	164	164	1	0
155	Dx	204	328	328	3	0
155	EL	51	82	82	1	0
155	EM	51	82	82	2	0
155	EN	51	82	82	0	0
155	EO	51	82	82	1	0
155	El	51	82	82	1	0
155	Em	51	82	82	0	0
155	Eo	102	164	164	0	0
155	G	51	82	82	0	0
156	A6	44	67	67	0	0
156	AA	44	67	67	0	0
156	AC	44	67	67	0	0
156	AL	44	67	67	1	0
156	DA	44	67	67	0	0
156	DN	88	134	134	0	0
156	Dl	44	67	67	0	0
156	Dn	88	134	134	0	0
156	EI	44	67	67	0	0
156	Ed	44	67	67	1	0
157	A8	27	12	12	0	0
157	AQ	27	12	12	0	0
158	AB	4	0	0	0	0
158	AI	4	0	0	1	0
158	BI	4	0	0	0	0
158	CB	4	0	0	2	0
158	E	4	0	0	1	0
158	EF	8	0	0	0	0
158	Ef	8	0	0	0	0
158	e	4	0	0	1	0
159	AB	16	0	0	1	0
159	AD	8	0	0	0	0
159	AL	16	0	0	2	0
159	AT	8	0	0	1	0
159	CB	8	0	0	0	0
160	AD	31	18	19	1	0
161	AS	34	43	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
162	BR	1	0	0	0	0
162	DD	1	0	0	0	0
162	Dd	1	0	0	0	0
163	CA	1	0	0	0	0
163	CB	1	0	0	0	0
163	DA	1	0	0	0	0
163	Da	1	0	0	0	0
164	CA	53	31	29	2	0
165	CB	7	0	0	0	0
166	CE	43	32	32	0	0
166	D	43	30	31	0	0
166	d	43	30	32	2	0
167	C	106	0	148	17	0
167	CC	53	74	74	1	0
167	DS	53	74	74	3	0
167	Ds	53	74	74	3	0
167	ED	53	74	74	2	0
167	EL	53	74	74	1	0
167	EN	53	74	74	3	0
167	Ed	53	74	74	3	0
167	El	53	74	74	2	0
167	En	53	74	74	4	0
167	c	53	0	74	8	0
168	C	86	60	60	11	0
168	ED	43	22	30	4	0
168	Ed	43	24	30	5	0
168	c	86	60	60	10	0
169	DA	120	108	108	2	0
169	Da	120	108	108	1	0
170	DA	1	0	0	0	0
170	Da	1	0	0	0	0
171	DB	2	0	0	0	0
171	Db	2	0	0	0	0
172	DD	1	0	0	0	0
173	ER	31	12	12	2	0
173	Er	31	12	12	1	0
All	All	399628	406234	406069	3417	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 3417 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:45:ARG:NH2	85:A:276:THR:O	2.03	0.91
88:d:288:GLU:OE1	88:d:290:TYR:OH	1.89	0.90
13:AC:215:ILE:HD11	51:BH:105:THR:HG21	1.52	0.89
122:EA:138:ARG:O	122:EA:151:ARG:NH2	2.06	0.88
75:CB:206:ARG:NH1	75:CB:210:ASP:OD1	2.07	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	501/516 (97%)	487 (97%)	14 (3%)	0	100	100
2	A1	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
3	A2	263/317 (83%)	257 (98%)	6 (2%)	0	100	100
4	A3	289/333 (87%)	287 (99%)	2 (1%)	0	100	100
5	A4	309/311 (99%)	305 (99%)	4 (1%)	0	100	100
6	A5	280/282 (99%)	279 (100%)	1 (0%)	0	100	100
7	A6	228/251 (91%)	224 (98%)	4 (2%)	0	100	100
8	A7	131/238 (55%)	129 (98%)	2 (2%)	0	100	100
9	A8	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
10	A9	229/231 (99%)	226 (99%)	3 (1%)	0	100	100
11	AA	711/750 (95%)	694 (98%)	16 (2%)	1 (0%)	48	77
12	AB	686/718 (96%)	674 (98%)	12 (2%)	0	100	100
13	AC	503/505 (100%)	489 (97%)	14 (3%)	0	100	100
14	AD	439/474 (93%)	427 (97%)	12 (3%)	0	100	100
15	AE	439/442 (99%)	431 (98%)	8 (2%)	0	100	100
16	AF	357/360 (99%)	349 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	43	72
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
79	CE	319/322 (99%)	301 (94%)	16 (5%)	2 (1%)	21 51
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
98	Db	602/604 (100%)	591 (98%)	11 (2%)	0	100	100
99	DC	580/594 (98%)	569 (98%)	10 (2%)	1 (0%)	43	72
99	Dc	580/594 (98%)	568 (98%)	12 (2%)	0	100	100
100	DD	554/637 (87%)	551 (100%)	3 (0%)	0	100	100
100	Dd	554/637 (87%)	550 (99%)	4 (1%)	0	100	100
101	DE	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
101	De	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
102	DF	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
102	Df	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
103	DG	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
103	Dg	96/103 (93%)	93 (97%)	3 (3%)	0	100	100
104	DH	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
104	Dh	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
105	DI	203/236 (86%)	198 (98%)	4 (2%)	1 (0%)	24	54
105	Di	203/236 (86%)	196 (97%)	6 (3%)	1 (0%)	24	54
106	DJ	218/220 (99%)	217 (100%)	1 (0%)	0	100	100
106	Dj	218/220 (99%)	216 (99%)	2 (1%)	0	100	100
107	DK	128/990 (13%)	121 (94%)	7 (6%)	0	100	100
107	Dk	128/990 (13%)	121 (94%)	7 (6%)	0	100	100
108	DM	453/490 (92%)	449 (99%)	4 (1%)	0	100	100
108	Dm	453/490 (92%)	448 (99%)	5 (1%)	0	100	100
109	DN	451/453 (100%)	443 (98%)	8 (2%)	0	100	100
109	Dn	451/453 (100%)	442 (98%)	9 (2%)	0	100	100
110	DO	431/473 (91%)	428 (99%)	3 (1%)	0	100	100
110	Do	431/473 (91%)	428 (99%)	3 (1%)	0	100	100
111	DP	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
111	Dp	288/402 (72%)	279 (97%)	9 (3%)	0	100	100
112	DQ	382/386 (99%)	376 (98%)	6 (2%)	0	100	100
112	Dq	382/386 (99%)	369 (97%)	13 (3%)	0	100	100
113	DR	241/348 (69%)	234 (97%)	7 (3%)	0	100	100
113	Dr	241/348 (69%)	238 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
114	DS	345/347 (99%)	344 (100%)	1 (0%)	0	100	100
114	Ds	345/347 (99%)	343 (99%)	2 (1%)	0	100	100
115	DT	291/318 (92%)	287 (99%)	4 (1%)	0	100	100
115	Dt	291/318 (92%)	288 (99%)	3 (1%)	0	100	100
116	DU	327/330 (99%)	322 (98%)	5 (2%)	0	100	100
116	Du	327/330 (99%)	321 (98%)	6 (2%)	0	100	100
117	DV	317/319 (99%)	315 (99%)	2 (1%)	0	100	100
117	Dv	317/319 (99%)	312 (98%)	5 (2%)	0	100	100
118	DW	299/318 (94%)	297 (99%)	2 (1%)	0	100	100
118	Dw	299/318 (94%)	297 (99%)	2 (1%)	0	100	100
119	DX	249/252 (99%)	248 (100%)	1 (0%)	0	100	100
119	Dx	249/252 (99%)	248 (100%)	1 (0%)	0	100	100
120	DY	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
120	Dy	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
121	DZ	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
121	Dz	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
122	EA	191/215 (89%)	189 (99%)	2 (1%)	0	100	100
122	Ea	191/215 (89%)	187 (98%)	4 (2%)	0	100	100
123	EB	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
123	Eb	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
124	EC	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
124	Ec	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
125	ED	188/190 (99%)	186 (99%)	2 (1%)	0	100	100
125	Ed	188/190 (99%)	185 (98%)	3 (2%)	0	100	100
126	EE	123/193 (64%)	122 (99%)	1 (1%)	0	100	100
126	Ee	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
127	EF	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
127	Ef	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
128	EG	96/100 (96%)	96 (100%)	0	0	100	100
128	Eg	96/100 (96%)	96 (100%)	0	0	100	100
129	EH	172/174 (99%)	171 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
129	Eh	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
130	EI	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
130	Ei	170/173 (98%)	165 (97%)	5 (3%)	0	100	100
131	EV	77/89 (86%)	76 (99%)	1 (1%)	0	100	100
131	Ev	77/89 (86%)	76 (99%)	1 (1%)	0	100	100
132	EK	167/170 (98%)	167 (100%)	0	0	100	100
132	Ek	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
133	EL	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
133	El	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
134	EM	151/154 (98%)	147 (97%)	4 (3%)	0	100	100
134	Em	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
135	EN	143/149 (96%)	140 (98%)	3 (2%)	0	100	100
135	En	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
136	EO	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
136	Eo	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
137	EP	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
137	Ep	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
138	EQ	121/123 (98%)	121 (100%)	0	0	100	100
138	Eq	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
139	ER	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
139	Er	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
140	ES	87/89 (98%)	87 (100%)	0	0	100	100
140	Es	87/89 (98%)	87 (100%)	0	0	100	100
141	ET	80/93 (86%)	80 (100%)	0	0	100	100
141	Et	80/93 (86%)	80 (100%)	0	0	100	100
142	EU	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
142	Eu	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
143	EJ	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
143	Ej	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
144	EW	61/81 (75%)	61 (100%)	0	0	100	100
144	Ew	61/81 (75%)	60 (98%)	1 (2%)	0	100	100

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

5 of 7 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	441/454 (97%)	437 (99%)	4 (1%)	70	90
2	A1	288/311 (93%)	287 (100%)	1 (0%)	86	96
3	A2	225/270 (83%)	224 (100%)	1 (0%)	84	94
4	A3	244/280 (87%)	242 (99%)	2 (1%)	73	90
5	A4	275/275 (100%)	275 (100%)	0	100	100
6	A5	257/257 (100%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	A6	207/223 (93%)	206 (100%)	1 (0%)	81 93
8	A7	122/224 (54%)	122 (100%)	0	100 100
9	A8	195/195 (100%)	194 (100%)	1 (0%)	81 93
10	A9	199/199 (100%)	197 (99%)	2 (1%)	68 89
11	AA	657/694 (95%)	650 (99%)	7 (1%)	65 88
12	AB	589/617 (96%)	588 (100%)	1 (0%)	87 96
13	AC	463/463 (100%)	459 (99%)	4 (1%)	70 90
14	AD	361/392 (92%)	360 (100%)	1 (0%)	86 96
15	AE	398/399 (100%)	395 (99%)	3 (1%)	73 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%)	244 (98%)	5 (2%)	48 78
19	AI	206/236 (87%)	205 (100%)	1 (0%)	81 93
20	AJ	243/244 (100%)	243 (100%)	0	100 100
21	AK	196/218 (90%)	195 (100%)	1 (0%)	81 93
22	AL	197/215 (92%)	193 (98%)	4 (2%)	48 78
23	AM	196/197 (100%)	195 (100%)	1 (0%)	81 93
24	AN	146/186 (78%)	146 (100%)	0	100 100
25	AO	191/191 (100%)	190 (100%)	1 (0%)	81 93
26	AP	168/170 (99%)	168 (100%)	0	100 100
27	AQ	170/172 (99%)	169 (99%)	1 (1%)	78 93
28	AR	159/163 (98%)	158 (99%)	1 (1%)	78 93
29	AS	154/154 (100%)	153 (99%)	1 (1%)	78 93
30	AT	136/137 (99%)	133 (98%)	3 (2%)	45 77
31	AU	132/133 (99%)	130 (98%)	2 (2%)	57 84
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%)	109 (97%)	3 (3%)	39 73
35	AY	108/108 (100%)	107 (99%)	1 (1%)	70 90
36	AZ	84/93 (90%)	84 (100%)	0	100 100
37	B0	88/89 (99%)	88 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	B1	83/84 (99%)	82 (99%)	1 (1%)	63 86
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%)	55 (100%)	0	100 100
44	BA	179/190 (94%)	179 (100%)	0	100 100
45	BB	145/182 (80%)	145 (100%)	0	100 100
46	BC	155/180 (86%)	155 (100%)	0	100 100
47	BD	124/179 (69%)	123 (99%)	1 (1%)	73 90
48	BE	159/178 (89%)	157 (99%)	2 (1%)	61 86
49	BF	161/172 (94%)	160 (99%)	1 (1%)	78 93
50	BG	142/156 (91%)	142 (100%)	0	100 100
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%)	128 (100%)	0	100 100
54	BK	97/131 (74%)	97 (100%)	0	100 100
55	BL	124/125 (99%)	123 (99%)	1 (1%)	73 90
56	BM	108/114 (95%)	107 (99%)	1 (1%)	70 90
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%)	91 (98%)	2 (2%)	45 77
61	BR	81/116 (70%)	80 (99%)	1 (1%)	63 86
62	BS	103/109 (94%)	103 (100%)	0	100 100
63	BT	110/110 (100%)	104 (94%)	6 (6%)	19 50
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	479 (100%)	2 (0%)	84	94
74	CI	97/97 (100%)	97 (100%)	0	100	100
75	CB	259/283 (92%)	257 (99%)	2 (1%)	73	90
76	CF	194/268 (72%)	194 (100%)	0	100	100
77	CG	179/181 (99%)	177 (99%)	2 (1%)	65	88
78	CK	85/85 (100%)	84 (99%)	1 (1%)	63	86
79	CE	286/287 (100%)	284 (99%)	2 (1%)	76	92
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%)	411 (100%)	0	100	100
85	a	411/440 (93%)	407 (99%)	4 (1%)	68	89
86	B	389/409 (95%)	387 (100%)	2 (0%)	81	93
86	b	389/409 (95%)	385 (99%)	4 (1%)	68	89
87	C	386/386 (100%)	385 (100%)	1 (0%)	86	96
87	c	386/386 (100%)	383 (99%)	3 (1%)	73	90
88	D	255/274 (93%)	252 (99%)	3 (1%)	63	86
88	d	255/274 (93%)	254 (100%)	1 (0%)	84	94
89	E	215/237 (91%)	214 (100%)	1 (0%)	81	93
89	e	215/237 (91%)	213 (99%)	2 (1%)	70	90
90	F	76/76 (100%)	76 (100%)	0	100	100
90	f	75/76 (99%)	74 (99%)	1 (1%)	61	86
91	G	288/289 (100%)	286 (99%)	2 (1%)	76	92
91	g	288/289 (100%)	285 (99%)	3 (1%)	68	89
92	H	117/118 (99%)	116 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
92	h	117/118 (99%)	117 (100%)	0	100 100
93	I	107/109 (98%)	104 (97%)	3 (3%)	38 72
93	i	107/109 (98%)	106 (99%)	1 (1%)	70 90
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%)	30 64
96	l	27/36 (75%)	27 (100%)	0	100 100
97	DA	596/613 (97%)	591 (99%)	5 (1%)	73 90
97	Da	596/613 (97%)	588 (99%)	8 (1%)	61 86
98	DB	569/569 (100%)	562 (99%)	7 (1%)	63 86
98	Db	569/569 (100%)	562 (99%)	7 (1%)	63 86
99	DC	553/565 (98%)	553 (100%)	0	100 100
99	Dc	553/565 (98%)	552 (100%)	1 (0%)	87 96
100	DD	506/579 (87%)	503 (99%)	3 (1%)	78 93
100	Dd	506/579 (87%)	502 (99%)	4 (1%)	73 90
101	DE	114/116 (98%)	114 (100%)	0	100 100
101	De	114/116 (98%)	114 (100%)	0	100 100
102	DF	200/207 (97%)	198 (99%)	2 (1%)	68 89
102	Df	200/207 (97%)	199 (100%)	1 (0%)	81 93
103	DG	84/88 (96%)	83 (99%)	1 (1%)	63 86
103	Dg	84/88 (96%)	84 (100%)	0	100 100
104	DH	120/120 (100%)	120 (100%)	0	100 100
104	Dh	120/120 (100%)	119 (99%)	1 (1%)	73 90
105	DI	193/218 (88%)	191 (99%)	2 (1%)	68 89
105	Di	193/218 (88%)	191 (99%)	2 (1%)	68 89
106	DJ	199/199 (100%)	196 (98%)	3 (2%)	57 84
106	Dj	199/199 (100%)	197 (99%)	2 (1%)	68 89
107	DK	121/943 (13%)	120 (99%)	1 (1%)	73 90
107	Dk	121/943 (13%)	121 (100%)	0	100 100
108	DM	413/447 (92%)	411 (100%)	2 (0%)	81 93
108	Dm	413/447 (92%)	410 (99%)	3 (1%)	76 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
109	DN	442/442 (100%)	440 (100%)	2 (0%)	81 93
109	Dn	442/442 (100%)	437 (99%)	5 (1%)	65 88
110	DO	380/413 (92%)	379 (100%)	1 (0%)	86 96
110	Do	380/413 (92%)	379 (100%)	1 (0%)	86 96
111	DP	253/358 (71%)	252 (100%)	1 (0%)	84 94
111	Dp	253/358 (71%)	252 (100%)	1 (0%)	84 94
112	DQ	341/343 (99%)	339 (99%)	2 (1%)	78 93
112	Dq	341/343 (99%)	341 (100%)	0	100 100
113	DR	219/318 (69%)	218 (100%)	1 (0%)	81 93
113	Dr	219/318 (69%)	219 (100%)	0	100 100
114	DS	294/294 (100%)	291 (99%)	3 (1%)	68 89
114	Ds	294/294 (100%)	290 (99%)	4 (1%)	59 85
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%)	84 94
116	Du	275/276 (100%)	270 (98%)	5 (2%)	51 80
117	DV	260/260 (100%)	259 (100%)	1 (0%)	84 94
117	Dv	260/260 (100%)	257 (99%)	3 (1%)	63 86
118	DW	258/272 (95%)	257 (100%)	1 (0%)	84 94
118	Dw	258/272 (95%)	257 (100%)	1 (0%)	84 94
119	DX	218/219 (100%)	217 (100%)	1 (0%)	81 93
119	Dx	218/219 (100%)	214 (98%)	4 (2%)	51 80
120	DY	169/216 (78%)	169 (100%)	0	100 100
120	Dy	169/216 (78%)	169 (100%)	0	100 100
121	DZ	189/213 (89%)	188 (100%)	1 (0%)	81 93
121	Dz	189/213 (89%)	188 (100%)	1 (0%)	81 93
122	EA	180/201 (90%)	180 (100%)	0	100 100
122	Ea	180/201 (90%)	180 (100%)	0	100 100
123	EB	180/181 (99%)	179 (99%)	1 (1%)	78 93
123	Eb	180/181 (99%)	179 (99%)	1 (1%)	78 93
124	EC	178/178 (100%)	177 (99%)	1 (1%)	78 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
124	Ec	178/178 (100%)	177 (99%)	1 (1%)	78 93
125	ED	185/185 (100%)	183 (99%)	2 (1%)	65 88
125	Ed	185/185 (100%)	183 (99%)	2 (1%)	65 88
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%)	63 86
127	Ef	164/164 (100%)	163 (99%)	1 (1%)	78 93
128	EG	77/78 (99%)	77 (100%)	0	100 100
128	Eg	77/78 (99%)	77 (100%)	0	100 100
129	EH	157/157 (100%)	156 (99%)	1 (1%)	78 93
129	Eh	157/157 (100%)	157 (100%)	0	100 100
130	EI	156/157 (99%)	154 (99%)	2 (1%)	61 86
130	Ei	156/157 (99%)	153 (98%)	3 (2%)	50 79
131	EV	72/81 (89%)	72 (100%)	0	100 100
131	Ev	72/81 (89%)	72 (100%)	0	100 100
132	EK	153/154 (99%)	152 (99%)	1 (1%)	76 92
132	Ek	153/154 (99%)	150 (98%)	3 (2%)	48 78
133	EL	134/139 (96%)	134 (100%)	0	100 100
133	El	134/139 (96%)	134 (100%)	0	100 100
134	EM	137/138 (99%)	136 (99%)	1 (1%)	76 92
134	Em	137/138 (99%)	136 (99%)	1 (1%)	76 92
135	EN	132/135 (98%)	131 (99%)	1 (1%)	73 90
135	En	132/135 (98%)	131 (99%)	1 (1%)	73 90
136	EO	112/113 (99%)	111 (99%)	1 (1%)	70 90
136	Eo	112/113 (99%)	111 (99%)	1 (1%)	70 90
137	EP	87/113 (77%)	87 (100%)	0	100 100
137	Ep	87/113 (77%)	87 (100%)	0	100 100
138	EQ	105/105 (100%)	102 (97%)	3 (3%)	37 71
138	Eq	105/105 (100%)	102 (97%)	3 (3%)	37 71
139	ER	87/88 (99%)	87 (100%)	0	100 100
139	Er	87/88 (99%)	87 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	73 (97%)	2 (3%)	39	73
141	Et	75/83 (90%)	72 (96%)	3 (4%)	28	62
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%)	155 (99%)	2 (1%)	61	86
143	Ej	157/157 (100%)	155 (99%)	2 (1%)	61	86
144	EW	57/66 (86%)	56 (98%)	1 (2%)	51	80
144	Ew	57/66 (86%)	56 (98%)	1 (2%)	51	80
145	EX	64/67 (96%)	63 (98%)	1 (2%)	55	83
145	Ex	64/67 (96%)	63 (98%)	1 (2%)	55	83
146	EY	62/63 (98%)	61 (98%)	1 (2%)	55	83
146	Ey	62/63 (98%)	62 (100%)	0	100	100
147	EZ	55/63 (87%)	54 (98%)	1 (2%)	51	80
147	Ez	55/63 (87%)	54 (98%)	1 (2%)	51	80
148	FA	62/63 (98%)	61 (98%)	1 (2%)	55	83
148	Fa	62/63 (98%)	60 (97%)	2 (3%)	34	68
149	DL	308/386 (80%)	306 (99%)	2 (1%)	78	93
149	Dl	308/386 (80%)	307 (100%)	1 (0%)	86	96
All	All	40248/44802 (90%)	39987 (99%)	261 (1%)	76	93

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
123	Eb	63	ARG
130	Ei	132	VAL
149	DL	366	THR
86	b	175	ARG
85	a	492	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
97	Da	182	ASN
119	Dx	47	GLN
98	Db	548	GLN
109	Dn	88	HIS
132	Ek	163	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
100	TPO	Dd	387	100	8,10,11	1.57	1 (12%)	10,14,16	1.83	1 (10%)
100	SEP	DD	520	100	8,9,10	1.53	1 (12%)	8,12,14	1.64	2 (25%)
105	SEP	Di	120	105	8,9,10	1.53	1 (12%)	8,12,14	1.57	2 (25%)
105	SEP	DI	120	105	8,9,10	1.53	1 (12%)	8,12,14	1.49	2 (25%)
100	SEP	Dd	520	100	8,9,10	1.54	1 (12%)	8,12,14	1.62	2 (25%)
100	TPO	DD	387	100	8,10,11	1.57	1 (12%)	10,14,16	1.90	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	-
100	SEP	DD	520	100	-	0/5/8/10	-
105	SEP	Di	120	105	-	0/5/8/10	-
105	SEP	DI	120	105	-	0/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
100	SEP	Dd	520	100	-	0/5/8/10	-
100	TPO	DD	387	100	-	2/9/11/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
100	Dd	520	SEP	P-O1P	3.36	1.61	1.50
100	DD	520	SEP	P-O1P	3.35	1.61	1.50
100	DD	387	TPO	P-O1P	3.34	1.61	1.50
105	Di	120	SEP	P-O1P	3.33	1.61	1.50
105	DI	120	SEP	P-O1P	3.32	1.61	1.50

The worst 5 of 10 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
100	DD	520	SEP	P-OG-CB	-3.02	109.98	118.30
100	Dd	520	SEP	P-OG-CB	-3.01	110.02	118.30
100	DD	520	SEP	OG-CB-CA	2.96	111.03	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
100	Dd	387	TPO	2	0
100	DD	520	SEP	1	0
105	Di	120	SEP	1	0
105	DI	120	SEP	1	0
100	Dd	520	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 384 ligands modelled in this entry, 14 are monoatomic - leaving 370 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
167	UQ8	CC	303	-	53,53,53	0.50	0	64,67,67	0.71	4 (6%)
153	PC1	Eo	204	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	DA	707	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	C	506	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	A1	403	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	A9	603	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	CC	305	-	99,99,99	0.29	0	105,111,111	0.53	1 (0%)
166	HEC	d	802	88	50,50,50	2.91	28 (56%)	68,82,82	2.45	26 (38%)
153	PC1	Dc	609	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	K	501	-	53,53,53	0.29	0	59,61,61	0.27	0
169	HEA	Da	703	97	66,67,67	2.48	26 (39%)	78,103,103	2.38	33 (42%)
167	UQ8	EN	1205	-	53,53,53	0.51	0	64,67,67	0.67	2 (3%)
150	CDL	Dg	201	-	99,99,99	0.31	0	105,111,111	0.51	1 (0%)
150	CDL	DJ	305	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	DC	606	-	50,50,50	0.27	0	53,55,55	0.22	0
158	FES	EF	201	127	0,4,4	-	-	-		
153	PC1	Eb	301	-	53,53,53	0.28	0	59,61,61	0.25	0
150	CDL	Ep	701	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	BL	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Ed	205	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	El	903	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	Ds	403	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	EB	301	-	53,53,53	0.29	0	59,61,61	0.25	0
150	CDL	Dv	402	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
159	SF4	AL	302	22	0,12,12	-	-	-		
153	PC1	Eb	303	-	53,53,53	0.29	0	59,61,61	0.27	0
159	SF4	AB	803	12	0,12,12	-	-	-		
153	PC1	DQ	1503	-	53,53,53	0.29	0	59,61,61	0.26	0
156	LPP	Ed	203	-	43,43,43	0.22	0	47,48,48	0.27	0
171	CUA	Db	701	98	0,1,1	-	-	-		
153	PC1	C	509	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	EM	901	-	50,50,50	0.27	0	53,55,55	0.20	0
171	CUA	DB	701	98	0,1,1	-	-	-		
150	CDL	c	509	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
150	CDL	DN	502	-	99,99,99	0.31	0	105,111,111	0.51	1 (0%)
153	PC1	AU	201	-	53,53,53	0.28	0	59,61,61	0.27	0
159	SF4	AT	201	30	0,12,12	-	-	-		
153	PC1	DC	603	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	DX	304	-	50,50,50	0.27	0	53,55,55	0.20	0
155	3PE	BA	301	-	50,50,50	0.27	0	53,55,55	0.21	0
159	SF4	AL	301	22	0,12,12	-	-	-		
155	3PE	DI	301	-	50,50,50	0.26	0	53,55,55	0.23	0
150	CDL	DU	403	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Dj	407	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
155	3PE	Dx	1207	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	DN	507	-	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	DS	406	-	53,53,53	0.29	0	59,61,61	0.25	0
153	PC1	EO	206	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	Dv	404	-	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
150	CDL	A0	601	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
156	LPP	Dn	505	-	43,43,43	0.22	0	47,48,48	0.28	0
150	CDL	DV	402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DC	604	-	53,53,53	0.28	0	59,61,61	0.27	0
154	NDP	A1	401	-	49,52,52	0.28	0	66,80,80	0.34	0
153	PC1	AA	903	-	53,53,53	0.29	0	59,61,61	0.26	0
155	3PE	Dc	607	-	50,50,50	0.28	0	53,55,55	0.20	0
153	PC1	DC	602	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Dc	608	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	DD	705	-	99,99,99	0.31	0	105,111,111	0.53	0
156	LPP	DN	505	-	43,43,43	0.22	0	47,48,48	0.28	0
155	3PE	CD	303	-	50,50,50	0.27	0	53,55,55	0.22	0
153	PC1	DA	708	-	53,53,53	0.29	0	59,61,61	0.27	0
167	UQ8	Ed	202	-	53,53,53	0.52	0	64,67,67	0.72	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
150	CDL	DM	501	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	BS	1302	-	53,53,53	0.28	0	59,61,61	0.26	0
151	UDP	A0	603	152	24,26,26	0.38	0	37,40,40	0.76	2 (5%)
150	CDL	DJ	302	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	EN	1204	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	DD	703	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	Ds	407	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	DD	704	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
153	PC1	Da	707	-	53,53,53	0.29	0	59,61,61	0.28	0
153	PC1	B1	401	-	53,53,53	0.28	0	59,61,61	0.27	0
159	SF4	AB	802	12	0,12,12	-	-	-		
153	PC1	DV	404	-	53,53,53	0.29	0	59,61,61	0.27	0
158	FES	AB	801	12	0,4,4	-	-	-		
150	CDL	ED	601	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Dh	202	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
159	SF4	CB	1001	75	0,12,12	-	-	-		
150	CDL	C	504	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	h	501	-	99,99,99	0.30	0	105,111,111	0.54	2 (1%)
150	CDL	Dq	1402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Du	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Ds	406	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	DA	706	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
150	CDL	Dc	601	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	Dg	202	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	DX	301	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
155	3PE	DJ	301	-	50,50,50	0.27	0	53,55,55	0.21	0
160	FMN	AD	502	-	33,33,33	0.19	0	48,50,50	0.32	0
150	CDL	Eb	302	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
150	CDL	ES	1101	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
153	PC1	AC	804	-	53,53,53	0.30	0	59,61,61	0.27	0
153	PC1	BG	202	-	53,53,53	0.28	0	59,61,61	0.25	0
150	CDL	C	505	-	99,99,99	0.29	0	105,111,111	0.55	1 (0%)
150	CDL	H	1302	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	A9	602	-	50,50,50	0.28	0	53,55,55	0.22	0
150	CDL	Ea	502	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	BT	201	-	50,50,50	0.28	0	53,55,55	0.20	0
155	3PE	Eo	203	-	50,50,50	0.27	0	53,55,55	0.20	0
153	PC1	AU	202	-	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	$\#\|Z\|>2$
165	F3S	CB	1002	75	0,9,9	-	-	-		
150	CDL	AA	901	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Di	1103	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
150	CDL	AA	908	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
155	3PE	CK	101	-	50,50,50	0.26	0	53,55,55	0.21	0
150	CDL	AP	301	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	g	802	-	53,53,53	0.29	0	59,61,61	0.25	0
153	PC1	Da	706	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	DG	205	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	DM	502	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Dn	506	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	DV	401	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	DB	702	-	53,53,53	0.29	0	59,61,61	0.25	0
168	HEM	c	505	87	50,50,50	1.37	6 (12%)	66,82,82	1.22	7 (10%)
153	PC1	AQ	202	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	Dx	1204	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
158	FES	Ef	502	127	0,4,4	-	-	-		
155	3PE	Dx	1202	-	50,50,50	0.27	0	53,55,55	0.21	0
150	CDL	Dm	501	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Dc	603	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	A0	602	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
153	PC1	DX	305	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	BG	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	DC	605	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	A6	303	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	B0	102	-	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%)
150	CDL	DN	503	-	99,99,99	0.31	0	105,111,111	0.53	1 (0%)
150	CDL	EI	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	EN	1201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
156	LPP	A6	301	-	43,43,43	0.30	0	47,48,48	0.44	1 (2%)
153	PC1	A6	302	-	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	DJ	306	-	53,53,53	0.29	0	59,61,61	0.26	0
155	3PE	Dx	1208	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	Dj	404	-	99,99,99	0.31	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%)
150	CDL	Dx	1201	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	E	303	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	DQ	1504	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
157	ADP	AQ	201	-	27,29,29	0.25	0	42,45,45	0.27	0
153	PC1	C	508	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Do	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	EO	205	-	53,53,53	0.30	0	59,61,61	0.27	0
150	CDL	Dj	405	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
150	CDL	H	1301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	DX	306	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	EL	901	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	Dn	503	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
166	HEC	CE	401	79	50,50,50	3.07	28 (56%)	68,82,82	2.94	35 (51%)
150	CDL	EO	202	-	99,99,99	0.32	0	105,111,111	0.52	1 (0%)
153	PC1	AH	301	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	c	502	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	B1	402	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	EB	303	-	53,53,53	0.29	0	59,61,61	0.27	0
167	UQ8	c	510	-	53,53,53	0.50	0	64,67,67	0.70	2 (3%)
153	PC1	c	508	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	Dd	703	-	50,50,50	0.28	0	53,55,55	0.20	0
167	UQ8	El	906	-	53,53,53	0.53	0	64,67,67	0.84	3 (4%)
153	PC1	Dc	602	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DZ	501	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	A9	601	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	Dx	1209	-	53,53,53	0.28	0	59,61,61	0.27	0
153	PC1	DV	405	-	53,53,53	0.29	0	59,61,61	0.27	0
156	LPP	AL	304	-	43,43,43	0.22	0	47,48,48	0.28	0
153	PC1	EN	1203	-	53,53,53	0.29	0	59,61,61	0.25	0
155	3PE	Eo	202	-	50,50,50	0.27	0	53,55,55	0.20	0
155	3PE	BP	201	-	50,50,50	0.27	0	53,55,55	0.22	0
167	UQ8	EL	905	-	53,53,53	0.51	0	64,67,67	0.80	3 (4%)
150	CDL	DA	709	-	99,99,99	0.31	0	105,111,111	0.55	1 (0%)
168	HEM	c	504	87	50,50,50	1.35	6 (12%)	66,82,82	1.20	6 (9%)
150	CDL	DU	402	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	Dc	606	-	50,50,50	0.28	0	53,55,55	0.20	0
150	CDL	A1	402	-	99,99,99	0.30	0	105,111,111	0.50	0
150	CDL	AC	802	-	99,99,99	0.29	0	105,111,111	0.53	1 (0%)
150	CDL	Dd	705	-	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	$\#\|Z\|>2$
150	CDL	AF	401	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
168	HEM	Ed	201	125	50,50,50	1.39	6 (12%)	66,82,82	1.29	9 (13%)
153	PC1	BS	1301	-	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%)
150	CDL	EB	302	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
153	PC1	DG	203	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	EK	201	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	Dn	501	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
167	UQ8	DS	403	-	53,53,53	0.50	0	64,67,67	0.66	1 (1%)
153	PC1	Di	1104	-	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%)
150	CDL	DJ	303	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	e	1101	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	Dj	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	AJ	501	-	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%)
155	3PE	DC	607	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	DJ	304	-	99,99,99	0.30	0	105,111,111	0.49	1 (0%)
150	CDL	DR	402	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
155	3PE	Dx	1206	-	50,50,50	0.27	0	53,55,55	0.21	0
150	CDL	El	901	-	99,99,99	0.31	0	105,111,111	0.57	1 (0%)
150	CDL	C	507	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Dq	1403	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	DS	402	-	50,50,50	0.27	0	53,55,55	0.19	0
167	UQ8	C	511	-	53,53,53	0.51	0	64,67,67	0.75	3 (4%)
158	FES	BI	201	52	0,4,4	-	-	-		
153	PC1	c	507	-	53,53,53	0.29	0	59,61,61	0.26	0
150	CDL	Ed	204	-	99,99,99	0.30	0	105,111,111	0.47	1 (0%)
150	CDL	En	1201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
157	ADP	A8	401	152	27,29,29	0.24	0	42,45,45	0.26	0
150	CDL	Dd	702	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	BC	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	AM	302	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	CG	301	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Dj	401	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	CG	302	-	99,99,99	0.29	0	105,111,111	0.50	1 (0%)
173	ATP	Er	201	-	29,33,33	0.29	0	44,52,52	0.79	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
155	3PE	G	401	-	50,50,50	0.26	0	53,55,55	0.22	0
153	PC1	El	904	-	53,53,53	0.27	0	59,61,61	0.28	0
156	LPP	Dl	1101	-	43,43,43	0.23	0	47,48,48	0.26	0
150	CDL	BV	201	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
158	FES	AI	301	19	0,4,4	-	-	-		
153	PC1	Dq	1404	-	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	0.53	1 (0%)
153	PC1	AX	401	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	c	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
159	SF4	AD	501	14	0,12,12	-	-	-		
150	CDL	Dv	403	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	AM	301	-	99,99,99	0.30	0	105,111,111	0.51	0
150	CDL	DQ	1501	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
153	PC1	A	1201	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	DG	204	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	Dh	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	DO	501	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	c	503	-	53,53,53	0.28	0	59,61,61	0.30	0
150	CDL	DD	706	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
155	3PE	A2	401	-	50,50,50	0.27	0	53,55,55	0.21	0
155	3PE	EL	904	-	50,50,50	0.28	0	53,55,55	0.22	0
150	CDL	B0	101	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	EA	301	-	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	0.56	1 (0%)
153	PC1	C	510	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DV	403	-	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	d	801	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	Du	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	AA	907	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	CD	302	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	Da	709	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Eu	101	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Dg	203	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	AA	906	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	DX	302	-	50,50,50	0.26	0	53,55,55	0.19	0
155	3PE	AJ	502	-	50,50,50	0.26	0	53,55,55	0.23	0
168	HEM	C	501	87	50,50,50	1.35	6 (12%)	66,82,82	1.17	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
168	HEM	ED	602	125	50,50,50	1.39	6 (12%)	66,82,82	1.26	8 (12%)
153	PC1	Ef	501	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DX	307	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
150	CDL	DG	202	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	DS	405	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
155	3PE	DN	501	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	DJ	307	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
155	3PE	Ds	408	-	50,50,50	0.27	0	53,55,55	0.20	0
150	CDL	DS	401	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
167	UQ8	C	512	-	53,53,53	0.50	0	64,67,67	0.68	3 (4%)
150	CDL	Di	1101	-	99,99,99	0.31	0	105,111,111	0.56	1 (0%)
150	CDL	CJ	201	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	EL	903	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Dx	1203	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	DU	404	-	99,99,99	0.31	0	105,111,111	0.54	1 (0%)
150	CDL	E	301	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DR	403	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	El	902	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	DI	303	-	53,53,53	0.29	0	59,61,61	0.26	0
155	3PE	DX	303	-	50,50,50	0.26	0	53,55,55	0.21	0
153	PC1	B1	403	-	53,53,53	0.29	0	59,61,61	0.27	0
153	PC1	BT	203	-	53,53,53	0.28	0	59,61,61	0.27	0
167	UQ8	Ds	404	-	53,53,53	0.51	0	64,67,67	0.66	1 (1%)
150	CDL	Ek	201	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
156	LPP	EI	402	-	43,43,43	0.23	0	47,48,48	0.27	0
153	PC1	Dv	407	-	53,53,53	0.29	0	59,61,61	0.26	0
156	LPP	AA	902	-	43,43,43	0.22	0	47,48,48	0.29	0
150	CDL	Dr	403	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
169	HEA	DA	702	97	66,67,67	2.49	26 (39%)	78,103,103	2.34	32 (41%)
150	CDL	Dn	502	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	DG	201	-	99,99,99	0.30	0	105,111,111	0.51	1 (0%)
158	FES	e	1102	89	0,4,4	-	-	-		
153	PC1	DC	608	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	A0	605	-	53,53,53	0.28	0	59,61,61	0.26	0
155	3PE	CC	301	-	50,50,50	0.26	0	53,55,55	0.22	0
150	CDL	DY	301	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
164	FAD	CA	702	73	56,58,58	0.49	0	81,89,89	0.56	1 (1%)
153	PC1	k	301	-	53,53,53	0.28	0	59,61,61	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
155	3PE	C	513	-	50,50,50	0.26	0	53,55,55	0.21	0
173	ATP	ER	201	-	29,33,33	0.29	0	44,52,52	0.79	1 (2%)
153	PC1	Dc	604	-	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
153	PC1	Eo	201	-	53,53,53	0.29	0	59,61,61	0.28	0
150	CDL	Du	403	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	C	503	-	99,99,99	0.30	0	105,111,111	0.52	0
150	CDL	DN	506	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	EO	204	-	53,53,53	0.28	0	59,61,61	0.28	0
166	HEC	D	401	88	50,50,50	2.92	28 (56%)	68,82,82	2.47	27 (39%)
150	CDL	Ea	501	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
168	HEM	C	502	87	50,50,50	1.34	7 (14%)	66,82,82	1.21	6 (9%)
150	CDL	BE	201	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
169	HEA	DA	703	97	66,67,67	2.48	26 (39%)	78,103,103	2.40	32 (41%)
153	PC1	Dx	1205	-	53,53,53	0.29	0	59,61,61	0.26	0
153	PC1	Dj	406	-	53,53,53	0.29	0	59,61,61	0.26	0
155	3PE	Dr	401	-	50,50,50	0.26	0	53,55,55	0.22	0
150	CDL	ED	604	-	99,99,99	0.30	0	105,111,111	0.47	1 (0%)
158	FES	Ef	503	127	0,4,4	-	-	-		
167	UQ8	En	1202	-	53,53,53	0.51	0	64,67,67	0.63	2 (3%)
153	PC1	D	402	-	53,53,53	0.28	0	59,61,61	0.26	0
156	LPP	Dn	504	-	43,43,43	0.23	0	47,48,48	0.33	0
150	CDL	Ei	401	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
155	3PE	Di	1102	-	50,50,50	0.26	0	53,55,55	0.24	0
155	3PE	EO	203	-	50,50,50	0.27	0	53,55,55	0.21	0
150	CDL	ED	605	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
153	PC1	DV	406	-	53,53,53	0.28	0	59,61,61	0.27	0
155	3PE	Em	901	-	50,50,50	0.27	0	53,55,55	0.19	0
153	PC1	Dv	406	-	53,53,53	0.29	0	59,61,61	0.26	0
156	LPP	AC	803	-	43,43,43	0.23	0	47,48,48	0.28	0
153	PC1	CC	302	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	Dy	301	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	K	502	-	53,53,53	0.28	0	59,61,61	0.27	0
156	LPP	DA	710	-	43,43,43	0.23	0	47,48,48	0.28	0
150	CDL	Ds	401	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
150	CDL	Dd	704	-	99,99,99	0.31	0	105,111,111	0.47	0
155	3PE	Dg	204	-	50,50,50	0.26	0	53,55,55	0.22	0
150	CDL	BC	302	-	99,99,99	0.30	0	105,111,111	0.57	2 (1%)
150	CDL	DH	202	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	PC1	AL	303	-	53,53,53	0.28	0	59,61,61	0.28	0
150	CDL	AF	402	-	99,99,99	0.30	0	105,111,111	0.55	1 (0%)
153	PC1	Db	702	-	53,53,53	0.29	0	59,61,61	0.25	0
158	FES	EF	202	127	0,4,4	-	-	-		
156	LPP	DN	504	-	43,43,43	0.23	0	47,48,48	0.35	0
153	PC1	AA	904	-	53,53,53	0.28	0	59,61,61	0.30	0
161	8Q1	AS	200	-	27,33,34	0.12	0	32,40,43	0.33	0
155	3PE	DR	401	-	50,50,50	0.27	0	53,55,55	0.22	0
155	3PE	Dr	404	-	50,50,50	0.26	0	53,55,55	0.20	0
150	CDL	Eg	101	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	DQ	1502	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
153	PC1	Eo	205	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	Dv	405	-	53,53,53	0.29	0	59,61,61	0.25	0
150	CDL	DH	201	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	AA	905	-	53,53,53	0.28	0	59,61,61	0.27	0
150	CDL	Dj	403	-	99,99,99	0.30	0	105,111,111	0.57	1 (0%)
150	CDL	BY	201	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	EL	902	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
150	CDL	Eh	1601	-	99,99,99	0.31	0	105,111,111	0.51	1 (0%)
155	3PE	El	905	-	50,50,50	0.28	0	53,55,55	0.21	0
150	CDL	g	801	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
167	UQ8	ED	603	-	53,53,53	0.51	0	64,67,67	0.70	3 (4%)
150	CDL	Dd	706	-	99,99,99	0.30	0	105,111,111	0.56	1 (0%)
150	CDL	Dr	402	-	99,99,99	0.30	0	105,111,111	0.54	1 (0%)
153	PC1	Dy	302	-	53,53,53	0.28	0	59,61,61	0.26	0
153	PC1	EO	201	-	53,53,53	0.29	0	59,61,61	0.27	0
150	CDL	Dv	401	-	99,99,99	0.30	0	105,111,111	0.52	2 (1%)
155	3PE	Da	708	-	50,50,50	0.25	0	53,55,55	0.21	0
153	PC1	A2	402	-	53,53,53	0.28	0	59,61,61	0.26	0
150	CDL	Ds	402	-	99,99,99	0.31	0	105,111,111	0.52	1 (0%)
158	FES	CB	1000	75	0,4,4	-	-	-		
169	HEA	Da	702	97	66,67,67	2.49	26 (39%)	78,103,103	2.37	32 (41%)
150	CDL	CC	304	-	99,99,99	0.29	0	105,111,111	0.54	1 (0%)
158	FES	E	302	89	0,4,4	-	-	-		
150	CDL	DS	404	-	99,99,99	0.30	0	105,111,111	0.52	1 (0%)
150	CDL	c	506	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)
150	CDL	CD	301	-	99,99,99	0.29	0	105,111,111	0.51	1 (0%)
150	CDL	BT	202	-	99,99,99	0.30	0	105,111,111	0.53	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
150	CDL	EH	1601	-	99,99,99	0.30	0	105,111,111	0.54	1 (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
167	UQ8	CC	303	-	-	10/51/75/75	0/1/1/1
153	PC1	Eo	204	-	-	20/57/57/57	-
153	PC1	DA	707	-	-	18/57/57/57	-
150	CDL	C	506	-	-	31/110/110/110	-
153	PC1	A1	403	-	-	14/57/57/57	-
153	PC1	A9	603	-	-	21/57/57/57	-
150	CDL	CC	305	-	-	29/110/110/110	-
166	HEC	d	802	88	1/1/7/7	6/14/54/54	-
153	PC1	Dc	609	-	-	17/57/57/57	-
153	PC1	K	501	-	-	15/57/57/57	-
169	HEA	Da	703	97	-	9/36/76/76	-
167	UQ8	EN	1205	-	-	15/51/75/75	0/1/1/1
150	CDL	Dg	201	-	-	46/110/110/110	-
150	CDL	DJ	305	-	-	25/110/110/110	-
155	3PE	DC	606	-	-	10/54/54/54	-
158	FES	EF	201	127	-	-	0/1/1/1
153	PC1	Eb	301	-	-	12/57/57/57	-
150	CDL	Ep	701	-	-	33/110/110/110	-
150	CDL	BL	301	-	-	21/110/110/110	-
150	CDL	Ed	205	-	-	30/110/110/110	-
150	CDL	El	903	-	-	38/110/110/110	-
155	3PE	Ds	403	-	-	20/54/54/54	-
153	PC1	EB	301	-	-	13/57/57/57	-
150	CDL	Dv	402	-	-	39/110/110/110	-
159	SF4	AL	302	22	-	-	0/6/5/5
153	PC1	Eb	303	-	-	6/57/57/57	-
159	SF4	AB	803	12	-	-	0/6/5/5
153	PC1	DQ	1503	-	-	11/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
156	LPP	Ed	203	-	-	2/45/45/45	-
153	PC1	C	509	-	-	24/57/57/57	-
155	3PE	EM	901	-	-	13/54/54/54	-
150	CDL	c	509	-	-	33/110/110/110	-
150	CDL	DN	502	-	-	40/110/110/110	-
153	PC1	AU	201	-	-	12/57/57/57	-
159	SF4	AT	201	30	-	-	0/6/5/5
153	PC1	DC	603	-	-	14/57/57/57	-
155	3PE	DX	304	-	-	13/54/54/54	-
155	3PE	BA	301	-	-	17/54/54/54	-
159	SF4	AL	301	22	-	-	0/6/5/5
155	3PE	DI	301	-	-	18/54/54/54	-
150	CDL	DU	403	-	-	30/110/110/110	-
150	CDL	Dj	407	-	-	32/110/110/110	-
155	3PE	Dx	1207	-	-	19/54/54/54	-
150	CDL	DN	507	-	-	38/110/110/110	-
150	CDL	DI	302	-	-	41/110/110/110	-
153	PC1	DS	406	-	-	19/57/57/57	-
153	PC1	EO	206	-	-	17/57/57/57	-
153	PC1	Dv	404	-	-	11/57/57/57	-
153	PC1	DY	302	-	-	9/57/57/57	-
150	CDL	A0	601	-	-	23/110/110/110	-
156	LPP	Dn	505	-	-	6/45/45/45	-
150	CDL	DV	402	-	-	32/110/110/110	-
153	PC1	DC	604	-	-	15/57/57/57	-
154	NDP	A1	401	-	-	6/34/77/77	0/5/5/5
153	PC1	AA	903	-	-	13/57/57/57	-
155	3PE	Dc	607	-	-	18/54/54/54	-
153	PC1	DC	602	-	-	15/57/57/57	-
150	CDL	Dc	608	-	-	27/110/110/110	-
150	CDL	DD	705	-	-	34/110/110/110	-
156	LPP	DN	505	-	-	1/45/45/45	-
155	3PE	CD	303	-	-	12/54/54/54	-
153	PC1	DA	708	-	-	10/57/57/57	-
167	UQ8	Ed	202	-	-	9/51/75/75	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	DM	501	-	-	41/110/110/110	-
153	PC1	BS	1302	-	-	10/57/57/57	-
151	UDP	A0	603	152	-	7/16/32/32	0/2/2/2
150	CDL	DJ	302	-	-	29/110/110/110	-
155	3PE	EN	1204	-	-	14/54/54/54	-
150	CDL	DD	703	-	-	31/110/110/110	-
153	PC1	Ds	407	-	-	9/57/57/57	-
150	CDL	DD	704	-	-	32/110/110/110	-
153	PC1	Da	707	-	-	12/57/57/57	-
153	PC1	B1	401	-	-	18/57/57/57	-
159	SF4	AB	802	12	-	-	0/6/5/5
153	PC1	DV	404	-	-	14/57/57/57	-
158	FES	AB	801	12	-	-	0/1/1/1
150	CDL	ED	601	-	-	32/110/110/110	-
150	CDL	Dh	202	-	-	39/110/110/110	-
159	SF4	CB	1001	75	-	-	0/6/5/5
150	CDL	C	504	-	-	39/110/110/110	-
150	CDL	h	501	-	-	26/110/110/110	-
150	CDL	Dq	1402	-	-	31/110/110/110	-
150	CDL	Du	401	-	-	38/110/110/110	-
150	CDL	Ds	406	-	-	35/110/110/110	-
150	CDL	DA	706	-	-	33/110/110/110	-
150	CDL	Dc	601	-	-	37/110/110/110	-
150	CDL	Dg	202	-	-	32/110/110/110	-
150	CDL	DX	301	-	-	33/110/110/110	-
155	3PE	DJ	301	-	-	15/54/54/54	-
160	FMN	AD	502	-	-	1/18/18/18	0/3/3/3
150	CDL	Eb	302	-	-	37/110/110/110	-
150	CDL	ES	1101	-	-	39/110/110/110	-
153	PC1	AC	804	-	-	12/57/57/57	-
153	PC1	BG	202	-	-	22/57/57/57	-
150	CDL	C	505	-	-	36/110/110/110	-
150	CDL	H	1302	-	-	29/110/110/110	-
155	3PE	A9	602	-	-	8/54/54/54	-
150	CDL	Ea	502	-	-	26/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
155	3PE	BT	201	-	-	21/54/54/54	-
155	3PE	Eo	203	-	-	8/54/54/54	-
153	PC1	AU	202	-	-	14/57/57/57	-
165	F3S	CB	1002	75	-	-	0/3/3/3
150	CDL	AA	901	-	-	32/110/110/110	-
150	CDL	Di	1103	-	-	35/110/110/110	-
150	CDL	AA	908	-	-	29/110/110/110	-
155	3PE	CK	101	-	-	3/54/54/54	-
150	CDL	AP	301	-	-	25/110/110/110	-
153	PC1	g	802	-	-	13/57/57/57	-
153	PC1	Da	706	-	-	16/57/57/57	-
155	3PE	DG	205	-	-	15/54/54/54	-
150	CDL	DM	502	-	-	24/110/110/110	-
150	CDL	Dn	506	-	-	35/110/110/110	-
150	CDL	DV	401	-	-	32/110/110/110	-
153	PC1	DB	702	-	-	21/57/57/57	-
168	HEM	c	505	87	-	1/14/54/54	-
153	PC1	AQ	202	-	-	15/57/57/57	-
150	CDL	Dx	1204	-	-	46/110/110/110	-
158	FES	Ef	502	127	-	-	0/1/1/1
155	3PE	Dx	1202	-	-	18/54/54/54	-
150	CDL	Dm	501	-	-	39/110/110/110	-
153	PC1	Dc	603	-	-	14/57/57/57	-
150	CDL	A0	602	-	-	36/110/110/110	-
153	PC1	DX	305	-	-	11/57/57/57	-
150	CDL	BG	201	-	-	34/110/110/110	-
153	PC1	DC	605	-	-	12/57/57/57	-
153	PC1	A6	303	-	-	11/57/57/57	-
150	CDL	B0	102	-	-	25/110/110/110	-
150	CDL	EN	1202	-	-	29/110/110/110	-
150	CDL	DN	503	-	-	26/110/110/110	-
150	CDL	EI	401	-	-	23/110/110/110	-
150	CDL	EN	1201	-	-	28/110/110/110	-
156	LPP	A6	301	-	-	3/45/45/45	-
153	PC1	A6	302	-	-	11/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	PC1	DX	308	-	-	18/57/57/57	-
153	PC1	DJ	306	-	-	12/57/57/57	-
155	3PE	Dx	1208	-	-	13/54/54/54	-
150	CDL	Dj	404	-	-	35/110/110/110	-
150	CDL	Ds	405	-	-	40/110/110/110	-
150	CDL	Dx	1201	-	-	37/110/110/110	-
153	PC1	E	303	-	-	12/57/57/57	-
150	CDL	DQ	1504	-	-	36/110/110/110	-
157	ADP	AQ	201	-	-	2/16/32/32	0/3/3/3
153	PC1	C	508	-	-	20/57/57/57	-
150	CDL	Do	501	-	-	36/110/110/110	-
153	PC1	EO	205	-	-	25/57/57/57	-
150	CDL	Dj	405	-	-	29/110/110/110	-
150	CDL	H	1301	-	-	29/110/110/110	-
150	CDL	DX	306	-	-	34/110/110/110	-
150	CDL	EL	901	-	-	45/110/110/110	-
150	CDL	Dn	503	-	-	30/110/110/110	-
166	HEC	CE	401	79	1/1/7/7	9/14/54/54	-
150	CDL	EO	202	-	-	33/110/110/110	-
153	PC1	AH	301	-	-	9/57/57/57	-
150	CDL	c	502	-	-	29/110/110/110	-
150	CDL	B1	402	-	-	33/110/110/110	-
153	PC1	EB	303	-	-	6/57/57/57	-
167	UQ8	c	510	-	-	12/51/75/75	0/1/1/1
153	PC1	c	508	-	-	8/57/57/57	-
155	3PE	Dd	703	-	-	18/54/54/54	-
167	UQ8	El	906	-	-	13/51/75/75	0/1/1/1
153	PC1	Dc	602	-	-	16/57/57/57	-
150	CDL	DZ	501	-	-	37/110/110/110	-
153	PC1	A9	601	-	-	13/57/57/57	-
153	PC1	Dx	1209	-	-	5/57/57/57	-
153	PC1	DV	405	-	-	9/57/57/57	-
156	LPP	AL	304	-	-	3/45/45/45	-
153	PC1	EN	1203	-	-	16/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
155	3PE	Eo	202	-	-	14/54/54/54	-
155	3PE	BP	201	-	-	15/54/54/54	-
167	UQ8	EL	905	-	-	11/51/75/75	0/1/1/1
150	CDL	DA	709	-	-	23/110/110/110	-
168	HEM	c	504	87	-	2/14/54/54	-
150	CDL	DU	402	-	-	29/110/110/110	-
155	3PE	Dc	606	-	-	5/54/54/54	-
150	CDL	A1	402	-	-	40/110/110/110	-
150	CDL	AC	802	-	-	34/110/110/110	-
150	CDL	Dd	705	-	-	31/110/110/110	-
150	CDL	AF	401	-	-	22/110/110/110	-
168	HEM	Ed	201	125	-	0/14/54/54	-
153	PC1	BS	1301	-	-	16/57/57/57	-
150	CDL	AC	801	-	-	37/110/110/110	-
150	CDL	EB	302	-	-	33/110/110/110	-
153	PC1	DG	203	-	-	9/57/57/57	-
150	CDL	EK	201	-	-	31/110/110/110	-
150	CDL	Dn	501	-	-	38/110/110/110	-
167	UQ8	DS	403	-	-	8/51/75/75	0/1/1/1
153	PC1	Di	1104	-	-	19/57/57/57	-
150	CDL	DU	401	-	-	37/110/110/110	-
150	CDL	DJ	303	-	-	31/110/110/110	-
153	PC1	e	1101	-	-	12/57/57/57	-
150	CDL	Dj	402	-	-	34/110/110/110	-
153	PC1	AJ	501	-	-	15/57/57/57	-
150	CDL	Dq	1401	-	-	40/110/110/110	-
155	3PE	DC	607	-	-	13/54/54/54	-
150	CDL	DJ	304	-	-	40/110/110/110	-
150	CDL	DR	402	-	-	33/110/110/110	-
155	3PE	Dx	1206	-	-	15/54/54/54	-
150	CDL	El	901	-	-	42/110/110/110	-
150	CDL	C	507	-	-	34/110/110/110	-
150	CDL	Dq	1403	-	-	34/110/110/110	-
155	3PE	DS	402	-	-	20/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
167	UQ8	C	511	-	-	16/51/75/75	0/1/1/1
158	FES	BI	201	52	-	-	0/1/1/1
153	PC1	c	507	-	-	19/57/57/57	-
150	CDL	Ed	204	-	-	27/110/110/110	-
150	CDL	En	1201	-	-	32/110/110/110	-
157	ADP	A8	401	152	-	2/16/32/32	0/3/3/3
150	CDL	Dd	702	-	-	30/110/110/110	-
150	CDL	BC	301	-	-	22/110/110/110	-
153	PC1	AM	302	-	-	19/57/57/57	-
150	CDL	CG	301	-	-	27/110/110/110	-
150	CDL	Dj	401	-	-	38/110/110/110	-
150	CDL	CG	302	-	-	36/110/110/110	-
173	ATP	Er	201	-	-	2/22/38/38	0/3/3/3
155	3PE	G	401	-	-	8/54/54/54	-
153	PC1	El	904	-	-	10/57/57/57	-
156	LPP	Dl	1101	-	-	8/45/45/45	-
150	CDL	BV	201	-	-	24/110/110/110	-
158	FES	AI	301	19	-	-	0/1/1/1
153	PC1	Dq	1404	-	-	10/57/57/57	-
150	CDL	DC	601	-	-	39/110/110/110	-
153	PC1	AX	401	-	-	8/57/57/57	-
150	CDL	c	501	-	-	34/110/110/110	-
159	SF4	AD	501	14	-	-	0/6/5/5
150	CDL	Dv	403	-	-	40/110/110/110	-
150	CDL	AM	301	-	-	31/110/110/110	-
150	CDL	DQ	1501	-	-	31/110/110/110	-
153	PC1	A	1201	-	-	13/57/57/57	-
155	3PE	DG	204	-	-	16/54/54/54	-
150	CDL	Dh	201	-	-	34/110/110/110	-
150	CDL	DO	501	-	-	29/110/110/110	-
153	PC1	c	503	-	-	16/57/57/57	-
150	CDL	DD	706	-	-	31/110/110/110	-
155	3PE	A2	401	-	-	9/54/54/54	-
155	3PE	EL	904	-	-	17/54/54/54	-
150	CDL	B0	101	-	-	34/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	EA	301	-	-	28/110/110/110	-
150	CDL	Dm	502	-	-	27/110/110/110	-
153	PC1	C	510	-	-	12/57/57/57	-
150	CDL	DV	403	-	-	37/110/110/110	-
150	CDL	BT	204	-	-	39/110/110/110	-
153	PC1	d	801	-	-	18/57/57/57	-
150	CDL	Du	402	-	-	33/110/110/110	-
153	PC1	AA	907	-	-	21/57/57/57	-
150	CDL	CD	302	-	-	28/110/110/110	-
150	CDL	Da	709	-	-	41/110/110/110	-
150	CDL	Eu	101	-	-	32/110/110/110	-
153	PC1	Dg	203	-	-	13/57/57/57	-
153	PC1	AA	906	-	-	20/57/57/57	-
155	3PE	DX	302	-	-	14/54/54/54	-
155	3PE	AJ	502	-	-	14/54/54/54	-
168	HEM	C	501	87	-	4/14/54/54	-
168	HEM	ED	602	125	-	0/14/54/54	-
153	PC1	Ef	501	-	-	14/57/57/57	-
150	CDL	DX	307	-	-	29/110/110/110	-
150	CDL	DG	202	-	-	27/110/110/110	-
150	CDL	DS	405	-	-	32/110/110/110	-
155	3PE	DN	501	-	-	12/54/54/54	-
150	CDL	DJ	307	-	-	34/110/110/110	-
155	3PE	Ds	408	-	-	12/54/54/54	-
150	CDL	DS	401	-	-	29/110/110/110	-
167	UQ8	C	512	-	-	10/51/75/75	0/1/1/1
150	CDL	Di	1101	-	-	40/110/110/110	-
150	CDL	CJ	201	-	-	24/110/110/110	-
150	CDL	EL	903	-	-	37/110/110/110	-
153	PC1	Dx	1203	-	-	18/57/57/57	-
150	CDL	DU	404	-	-	26/110/110/110	-
150	CDL	E	301	-	-	28/110/110/110	-
150	CDL	DR	403	-	-	29/110/110/110	-
150	CDL	El	902	-	-	39/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	PC1	DI	303	-	-	18/57/57/57	-
155	3PE	DX	303	-	-	18/54/54/54	-
153	PC1	B1	403	-	-	16/57/57/57	-
153	PC1	BT	203	-	-	16/57/57/57	-
167	UQ8	Ds	404	-	-	12/51/75/75	0/1/1/1
150	CDL	Ek	201	-	-	30/110/110/110	-
156	LPP	EI	402	-	-	7/45/45/45	-
153	PC1	Dv	407	-	-	9/57/57/57	-
156	LPP	AA	902	-	-	11/45/45/45	-
150	CDL	Dr	403	-	-	30/110/110/110	-
169	HEA	DA	702	97	-	4/36/76/76	-
150	CDL	Dn	502	-	-	41/110/110/110	-
150	CDL	DG	201	-	-	37/110/110/110	-
158	FES	e	1102	89	-	-	0/1/1/1
153	PC1	DC	608	-	-	16/57/57/57	-
153	PC1	A0	605	-	-	13/57/57/57	-
155	3PE	CC	301	-	-	5/54/54/54	-
150	CDL	DY	301	-	-	35/110/110/110	-
164	FAD	CA	702	73	-	15/34/50/50	0/6/6/6
153	PC1	k	301	-	-	17/57/57/57	-
155	3PE	C	513	-	-	11/54/54/54	-
173	ATP	ER	201	-	-	6/22/38/38	0/3/3/3
153	PC1	Dc	604	-	-	11/57/57/57	-
153	PC1	Dc	605	-	-	18/57/57/57	-
153	PC1	Eo	201	-	-	15/57/57/57	-
150	CDL	Du	403	-	-	30/110/110/110	-
150	CDL	C	503	-	-	35/110/110/110	-
150	CDL	DN	506	-	-	37/110/110/110	-
166	HEC	D	401	88	1/1/7/7	5/14/54/54	-
153	PC1	EO	204	-	-	10/57/57/57	-
150	CDL	Ea	501	-	-	37/110/110/110	-
168	HEM	C	502	87	-	5/14/54/54	-
150	CDL	BE	201	-	-	29/110/110/110	-
169	HEA	DA	703	97	-	9/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	PC1	Dx	1205	-	-	14/57/57/57	-
153	PC1	Dj	406	-	-	10/57/57/57	-
155	3PE	Dr	401	-	-	15/54/54/54	-
150	CDL	ED	604	-	-	26/110/110/110	-
158	FES	Ef	503	127	-	-	0/1/1/1
167	UQ8	En	1202	-	-	11/51/75/75	0/1/1/1
153	PC1	D	402	-	-	18/57/57/57	-
156	LPP	Dn	504	-	-	9/45/45/45	-
150	CDL	Ei	401	-	-	26/110/110/110	-
155	3PE	Di	1102	-	-	17/54/54/54	-
155	3PE	EO	203	-	-	9/54/54/54	-
150	CDL	ED	605	-	-	36/110/110/110	-
153	PC1	DV	406	-	-	9/57/57/57	-
155	3PE	Em	901	-	-	15/54/54/54	-
153	PC1	Dv	406	-	-	13/57/57/57	-
156	LPP	AC	803	-	-	11/45/45/45	-
153	PC1	CC	302	-	-	15/57/57/57	-
150	CDL	Dy	301	-	-	40/110/110/110	-
153	PC1	K	502	-	-	12/57/57/57	-
156	LPP	DA	710	-	-	7/45/45/45	-
150	CDL	Ds	401	-	-	28/110/110/110	-
150	CDL	Dd	704	-	-	34/110/110/110	-
155	3PE	Dg	204	-	-	13/54/54/54	-
150	CDL	BC	302	-	-	32/110/110/110	-
150	CDL	DH	202	-	-	39/110/110/110	-
153	PC1	AL	303	-	-	9/57/57/57	-
150	CDL	AF	402	-	-	29/110/110/110	-
153	PC1	Db	702	-	-	22/57/57/57	-
158	FES	EF	202	127	-	-	0/1/1/1
156	LPP	DN	504	-	-	9/45/45/45	-
153	PC1	AA	904	-	-	14/57/57/57	-
161	8Q1	AS	200	-	-	12/38/40/41	-
155	3PE	DR	401	-	-	9/54/54/54	-
155	3PE	Dr	404	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
150	CDL	Eg	101	-	-	32/110/110/110	-
150	CDL	DQ	1502	-	-	33/110/110/110	-
153	PC1	Eo	205	-	-	14/57/57/57	-
153	PC1	Dv	405	-	-	19/57/57/57	-
150	CDL	DH	201	-	-	27/110/110/110	-
153	PC1	AA	905	-	-	15/57/57/57	-
150	CDL	Dj	403	-	-	35/110/110/110	-
150	CDL	BY	201	-	-	28/110/110/110	-
150	CDL	EL	902	-	-	44/110/110/110	-
150	CDL	Eh	1601	-	-	40/110/110/110	-
155	3PE	El	905	-	-	17/54/54/54	-
150	CDL	g	801	-	-	31/110/110/110	-
167	UQ8	ED	603	-	-	9/51/75/75	0/1/1/1
150	CDL	Dd	706	-	-	29/110/110/110	-
150	CDL	Dr	402	-	-	35/110/110/110	-
153	PC1	Dy	302	-	-	12/57/57/57	-
153	PC1	EO	201	-	-	12/57/57/57	-
150	CDL	Dv	401	-	-	37/110/110/110	-
155	3PE	Da	708	-	-	17/54/54/54	-
153	PC1	A2	402	-	-	9/57/57/57	-
150	CDL	Ds	402	-	-	33/110/110/110	-
158	FES	CB	1000	75	-	-	0/1/1/1
169	HEA	Da	702	97	-	5/36/76/76	-
150	CDL	CC	304	-	-	22/110/110/110	-
158	FES	E	302	89	-	-	0/1/1/1
150	CDL	DS	404	-	-	36/110/110/110	-
150	CDL	c	506	-	-	38/110/110/110	-
150	CDL	CD	301	-	-	38/110/110/110	-
150	CDL	BT	202	-	-	36/110/110/110	-
150	CDL	EH	1601	-	-	32/110/110/110	-

The worst 5 of 225 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	CE	401	HEC	C3B-C2B	7.09	1.51	1.36
169	Da	702	HEA	C3A-C2A	5.91	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	DA	702	HEA	C3A-C2A	5.85	1.49	1.36
166	CE	401	HEC	C2A-C3A	5.81	1.49	1.36
169	Da	703	HEA	C3A-C2A	5.77	1.49	1.36

The worst 5 of 456 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	CE	401	HEC	C2A-C1A-NA	8.73	118.82	110.32
169	DA	702	HEA	C3C-C4C-NC	6.93	114.51	110.25
169	DA	703	HEA	C3C-C4C-NC	6.85	114.46	110.25
166	D	401	HEC	C1B-C2B-C3B	-6.84	99.76	106.96
166	CE	401	HEC	C1C-C2C-C3C	-6.84	98.83	106.83

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
166	CE	401	HEC	NA
166	D	401	HEC	NA
166	d	802	HEC	NA

5 of 7642 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

There are no ring outliers.

186 monomers are involved in 320 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
167	CC	303	UQ8	1	0
153	Eo	204	PC1	3	0
150	C	506	CDL	3	0
166	d	802	HEC	2	0
153	Dc	609	PC1	2	0
167	EN	1205	UQ8	3	0
150	Dg	201	CDL	5	0
155	DC	606	3PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
150	El	903	CDL	1	0
155	Ds	403	3PE	1	0
150	Dv	402	CDL	1	0
159	AL	302	SF4	2	0
153	Eb	303	PC1	1	0
159	AB	803	SF4	1	0
153	DQ	1503	PC1	1	0
156	Ed	203	LPP	1	0
153	C	509	PC1	2	0
155	EM	901	3PE	2	0
150	c	509	CDL	2	0
150	DN	502	CDL	1	0
159	AT	201	SF4	1	0
155	DX	304	3PE	1	0
155	BA	301	3PE	1	0
155	Dx	1207	3PE	1	0
150	DN	507	CDL	3	0
150	DI	302	CDL	2	0
153	Dv	404	PC1	1	0
153	DC	602	PC1	2	0
150	Dc	608	CDL	2	0
155	CD	303	3PE	1	0
153	DA	708	PC1	1	0
167	Ed	202	UQ8	3	0
151	A0	603	UDP	1	0
150	DJ	302	CDL	1	0
150	DD	703	CDL	1	0
150	DD	704	CDL	4	0
153	Da	707	PC1	1	0
150	Dh	202	CDL	3	0
150	C	504	CDL	1	0
150	h	501	CDL	1	0
150	Du	401	CDL	1	0
150	Ds	406	CDL	1	0
150	Dc	601	CDL	1	0
150	Dg	202	CDL	1	0
150	DX	301	CDL	1	0
160	AD	502	FMN	1	0
150	ES	1101	CDL	1	0
153	AC	804	PC1	1	0
150	C	505	CDL	4	0
150	Ea	502	CDL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
155	BT	201	3PE	1	0
150	AA	901	CDL	1	0
150	Di	1103	CDL	3	0
150	AP	301	CDL	3	0
150	Dn	506	CDL	1	0
168	c	505	HEM	6	0
150	Dx	1204	CDL	3	0
150	Dm	501	CDL	1	0
153	DX	305	PC1	1	0
153	DC	605	PC1	1	0
153	A6	303	PC1	3	0
150	B0	102	CDL	1	0
150	EN	1202	CDL	1	0
150	EI	401	CDL	1	0
150	EN	1201	CDL	2	0
153	DX	308	PC1	1	0
150	Dj	404	CDL	3	0
150	Ds	405	CDL	2	0
150	Dx	1201	CDL	3	0
153	E	303	PC1	1	0
150	DQ	1504	CDL	1	0
150	Do	501	CDL	1	0
153	EO	205	PC1	1	0
150	H	1301	CDL	2	0
150	DX	306	CDL	1	0
150	EL	901	CDL	3	0
150	Dn	503	CDL	2	0
150	c	502	CDL	1	0
150	B1	402	CDL	1	0
153	EB	303	PC1	1	0
167	c	510	UQ8	8	0
155	Dd	703	3PE	1	0
167	El	906	UQ8	2	0
153	Dx	1209	PC1	1	0
156	AL	304	LPP	1	0
167	EL	905	UQ8	1	0
168	c	504	HEM	4	0
155	Dc	606	3PE	2	0
150	AC	802	CDL	2	0
150	Dd	705	CDL	4	0
150	AF	401	CDL	1	0
168	Ed	201	HEM	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	BS	1301	PC1	1	0
150	AC	801	CDL	2	0
150	EB	302	CDL	2	0
153	DG	203	PC1	2	0
150	Dn	501	CDL	1	0
167	DS	403	UQ8	3	0
153	Di	1104	PC1	2	0
150	DJ	303	CDL	1	0
155	DC	607	3PE	1	0
150	DJ	304	CDL	1	0
150	DR	402	CDL	1	0
155	Dx	1206	3PE	2	0
150	El	901	CDL	1	0
155	DS	402	3PE	1	0
167	C	511	UQ8	9	0
150	En	1201	CDL	2	0
150	Dd	702	CDL	1	0
150	CG	301	CDL	1	0
150	Dj	401	CDL	1	0
173	Er	201	ATP	1	0
158	AI	301	FES	1	0
150	DC	601	CDL	1	0
150	c	501	CDL	3	0
150	DQ	1501	CDL	1	0
155	DG	204	3PE	1	0
150	Dh	201	CDL	3	0
150	DO	501	CDL	2	0
153	c	503	PC1	1	0
155	A2	401	3PE	1	0
155	EL	904	3PE	1	0
150	EA	301	CDL	1	0
150	Dm	502	CDL	1	0
153	C	510	PC1	1	0
150	BT	204	CDL	3	0
150	Da	709	CDL	5	0
153	AA	906	PC1	1	0
168	C	501	HEM	5	0
168	ED	602	HEM	4	0
153	Ef	501	PC1	2	0
150	DX	307	CDL	1	0
150	DS	405	CDL	2	0
150	DS	401	CDL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
167	C	512	UQ8	8	0
150	CJ	201	CDL	2	0
153	Dx	1203	PC1	2	0
153	DI	303	PC1	1	0
155	DX	303	3PE	1	0
153	BT	203	PC1	1	0
167	Ds	404	UQ8	3	0
150	Ek	201	CDL	1	0
150	Dr	403	CDL	1	0
169	DA	702	HEA	1	0
150	Dn	502	CDL	1	0
150	DG	201	CDL	1	0
158	e	1102	FES	1	0
153	DC	608	PC1	3	0
164	CA	702	FAD	2	0
155	C	513	3PE	3	0
173	ER	201	ATP	2	0
153	Eo	201	PC1	1	0
150	DN	506	CDL	2	0
153	EO	204	PC1	1	0
168	C	502	HEM	6	0
169	DA	703	HEA	1	0
155	Dr	401	3PE	2	0
167	En	1202	UQ8	4	0
155	EO	203	3PE	1	0
153	DV	406	PC1	1	0
153	K	502	PC1	1	0
150	Ds	401	CDL	3	0
150	Dd	704	CDL	1	0
155	Dg	204	3PE	1	0
150	BC	302	CDL	2	0
150	DH	202	CDL	1	0
153	AL	303	PC1	1	0
150	AF	402	CDL	1	0
155	DR	401	3PE	1	0
150	Eg	101	CDL	3	0
150	DQ	1502	CDL	1	0
150	DH	201	CDL	4	0
150	Dj	403	CDL	1	0
150	Eh	1601	CDL	2	0
155	El	905	3PE	1	0
150	g	801	CDL	1	0

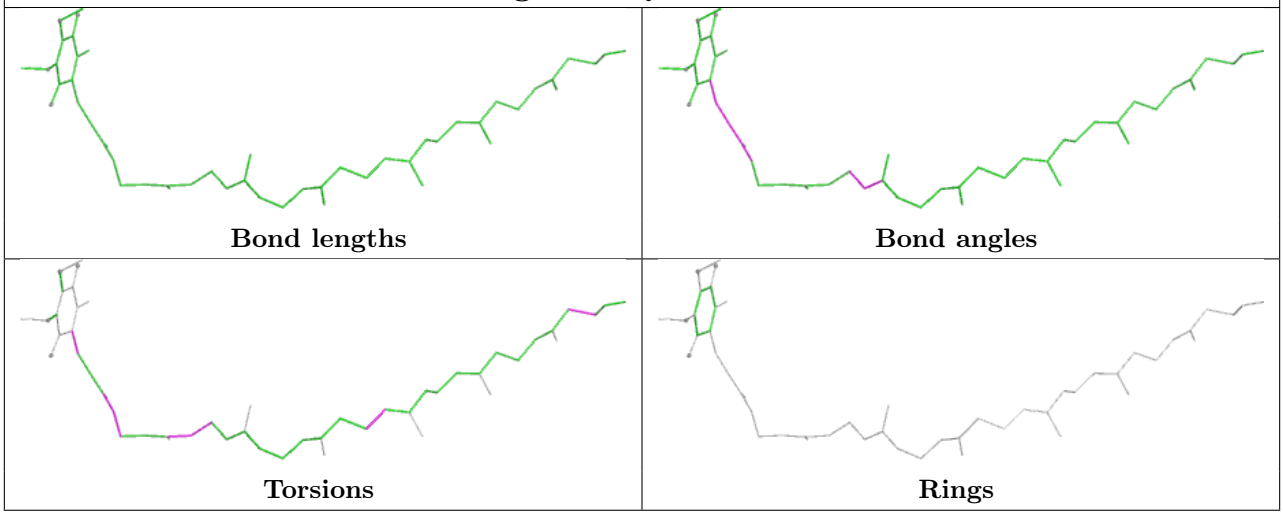
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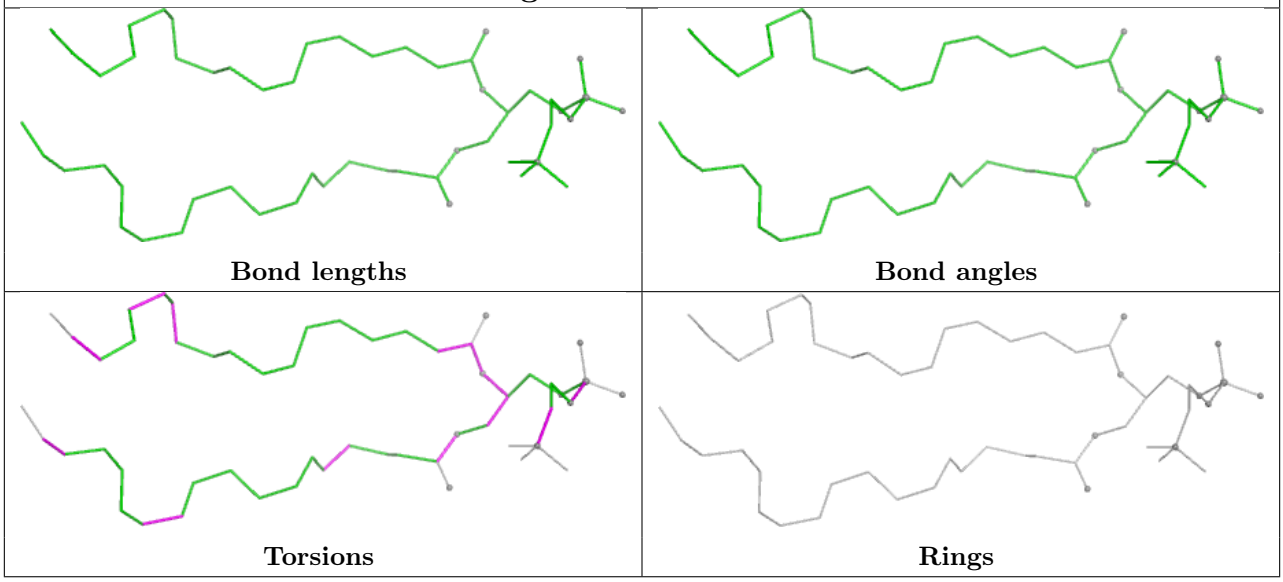
Mol	Chain	Res	Type	Clashes	Symm-Clashes
167	ED	603	UQ8	2	0
150	Dd	706	CDL	1	0
150	Dr	402	CDL	3	0
153	EO	201	PC1	2	0
158	CB	1000	FES	2	0
169	Da	702	HEA	1	0
158	E	302	FES	1	0
150	DS	404	CDL	2	0
150	CD	301	CDL	1	0
150	EH	1601	CDL	5	0

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

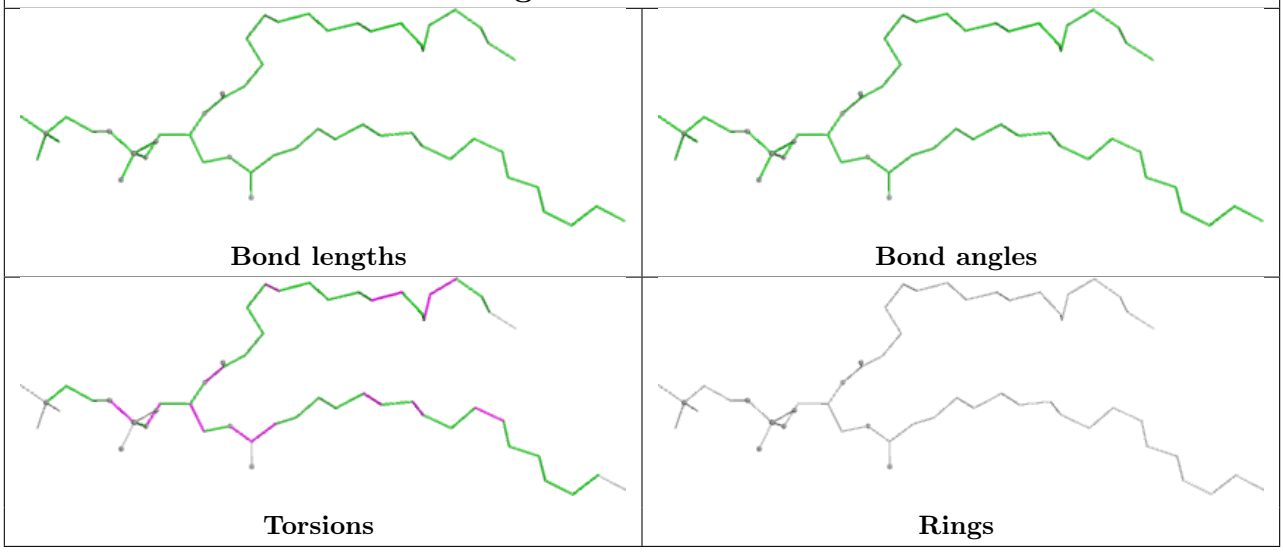
Ligand UQ8 CC 303



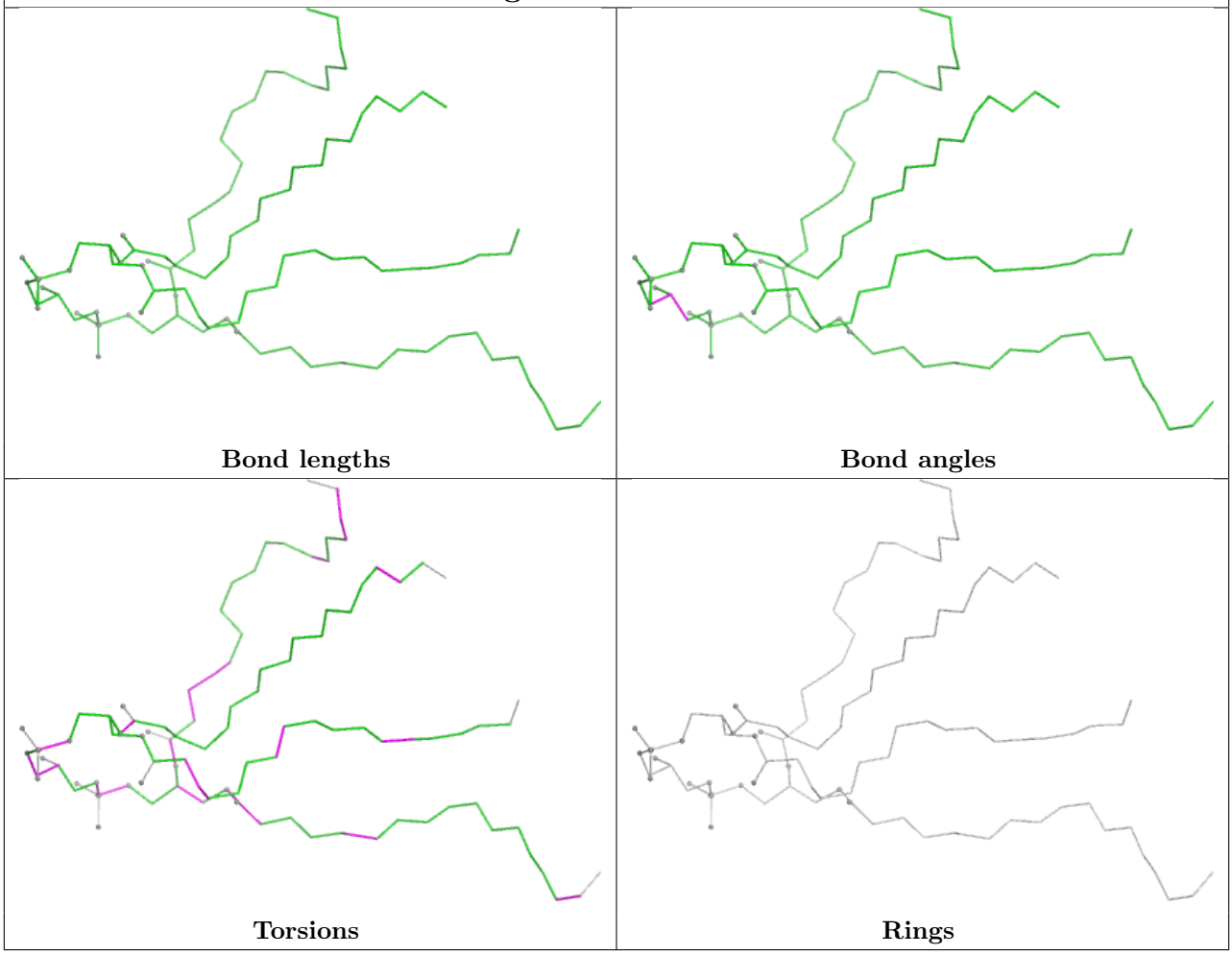
Ligand PC1 Eo 204



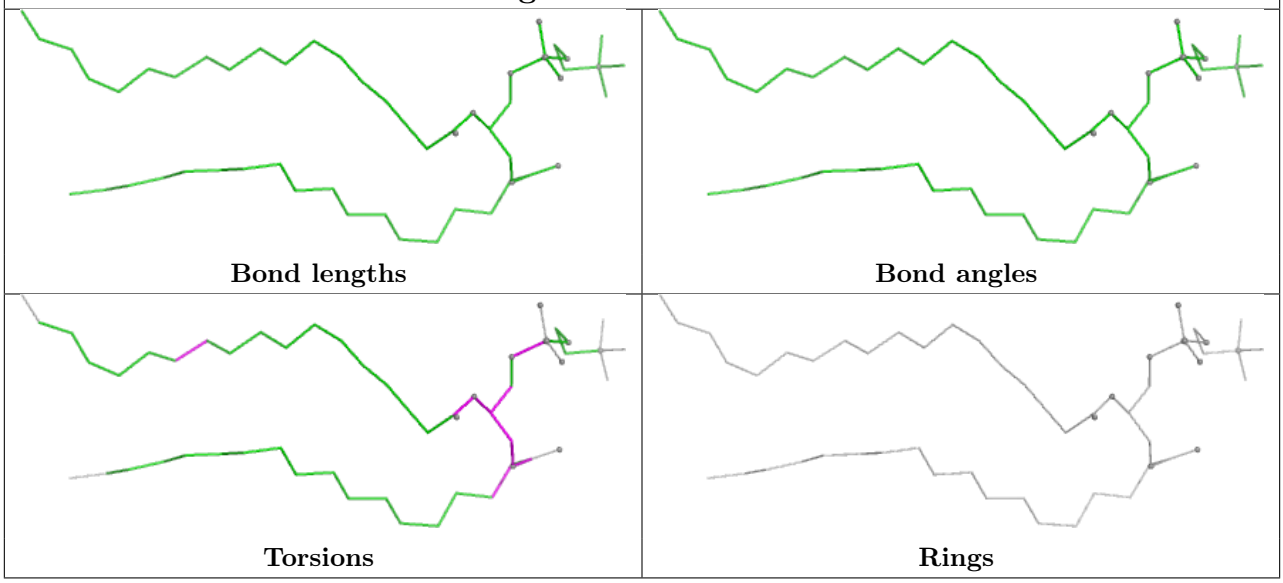
Ligand PC1 DA 707



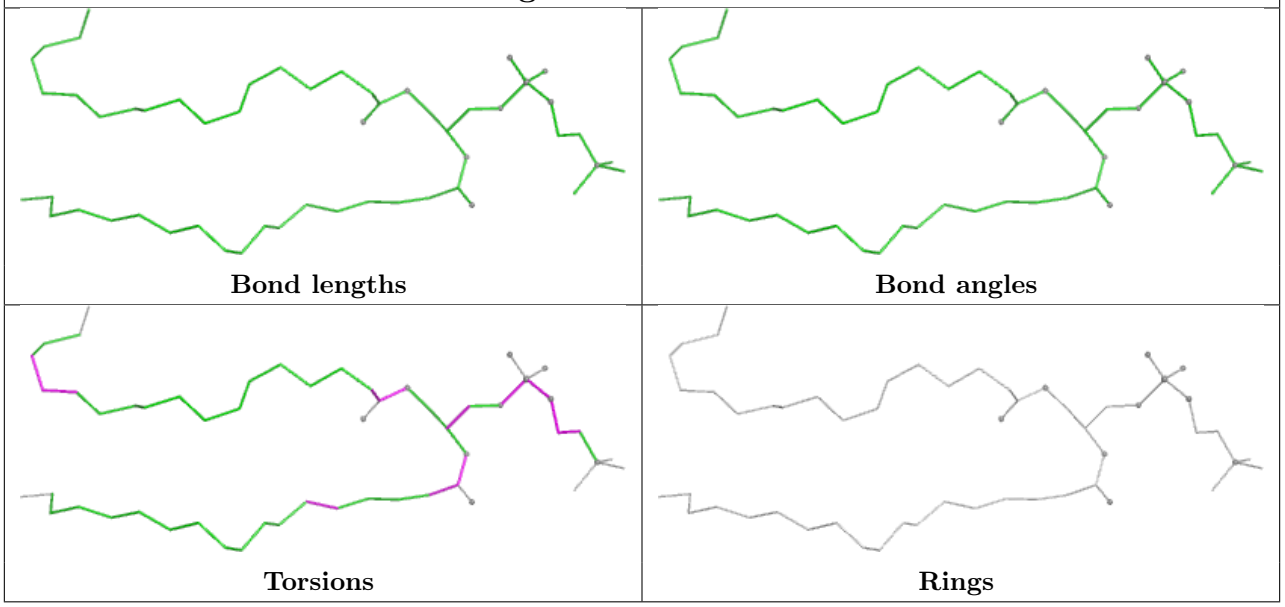
Ligand CDL C 506



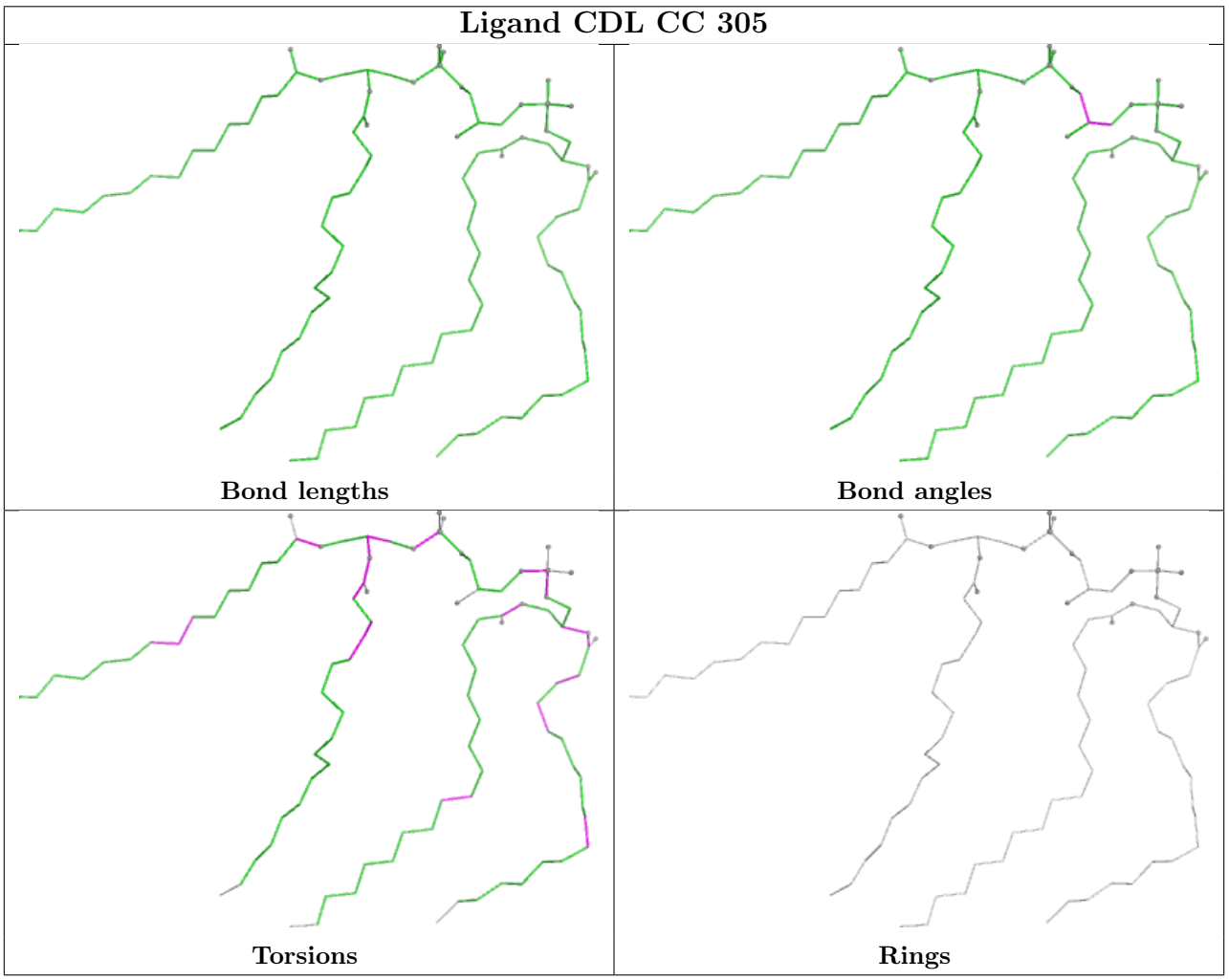
Ligand PC1 A1 403



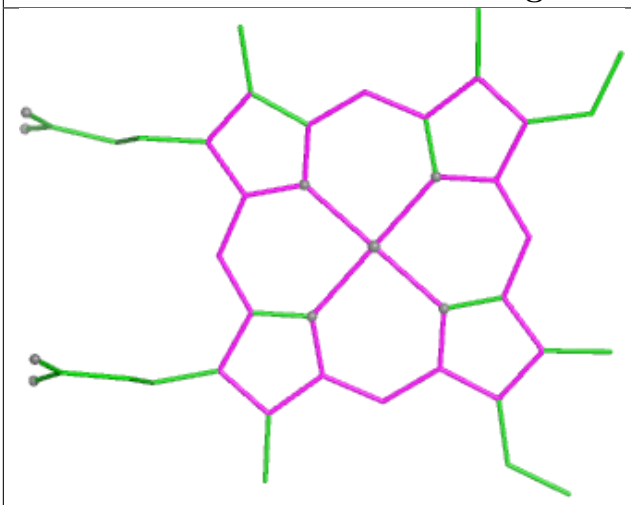
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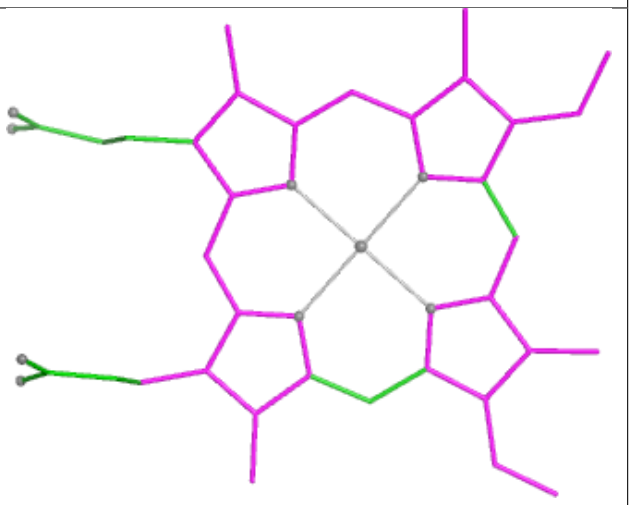
Ligand CDL CC 305



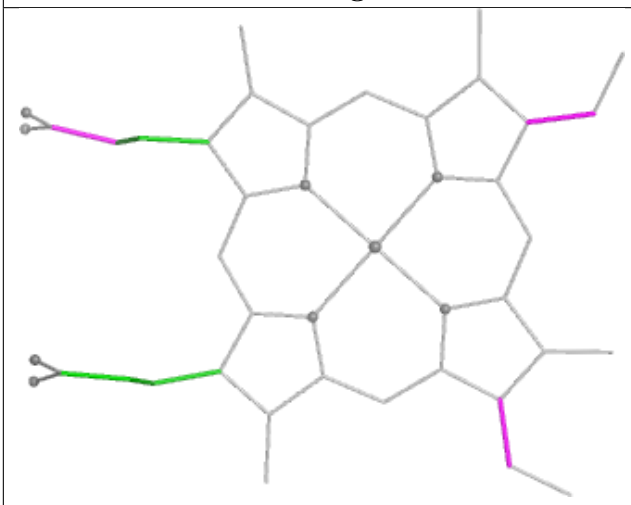
Ligand HEC d 802



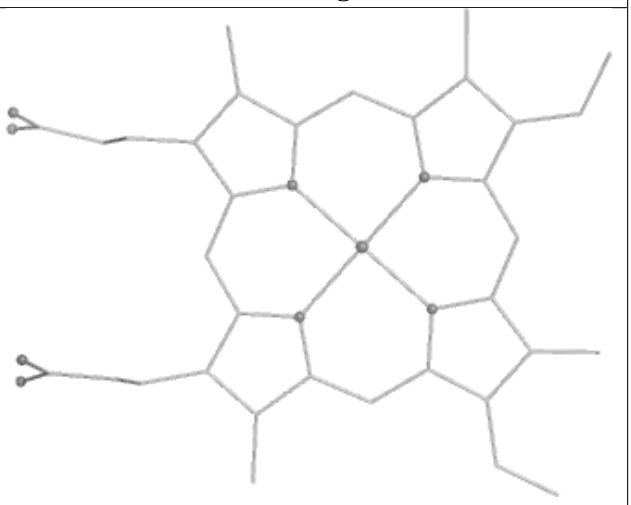
Bond lengths



Bond angles

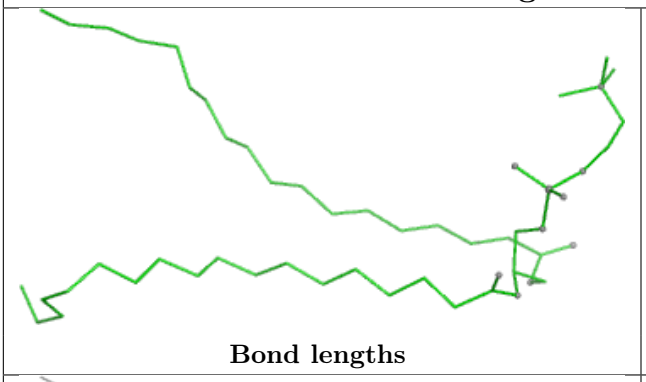


Torsions

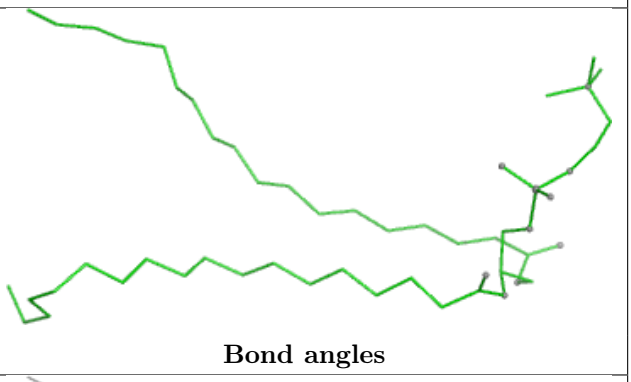


Rings

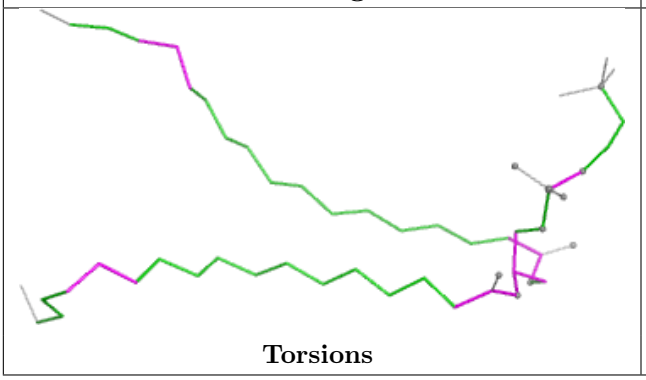
Ligand PC1 Dc 609



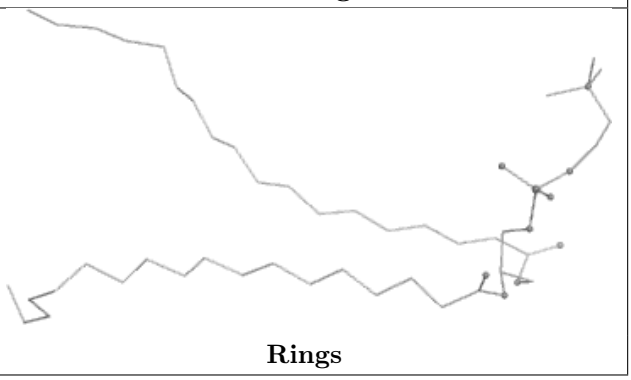
Bond lengths



Bond angles

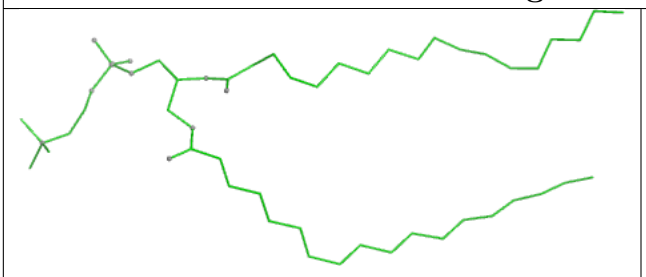


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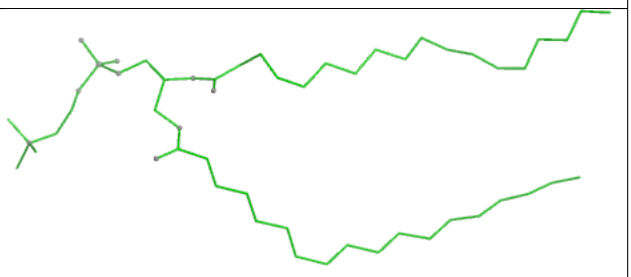


Rings

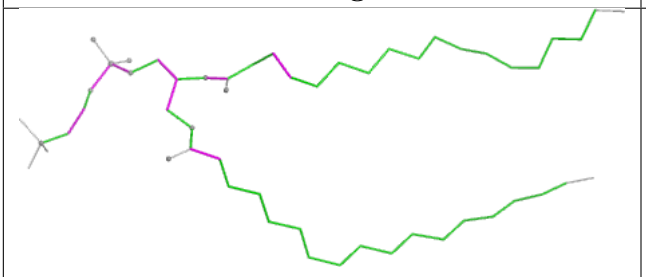
Ligand PC1 K 501



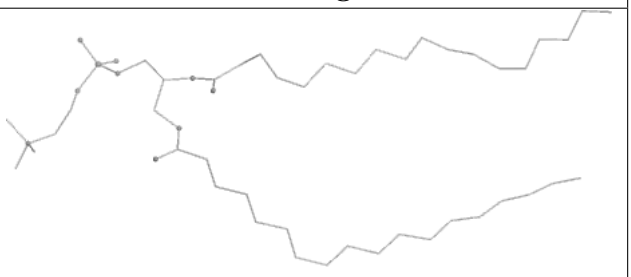
Bond lengths



Bond angles

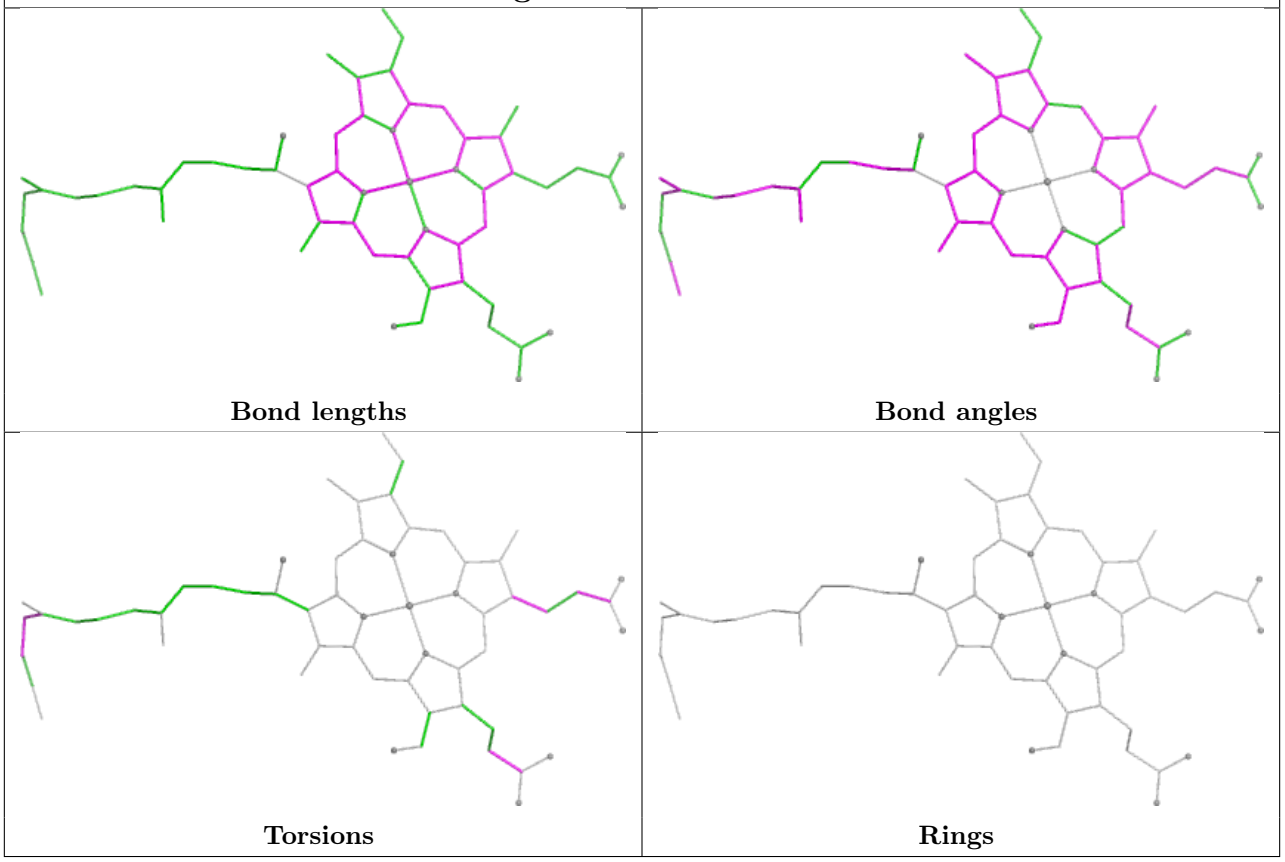


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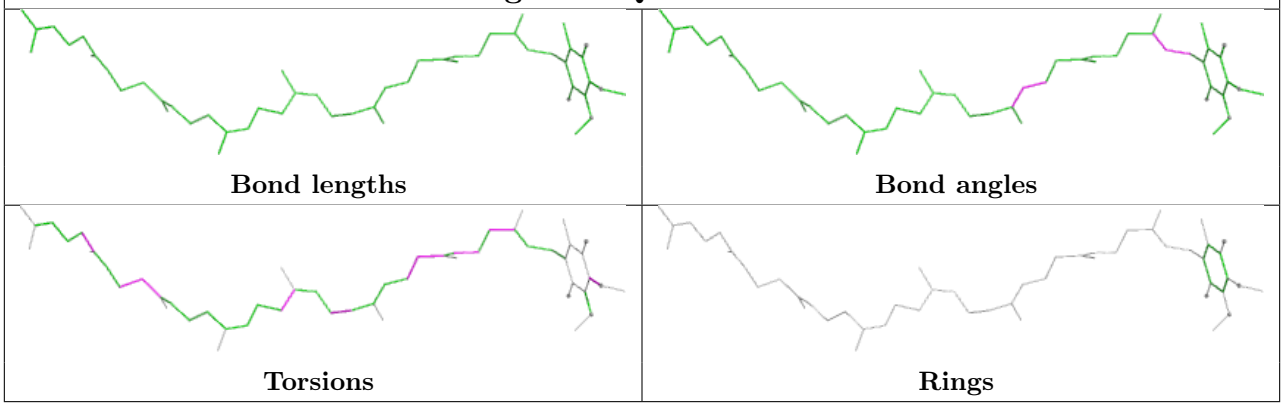


Rings

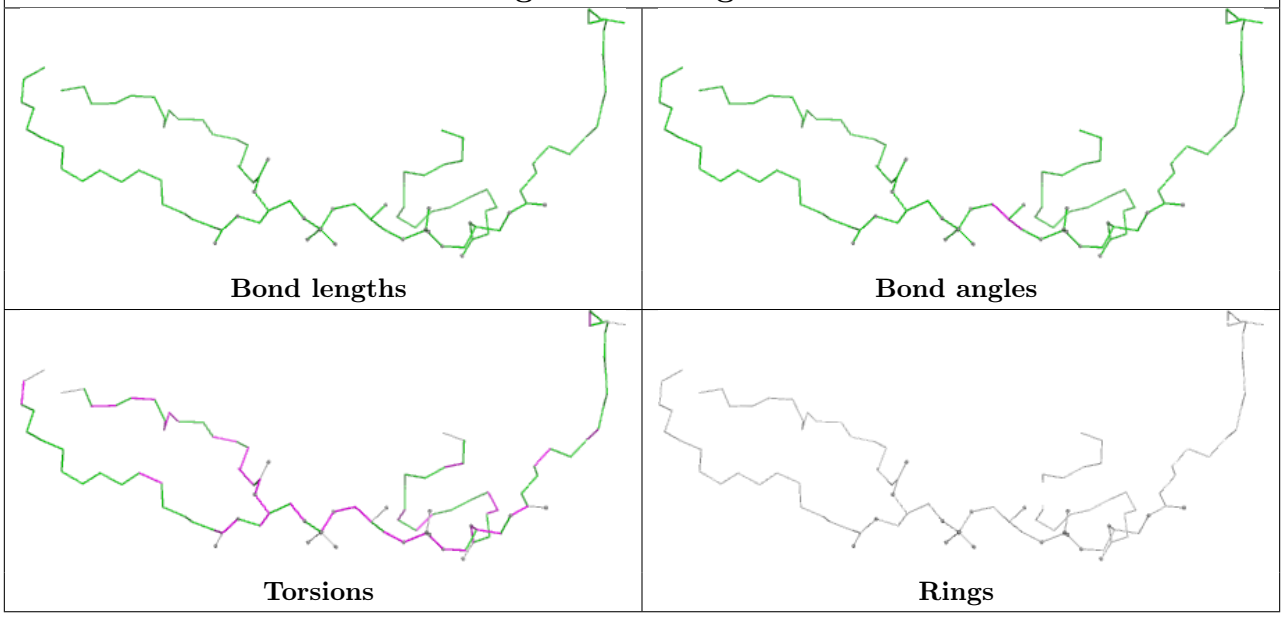
Ligand HEA Da 703



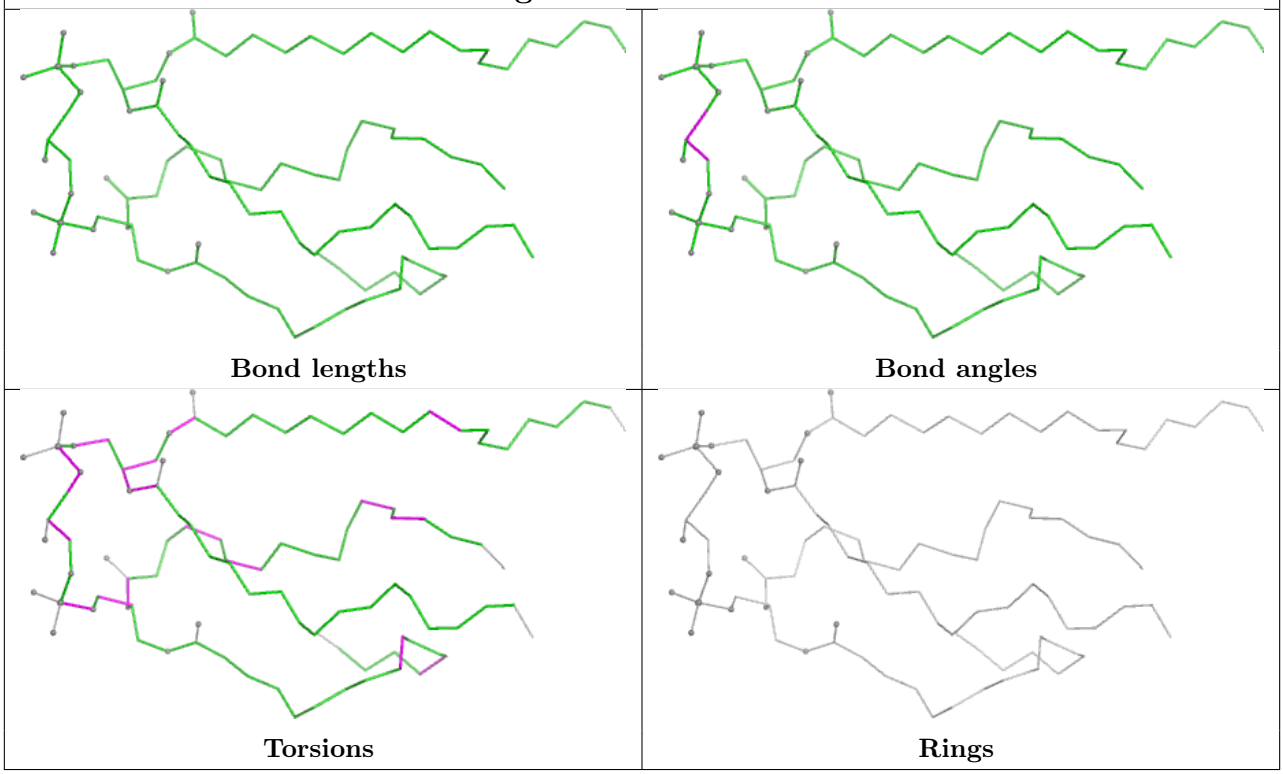
Ligand UQ8 EN 1205



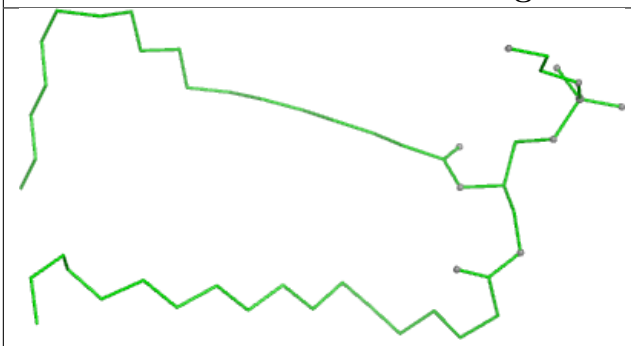
Ligand CDL Dg 201



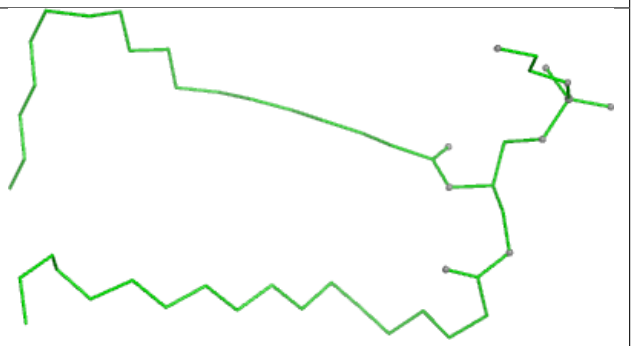
Ligand CDL DJ 305



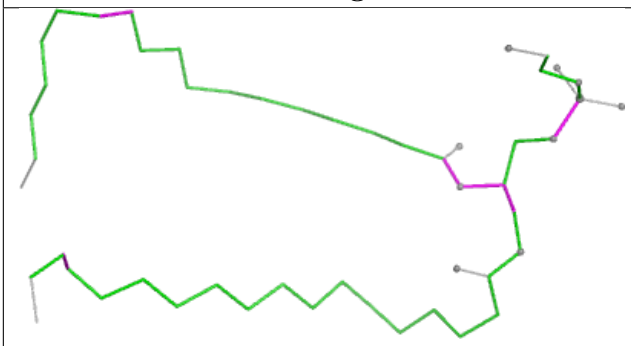
Ligand 3PE DC 606



Bond lengths



Bond angles

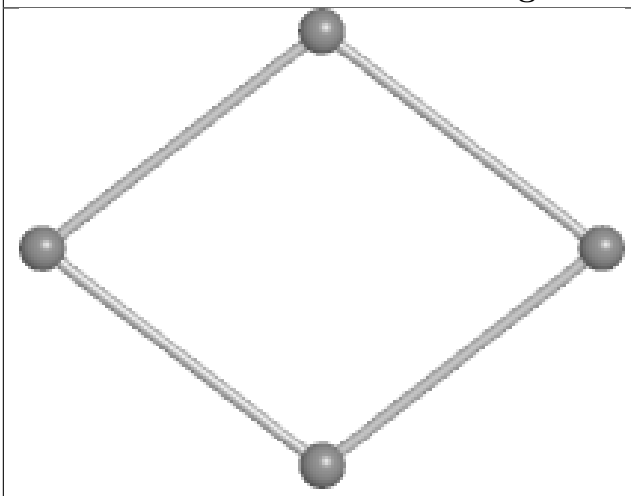


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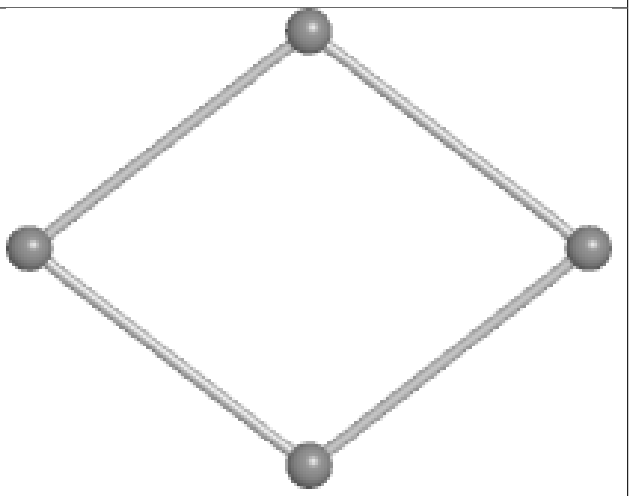


Rings

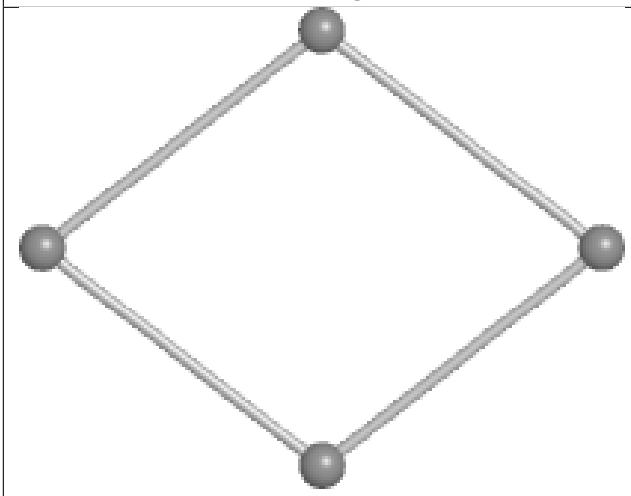
Ligand FES EF 201



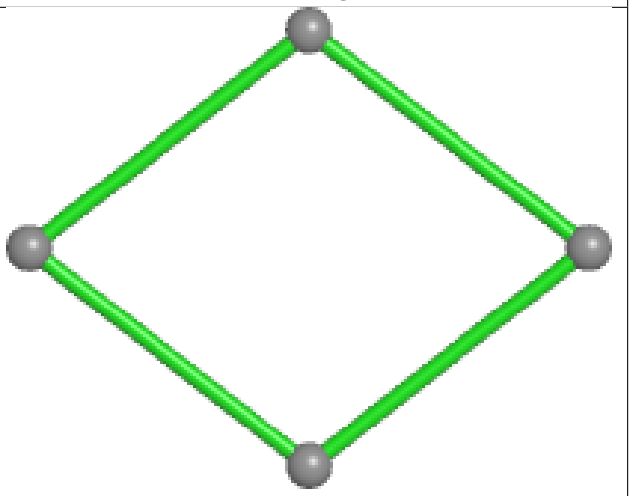
Bond lengths



Bond angles

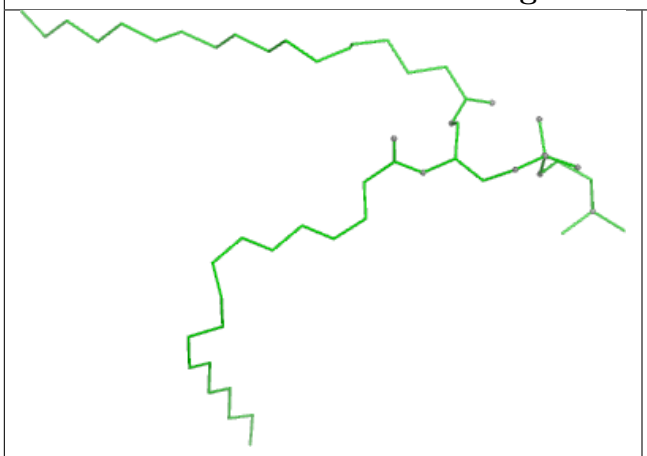


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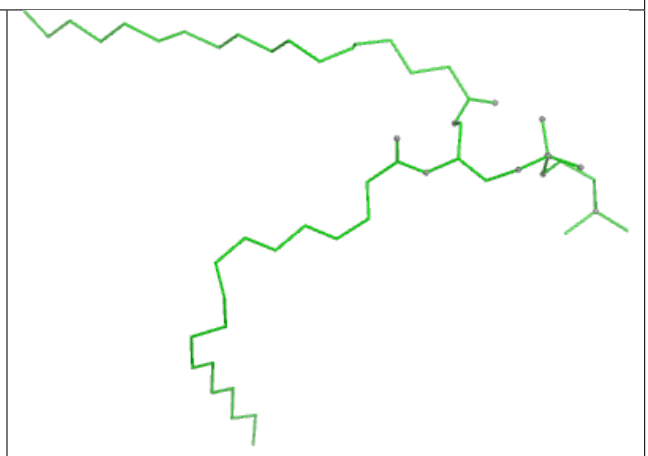


Rings

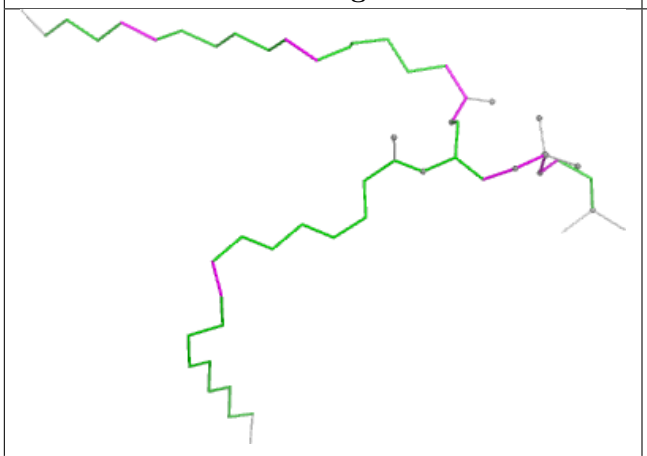
Ligand PC1 Eb 301



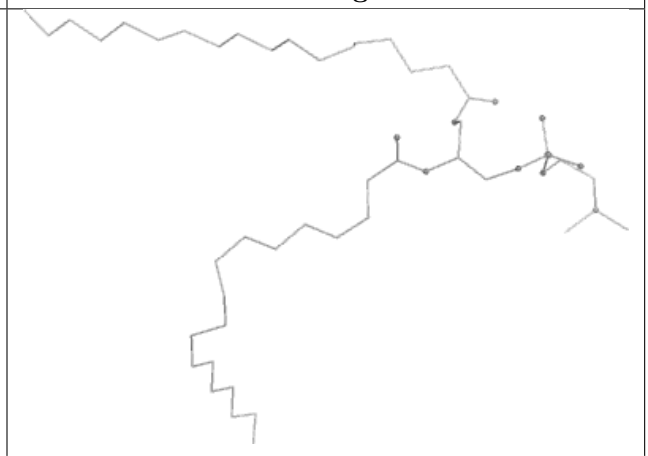
Bond lengths



Bond angles

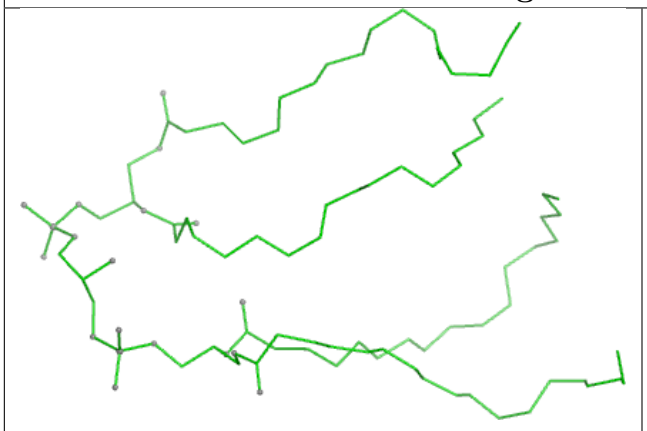


Torsions

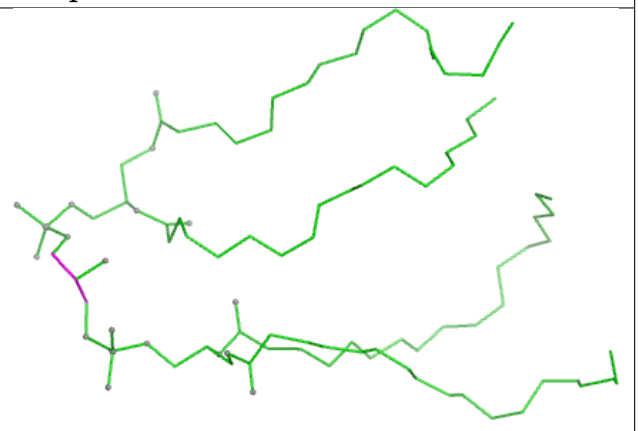


Rings

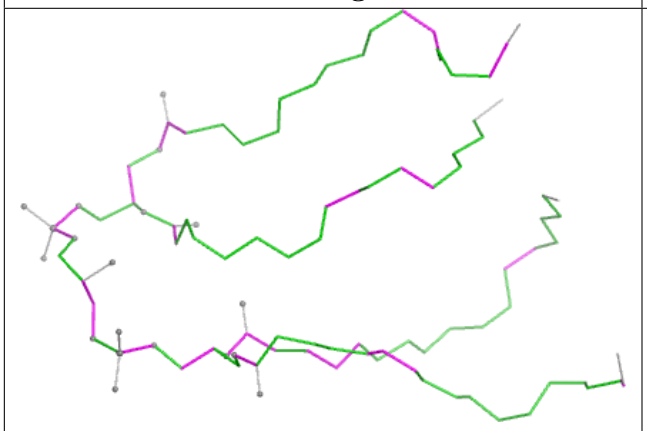
Ligand CDL Ep 701



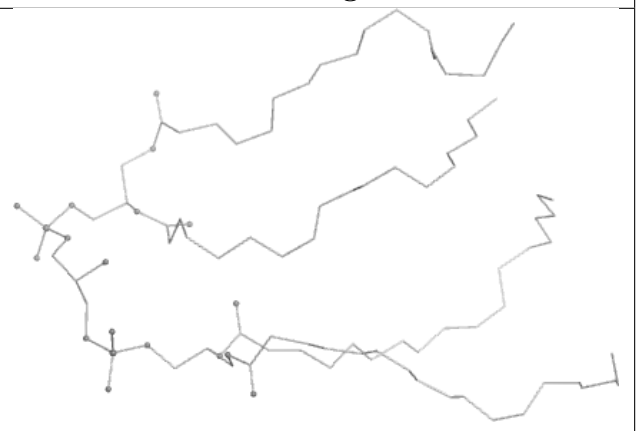
Bond lengths



Bond angles

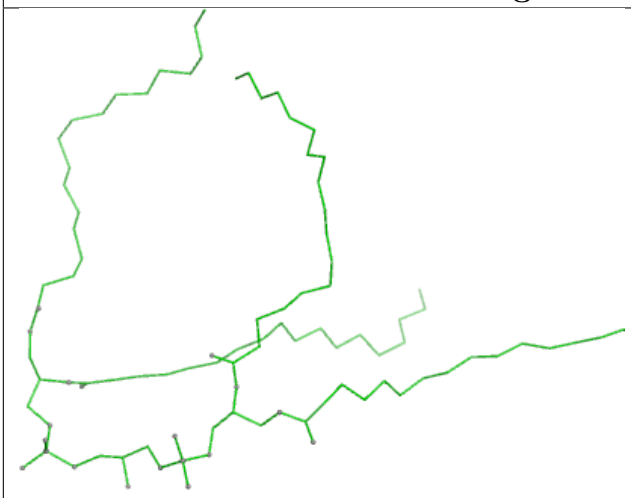


Torsions



Rings

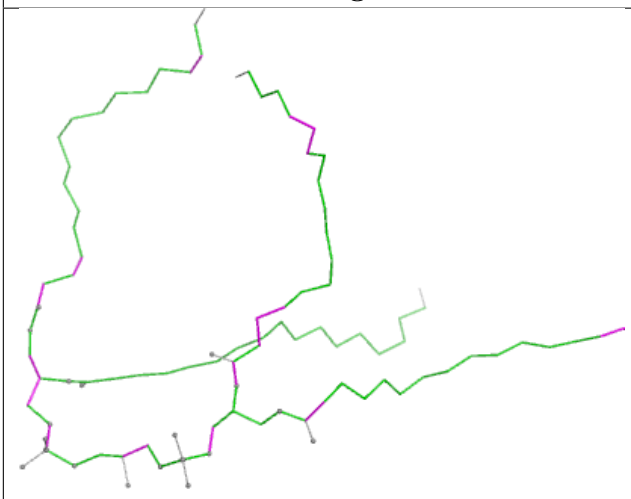
Ligand CDL BL 301



Bond lengths



Bond angles

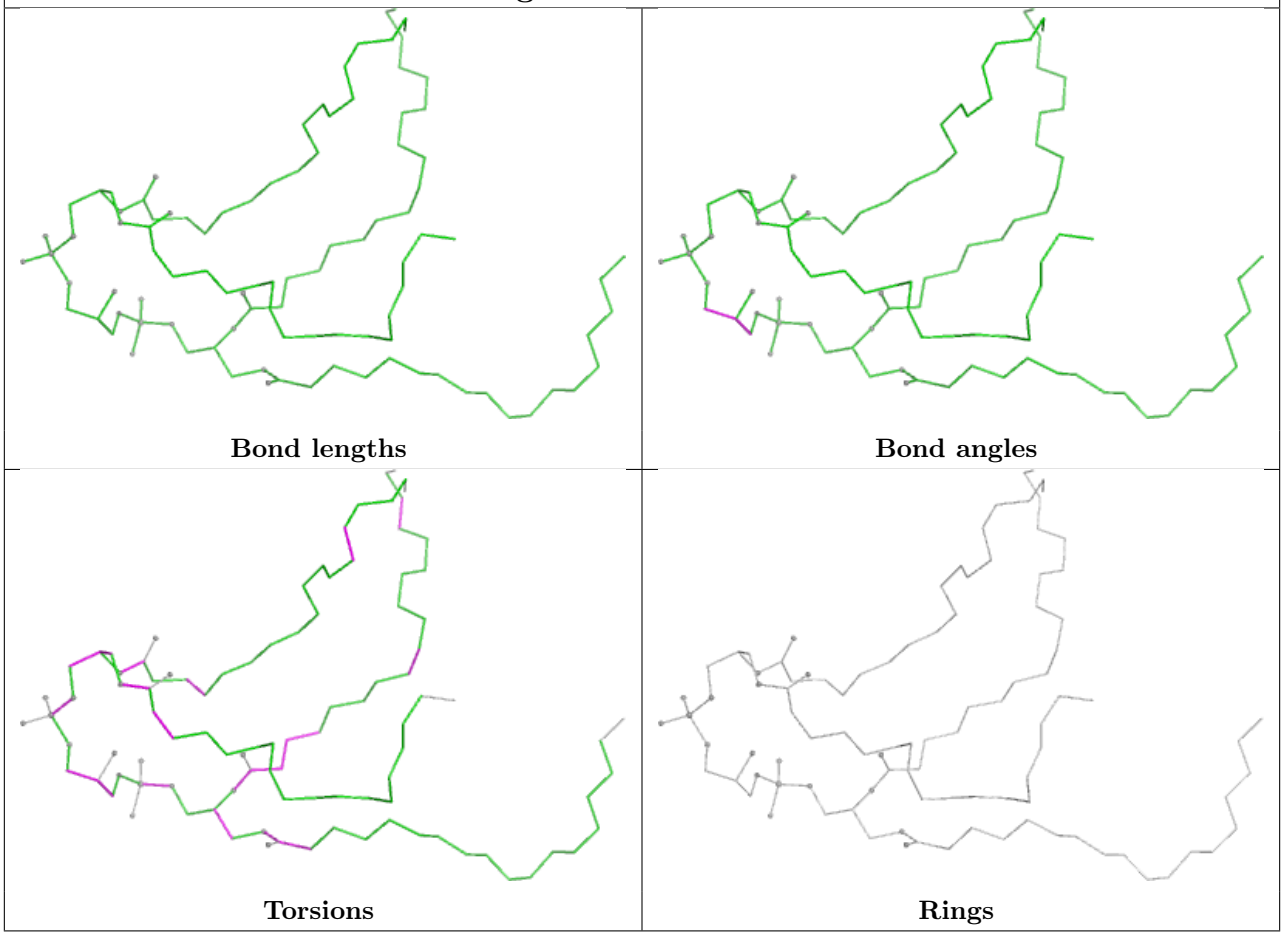


Torsions

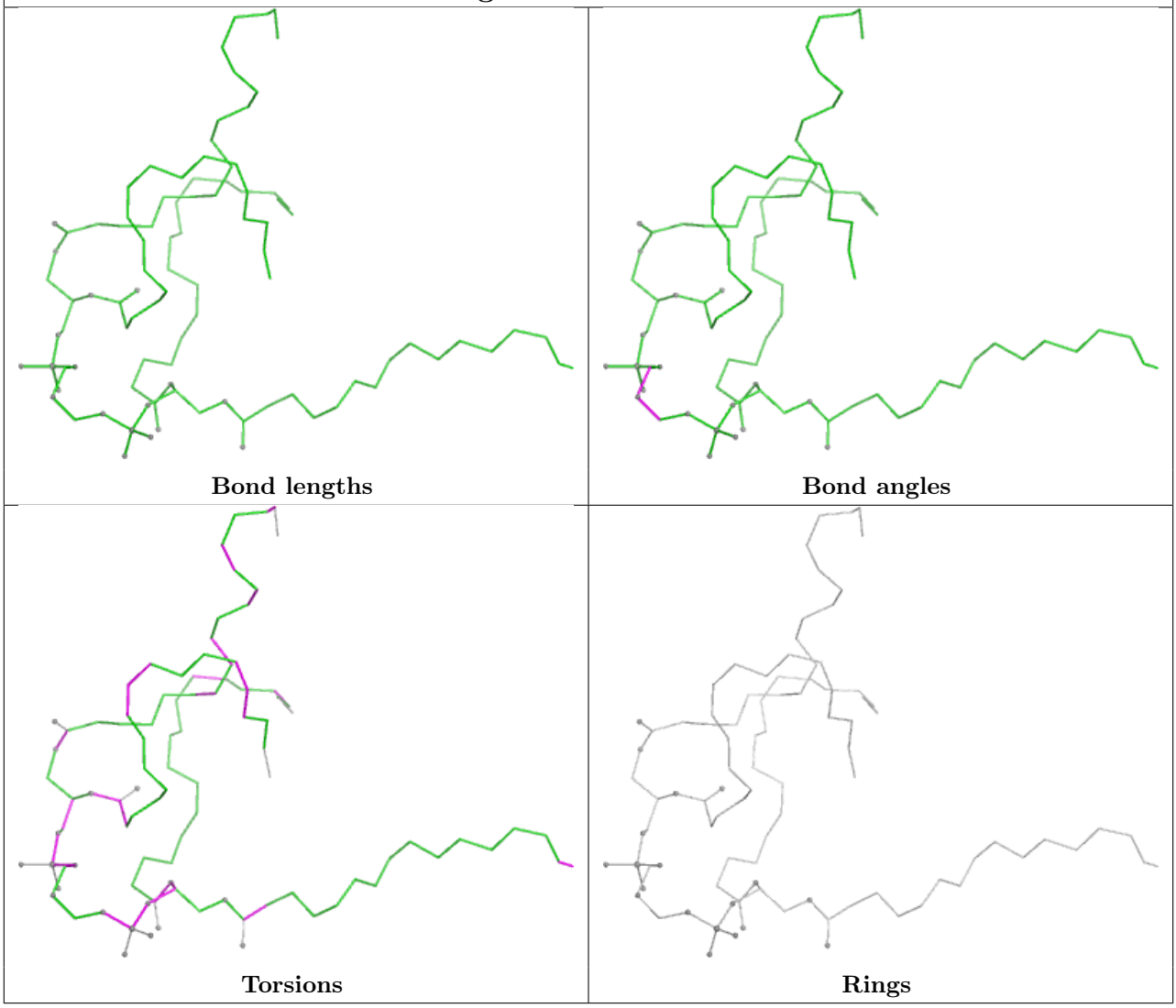


Rings

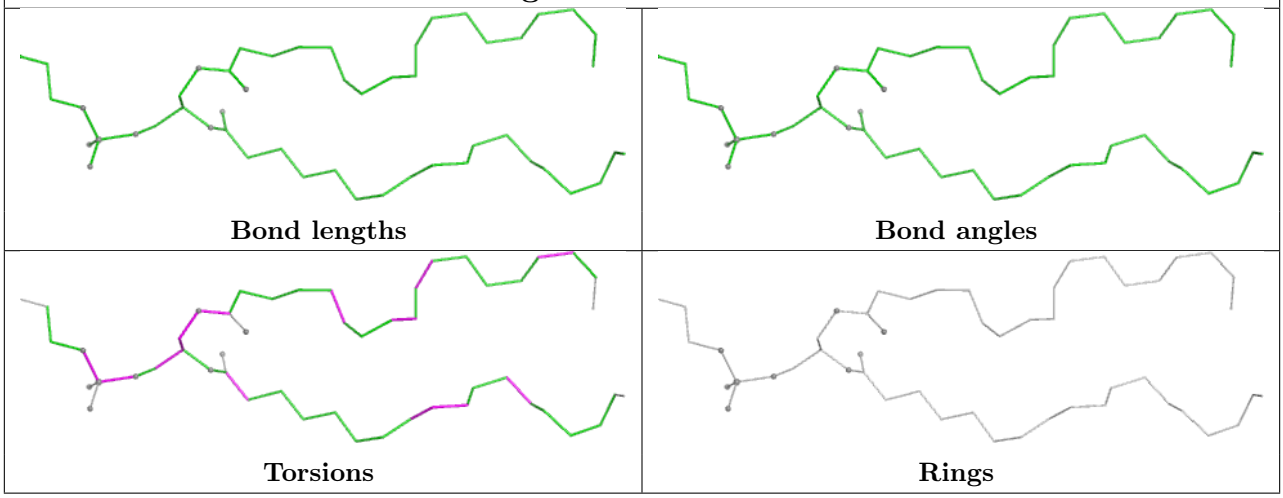
Ligand CDL Ed 205



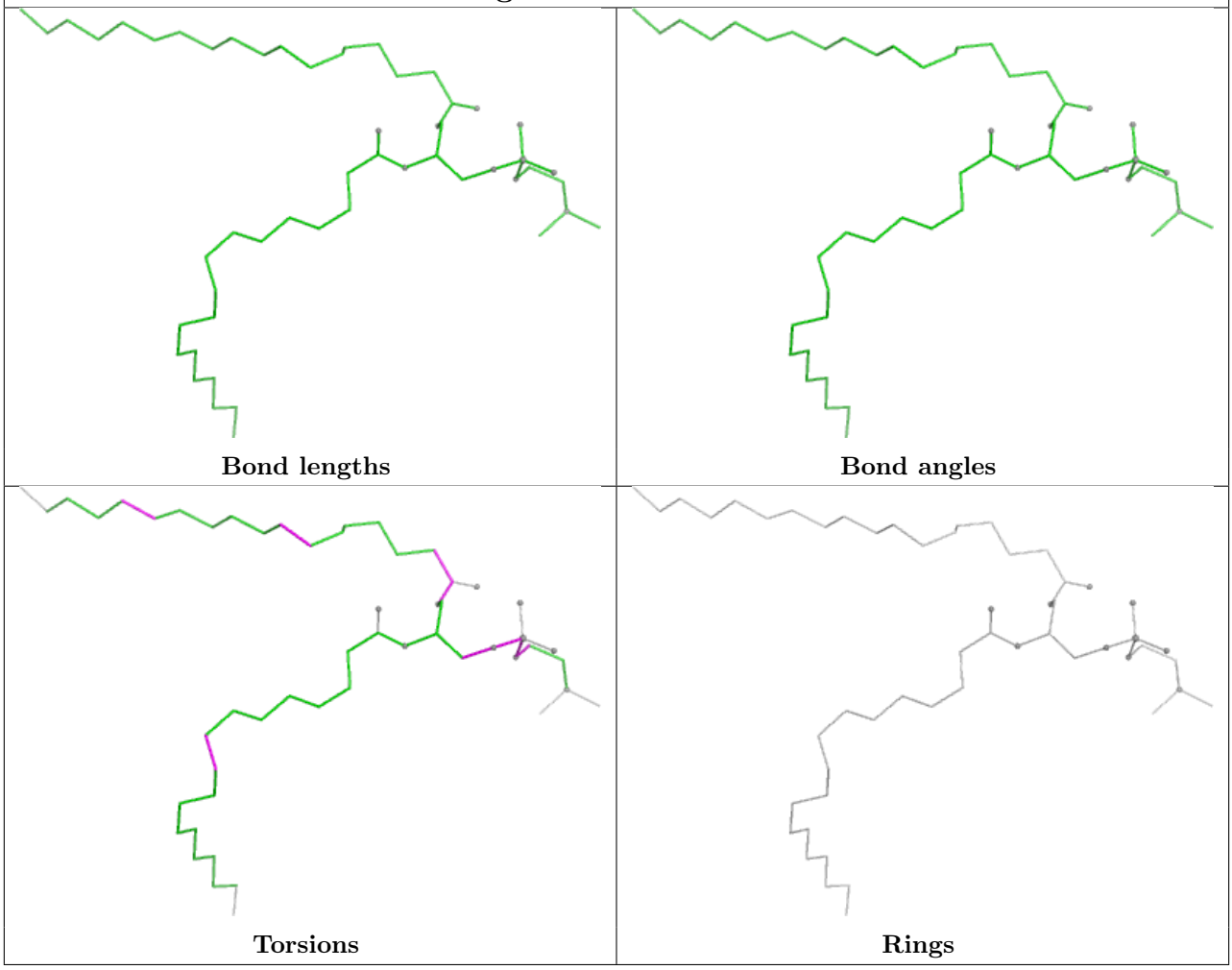
Ligand CDL El 903



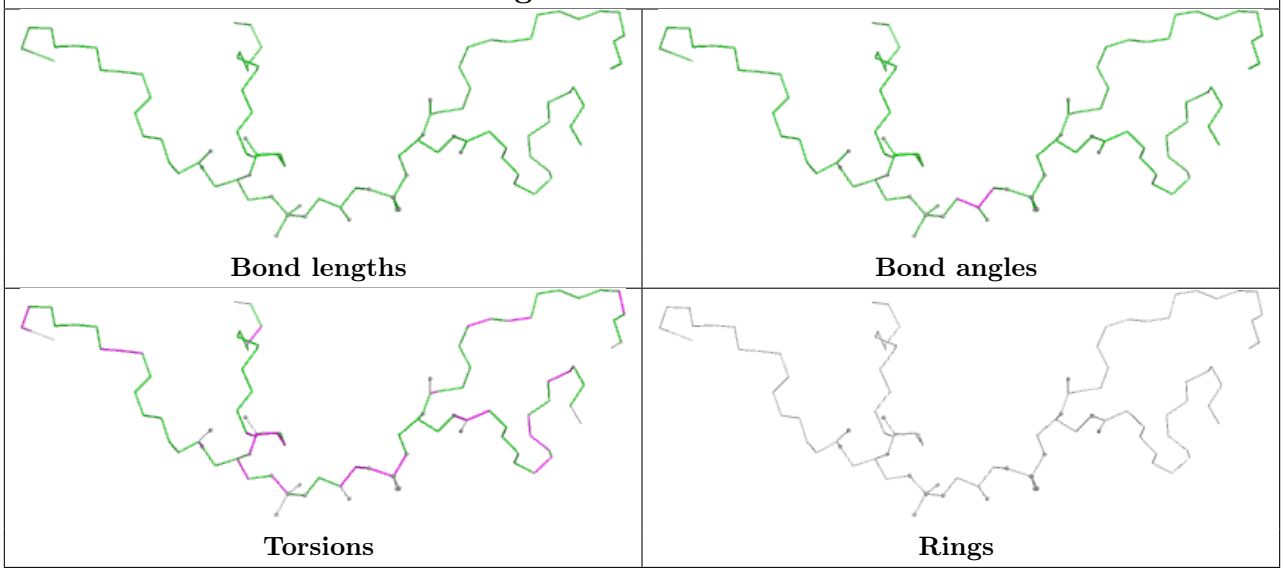
Ligand 3PE Ds 403



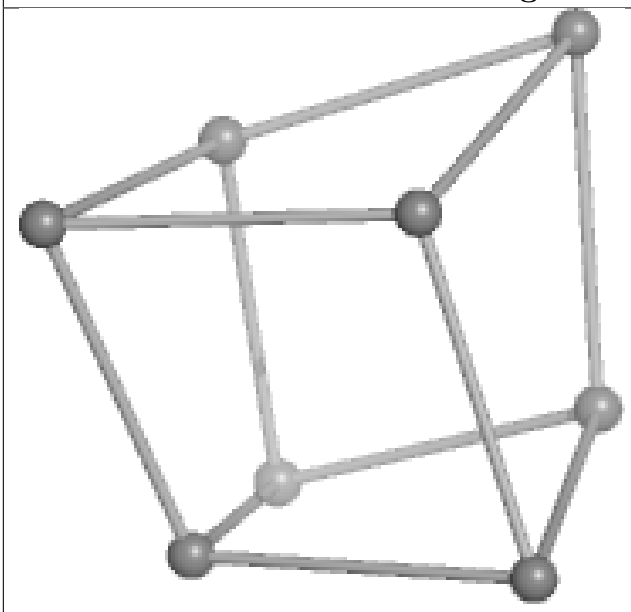
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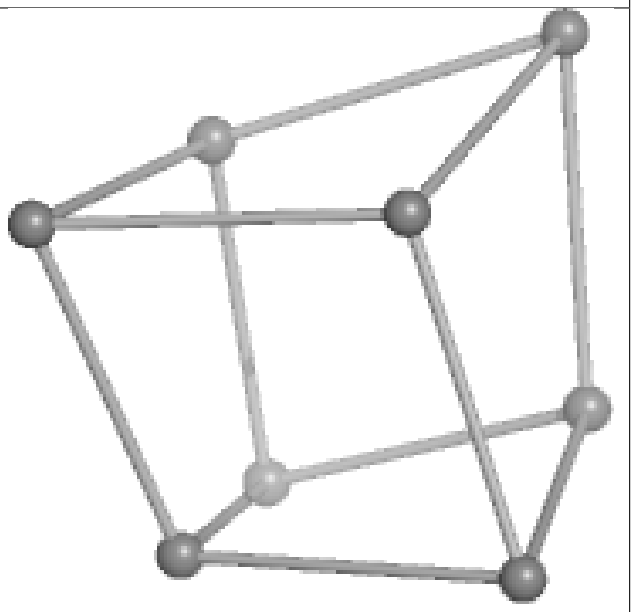
Ligand CDL Dv 402



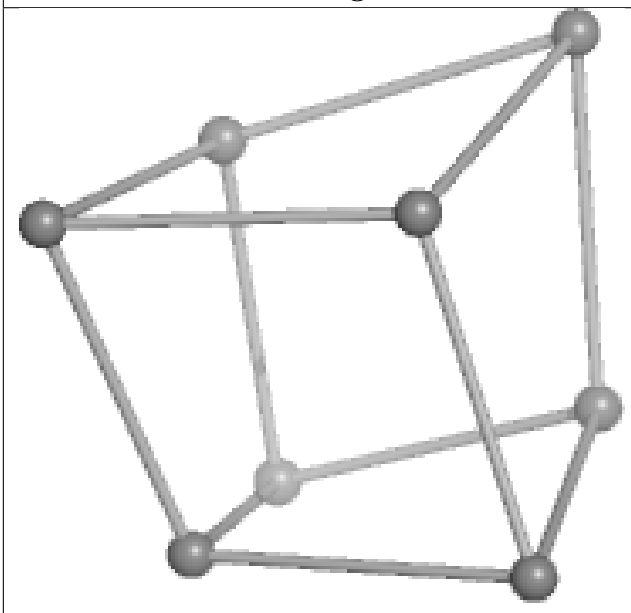
Ligand SF4 AL 302



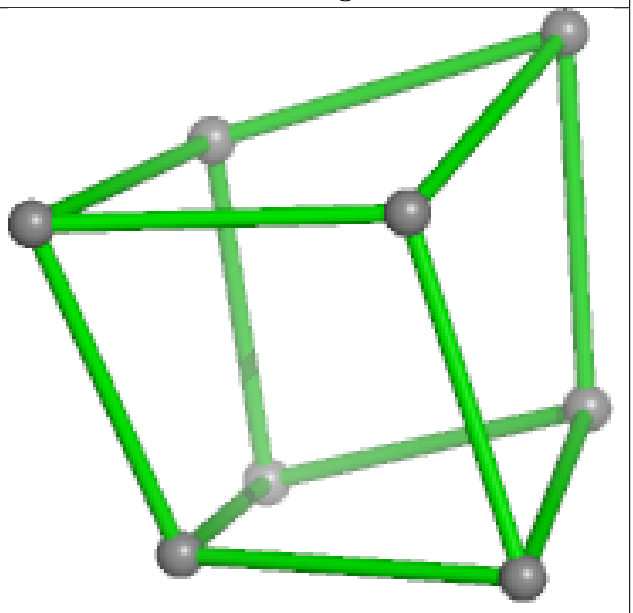
Bond lengths



Bond angles



Torsions



Rings

Ligand PC1 Eb 303



Bond lengths



Bond angles

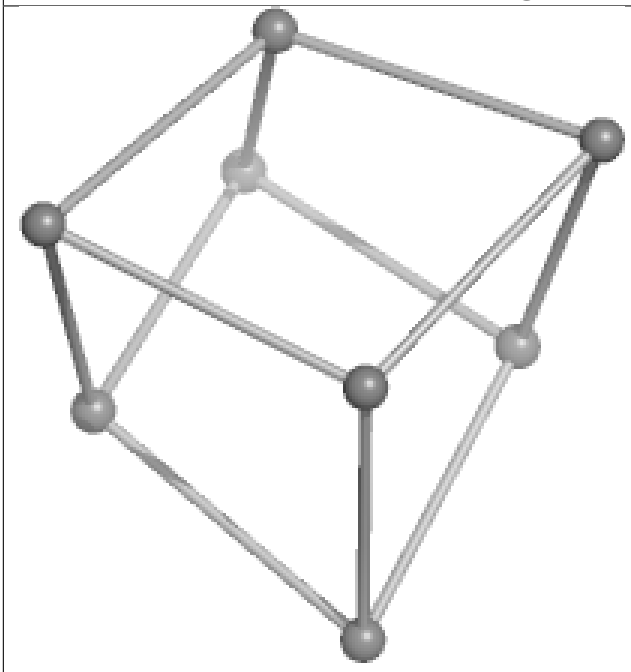


Torsions

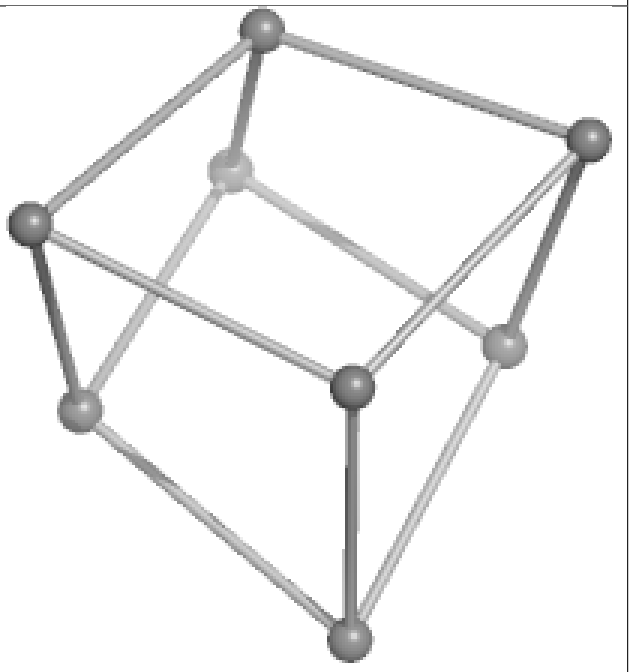


Rings

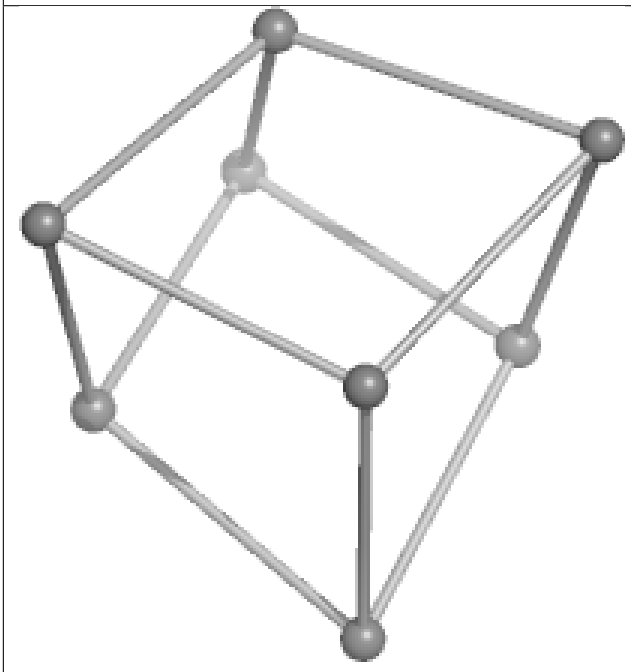
Ligand SF4 AB 803



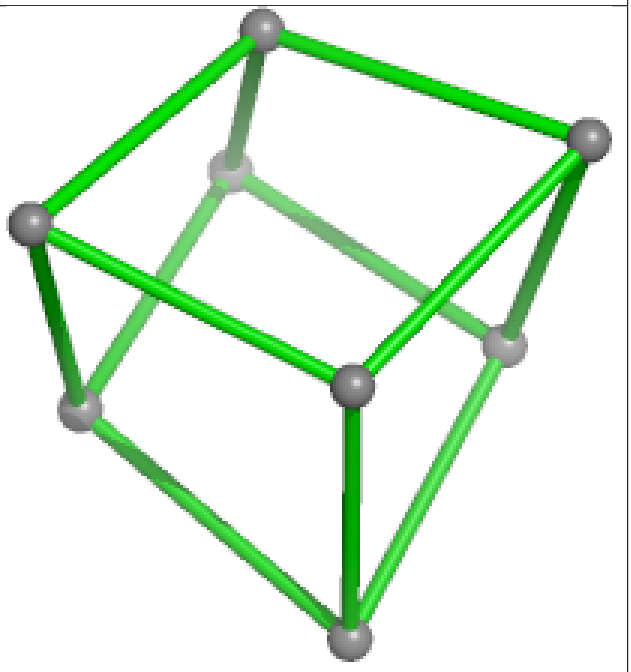
Bond lengths



Bond angles

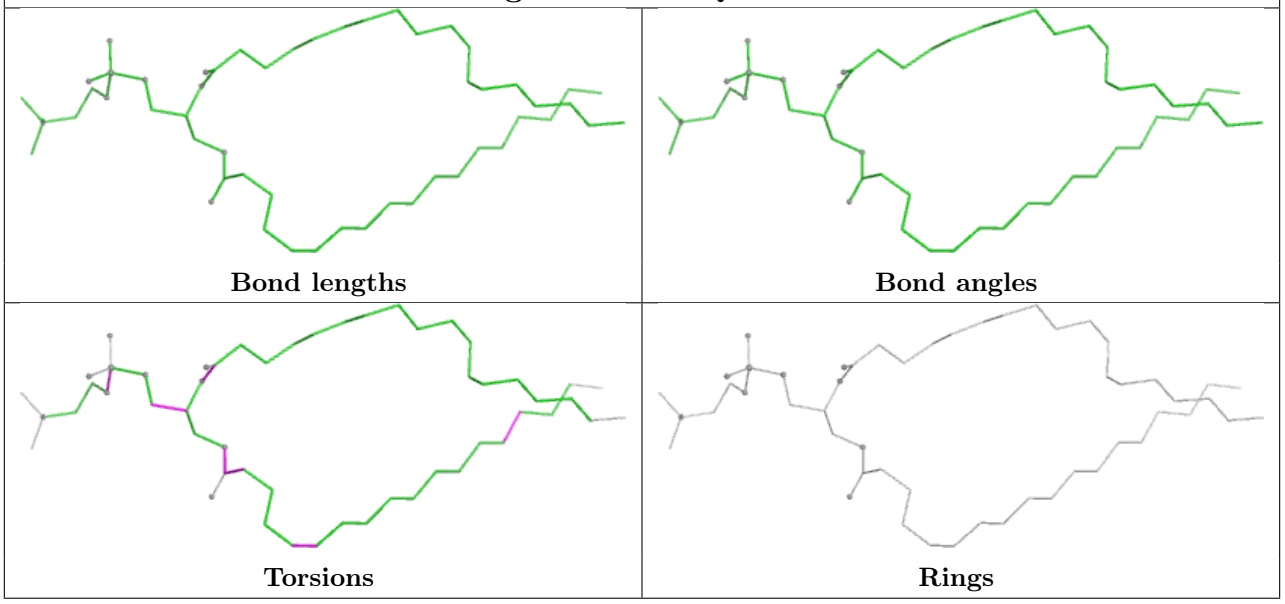


Torsions

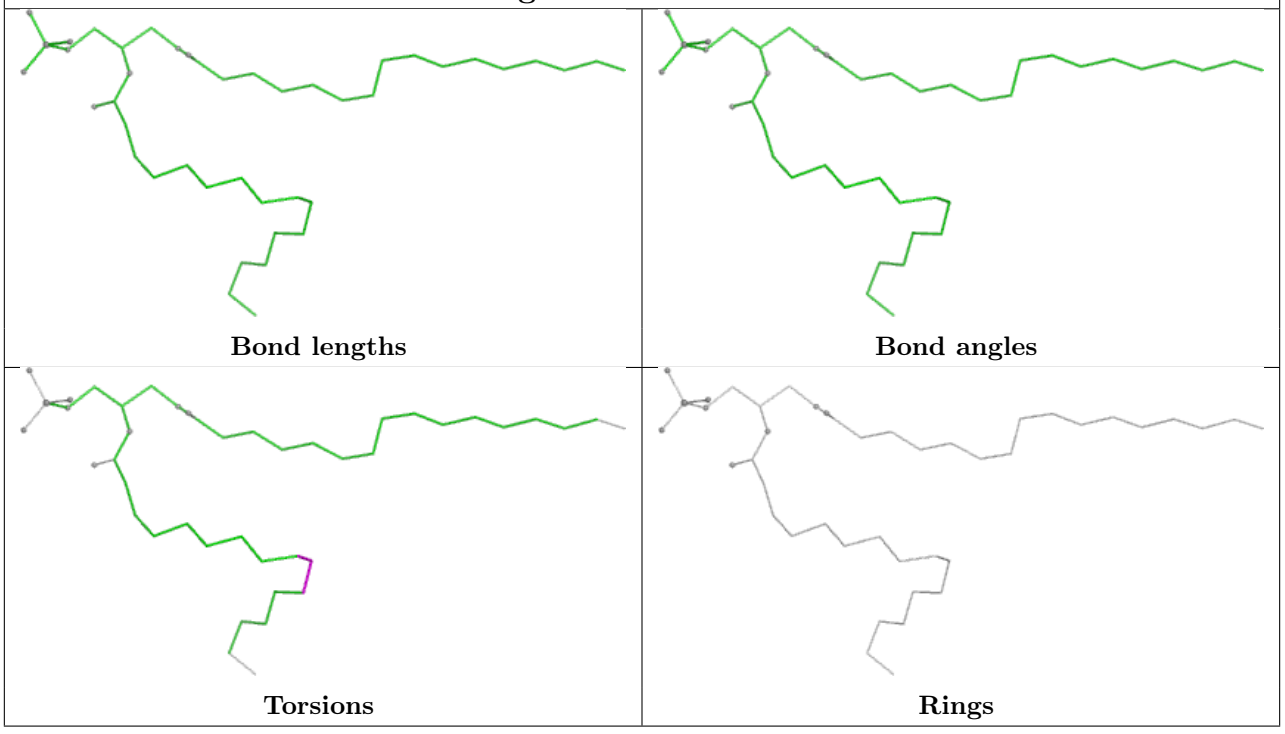


Rings

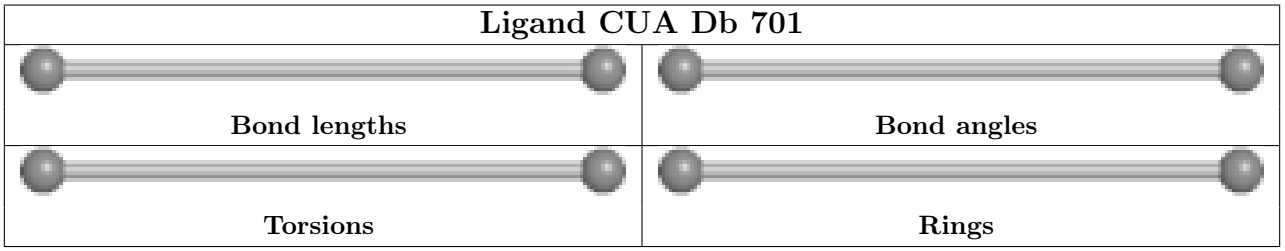
Ligand PC1 DQ 1503



Ligand LPP Ed 203



Ligand CUA Db 701



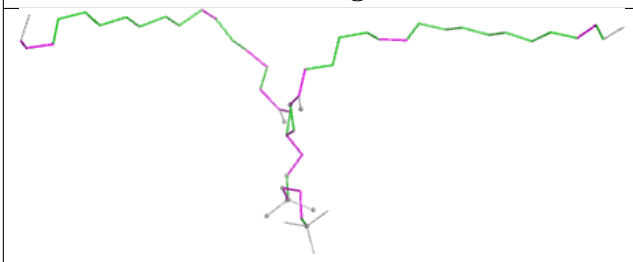
Ligand PC1 C 509



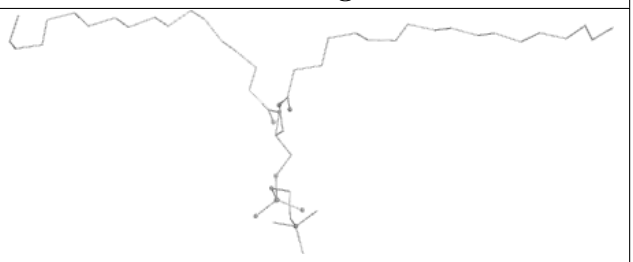
Bond lengths



Bond angles

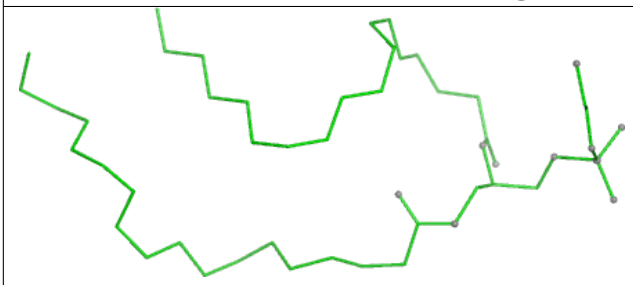


Torsions

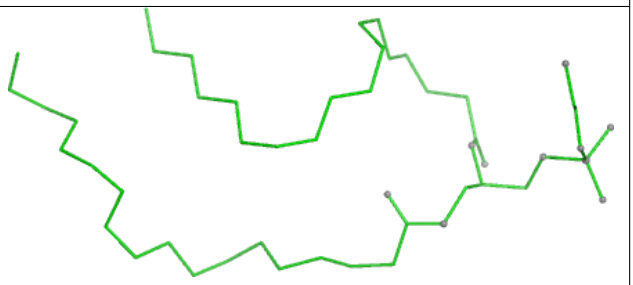


Rings

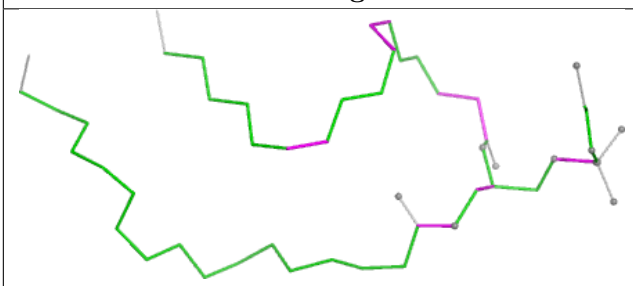
Ligand 3PE EM 901



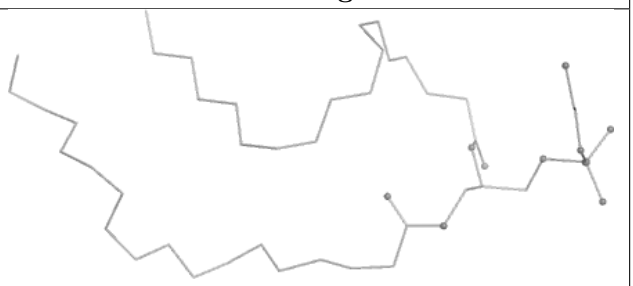
Bond lengths



Bond angles



Torsions



Rings

Ligand CUA DB 701



Bond lengths



Bond angles

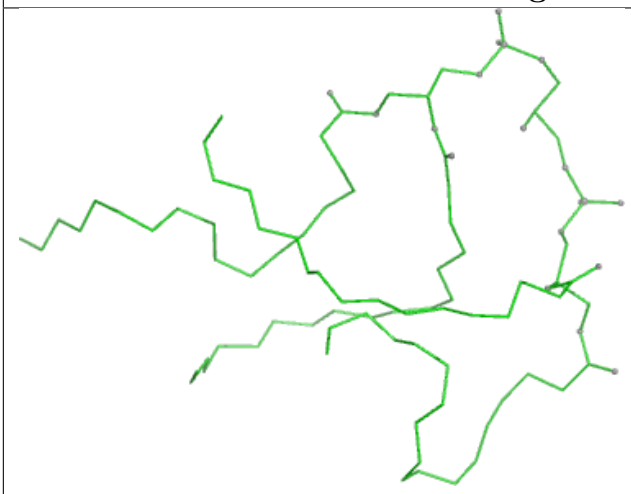


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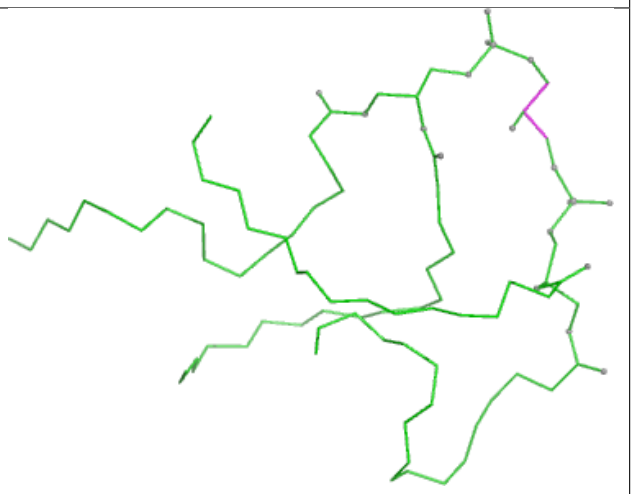


Rings

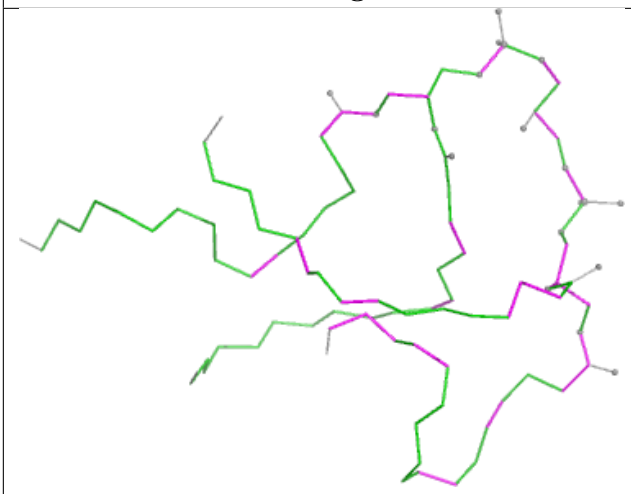
Ligand CDL c 509



Bond lengths



Bond angles

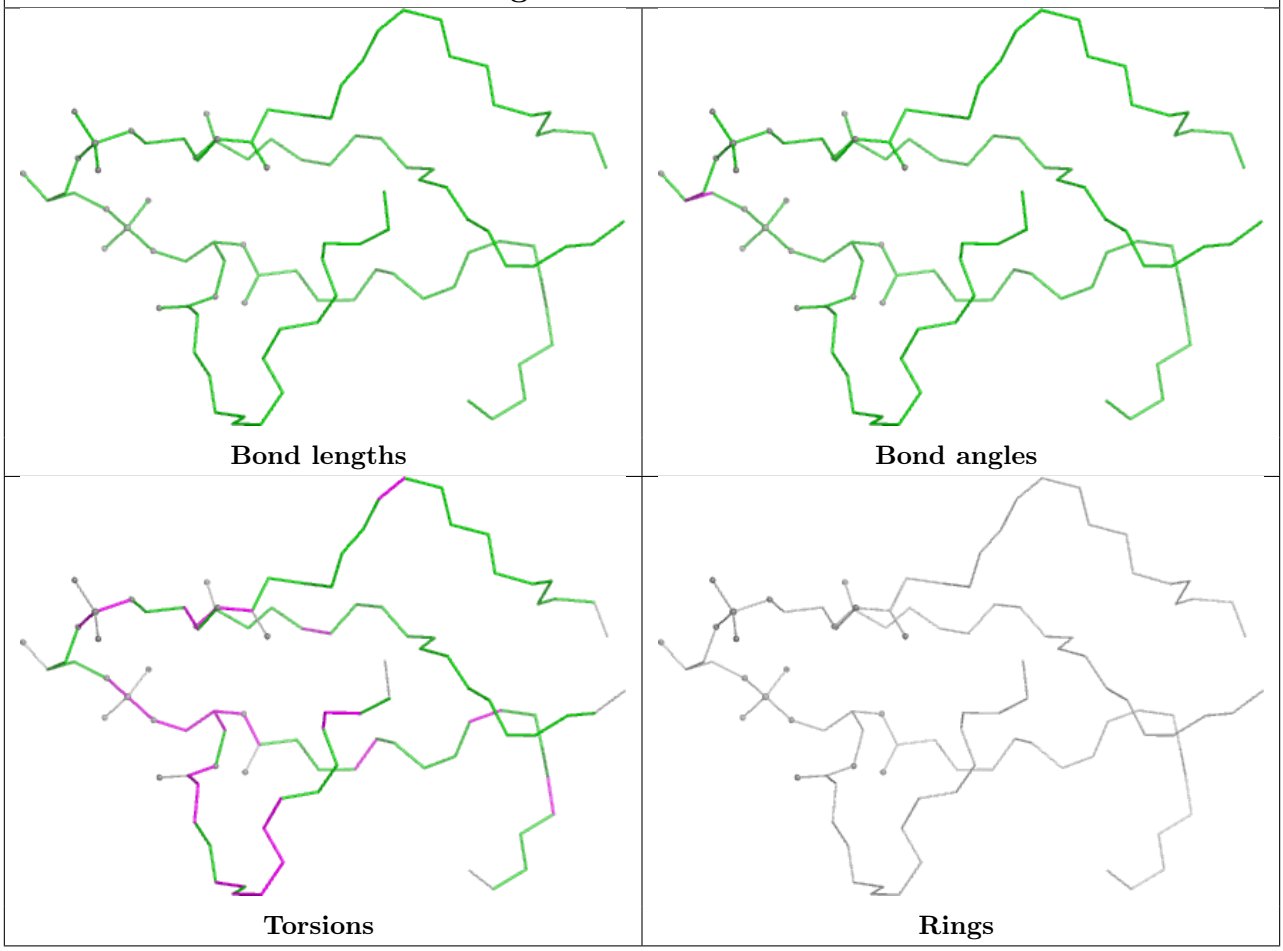


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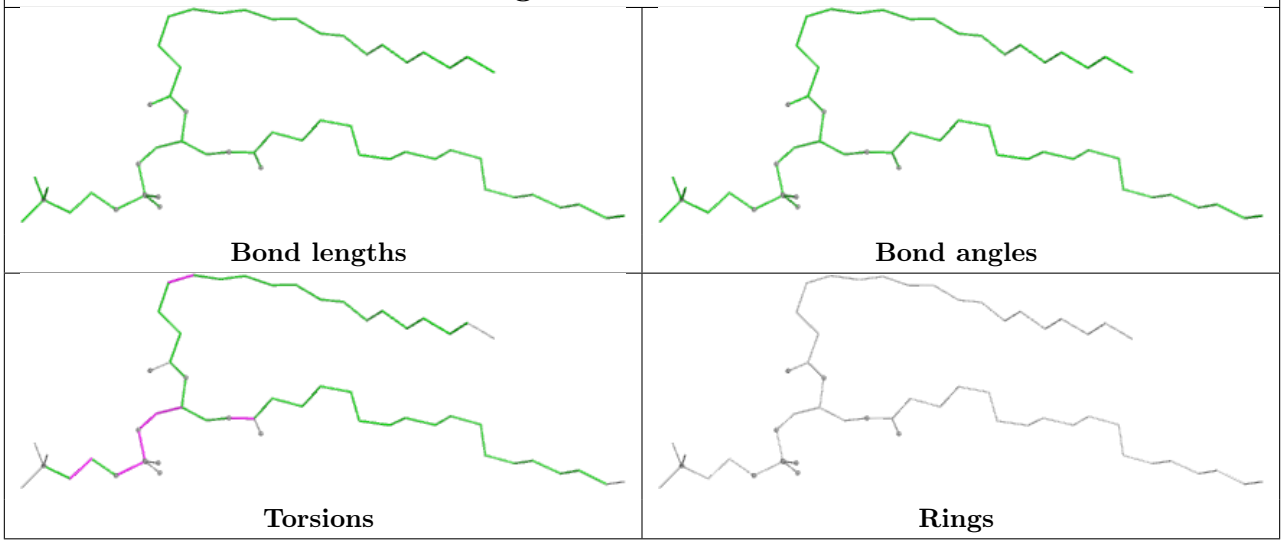


Rings

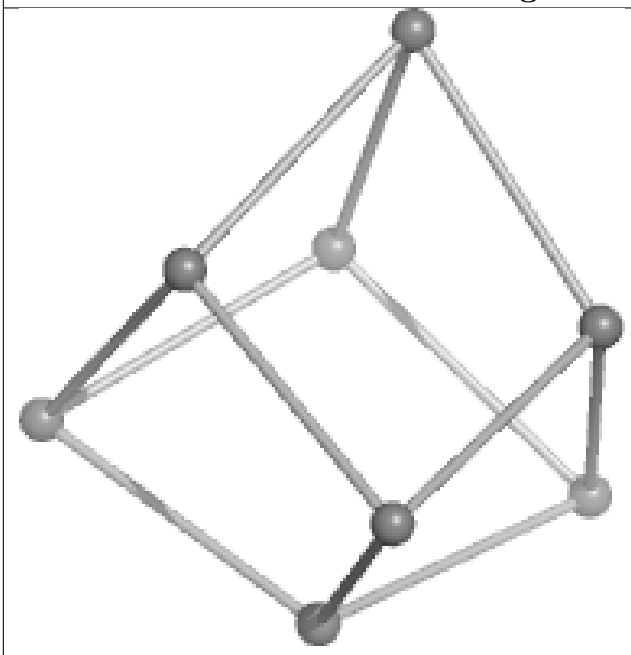
Ligand CDL DN 502



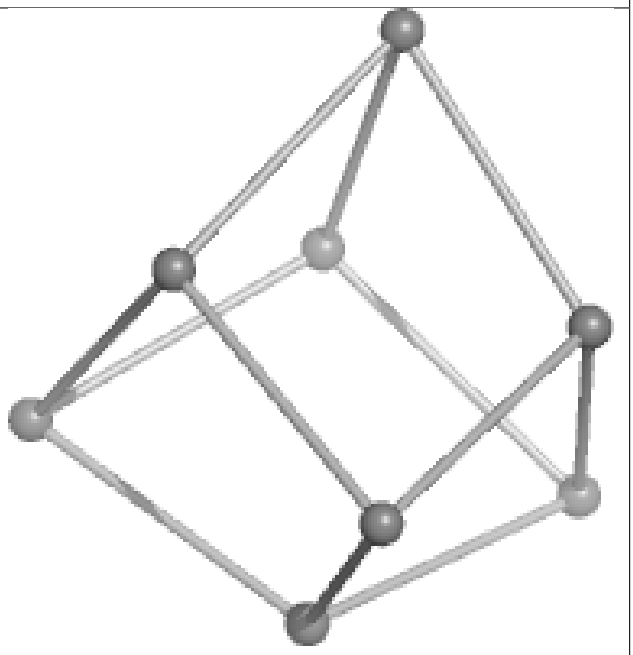
Ligand PC1 AU 201



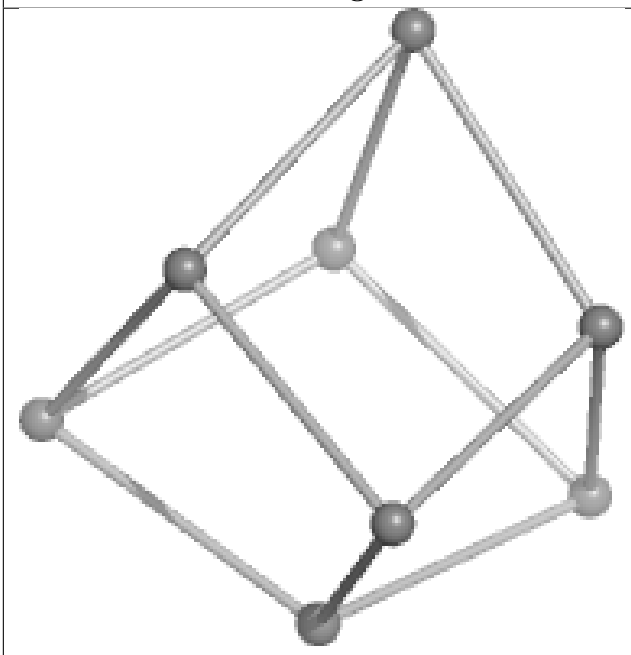
Ligand SF4 AT 201



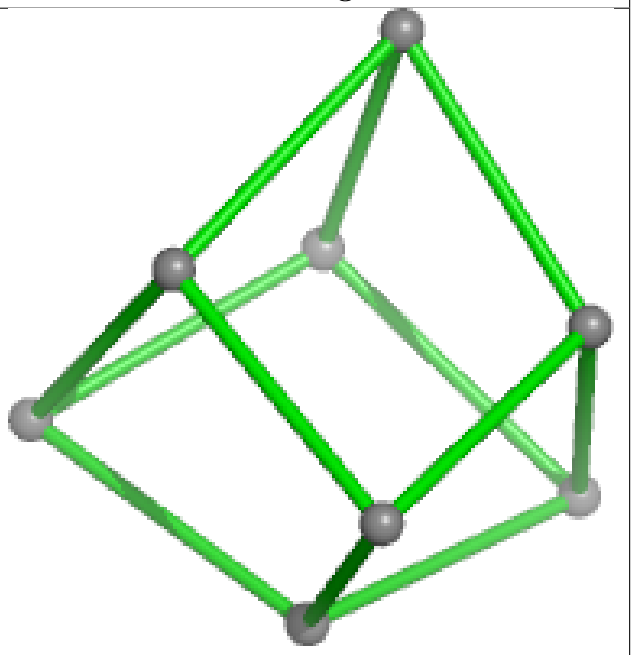
Bond lengths



Bond angles



Torsions



Rings

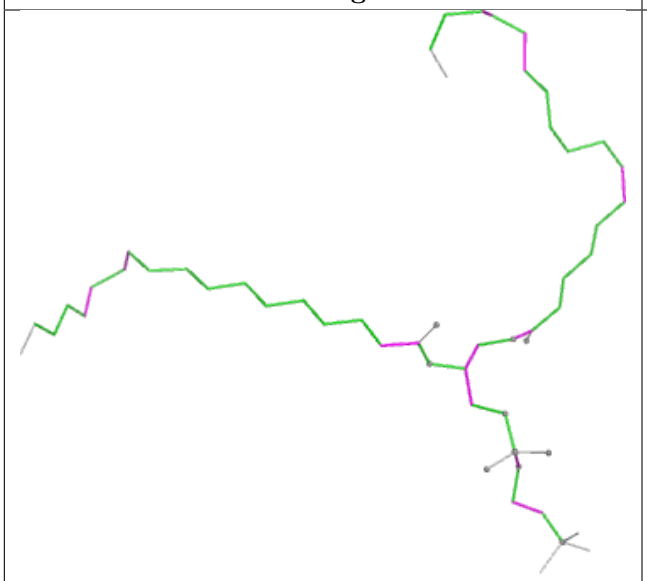
Ligand PC1 DC 603



Bond lengths



Bond angles

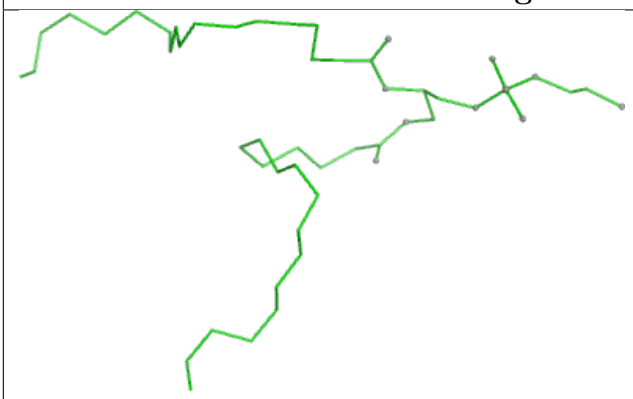


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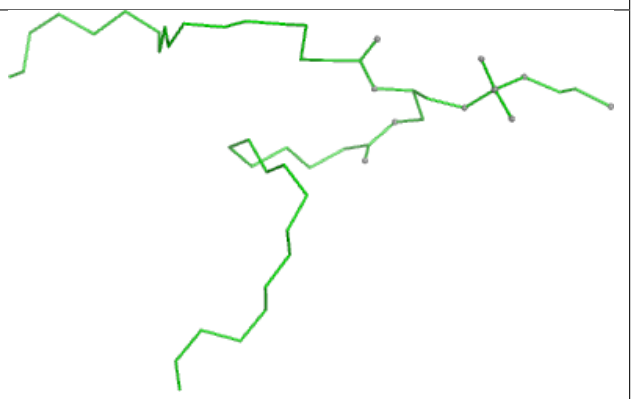


Rings

Ligand 3PE DX 304



Bond lengths



Bond angles



Torsions



Rings

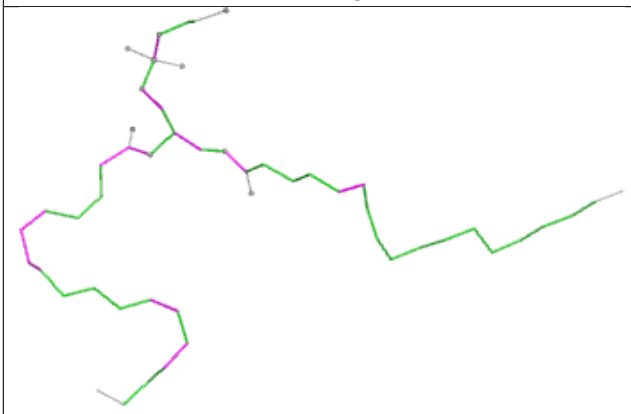
Ligand 3PE BA 301



Bond lengths



Bond angles

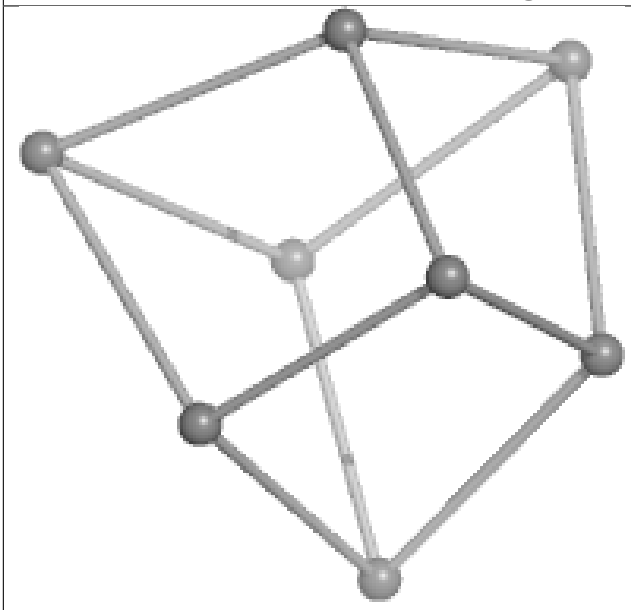


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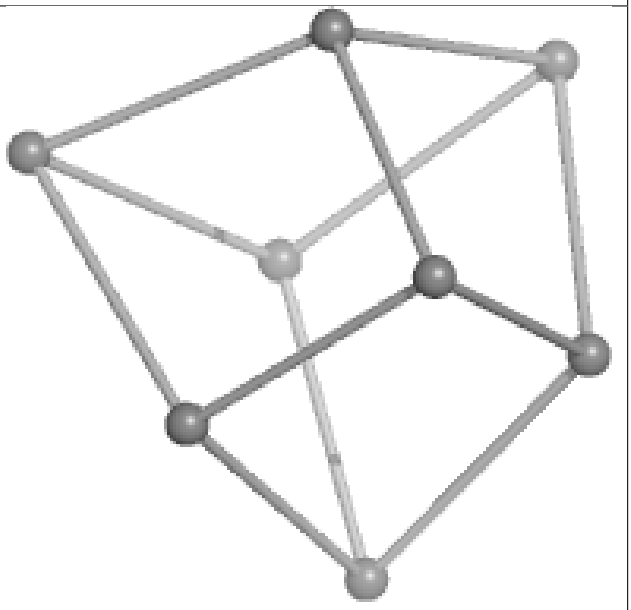


Rings

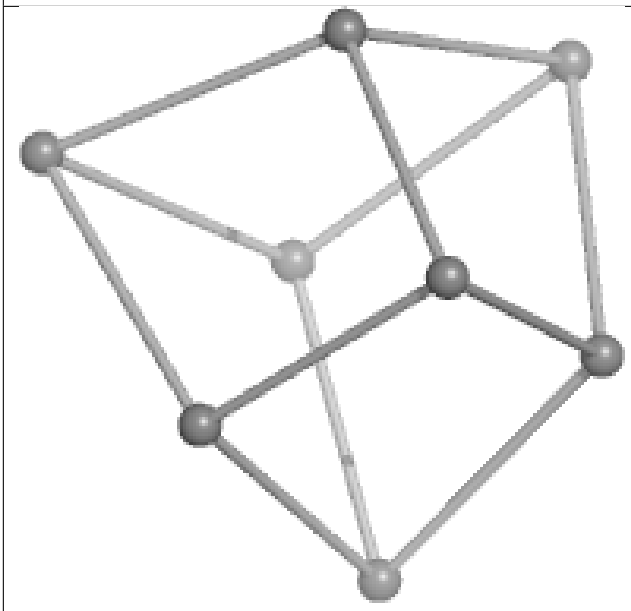
Ligand SF4 AL 301



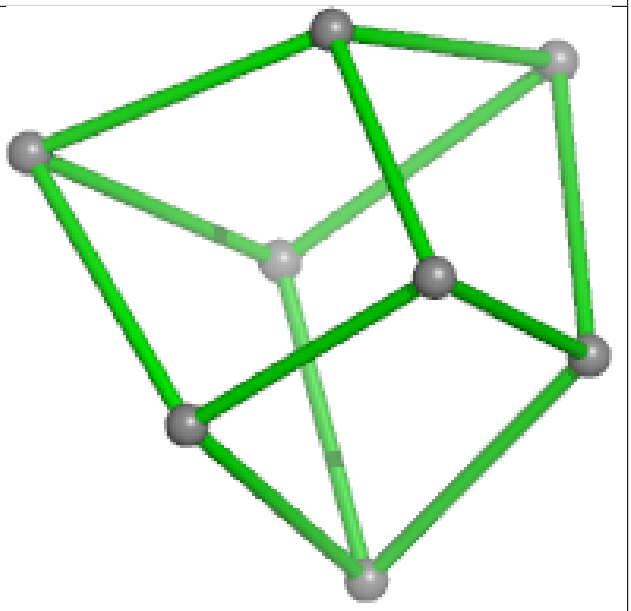
Bond lengths



Bond angles

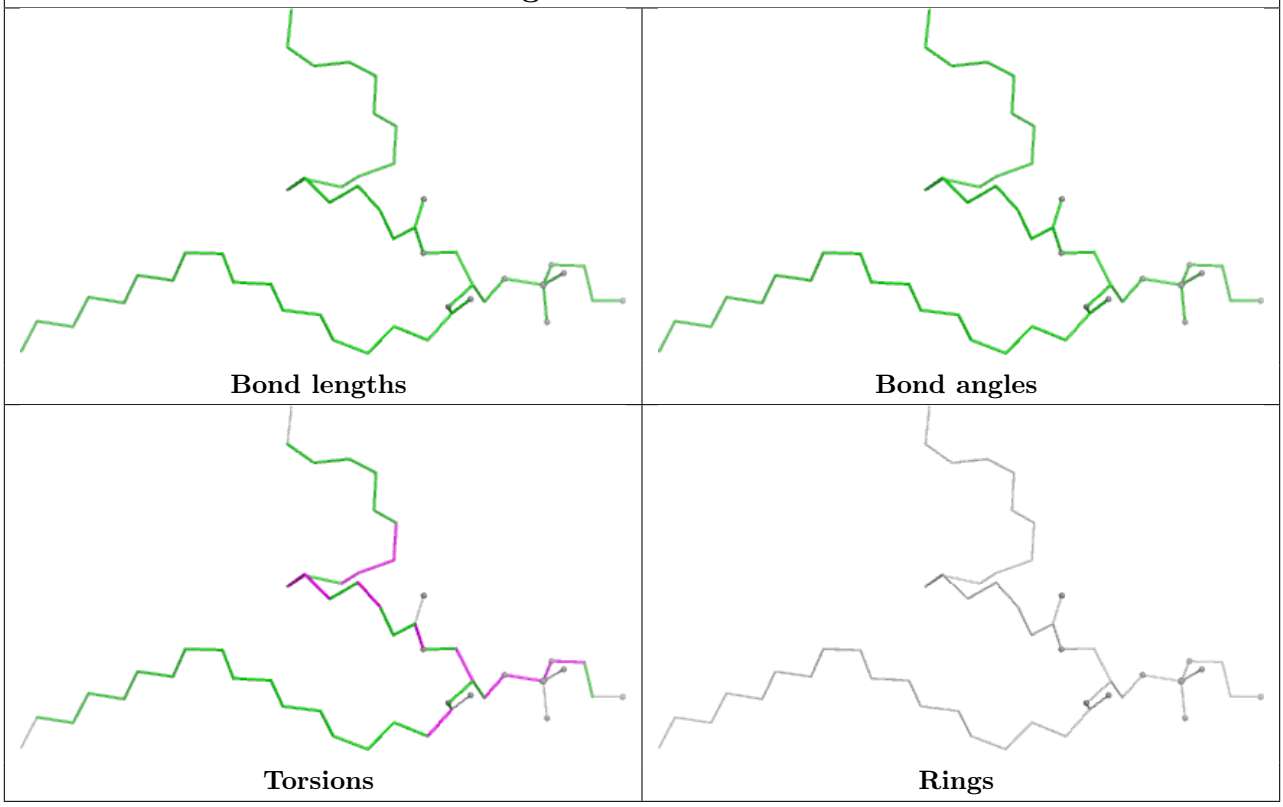


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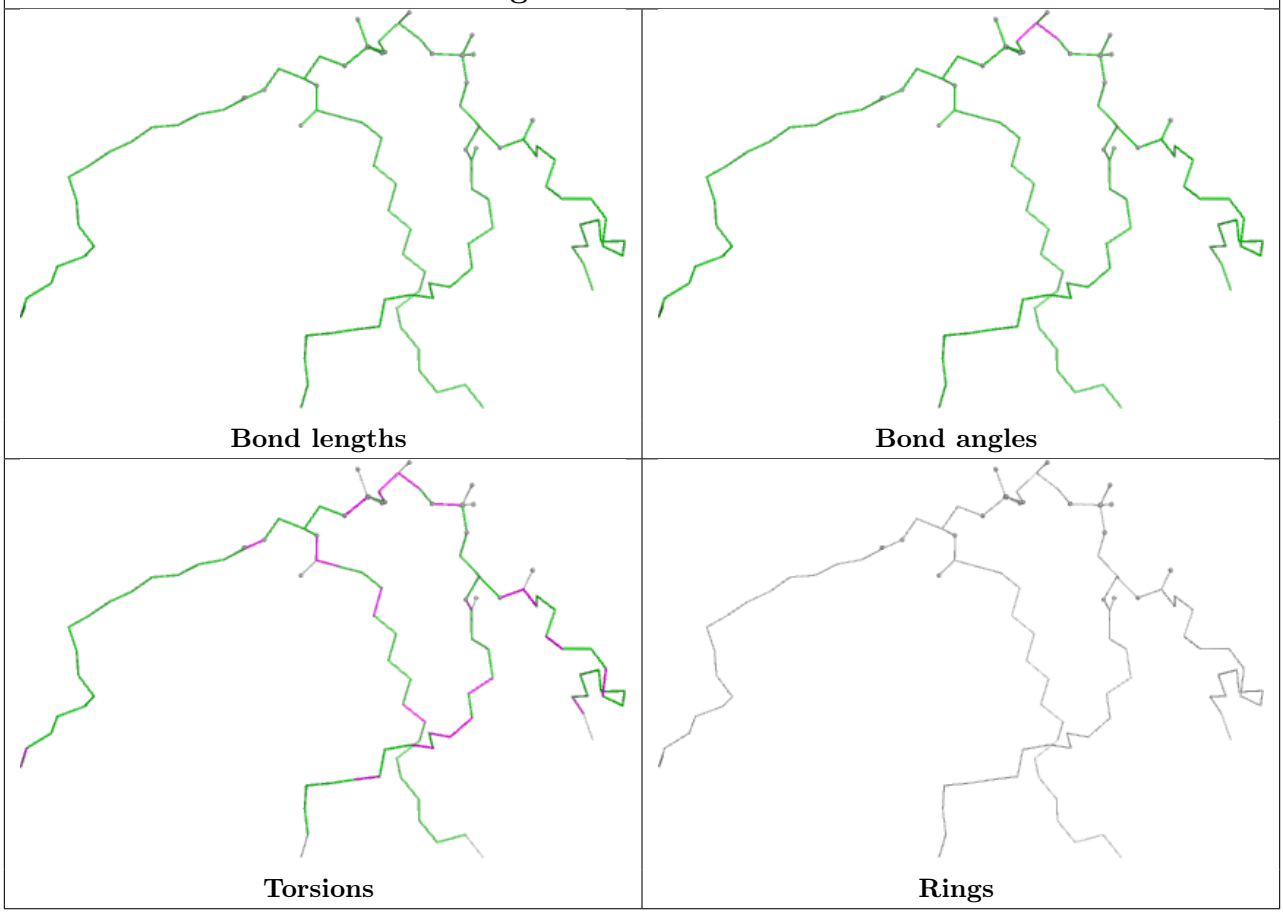


Rings

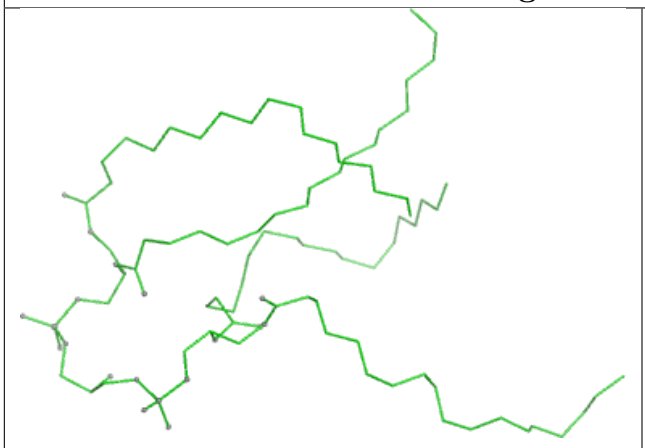
Ligand 3PE DI 301



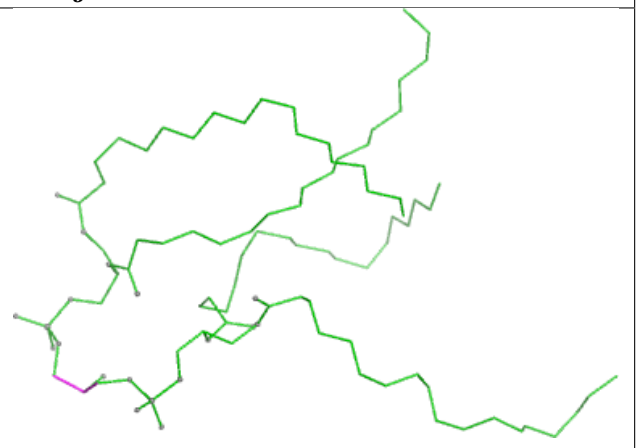
Ligand CDL DU 403



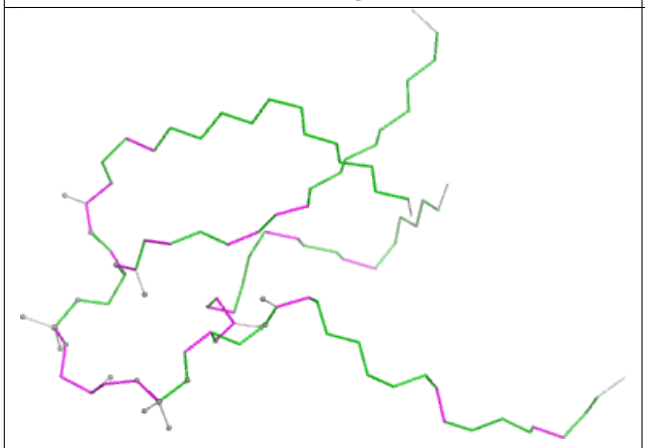
Ligand CDL Dj 407



Bond lengths



Bond angles

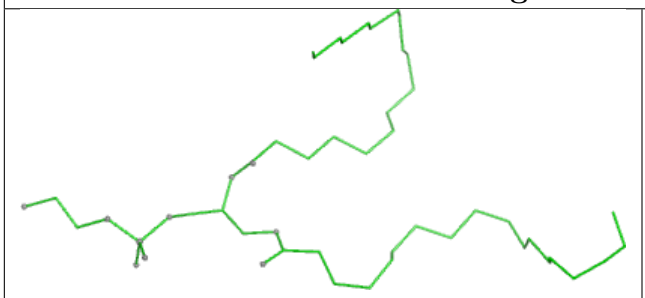


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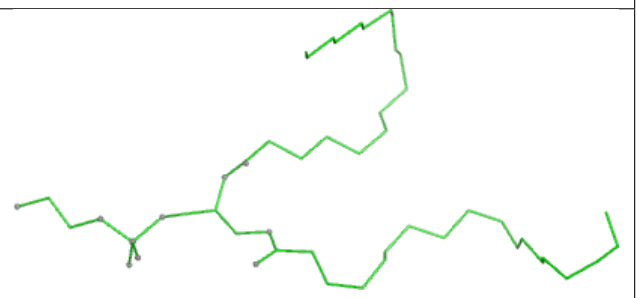


Rings

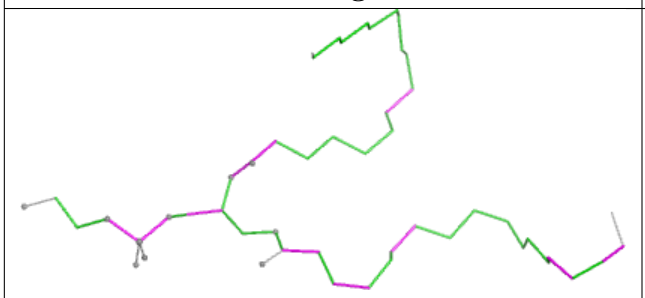
Ligand 3PE Dx 1207



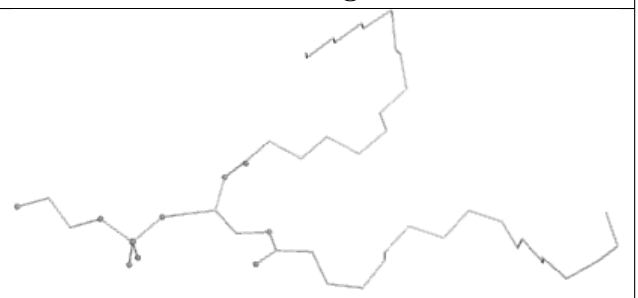
Bond lengths



Bond angles

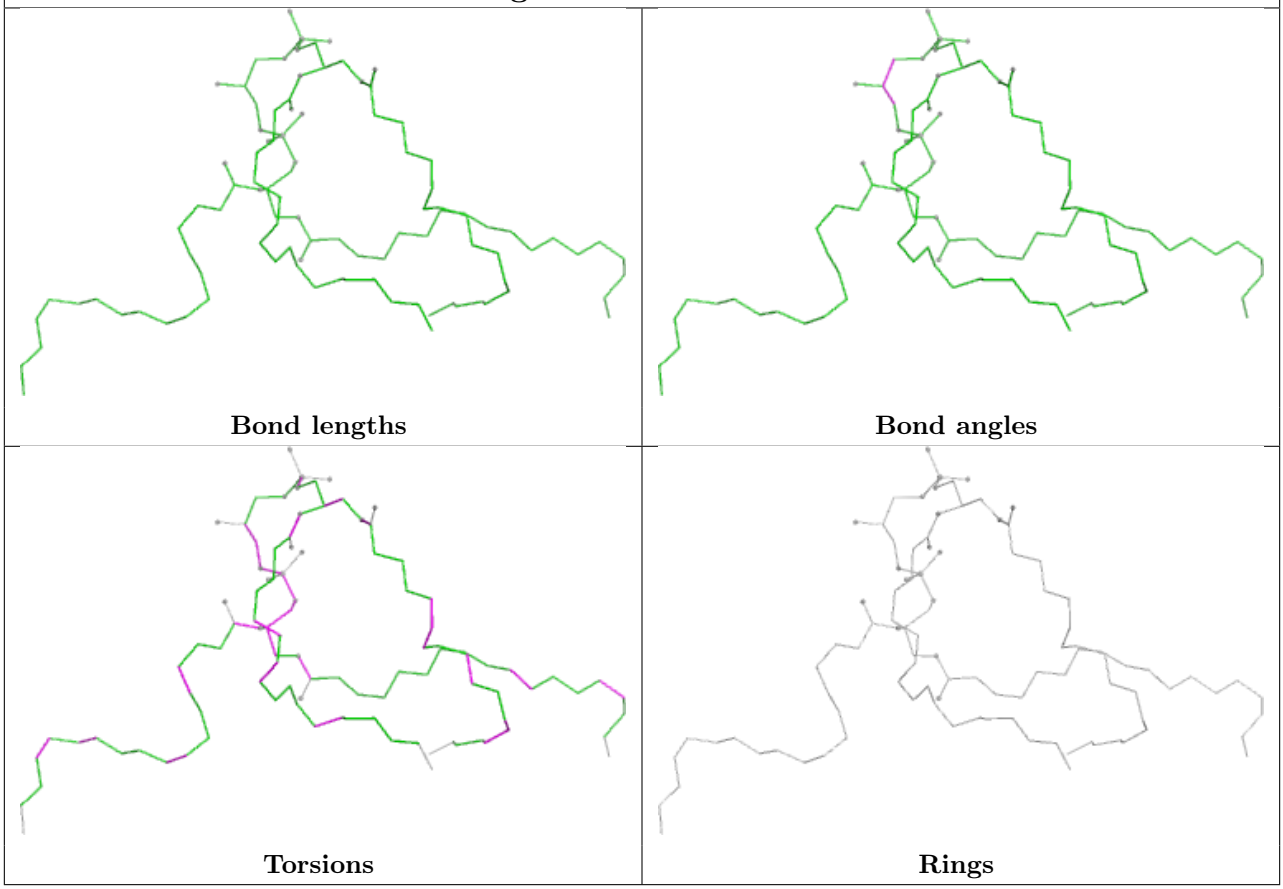


Torsions



Rings

Ligand CDL DN 507



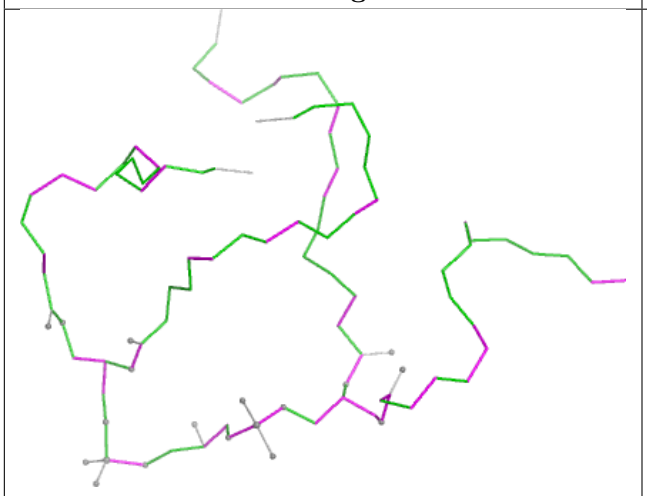
Ligand CDL DI 302



Bond lengths



Bond angles

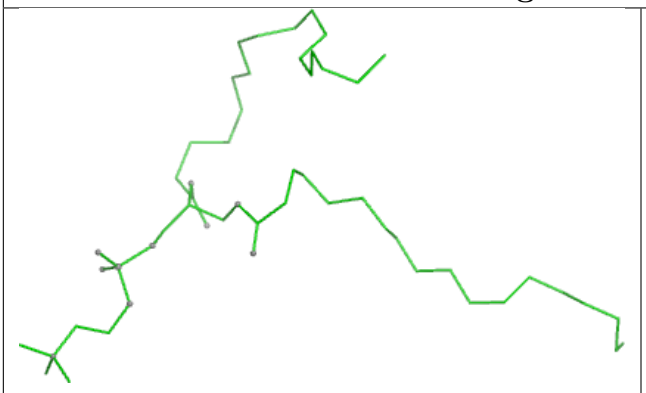


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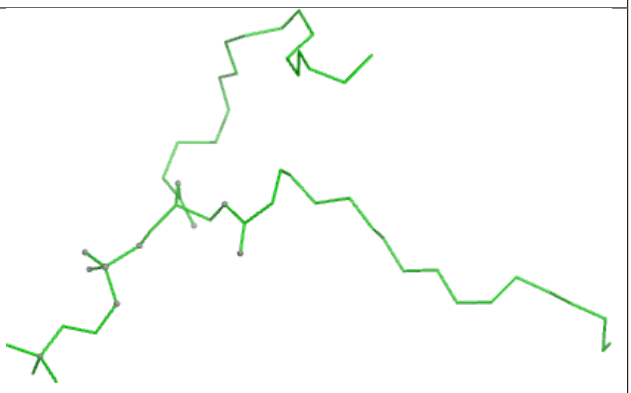


Rings

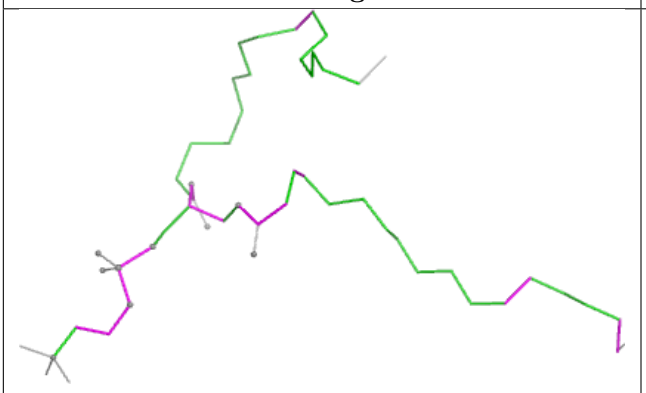
Ligand PC1 DS 406



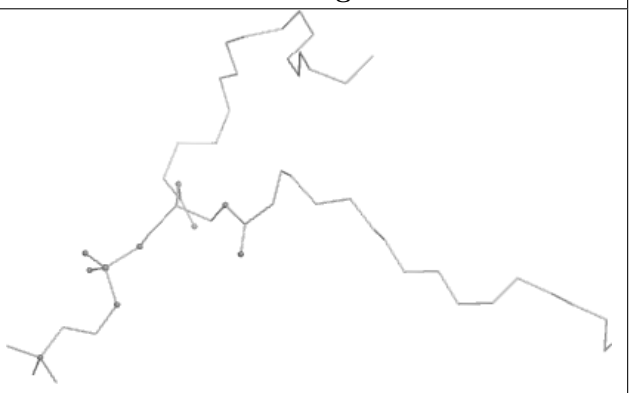
Bond lengths



Bond angles

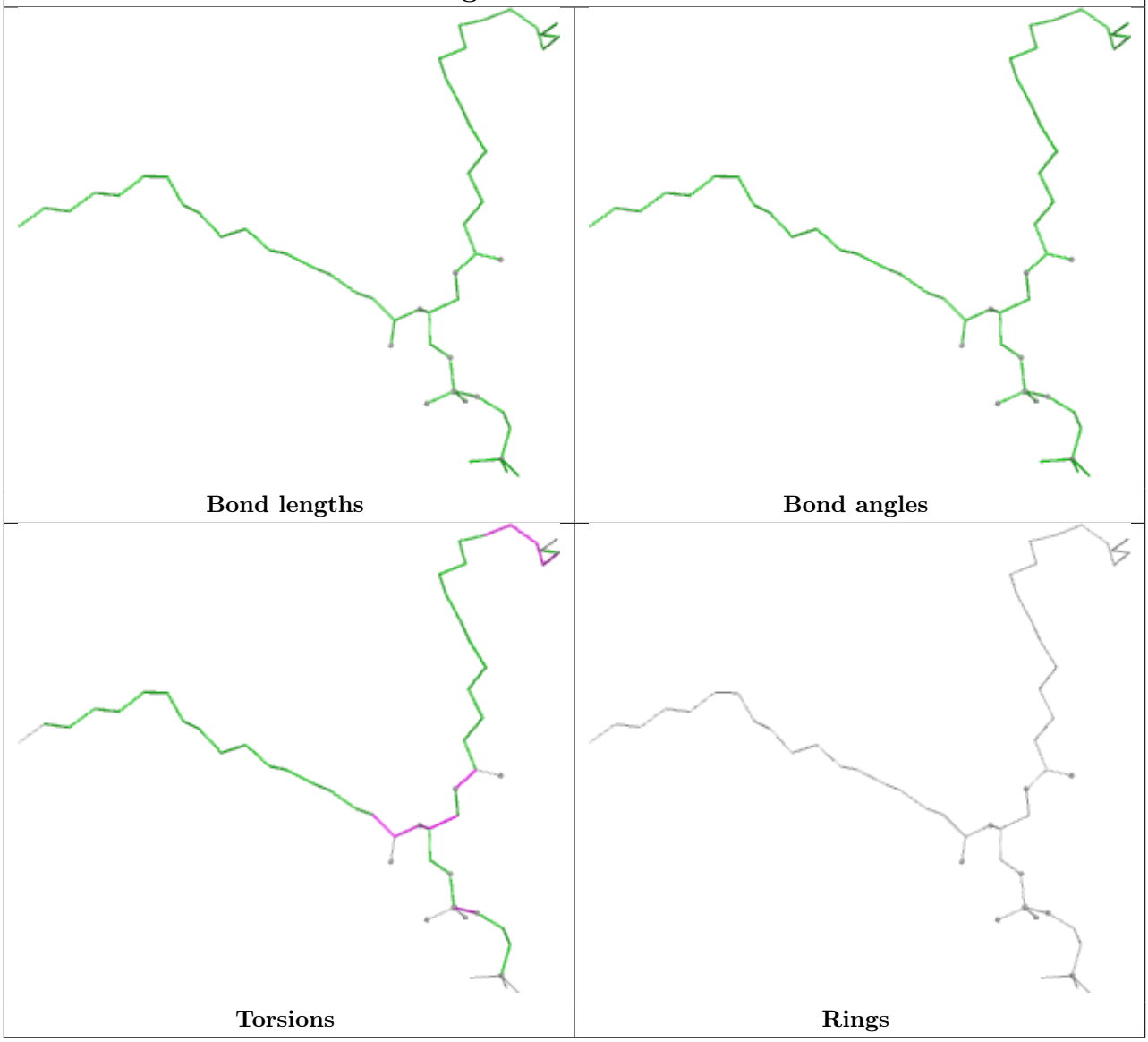


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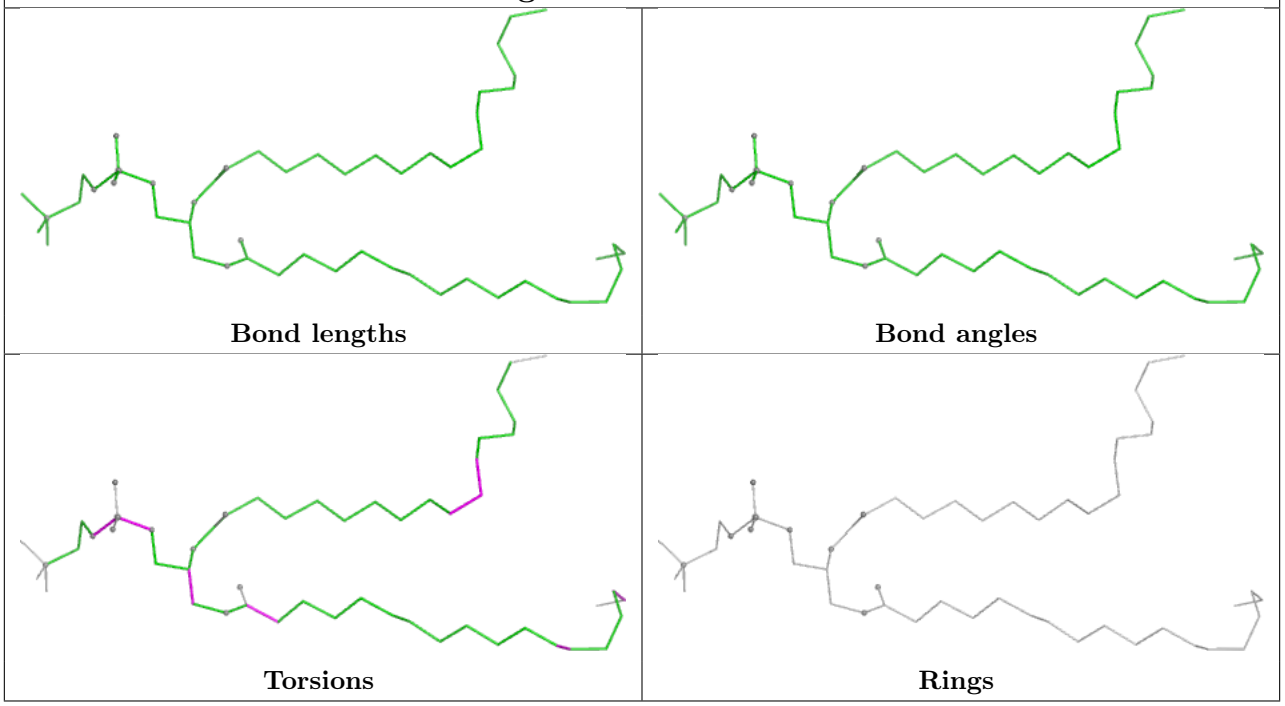


Rings

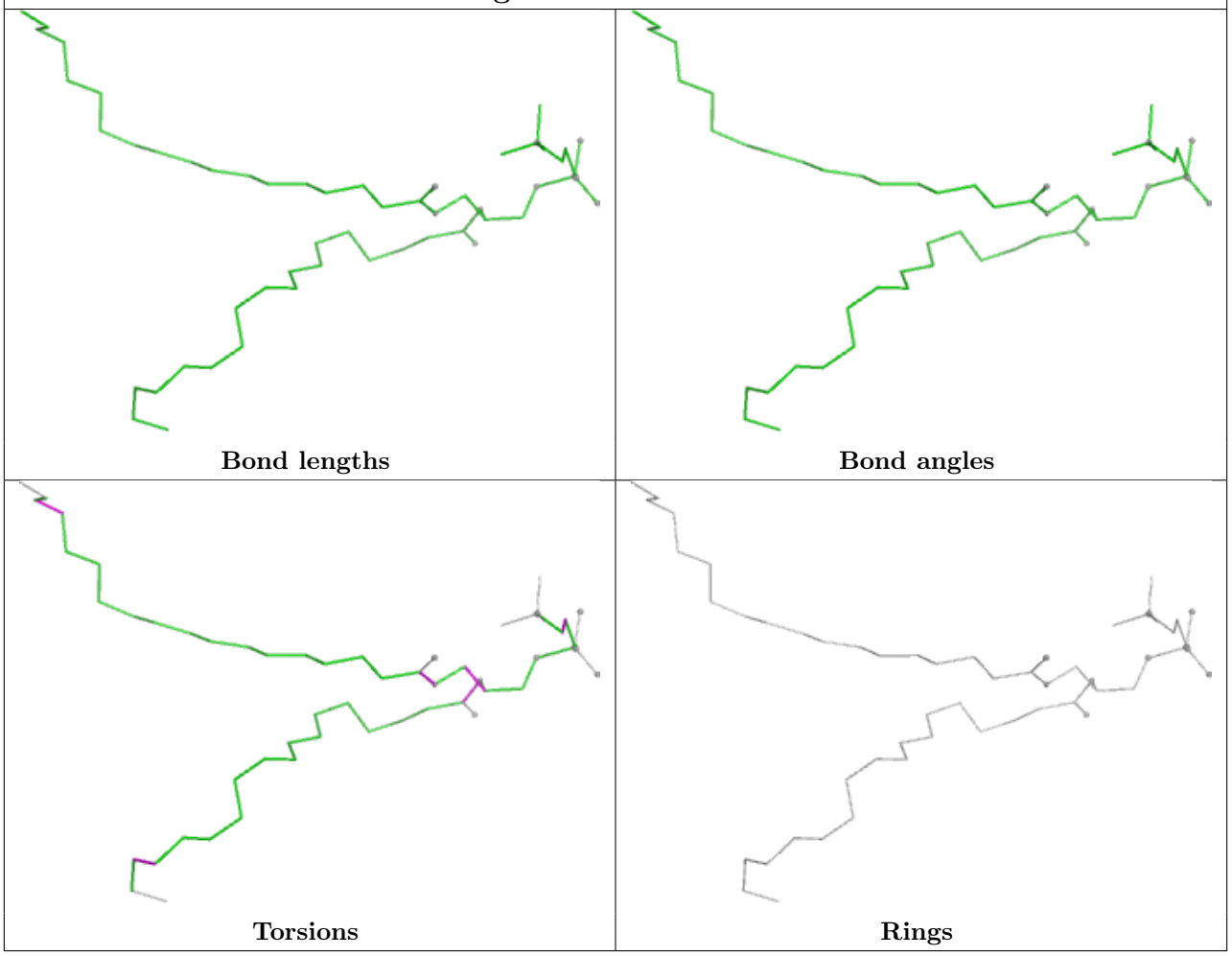
Ligand PC1 EO 206



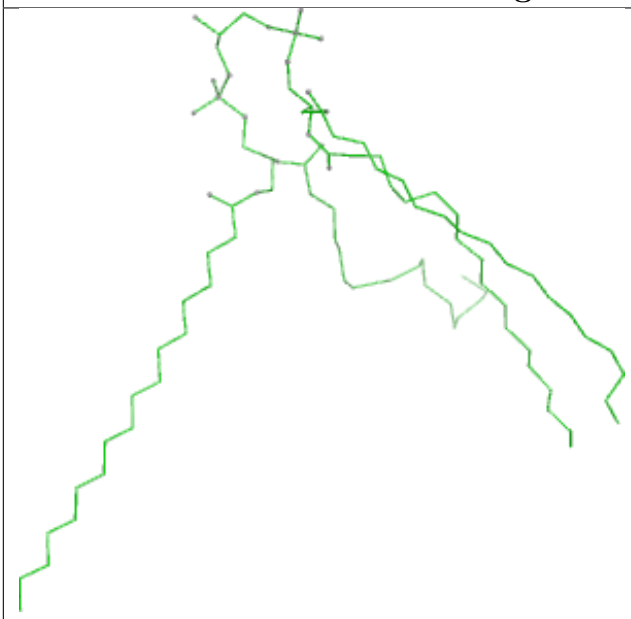
Ligand PC1 Dv 404



Ligand PC1 DY 302



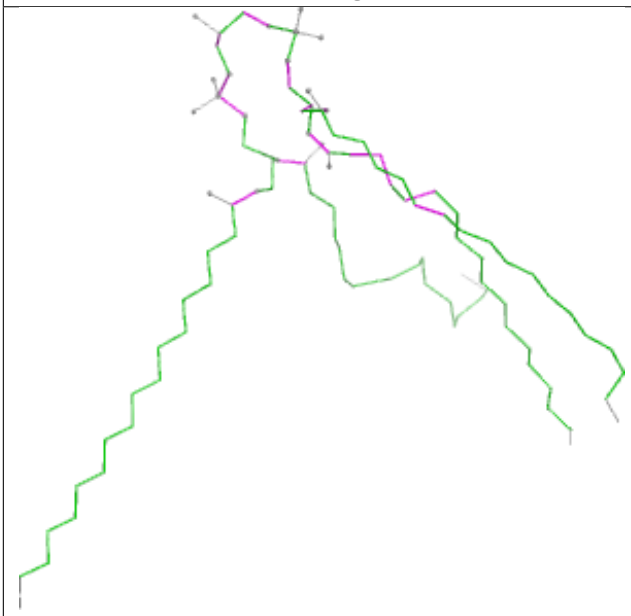
Ligand CDL A0 601



Bond lengths



Bond angles

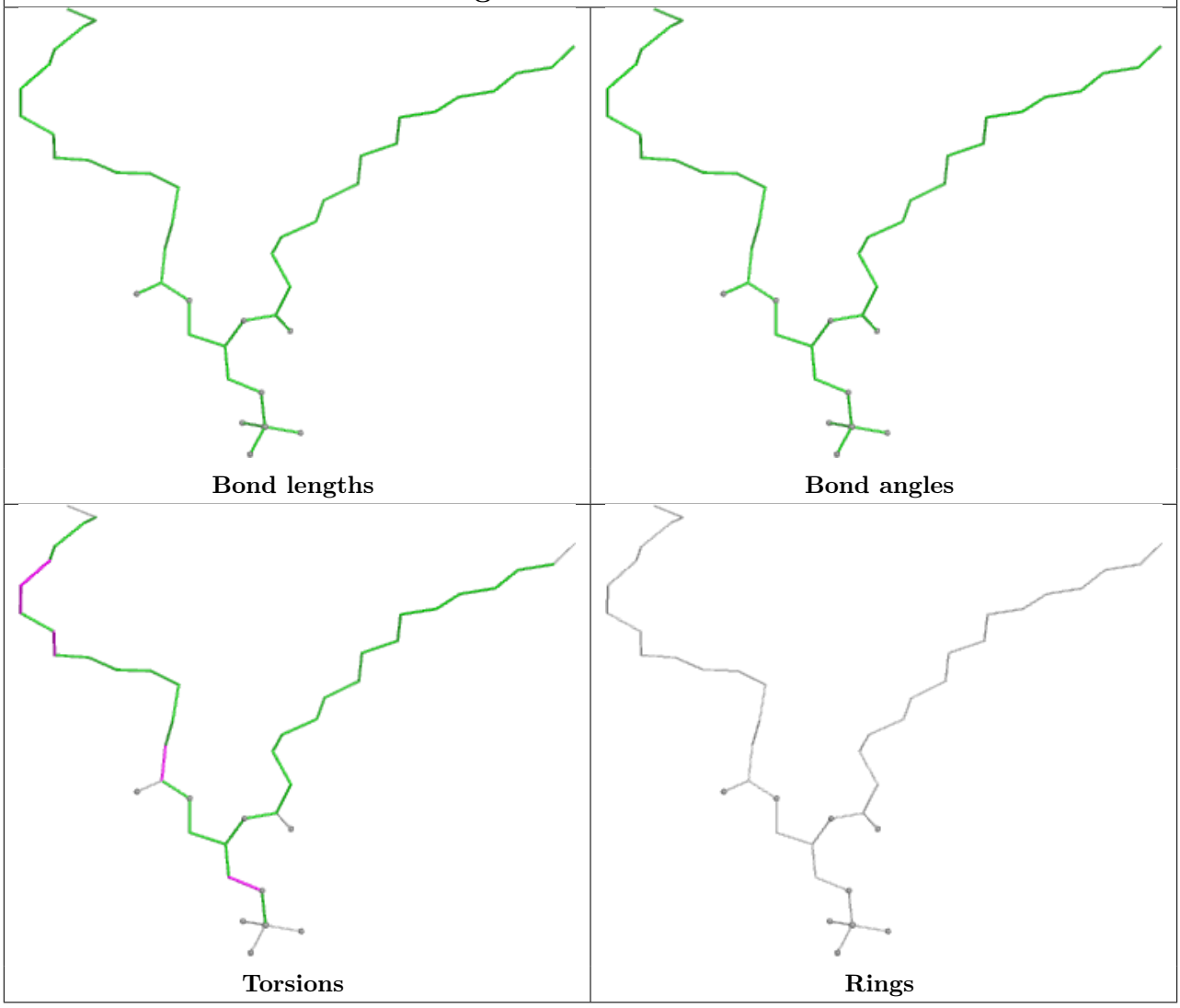


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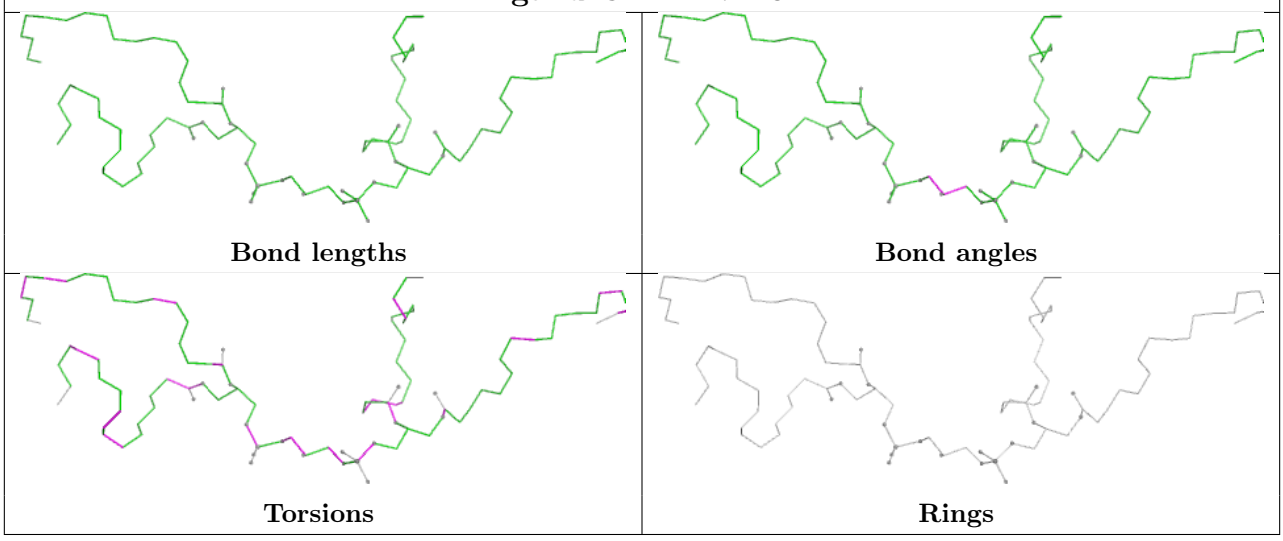


Rings

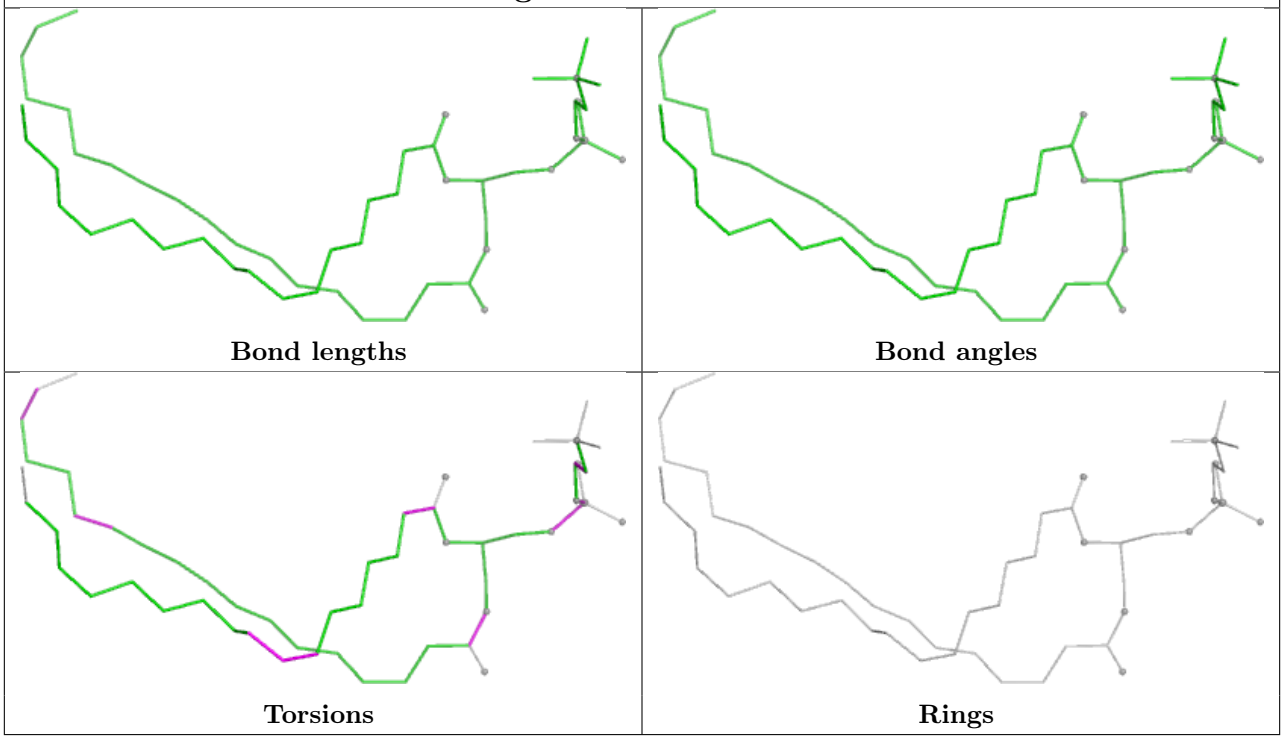
Ligand LPP Dn 505



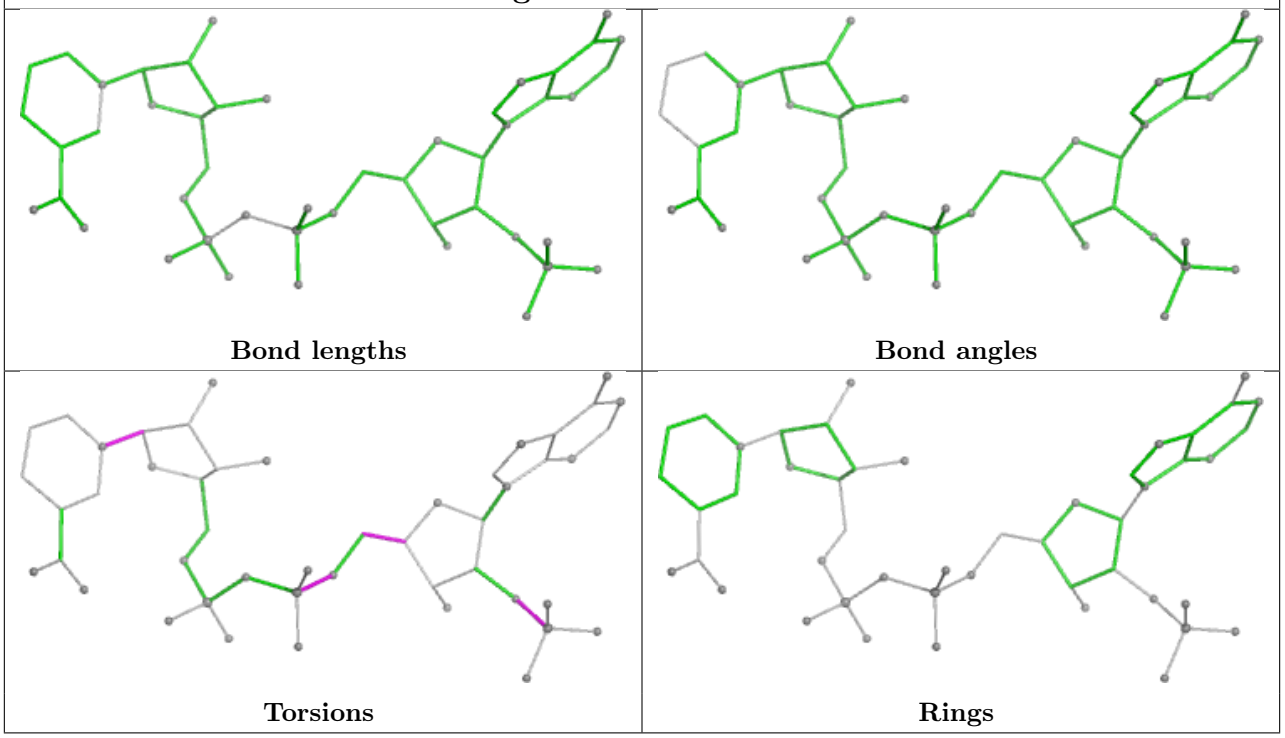
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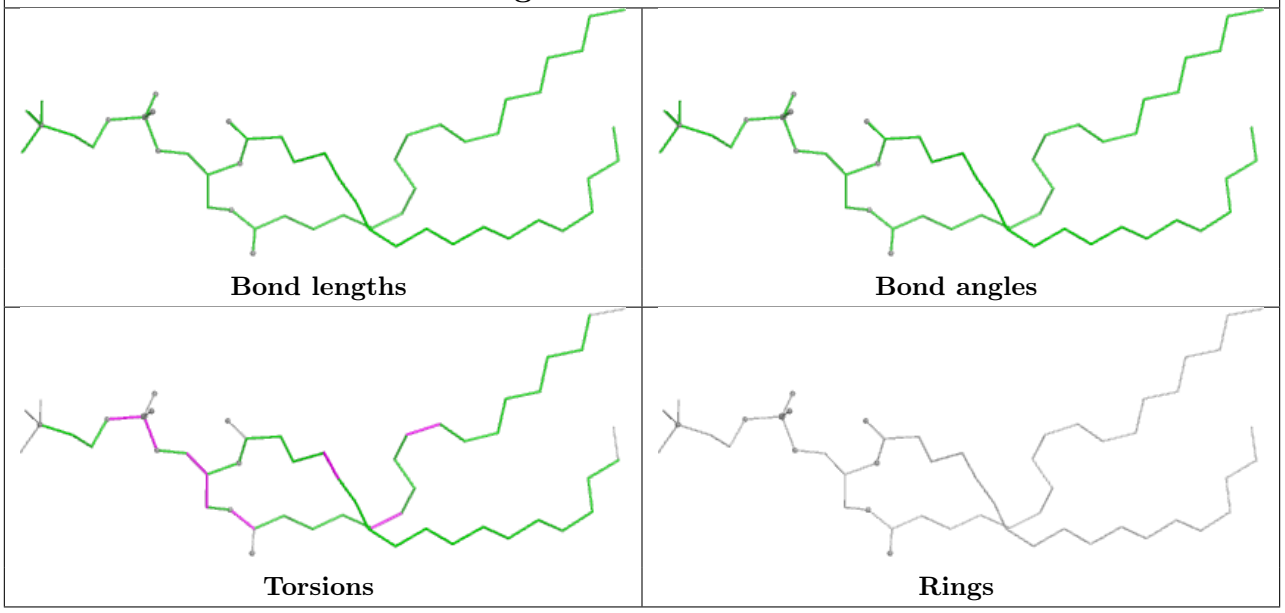
Ligand PC1 DC 604



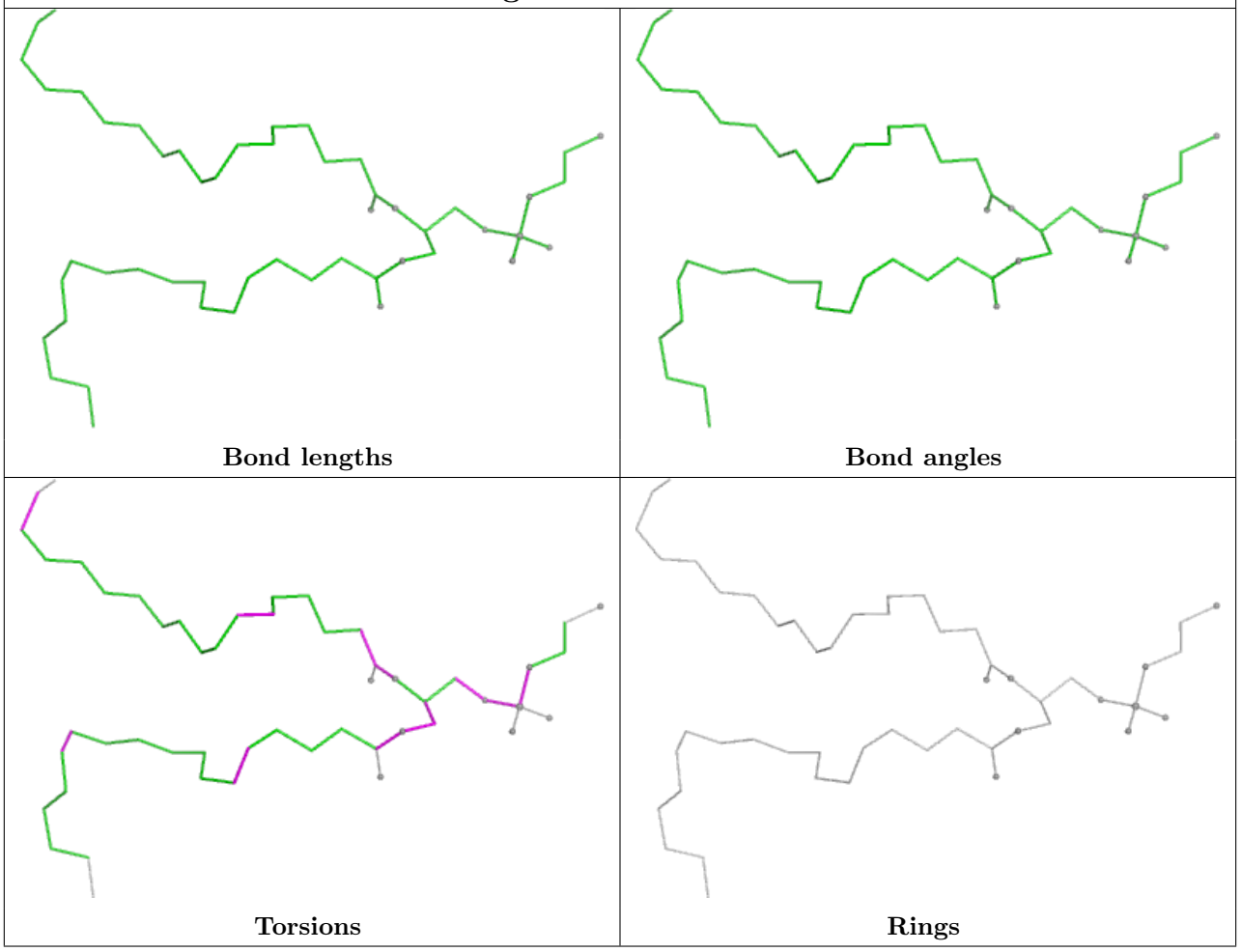
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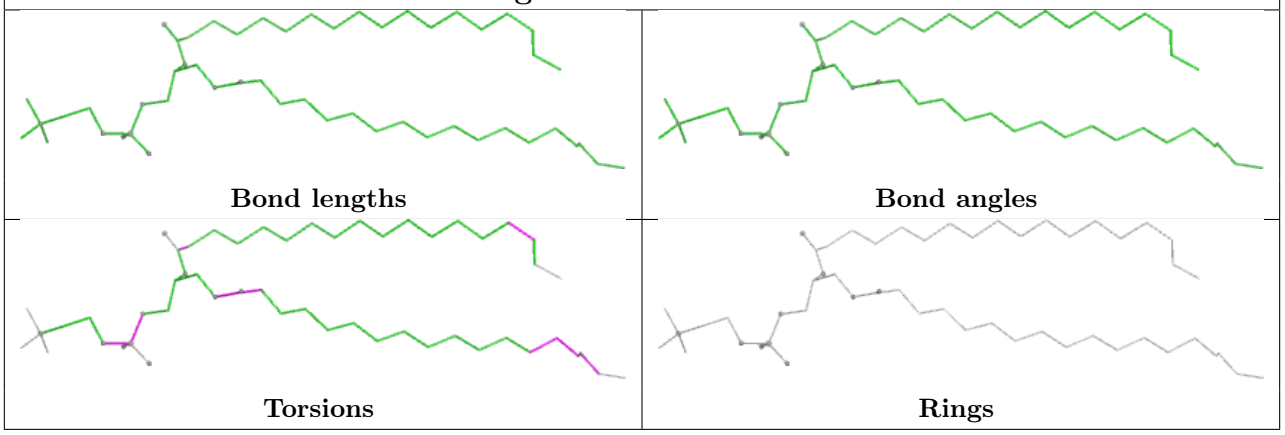
Ligand PC1 AA 903



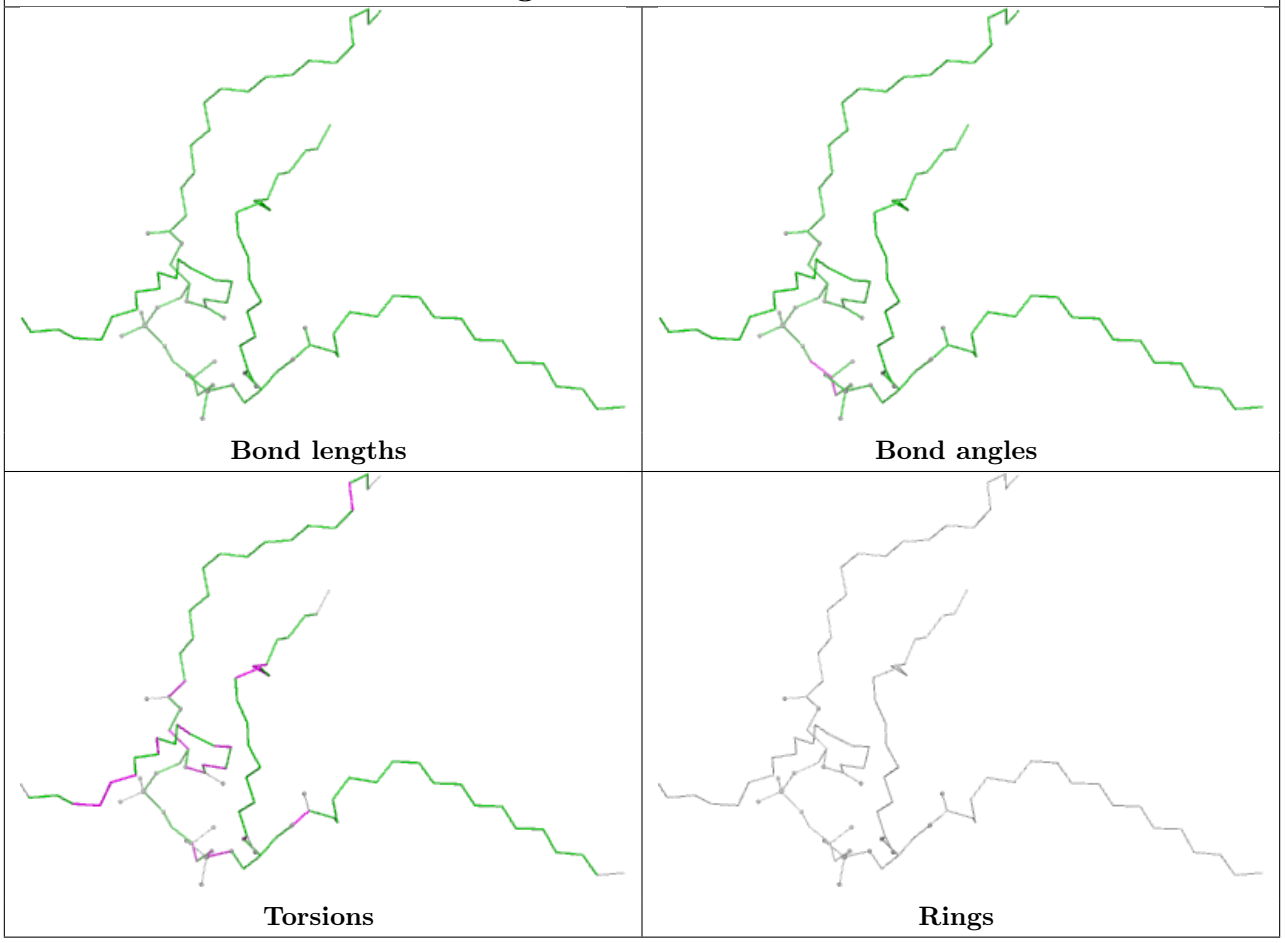
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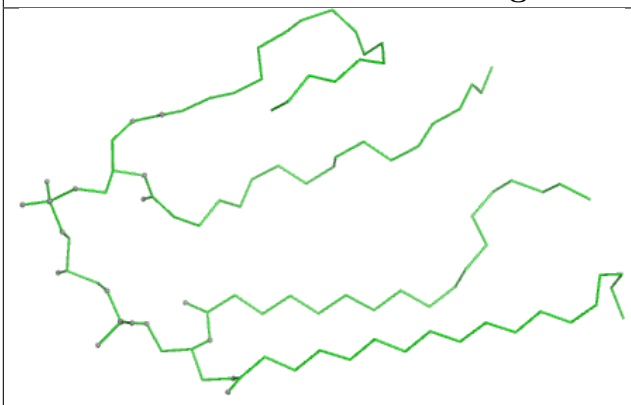
Ligand PC1 DC 602



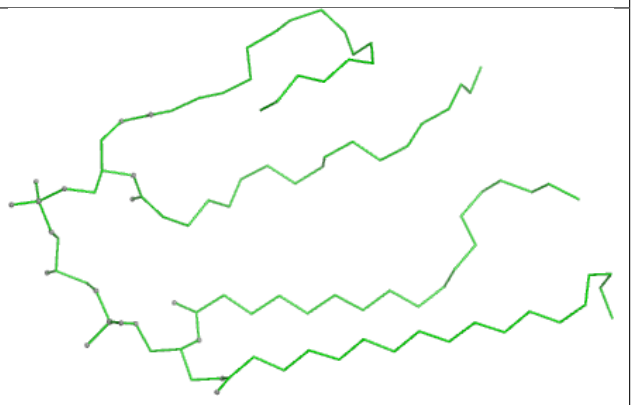
Ligand CDL Dc 608



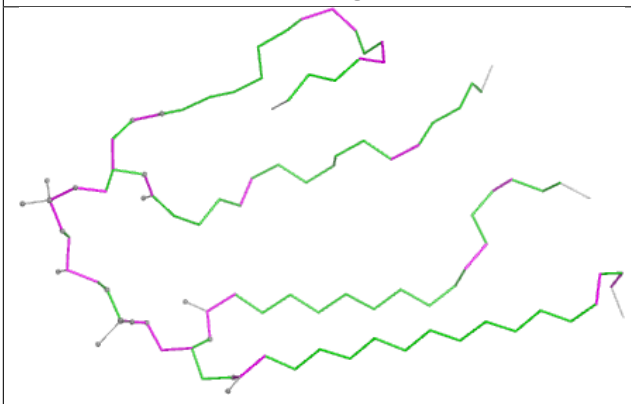
Ligand CDL DD 705



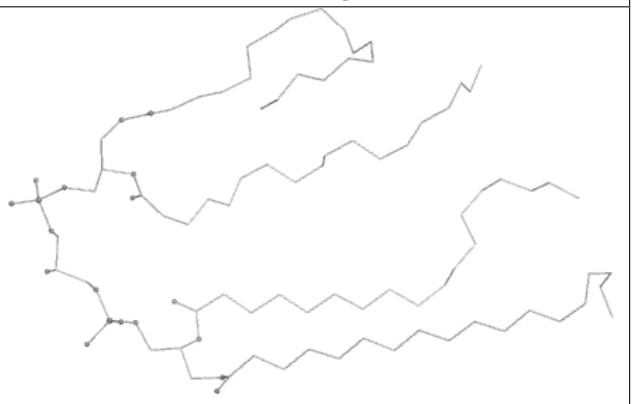
Bond lengths



Bond angles

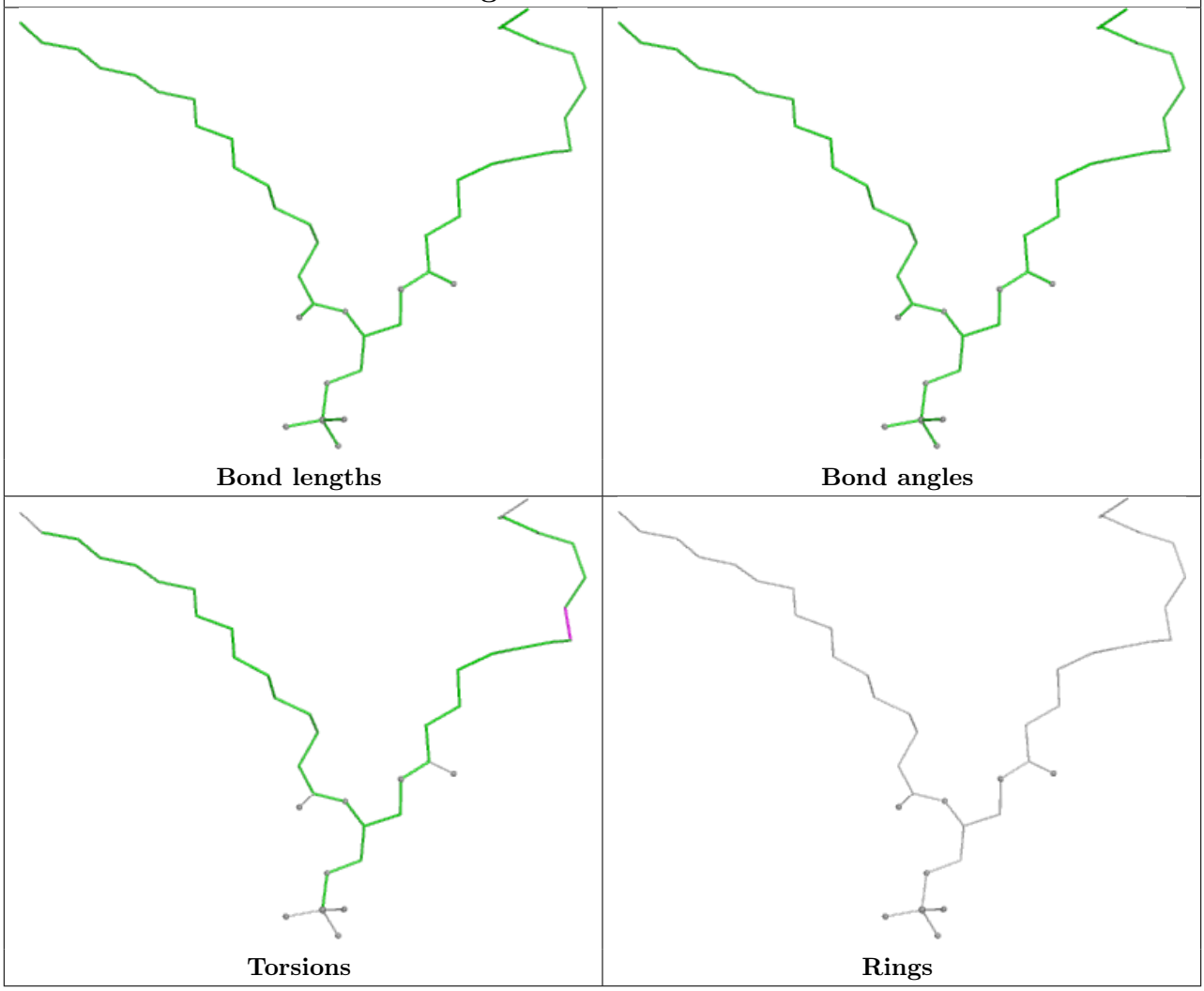


Torsions

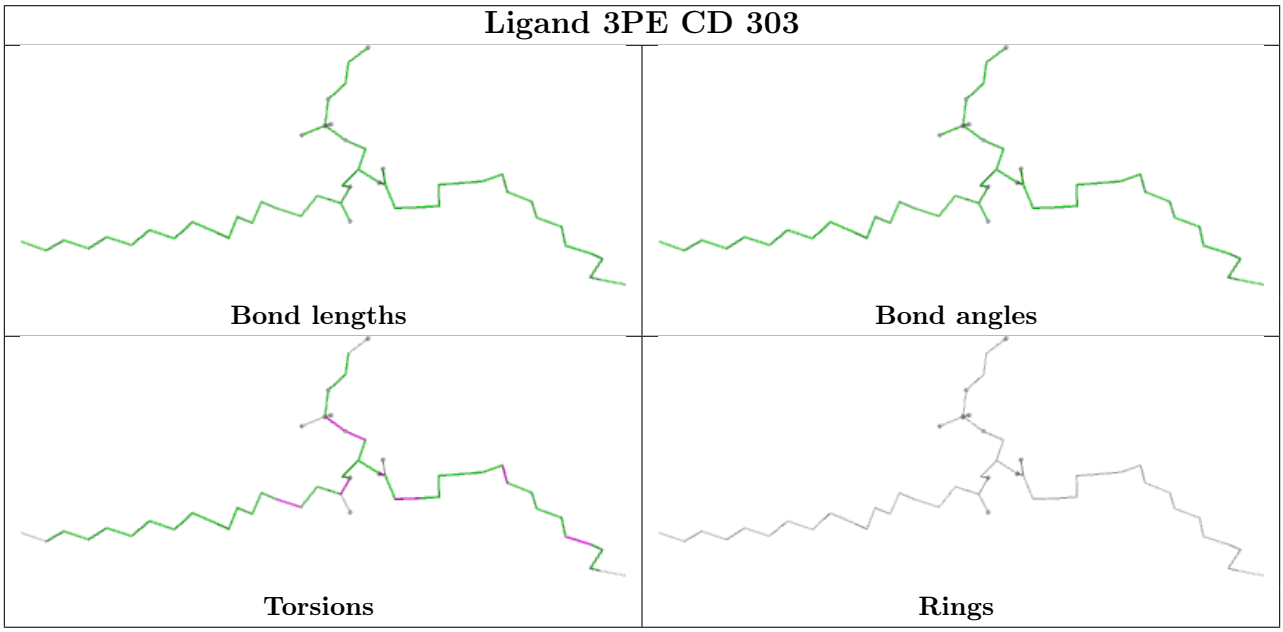


Rings

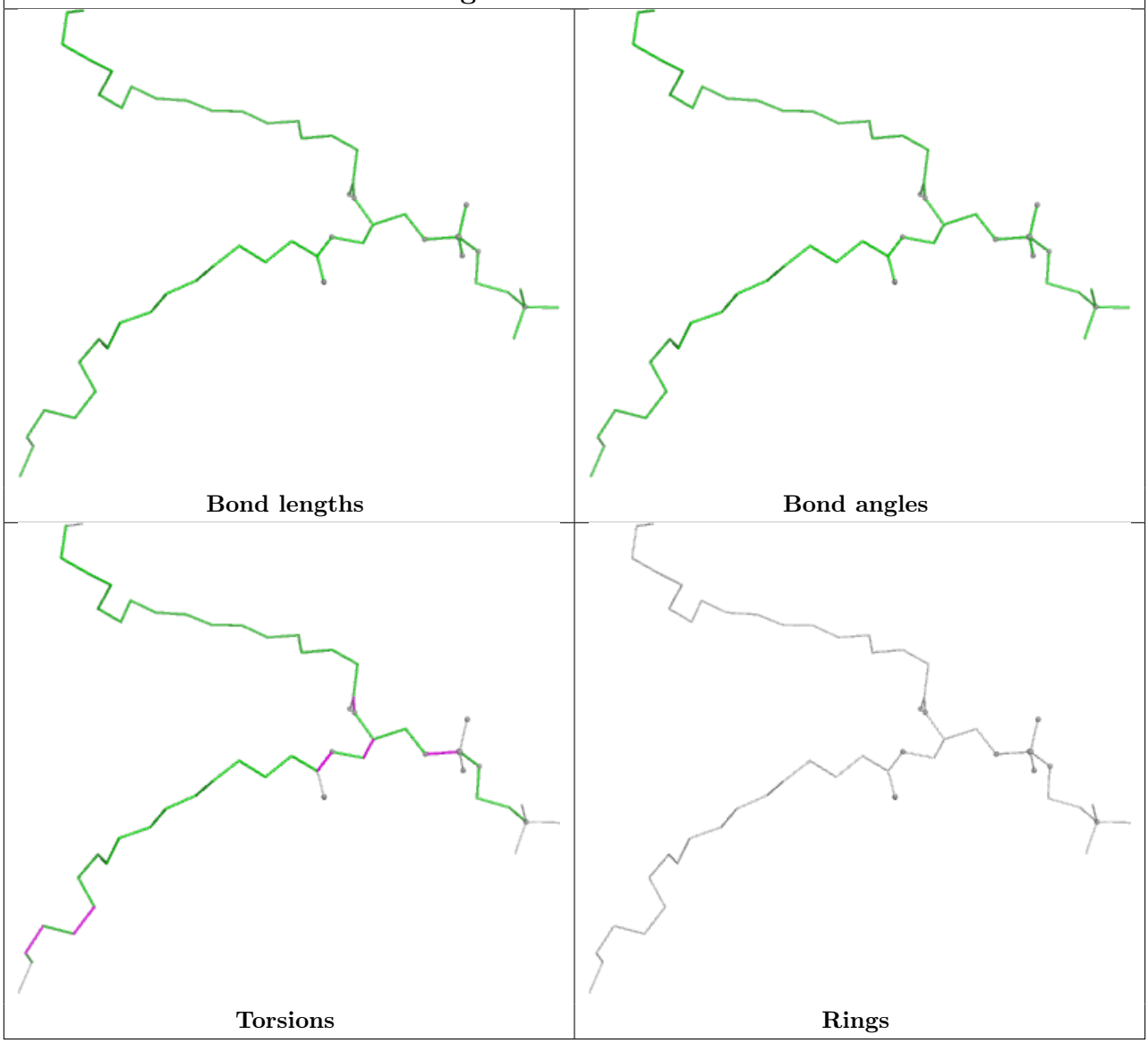
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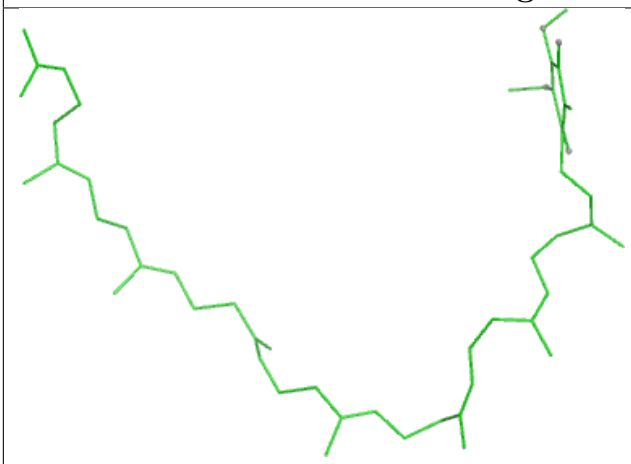
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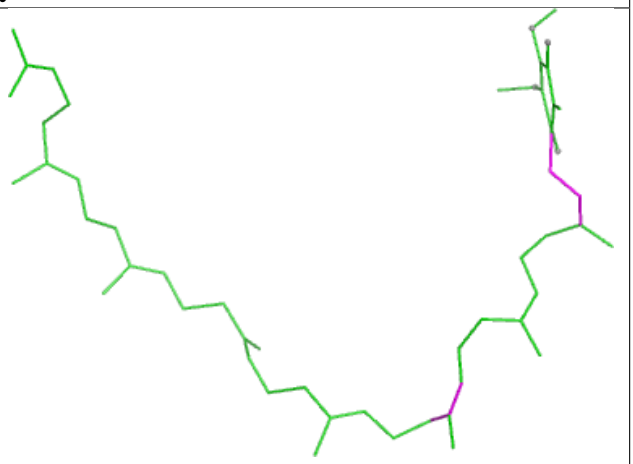
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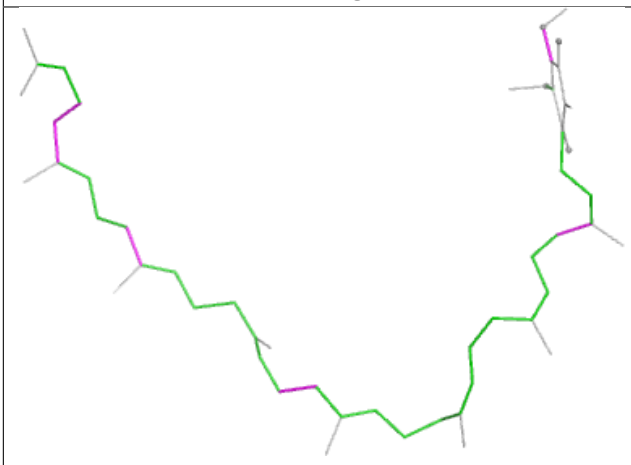
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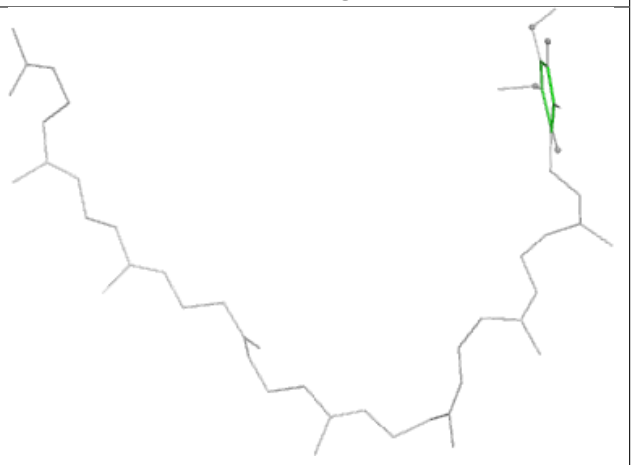
Bond lengths



Bond angles

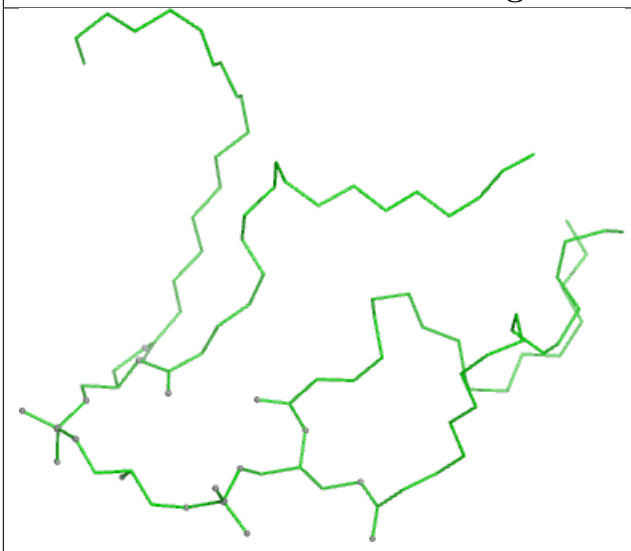


Torsions

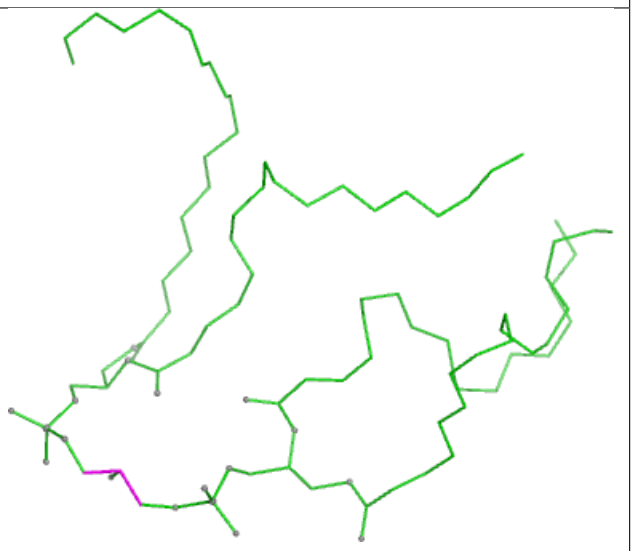


Rings

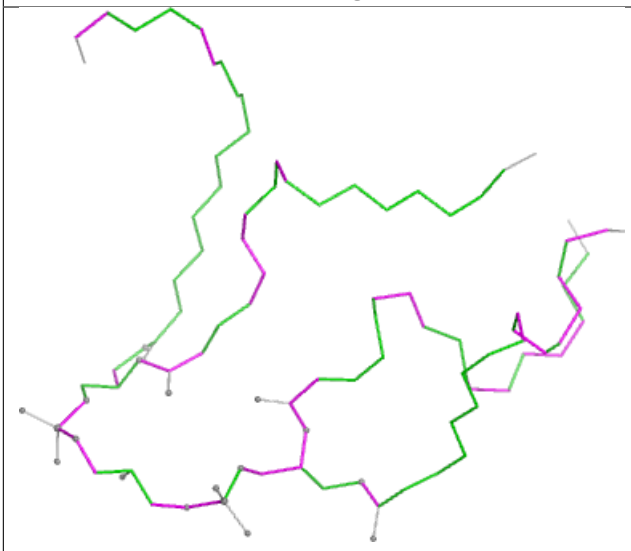
Ligand CDL DM 501



Bond lengths



Bond angles

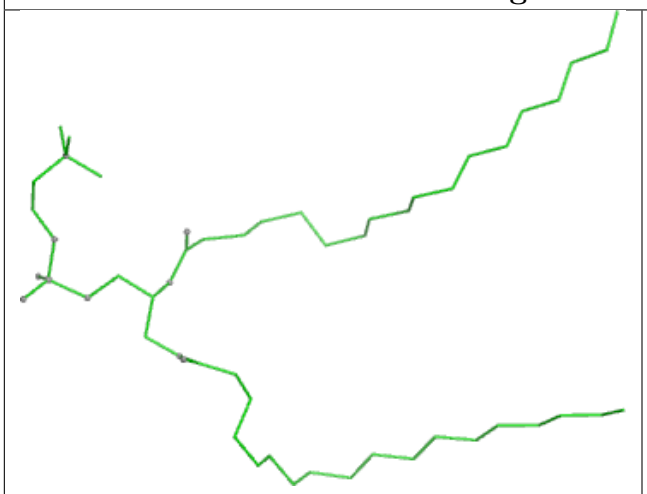


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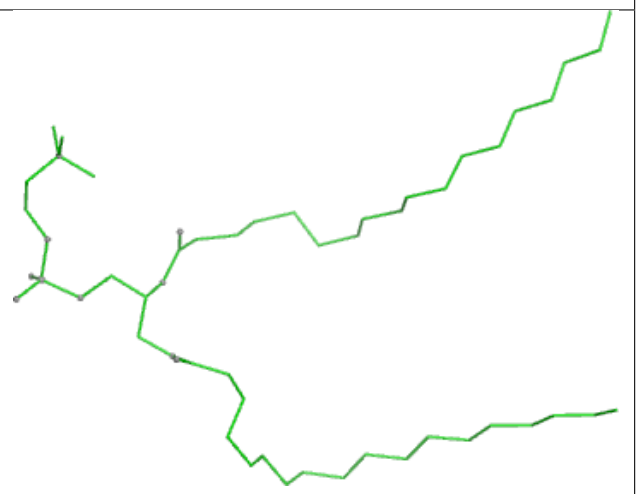


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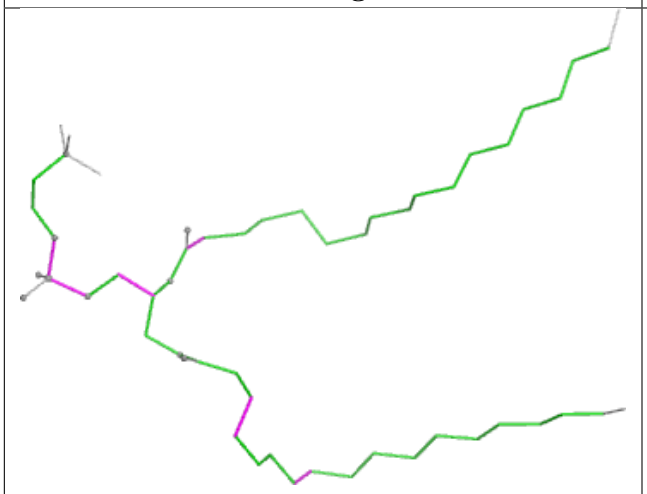
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Bond lengths



Bond angles

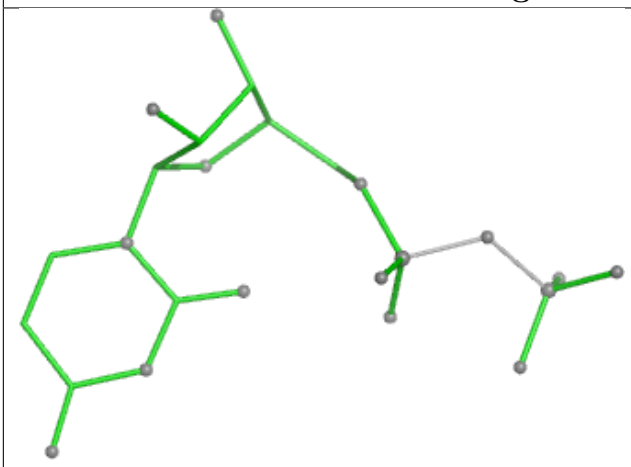


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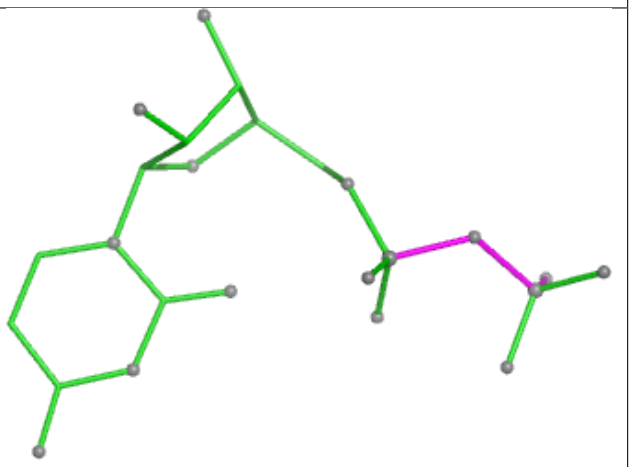


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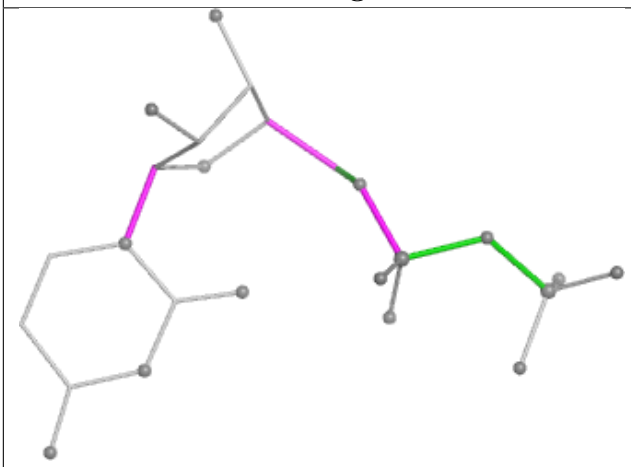
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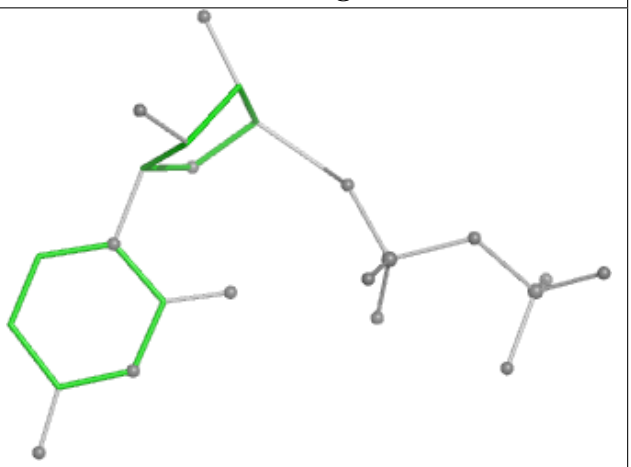
Bond lengths



Bond angles

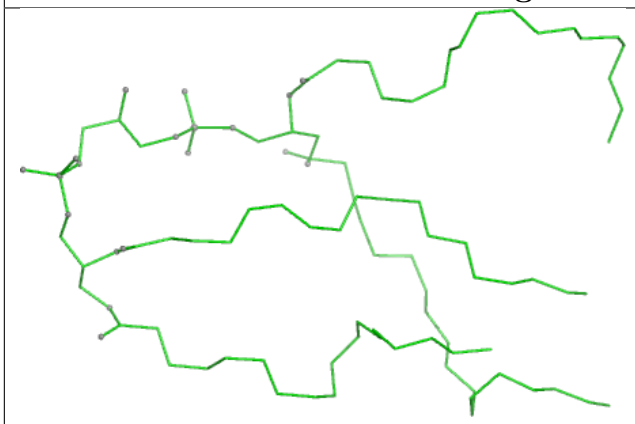


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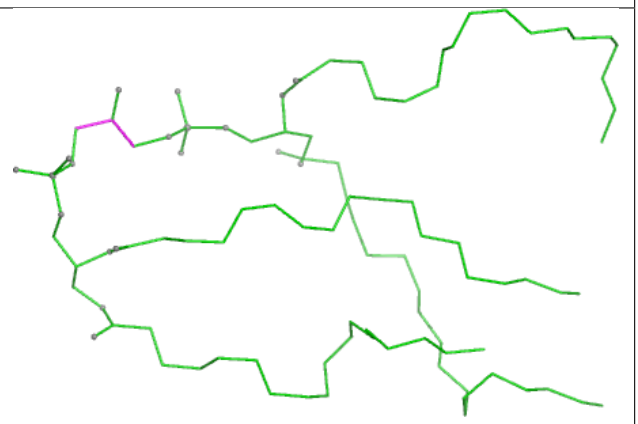


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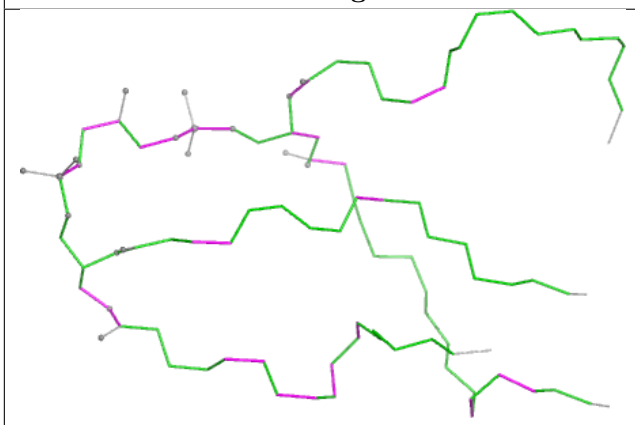
Ligand CDL DJ 302



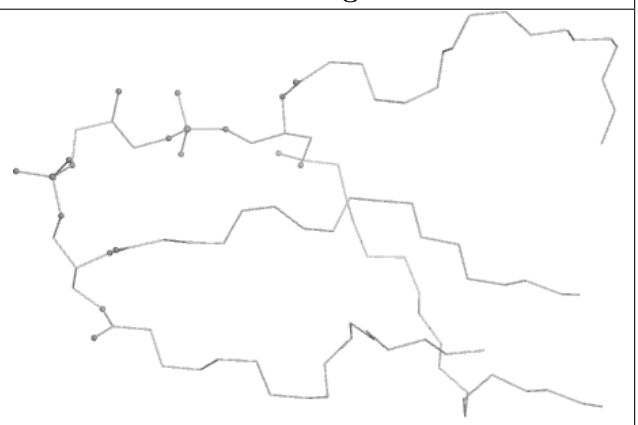
Bond lengths



Bond angles

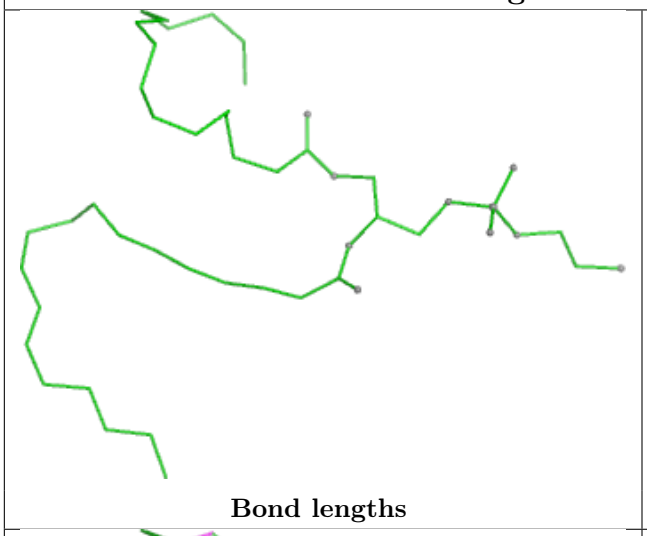


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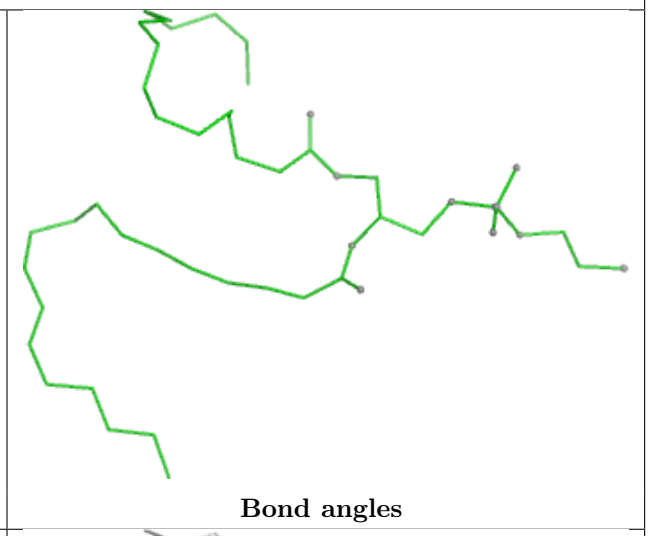


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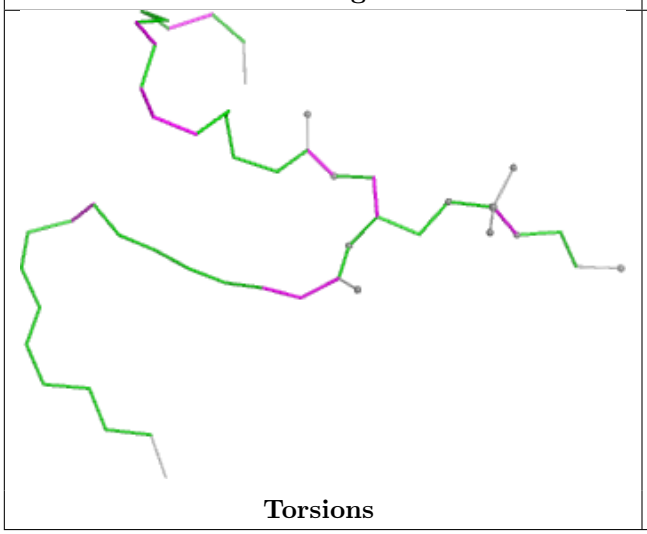
Ligand 3PE EN 1204



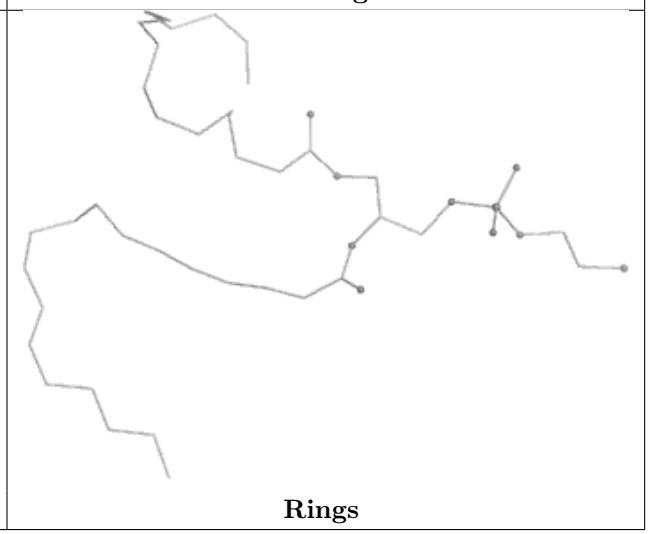
Bond lengths



Bond angles



Torsions

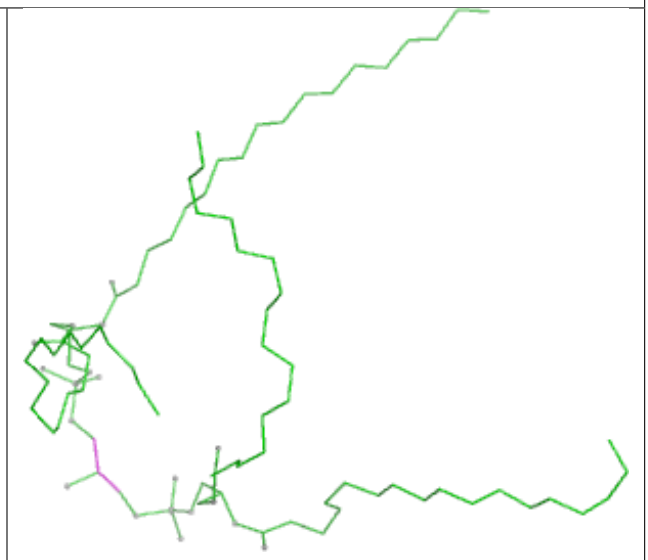


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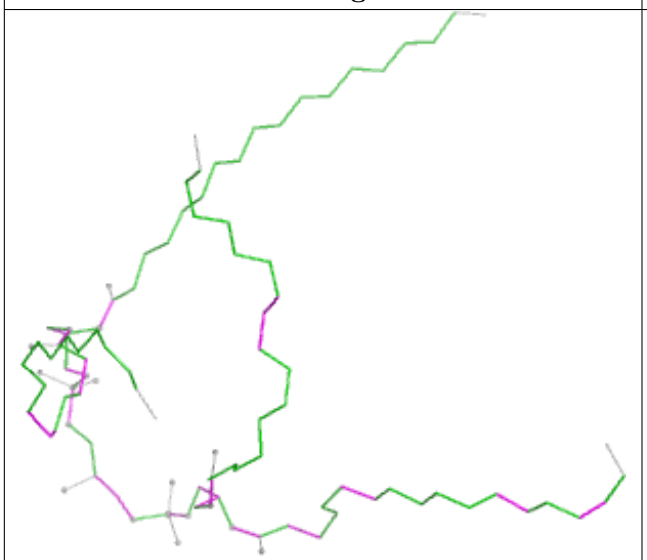
Ligand CDL DD 703



Bond lengths



Bond angles

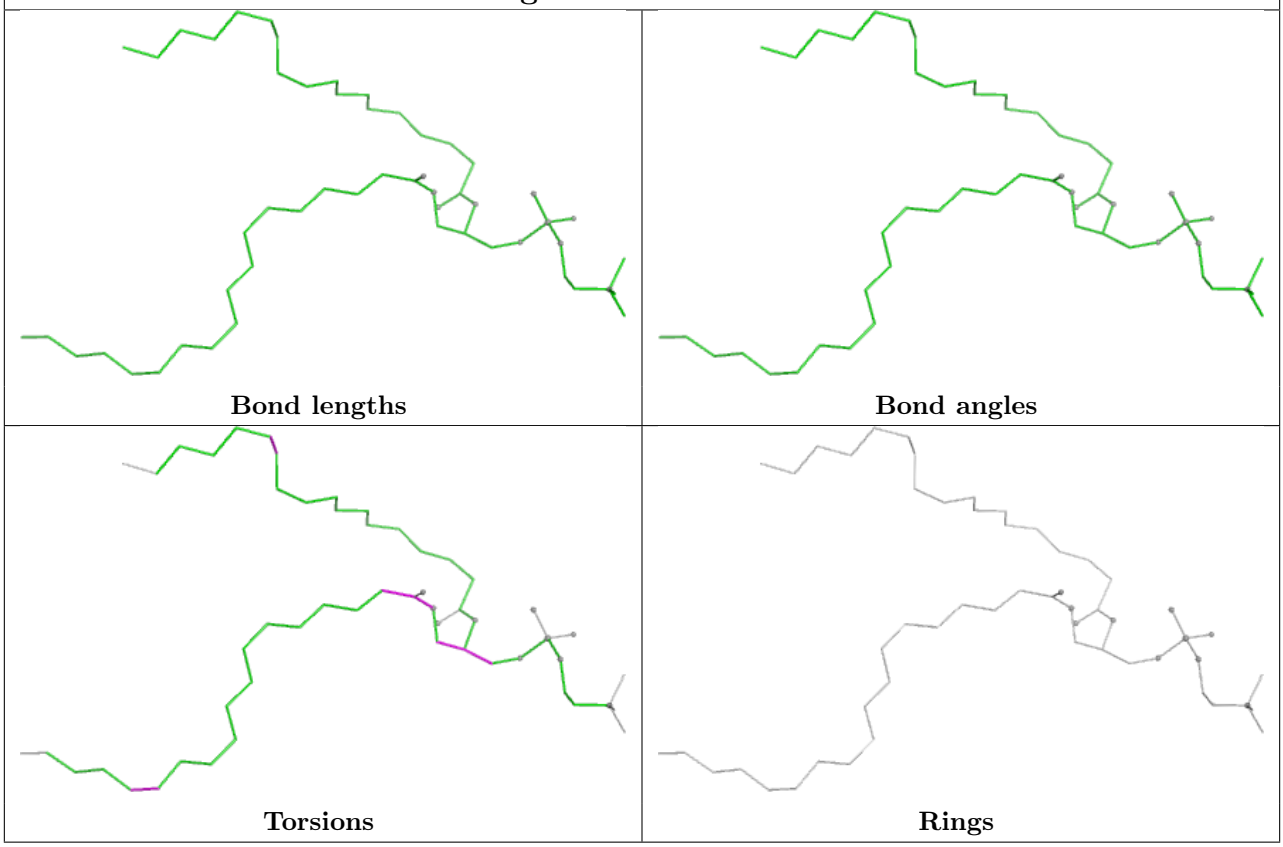


Torsions



Rings

Ligand PC1 Ds 407



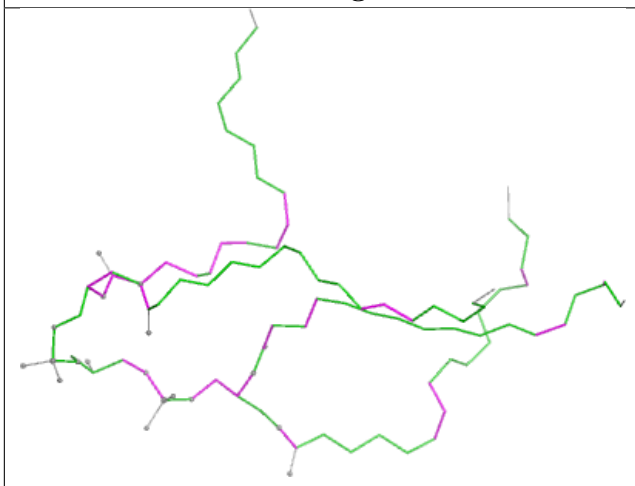
Ligand CDL DD 704



Bond lengths



Bond angles

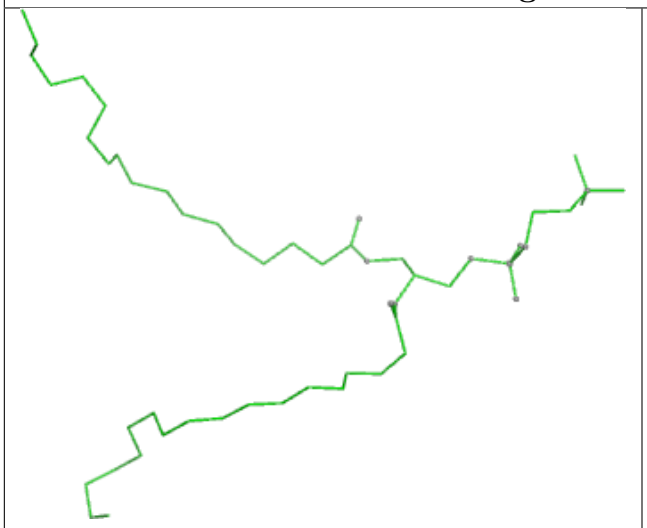


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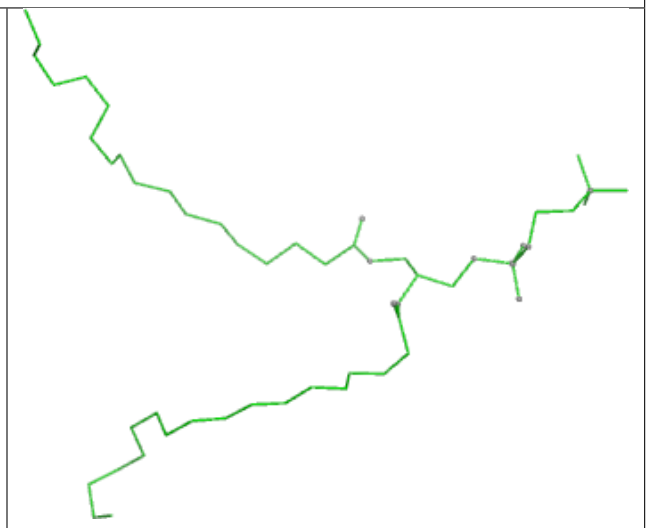


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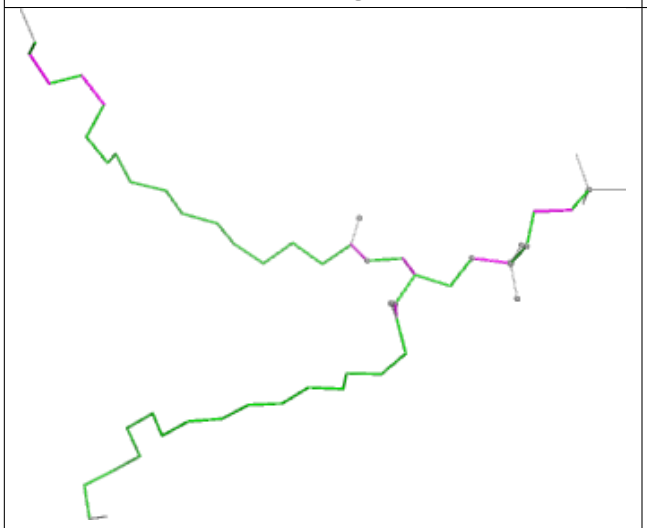
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Bond lengths



Bond angles

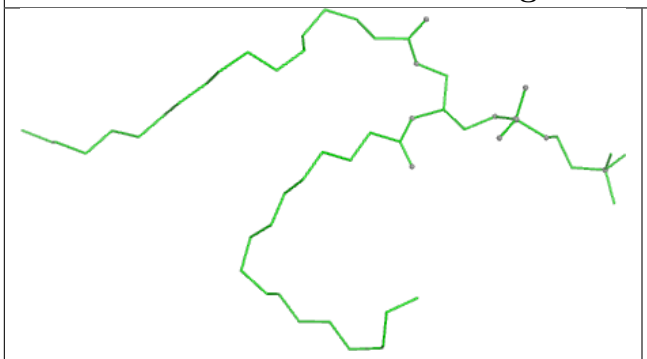


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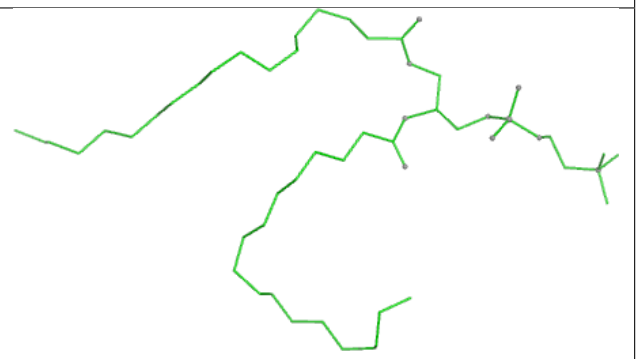


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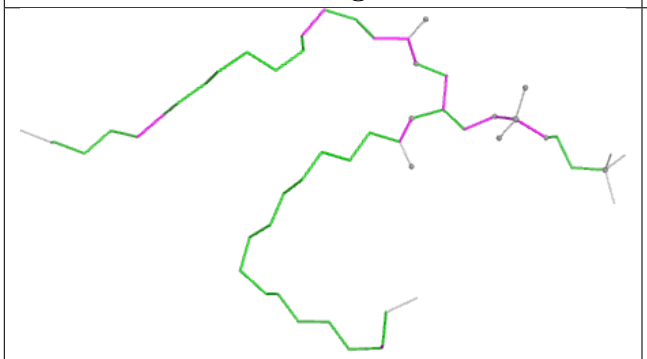
Ligand PC1 B1 401



Bond lengths



Bond angles

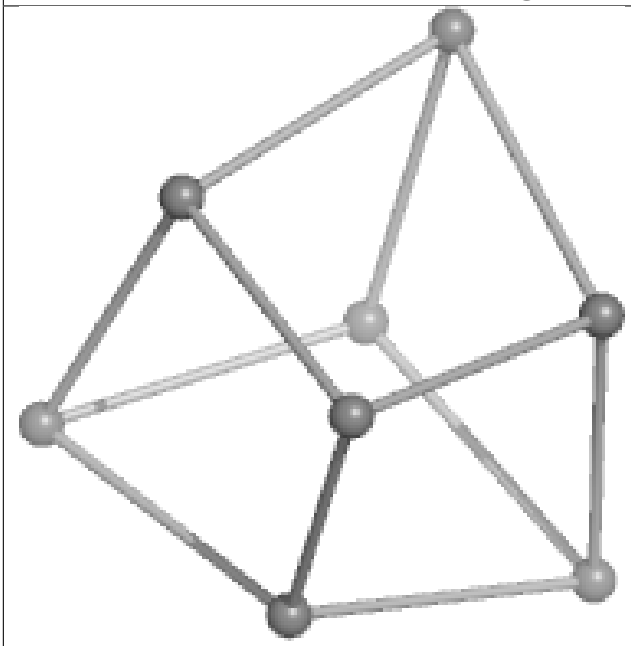


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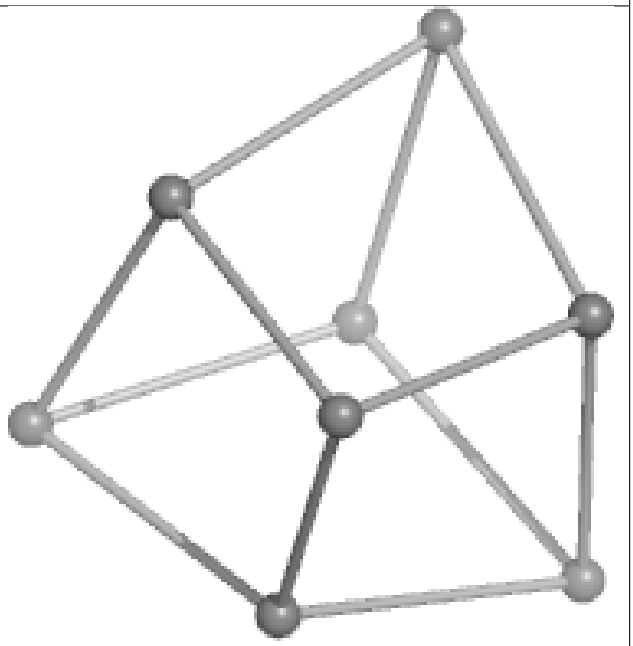


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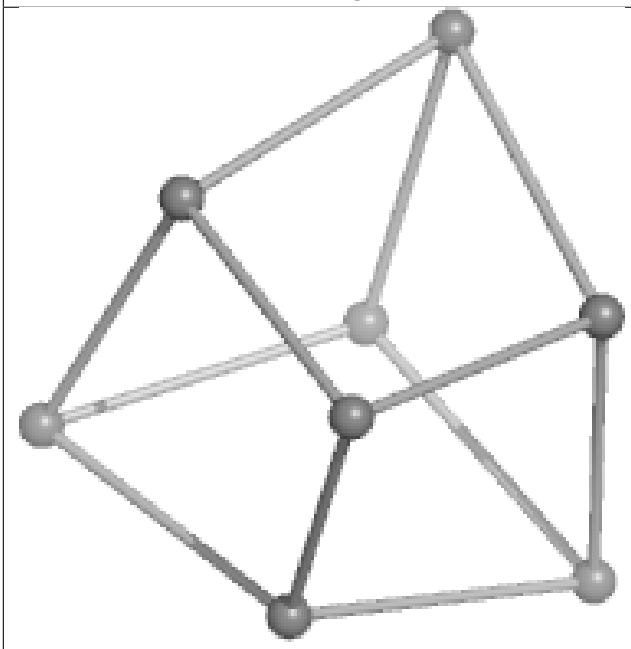
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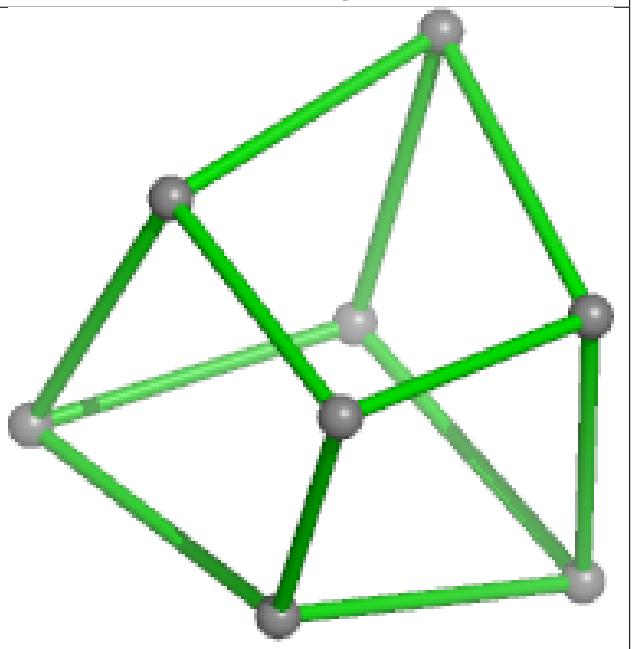
Bond lengths



Bond angles

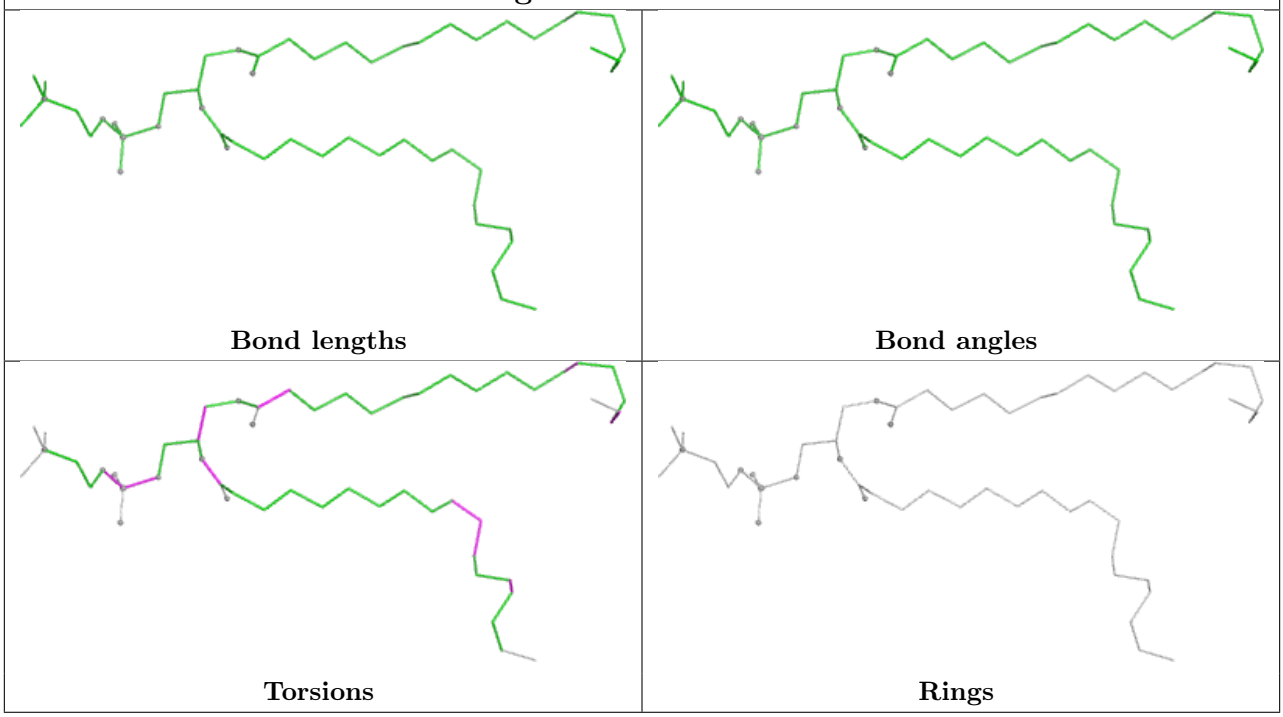


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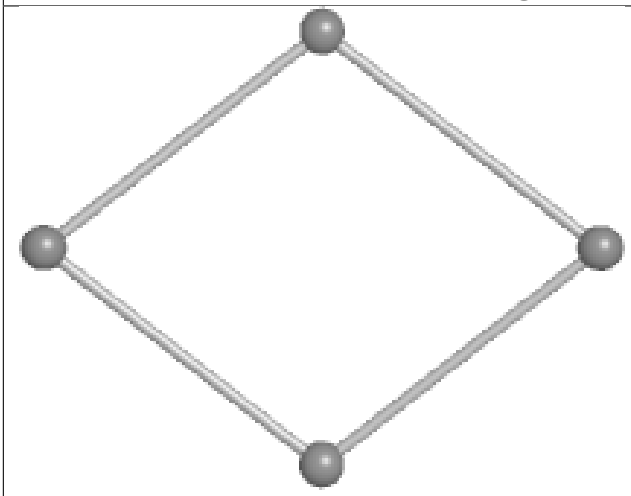


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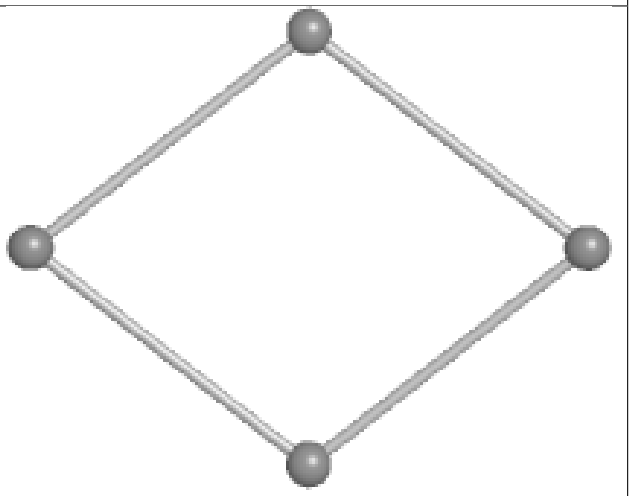
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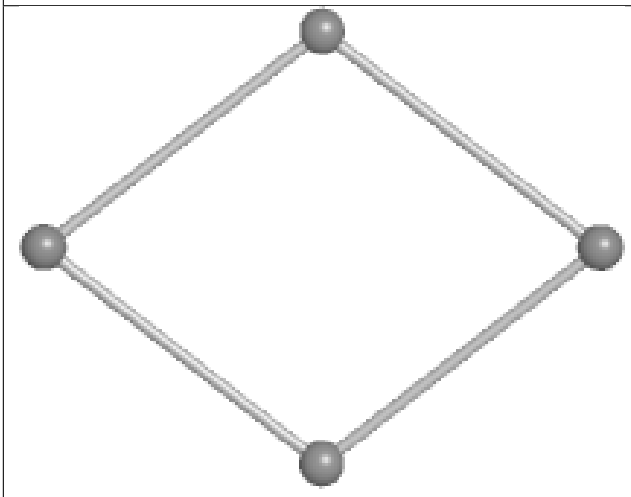
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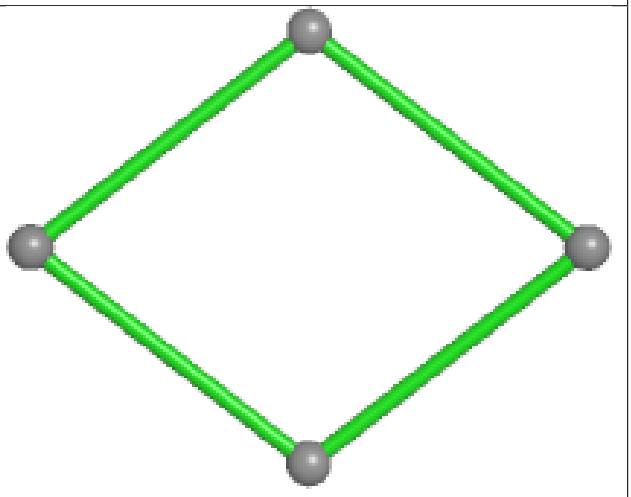
Bond lengths



Bond angles

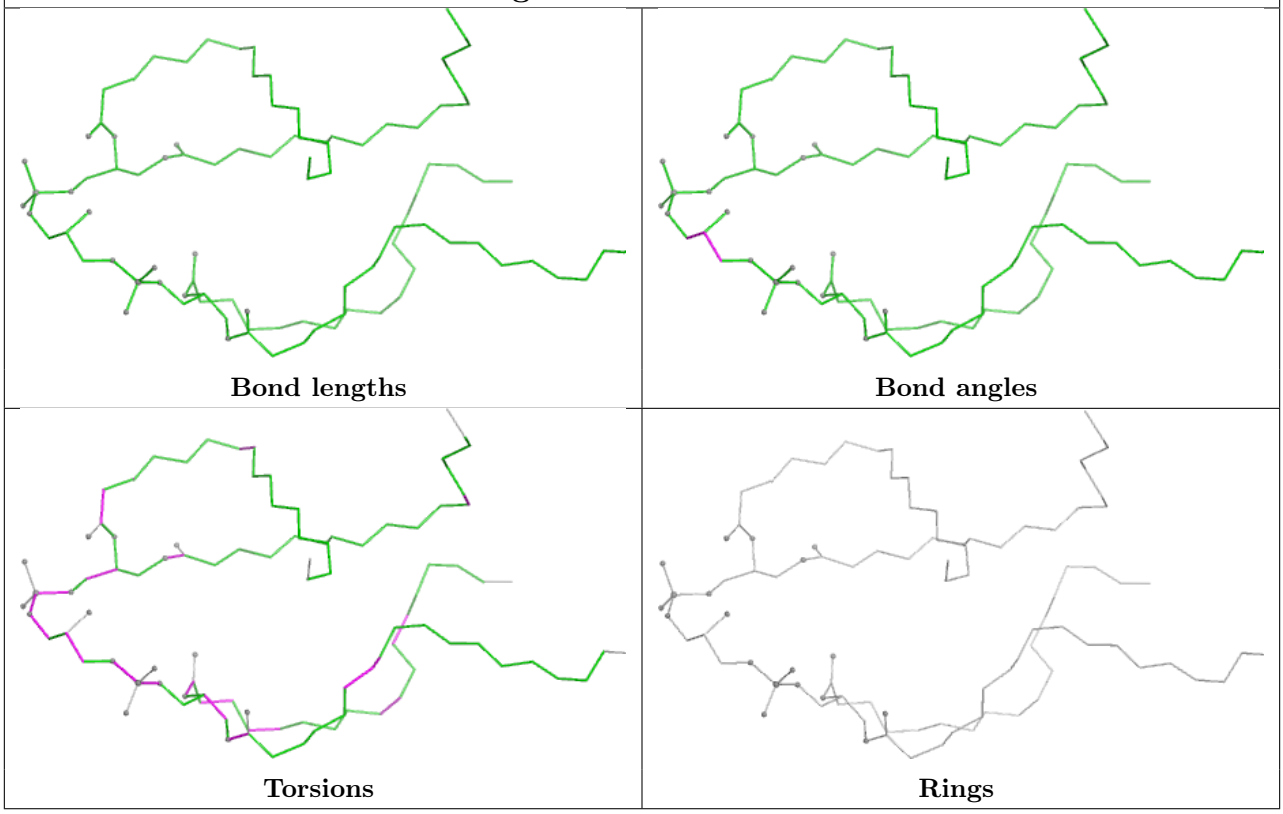


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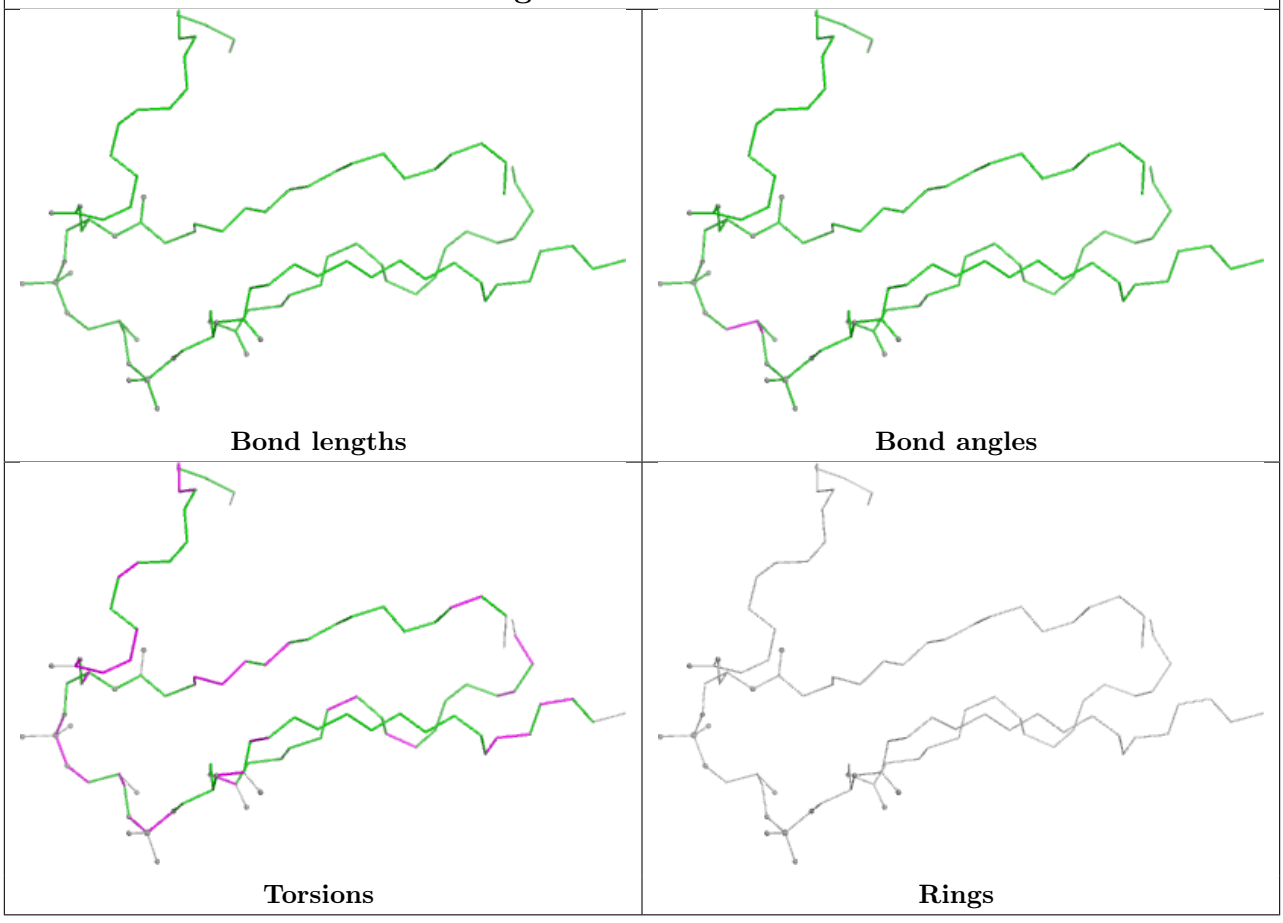


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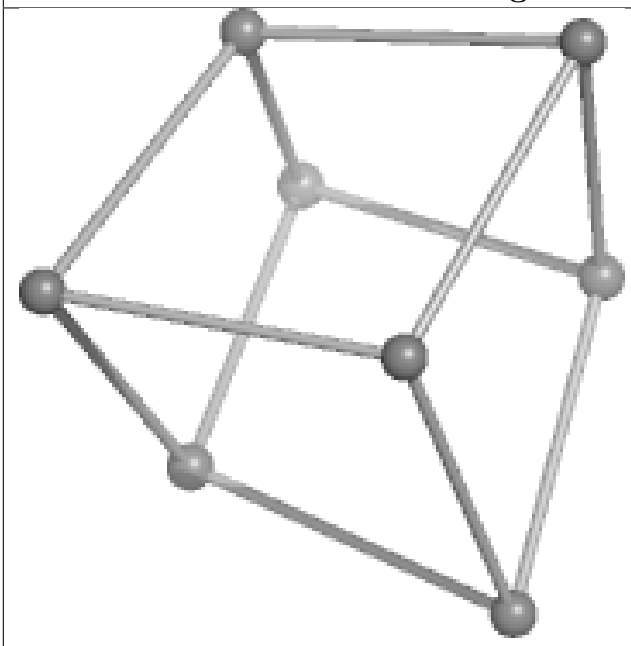
Ligand CDL ED 601



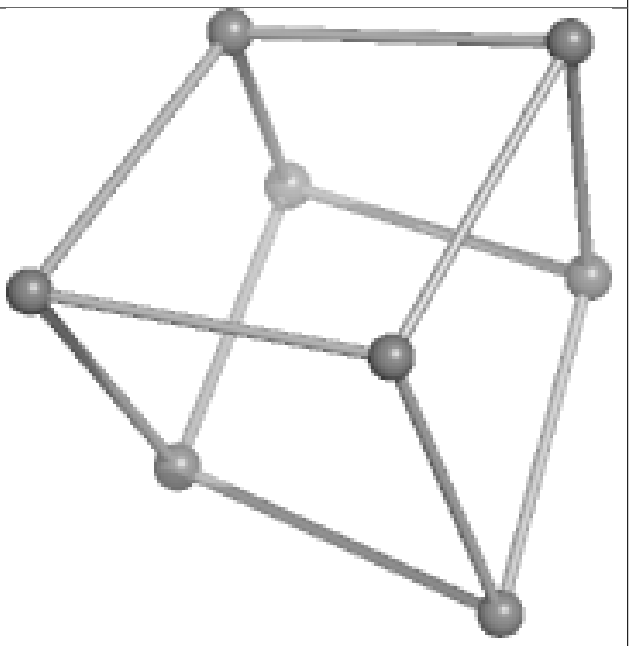
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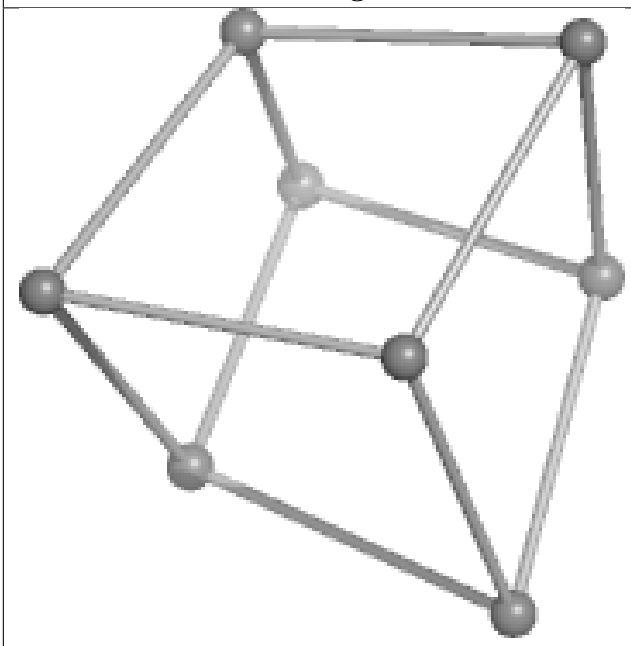
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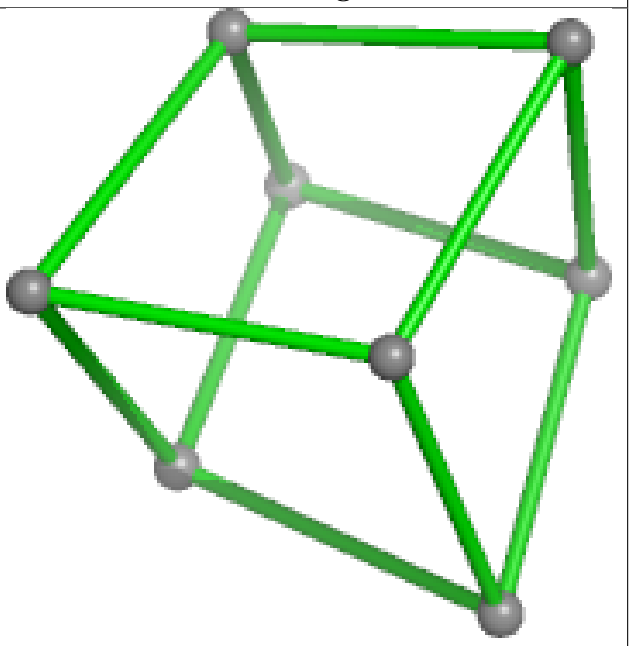
Bond lengths



Bond angles

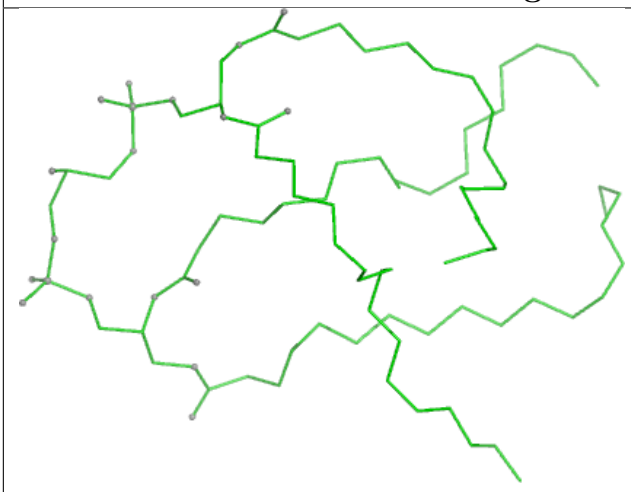


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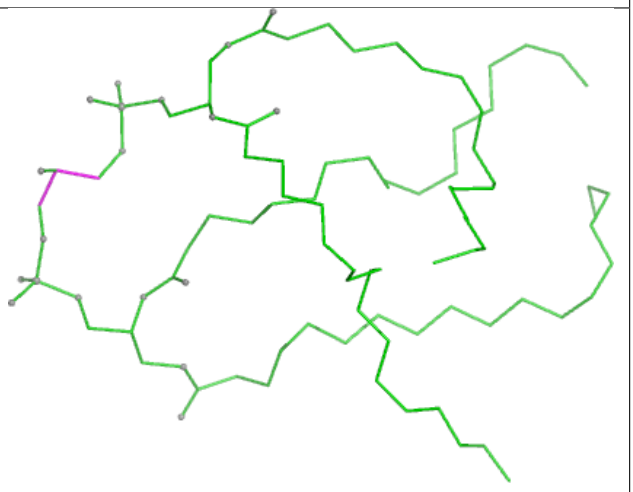


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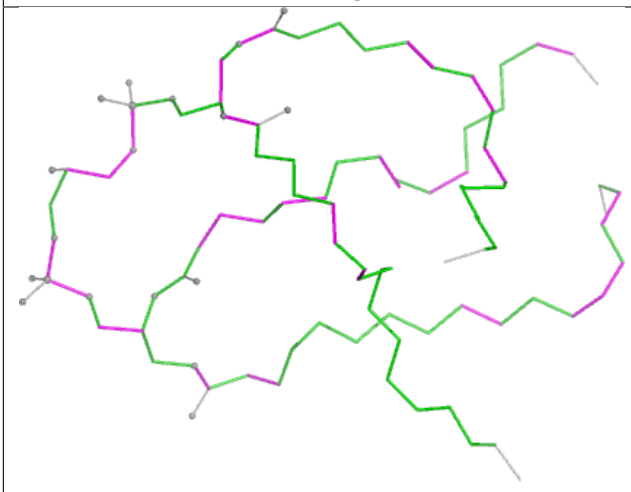
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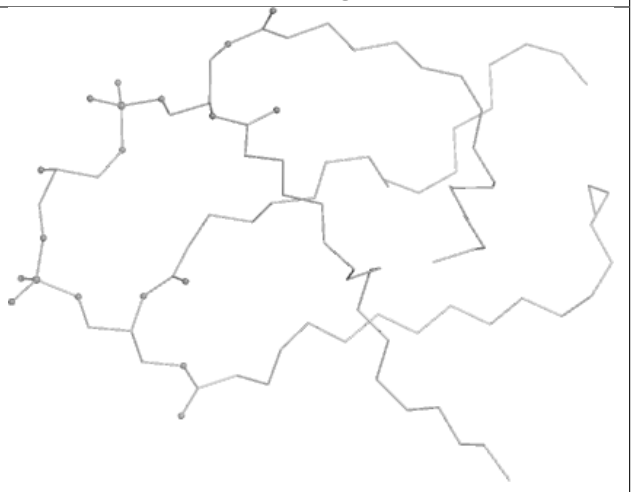
Bond lengths



Bond angles



Torsions



Rings

Ligand CDL h 501



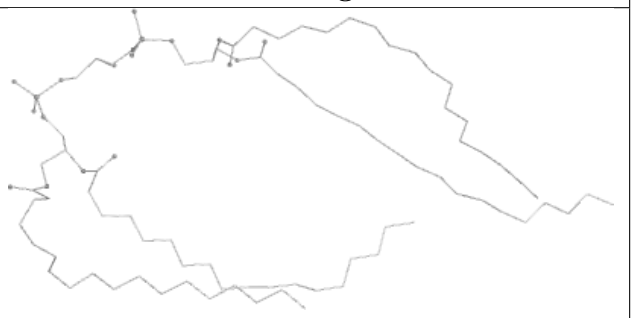
Bond lengths



Bond angles

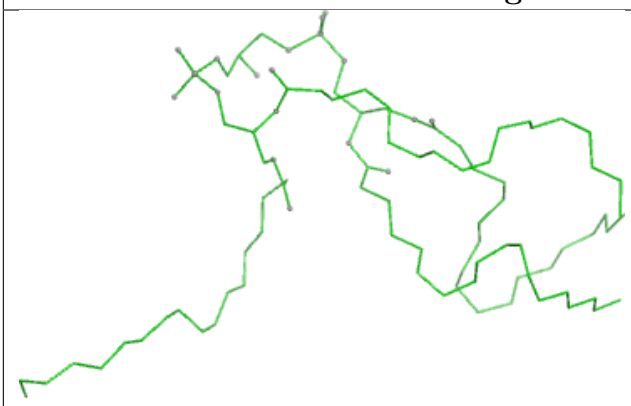


Torsions



Rings

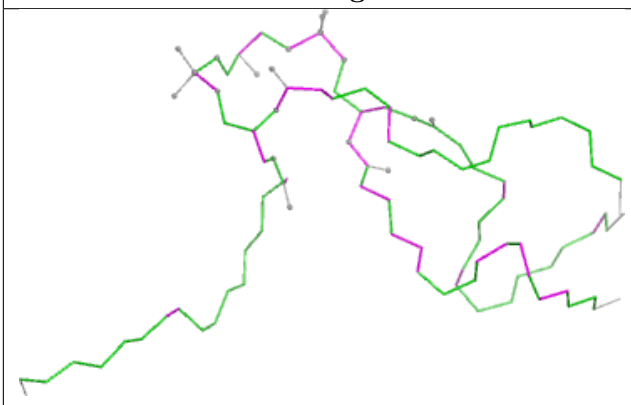
Ligand CDL Dq 1402



Bond lengths



Bond angles



Torsions



Rings

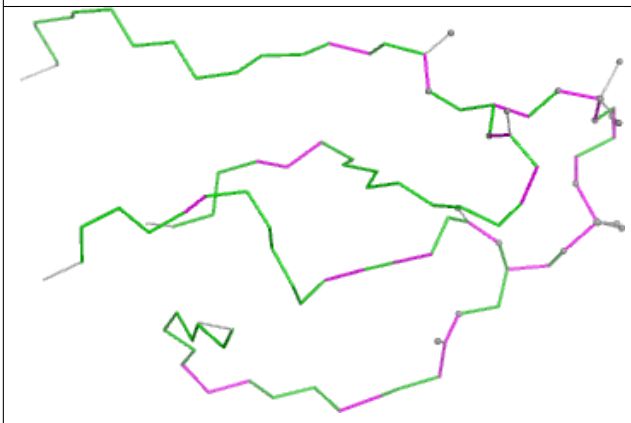
Ligand CDL Du 401



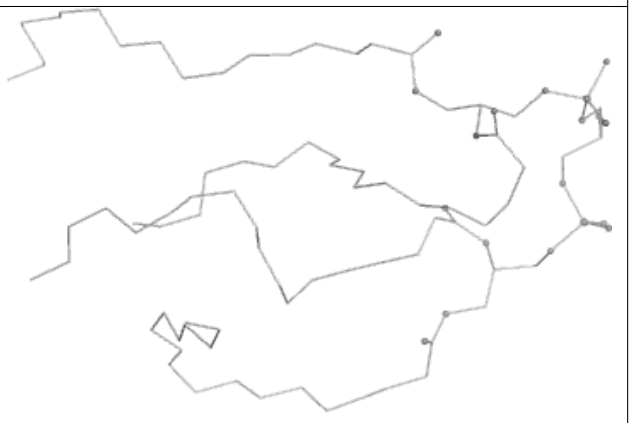
Bond lengths



Bond angles

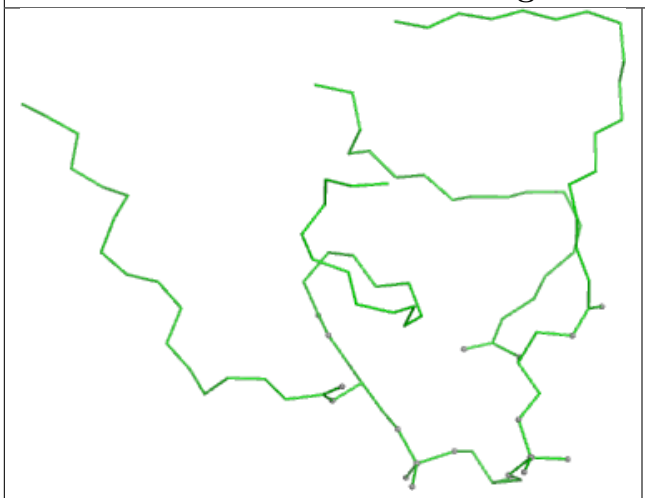


Torsions

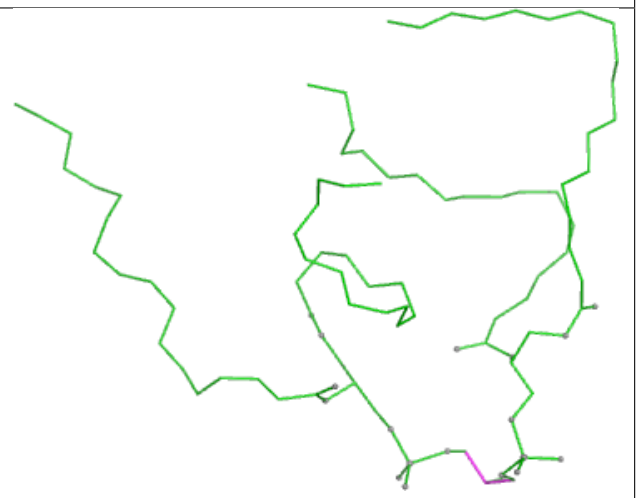


Rings

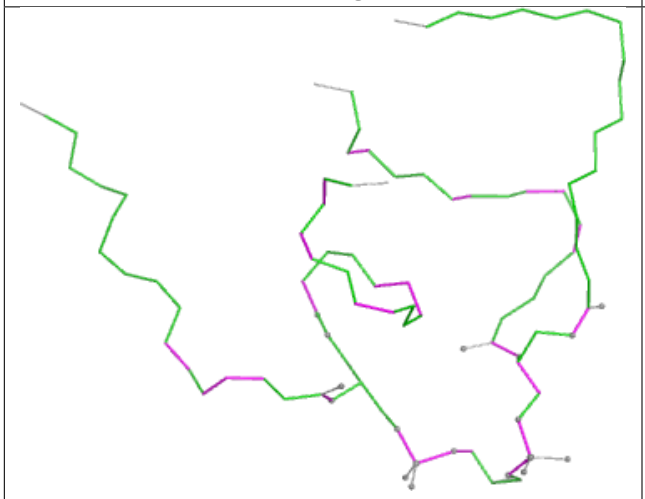
Ligand CDL Ds 406



Bond lengths



Bond angles

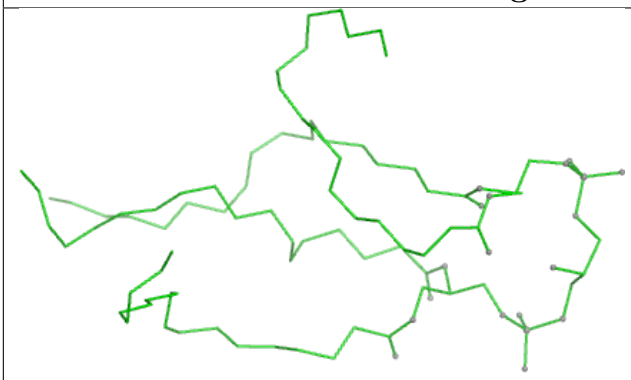


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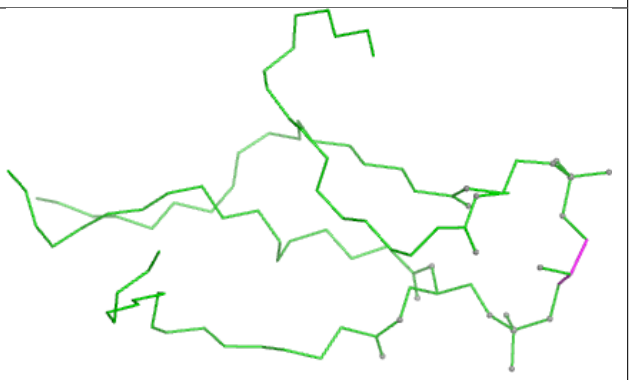


Rings

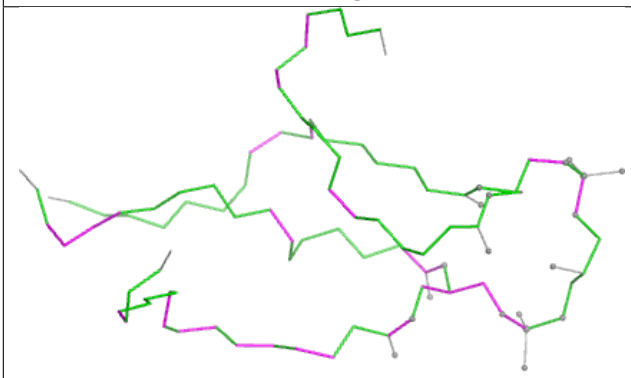
Ligand CDL DA 706



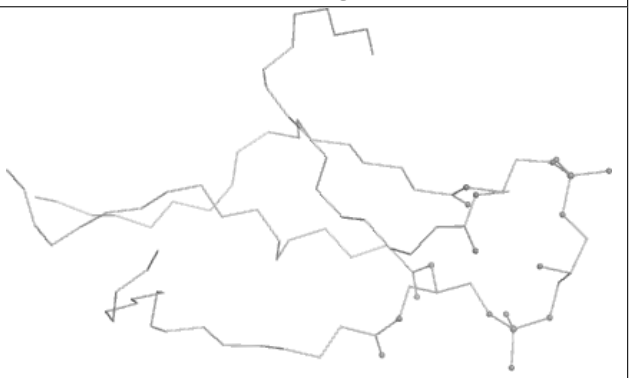
Bond lengths



Bond angles

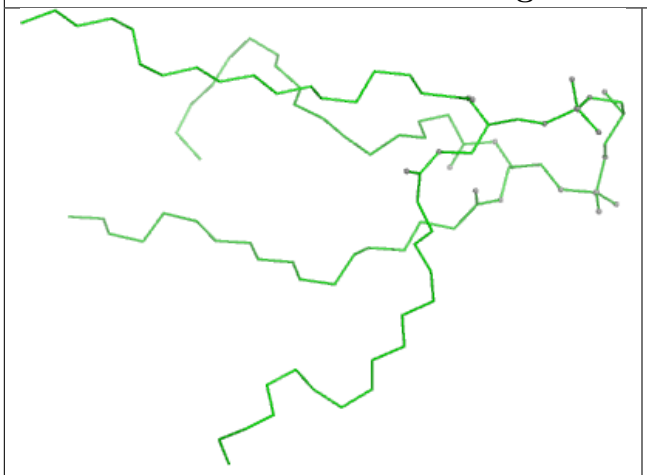


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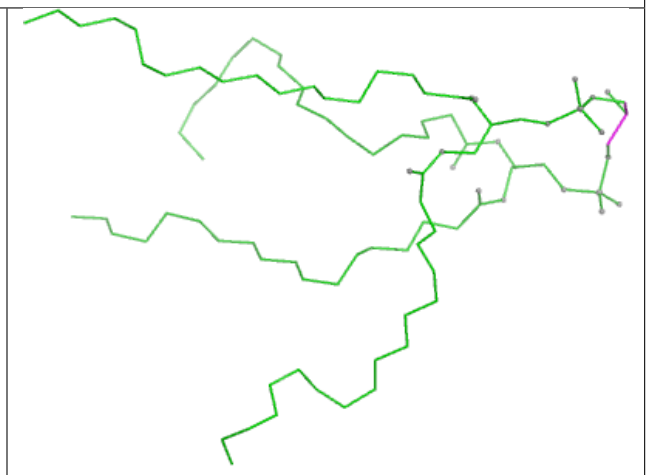


Rings

Ligand CDL Dc 601



Bond lengths



Bond angles

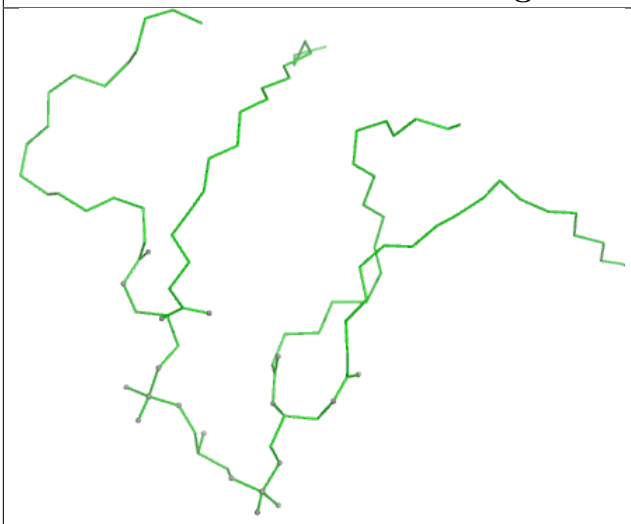


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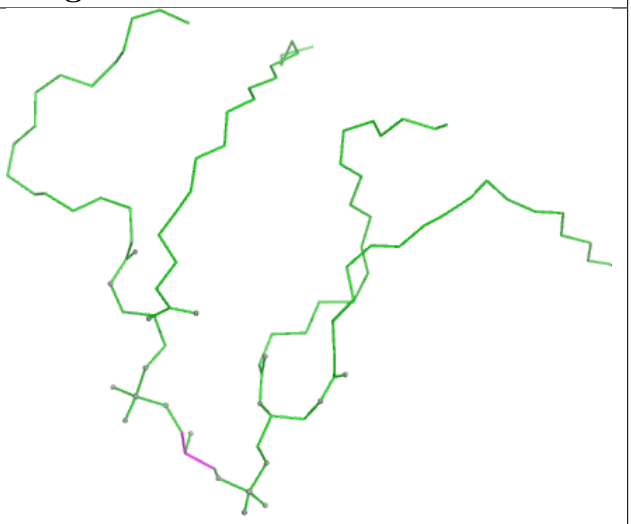


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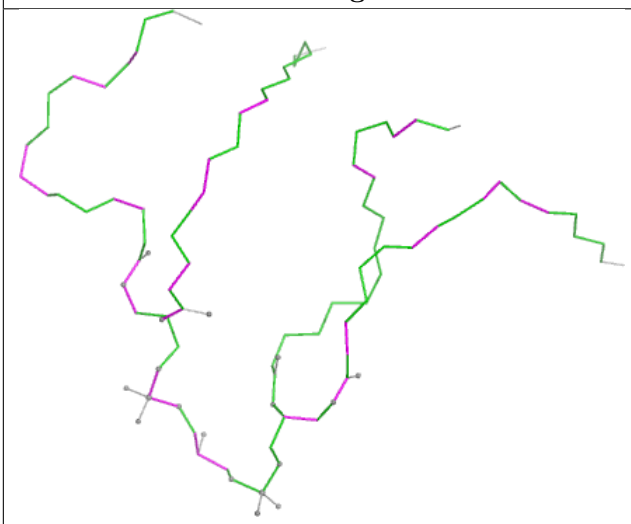
Ligand CDL Dg 202



Bond lengths



Bond angles

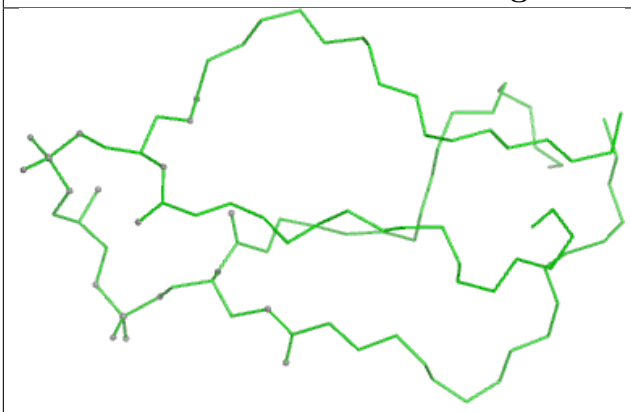


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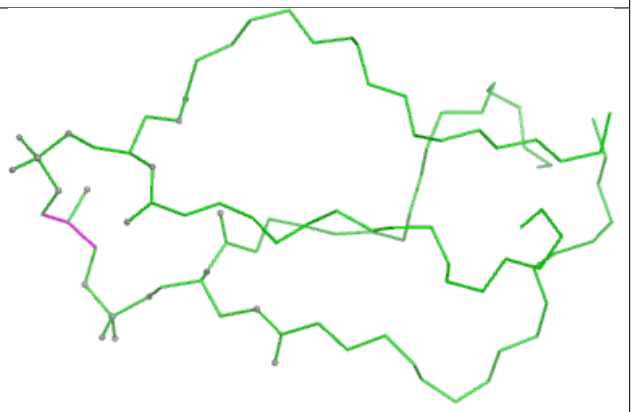


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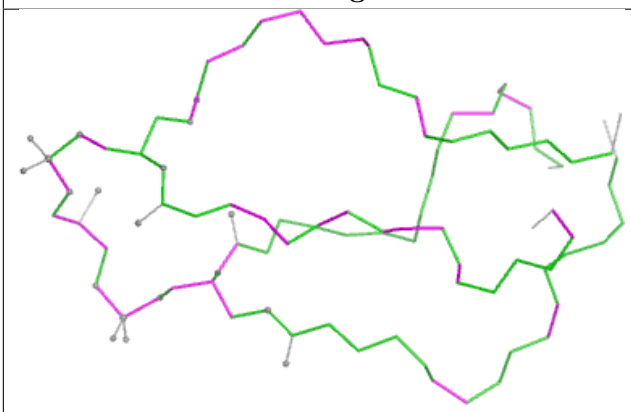
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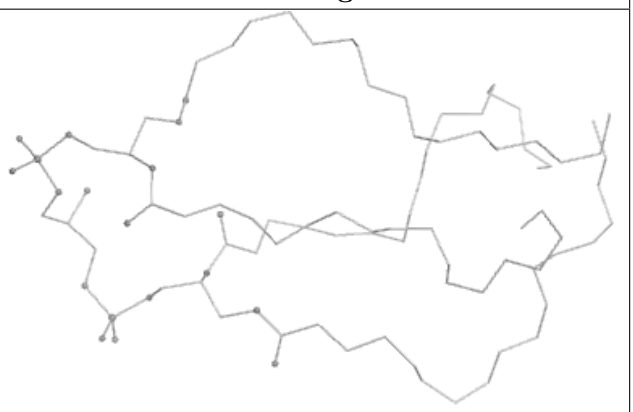
Bond lengths



Bond angles

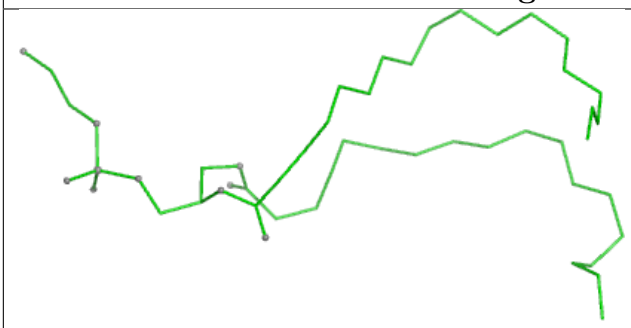


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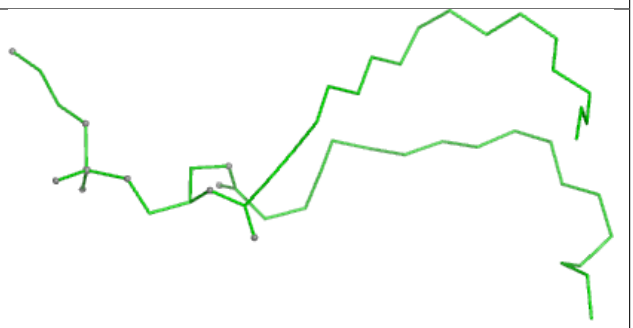


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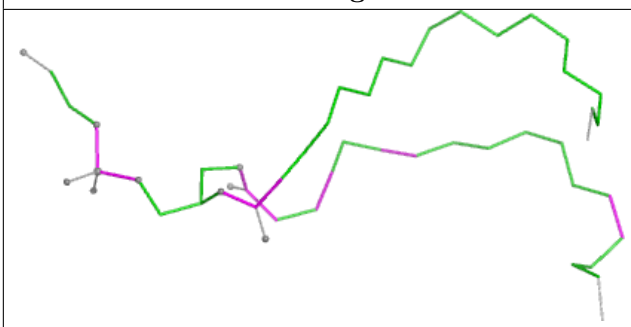
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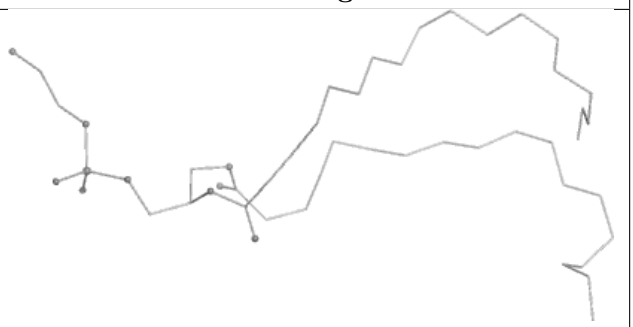
Bond lengths



Bond angles

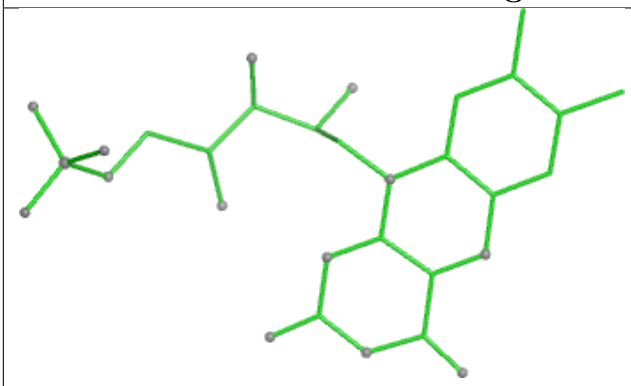


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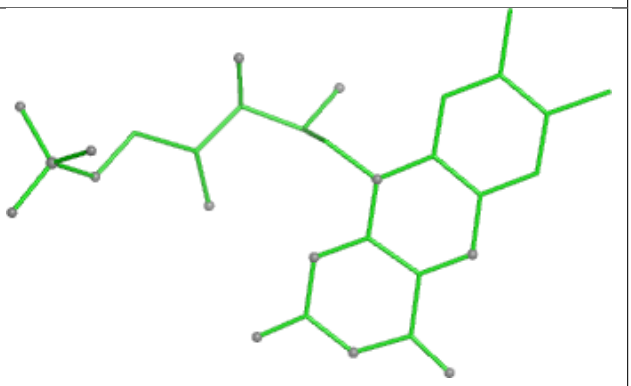


Rings

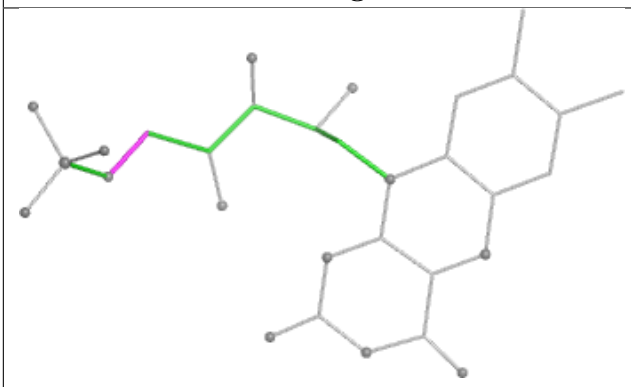
Ligand FMN AD 502



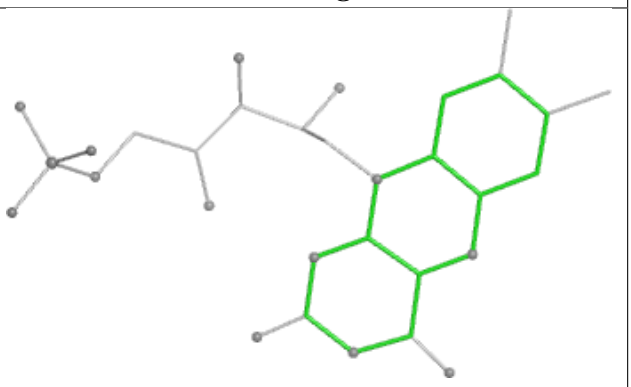
Bond lengths



Bond angles

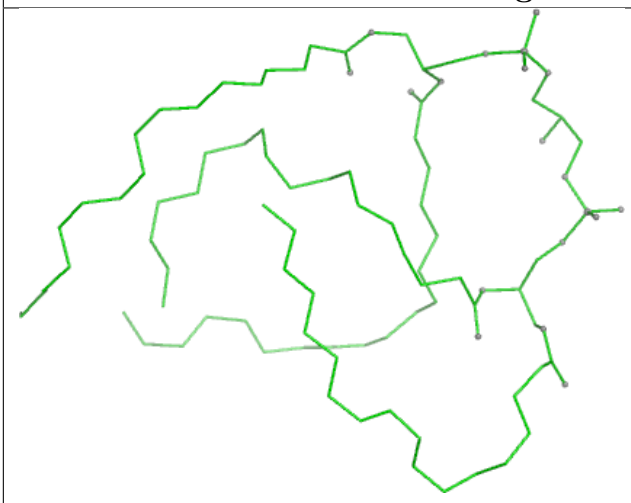


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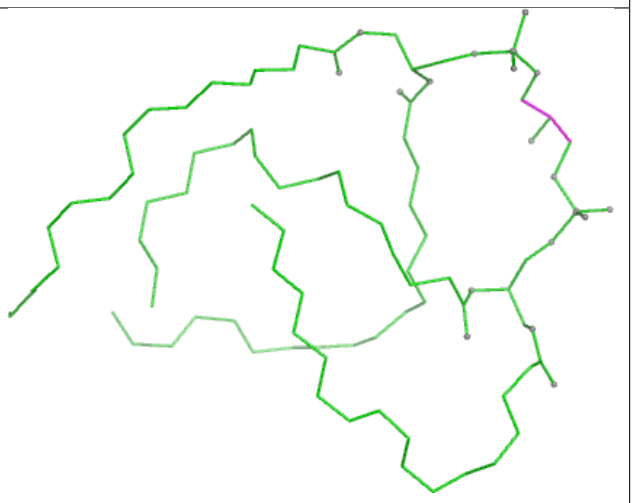


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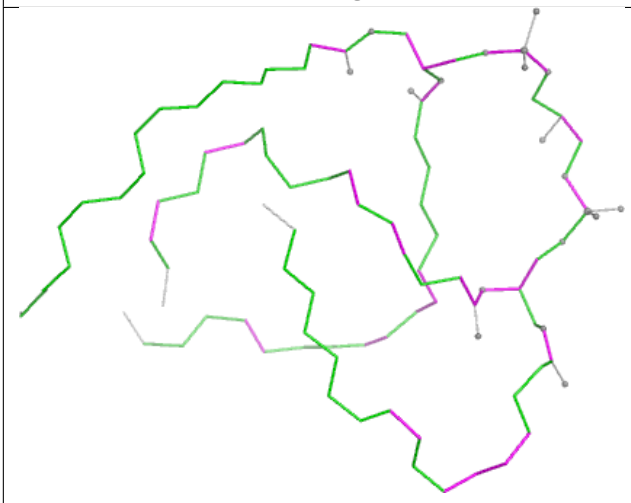
Ligand CDL Eb 302



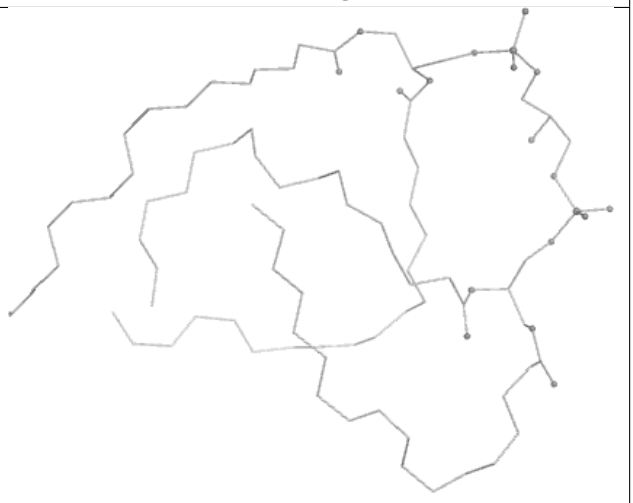
Bond lengths



Bond angles

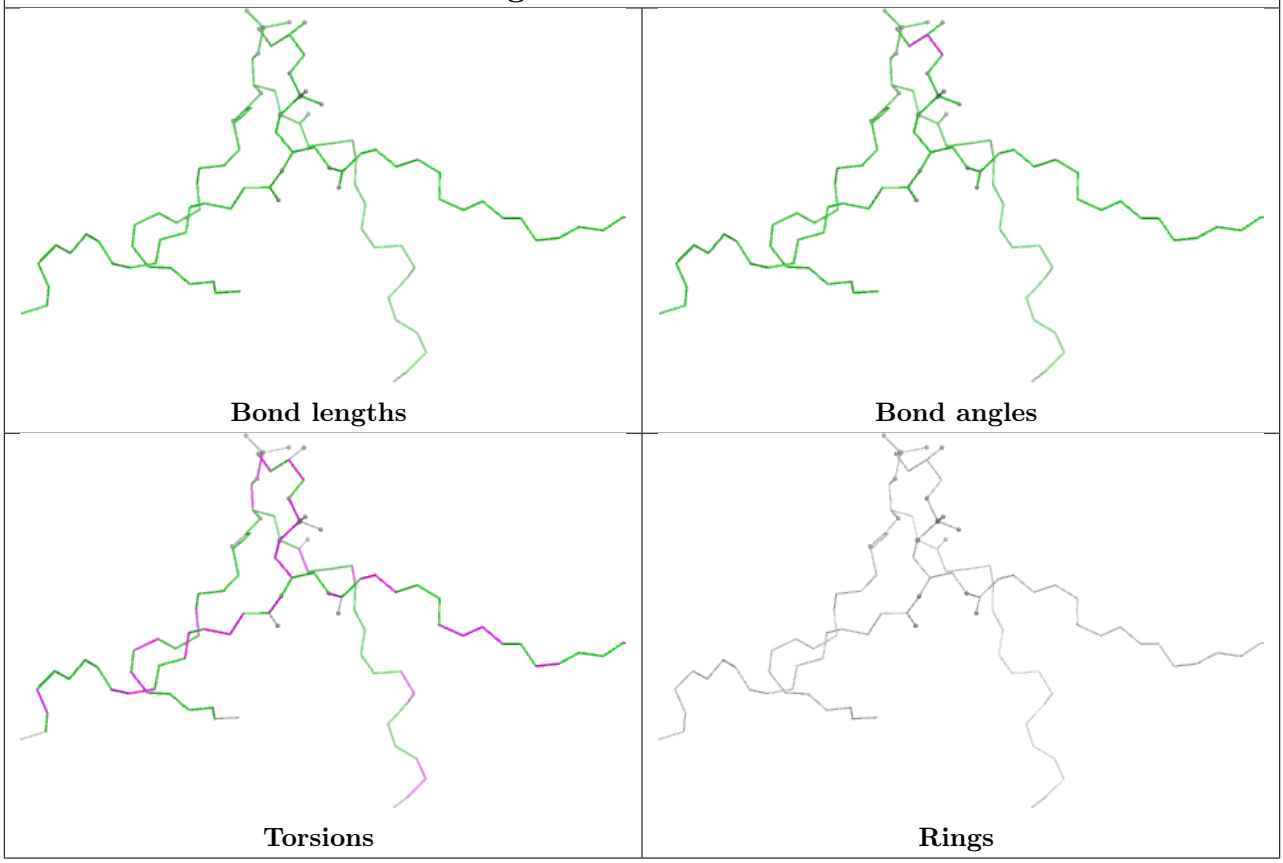


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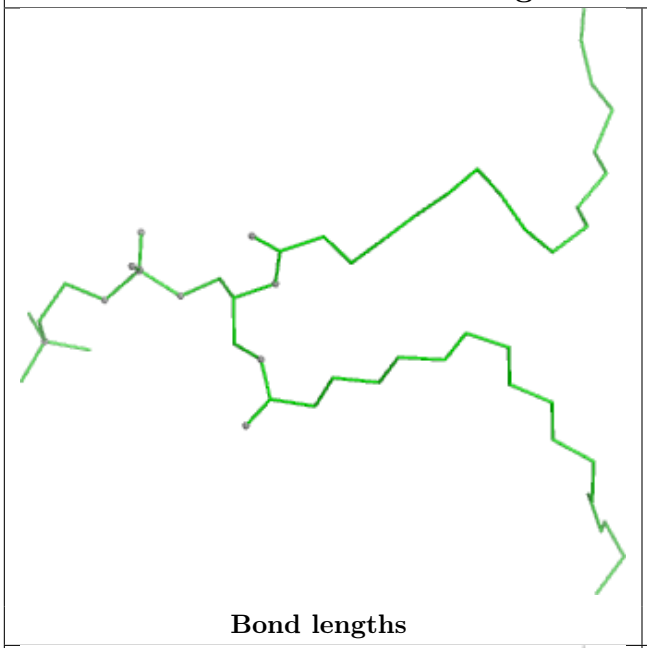


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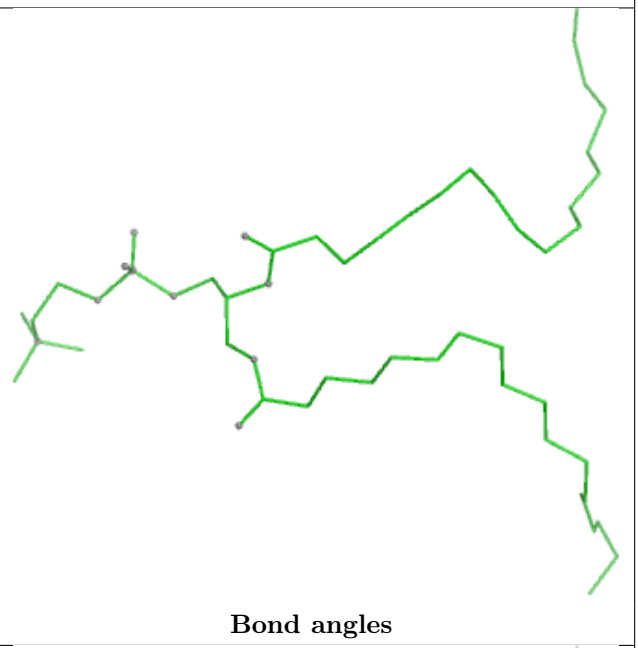
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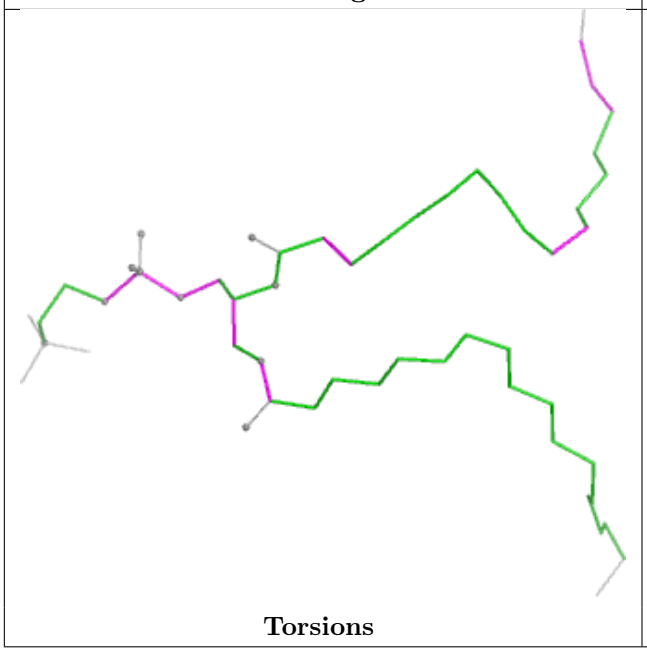
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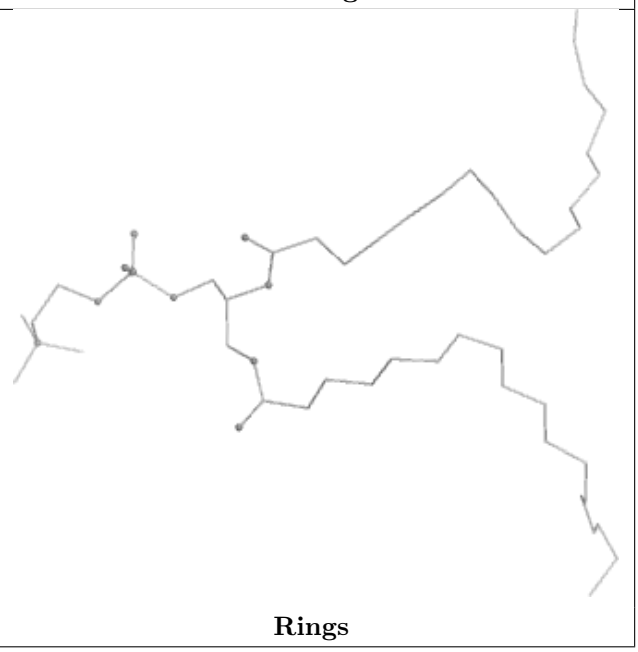
Bond lengths



Bond angles

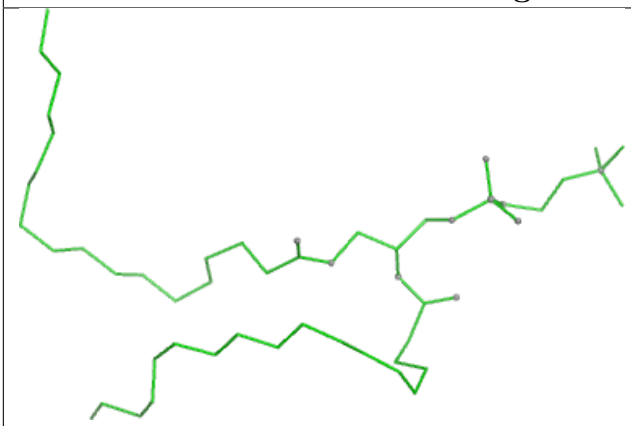


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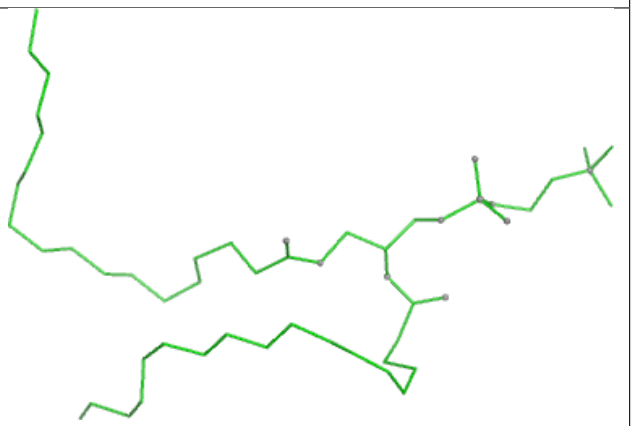


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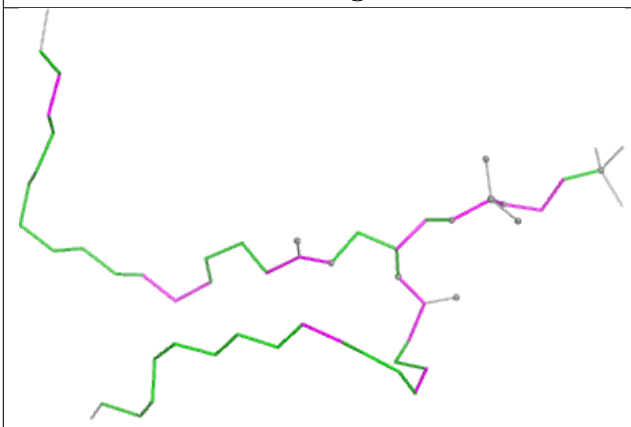
Ligand PC1 BG 202



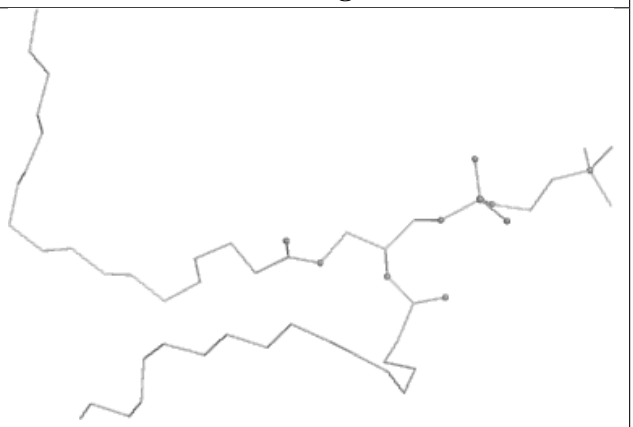
Bond lengths



Bond angles

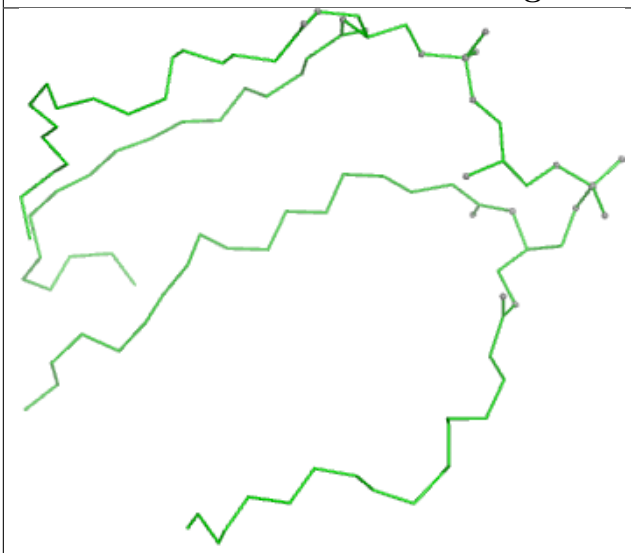


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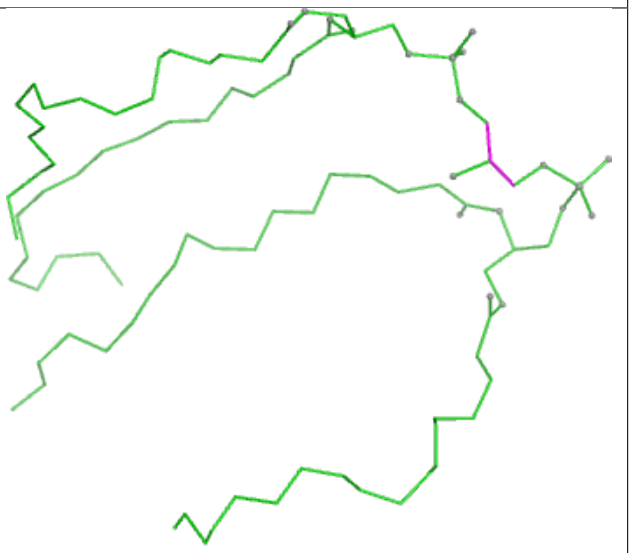


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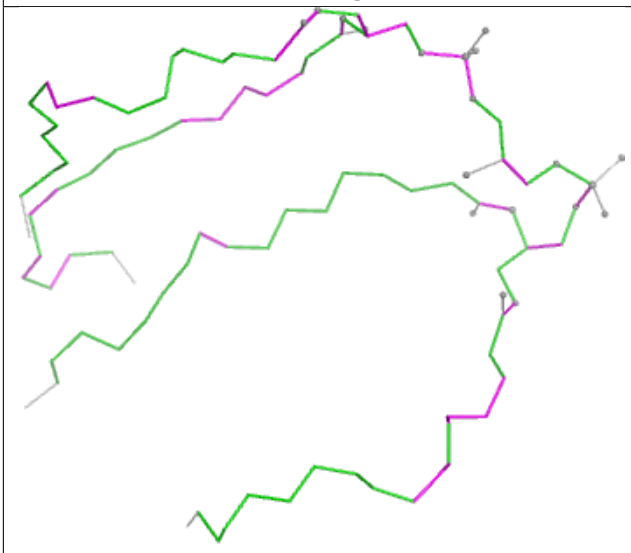
Ligand CDL C 505



Bond lengths



Bond angles

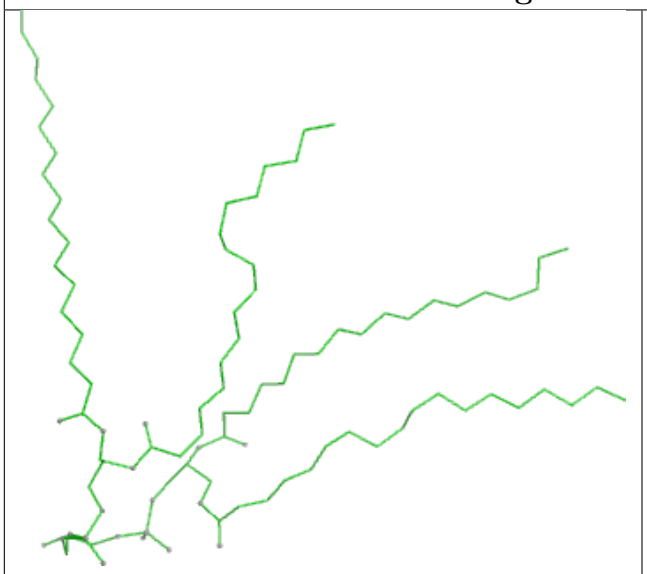


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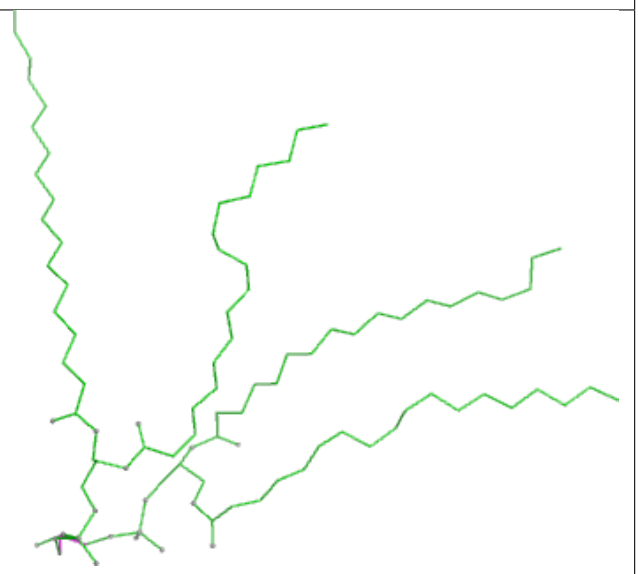


Rings

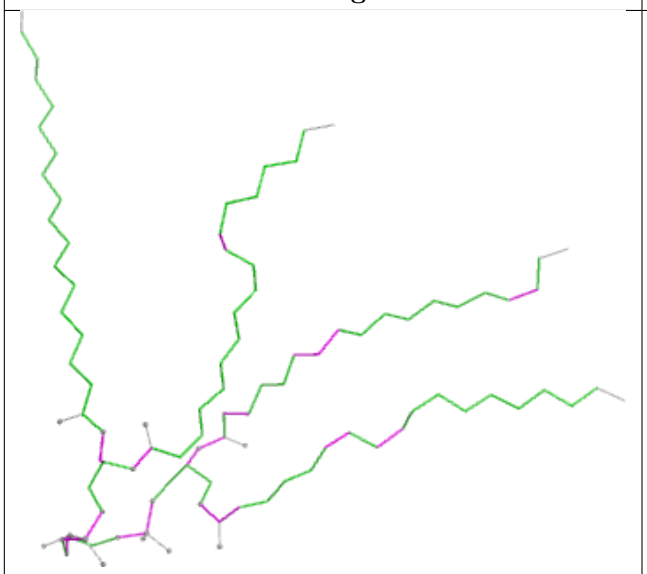
Ligand CDL H 1302



Bond lengths



Bond angles

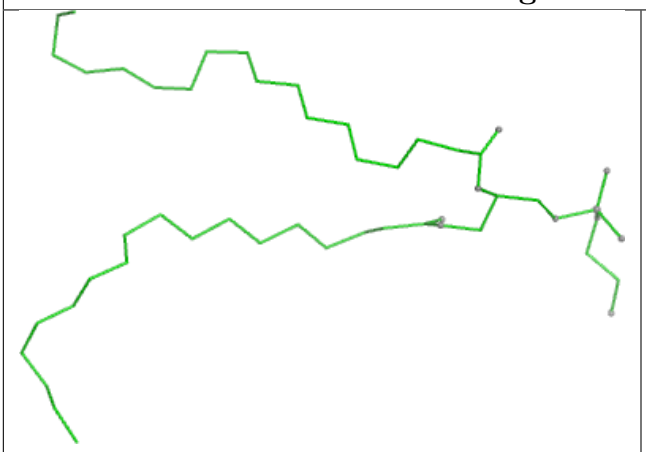


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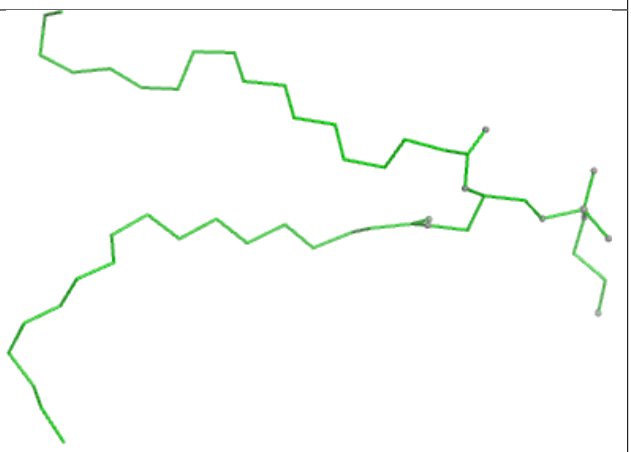


Rings

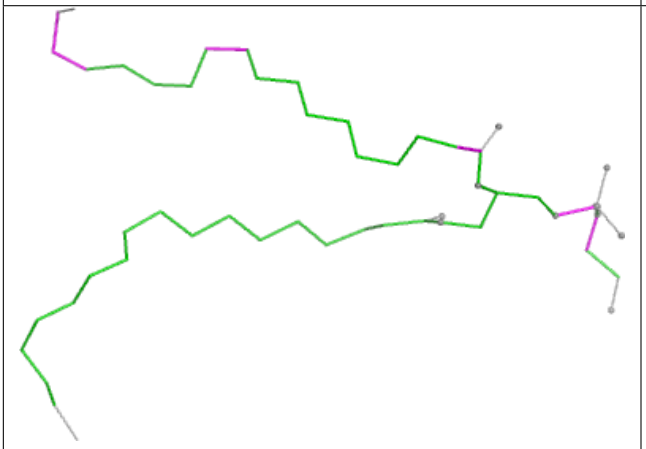
Ligand 3PE A9 602



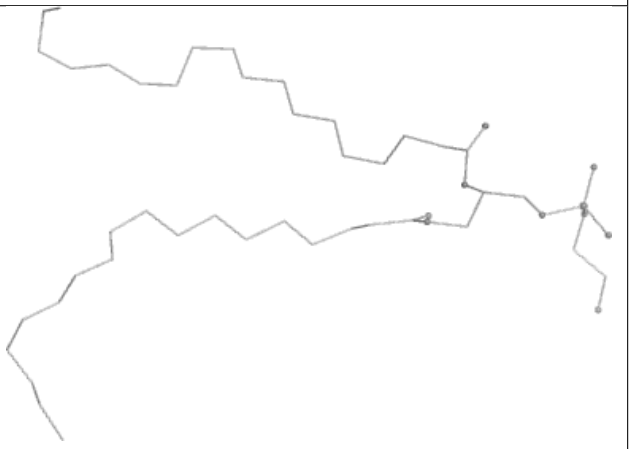
Bond lengths



Bond angles

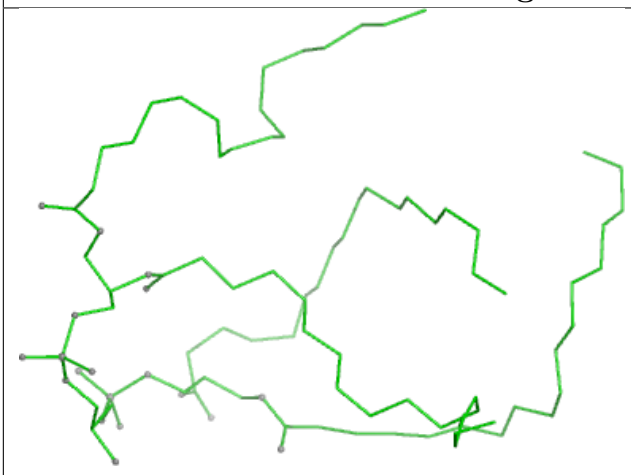


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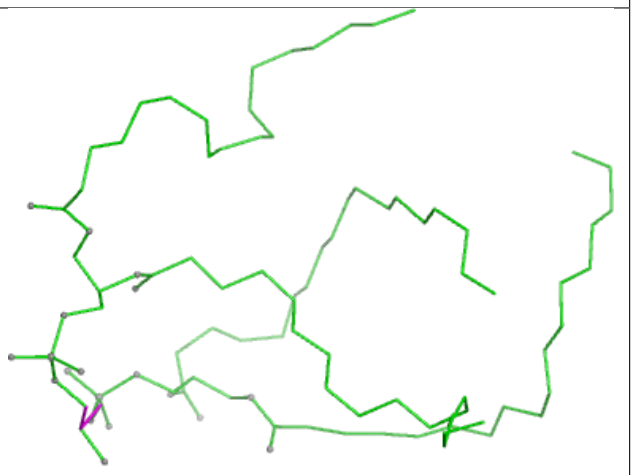


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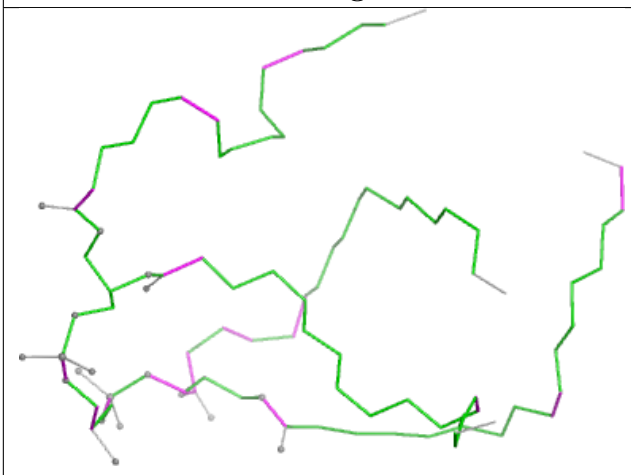
Ligand CDL Ea 502



Bond lengths



Bond angles

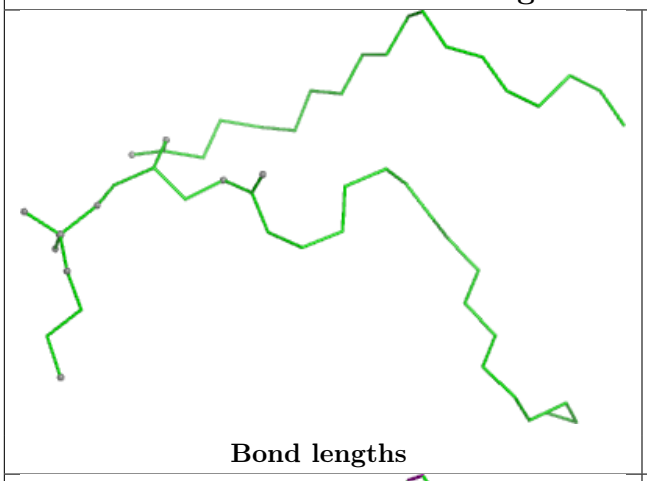


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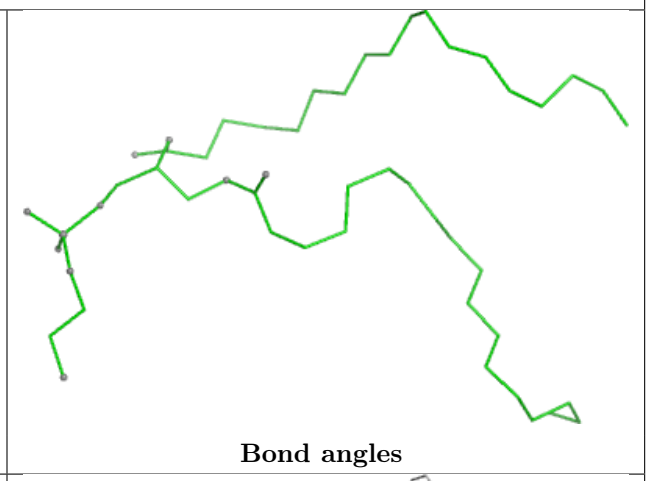


Rings

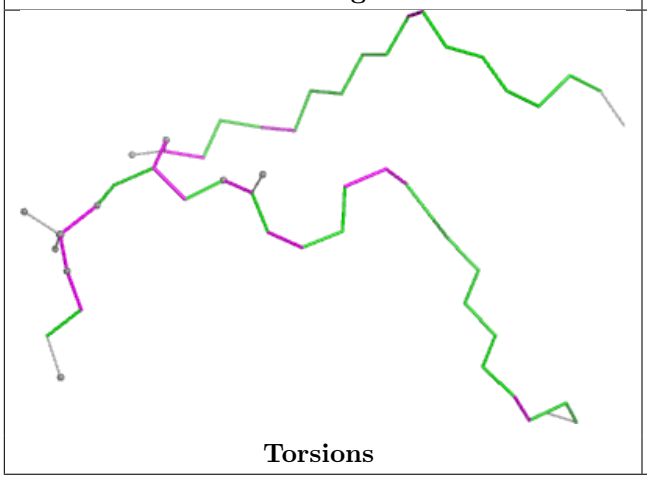
Ligand 3PE BT 201



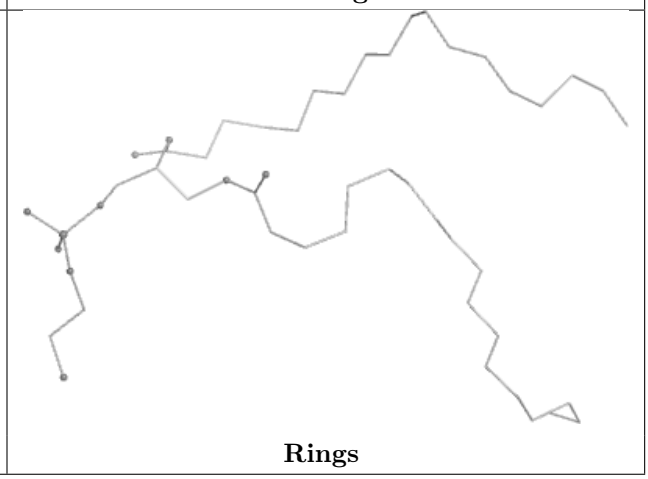
Bond lengths



Bond angles

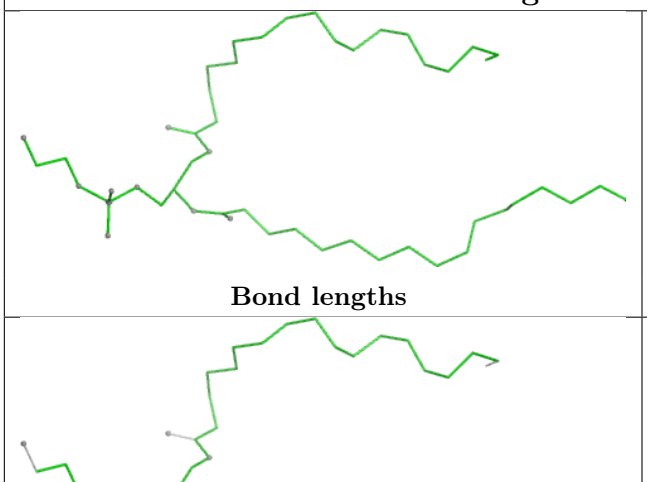


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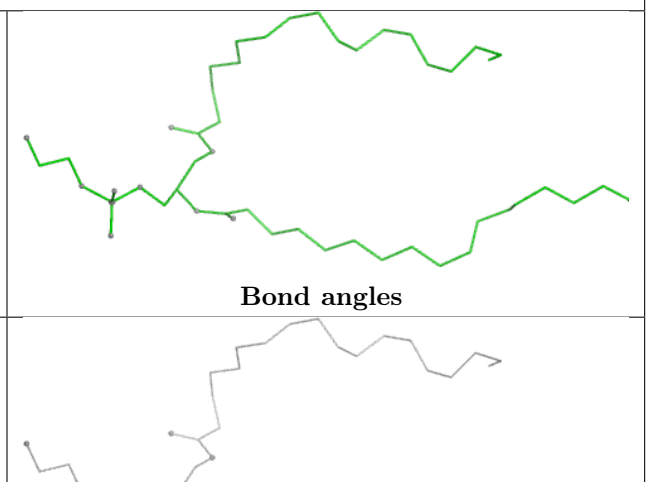


Rings

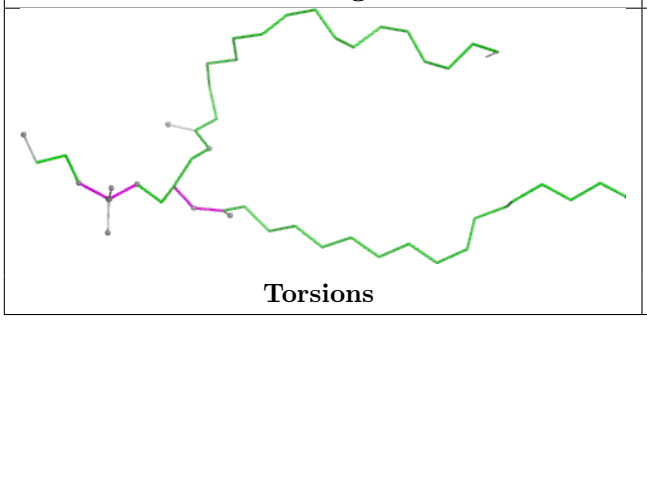
Ligand 3PE Eo 203



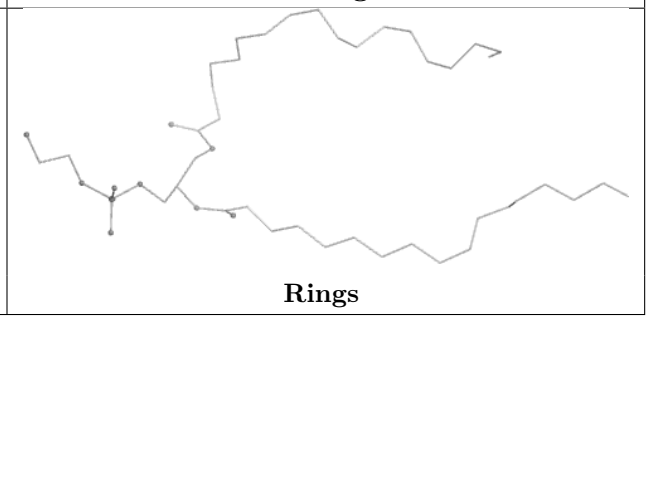
Bond lengths



Bond angles

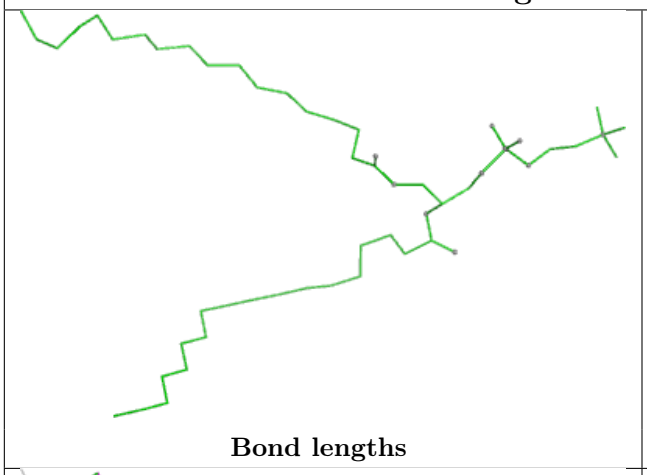


Torsions

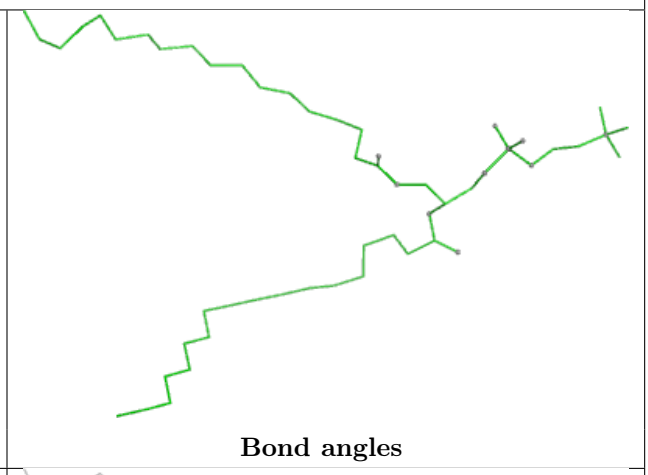


Rings

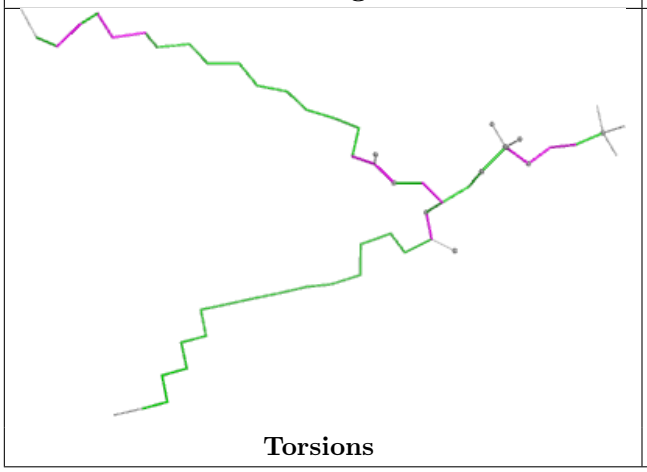
Ligand PC1 AU 202



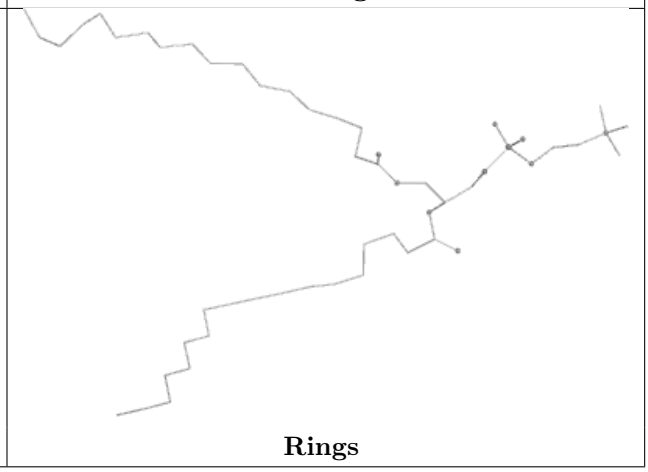
Bond lengths



Bond angles

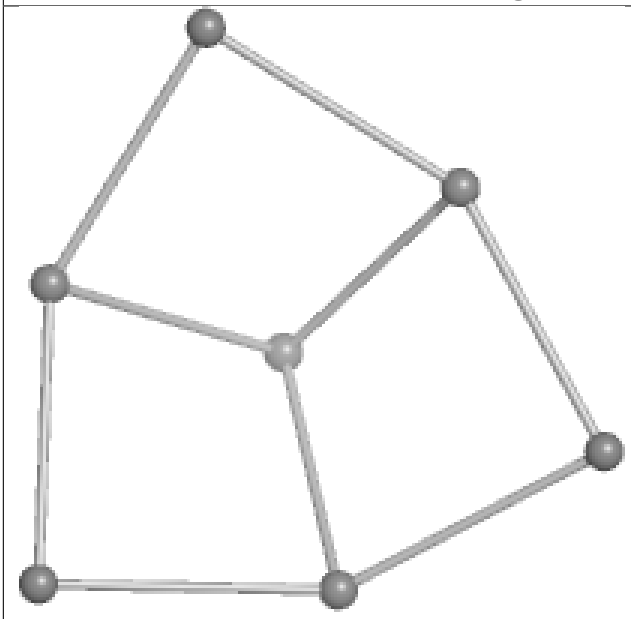


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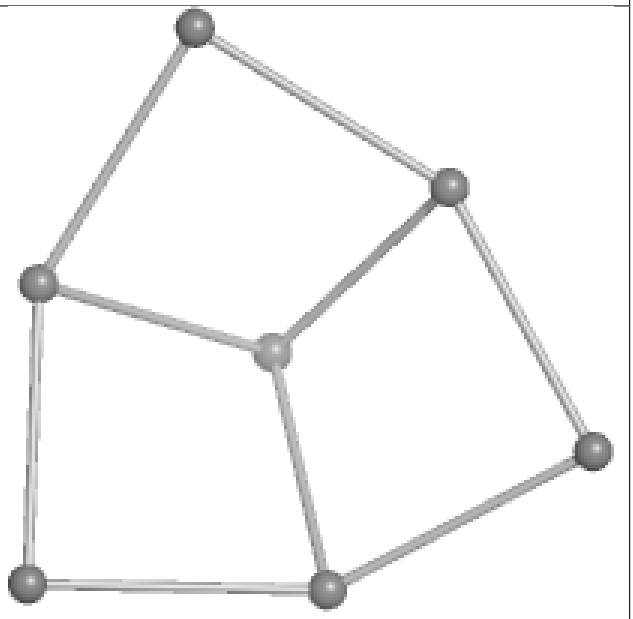


Rings

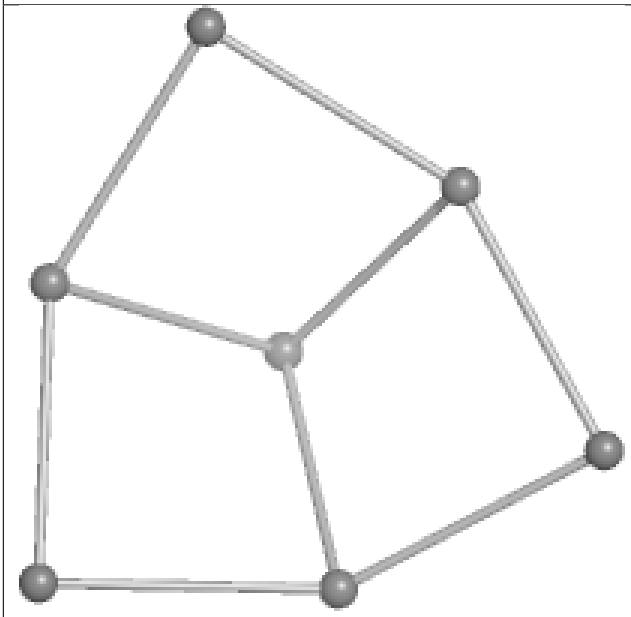
Ligand F3S CB 1002



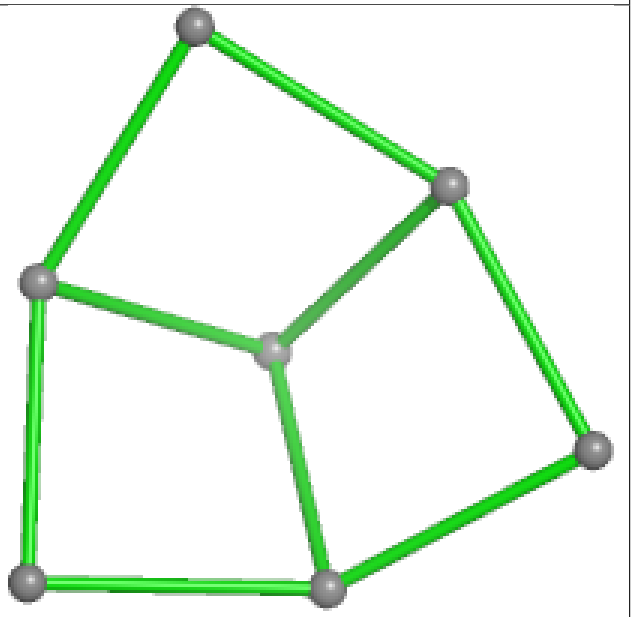
Bond lengths



Bond angles

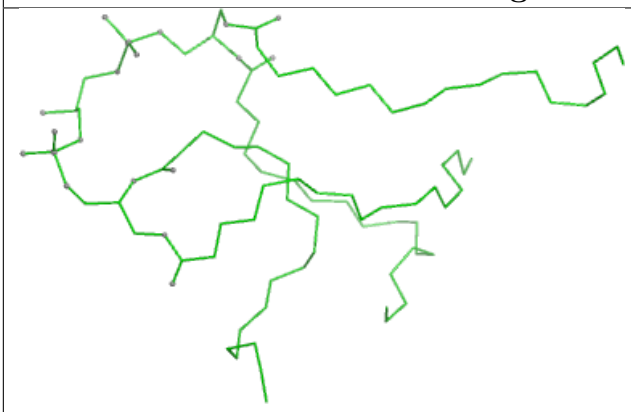


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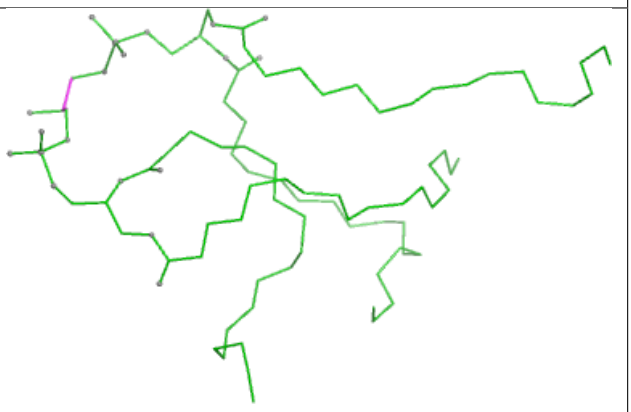


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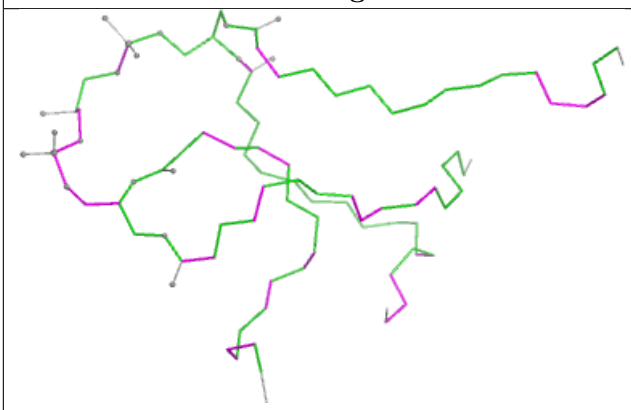
Ligand CDL AA 901



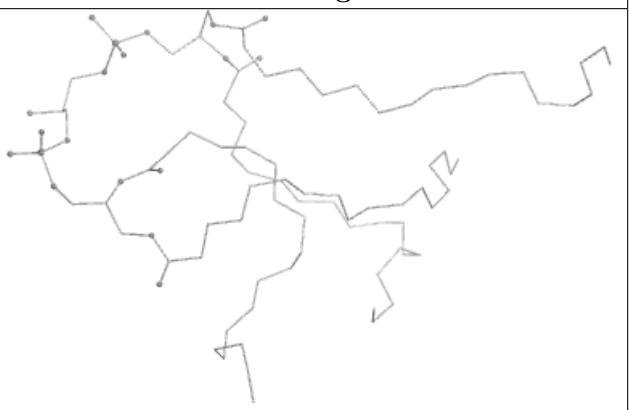
Bond lengths



Bond angles



Torsions

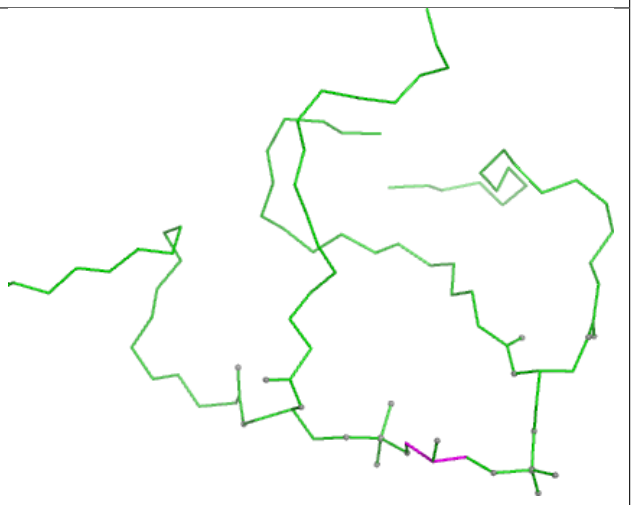


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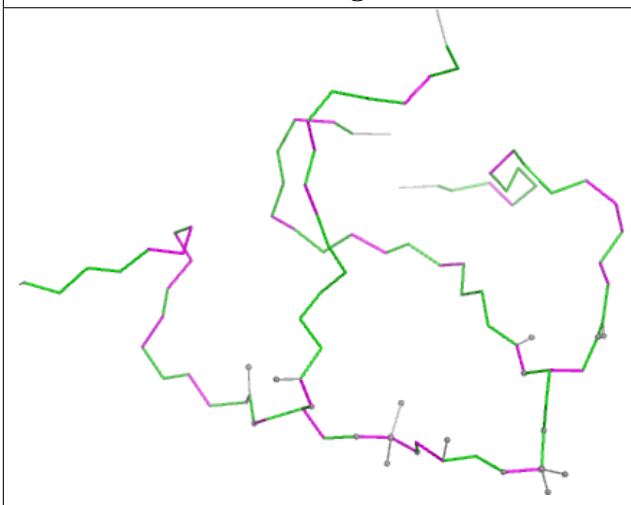
Ligand CDL Di 1103



Bond lengths



Bond angles

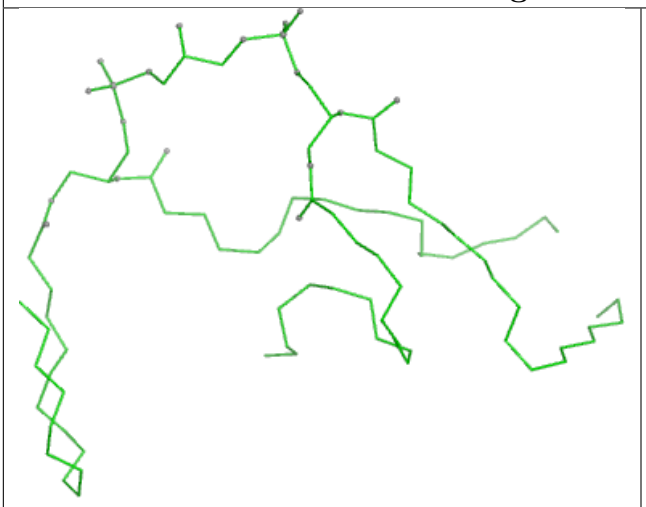


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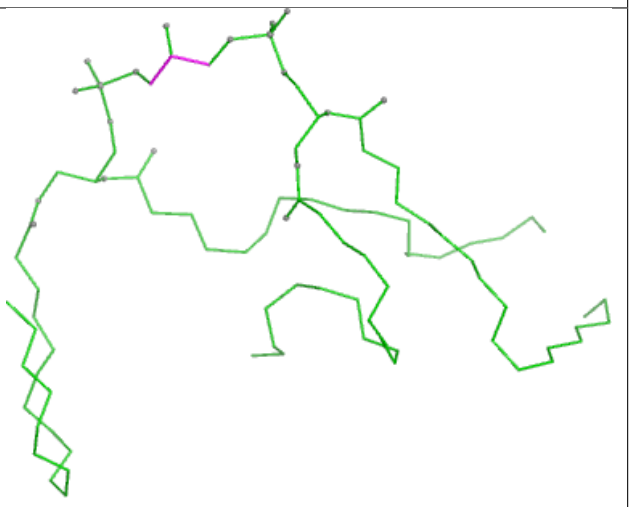


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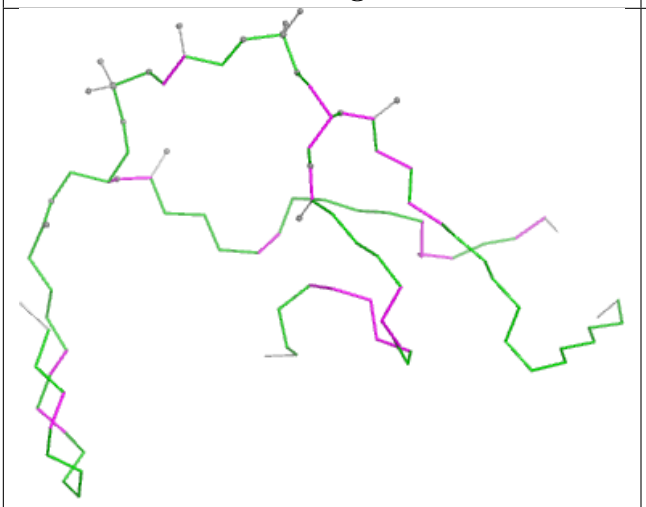
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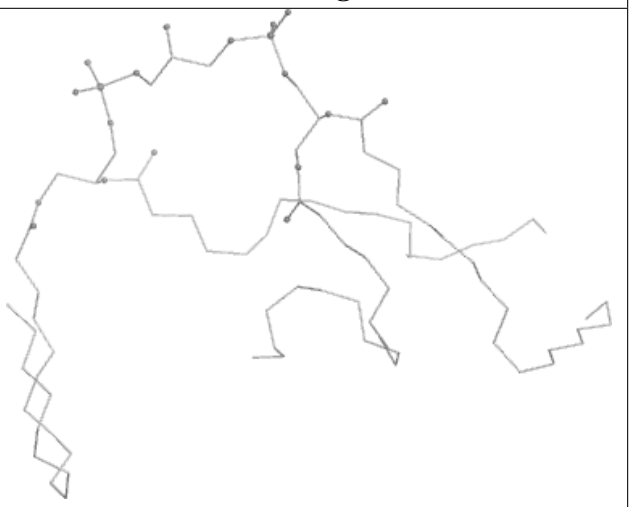
Bond lengths



Bond angles

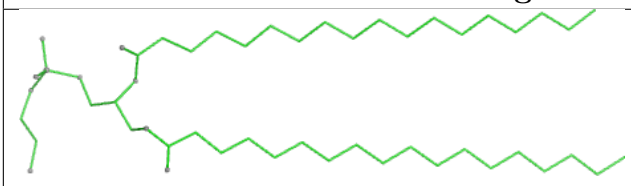


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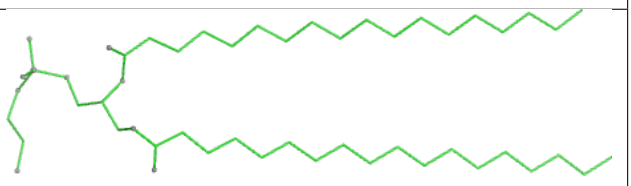


Rings

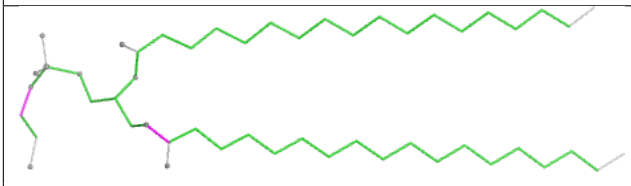
Ligand 3PE CK 101



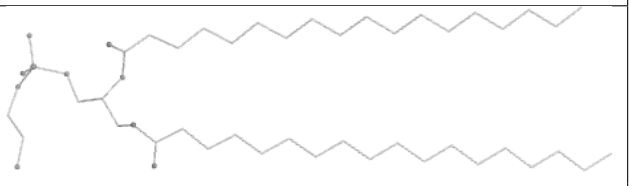
Bond lengths



Bond angles

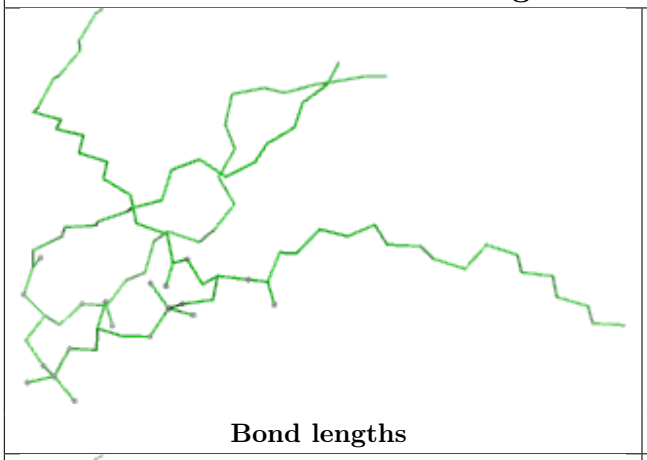


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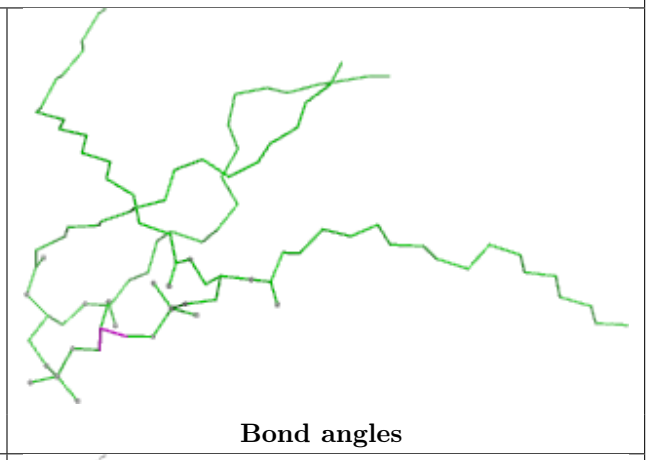


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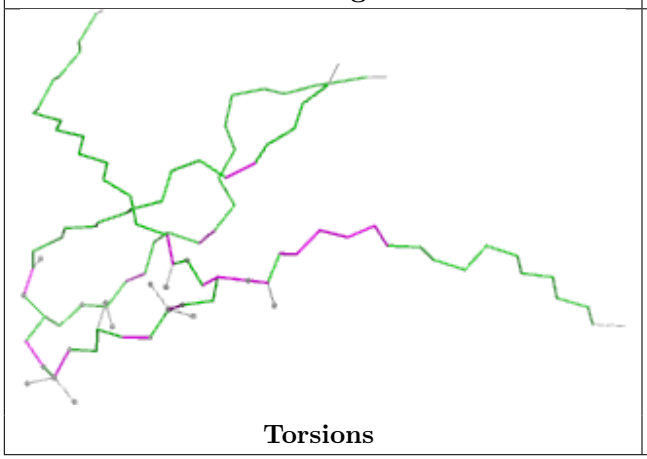
Ligand CDL AP 301



Bond lengths



Bond angles

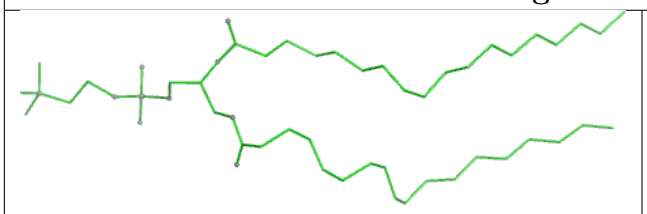


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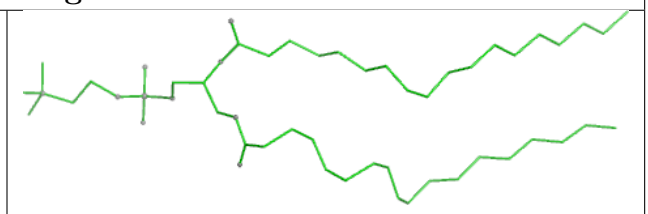


Rings

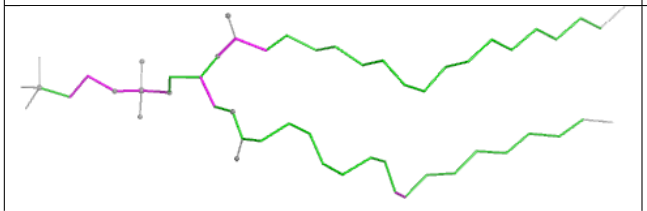
Ligand PC1 g 802



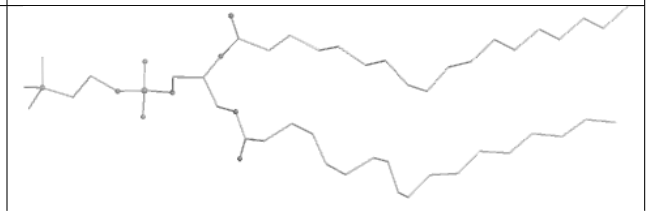
Bond lengths



Bond angles

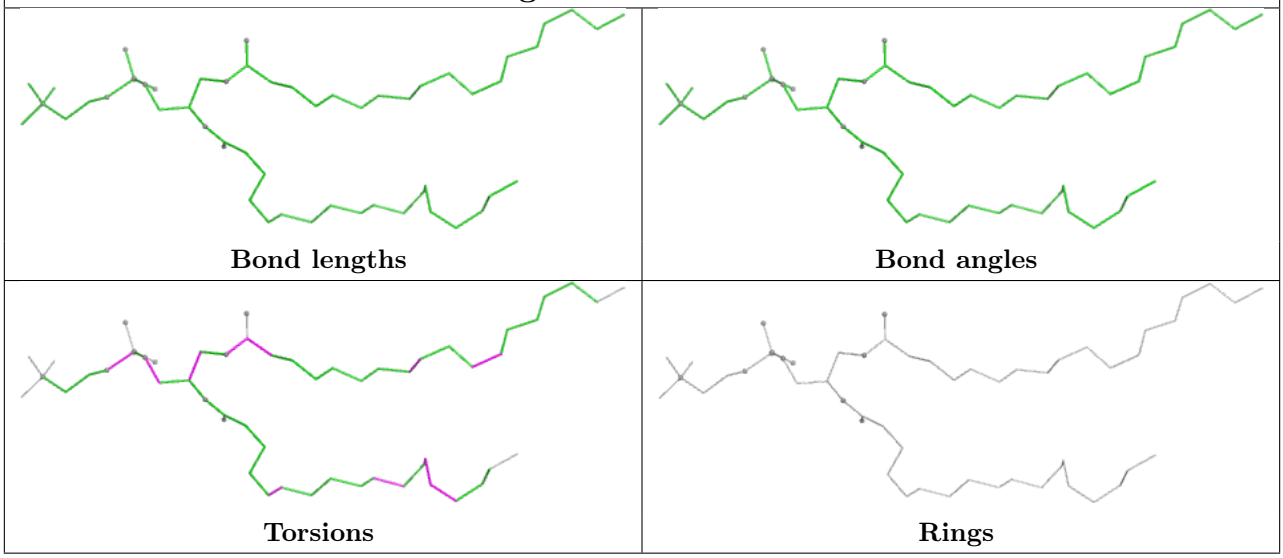


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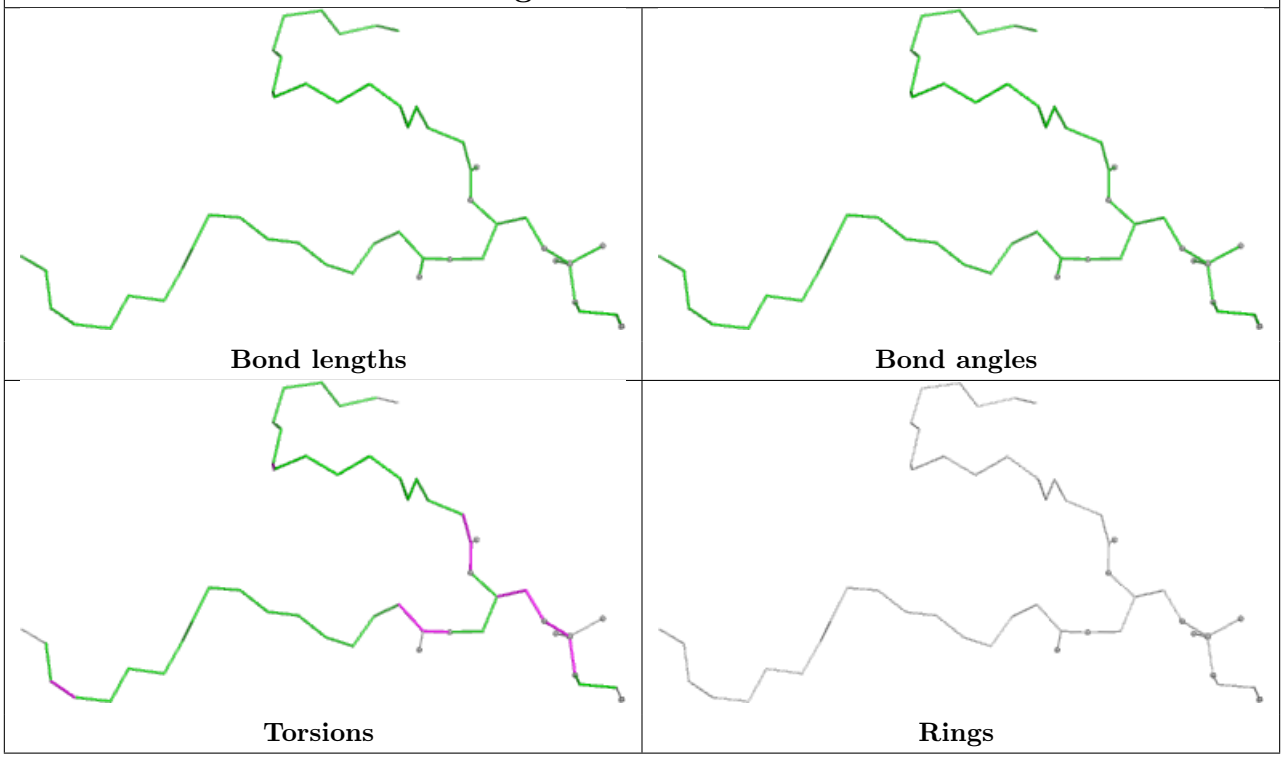


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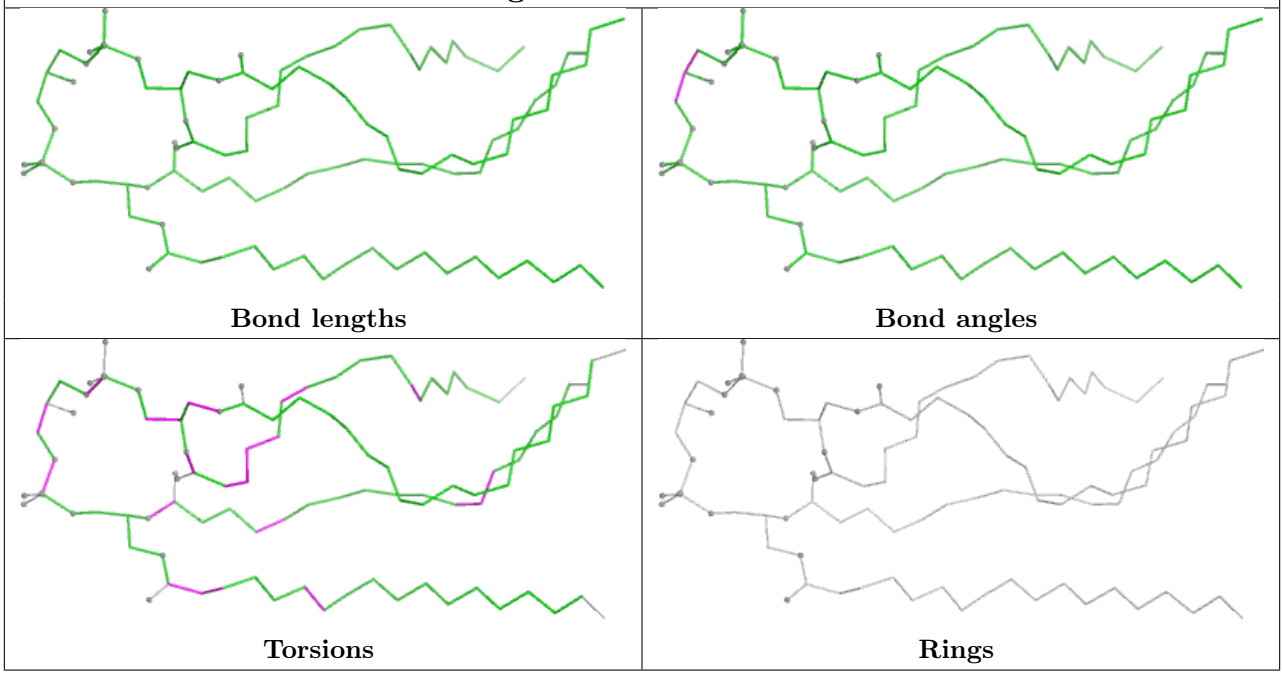
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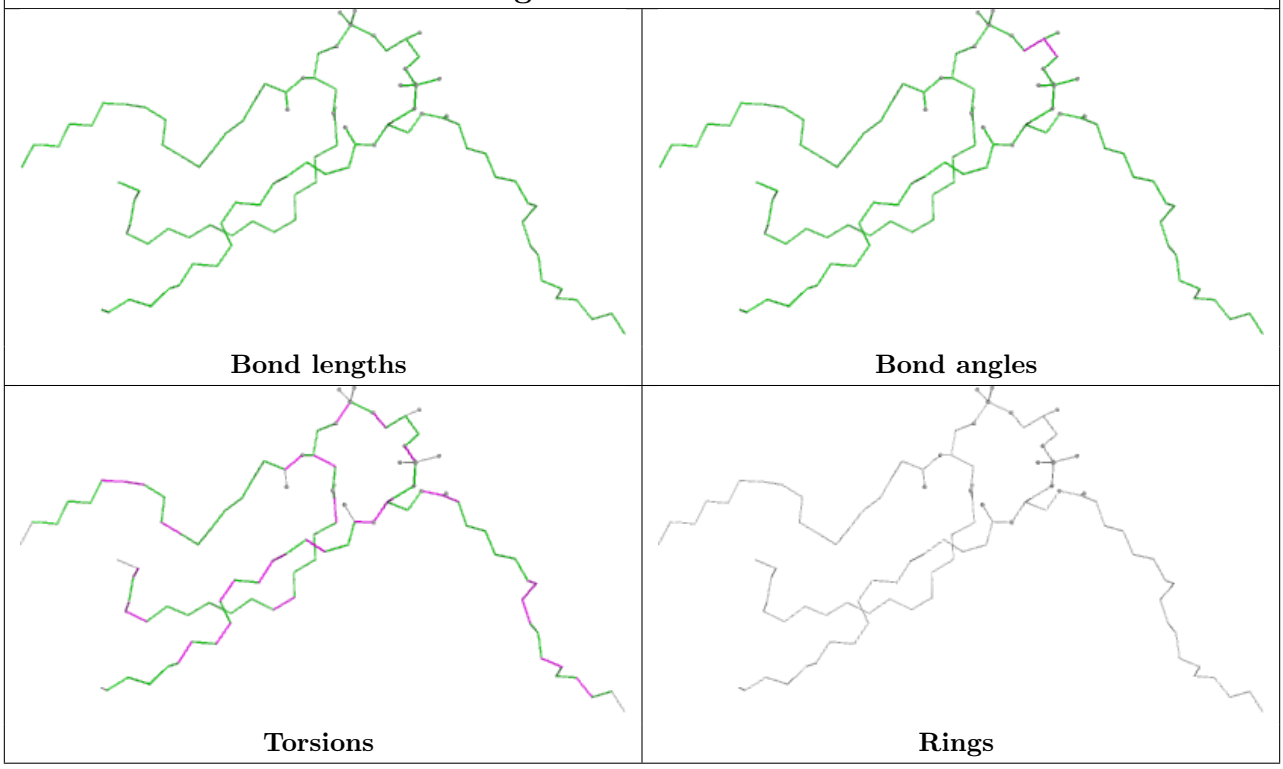
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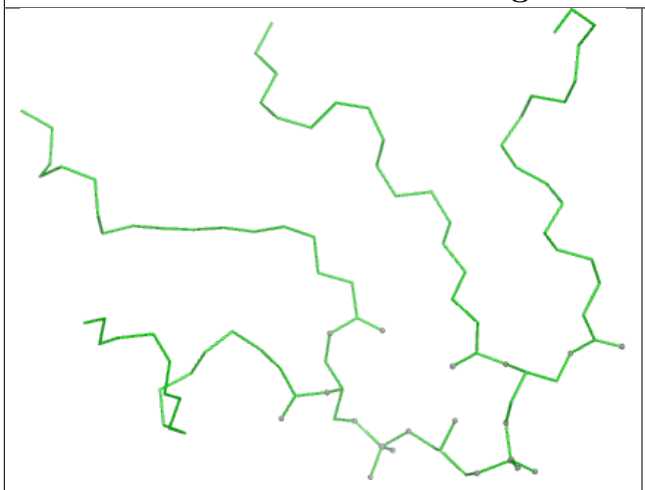
Ligand CDL DM 502



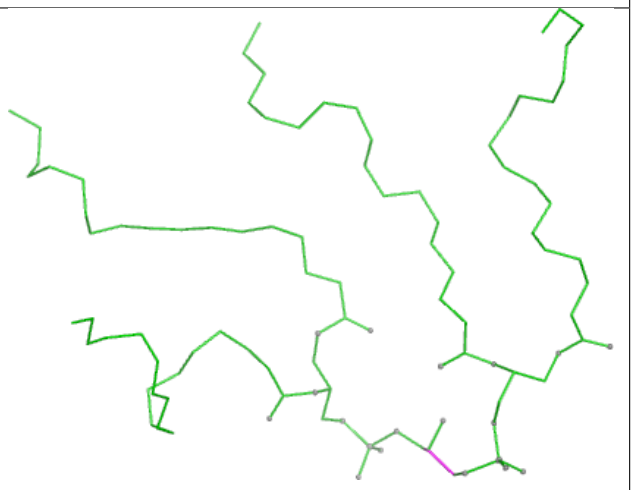
Ligand CDL Dn 506



Ligand CDL DV 401



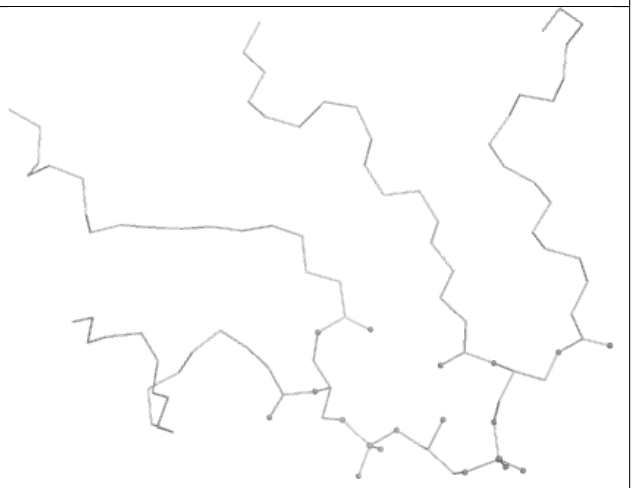
Bond lengths



Bond angles

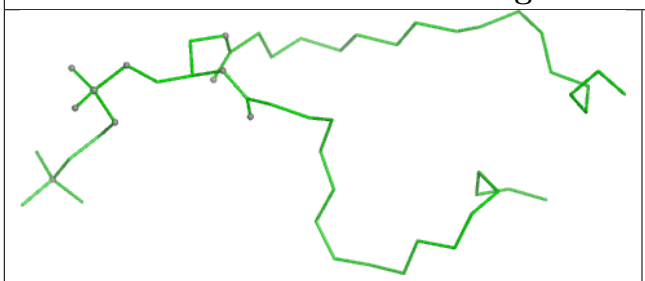


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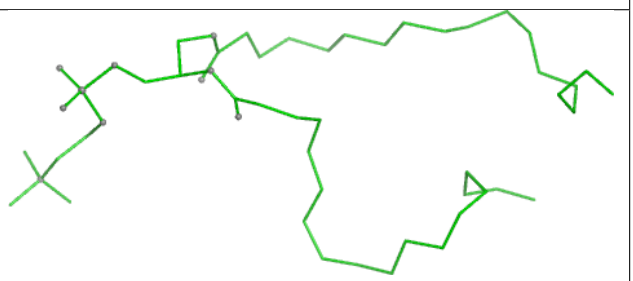


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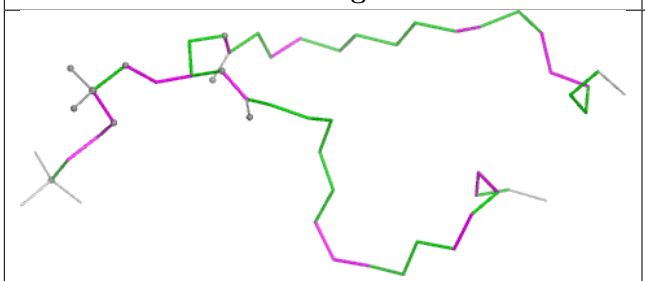
Ligand PC1 DB 702



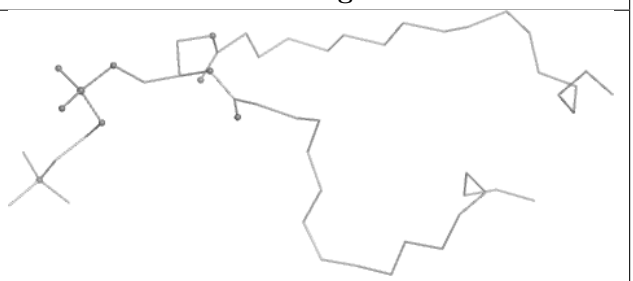
Bond lengths



Bond angles

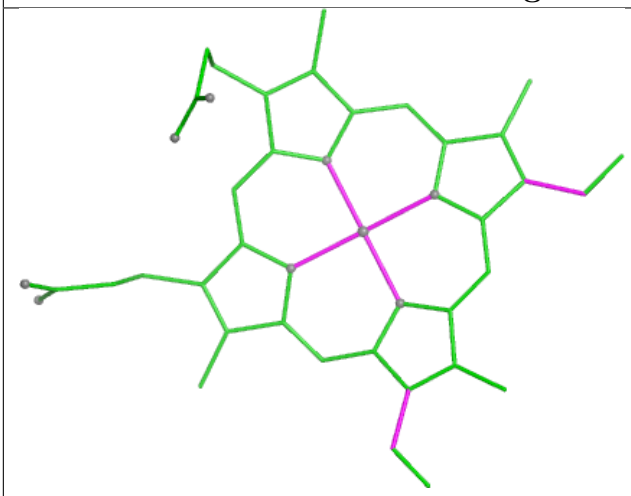


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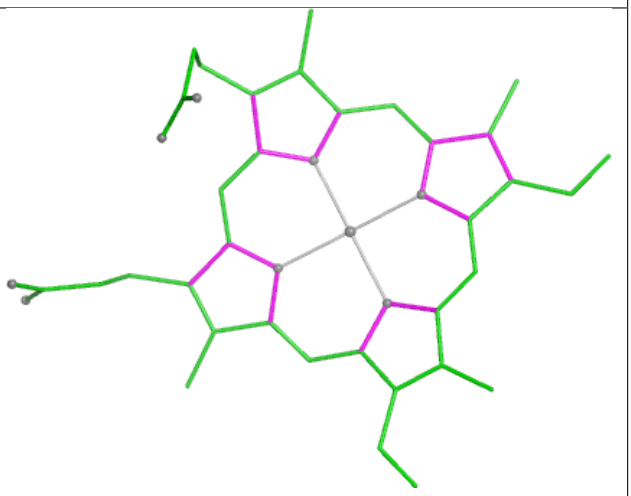


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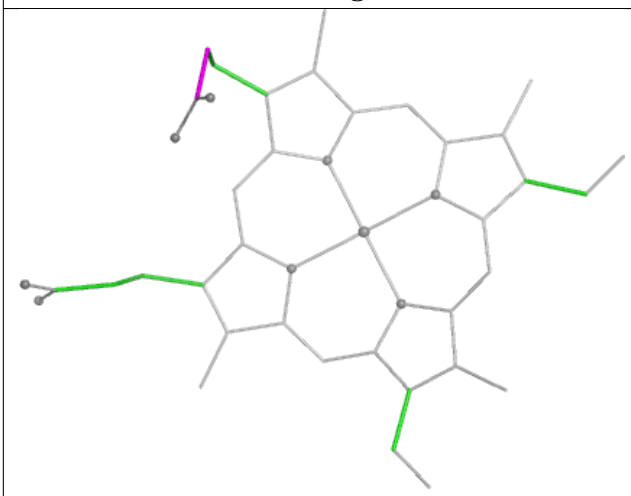
Ligand HEM c 505



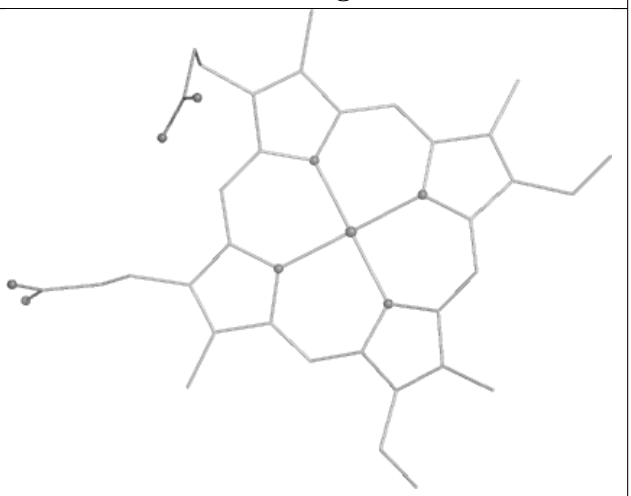
Bond lengths



Bond angles

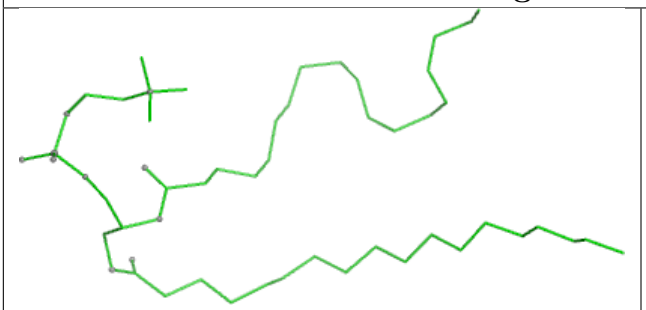


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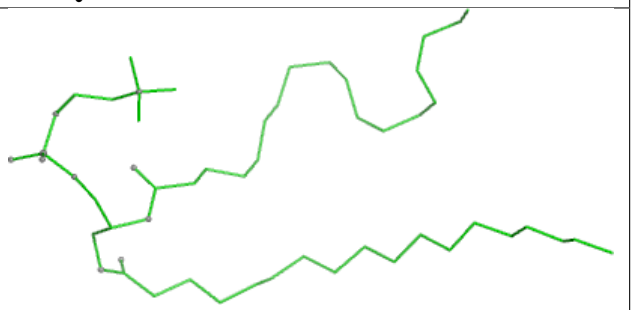


Rings

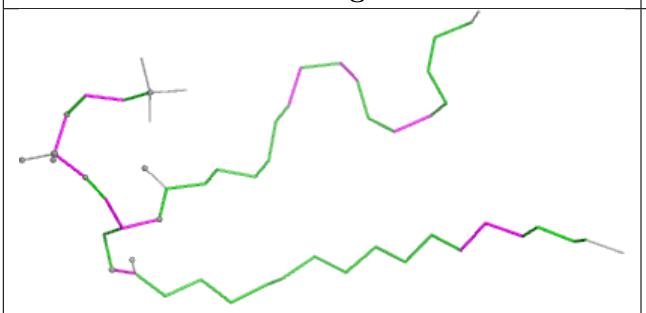
Ligand PC1 AQ 202



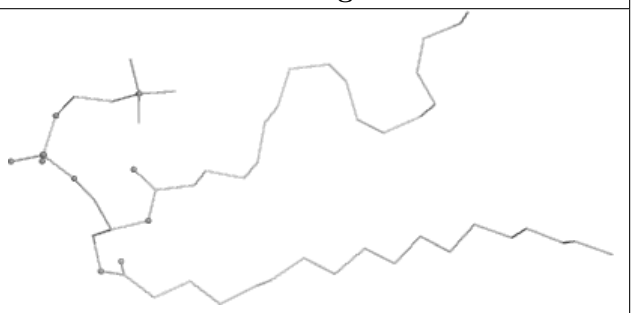
Bond lengths



Bond angles

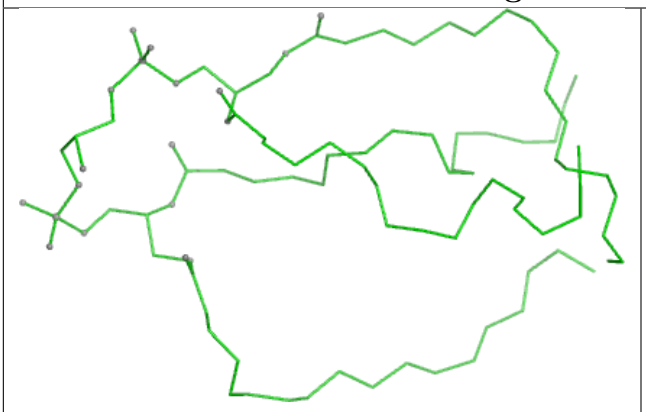


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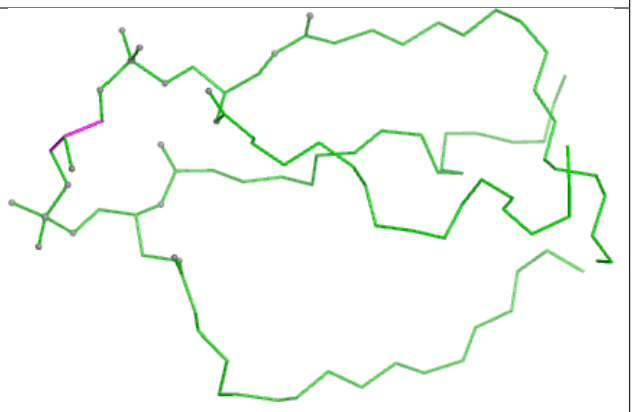


Rings

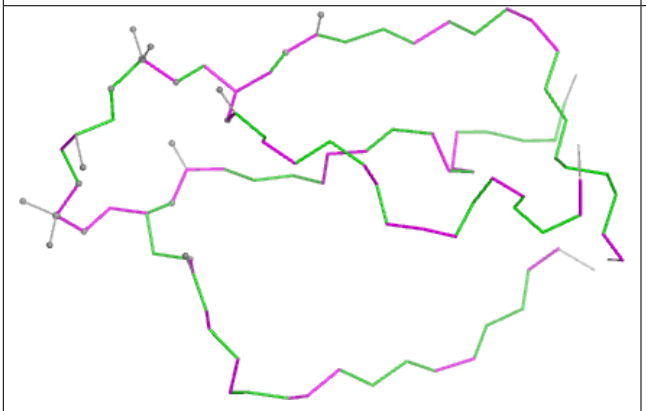
Ligand CDL Dx 1204



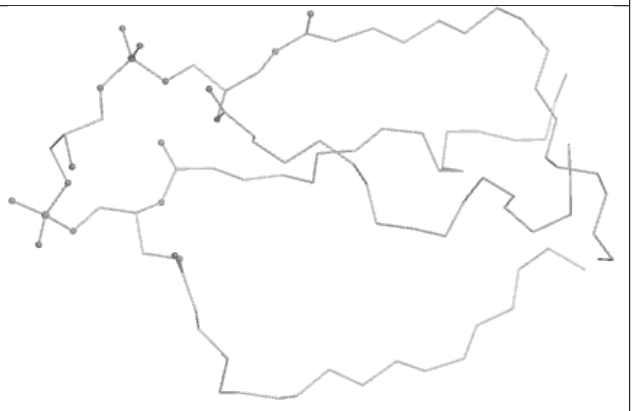
Bond lengths



Bond angles

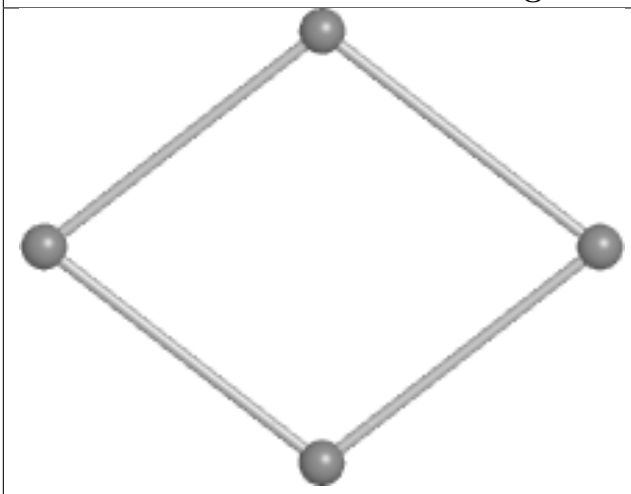


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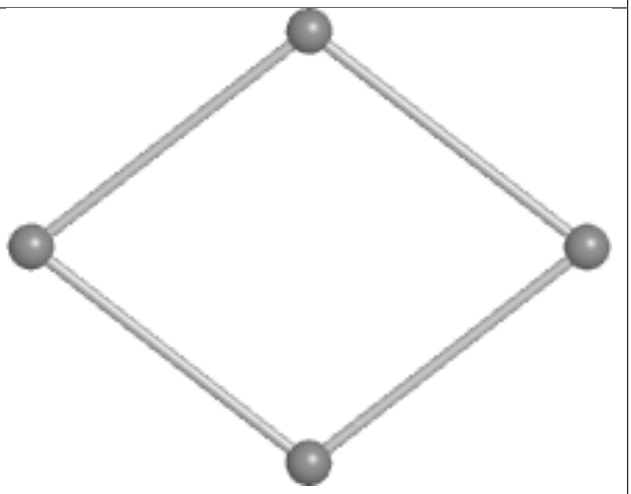


Rings

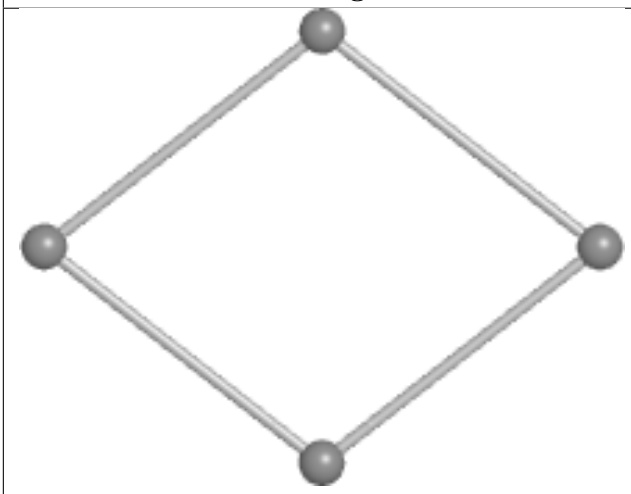
Ligand FES Ef 502



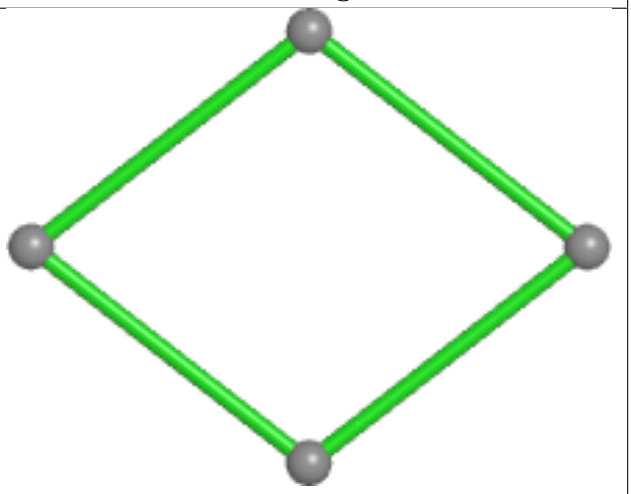
Bond lengths



Bond angles

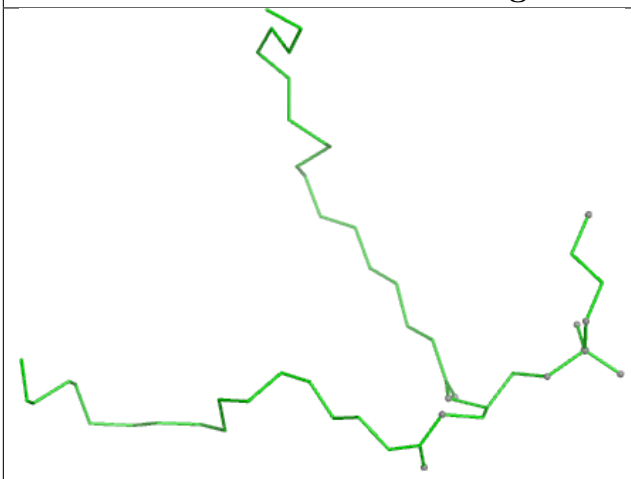


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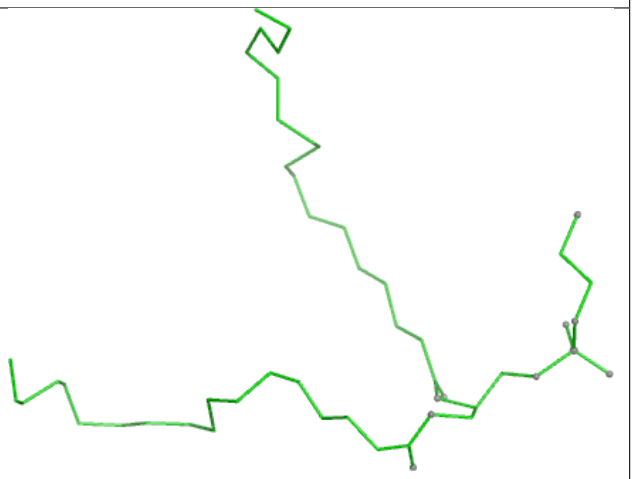


Rings

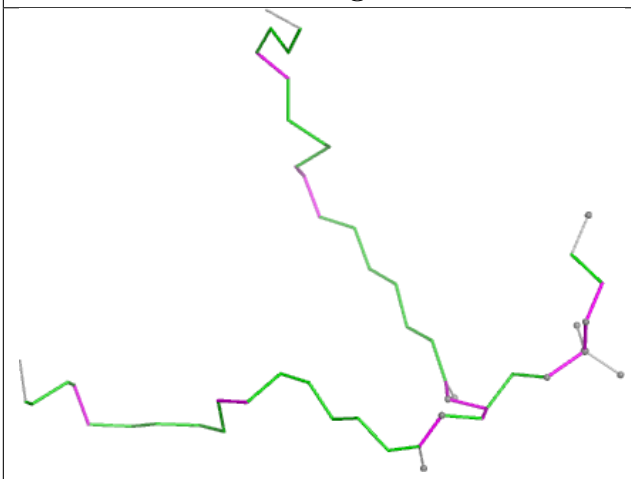
Ligand 3PE Dx 1202



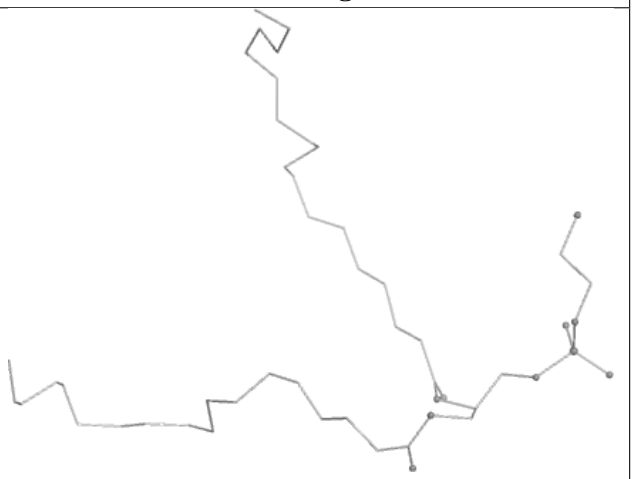
Bond lengths



Bond angles

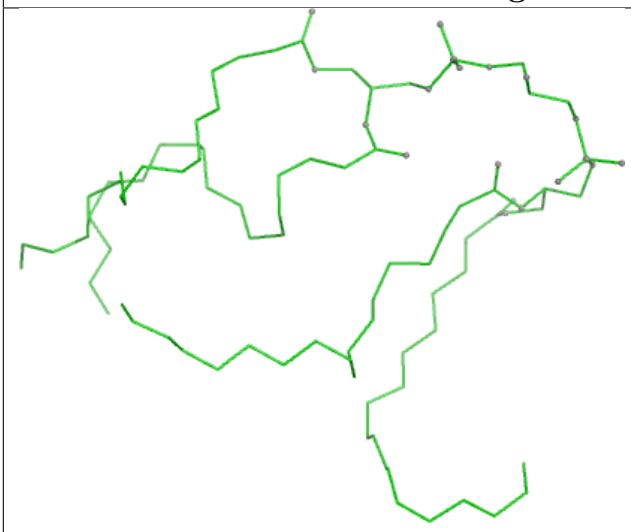


Torsions

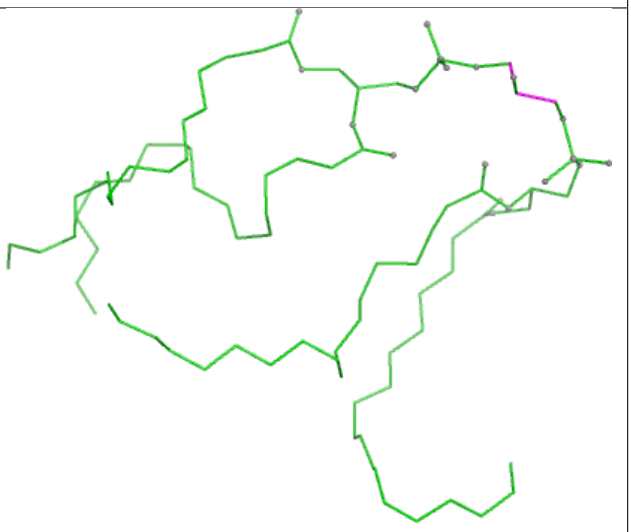


Rings

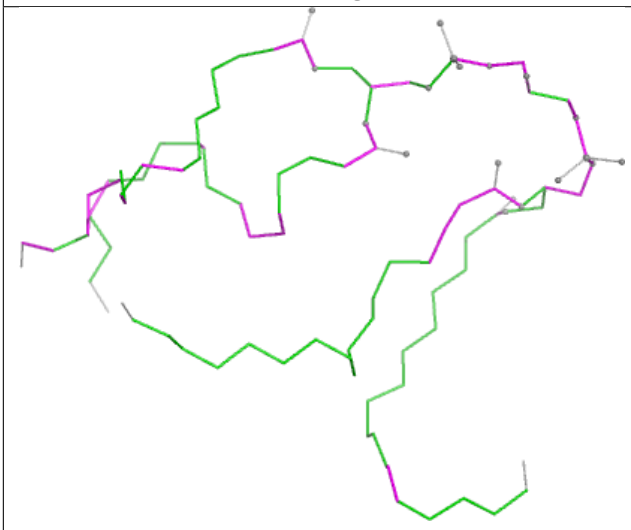
Ligand CDL Dm 501



Bond lengths



Bond angles



Torsions

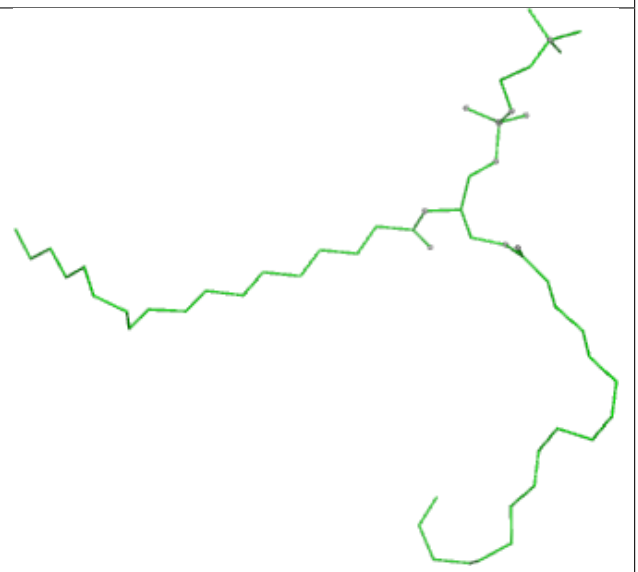


Rings

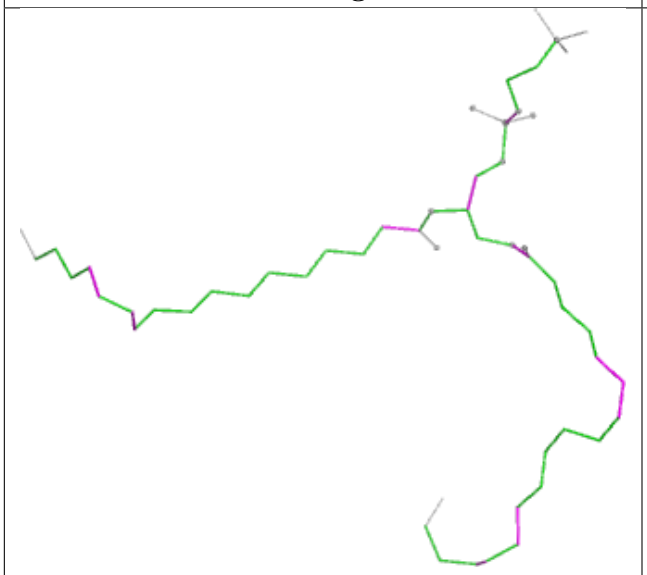
Ligand PC1 Dc 603



Bond lengths



Bond angles

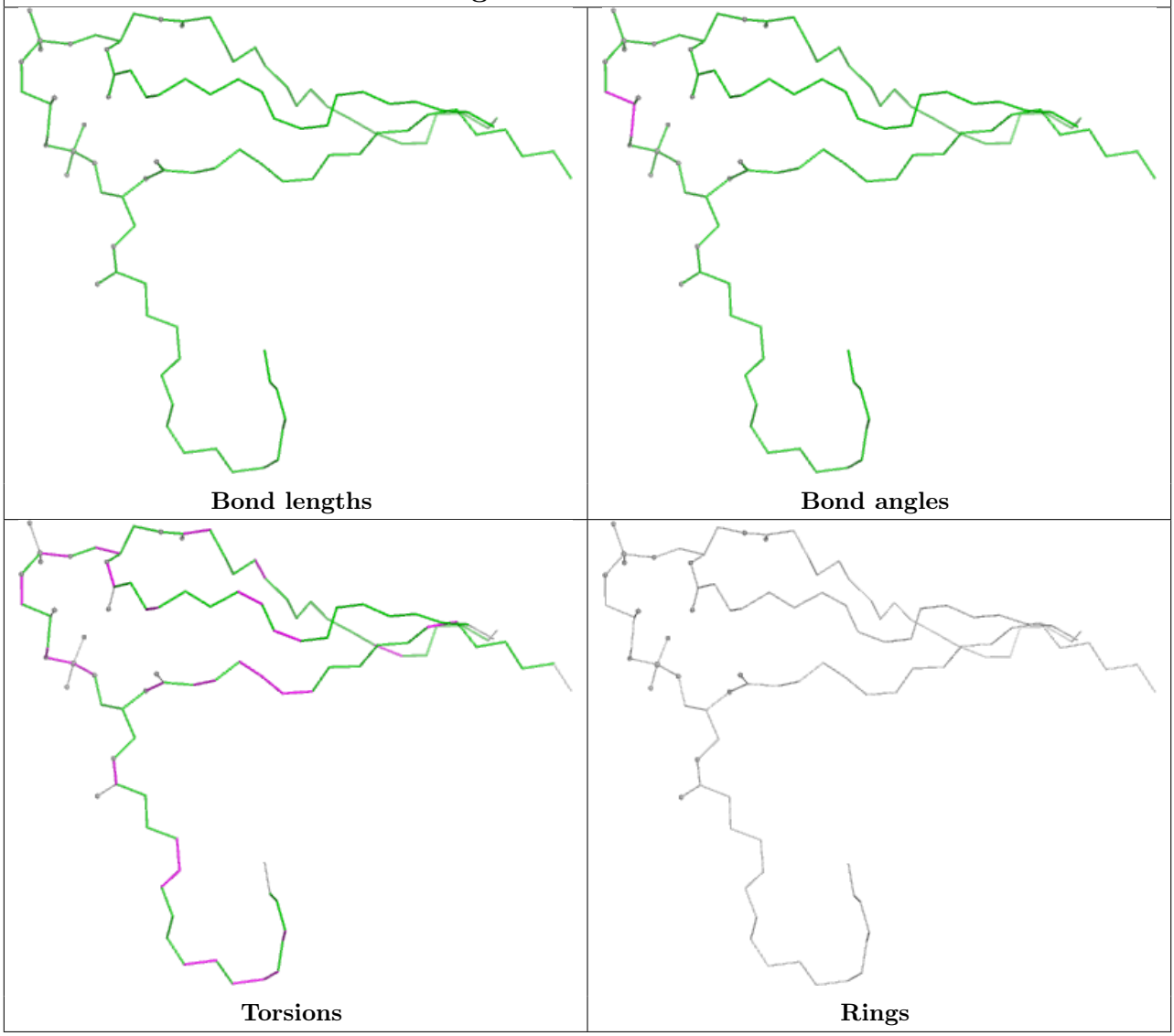


Torsions



Rings

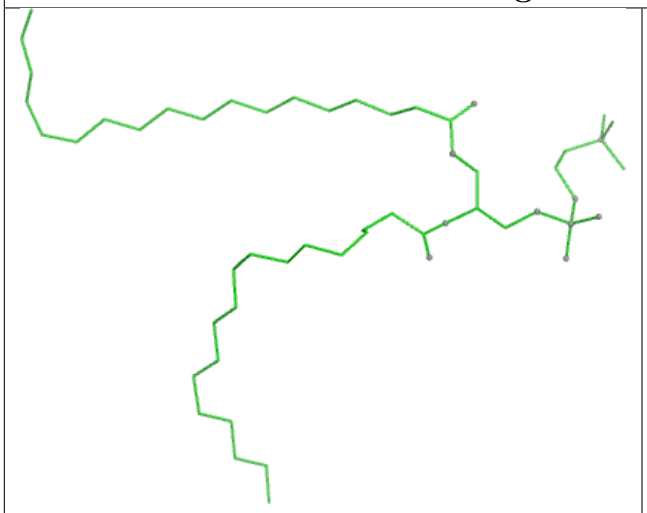
Ligand CDL A0 602



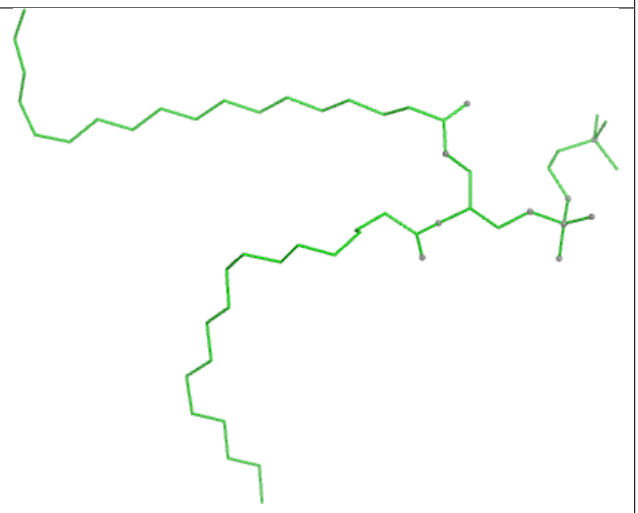
Bond lengths | **Bond angles**

Torsions | **Rings**

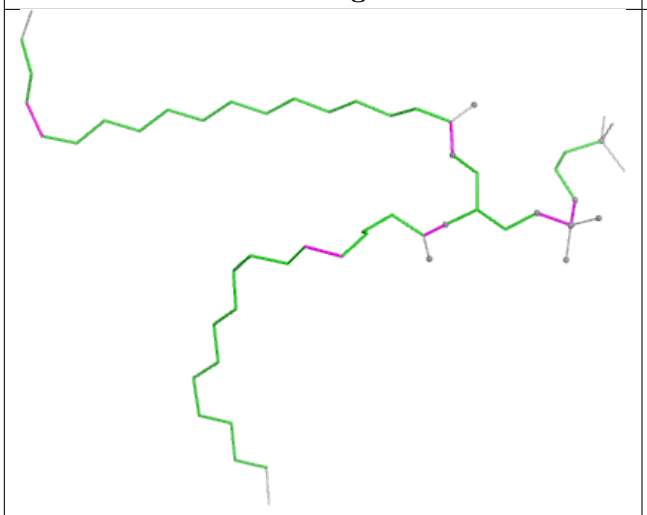
Ligand PC1 DX 305



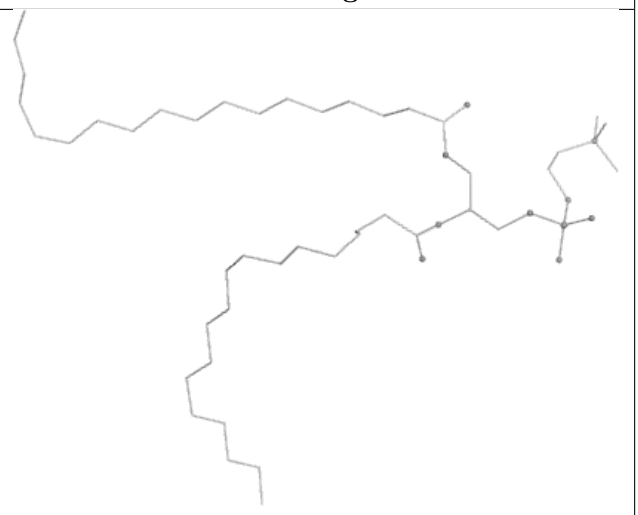
Bond lengths



Bond angles

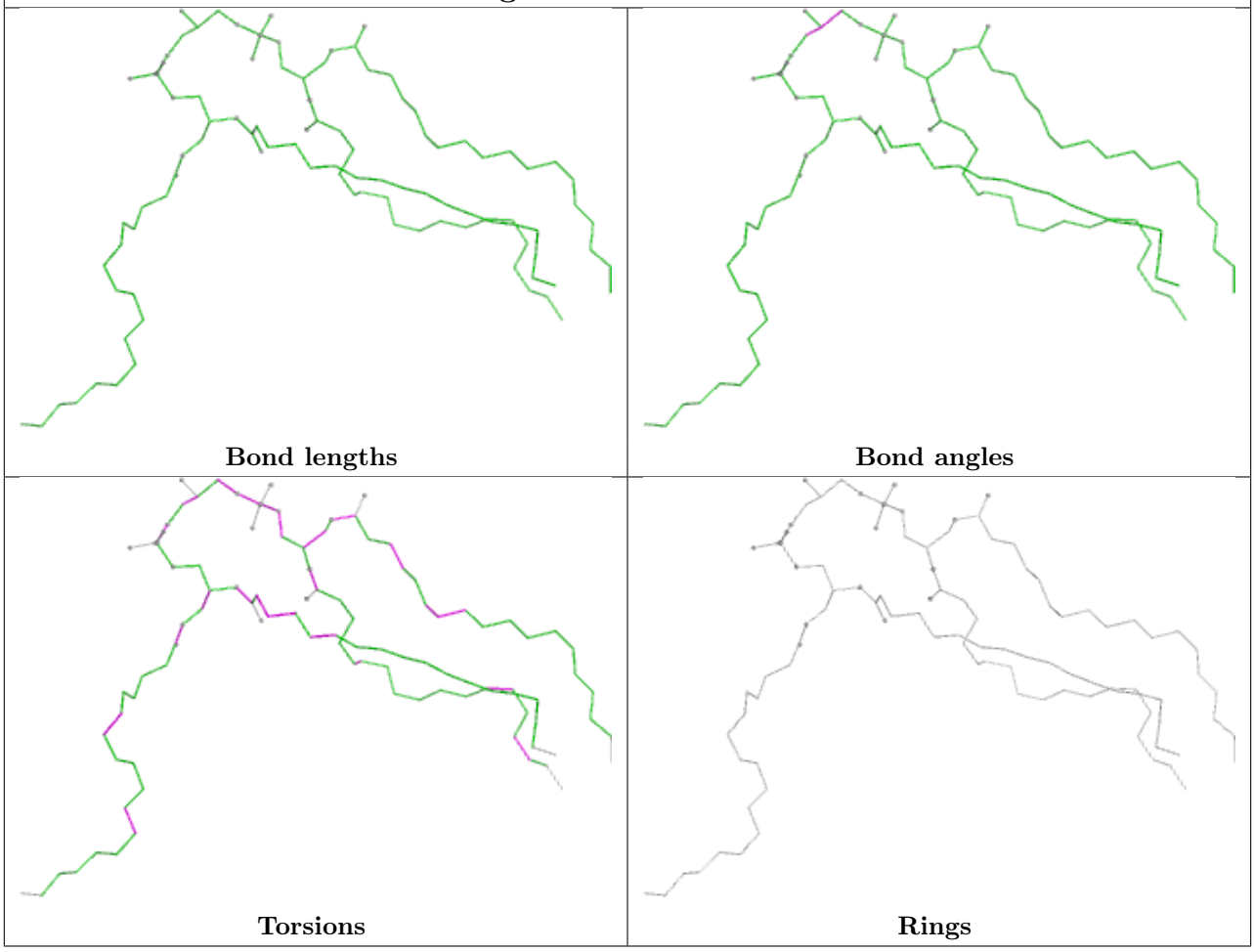


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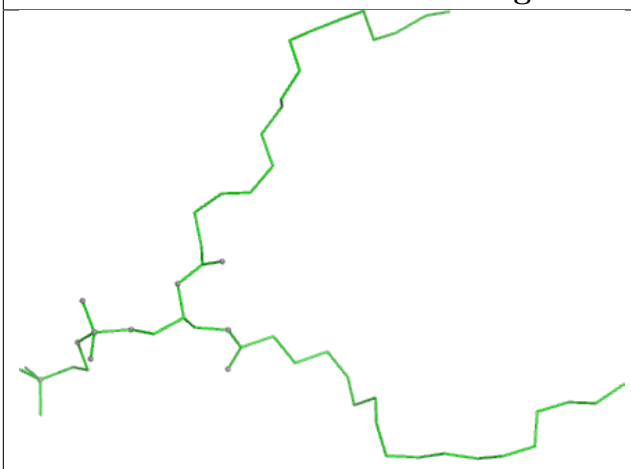


Rings

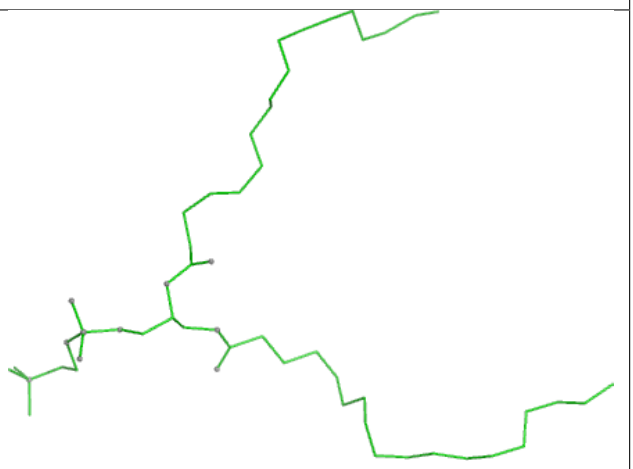
Ligand CDL BG 201



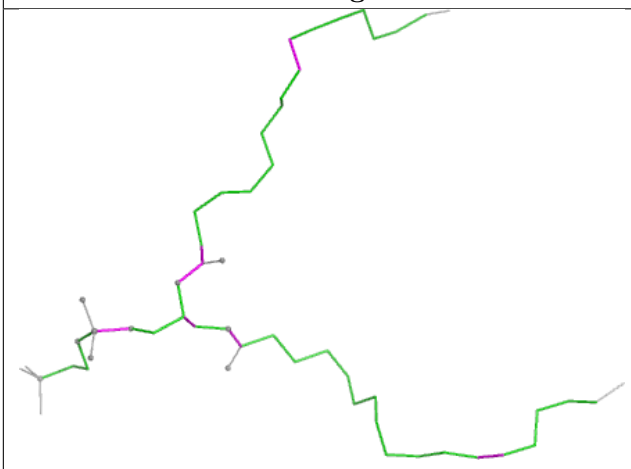
Ligand PC1 DC 605



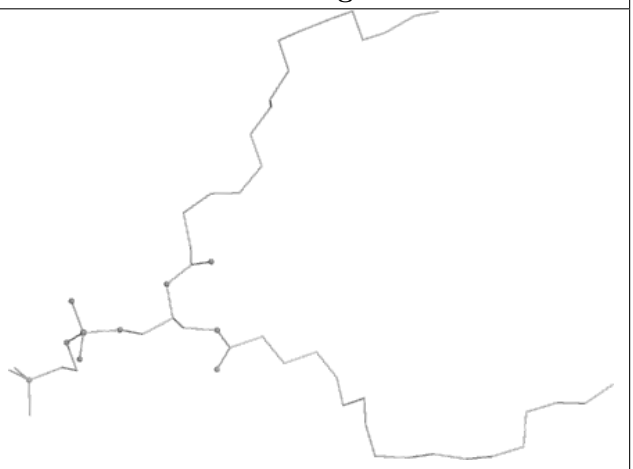
Bond lengths



Bond angles

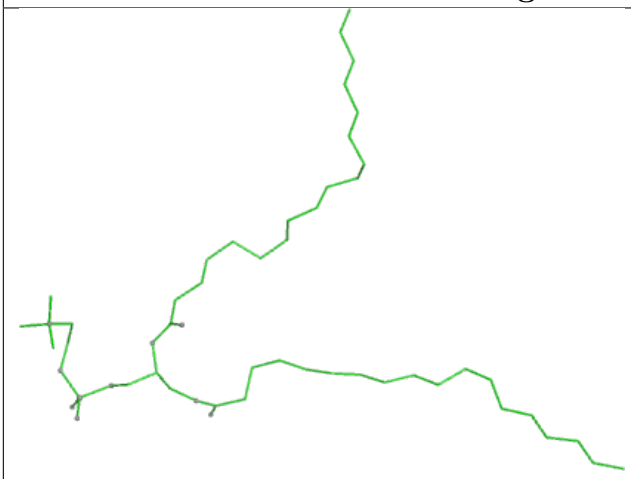


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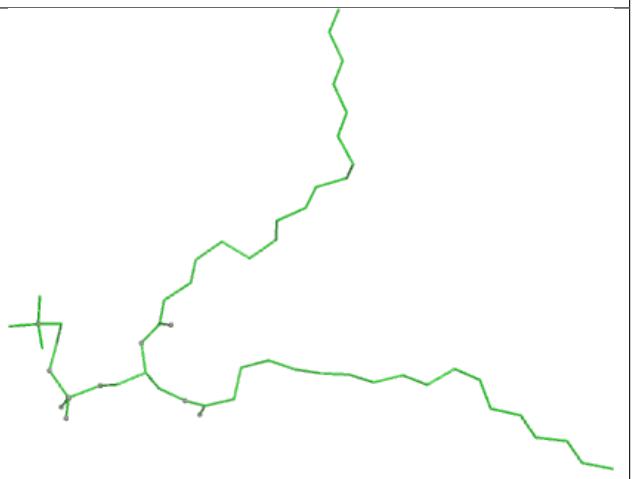


Rings

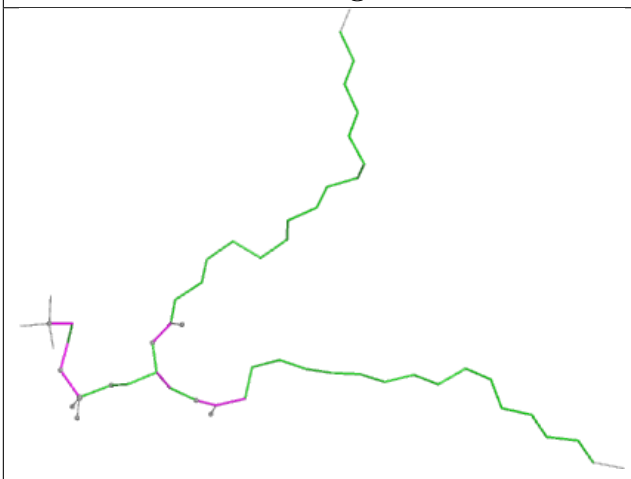
Ligand PC1 A6 303



Bond lengths



Bond angles

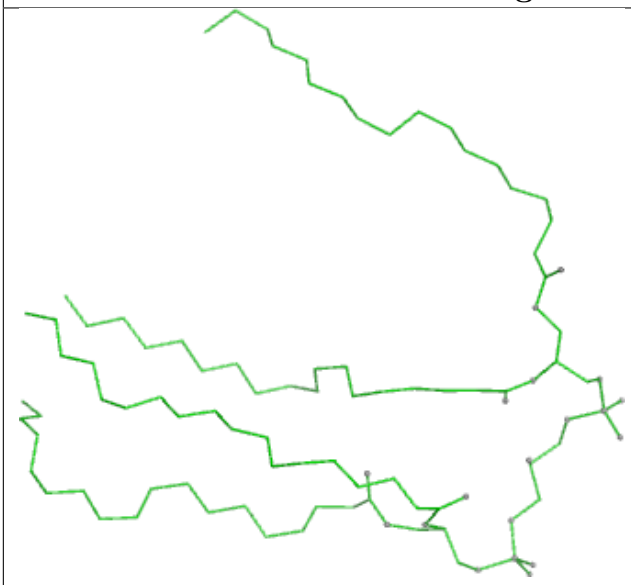


Torsions



Rings

Ligand CDL B0 102



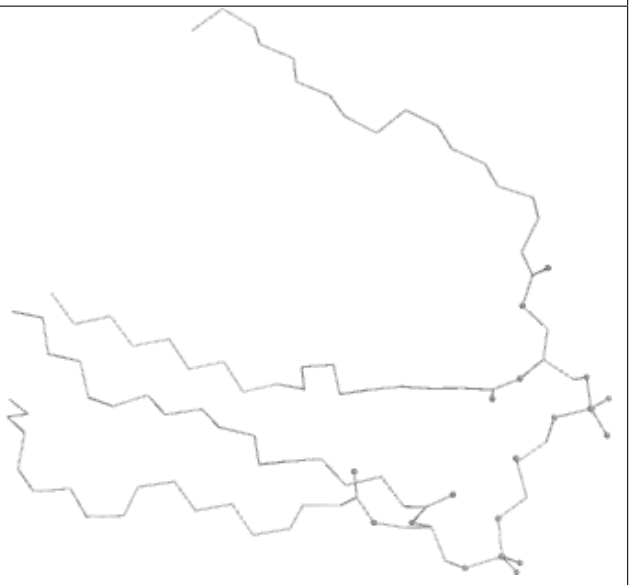
Bond lengths



Bond angles

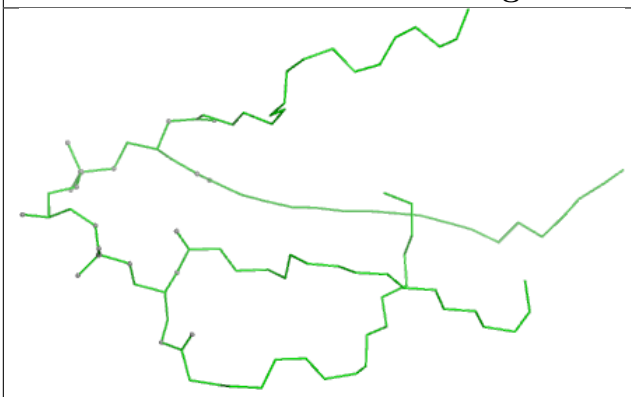


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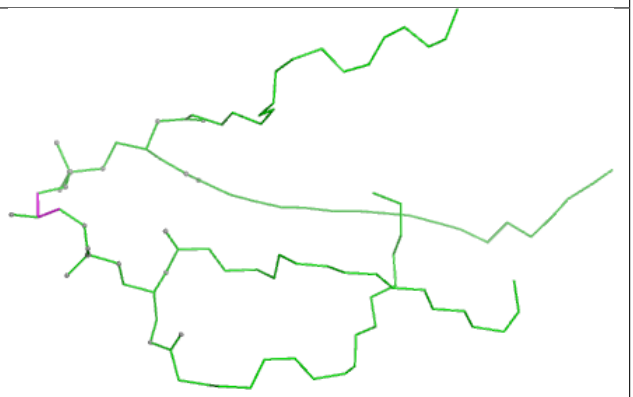


Rings

Ligand CDL EN 1202



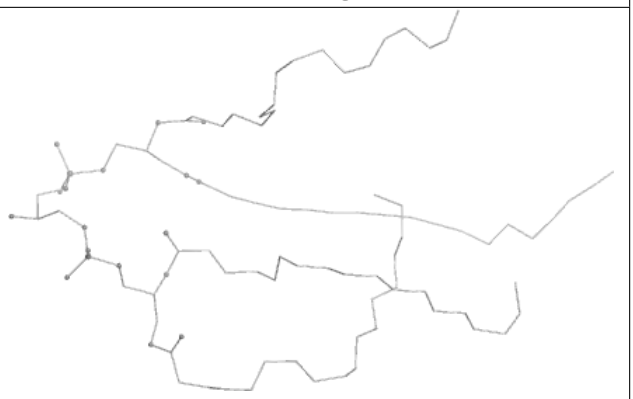
Bond lengths



Bond angles

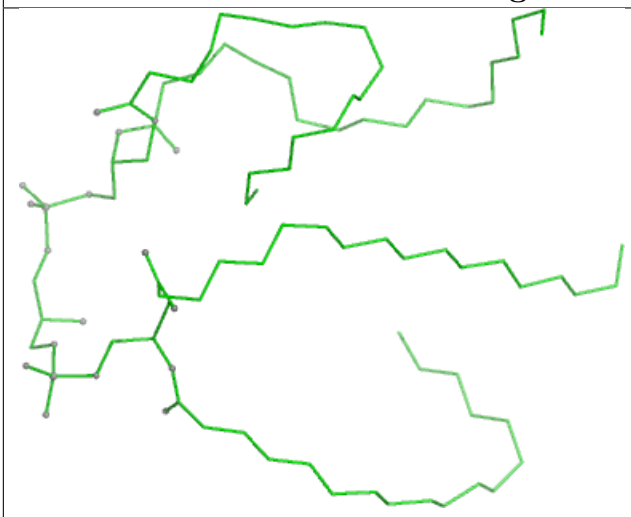


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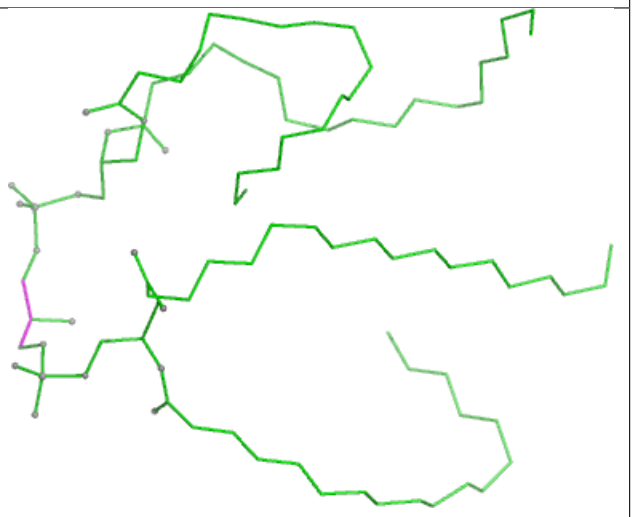


Rings

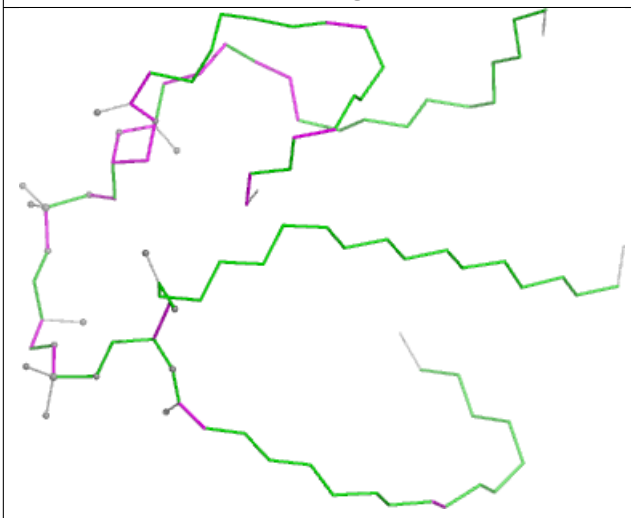
Ligand CDL DN 503



Bond lengths



Bond angles

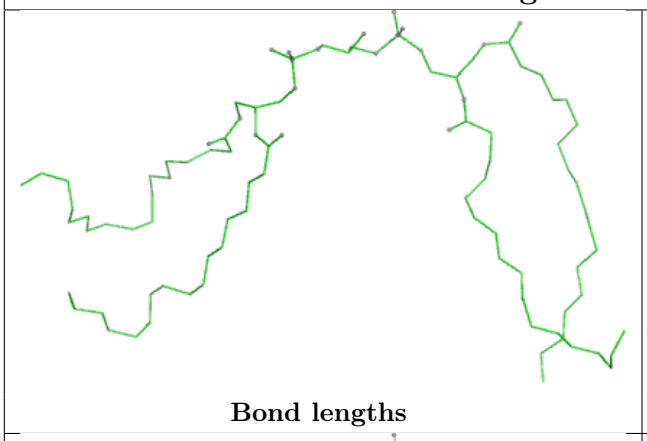


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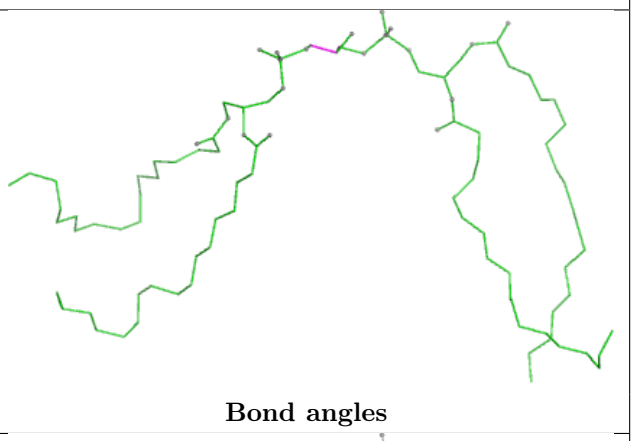


Rings

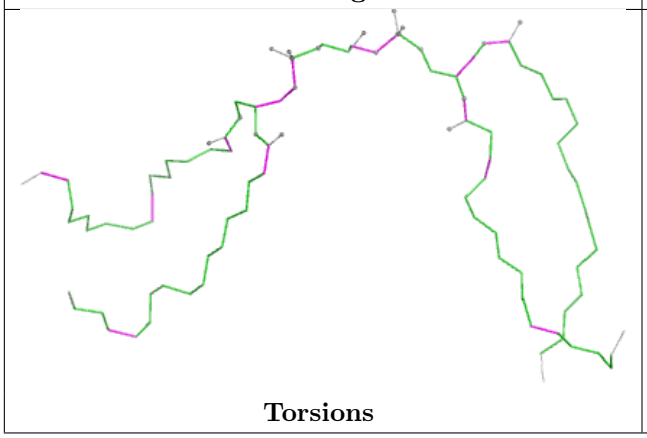
Ligand CDL EI 401



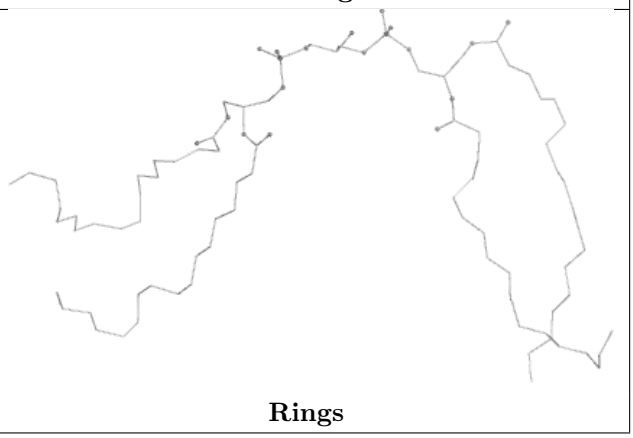
Bond lengths



Bond angles

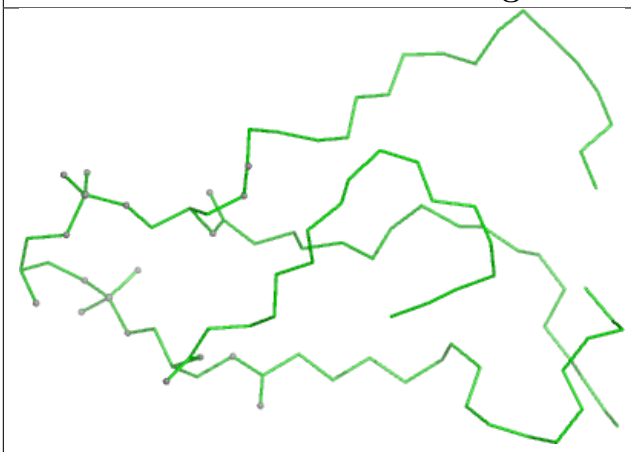


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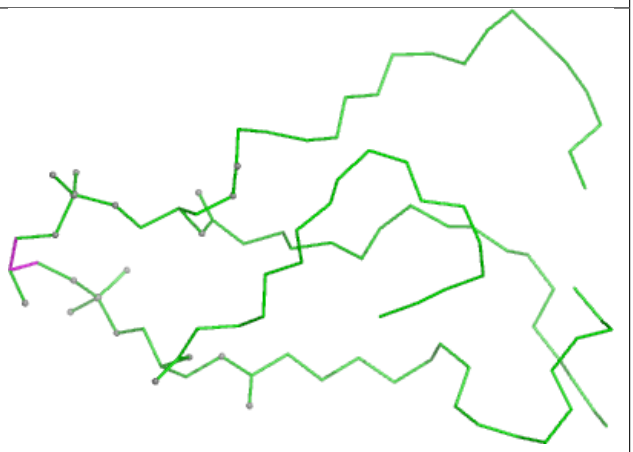


Rings

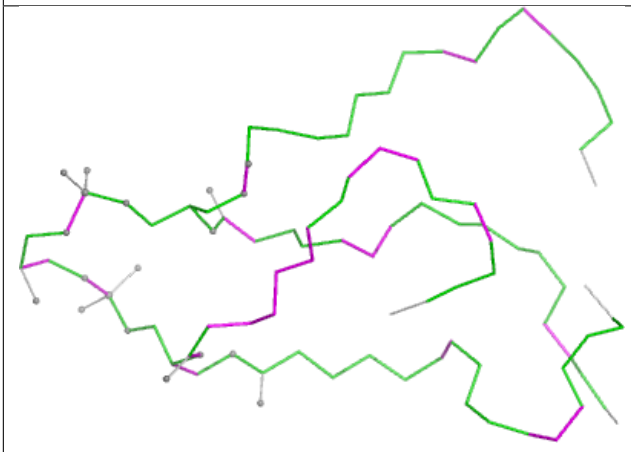
Ligand CDL EN 1201



Bond lengths



Bond angles

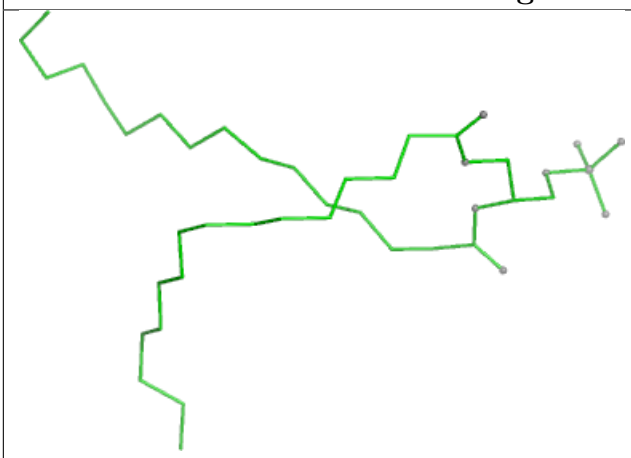


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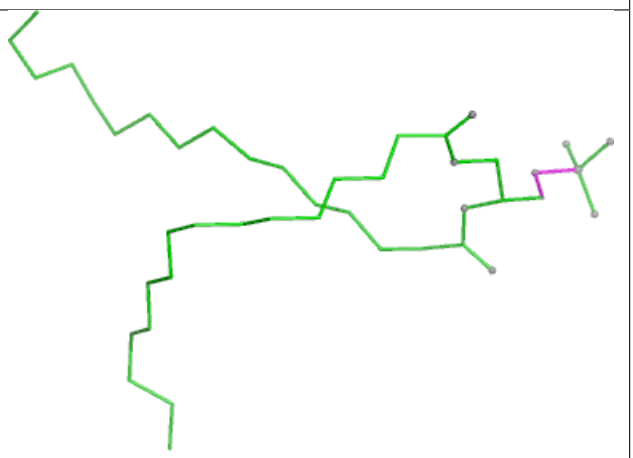


Rings

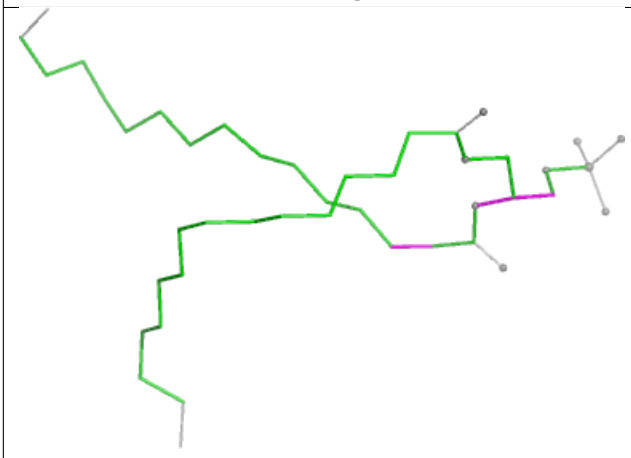
Ligand LPP A6 301



Bond lengths



Bond angles

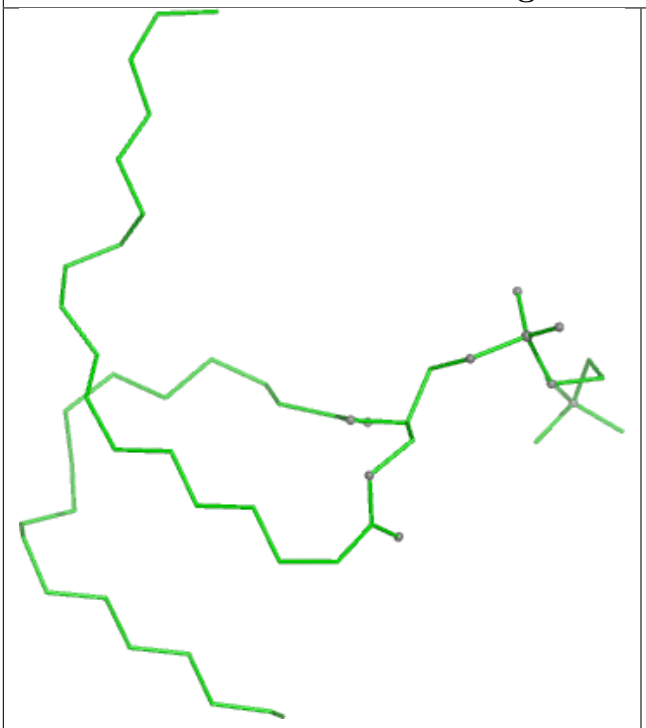


Torsions

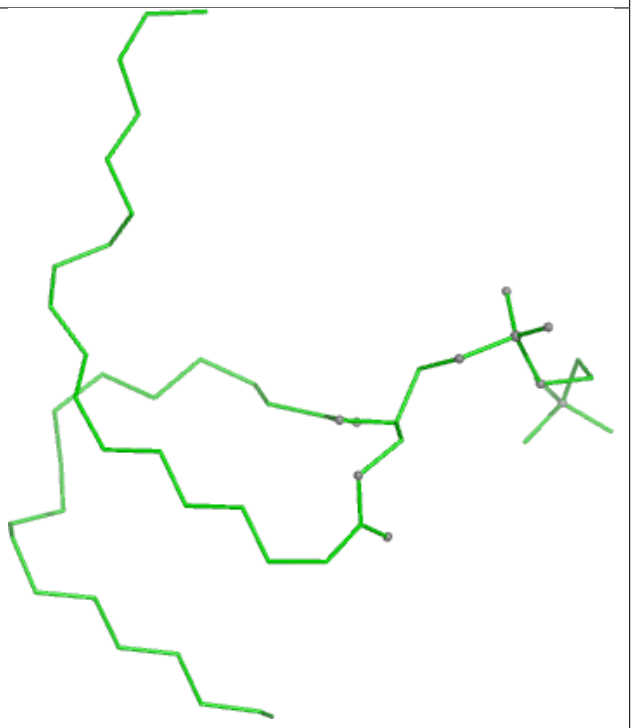


Rings

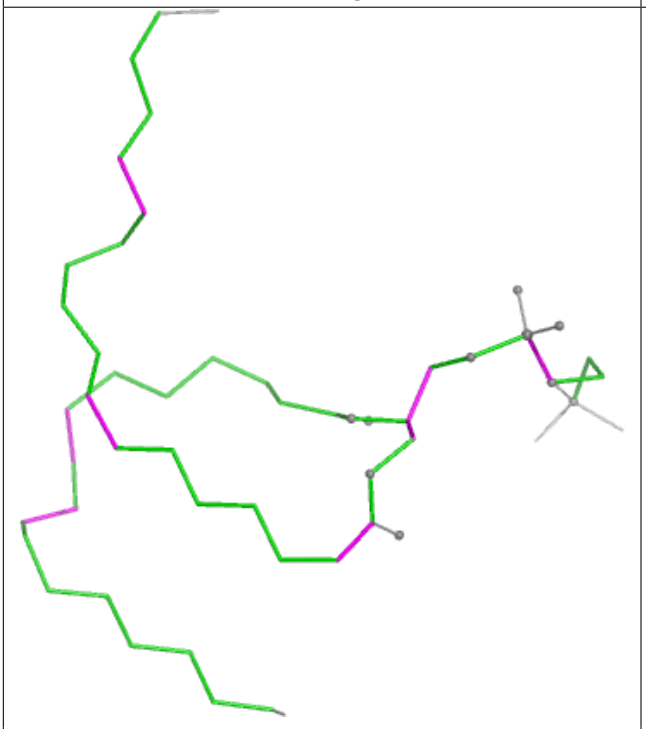
Ligand PC1 A6 302



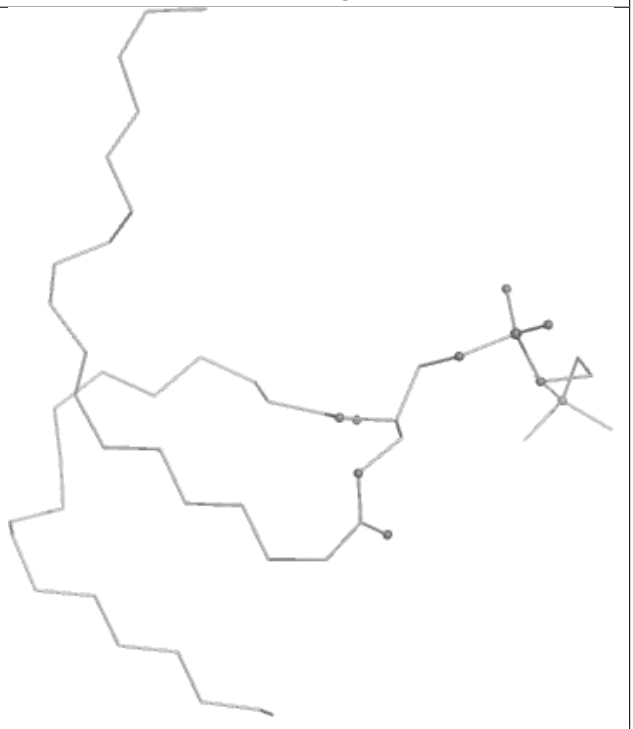
Bond lengths



Bond angles

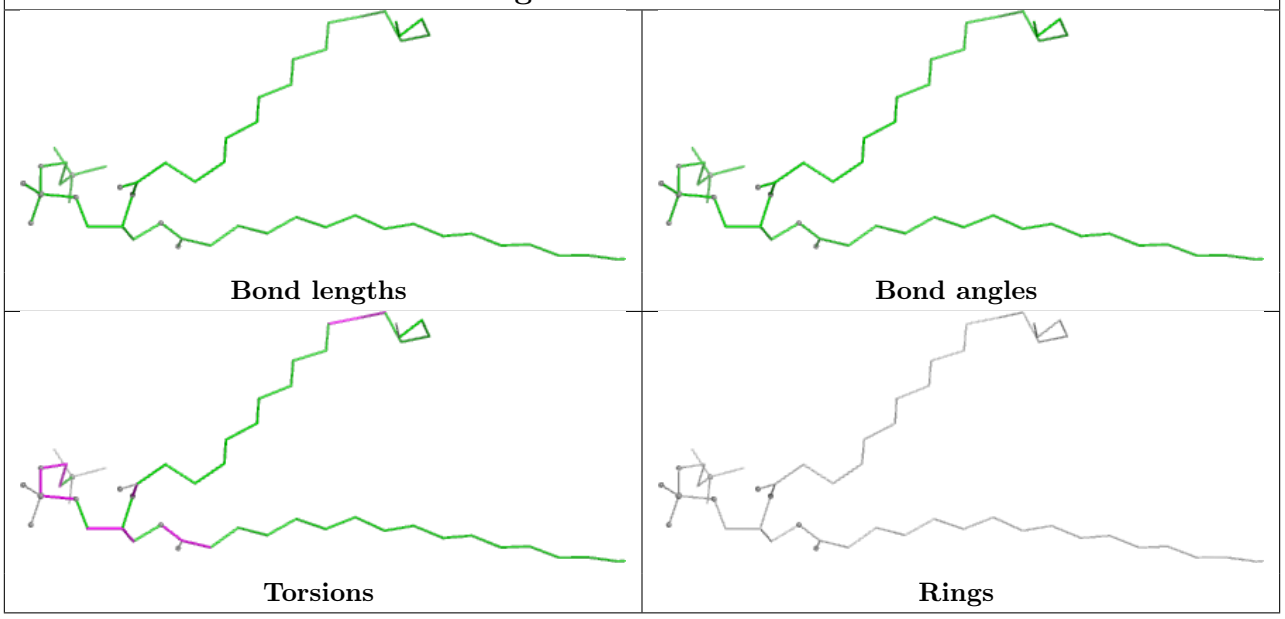


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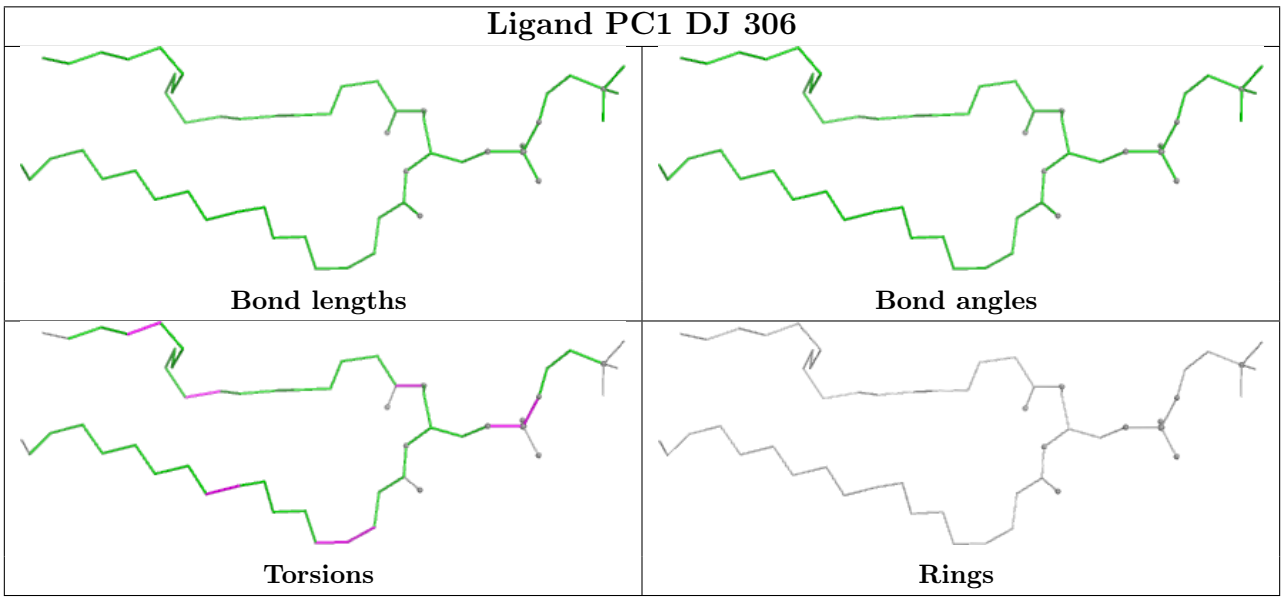


Rings

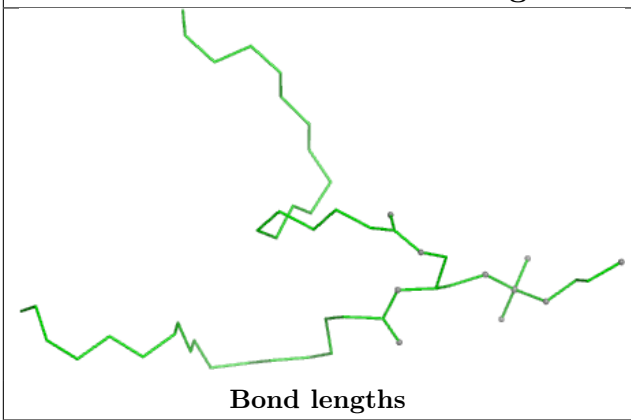
Ligand PC1 DX 308



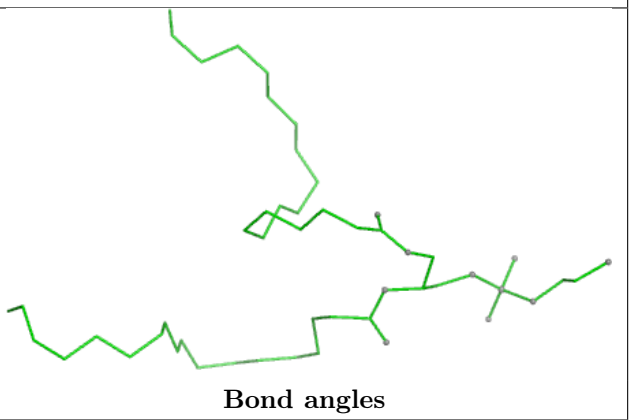
Ligand PC1 DJ 306



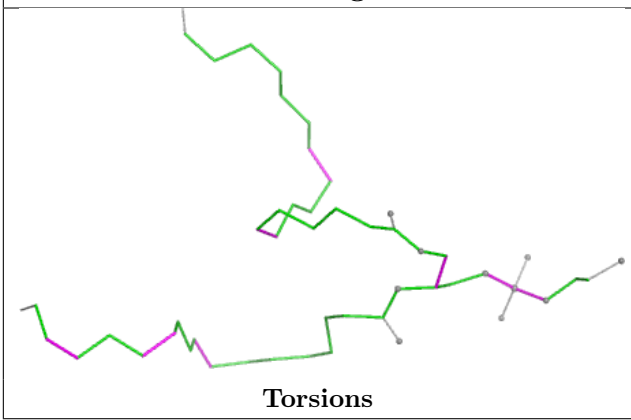
Ligand 3PE Dx 1208



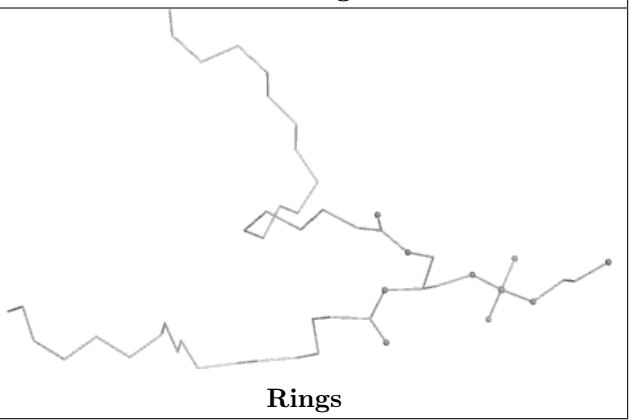
Bond lengths



Bond angles



Torsions



Rings

Ligand CDL Dj 404



Bond lengths



Bond angles

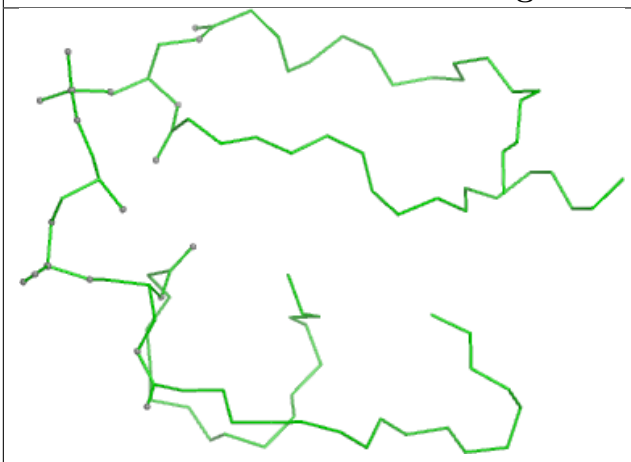


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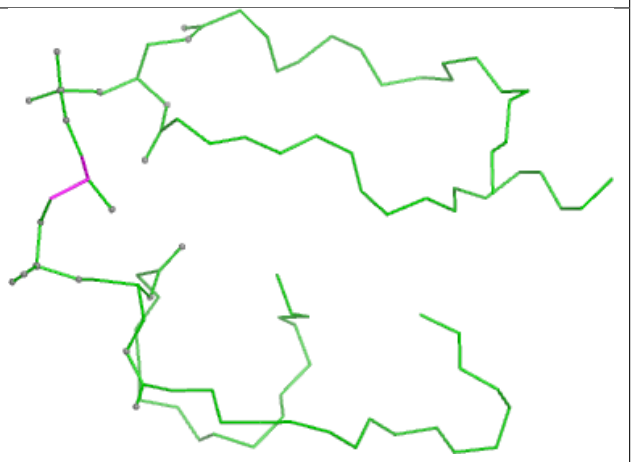


Rings

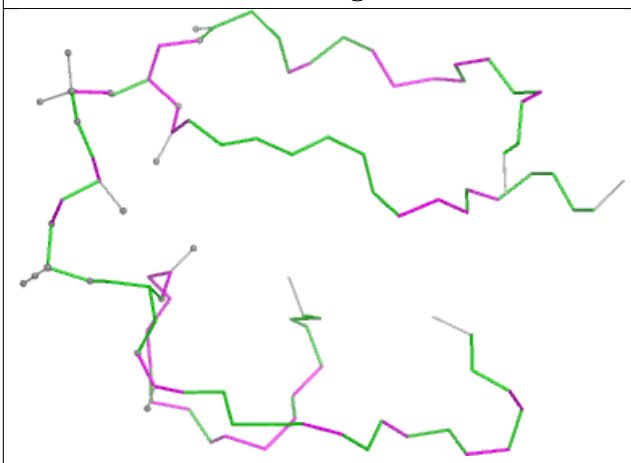
Ligand CDL Ds 405



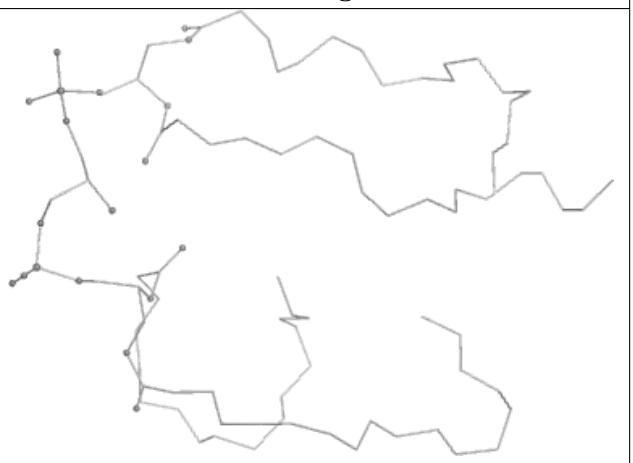
Bond lengths



Bond angles

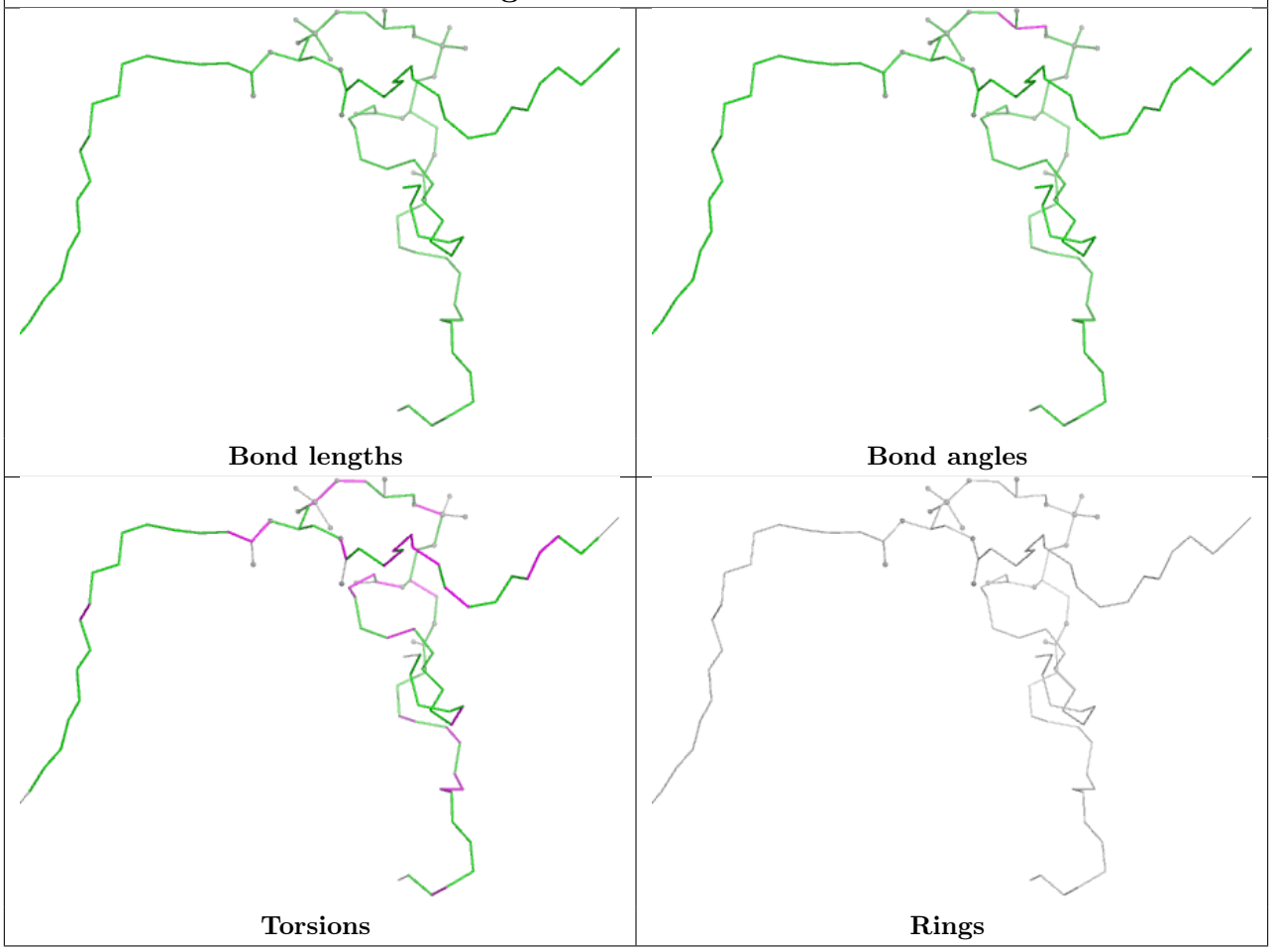


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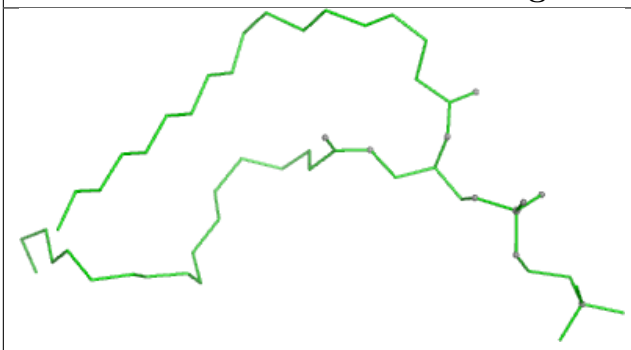


Rings

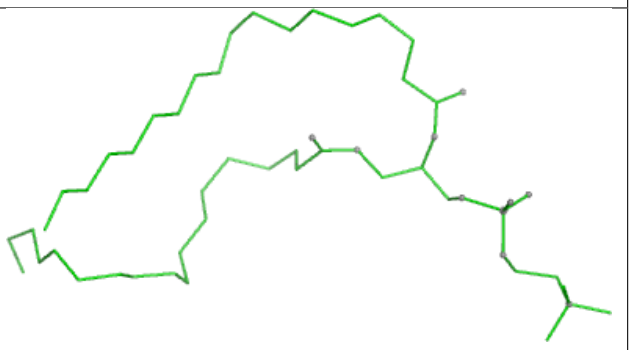
Ligand CDL Dx 1201



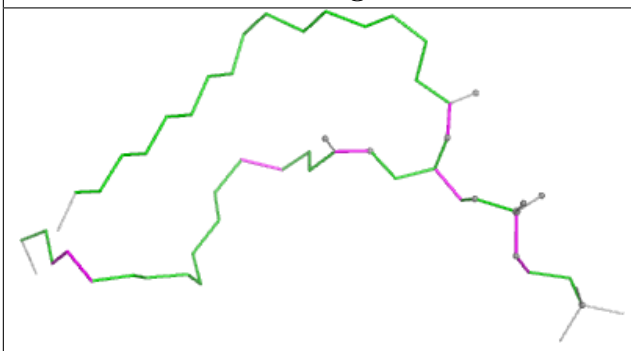
Ligand PC1 E 303



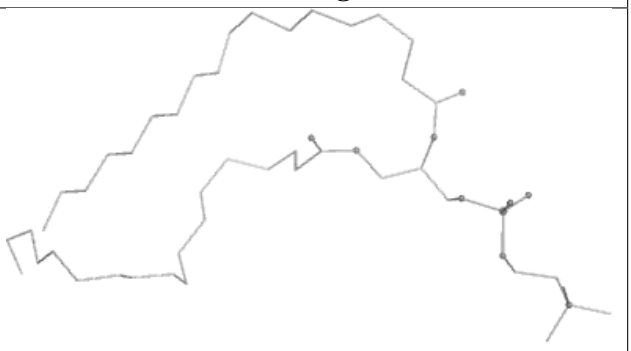
Bond lengths



Bond angles

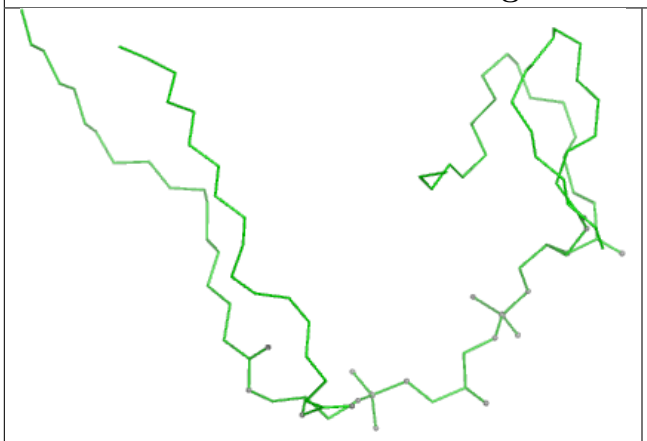


Torsions

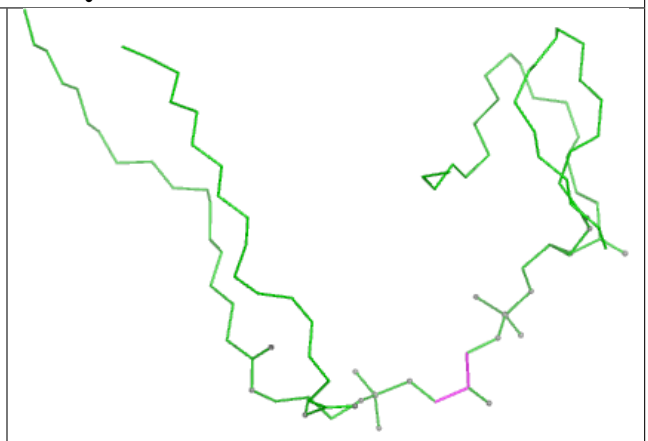


Rings

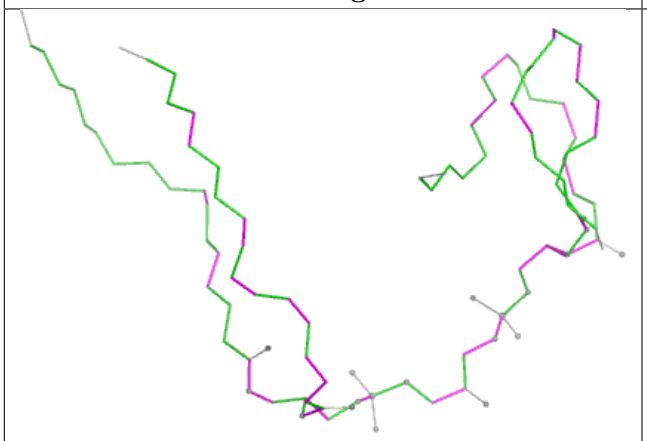
Ligand CDL DQ 1504



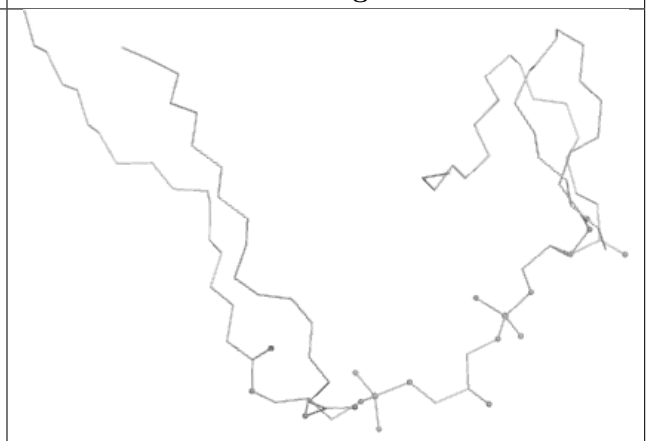
Bond lengths



Bond angles

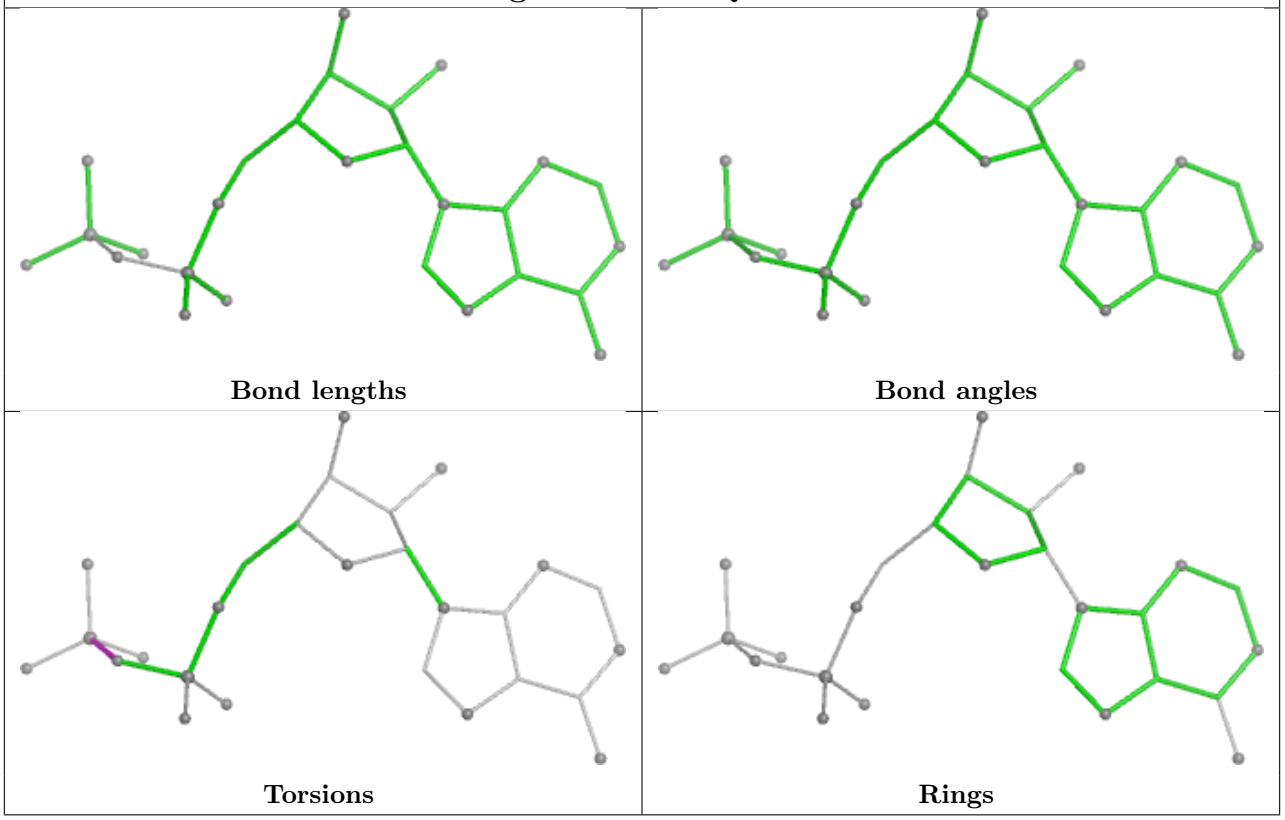


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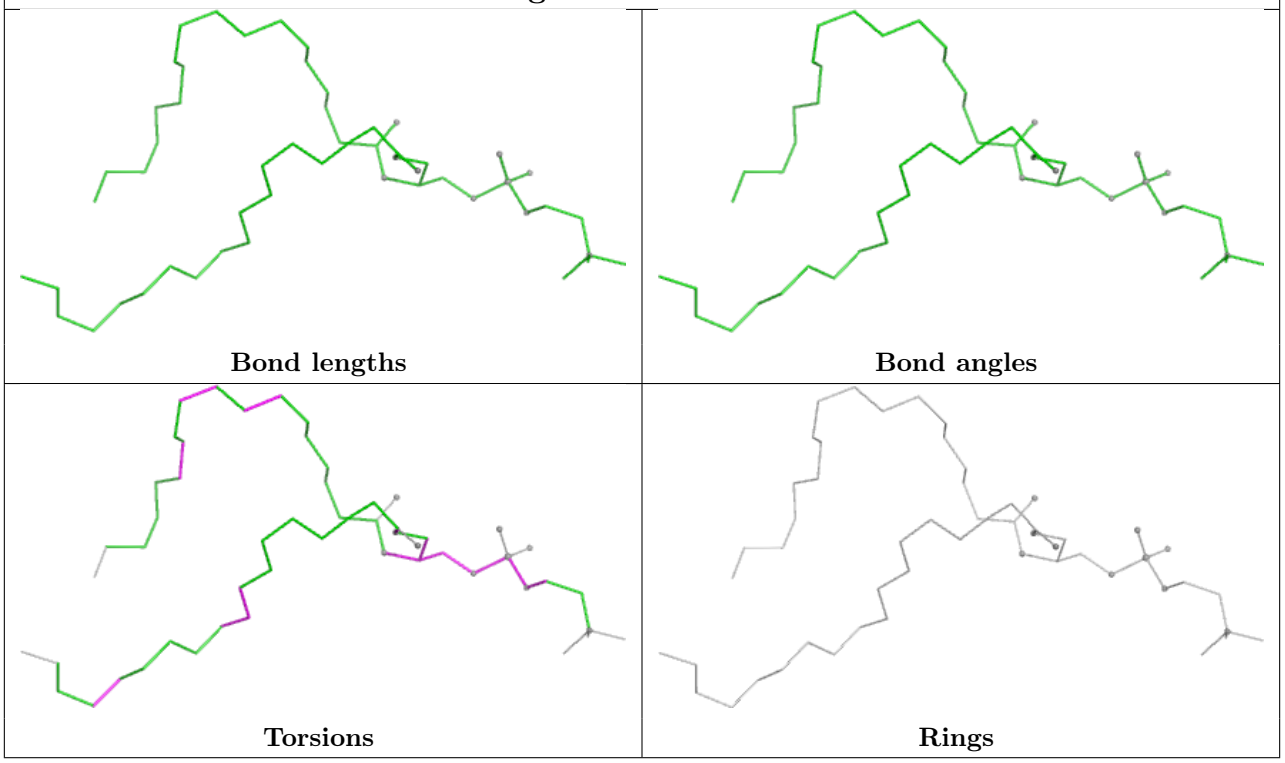


Rings

Ligand ADP AQ 201



Ligand PC1 C 508



Ligand CDL Do 501



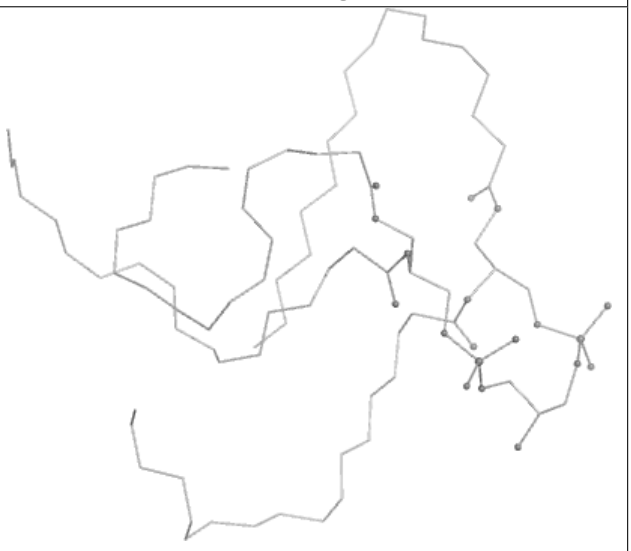
Bond lengths



Bond angles

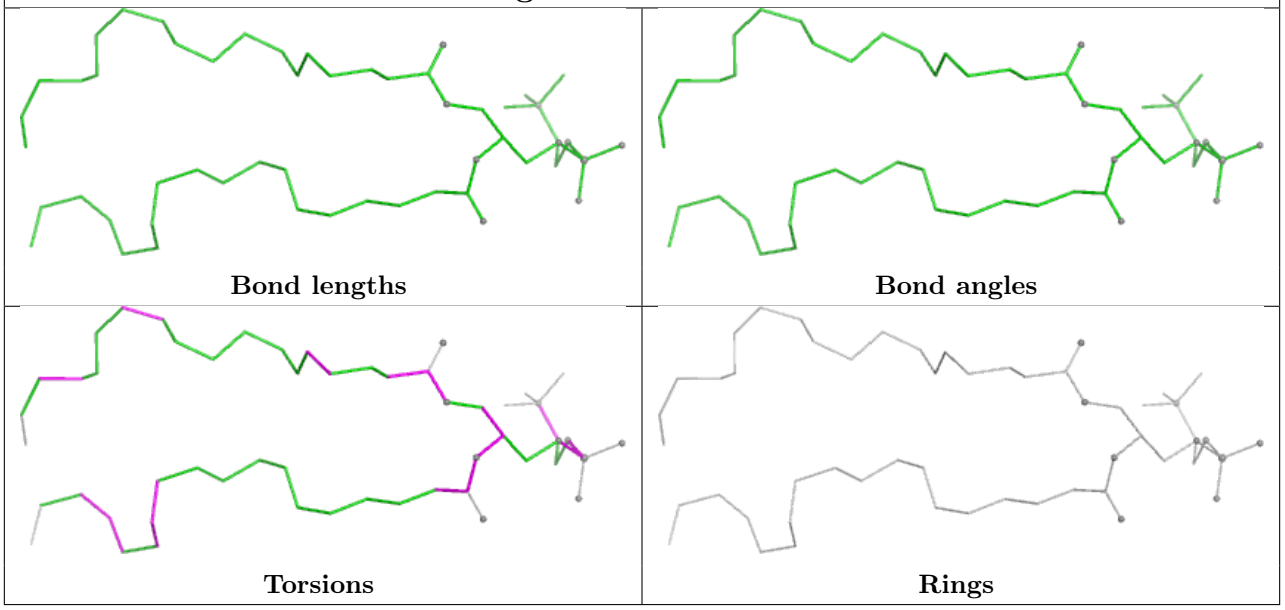


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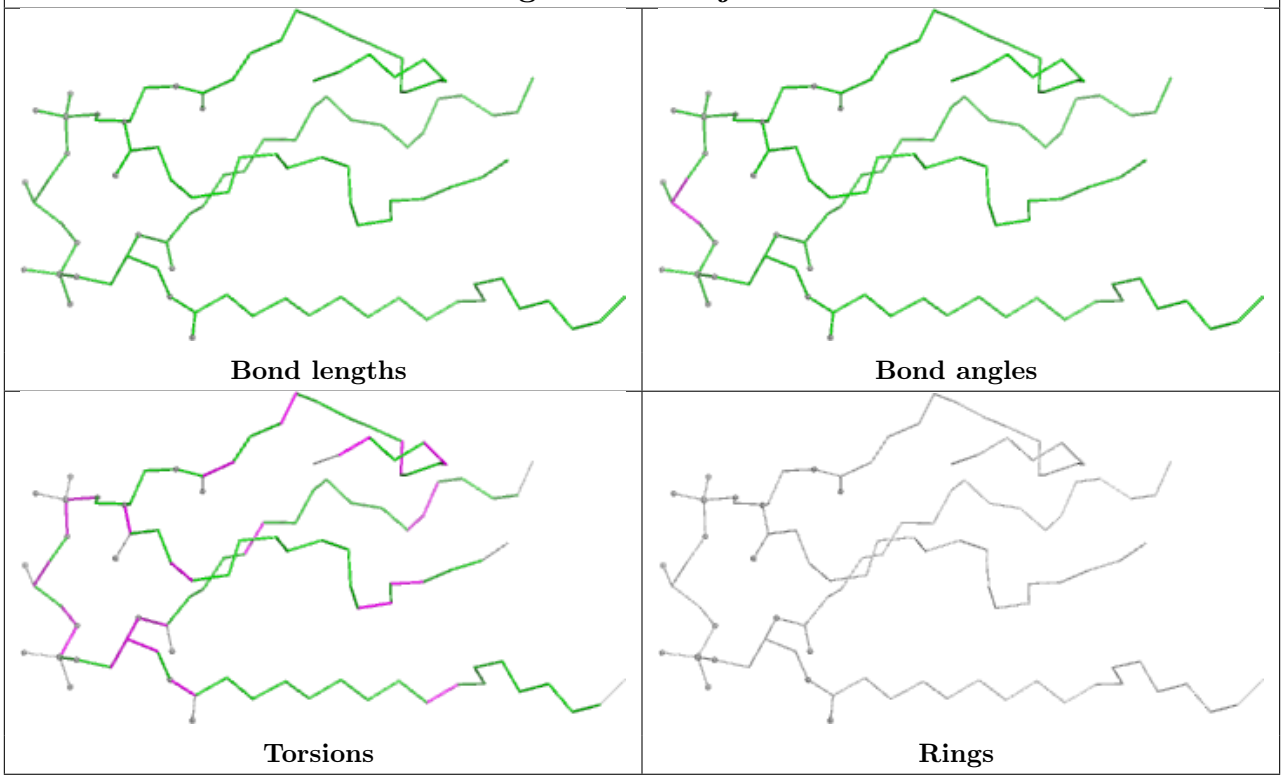


Rings

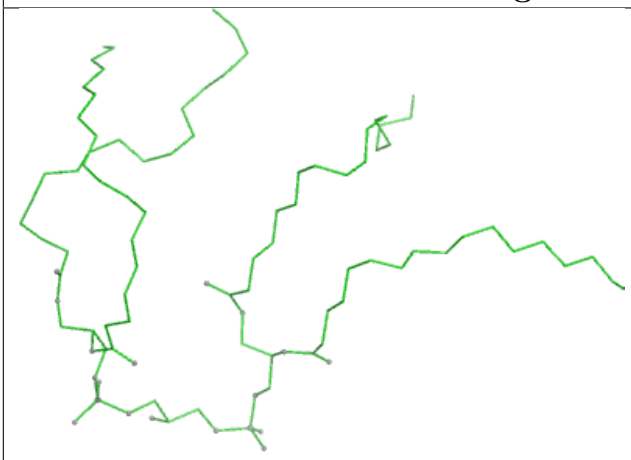
Ligand PC1 EO 205



Ligand CDL Dj 405



Ligand CDL H 1301



Bond lengths



Bond angles

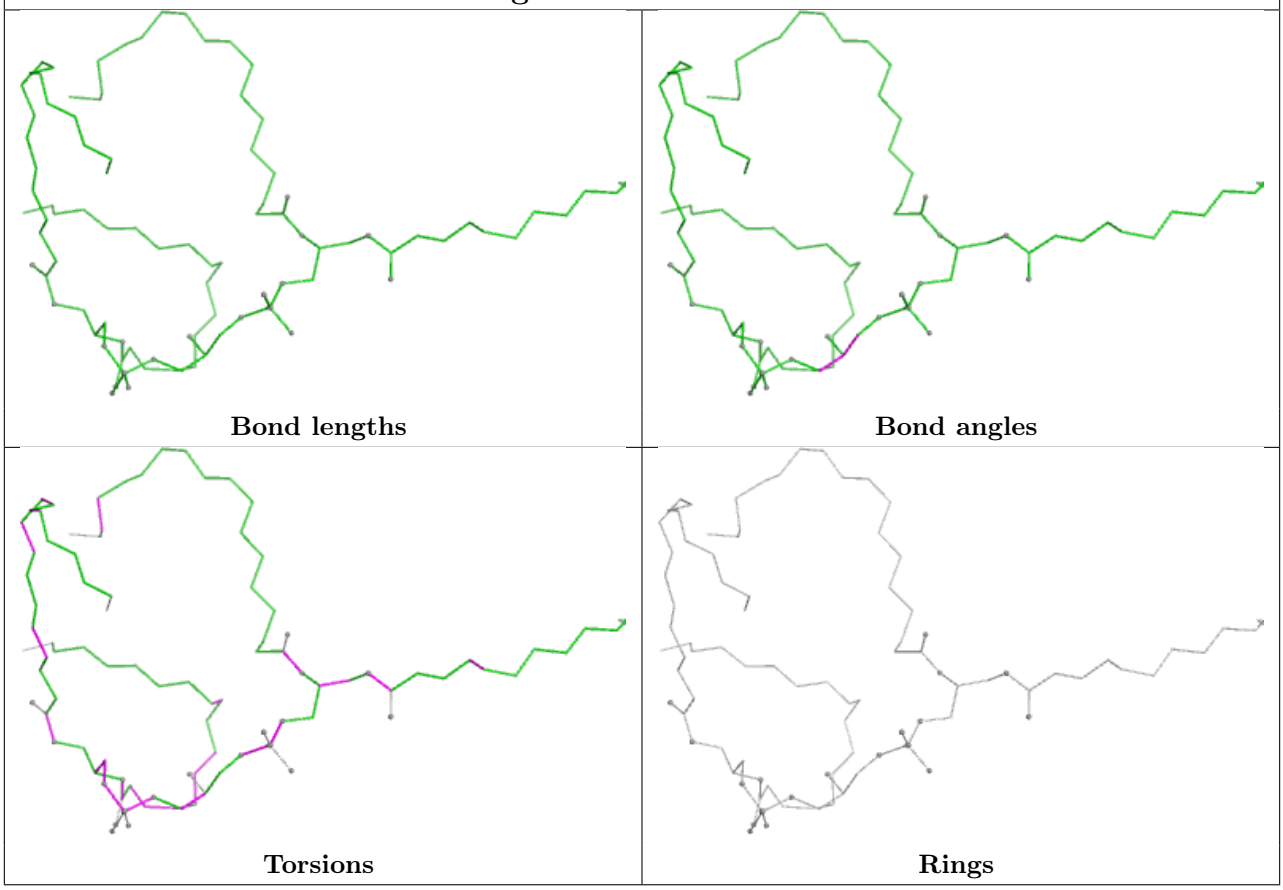


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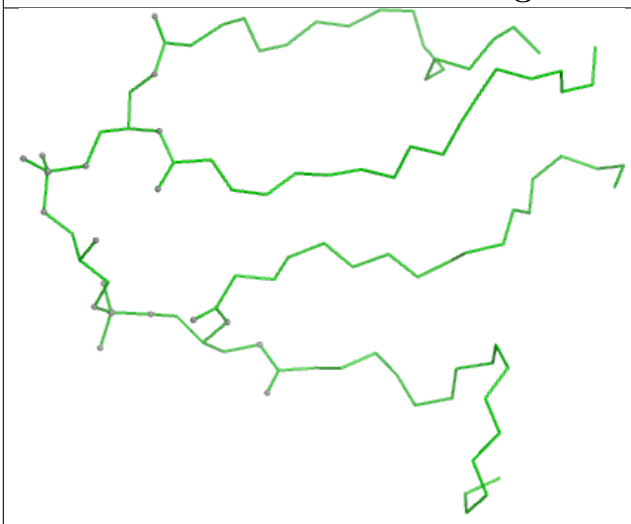


Rings

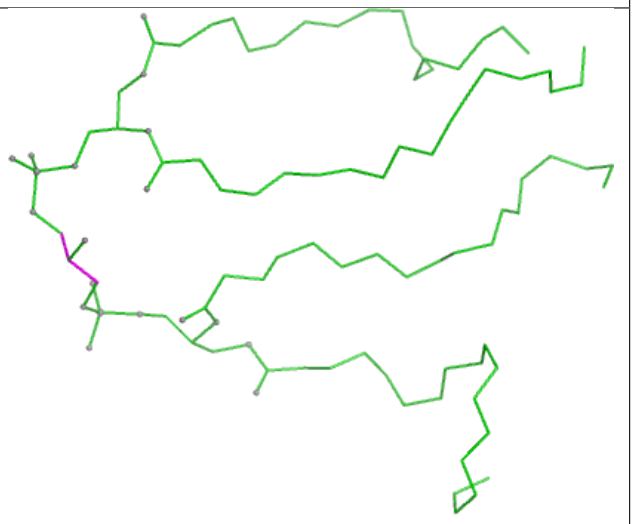
Ligand CDL DX 306



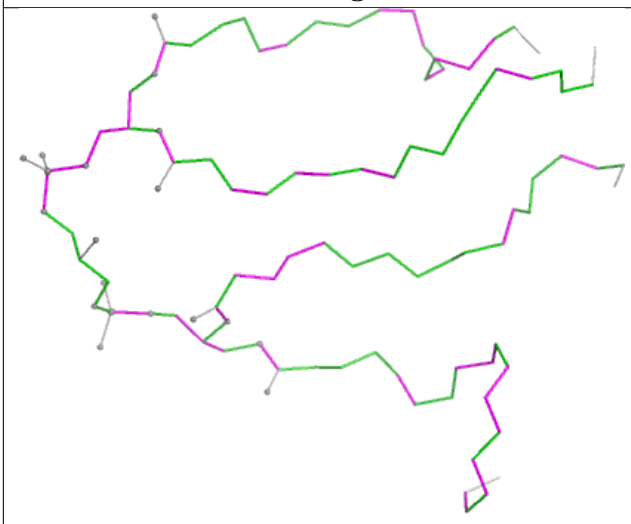
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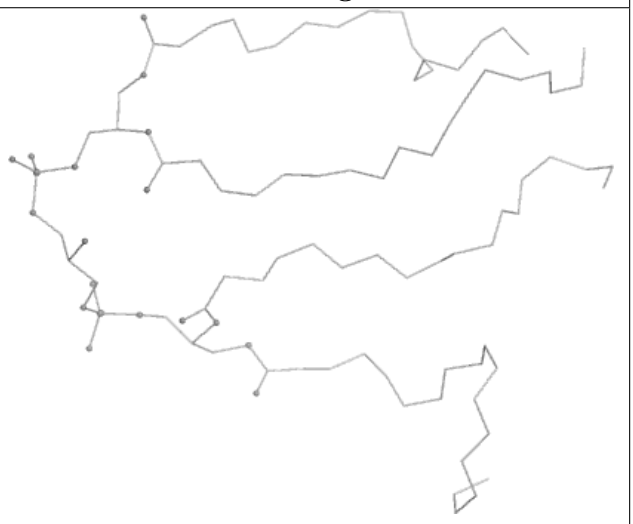
Bond lengths



Bond angles

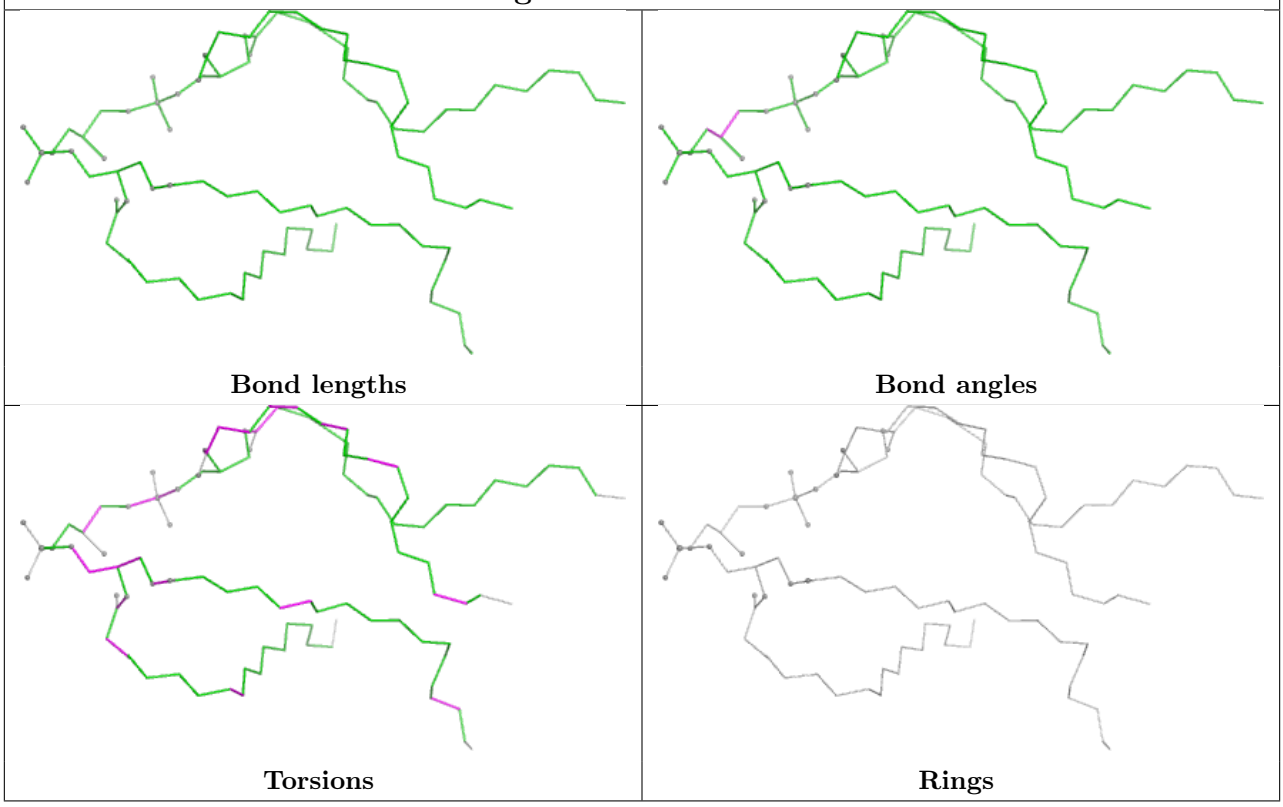


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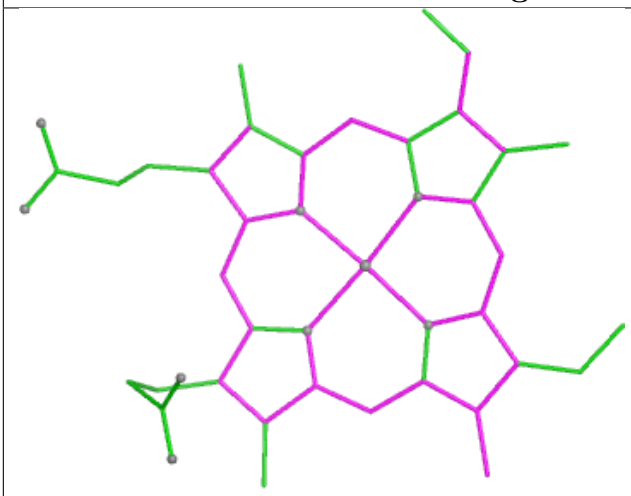


Rings

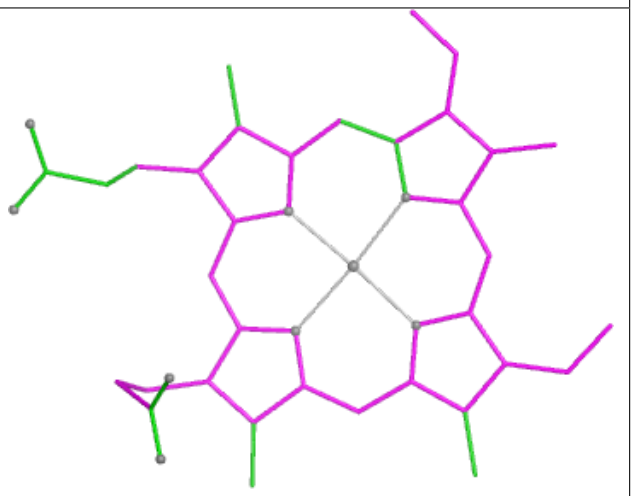
Ligand CDL Dn 503



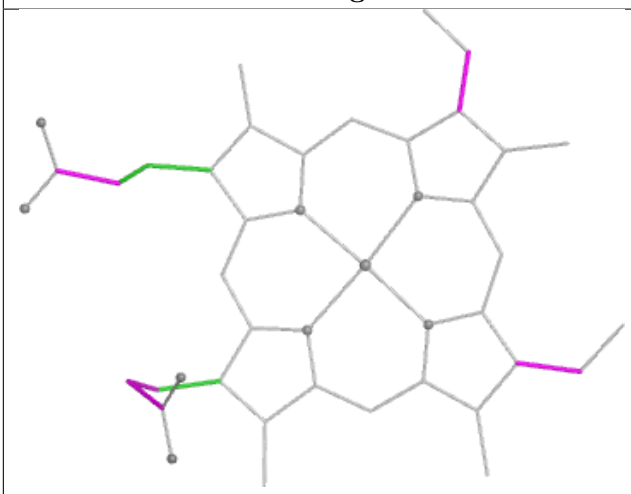
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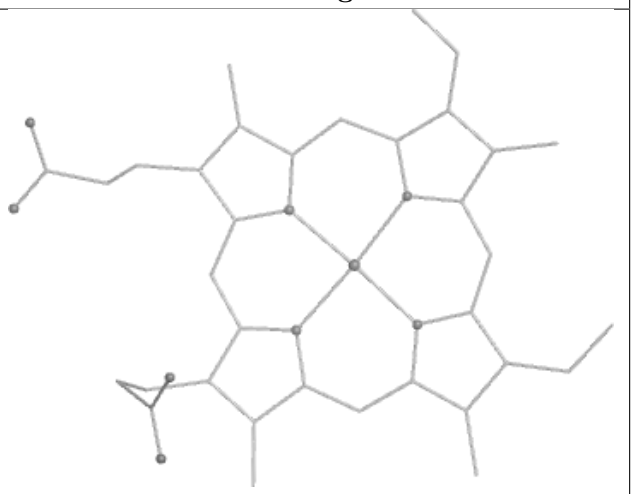
Bond lengths



Bond angles

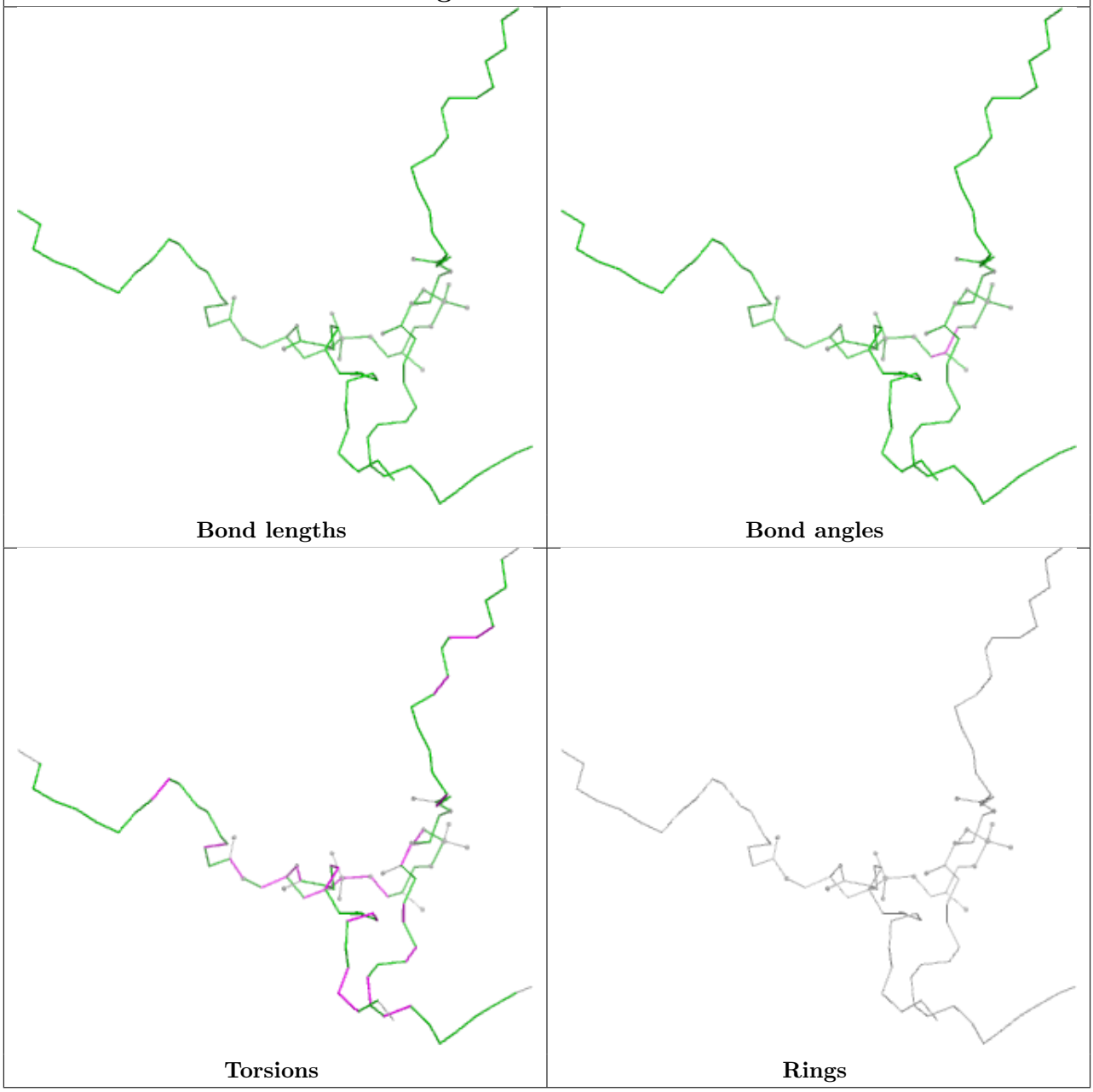


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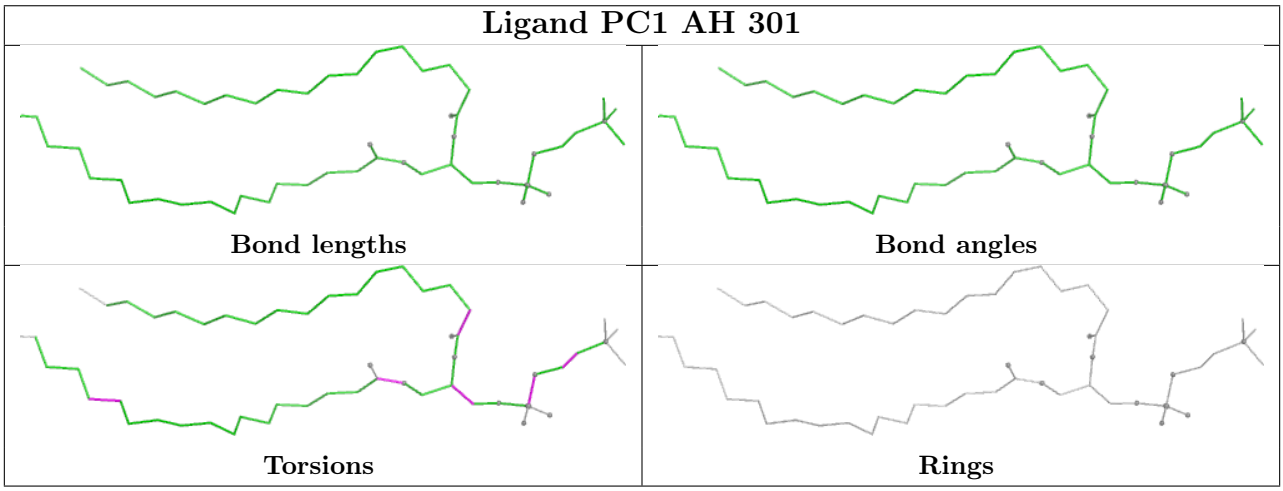


Rings

Ligand CDL EO 202



Ligand PC1 AH 301



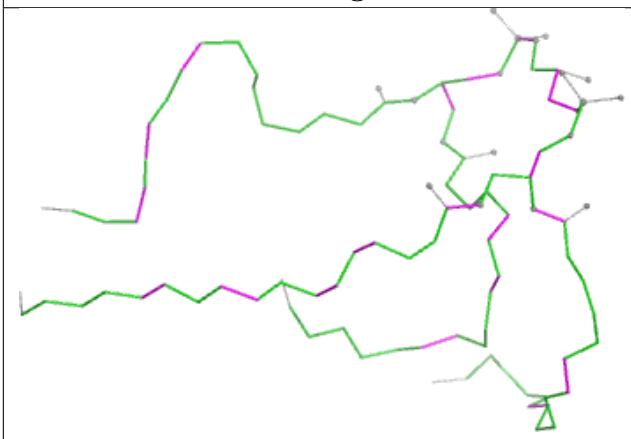
Ligand CDL c 502



Bond lengths



Bond angles

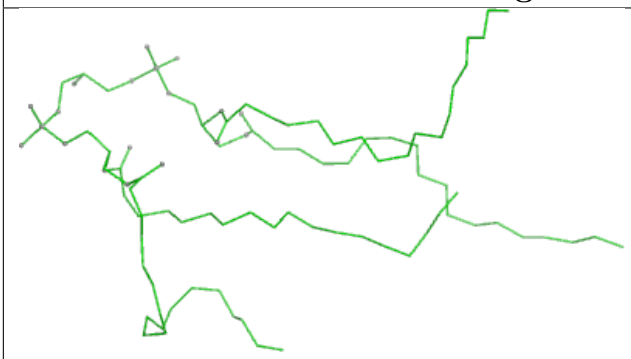


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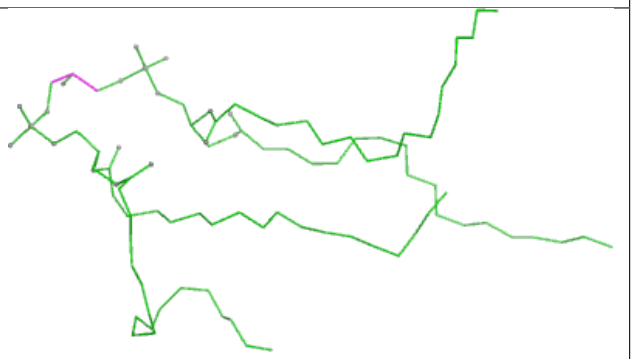


Rings

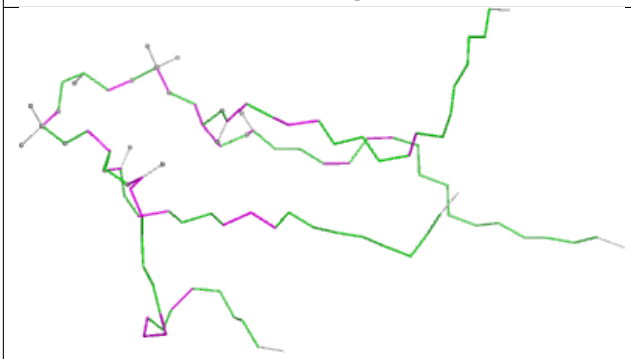
Ligand CDL B1 402



Bond lengths



Bond angles

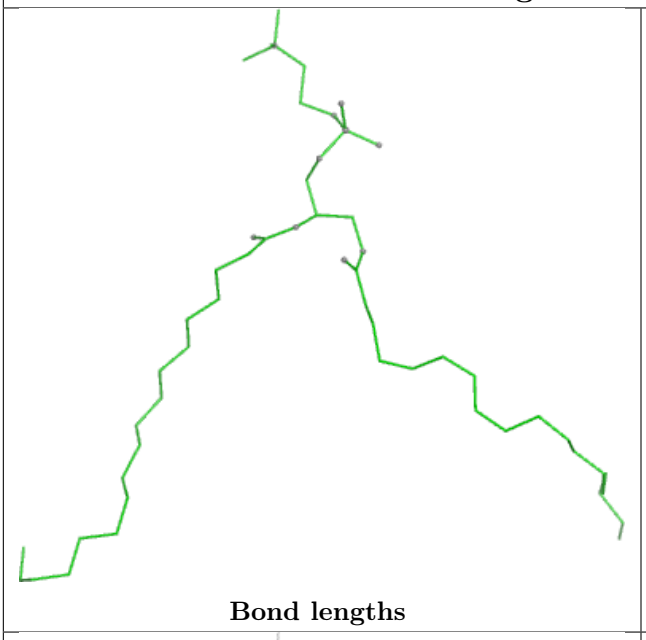


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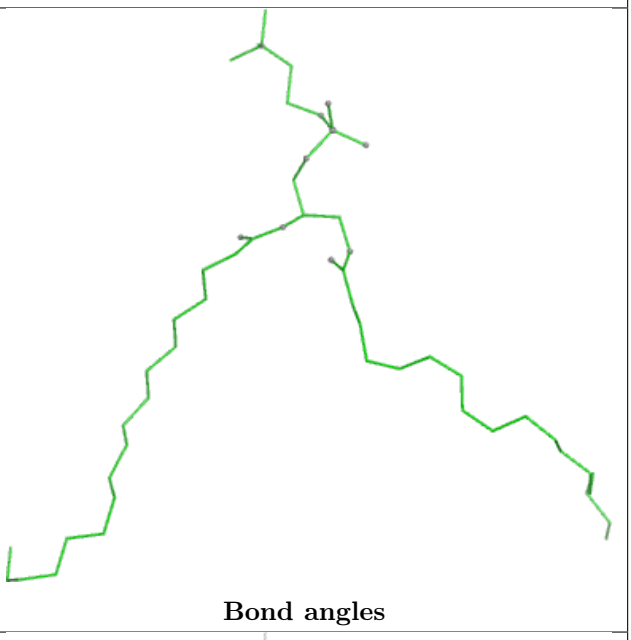


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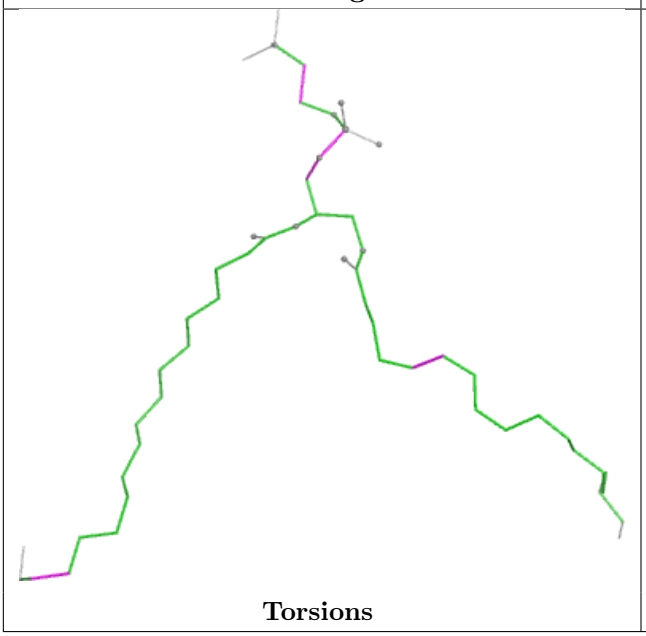
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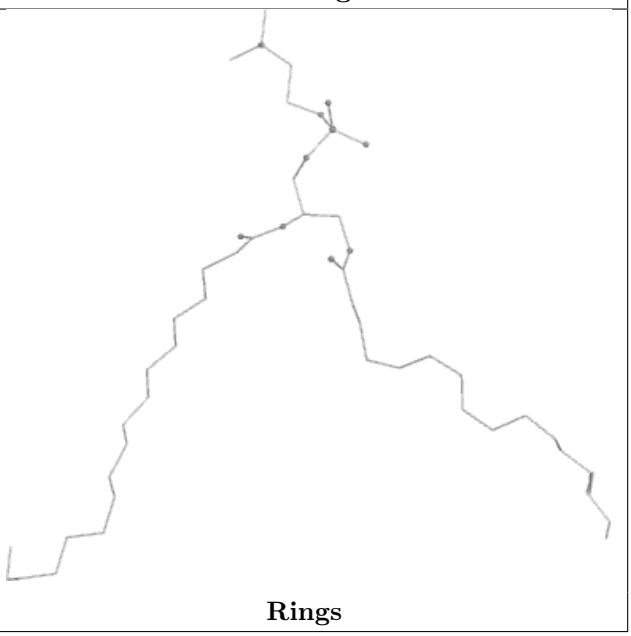
Bond lengths



Bond angles



Torsions

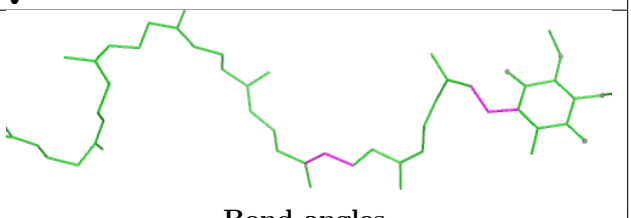


Rings

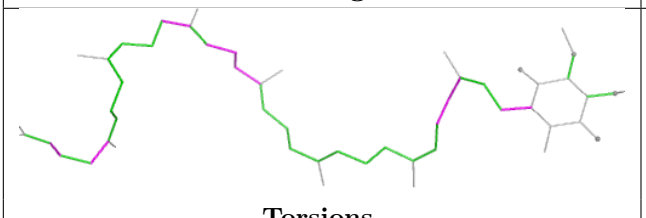
Ligand UQ8 c 510



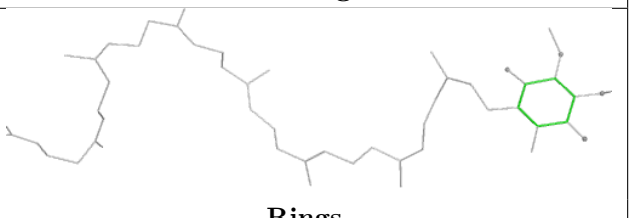
Bond lengths



Bond angles

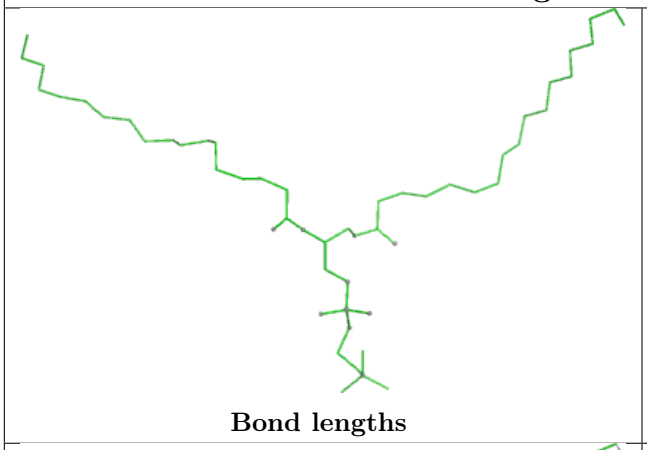


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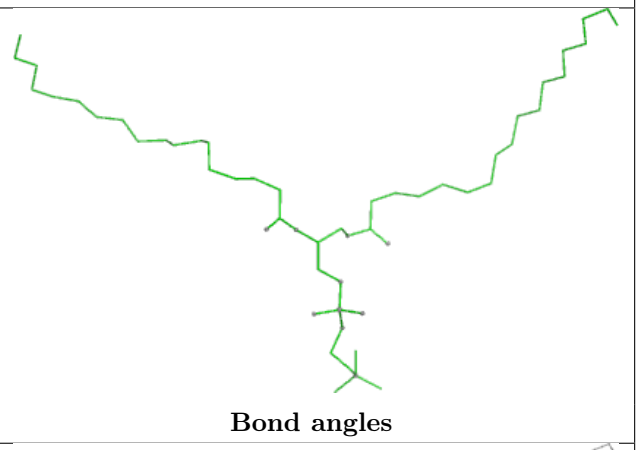


Rings

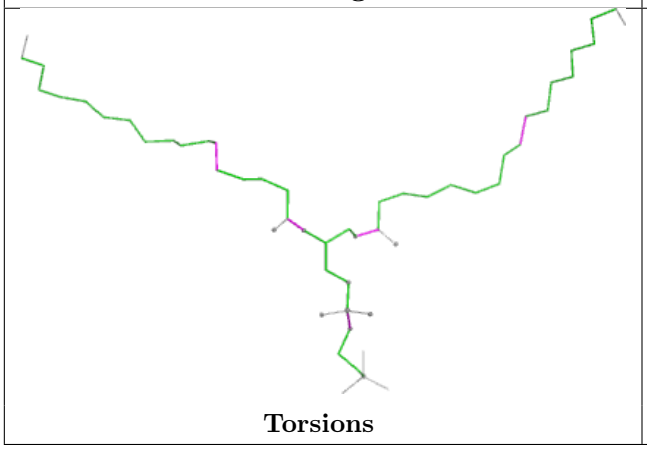
Ligand PC1 c 508



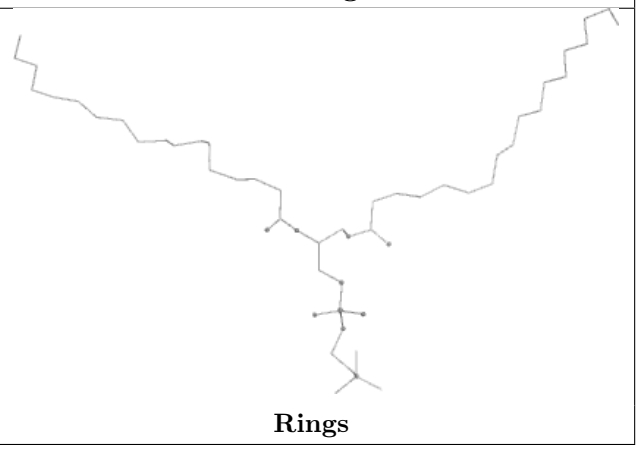
Bond lengths



Bond angles

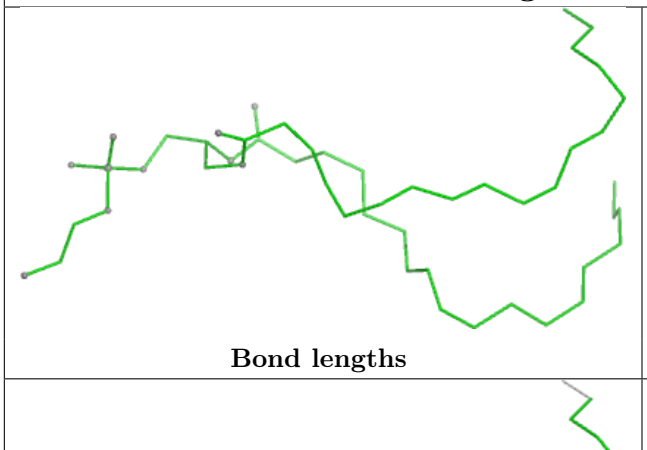


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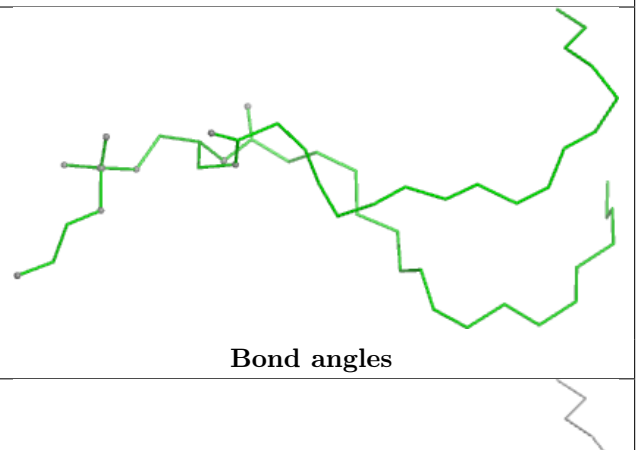


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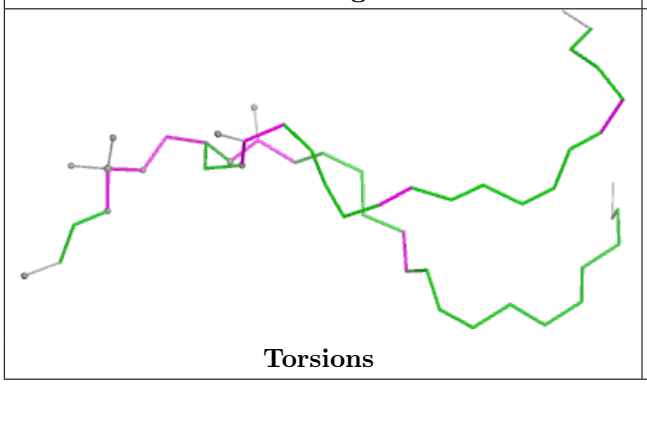
Ligand 3PE Dd 703



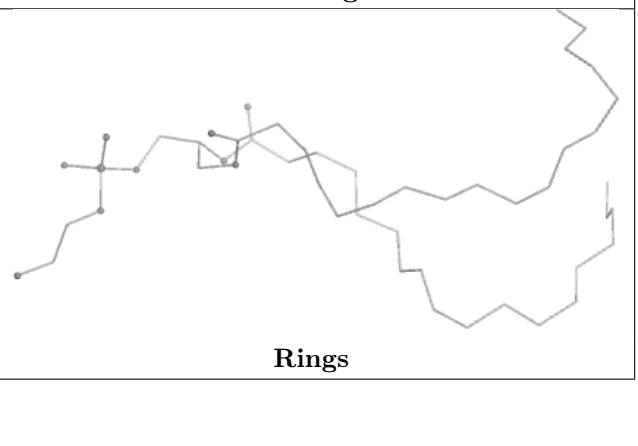
Bond lengths



Bond angles

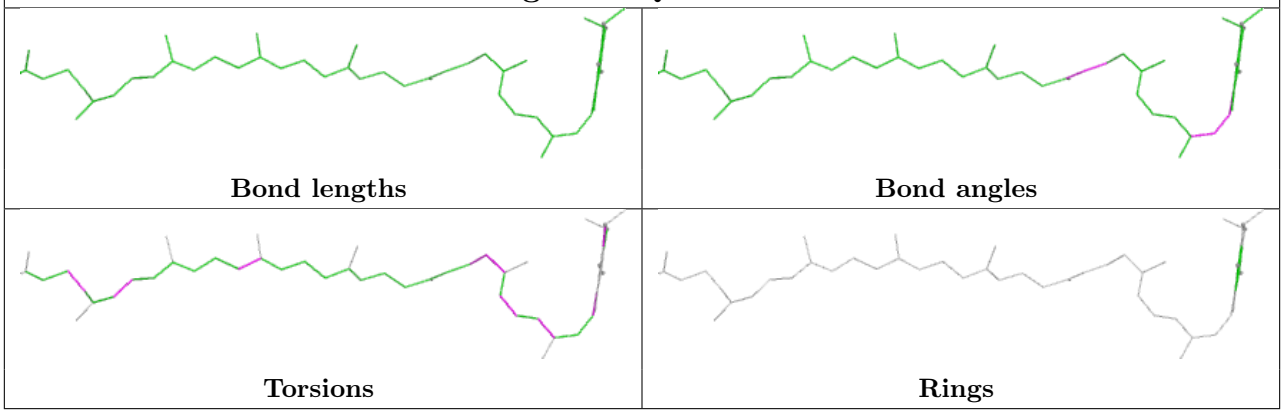


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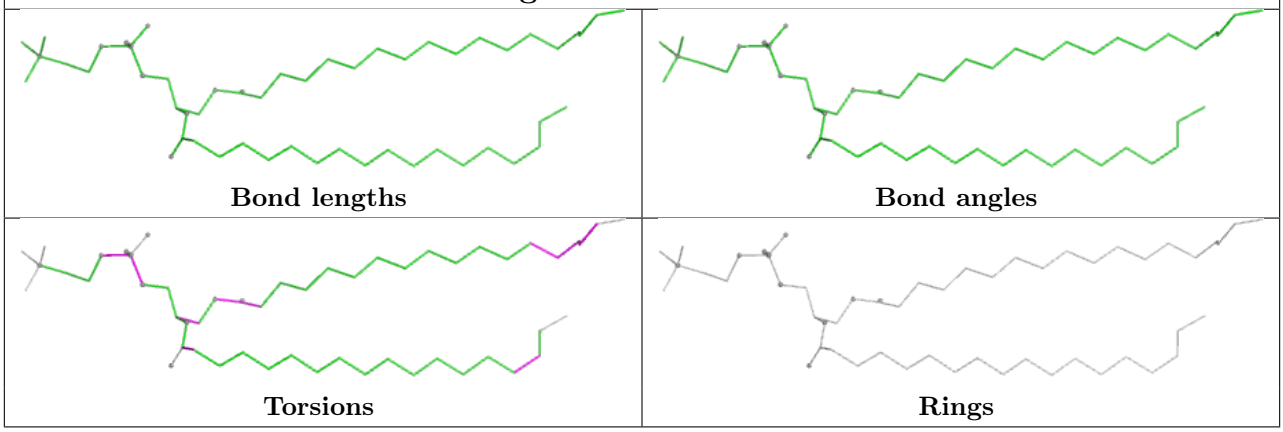


Rings

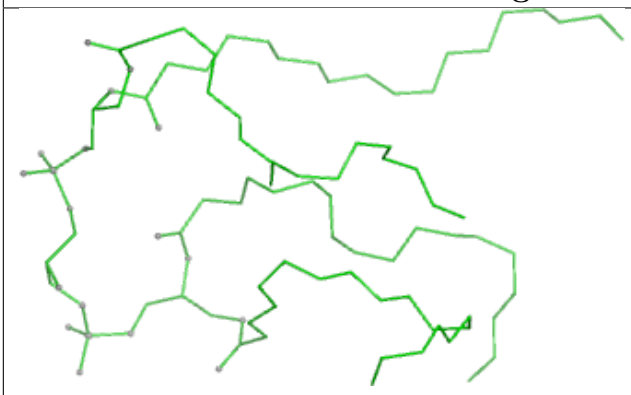
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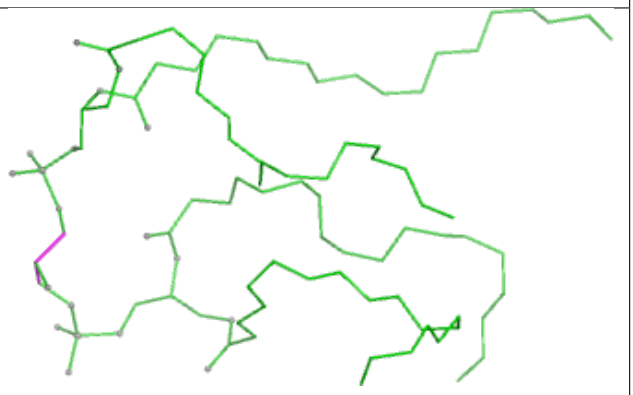
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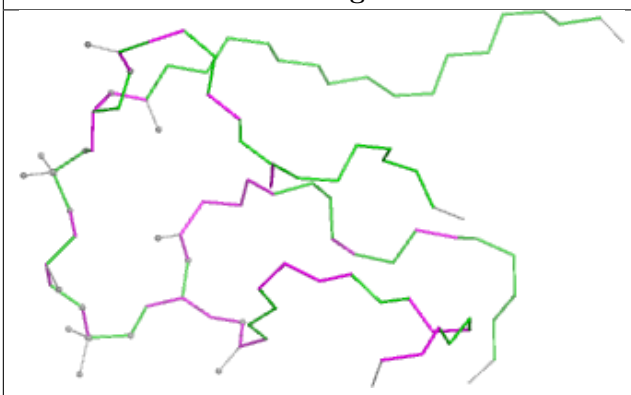
Ligand CDL DZ 501



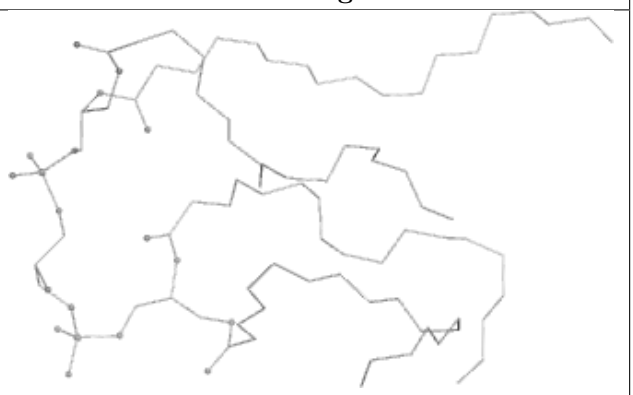
Bond lengths



Bond angles



Torsions

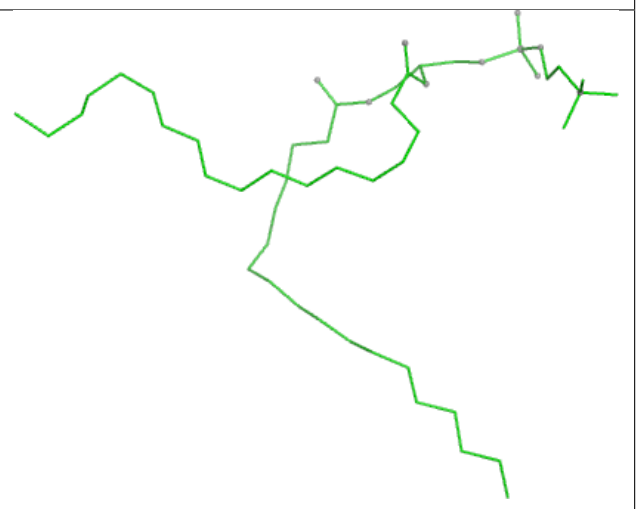


Rings

Ligand PC1 A9 601



Bond lengths



Bond angles

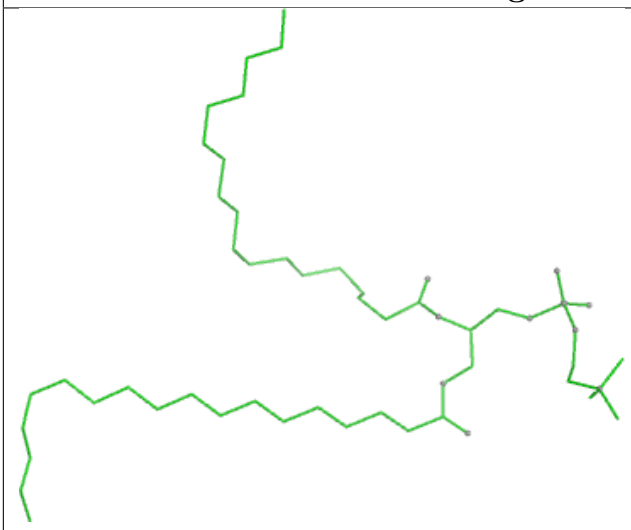


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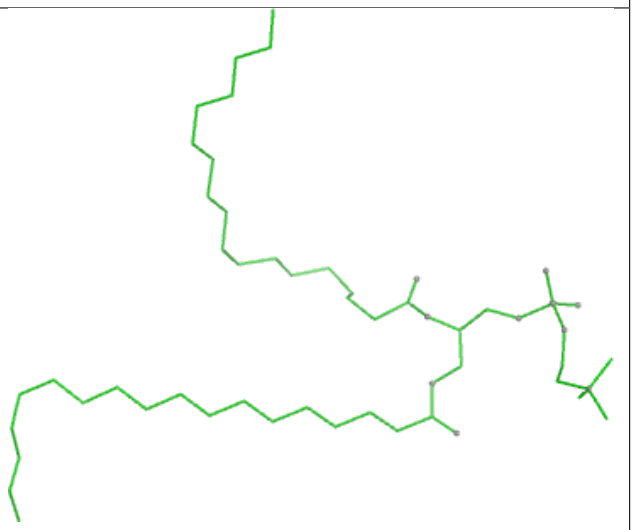


Rings

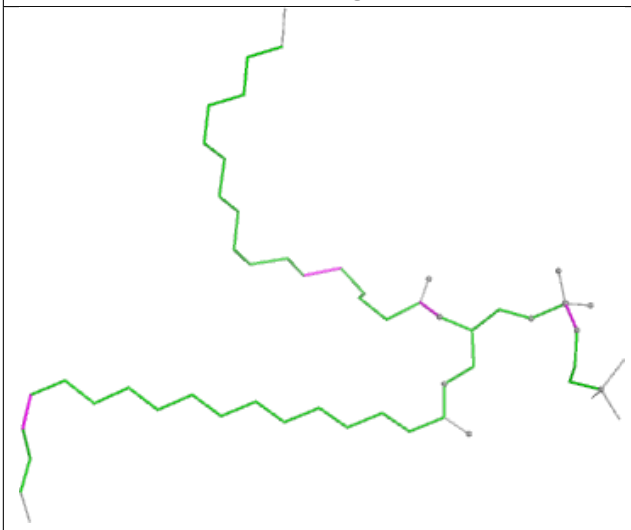
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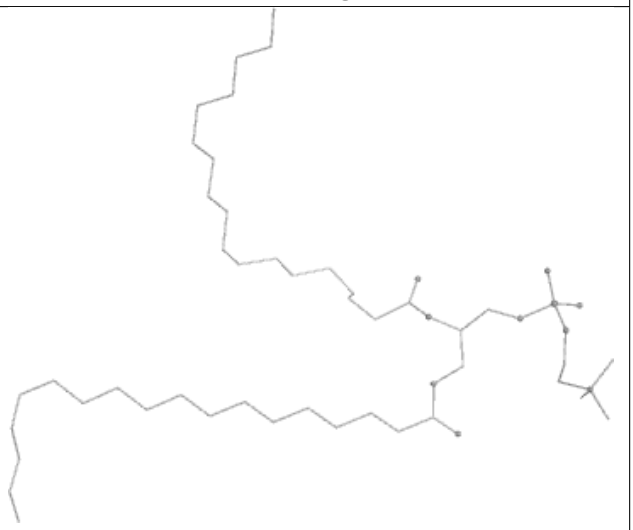
Bond lengths



Bond angles

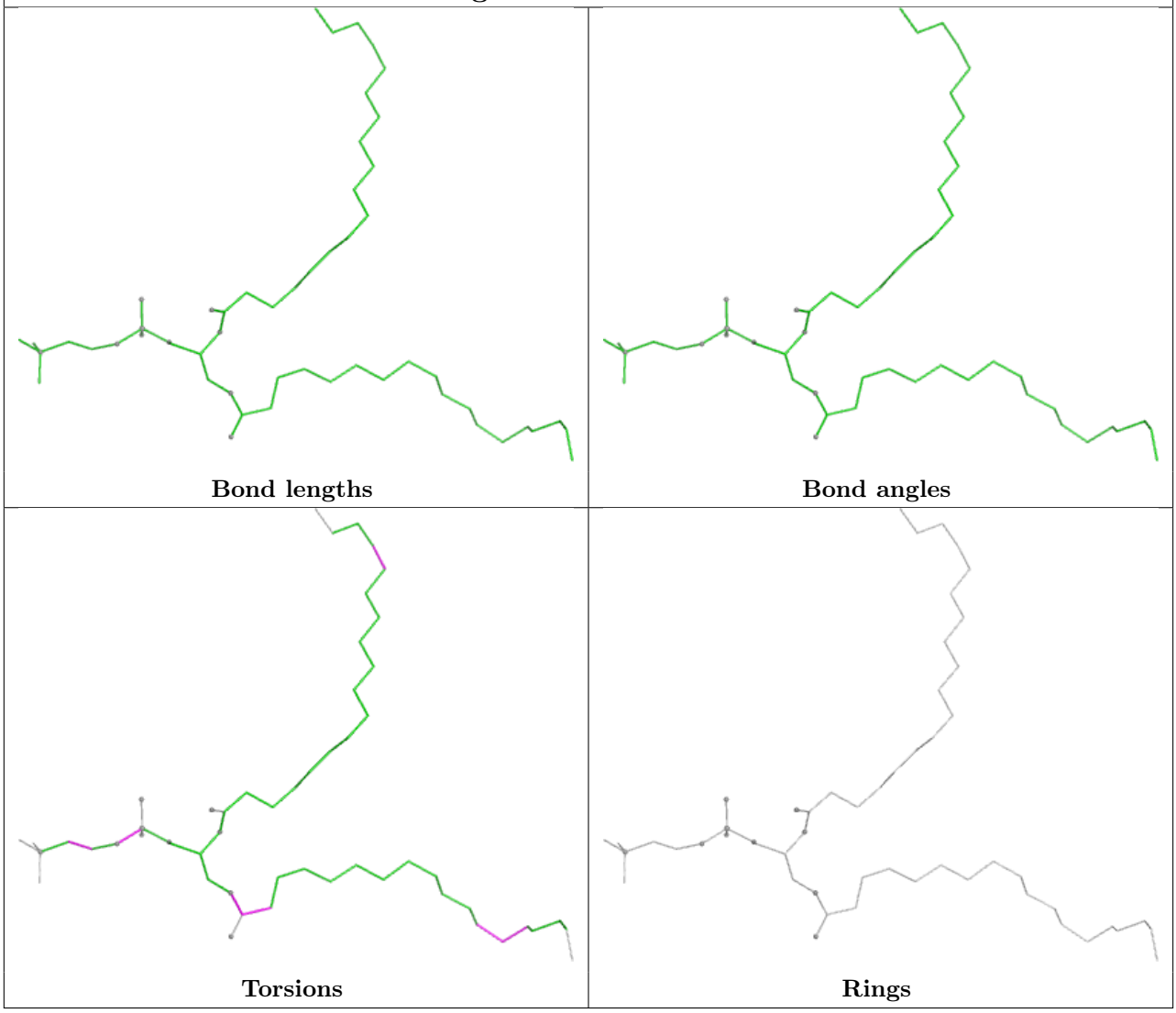


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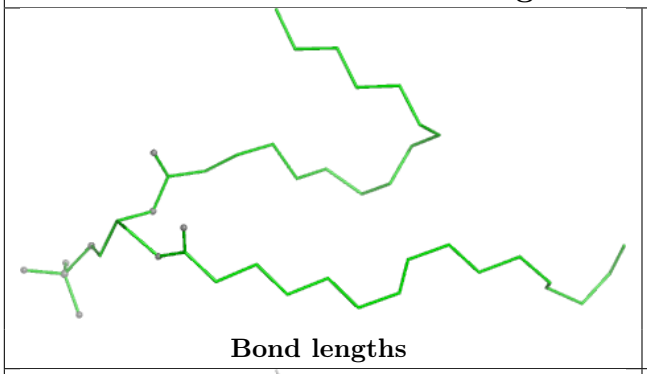


Rings

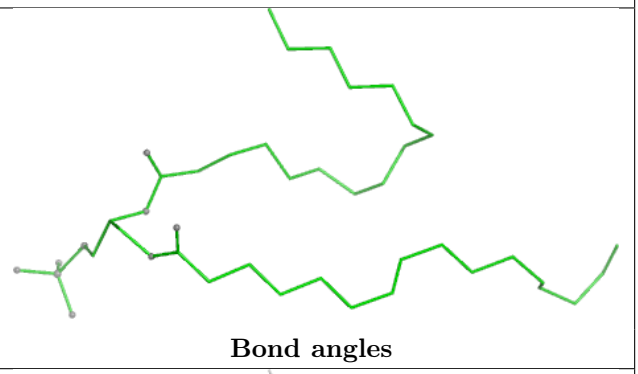
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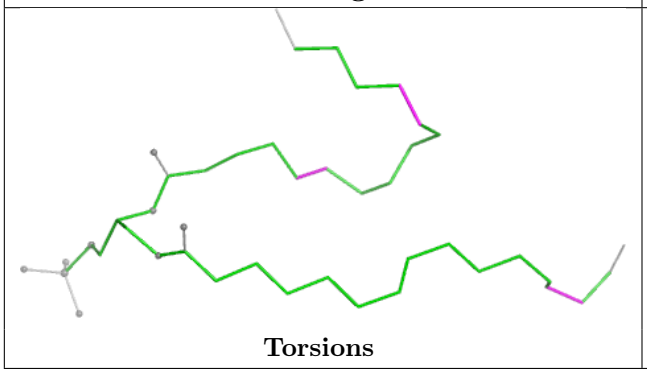
Ligand LPP AL 304



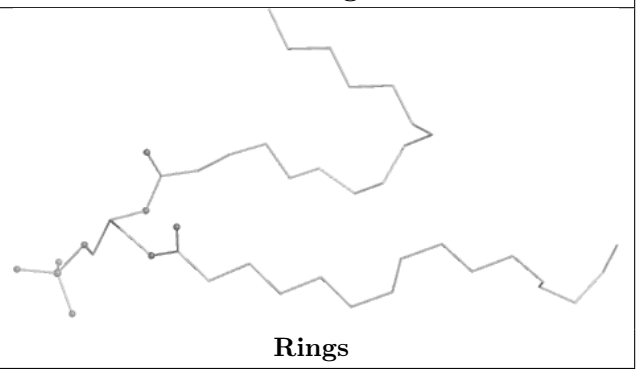
Bond lengths



Bond angles

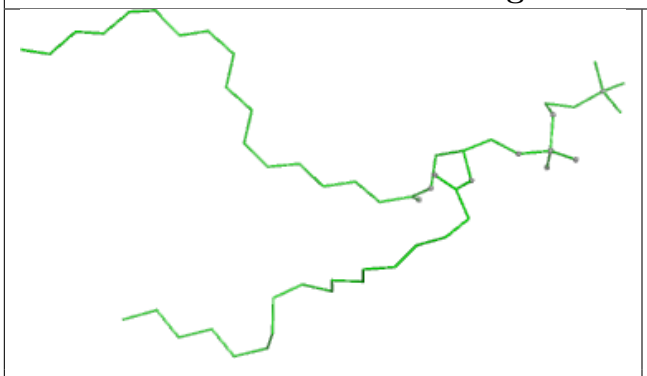


Torsions

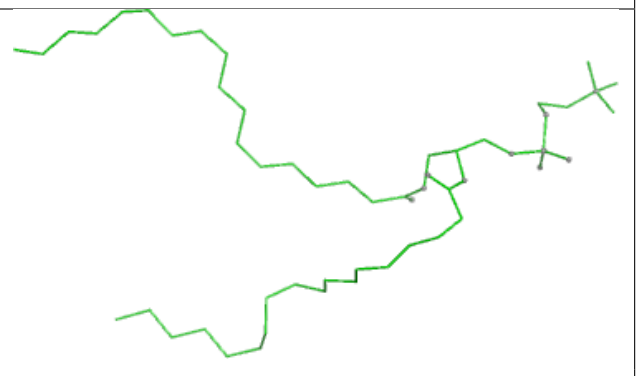


Rings

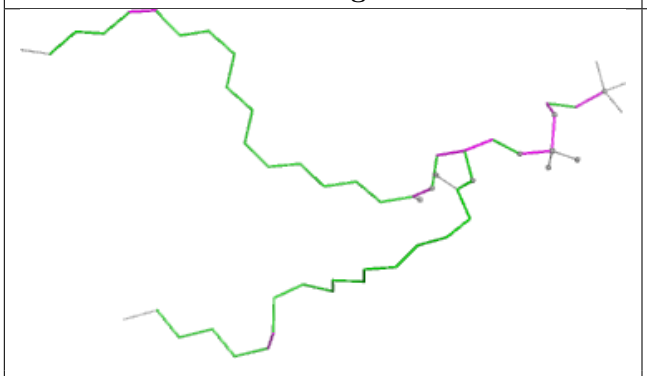
Ligand PC1 EN 1203



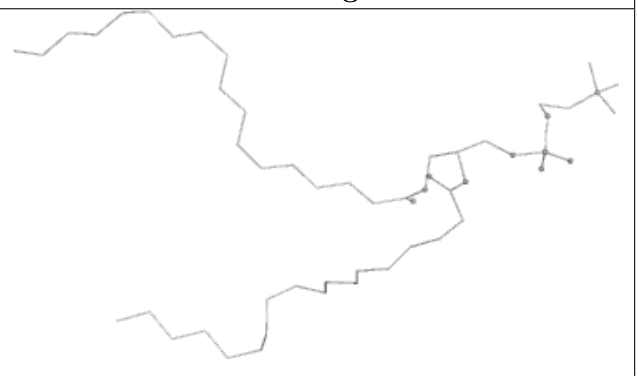
Bond lengths



Bond angles

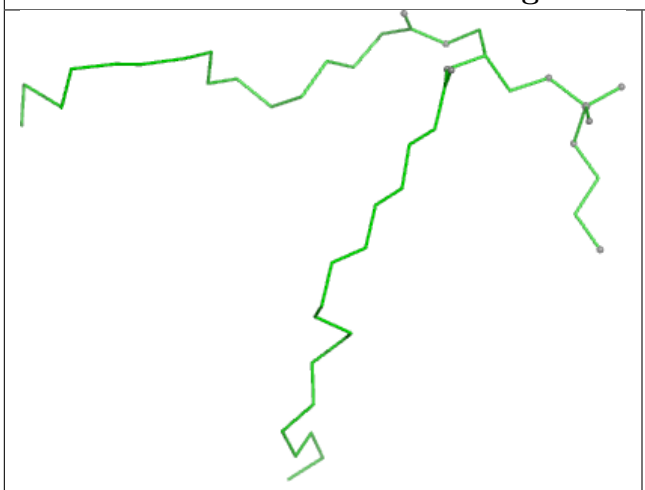


Torsions

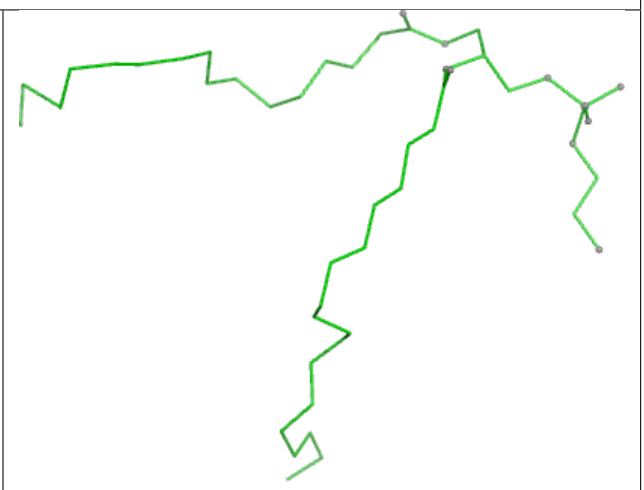


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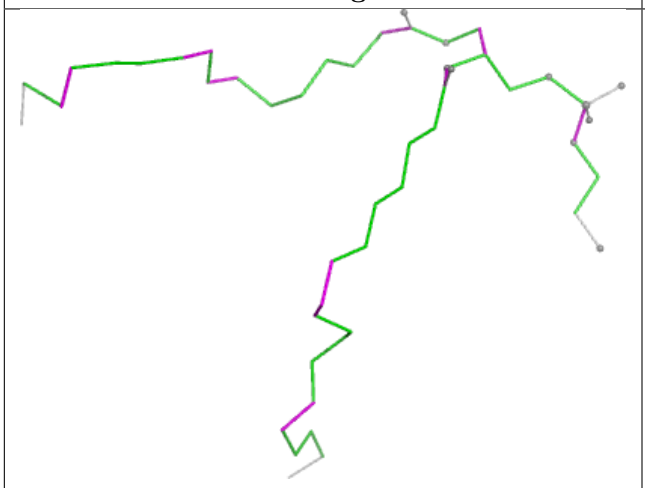
Ligand 3PE Eo 202



Bond lengths



Bond angles

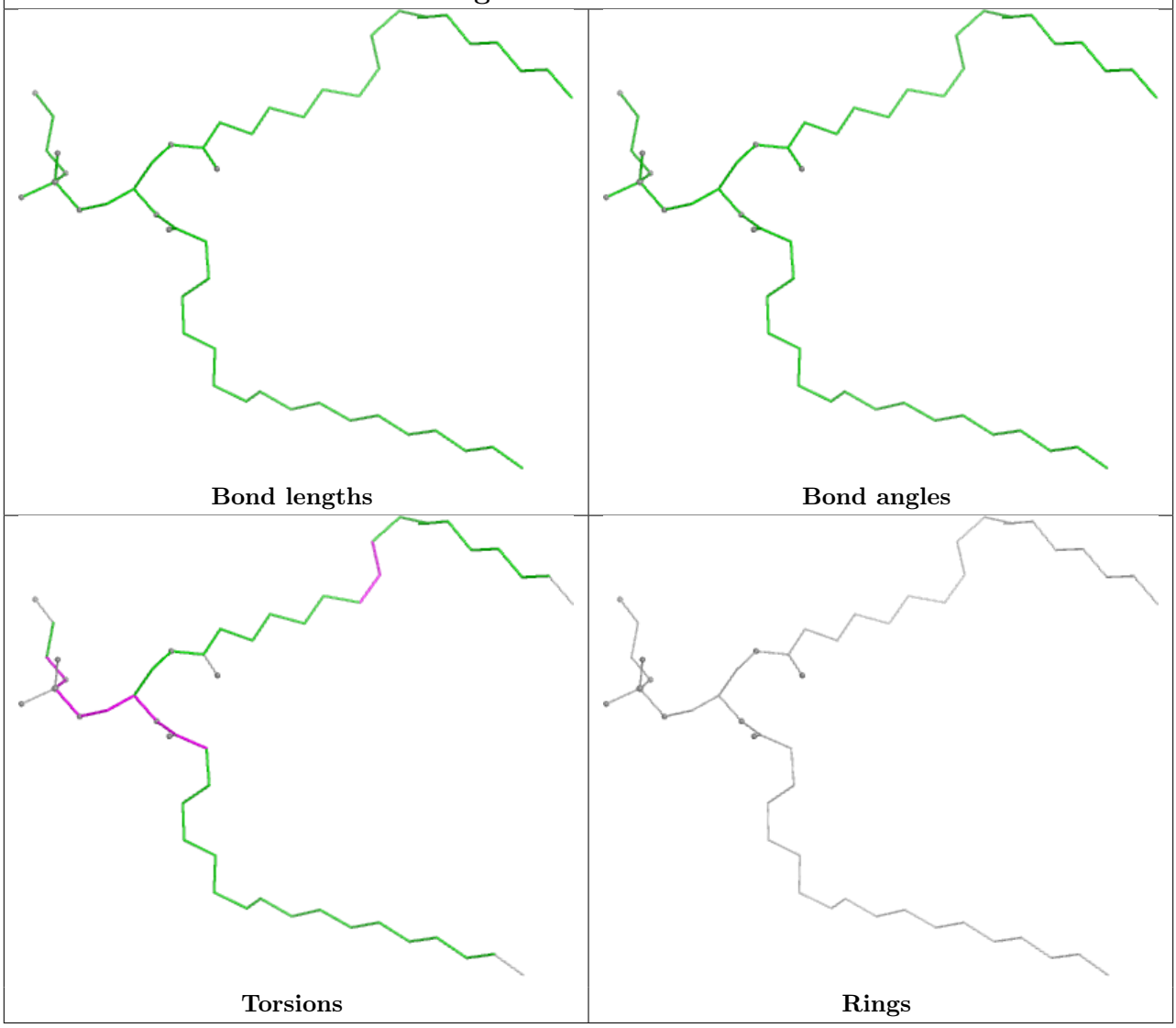


Torsions

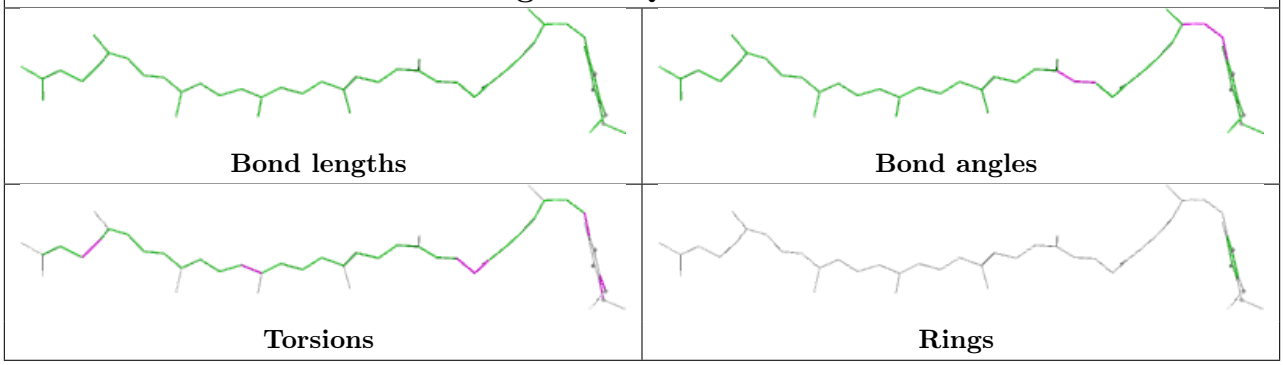


Rings

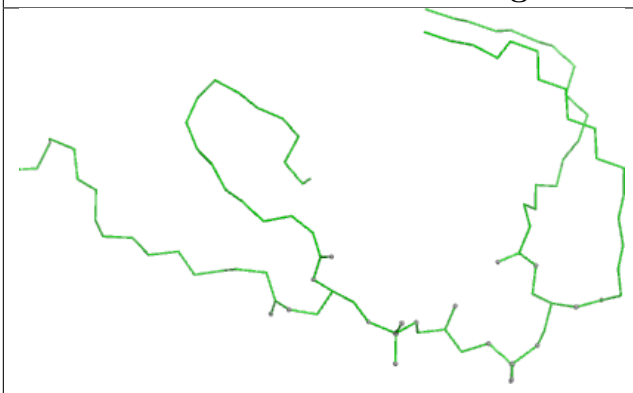
Ligand 3PE BP 201



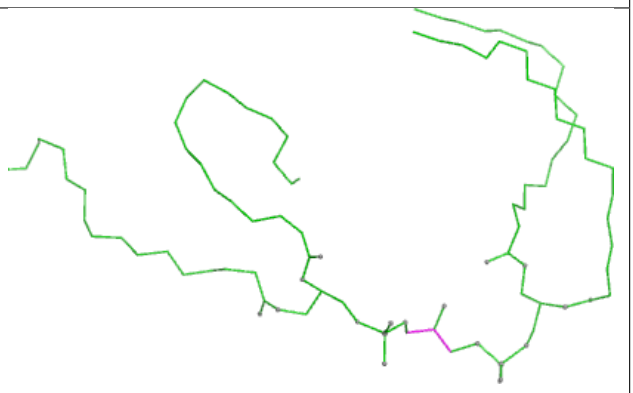
Ligand UQ8 EL 905



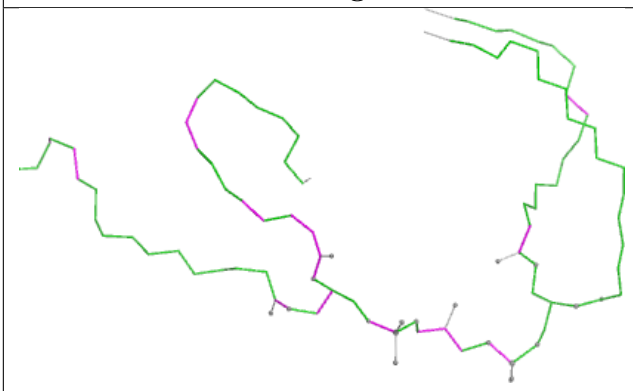
Ligand CDL DA 709



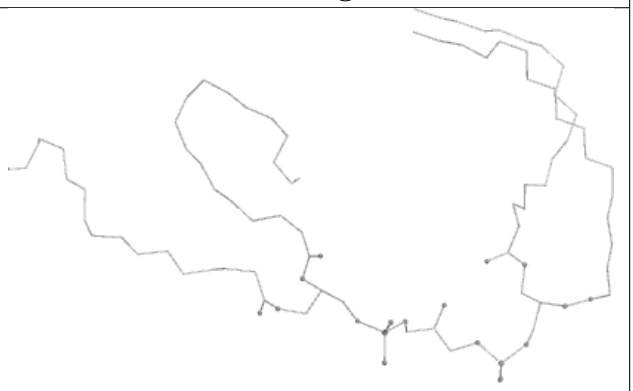
Bond lengths



Bond angles

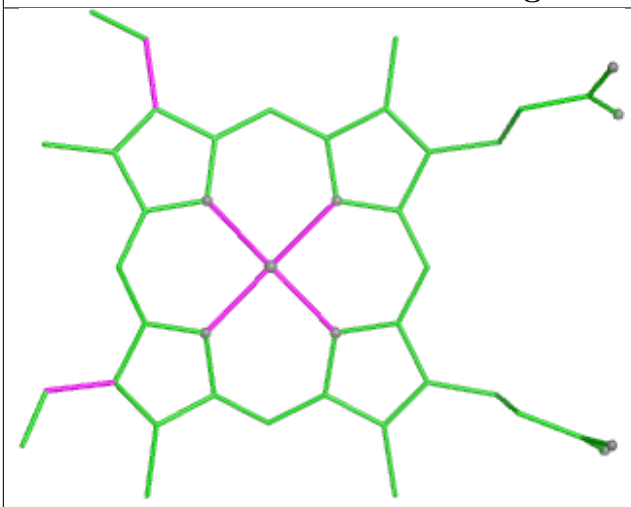


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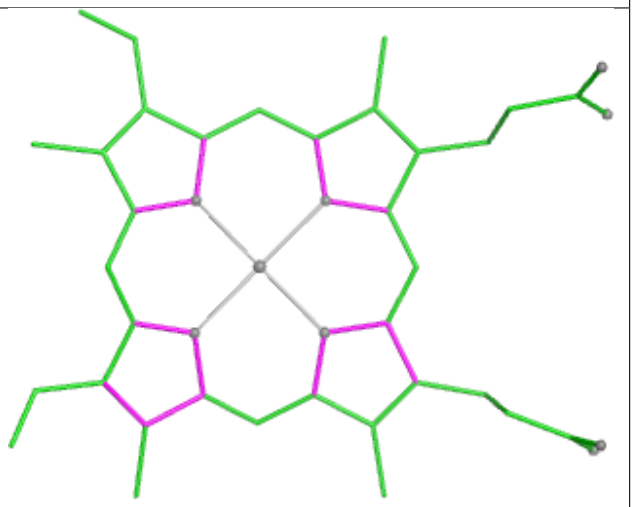


Rings

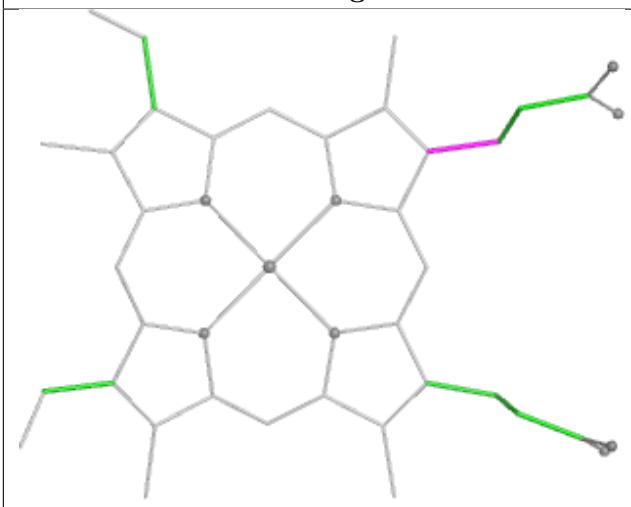
Ligand HEM c 504



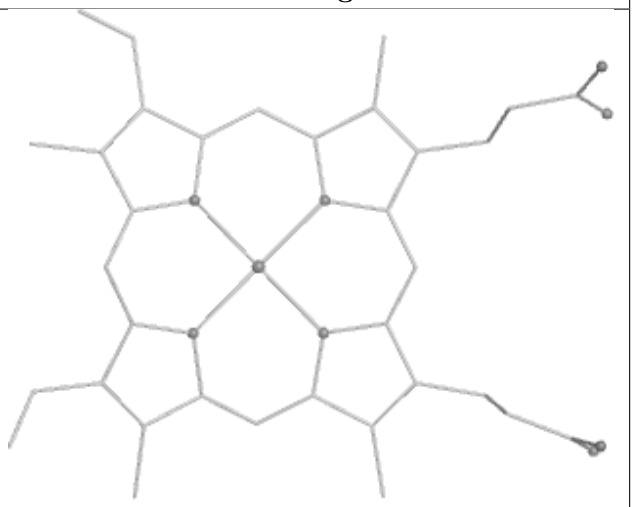
Bond lengths



Bond angles

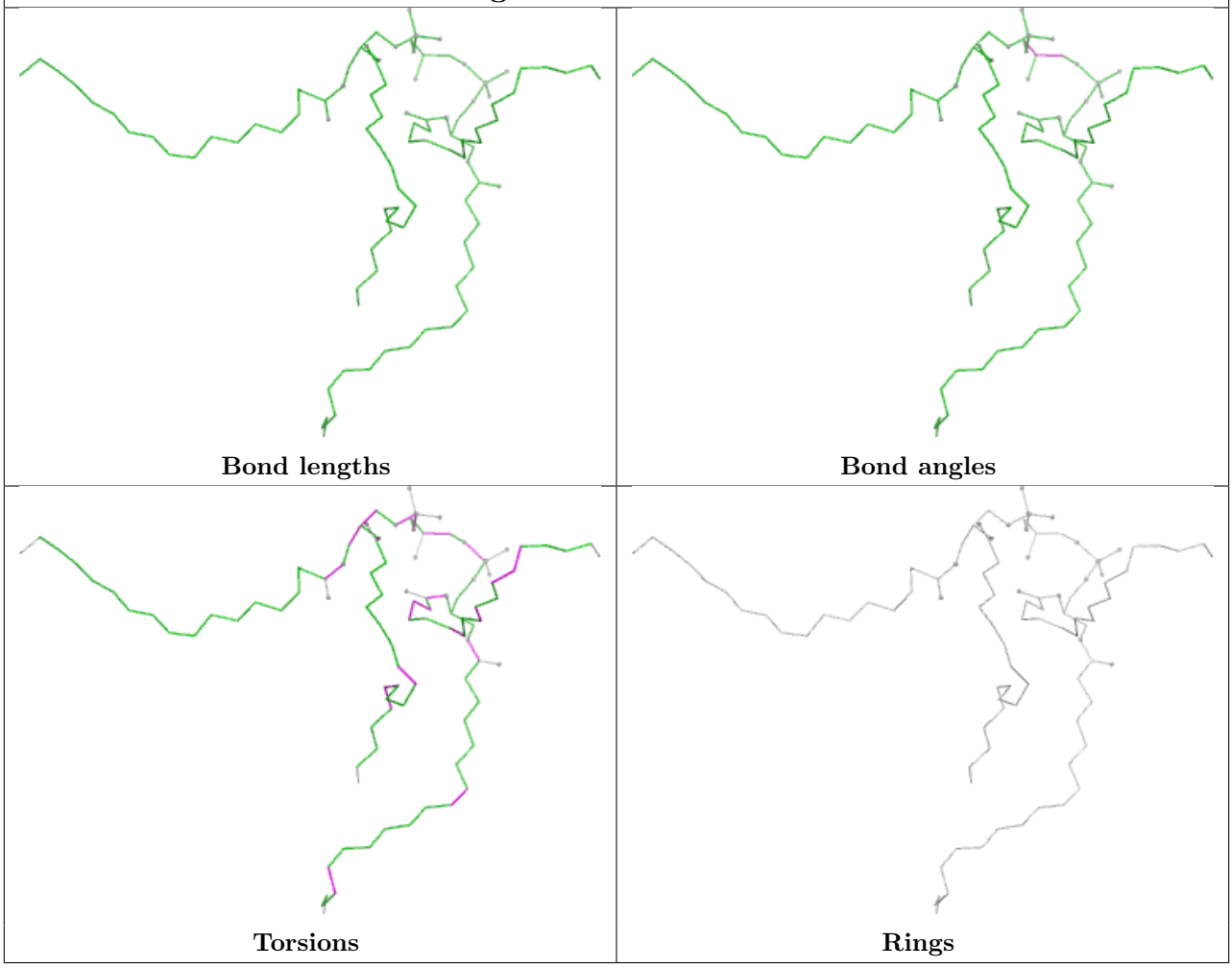


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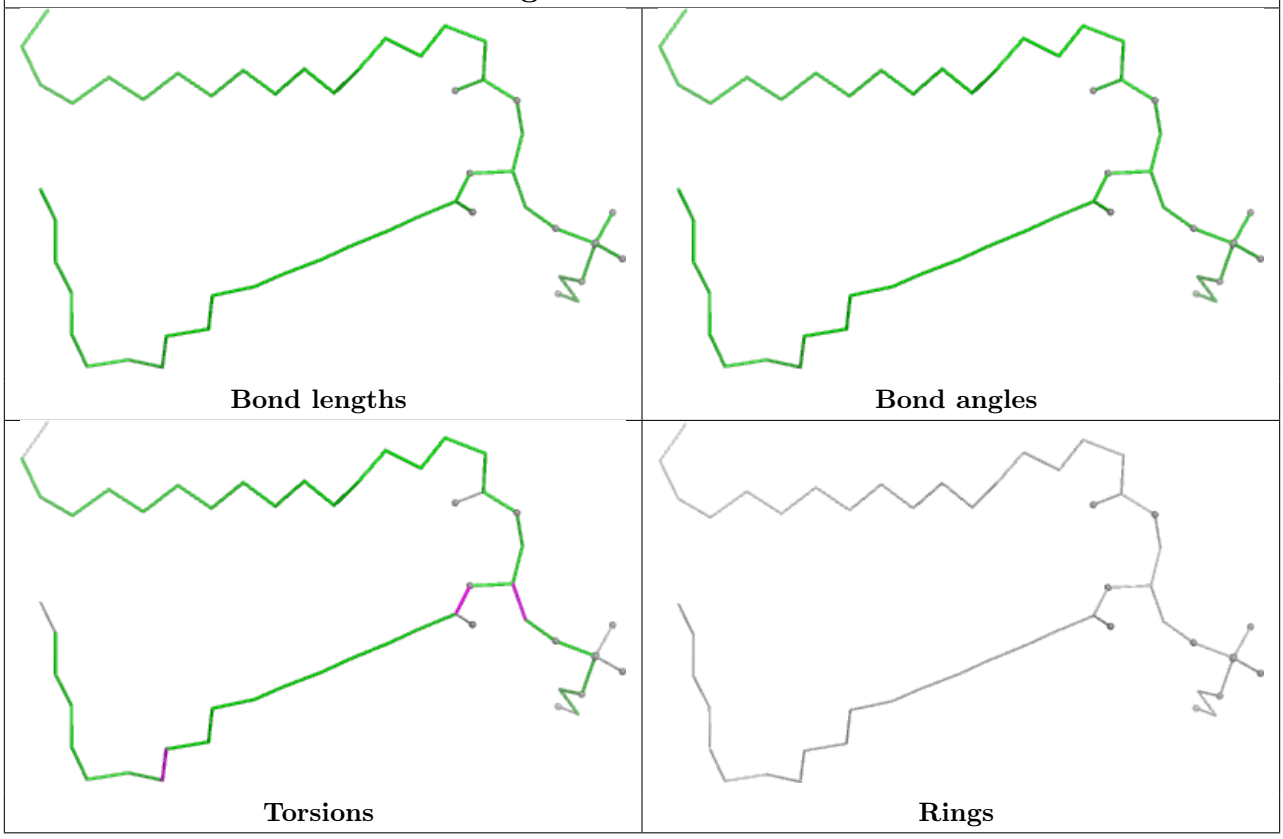


Rings

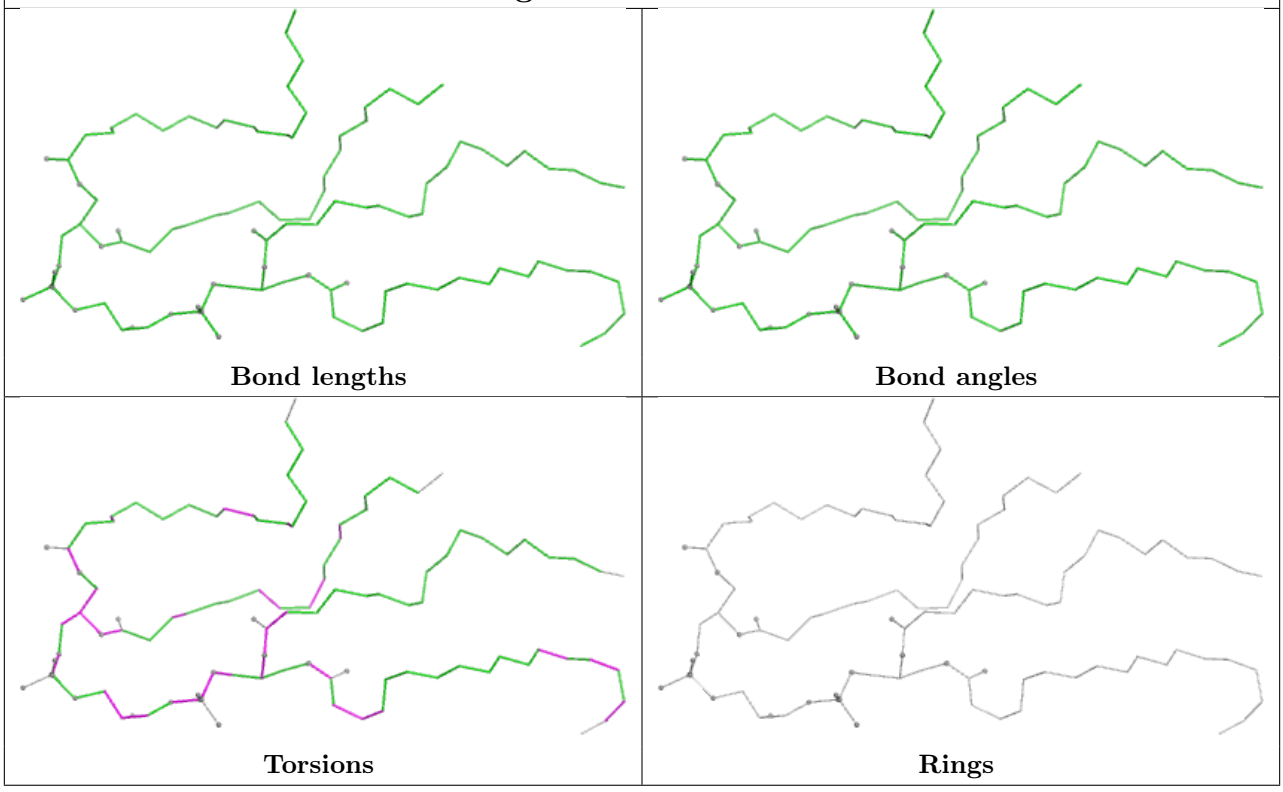
Ligand CDL DU 402



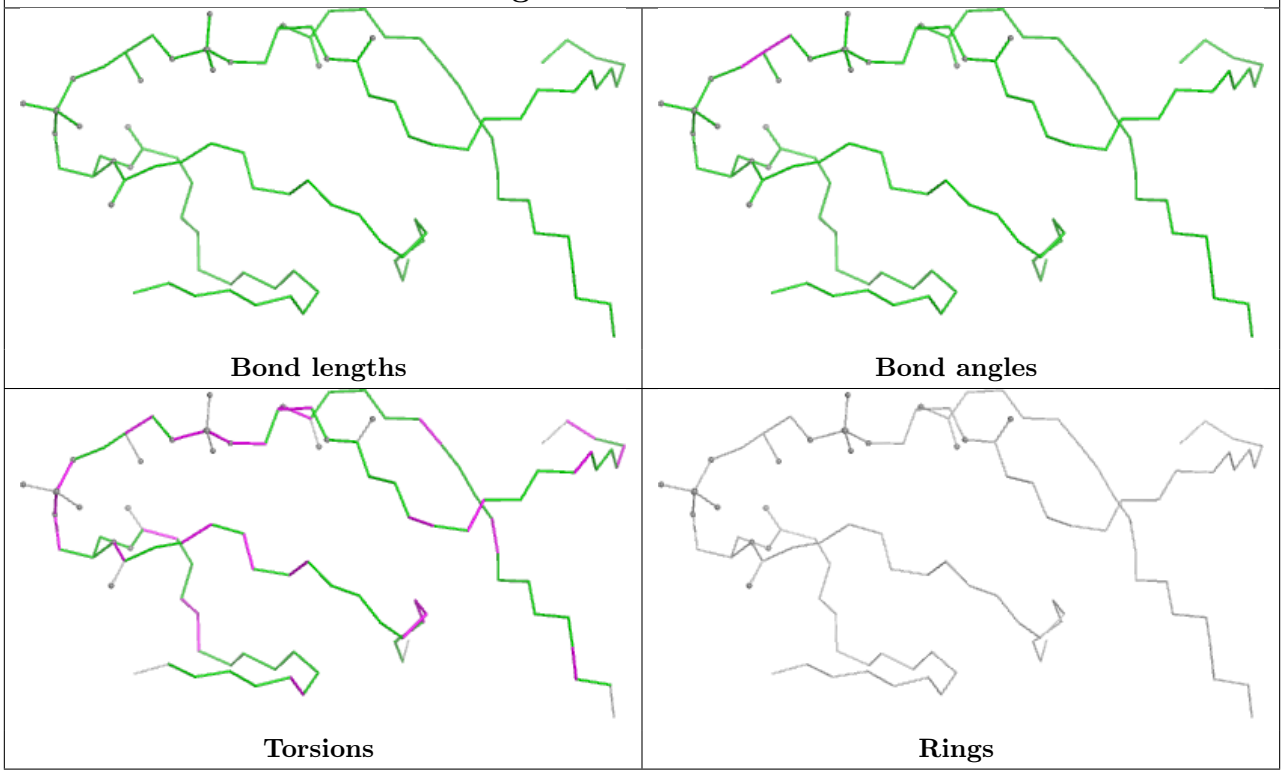
Ligand 3PE Dc 606



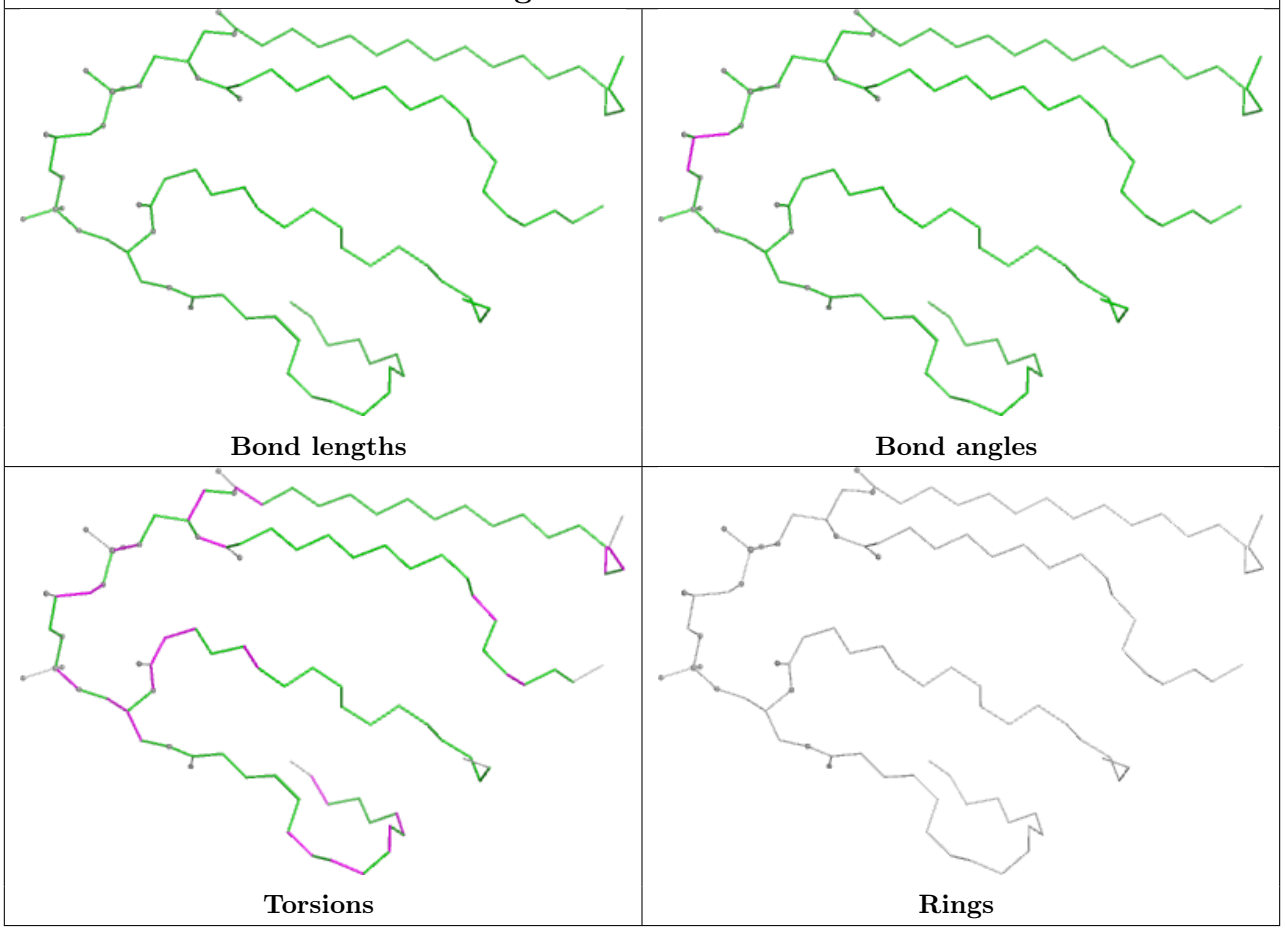
Ligand CDL A1 402



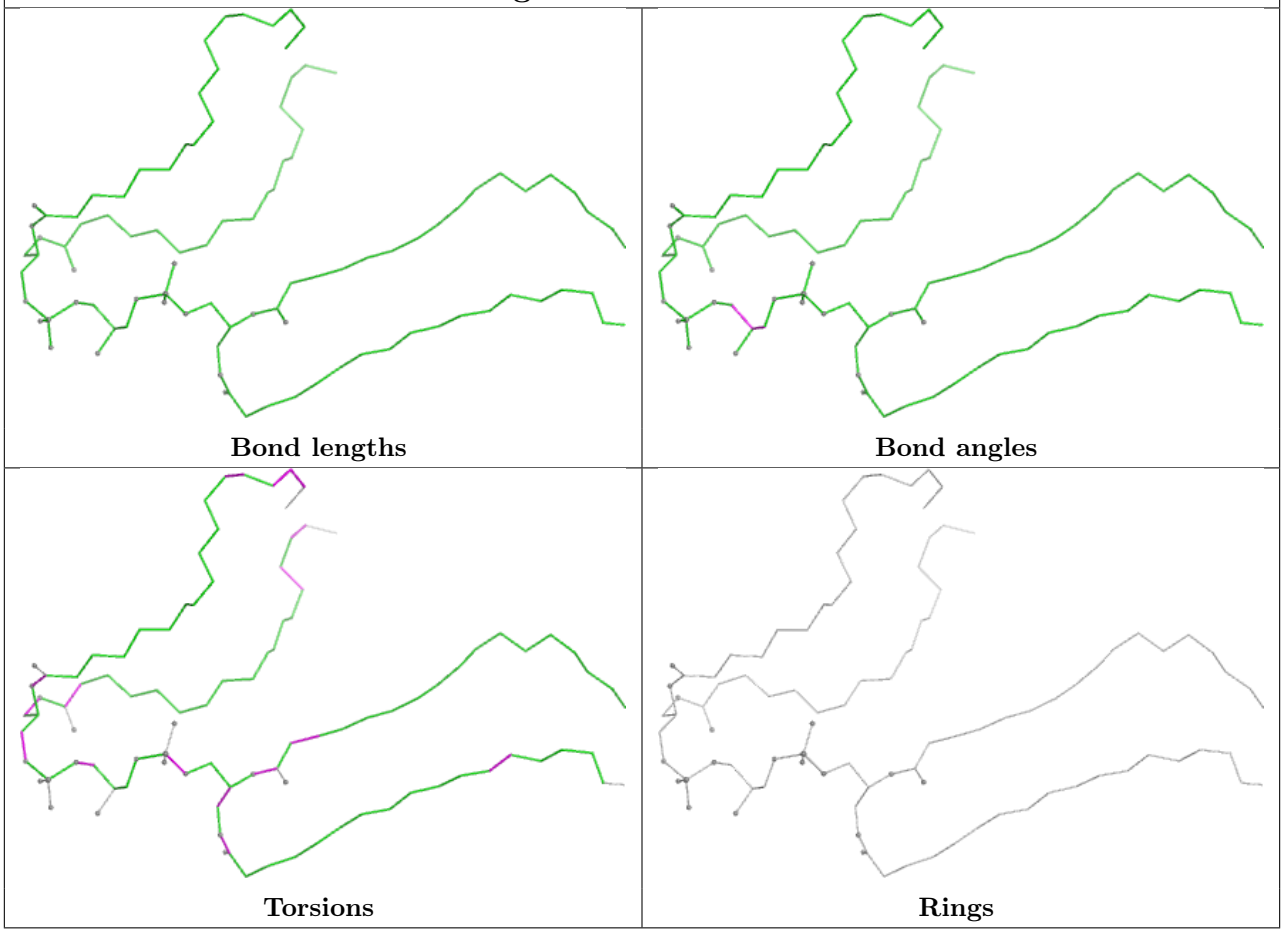
Ligand CDL AC 802



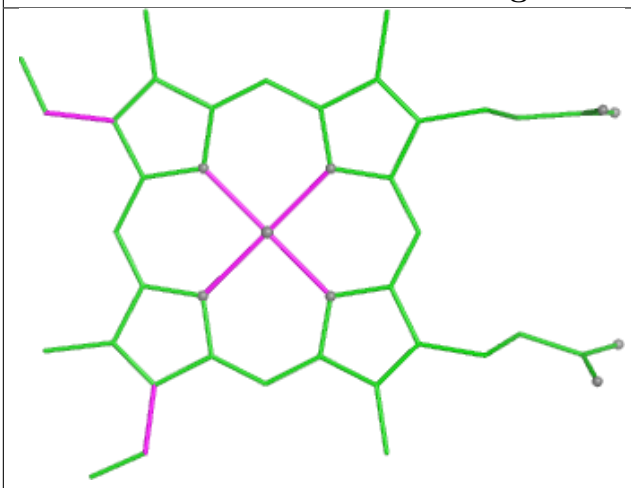
Ligand CDL Dd 705



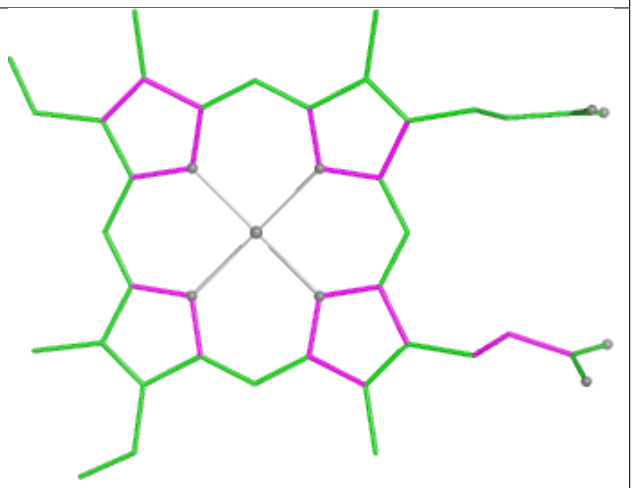
Ligand CDL AF 401



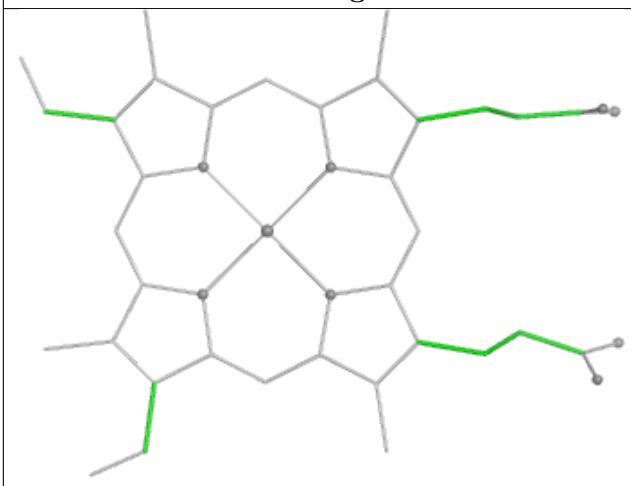
Ligand HEM Ed 201



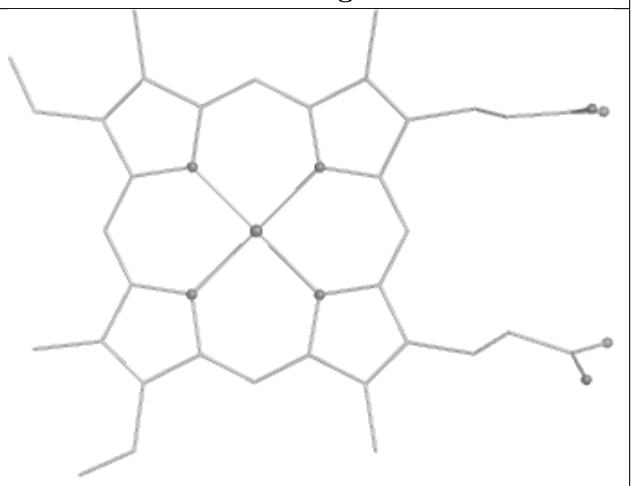
Bond lengths



Bond angles

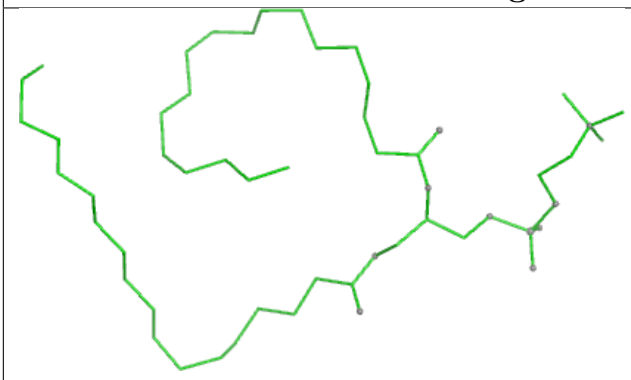


Torsions

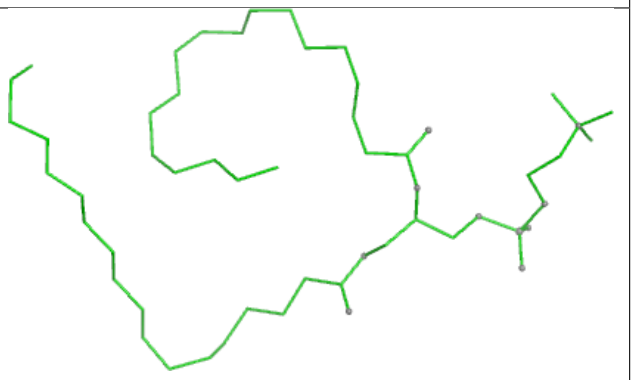


Rings

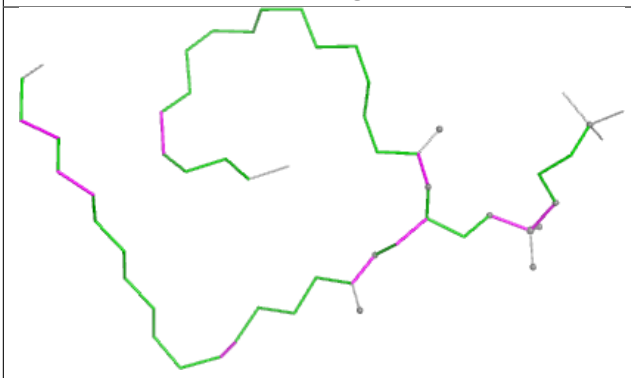
Ligand PC1 BS 1301



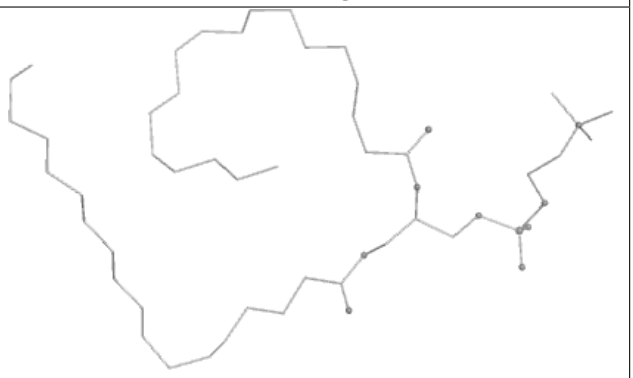
Bond lengths



Bond angles

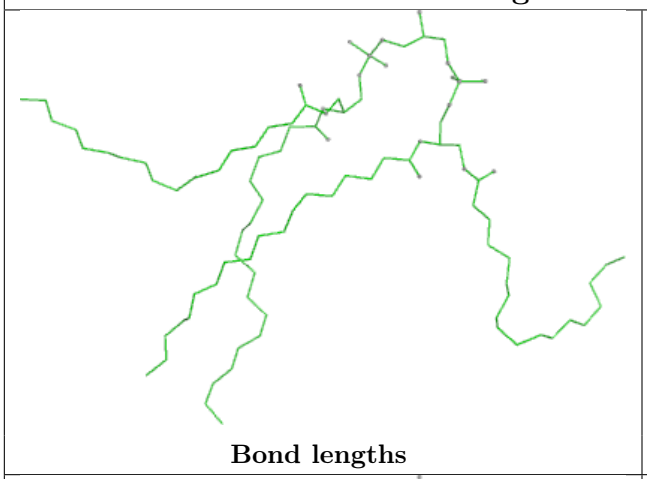


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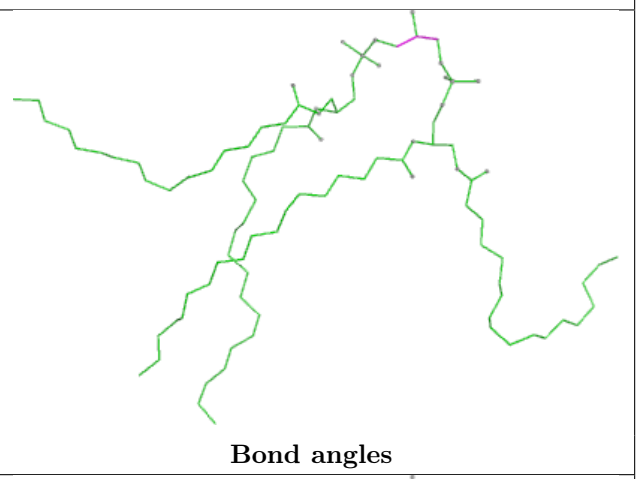


Rings

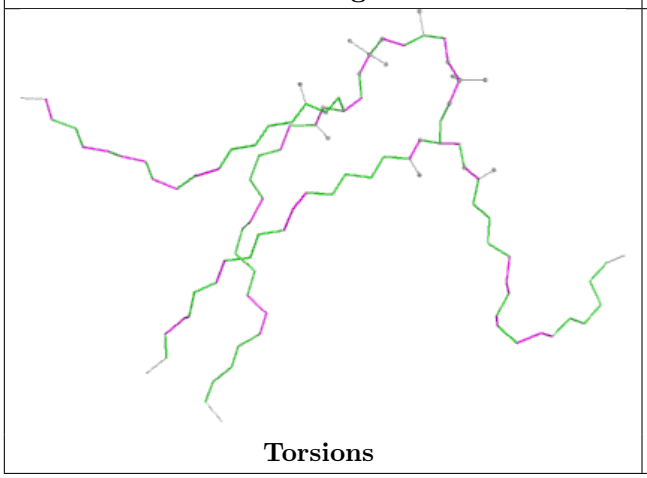
Ligand CDL AC 801



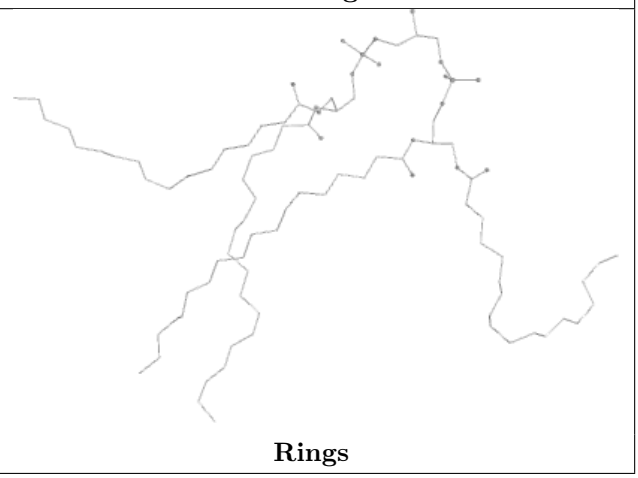
Bond lengths



Bond angles

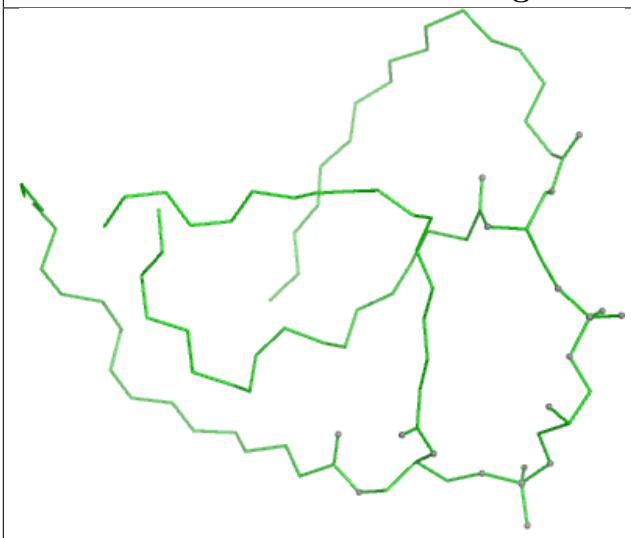


Torsions

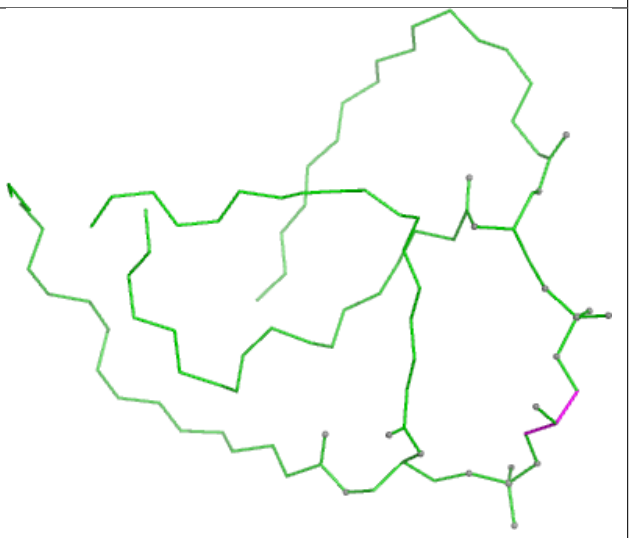


Rings

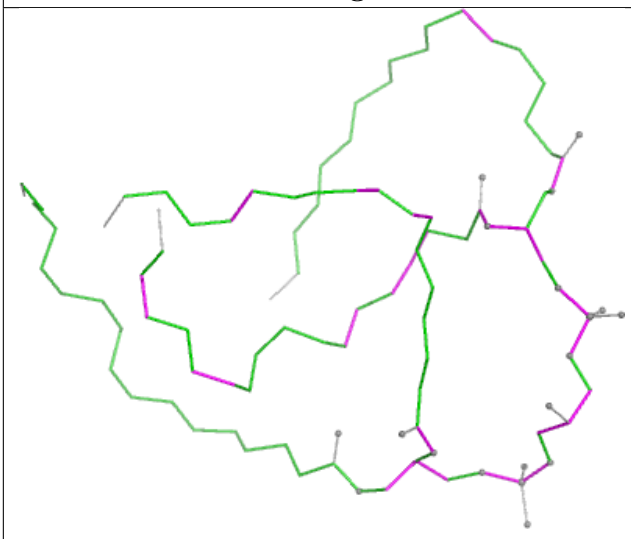
Ligand CDL EB 302



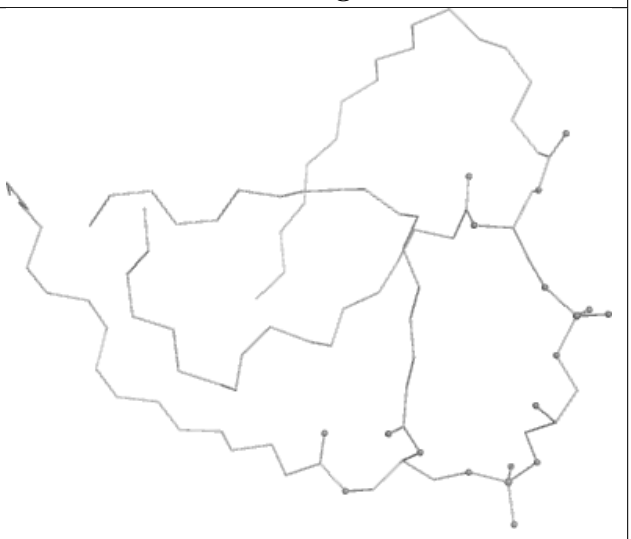
Bond lengths



Bond angles

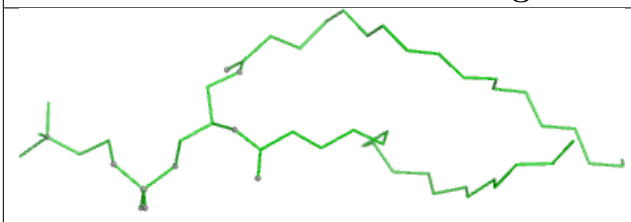


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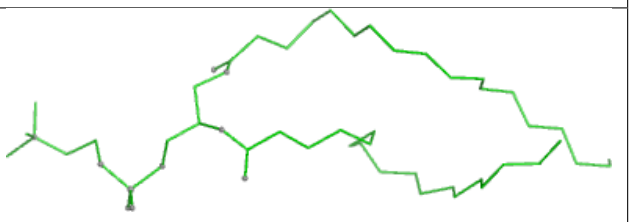


Rings

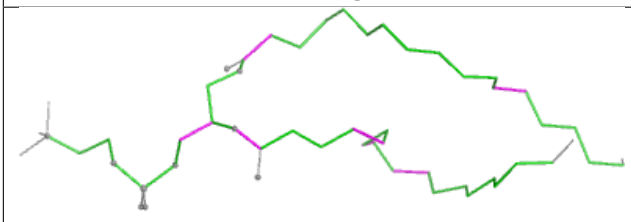
Ligand PC1 DG 203



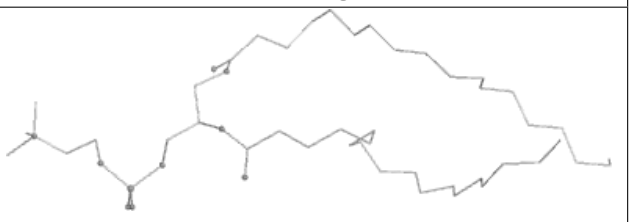
Bond lengths



Bond angles



Torsions

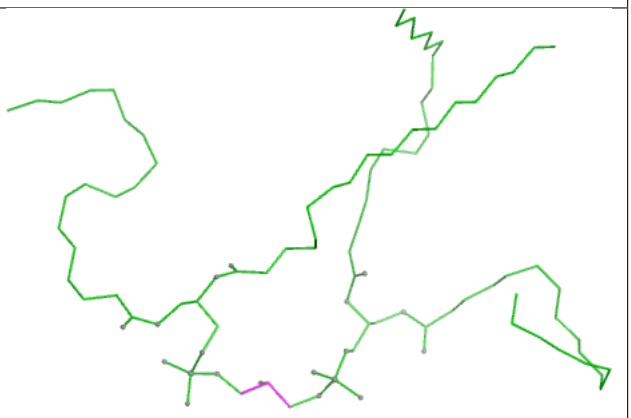


Rings

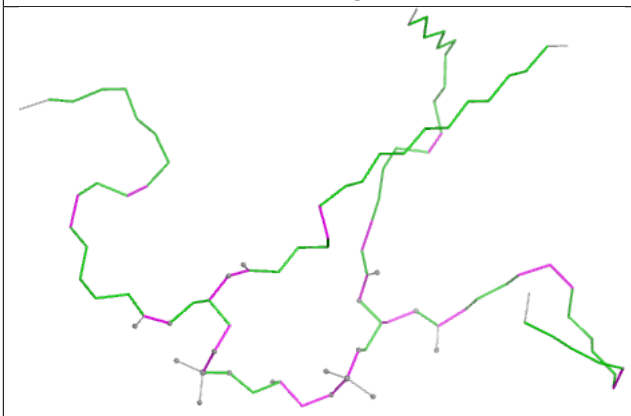
Ligand CDL EK 201



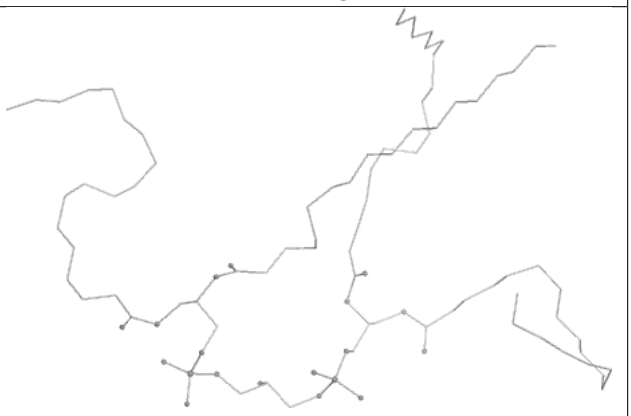
Bond lengths



Bond angles

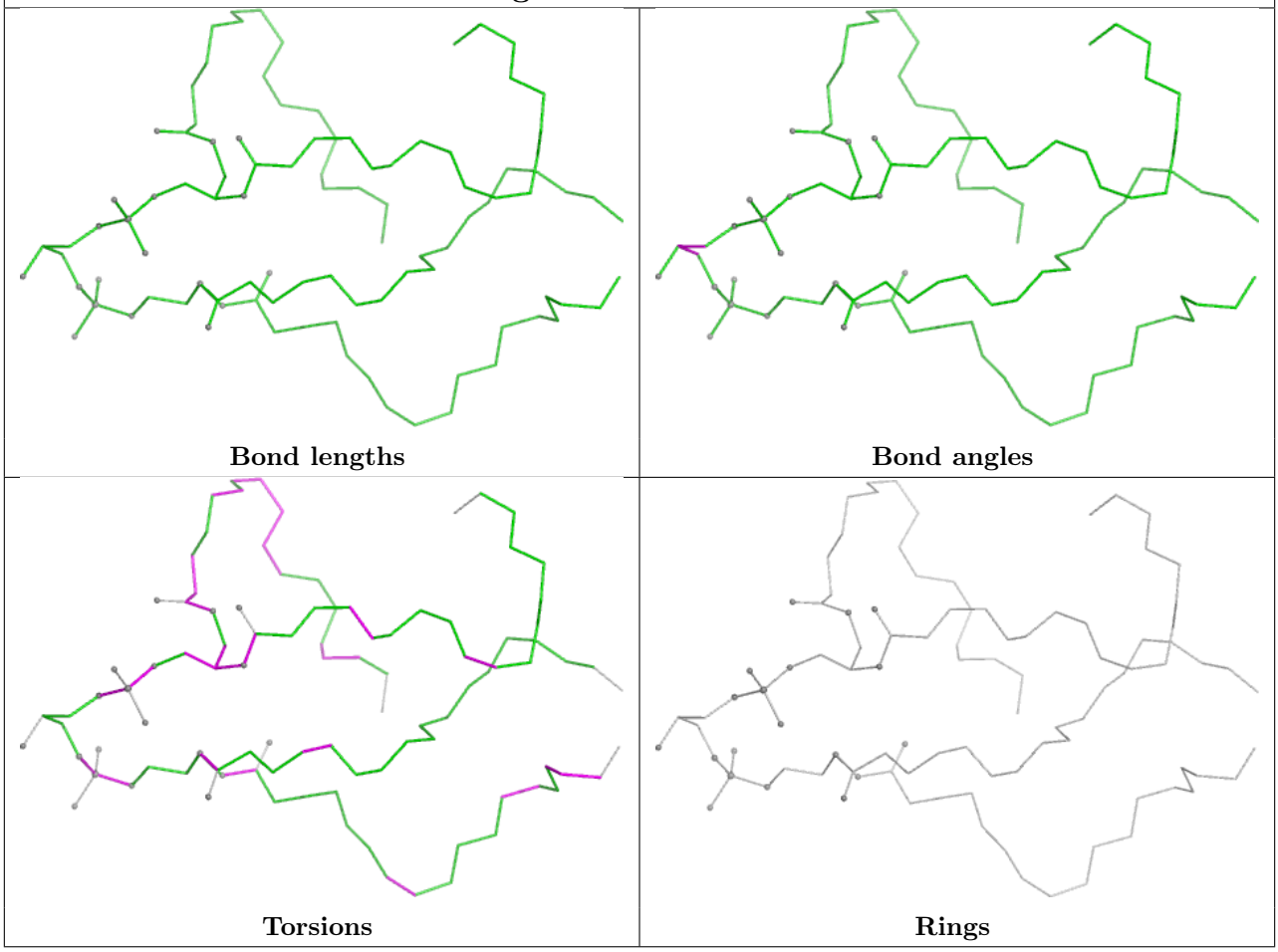


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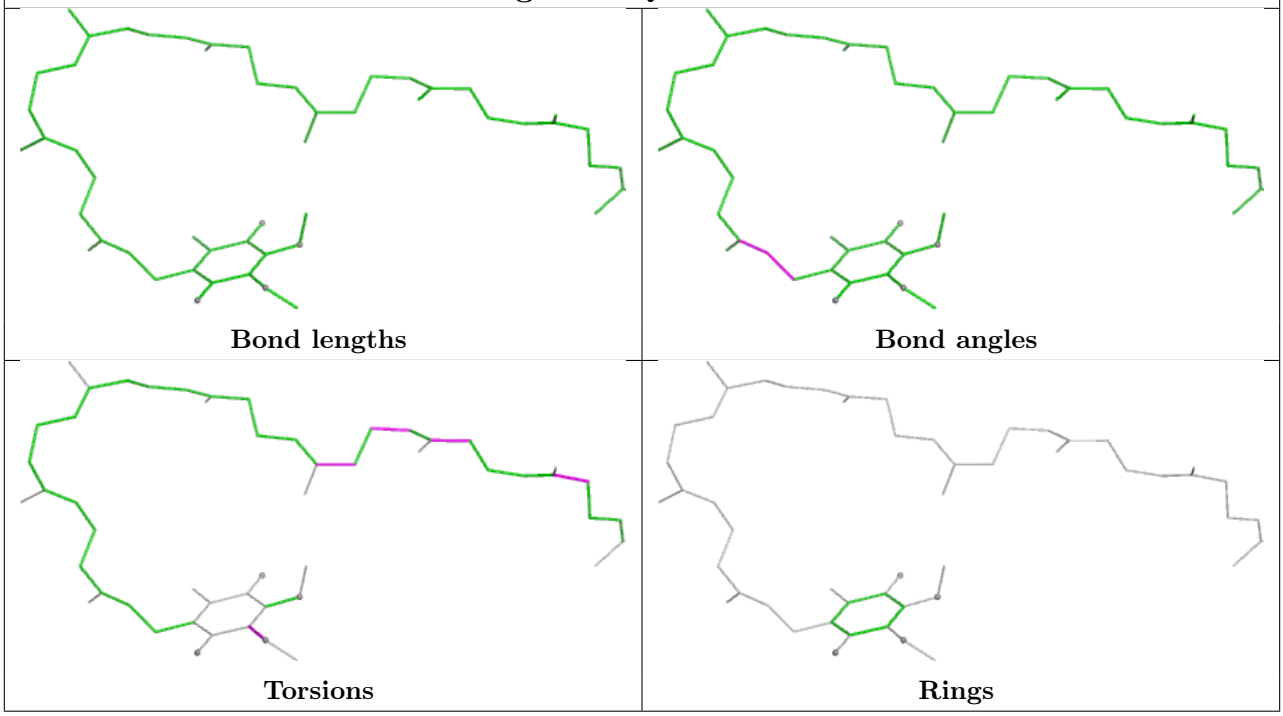


Rings

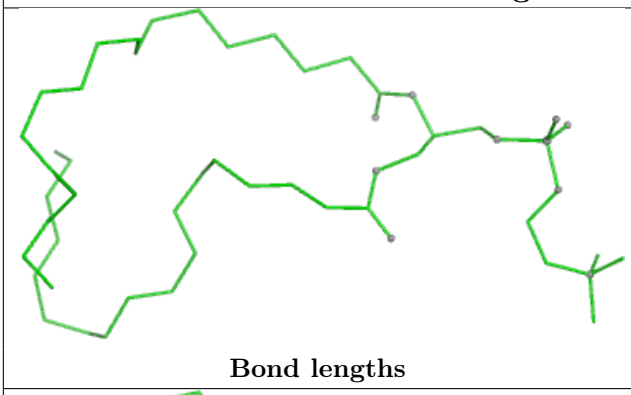
Ligand CDL Dn 501



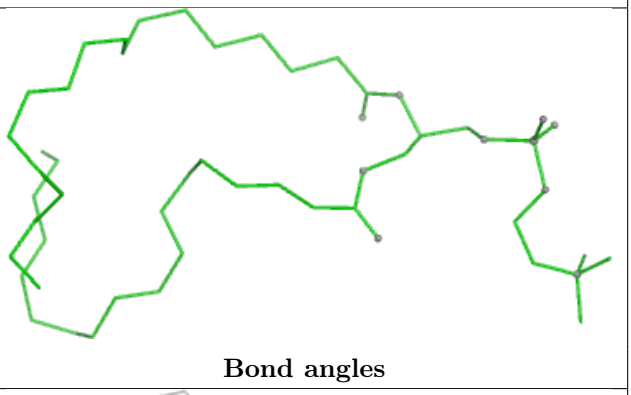
Ligand UQ8 DS 403



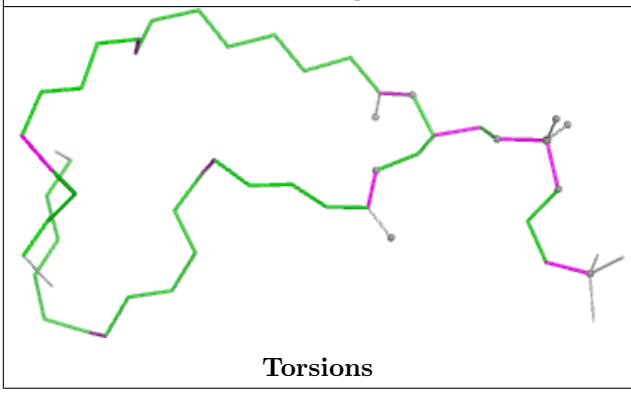
Ligand PC1 Di 1104



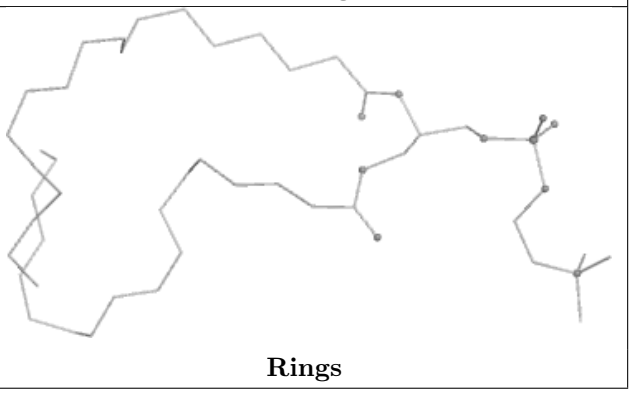
Bond lengths



Bond angles

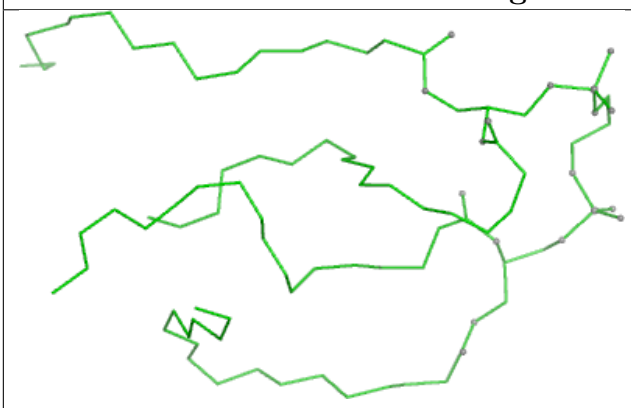


Torsions

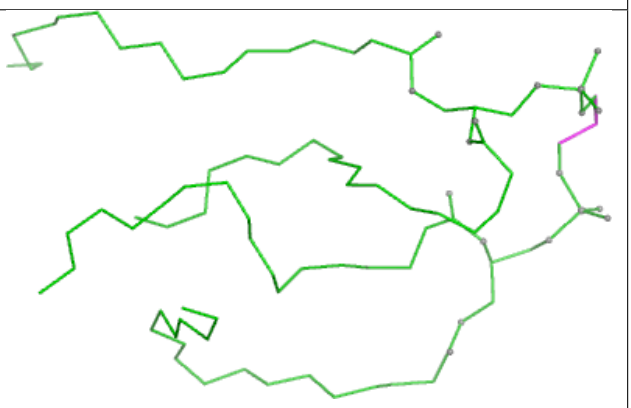


Rings

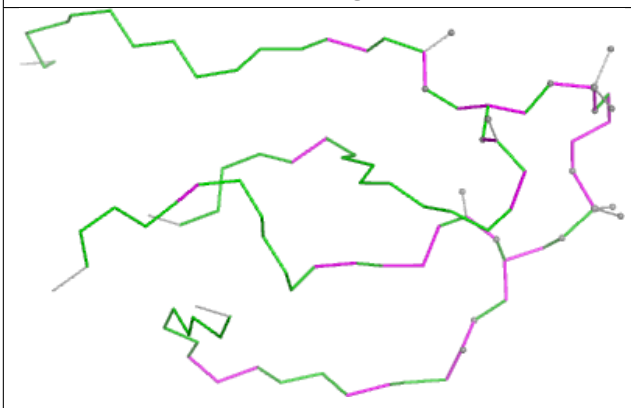
Ligand CDL DU 401



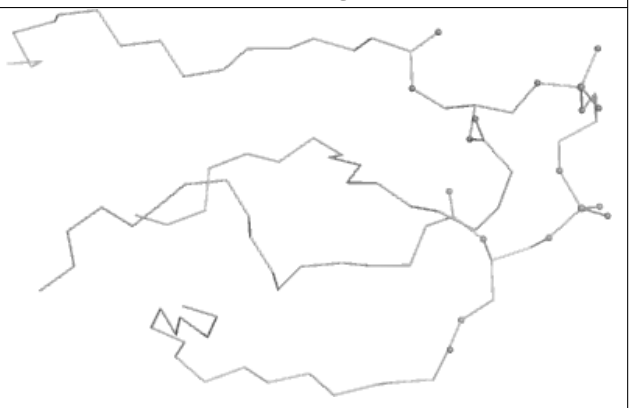
Bond lengths



Bond angles

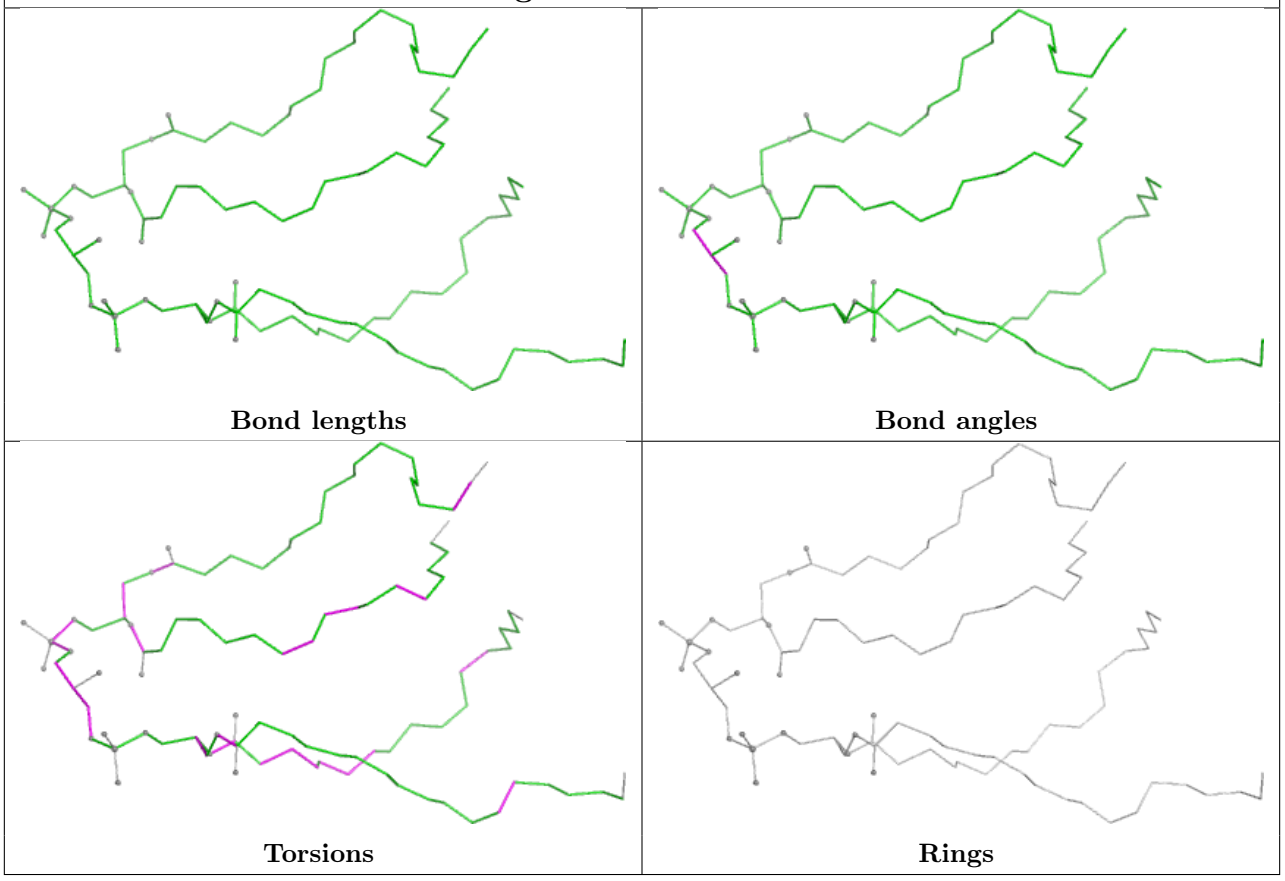


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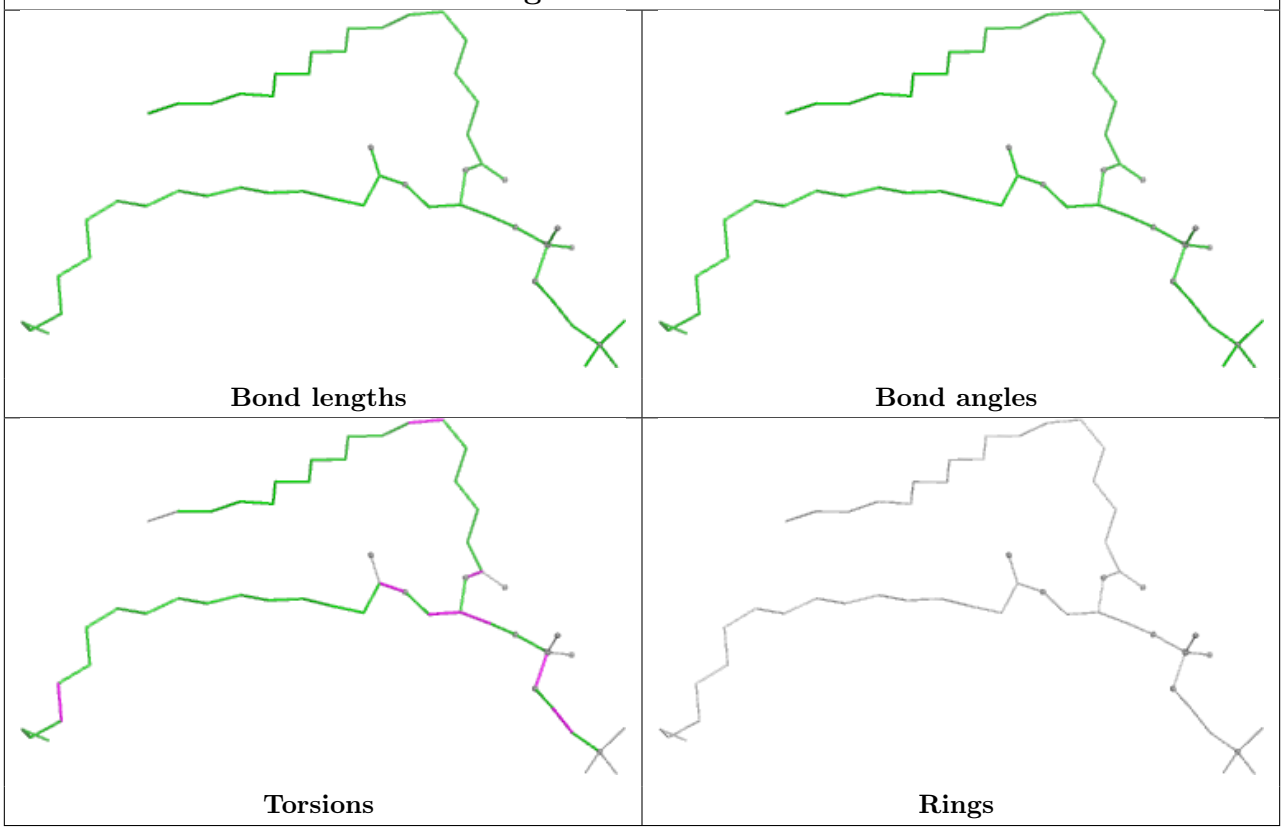


Rings

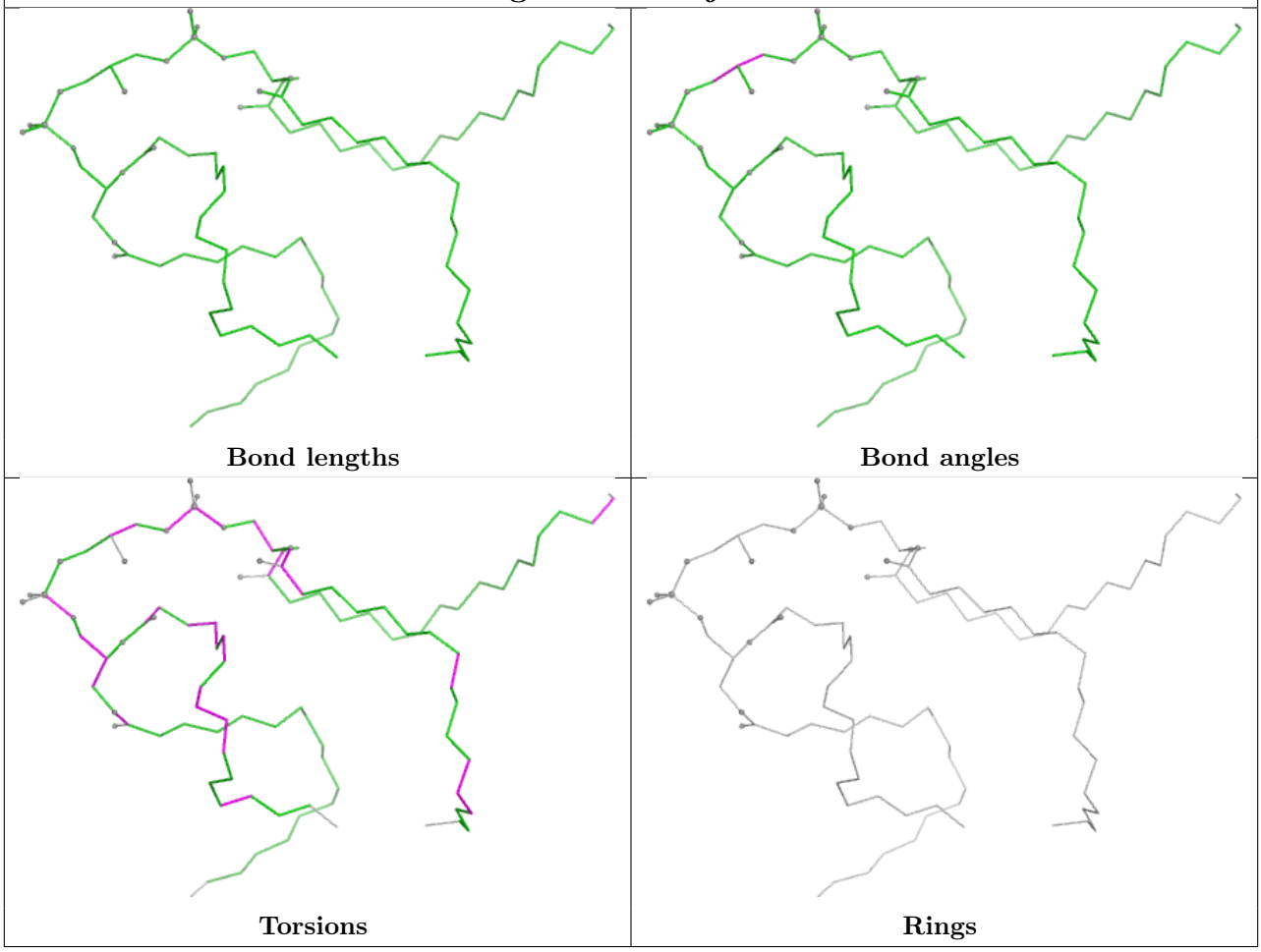
Ligand CDL DJ 303



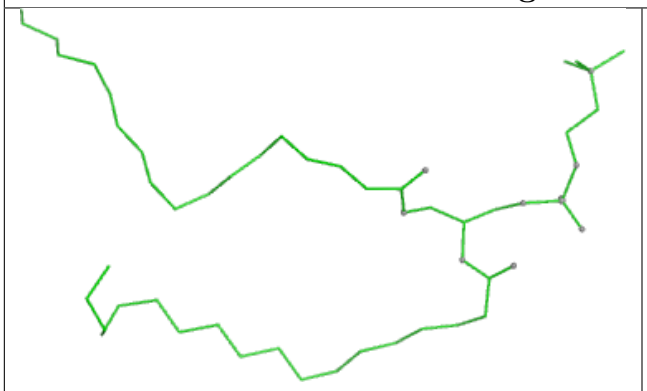
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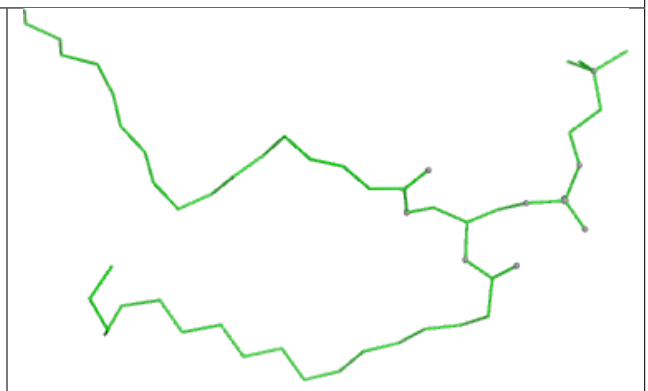
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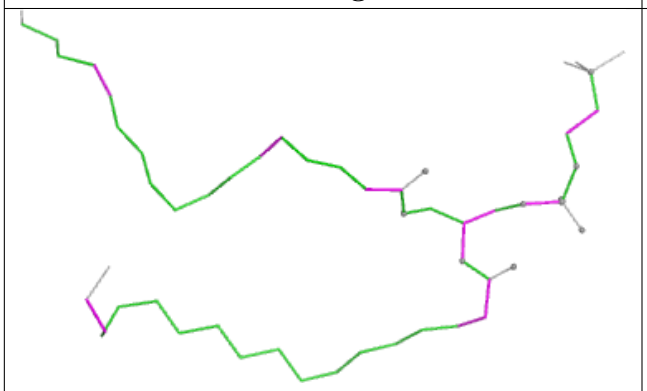
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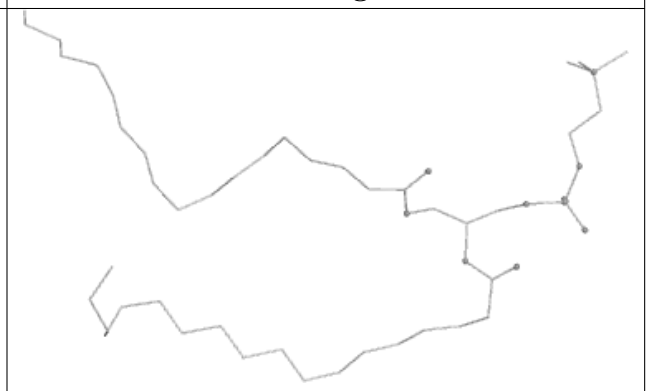
Bond lengths



Bond angles

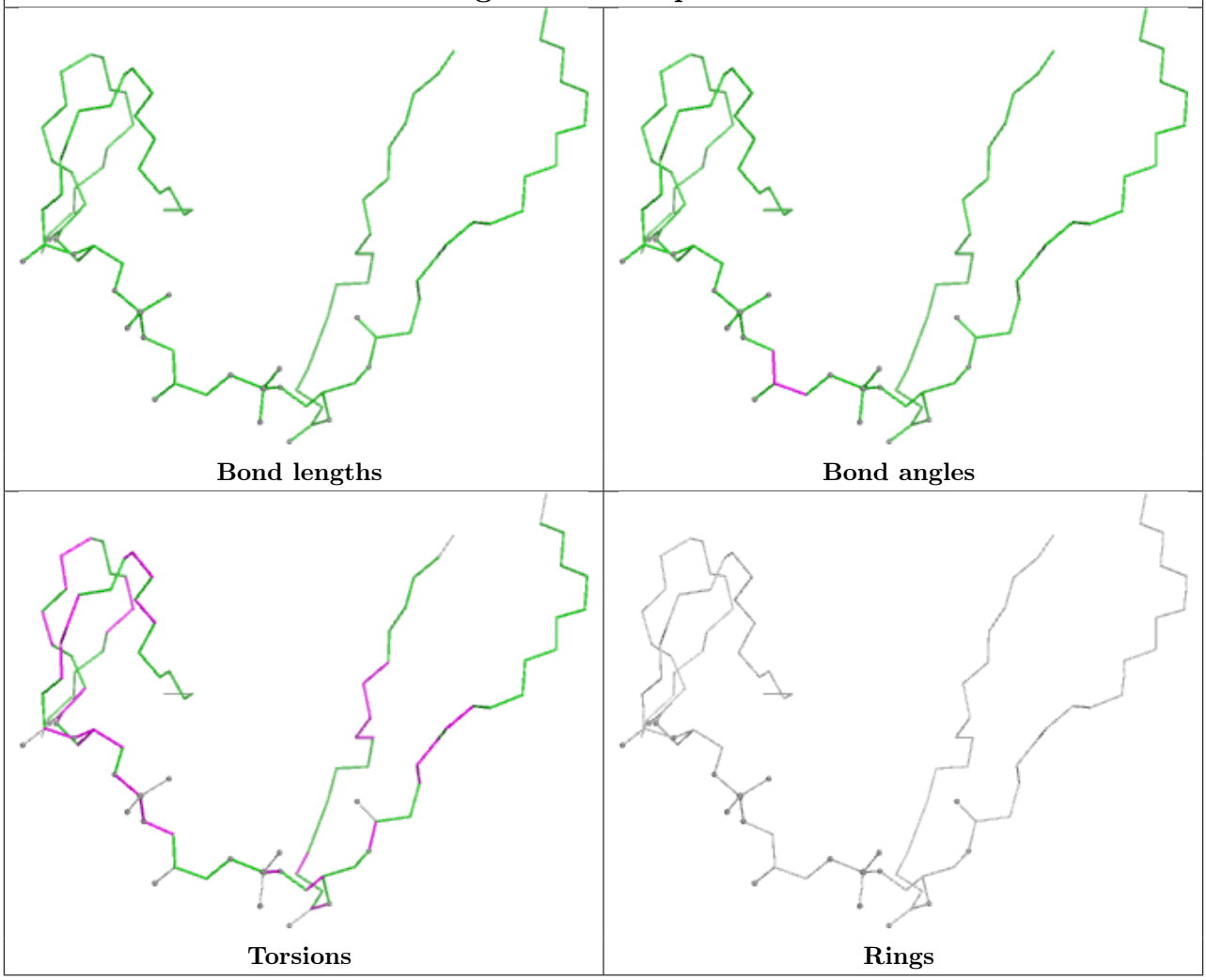


Torsions



Rings

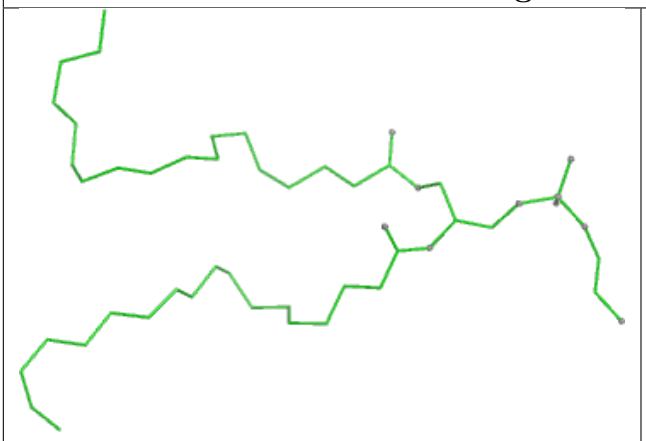
Ligand CDL Dq 1401



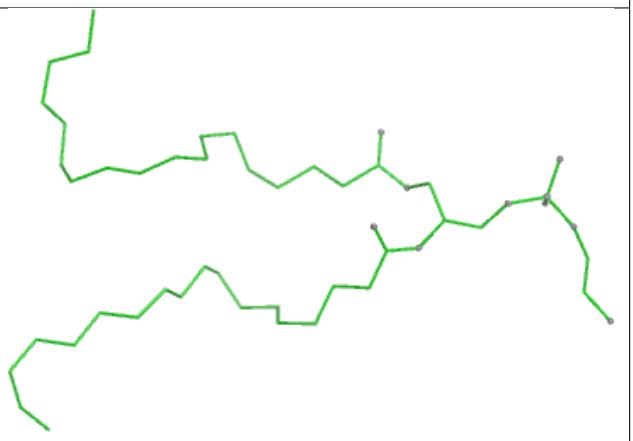
Bond lengths | **Bond angles**

Torsions | **Rings**

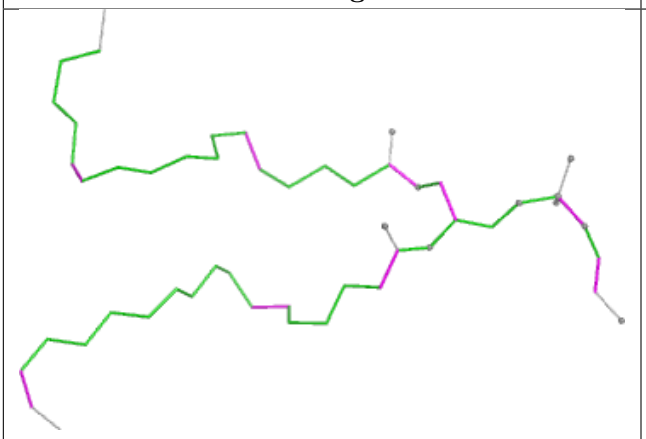
Ligand 3PE DC 607



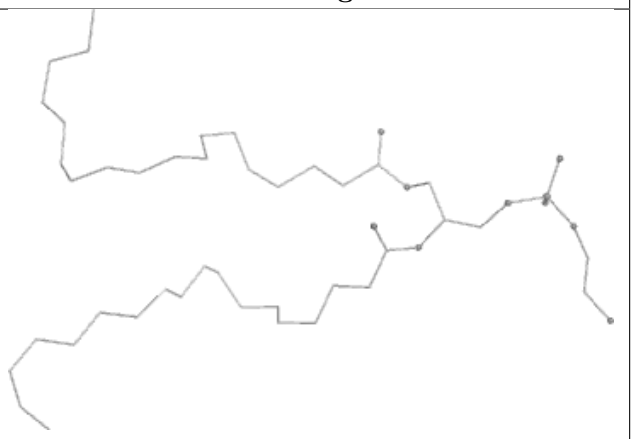
Bond lengths



Bond angles

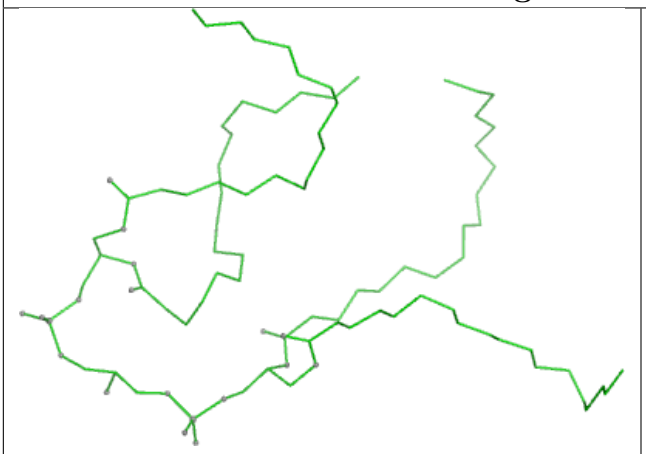


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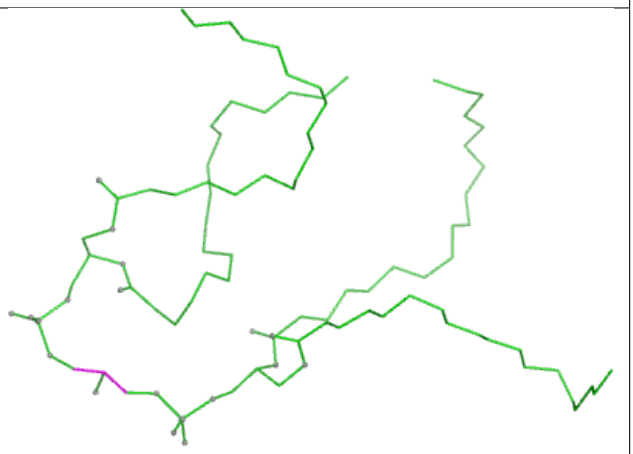


Rings

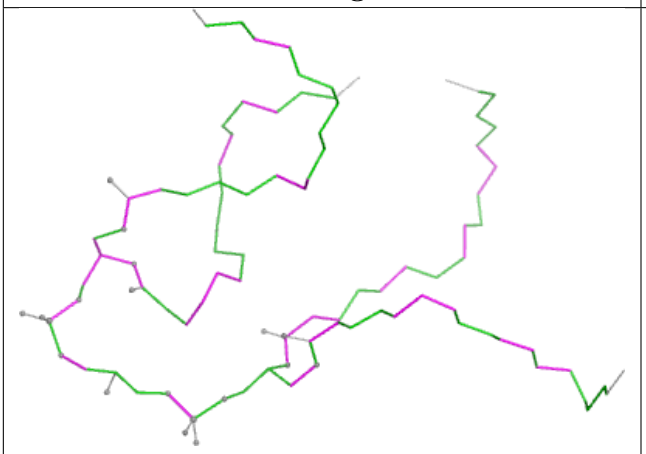
Ligand CDL DJ 304



Bond lengths



Bond angles

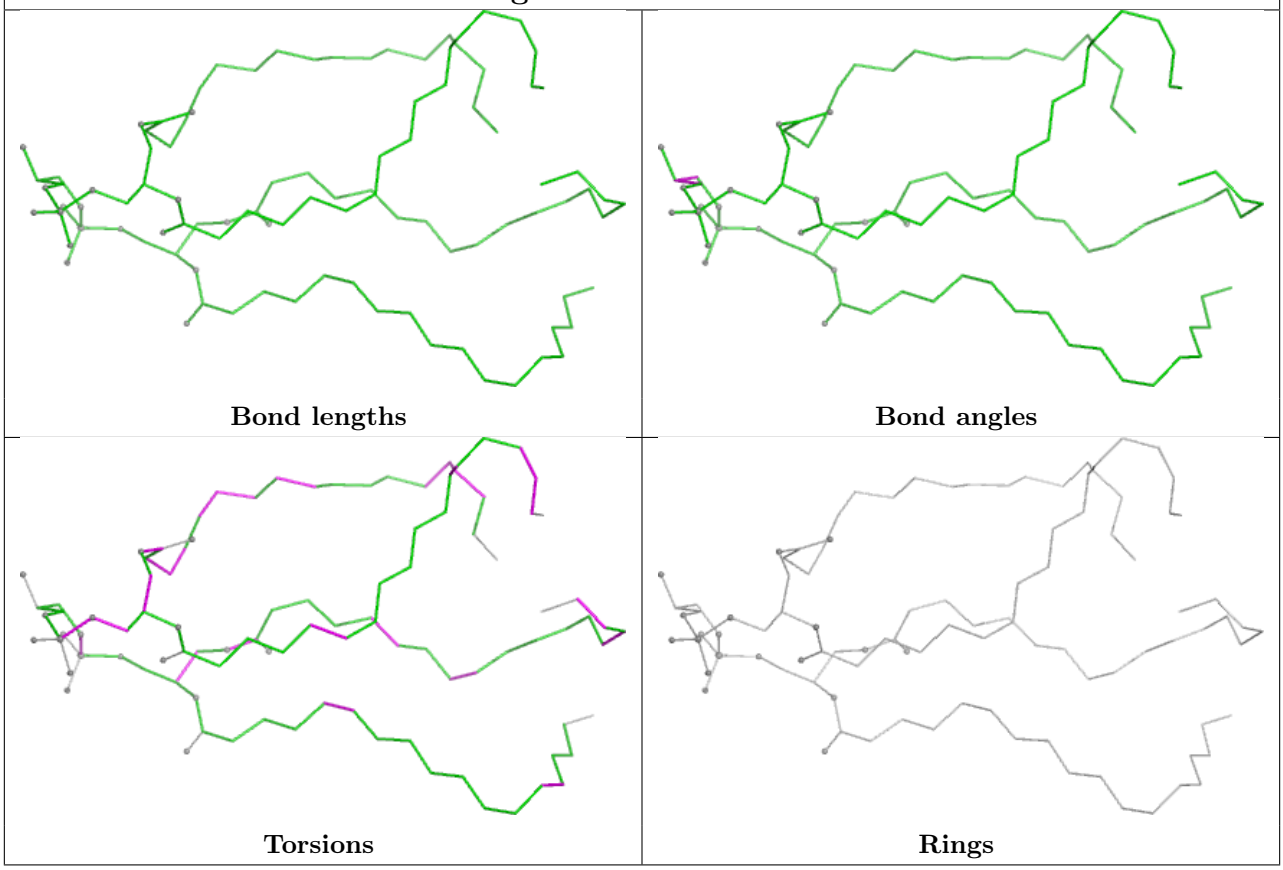


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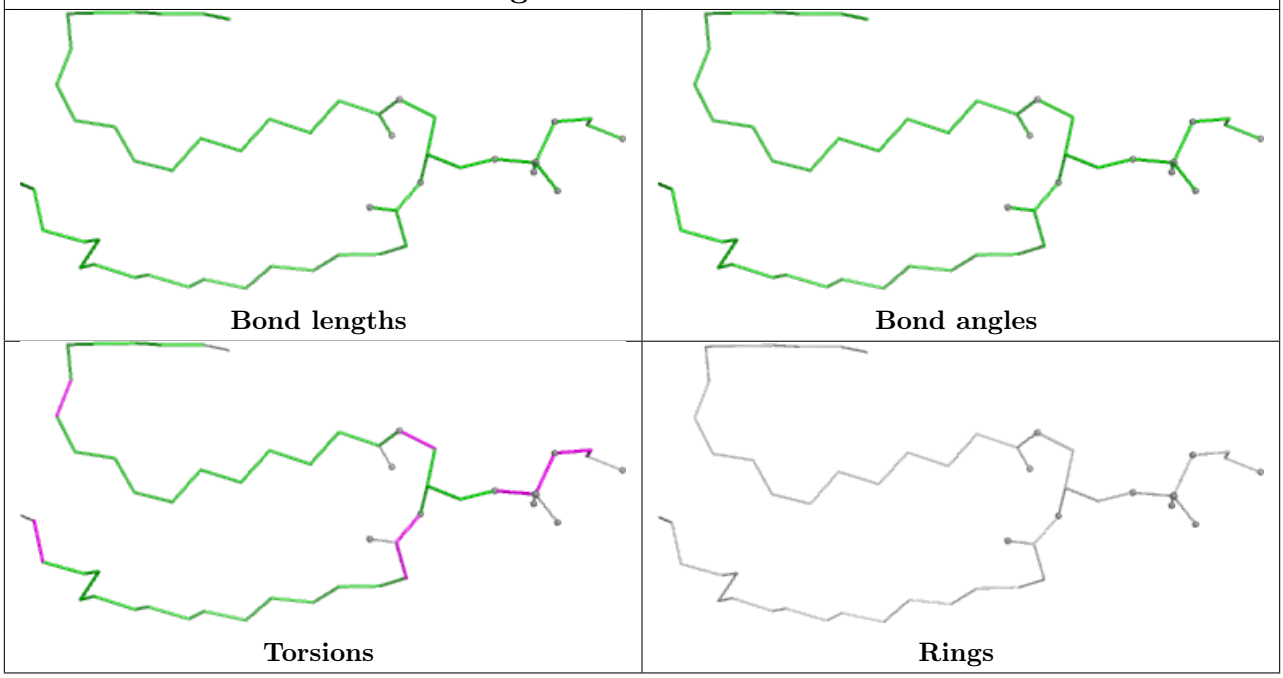


Rings

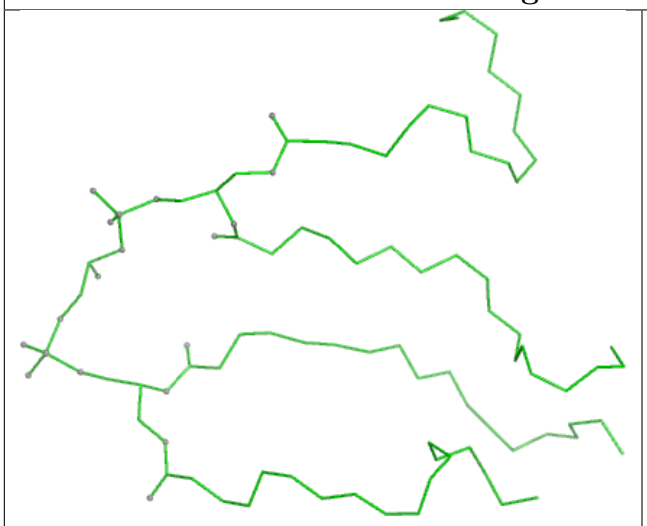
Ligand CDL DR 402



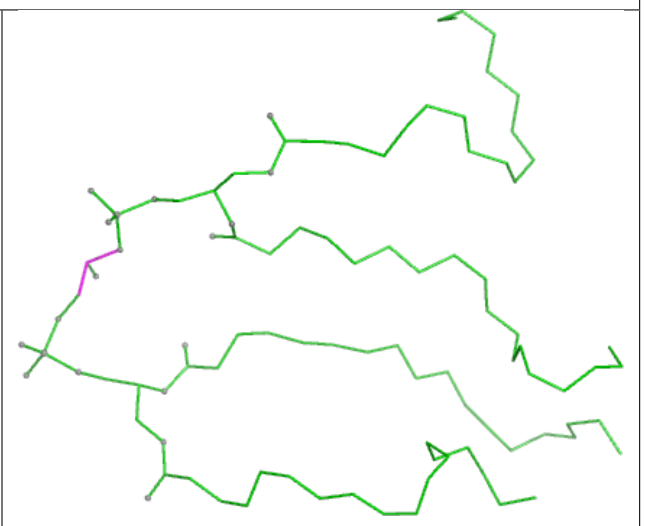
Ligand 3PE Dx 1206



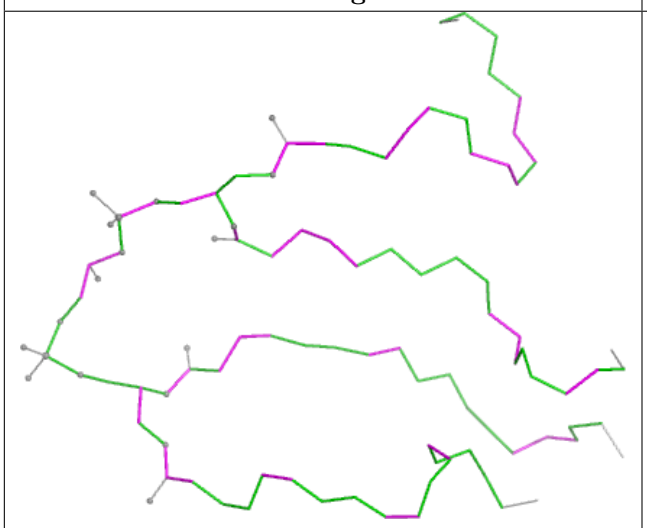
Ligand CDL El 901



Bond lengths



Bond angles

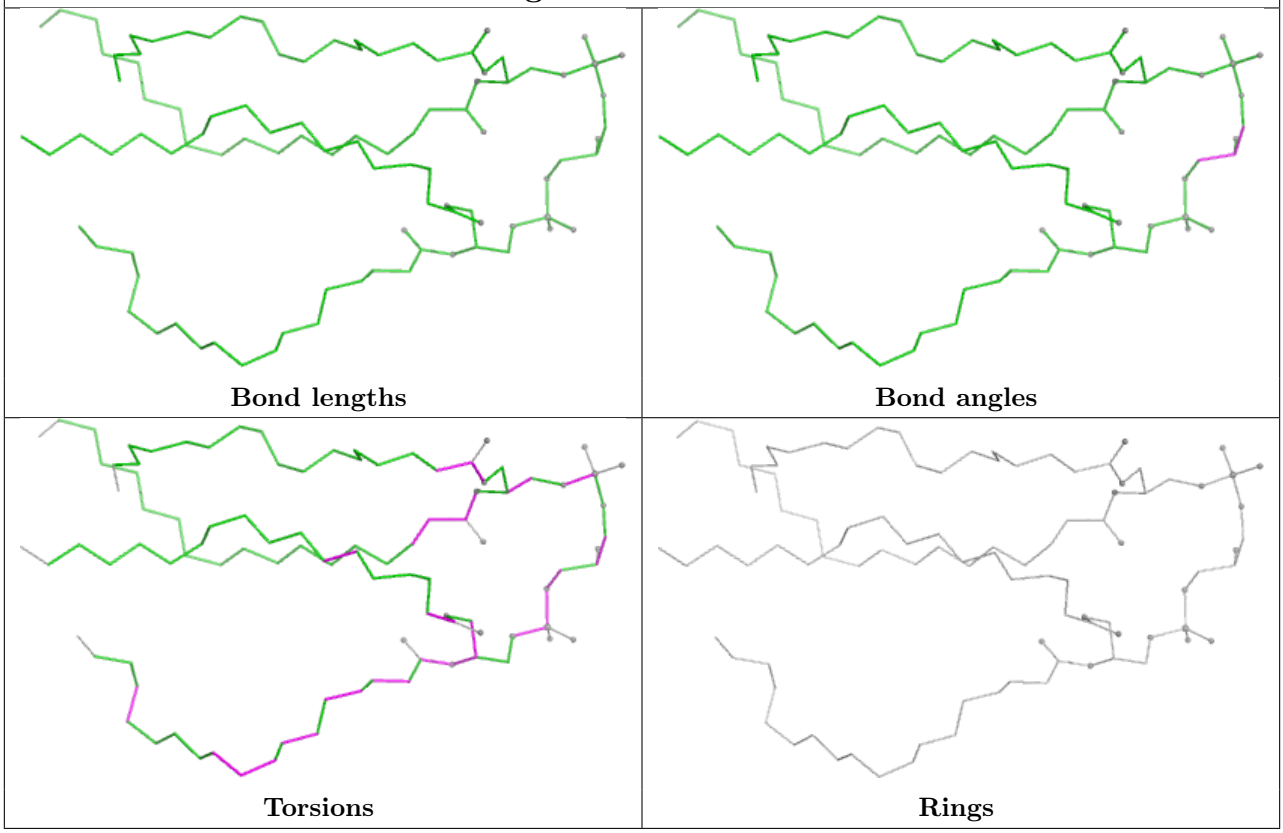


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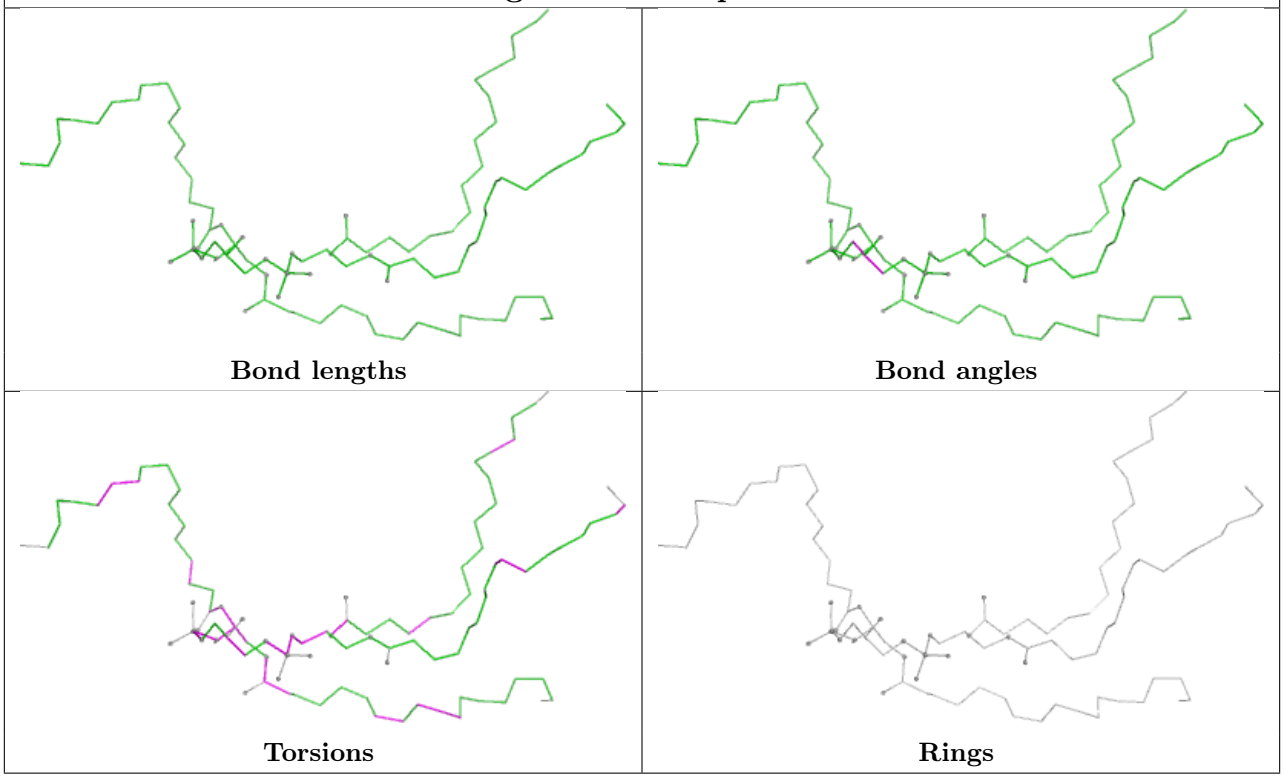


Rings

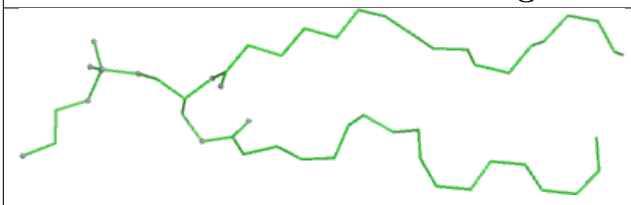
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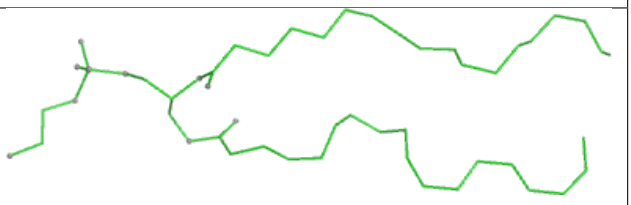
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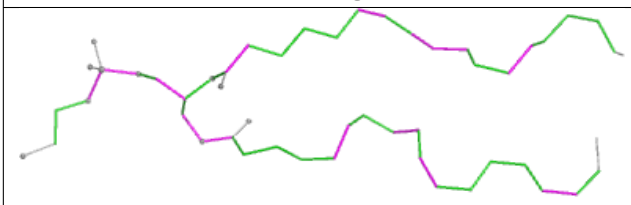
Ligand 3PE DS 402



Bond lengths



Bond angles

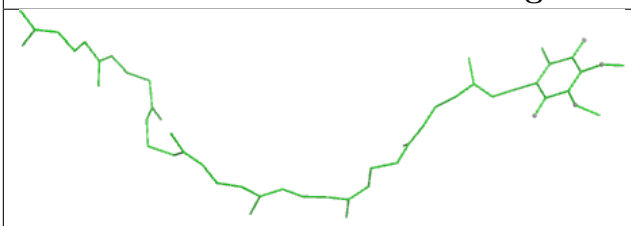


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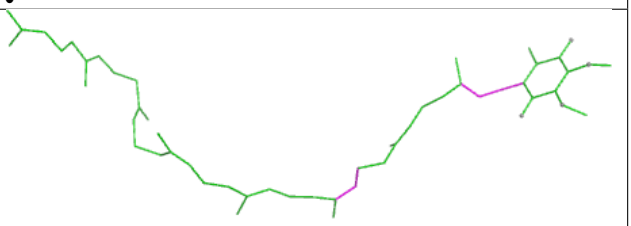


Rings

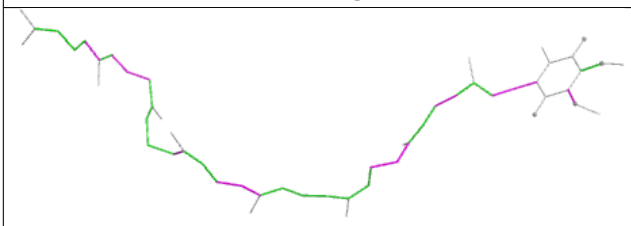
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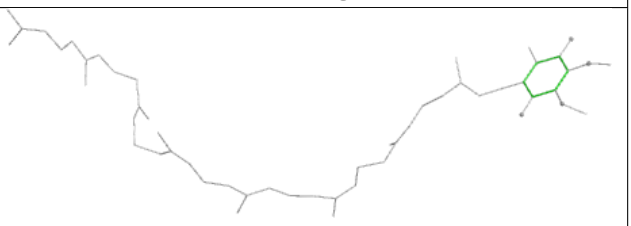
Bond lengths



Bond angles

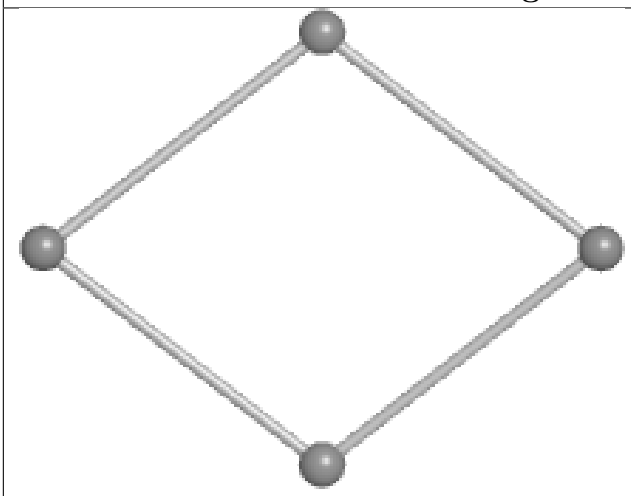


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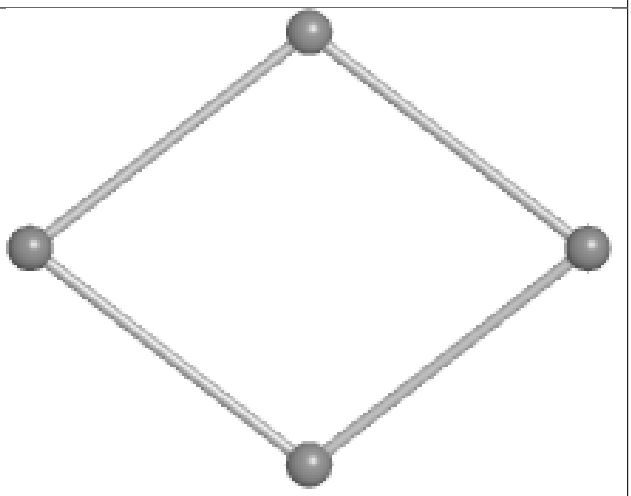


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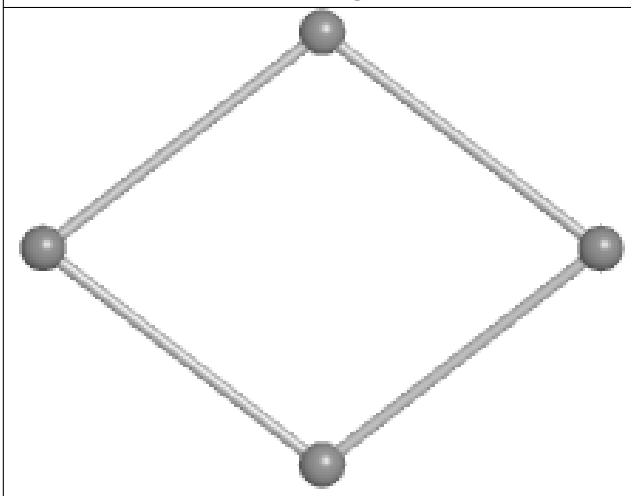
Ligand FES BI 201



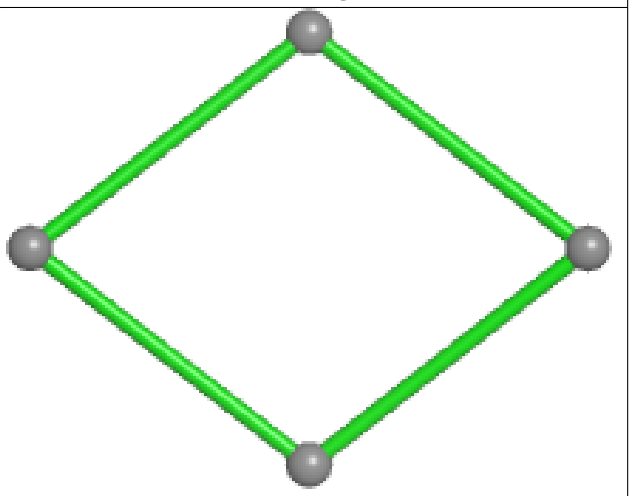
Bond lengths



Bond angles

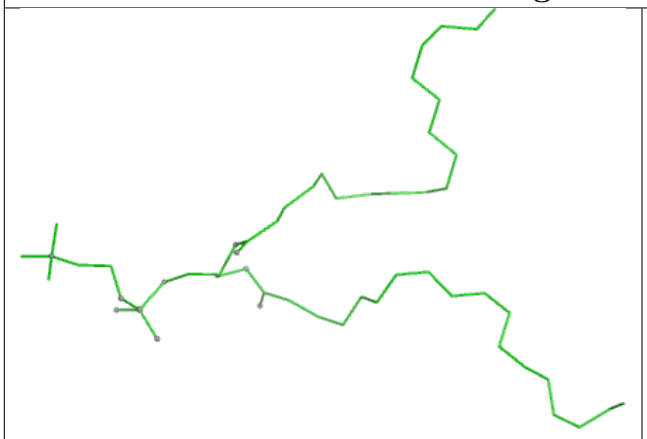


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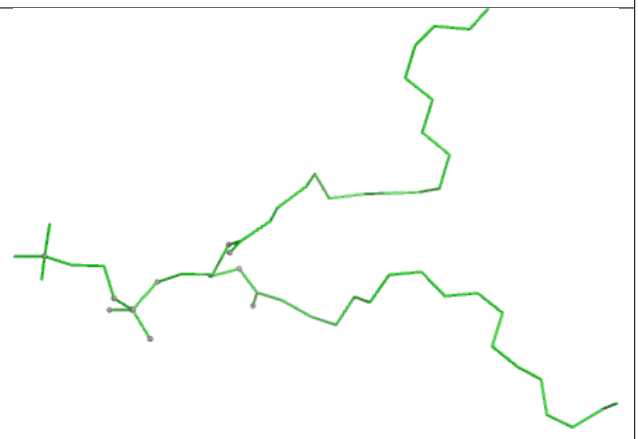


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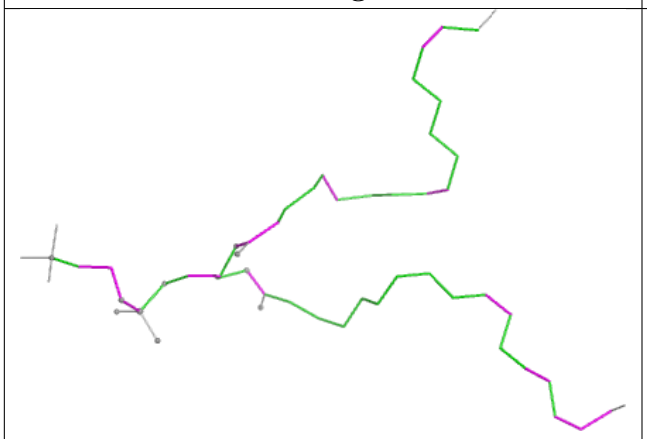
Ligand PC1 c 507



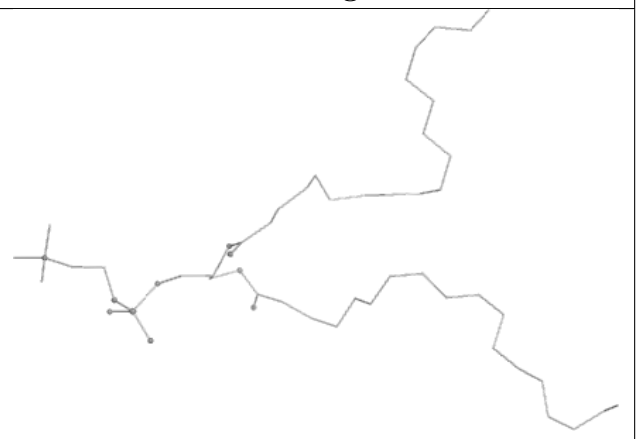
Bond lengths



Bond angles



Torsions

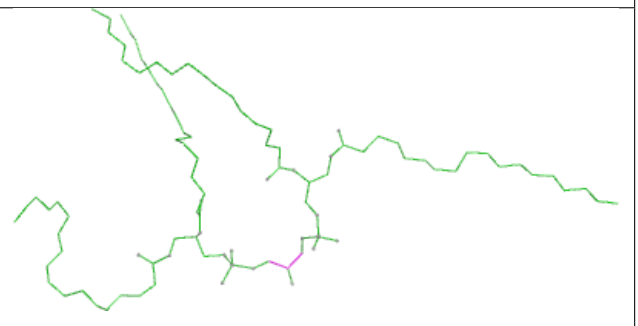


Rings

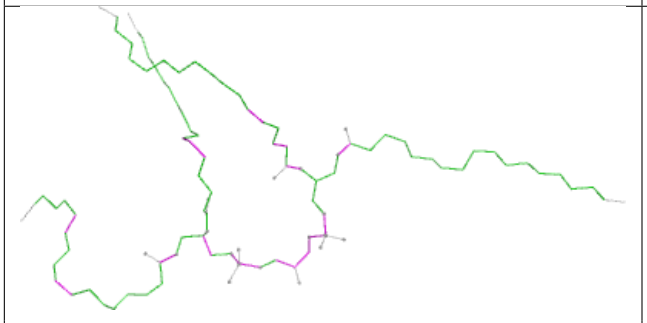
Ligand CDL Ed 204



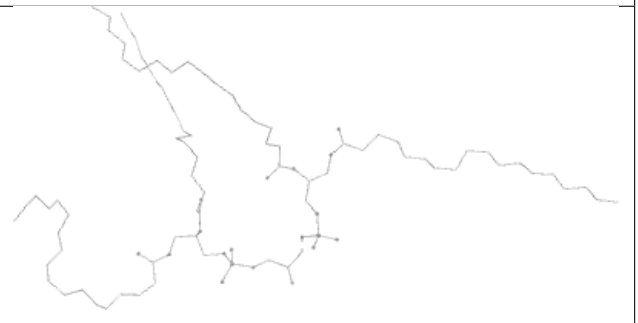
Bond lengths



Bond angles

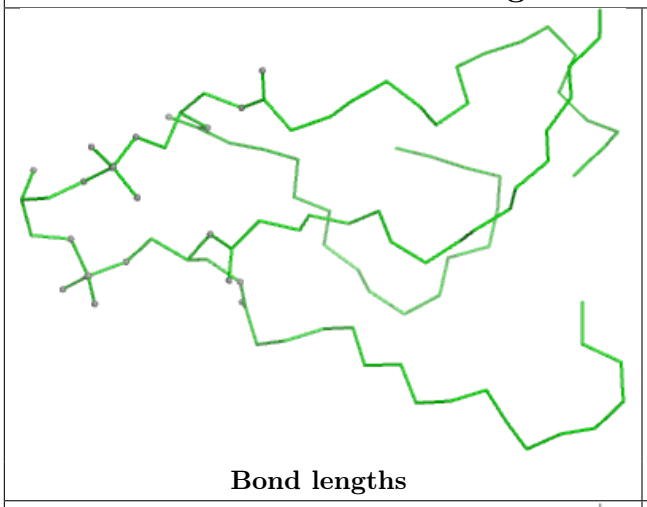


Torsions

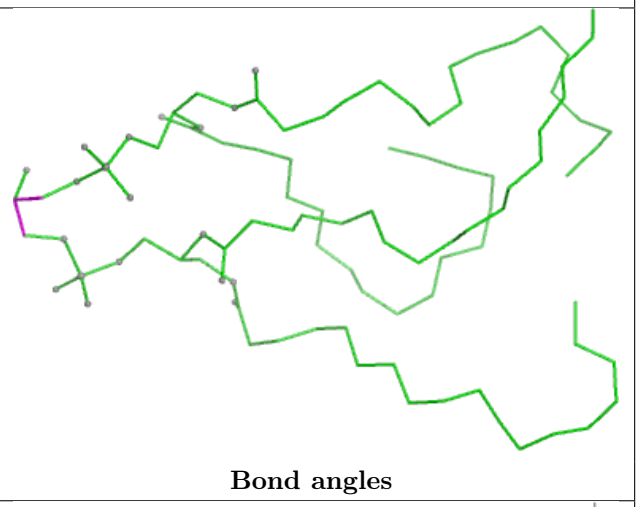


Rings

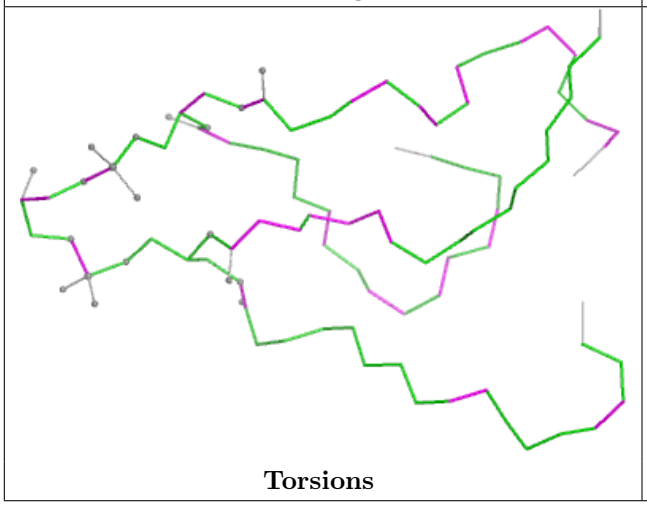
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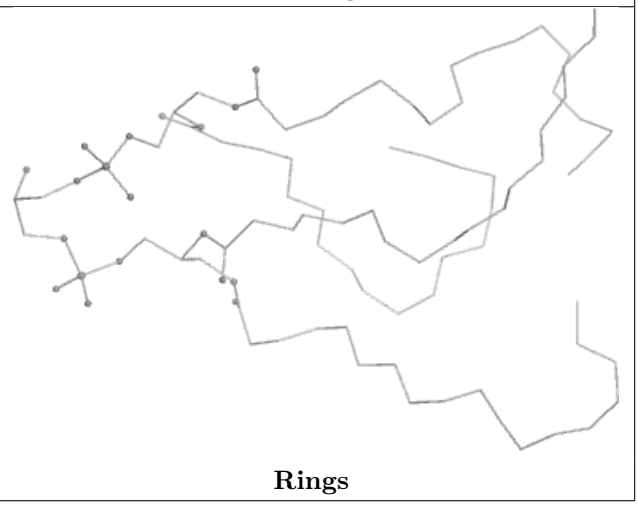
Bond lengths



Bond angles

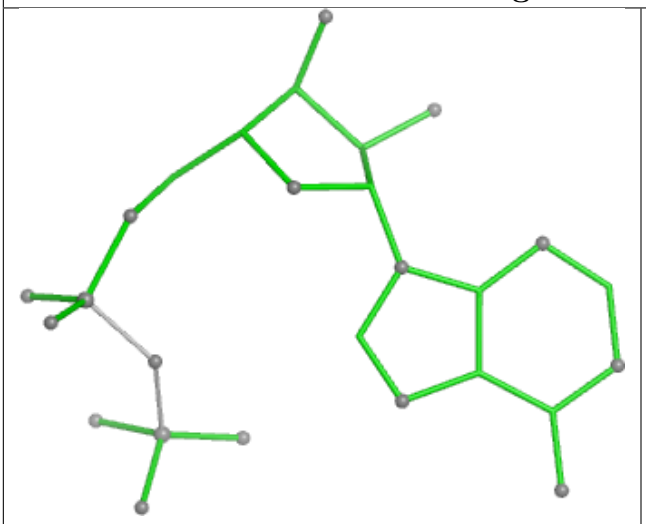


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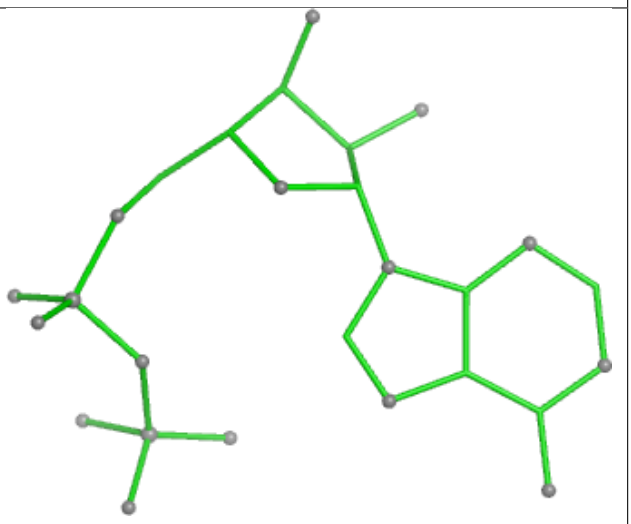


Rings

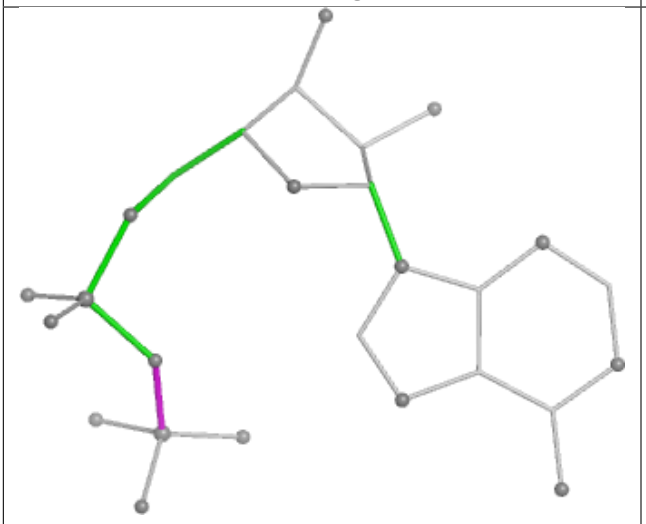
Ligand ADP A8 401



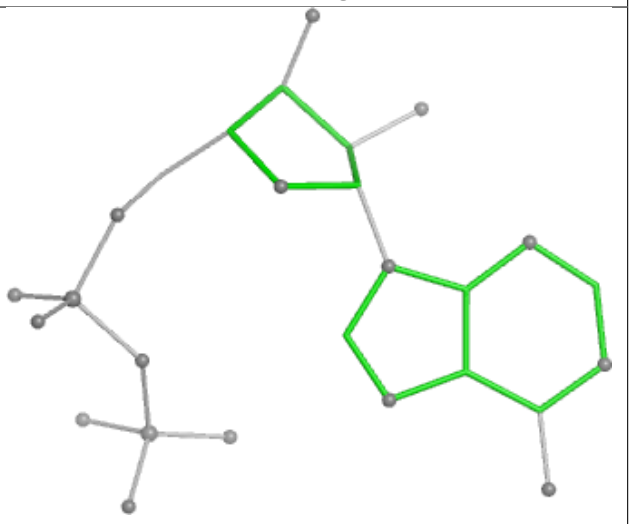
Bond lengths



Bond angles



Torsions



Rings

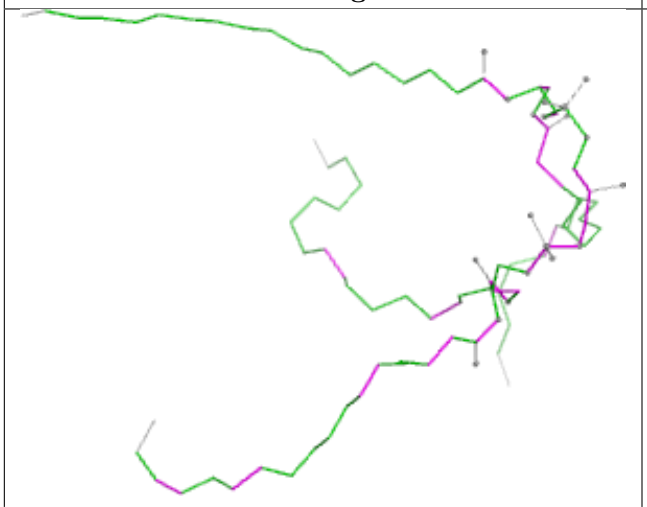
Ligand CDL Dd 702



Bond lengths



Bond angles

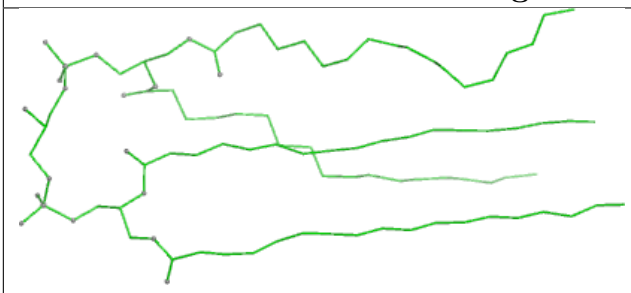


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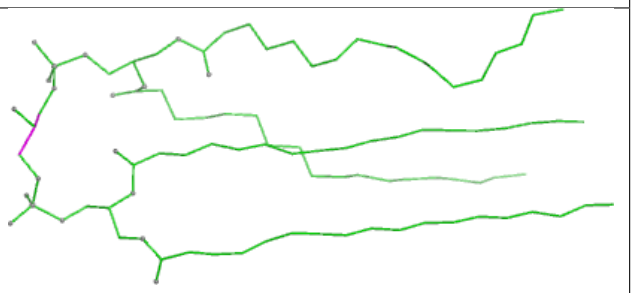


Rings

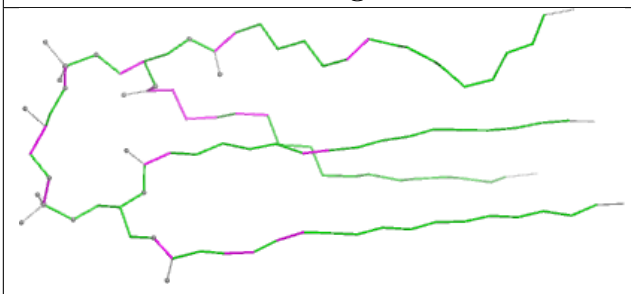
Ligand CDL BC 301



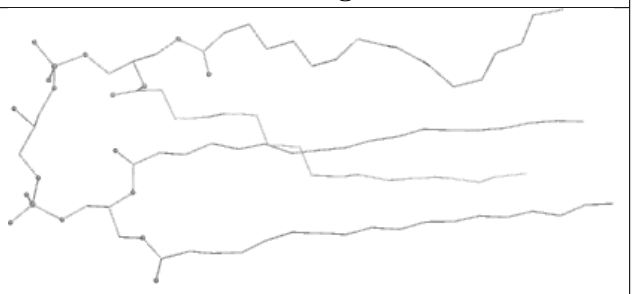
Bond lengths



Bond angles

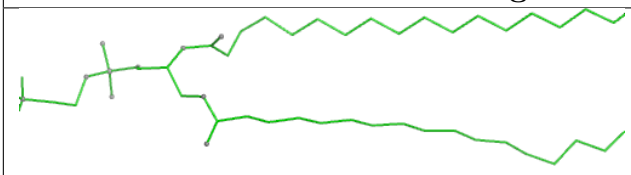


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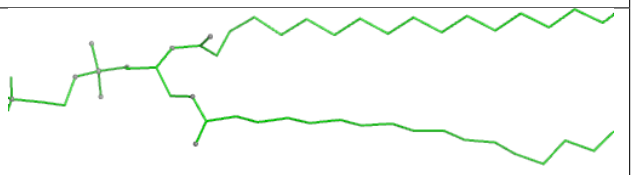


Rings

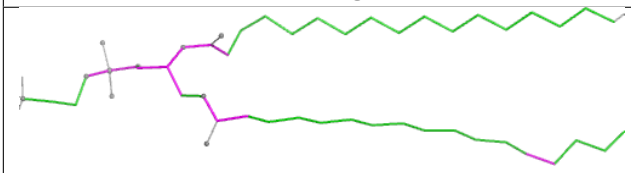
Ligand PC1 AM 302



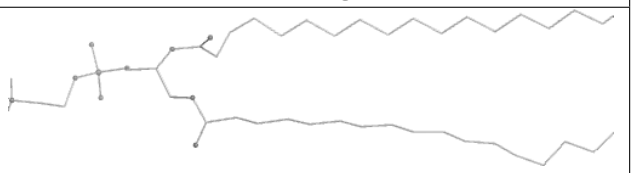
Bond lengths



Bond angles

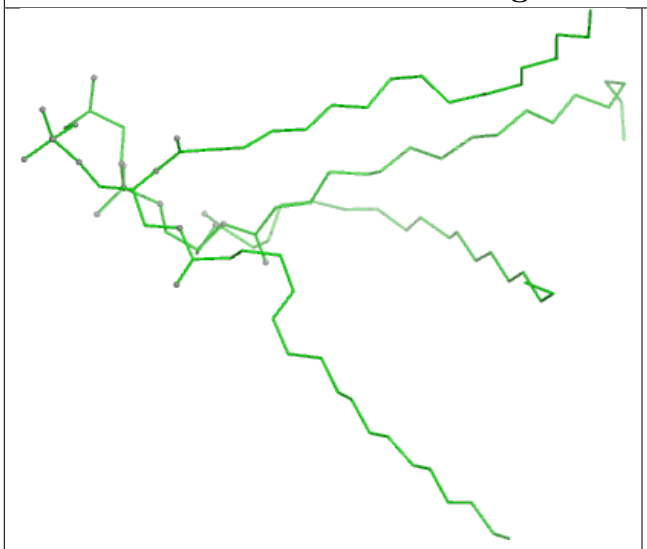


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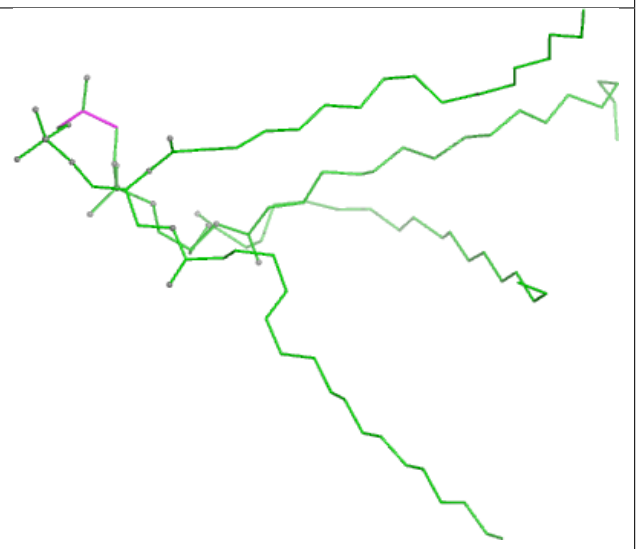


Rings

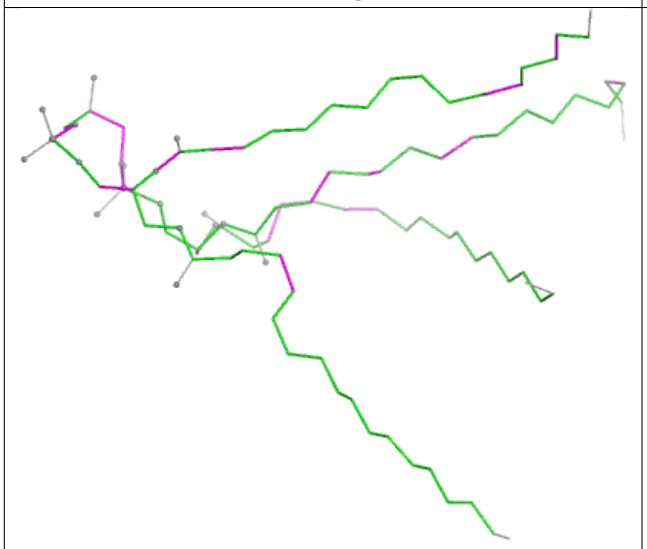
Ligand CDL CG 301



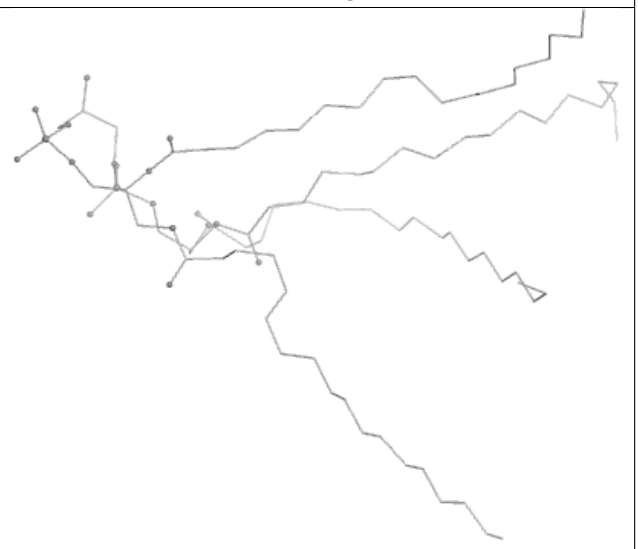
Bond lengths



Bond angles

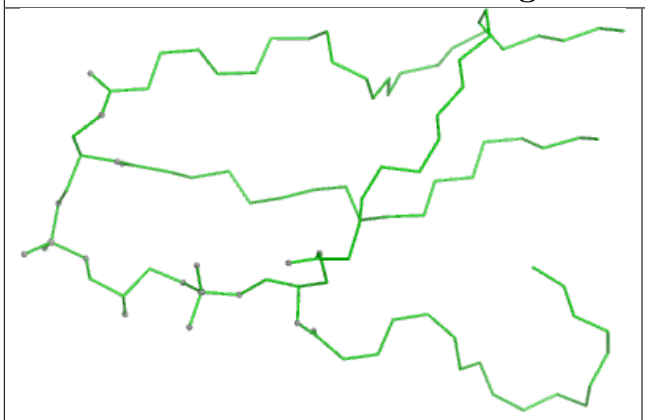


Torsions

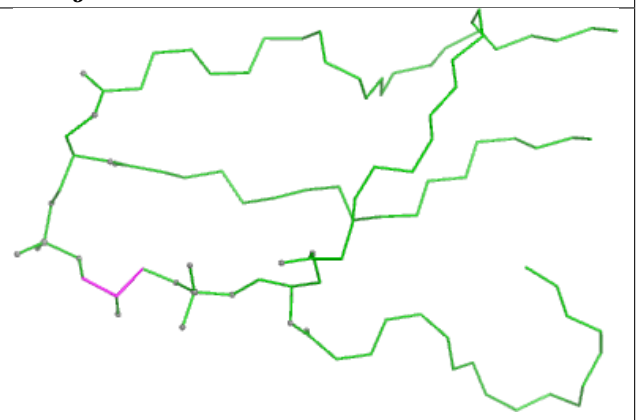


Rings

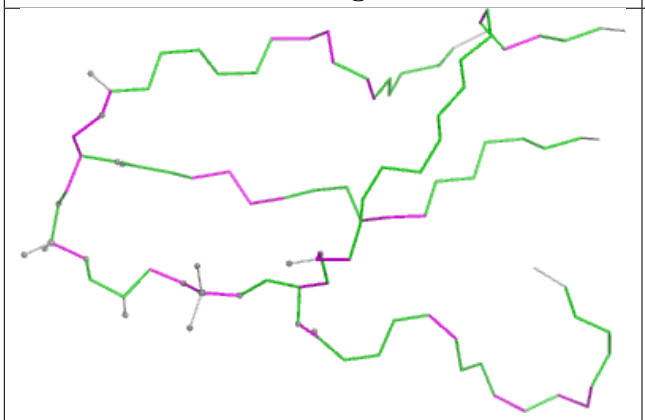
Ligand CDL Dj 401



Bond lengths



Bond angles

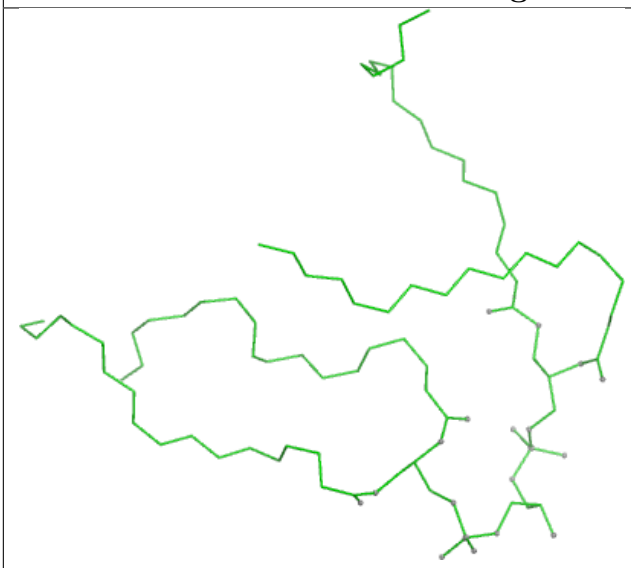


Torsions



Rings

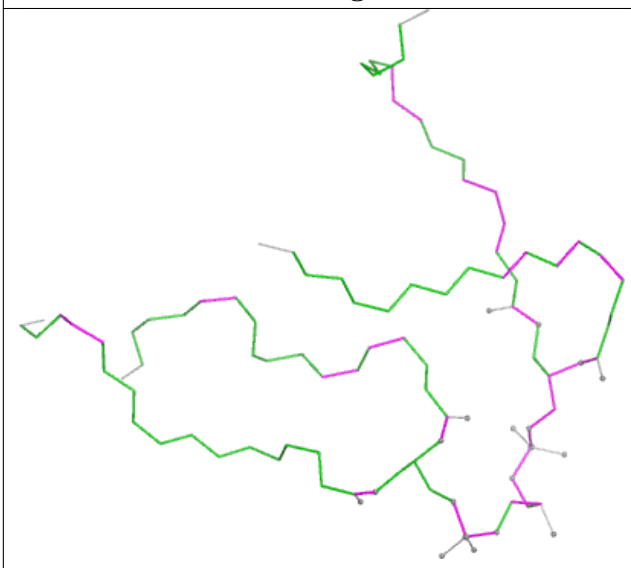
Ligand CDL CG 302



Bond lengths



Bond angles

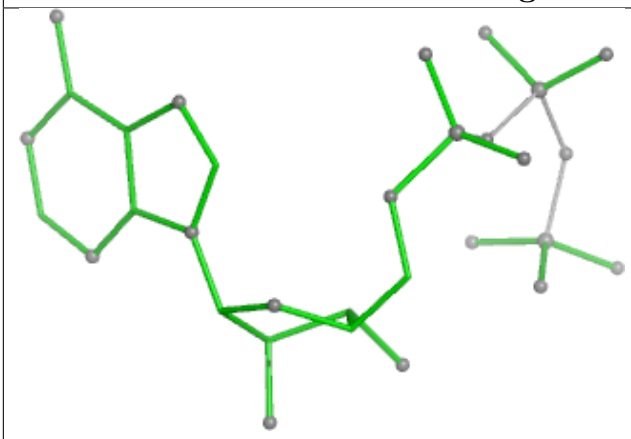


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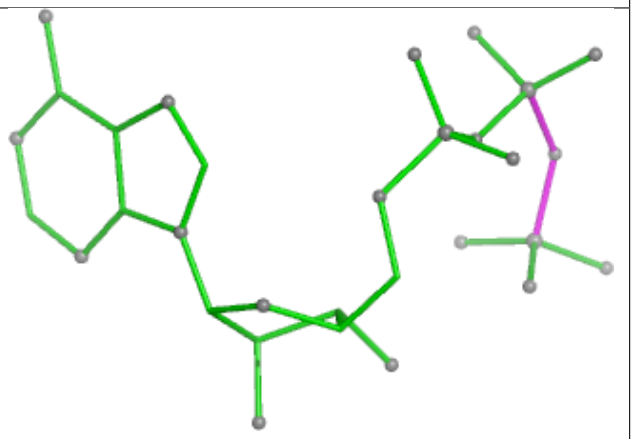


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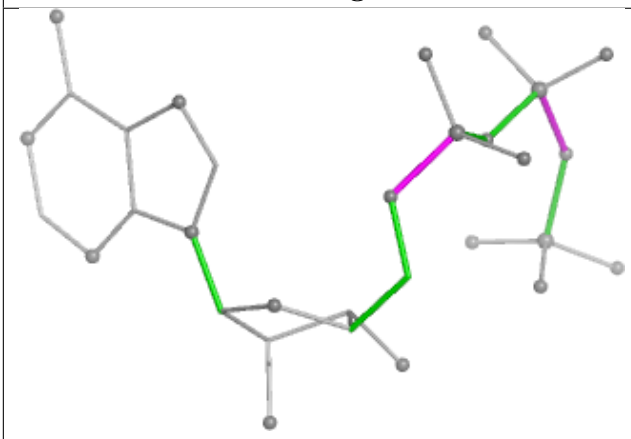
Ligand ATP Er 201



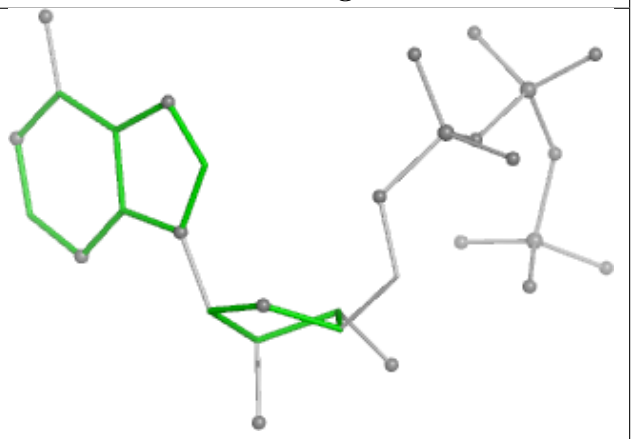
Bond lengths



Bond angles

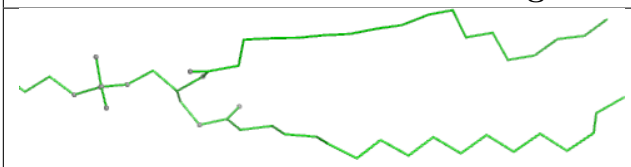


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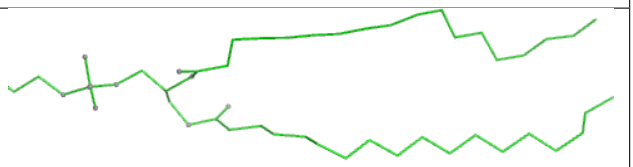


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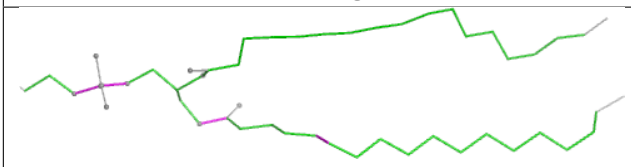
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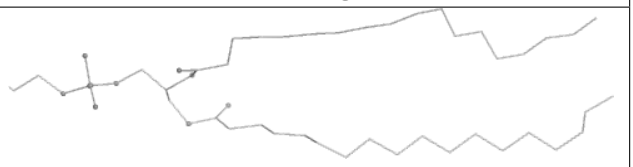
Bond lengths



Bond angles

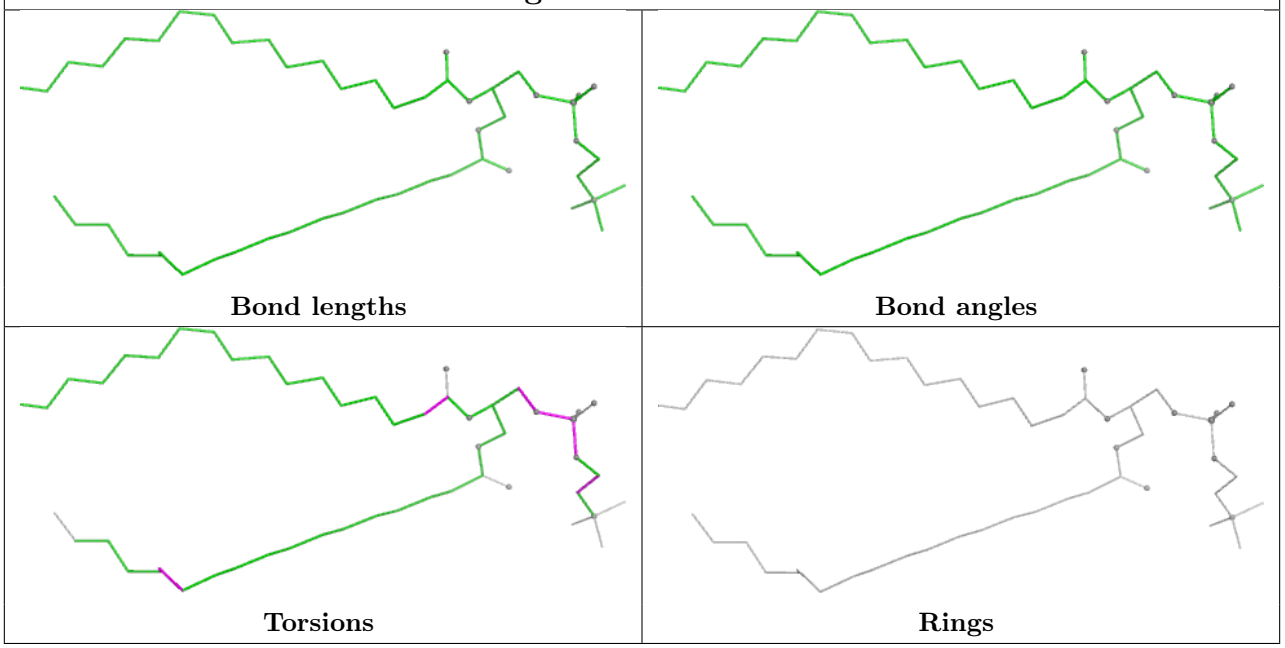


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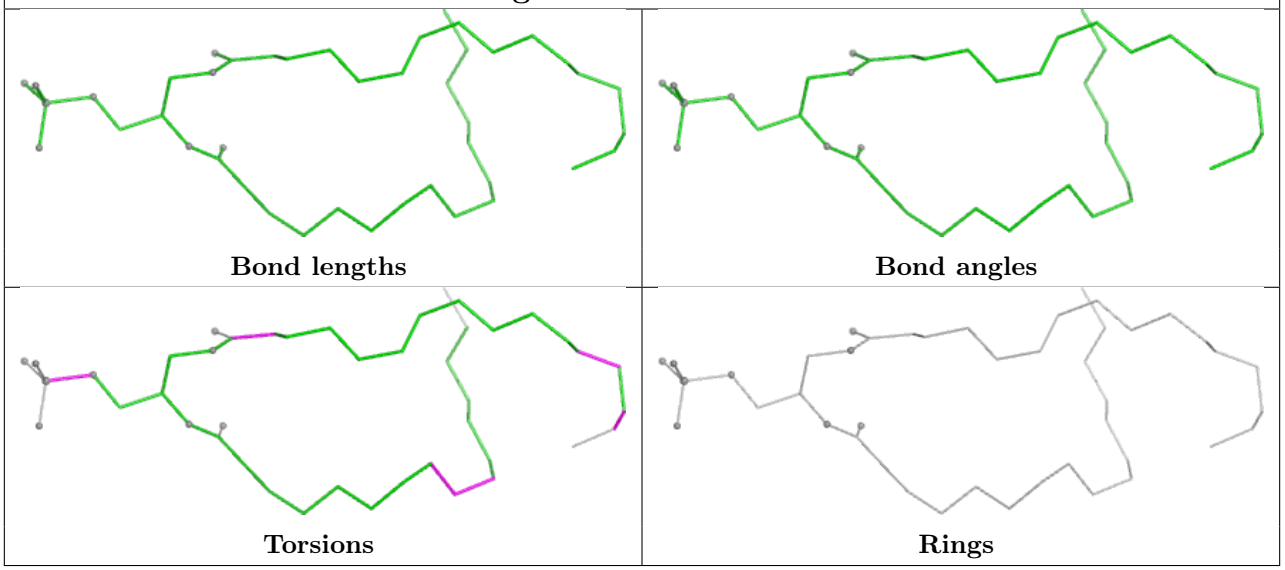


Rings

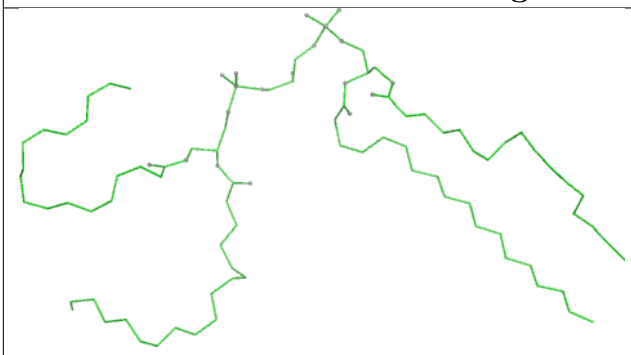
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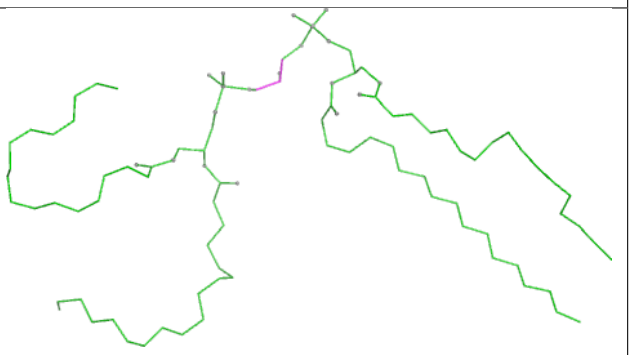
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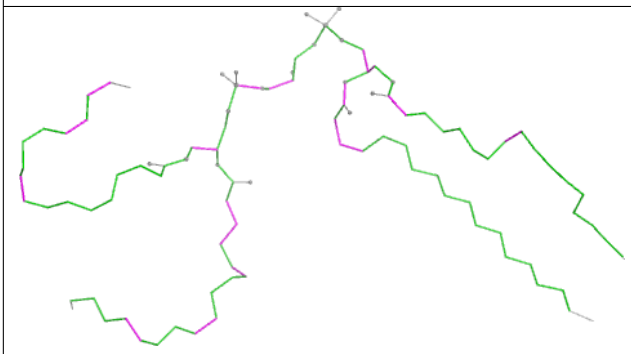
Ligand CDL BV 201



Bond lengths



Bond angles

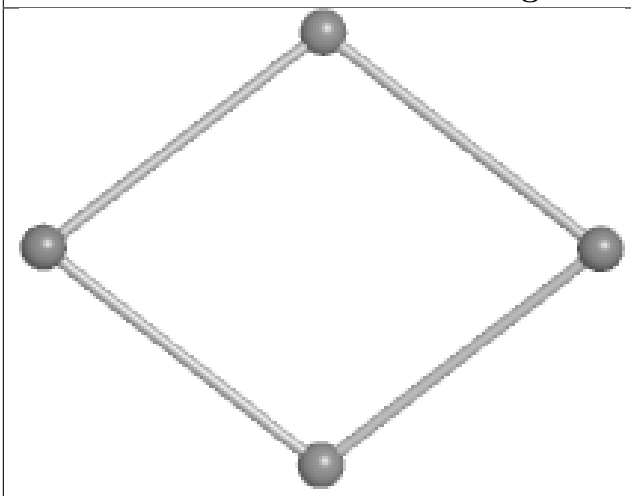


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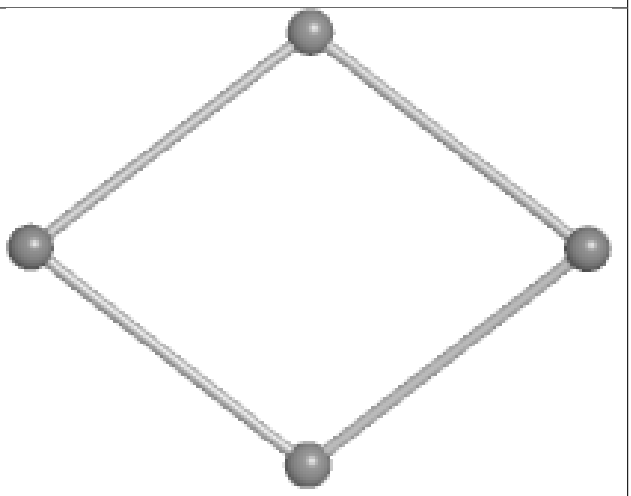


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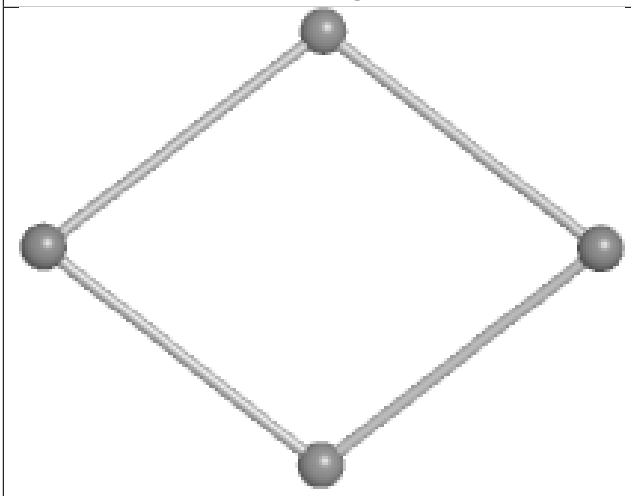
Ligand FES AI 301



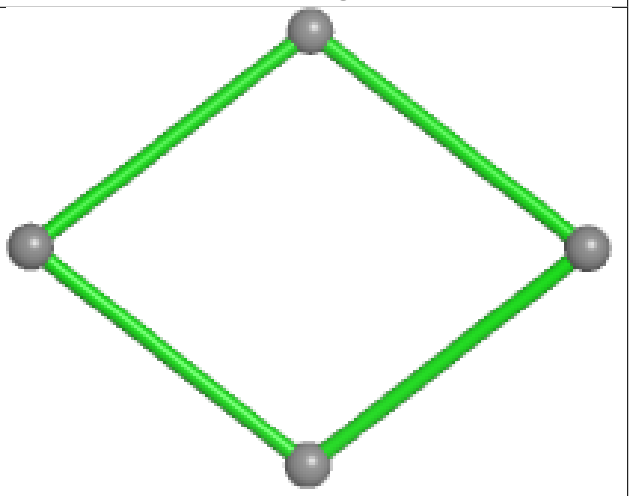
Bond lengths



Bond angles

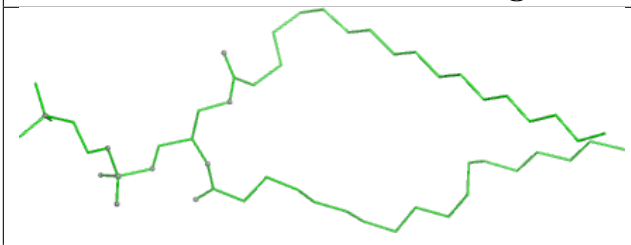


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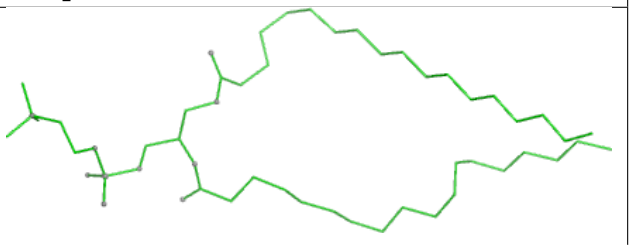


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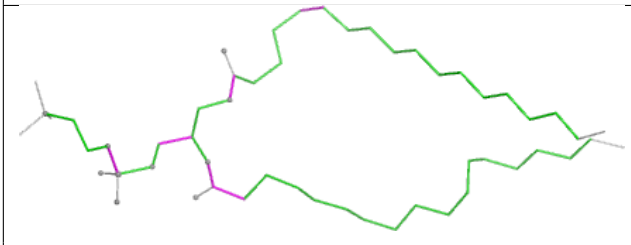
Ligand PC1 Dq 1404



Bond lengths



Bond angles

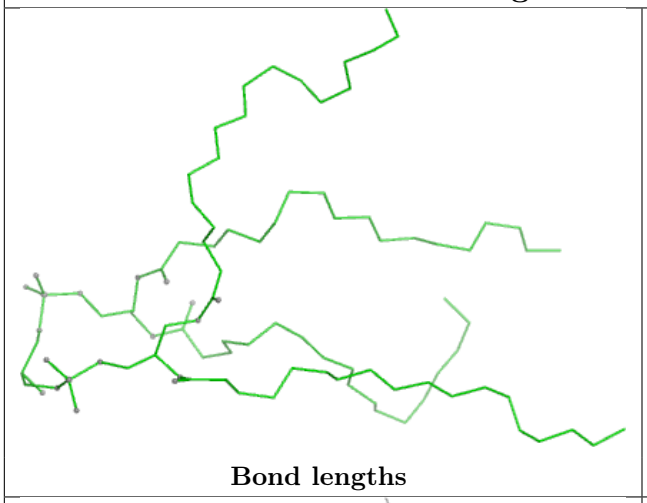


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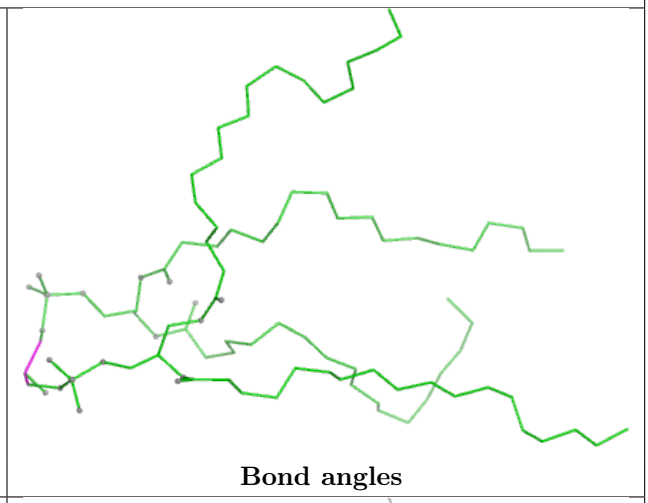


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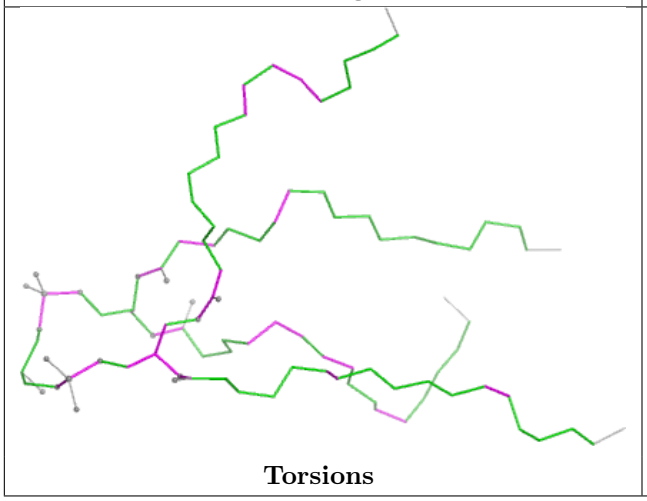
Ligand CDL DC 601



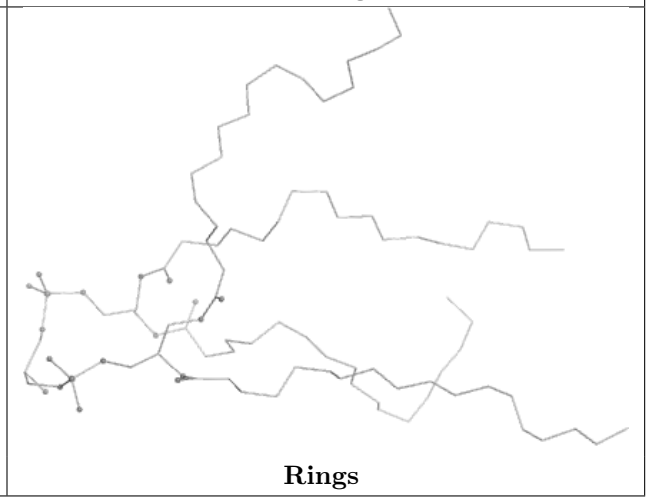
Bond lengths



Bond angles

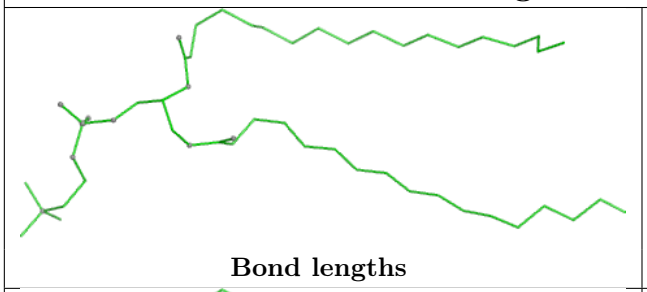


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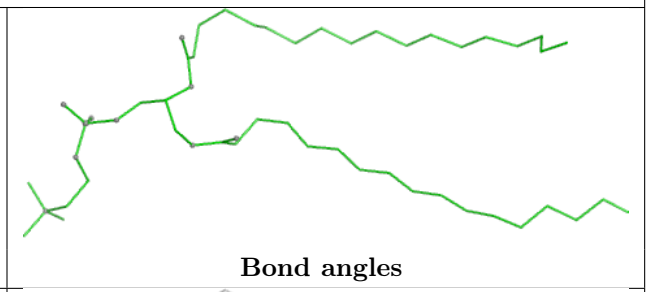


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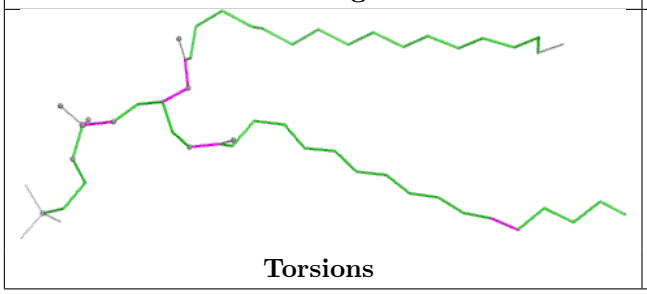
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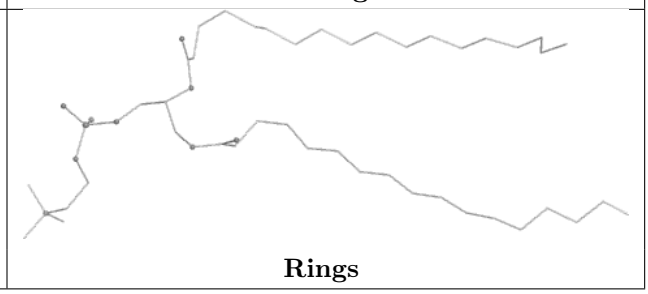
Bond lengths



Bond angles



Torsions

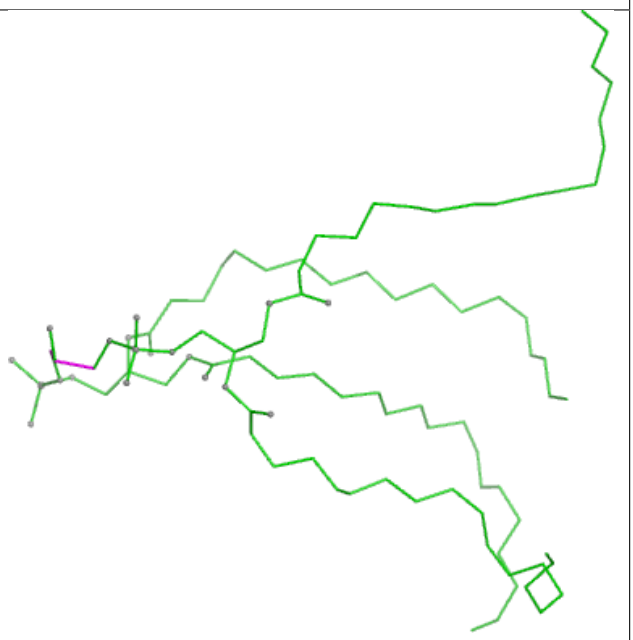


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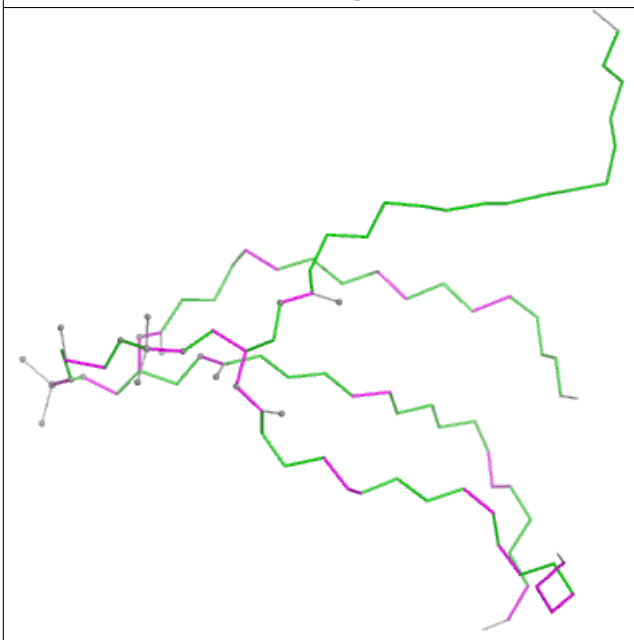
Ligand CDL c 501



Bond lengths



Bond angles

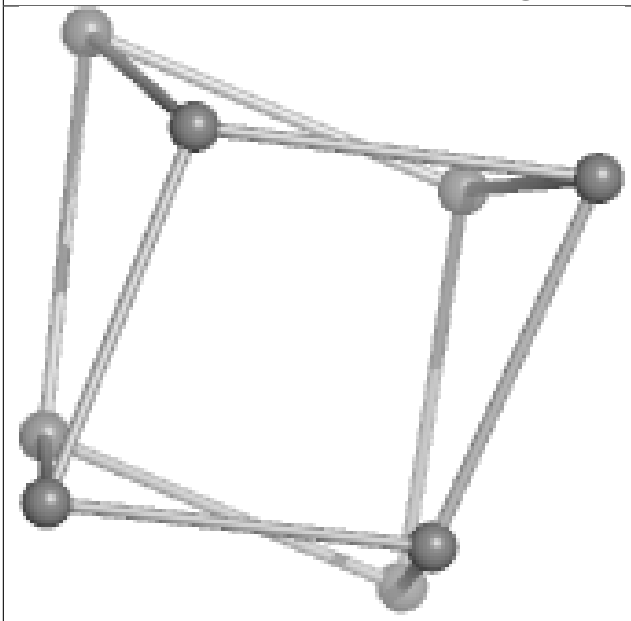


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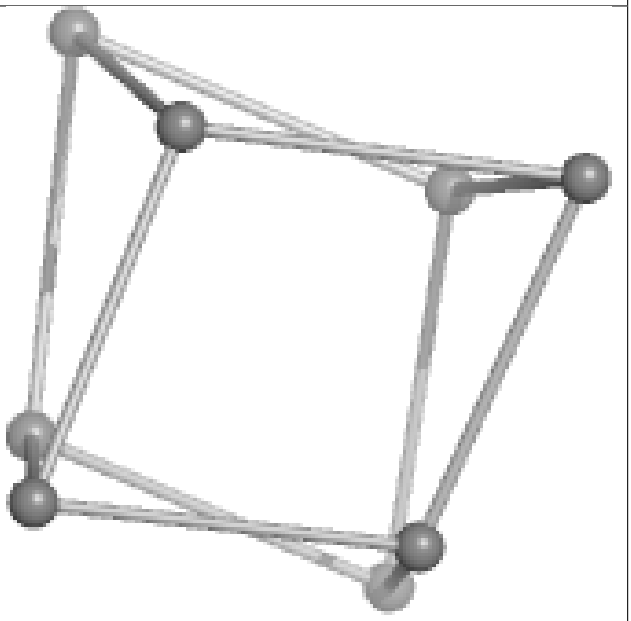


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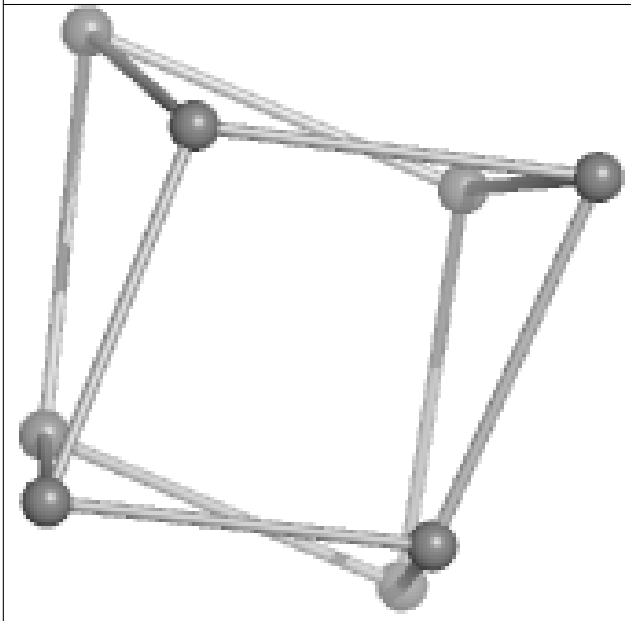
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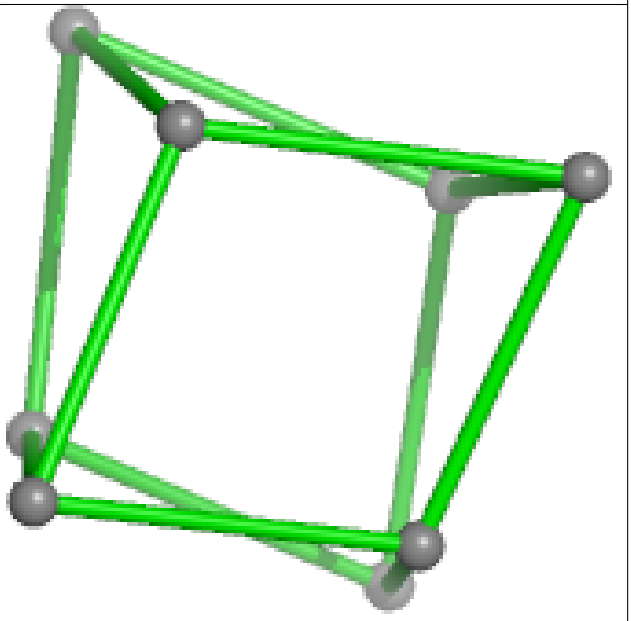
Bond lengths



Bond angles

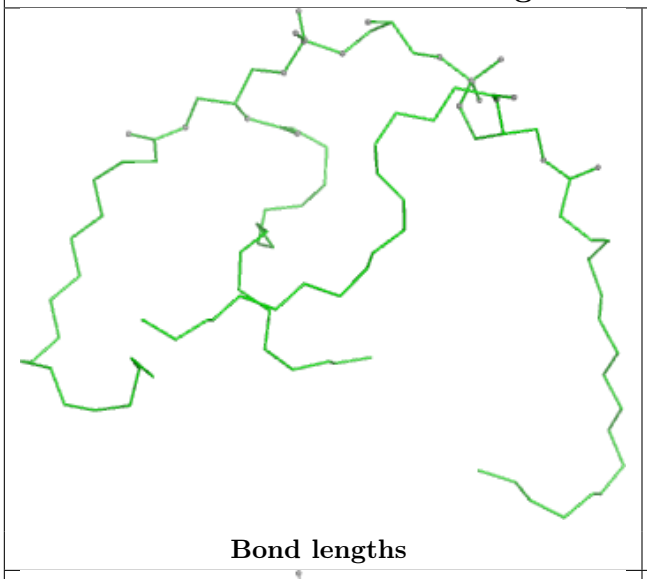


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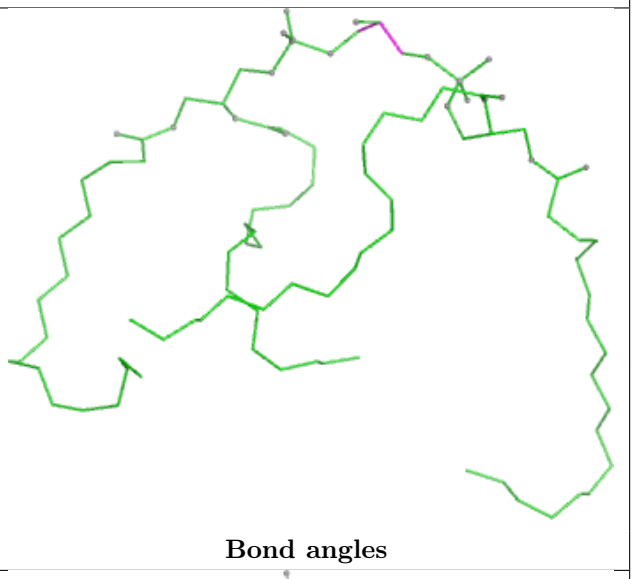


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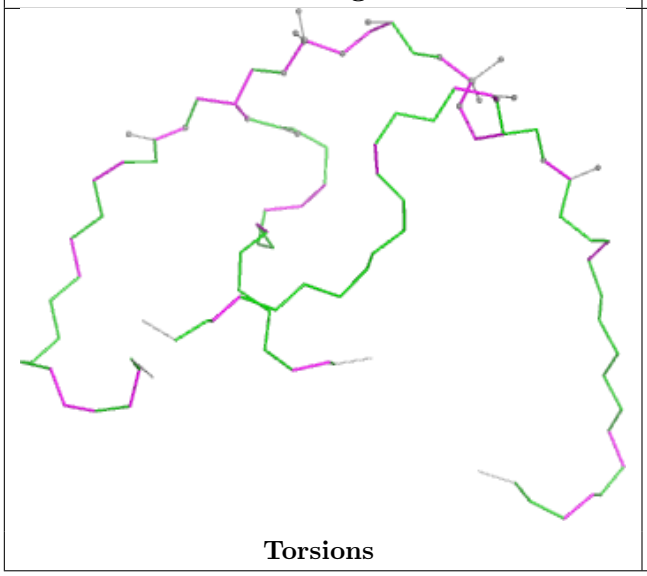
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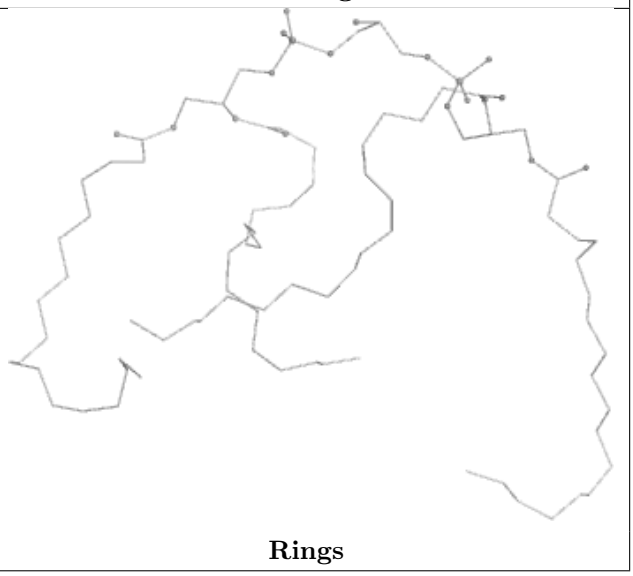
Bond lengths



Bond angles

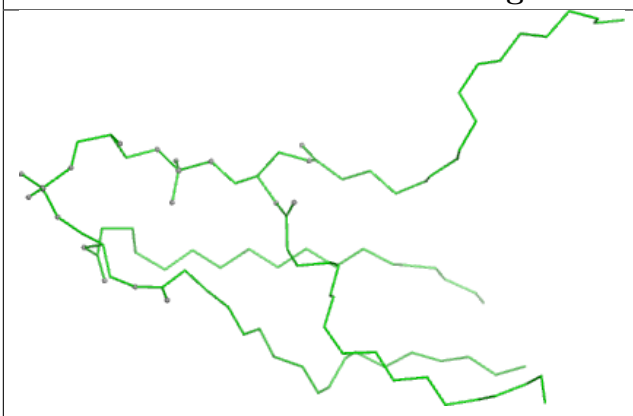


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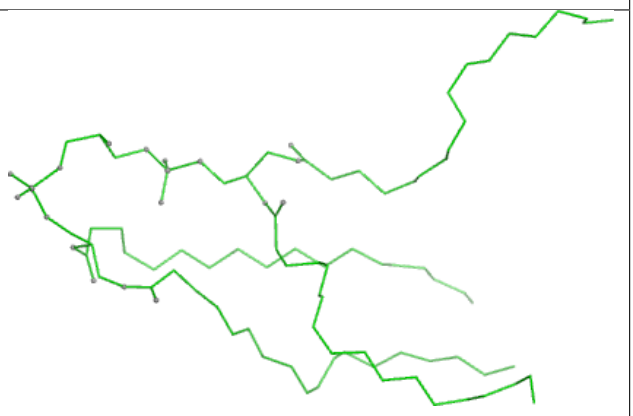


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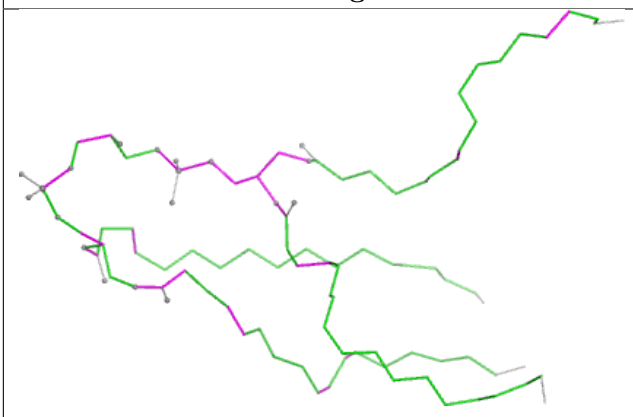
Ligand CDL AM 301



Bond lengths



Bond angles

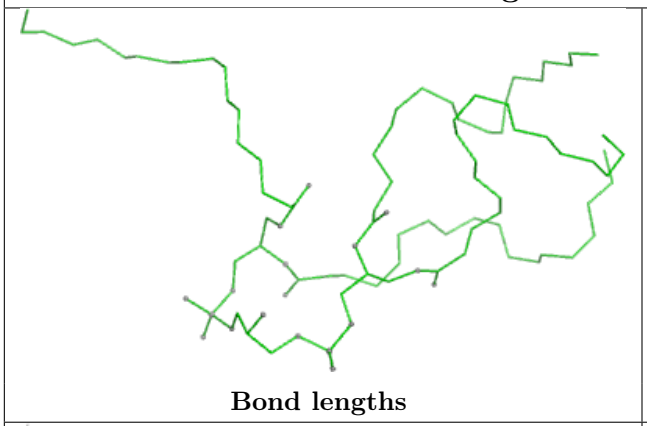


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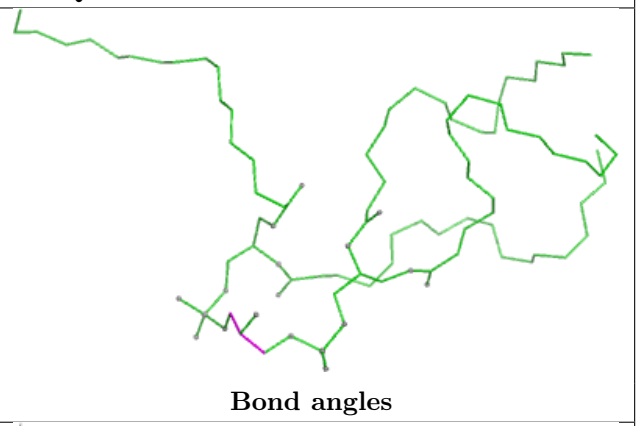


Rings

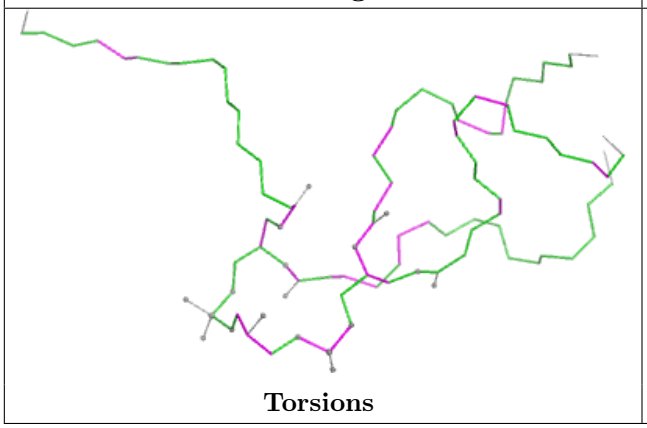
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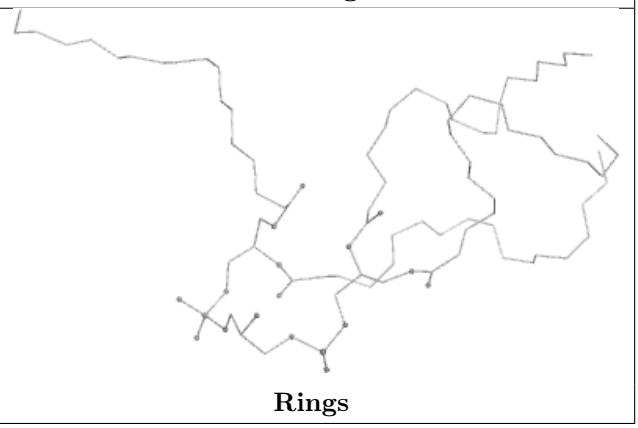
Bond lengths



Bond angles

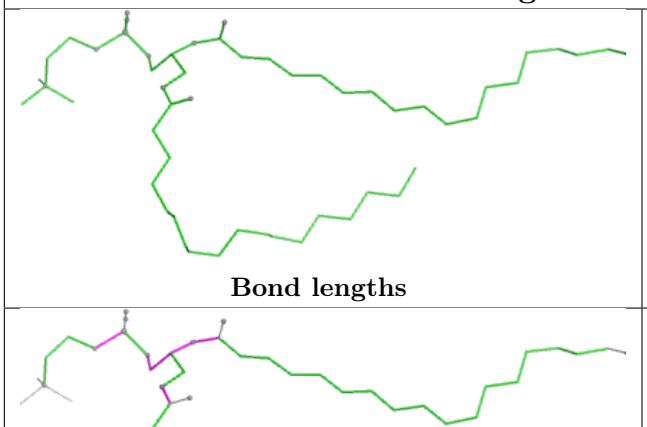


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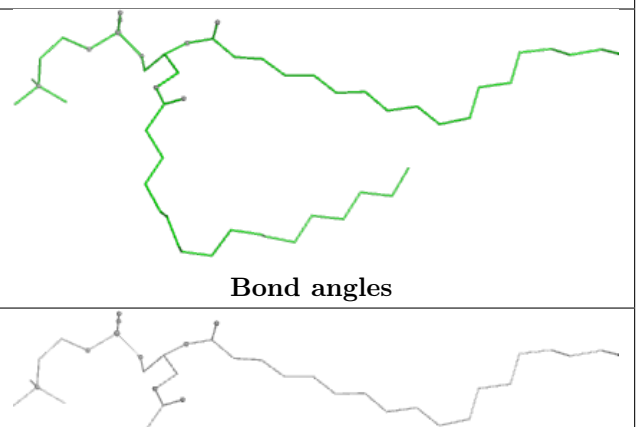


Rings

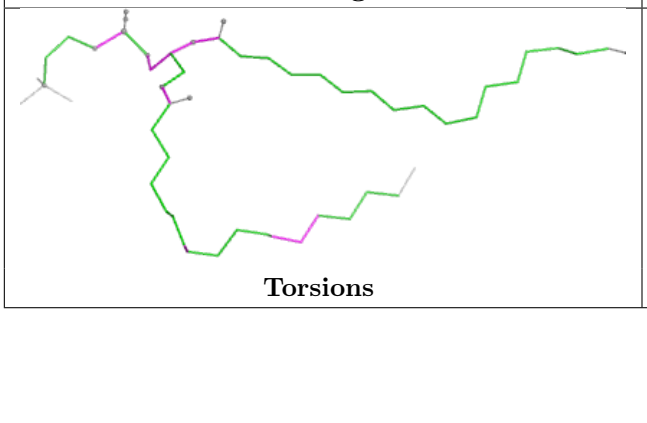
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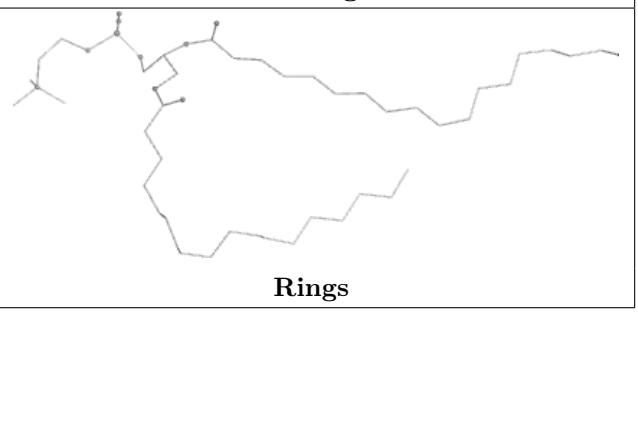
Bond lengths



Bond angles

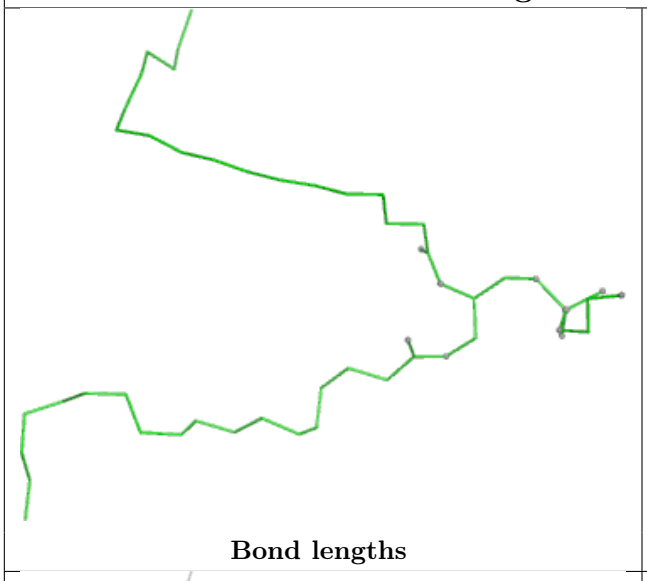


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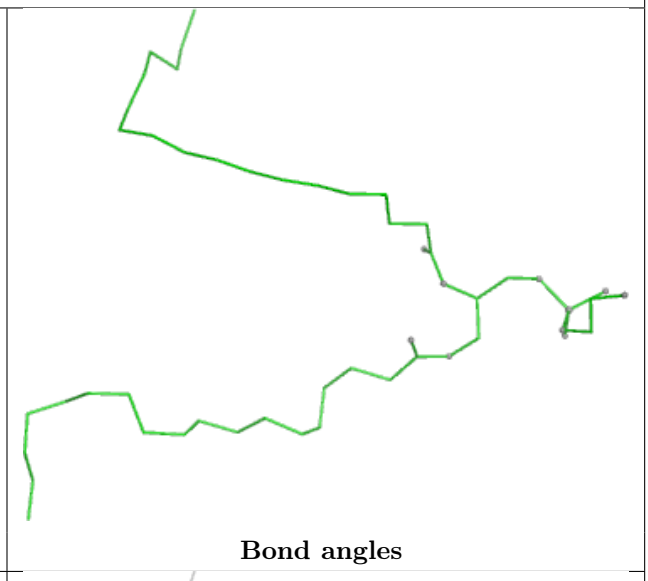


Rings

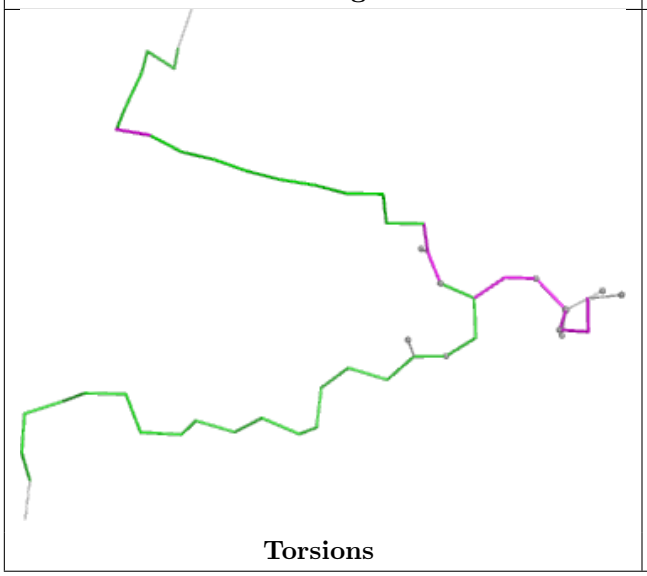
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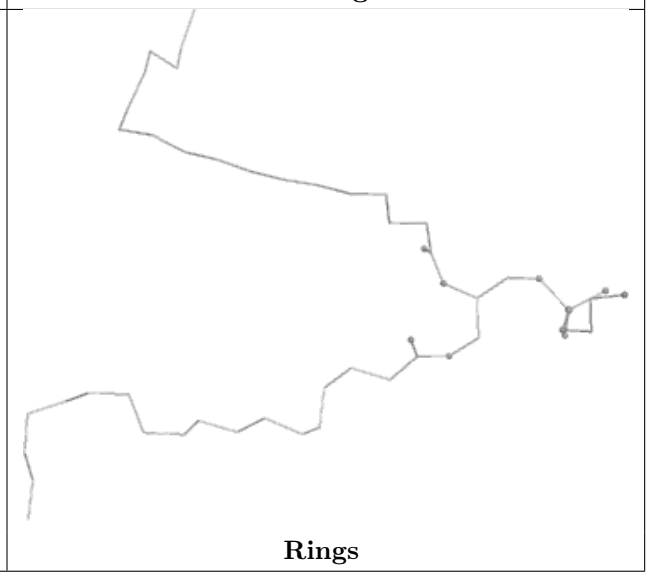
Bond lengths



Bond angles

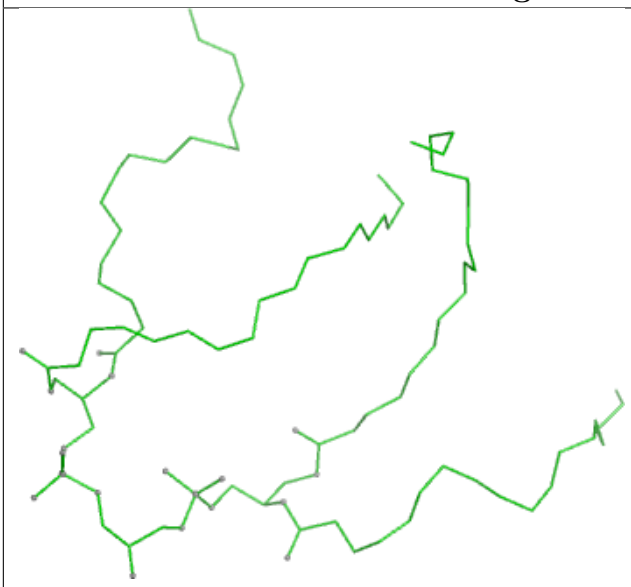


Torsions



Rings

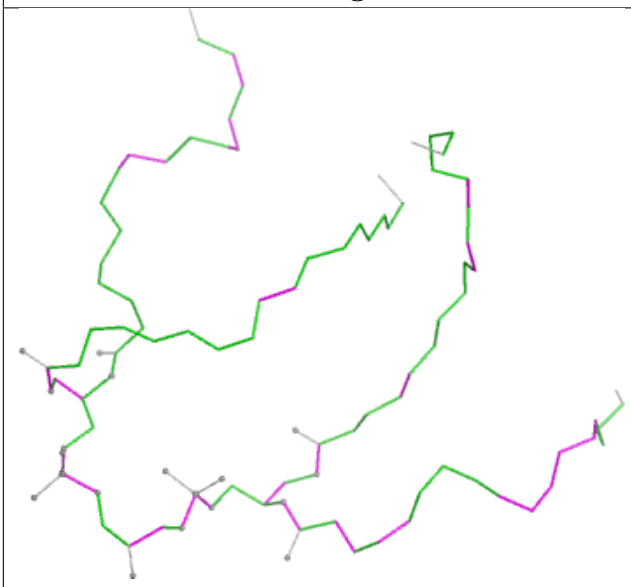
Ligand CDL Dh 201



Bond lengths



Bond angles

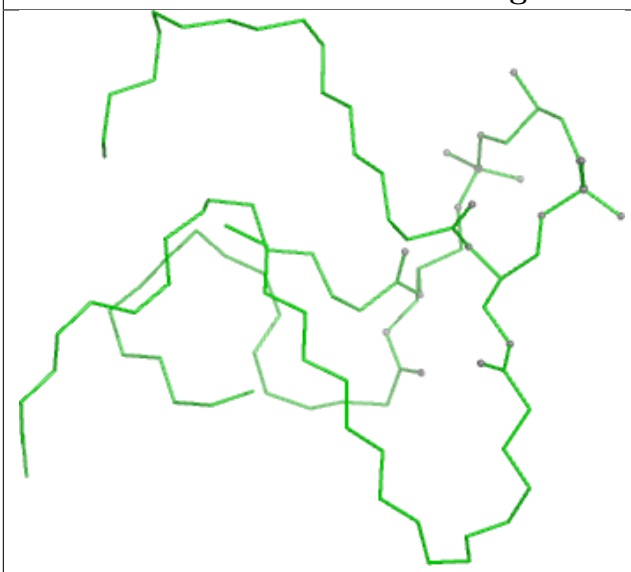


Torsions

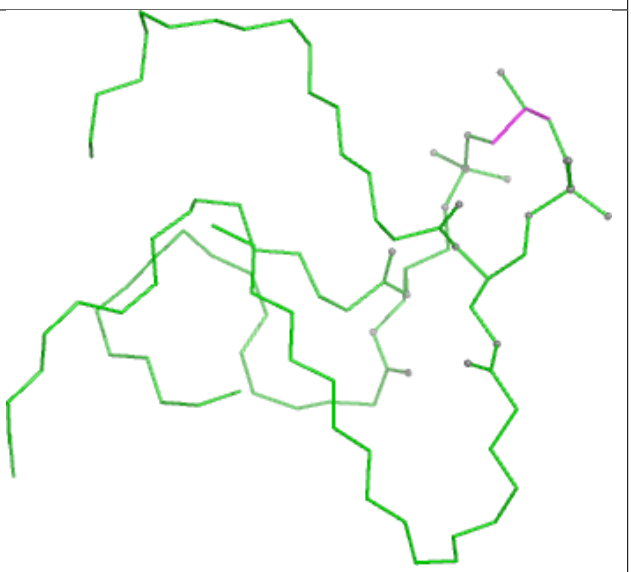


Rings

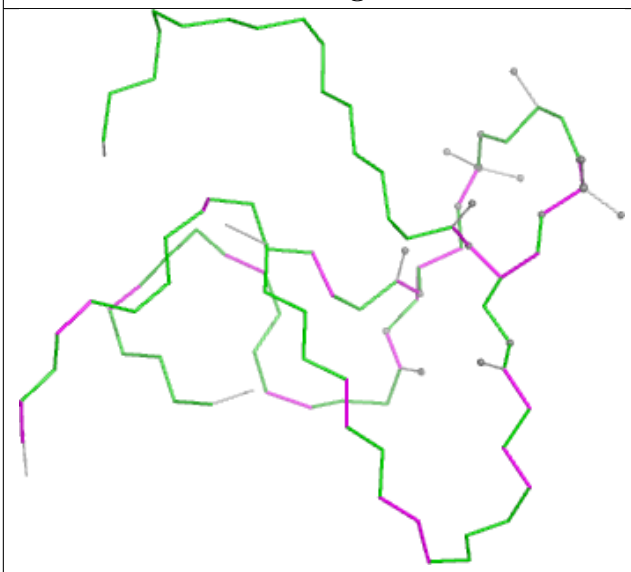
Ligand CDL DO 501



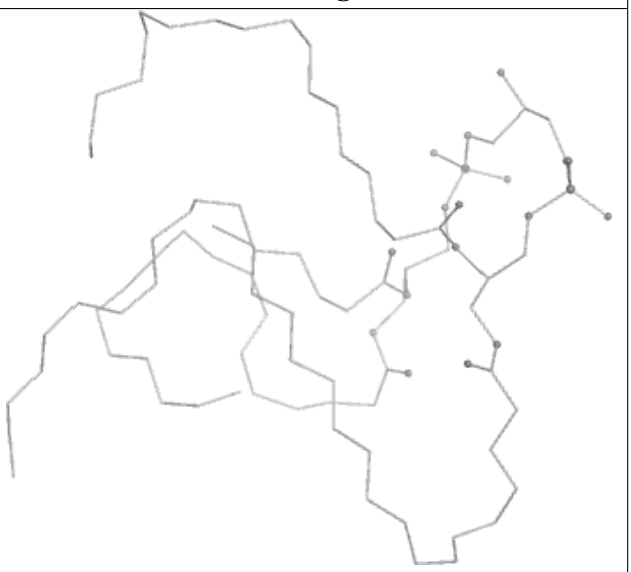
Bond lengths



Bond angles

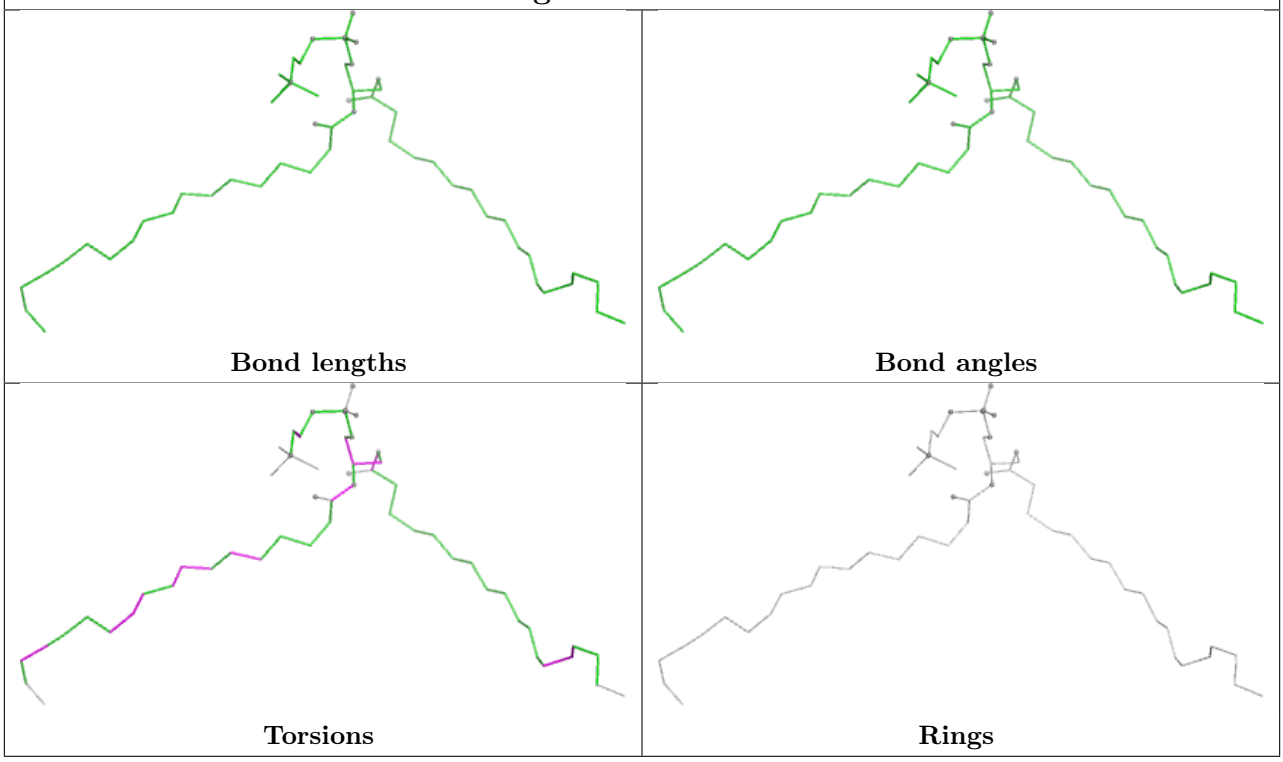


Torsions

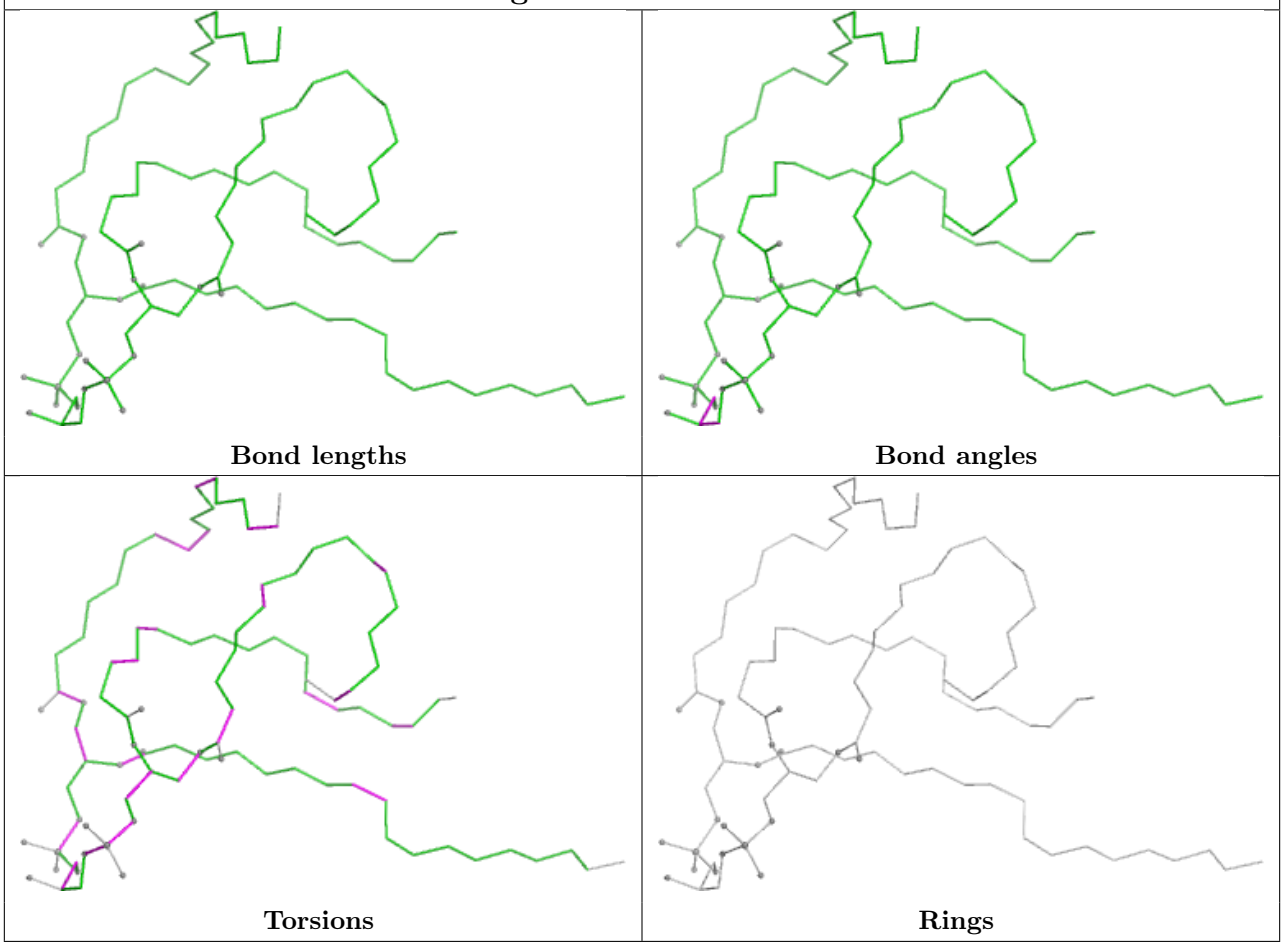


Rings

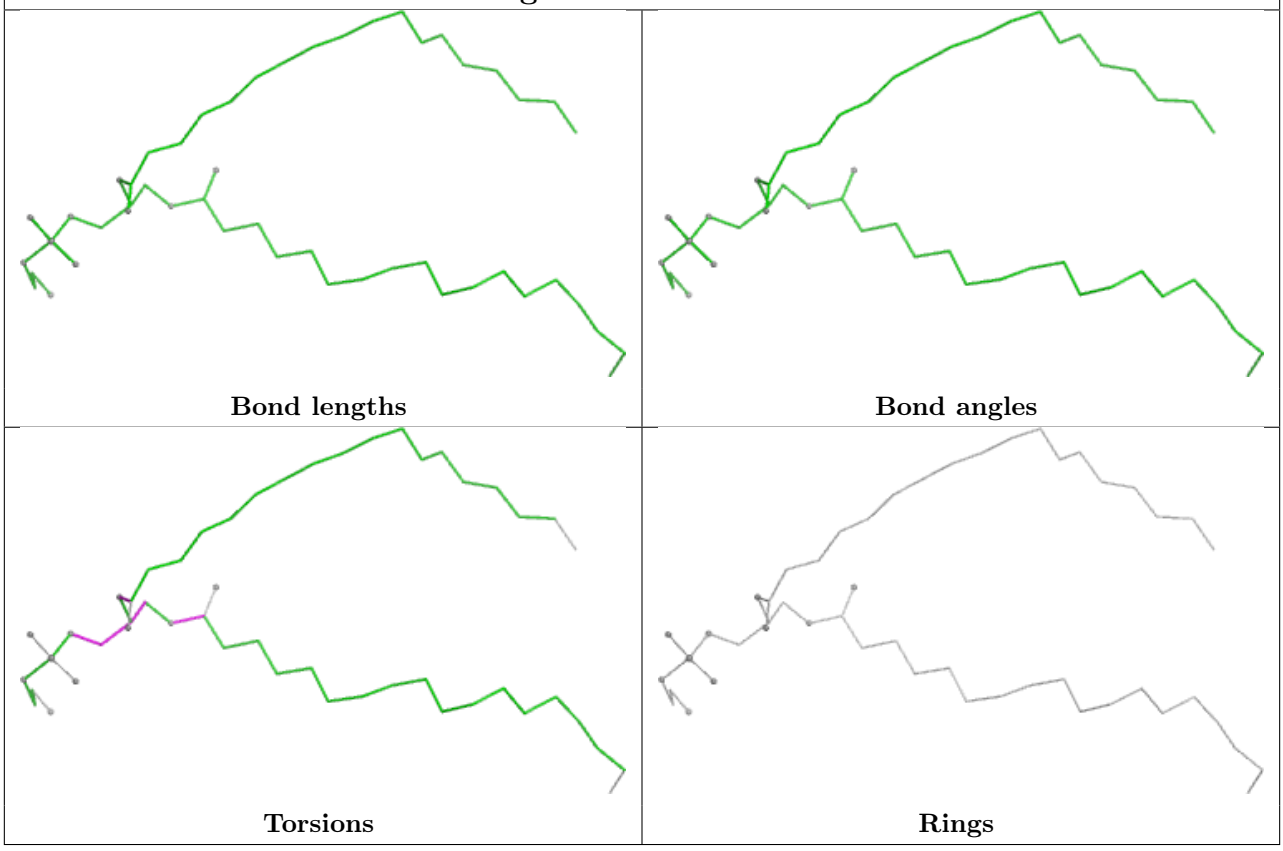
Ligand PC1 c 503



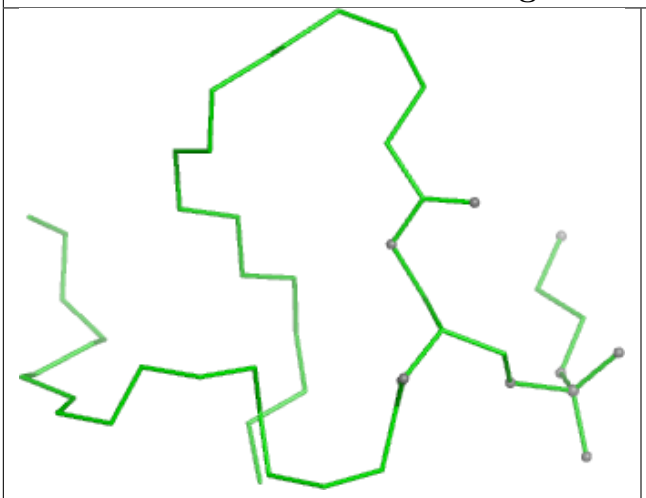
Ligand CDL DD 706



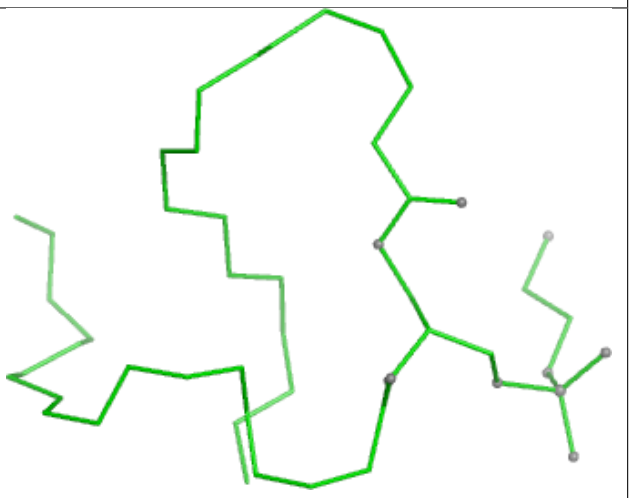
Ligand 3PE A2 401



Ligand 3PE EL 904



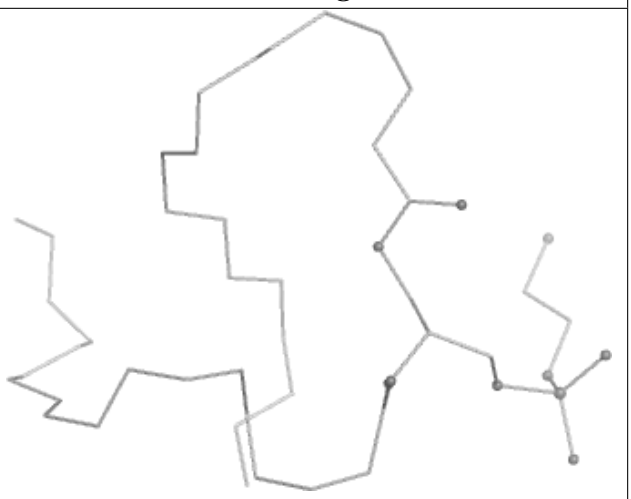
Bond lengths



Bond angles

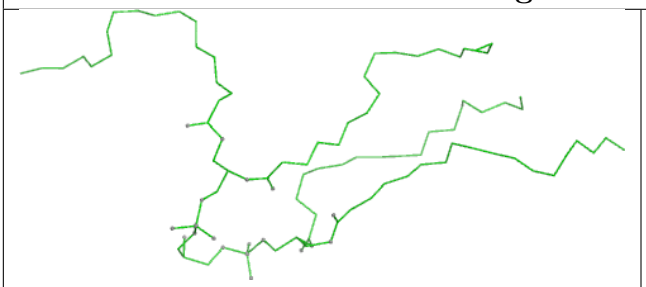


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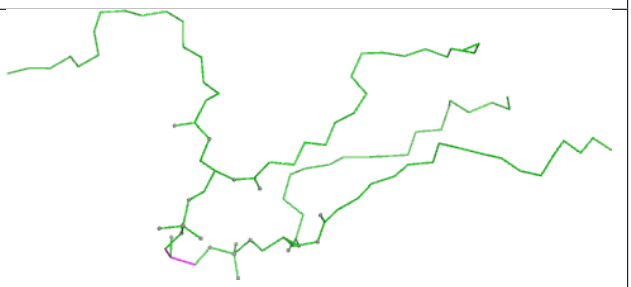


Rings

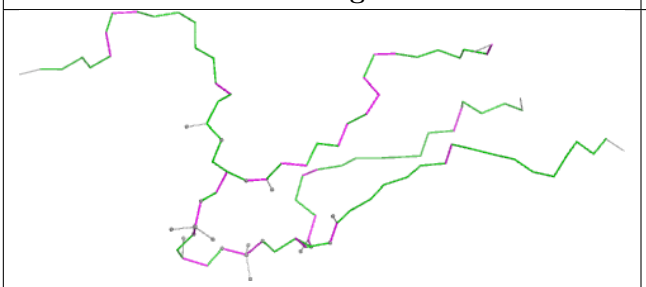
Ligand CDL B0 101



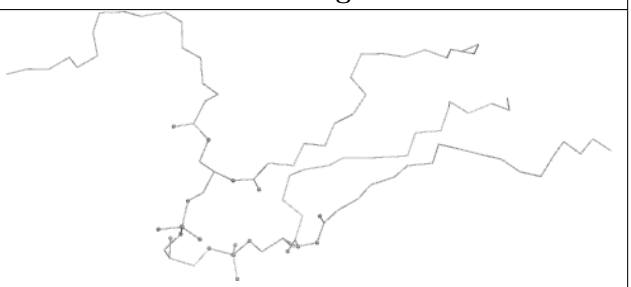
Bond lengths



Bond angles

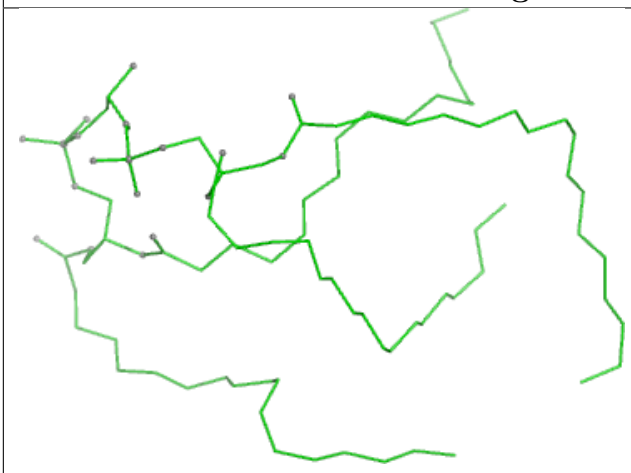


Torsions



Rings

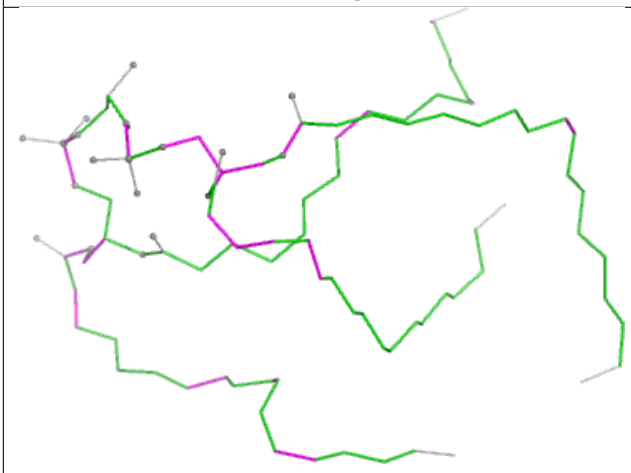
Ligand CDL EA 301



Bond lengths



Bond angles

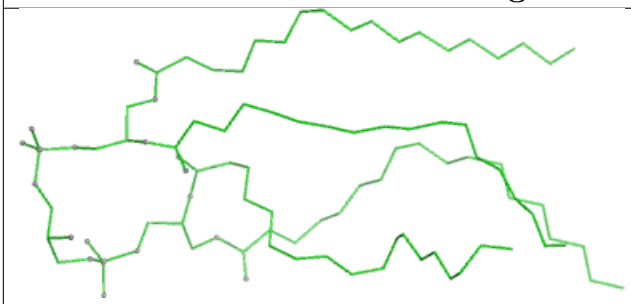


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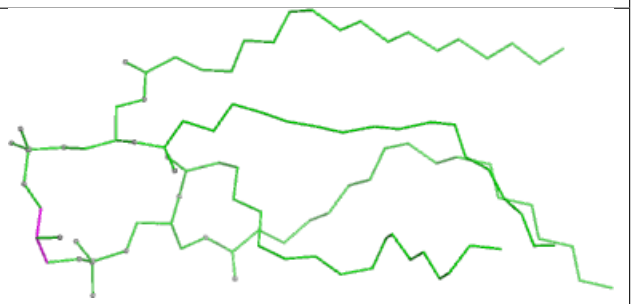


Rings

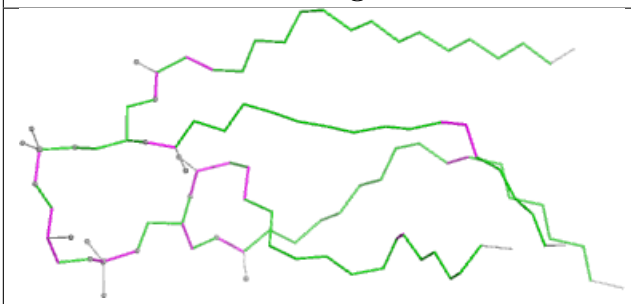
Ligand CDL Dm 502



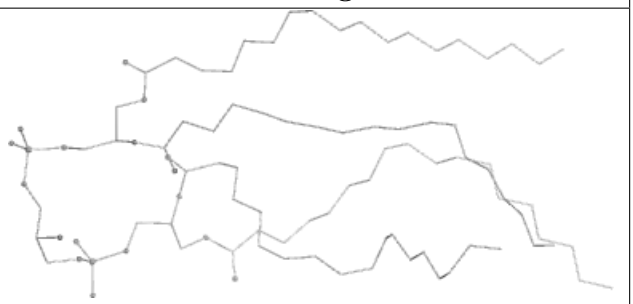
Bond lengths



Bond angles

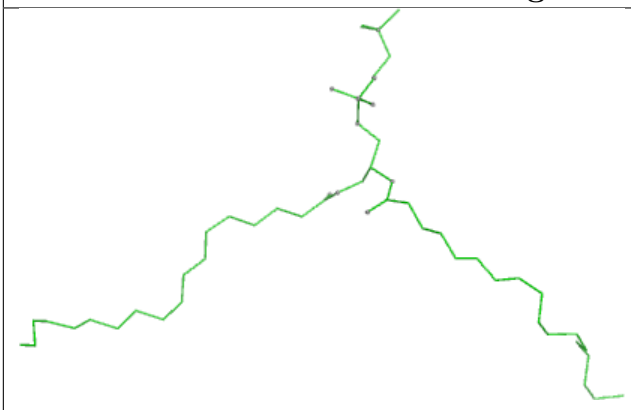


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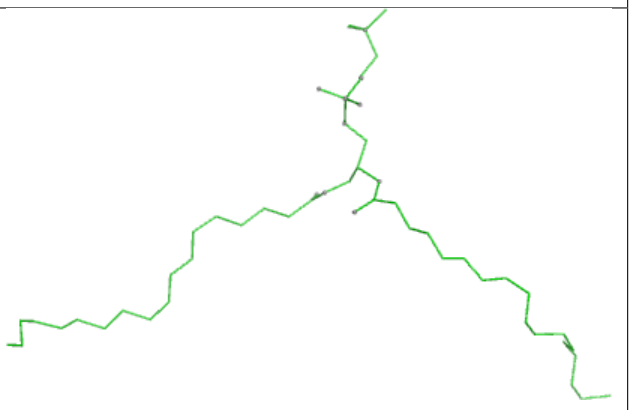


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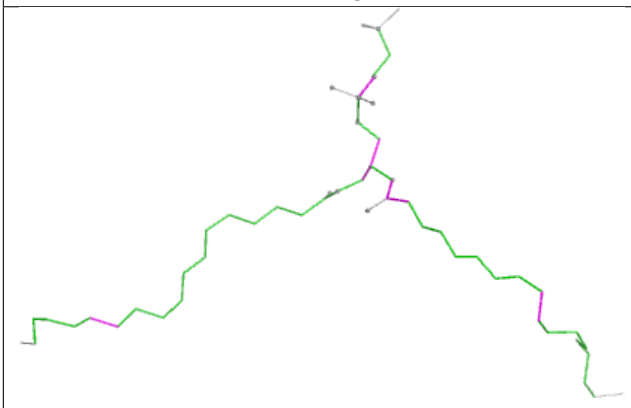
Ligand PC1 C 510



Bond lengths



Bond angles

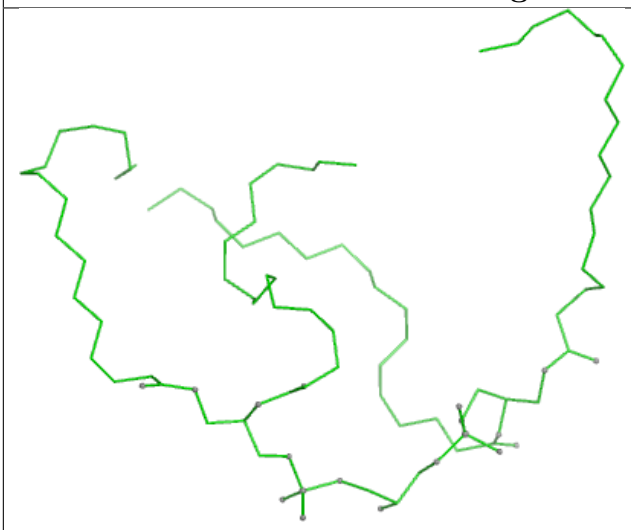


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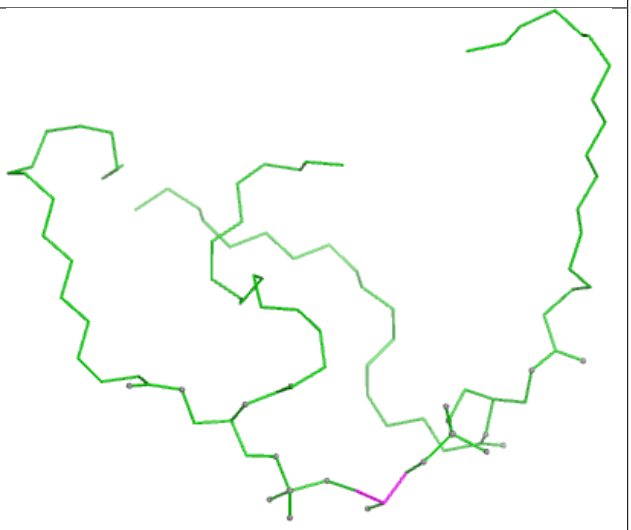


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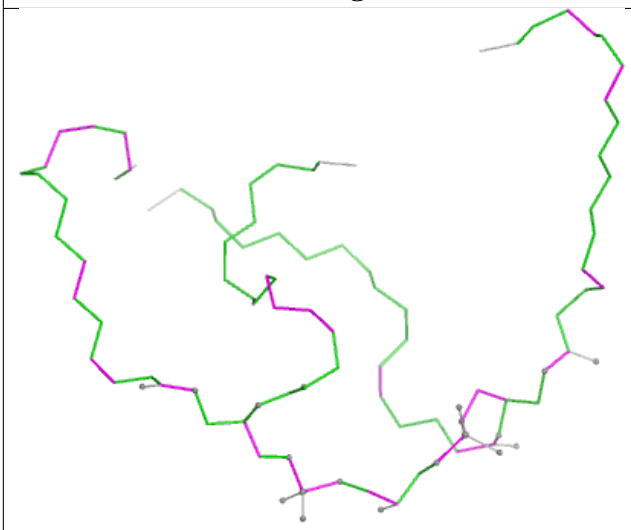
Ligand CDL DV 403



Bond lengths



Bond angles

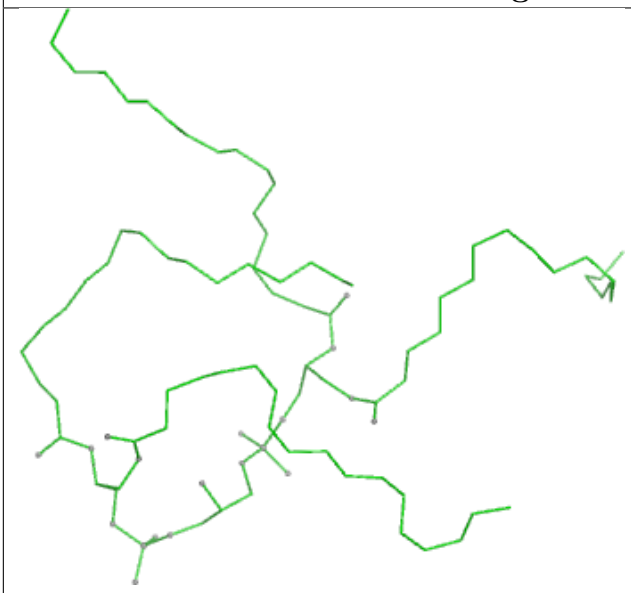


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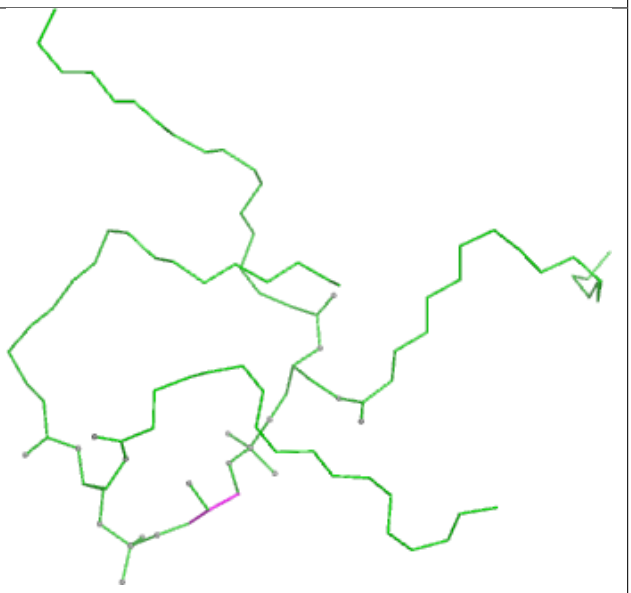


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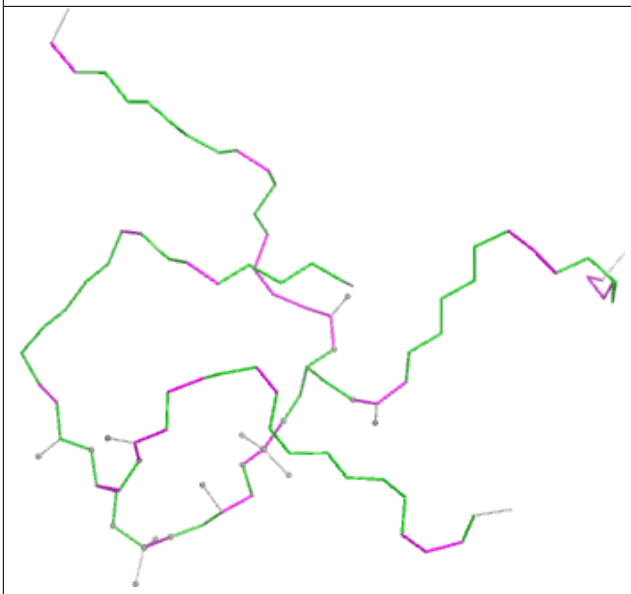
Ligand CDL BT 204



Bond lengths



Bond angles

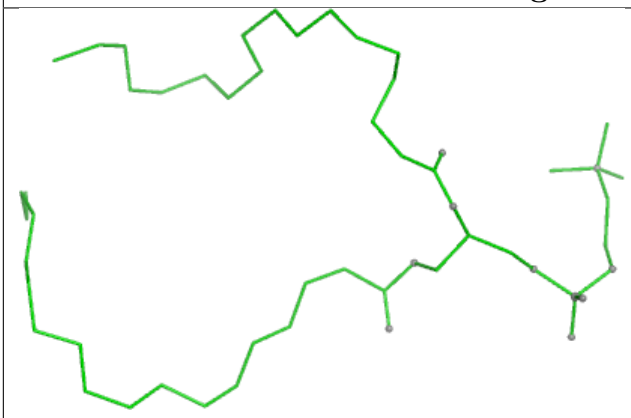


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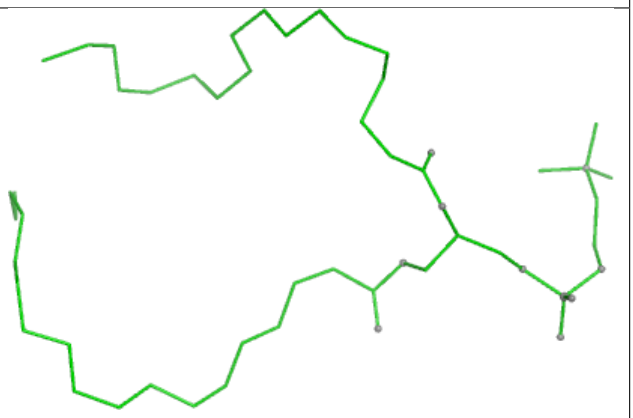


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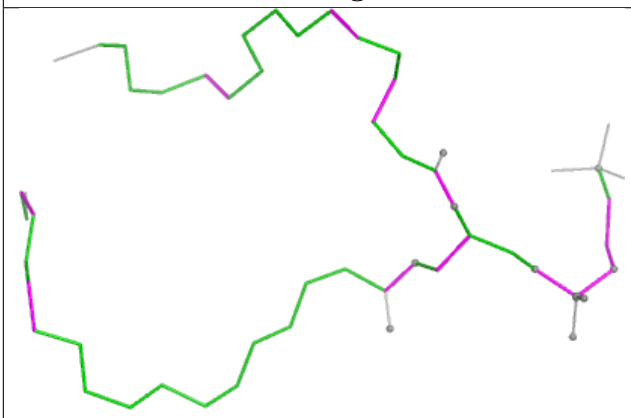
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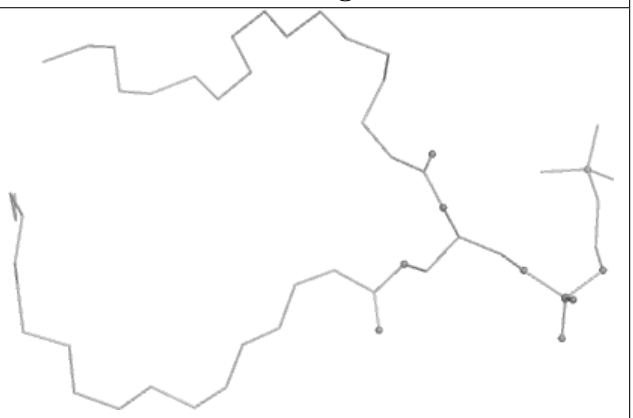
Bond lengths



Bond angles

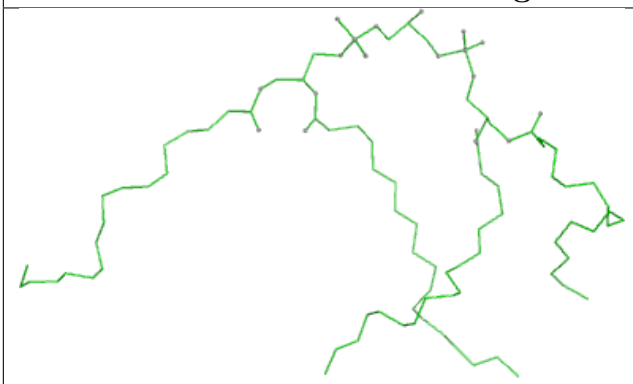


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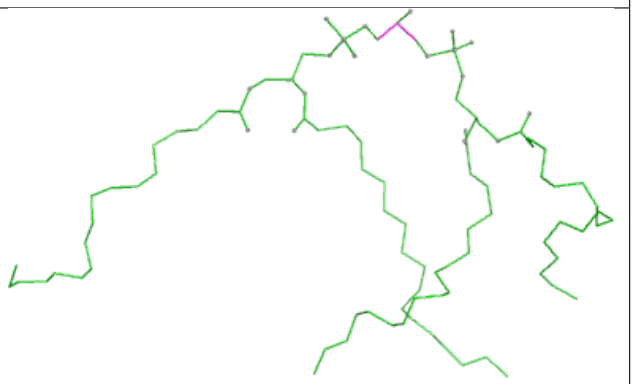


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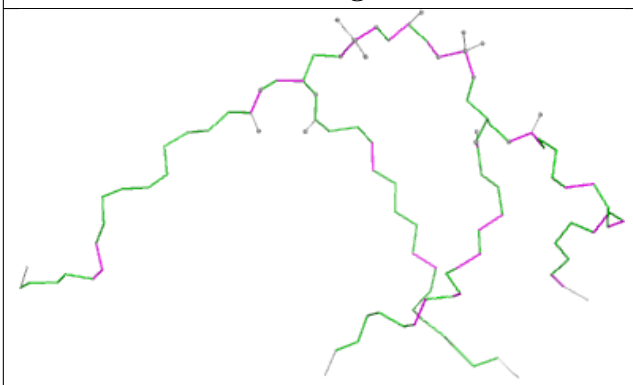
Ligand CDL Du 402



Bond lengths



Bond angles

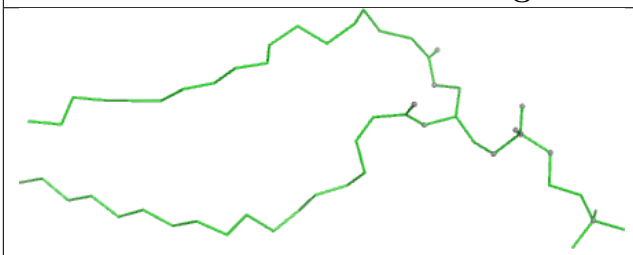


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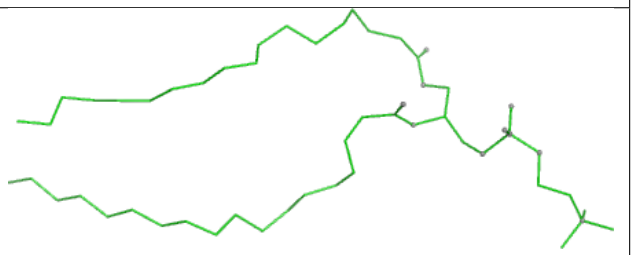


Rings

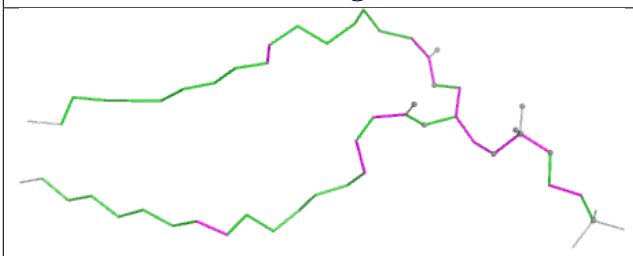
Ligand PC1 AA 907



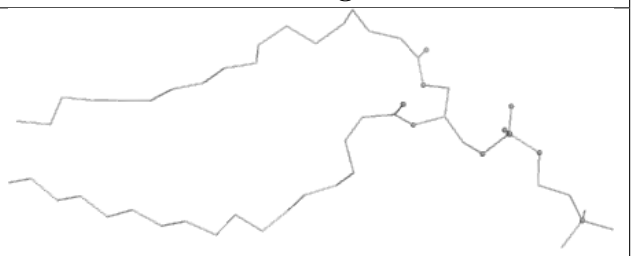
Bond lengths



Bond angles

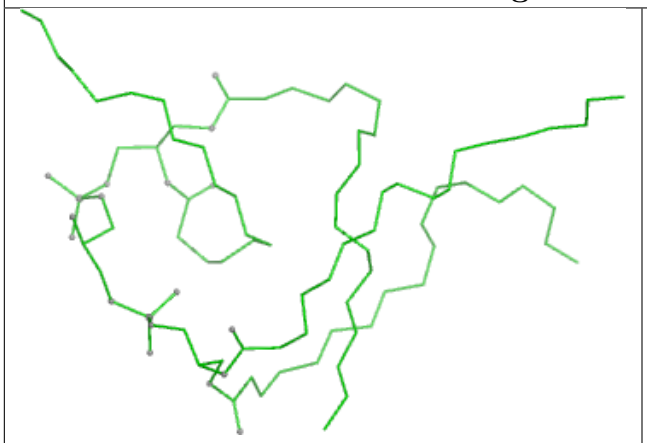


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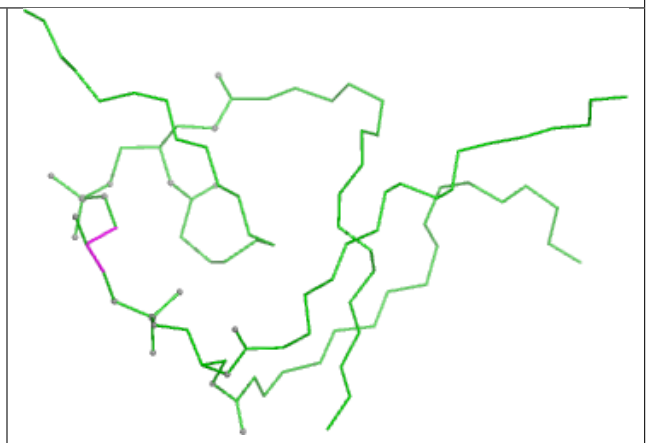


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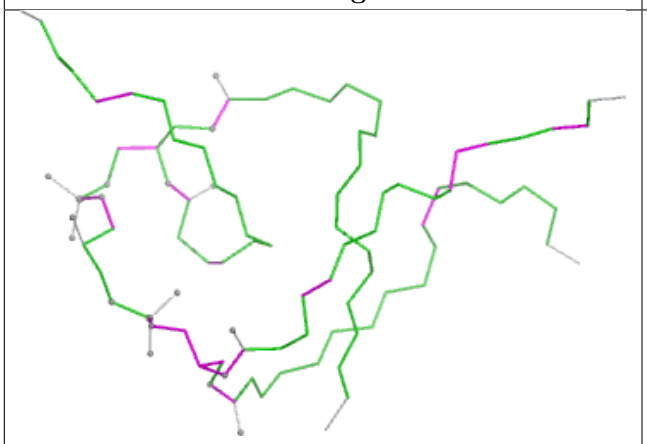
Ligand CDL CD 302



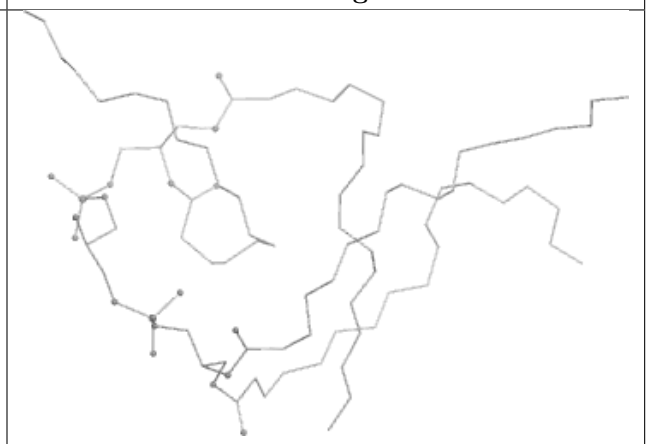
Bond lengths



Bond angles

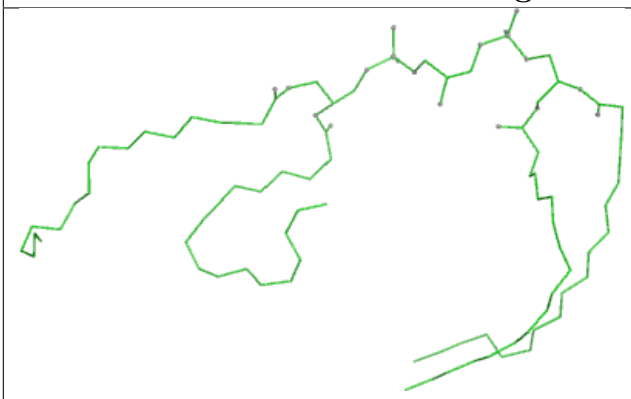


Torsions

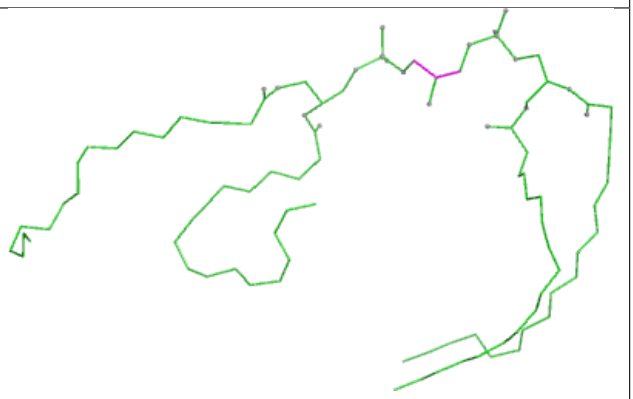


Rings

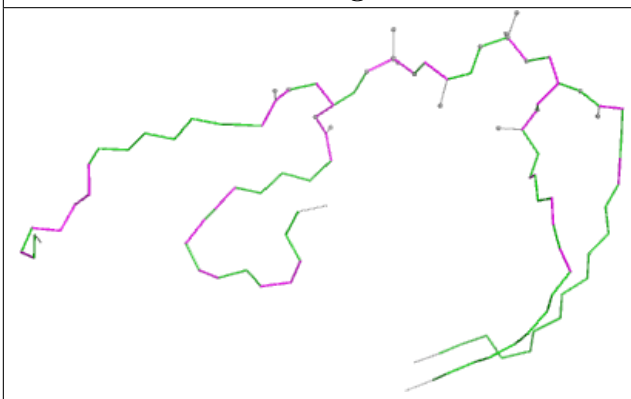
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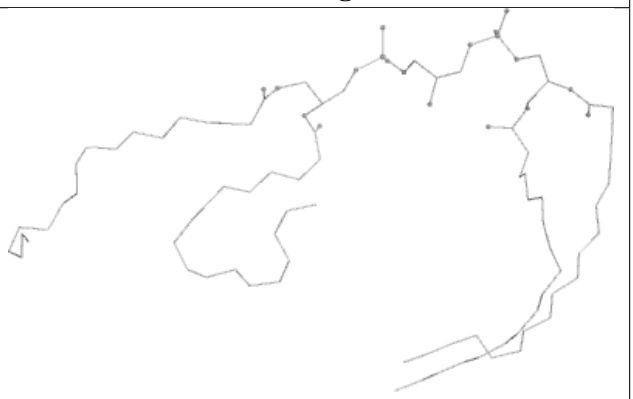
Bond lengths



Bond angles



Torsions

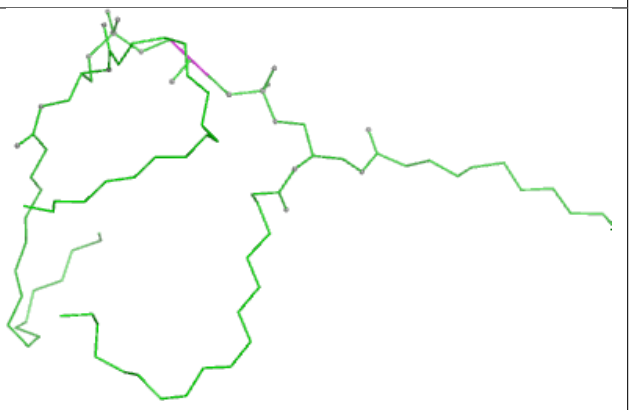


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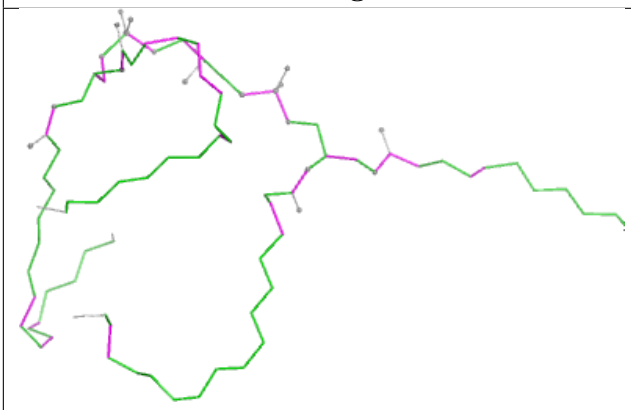
Ligand CDL Eu 101



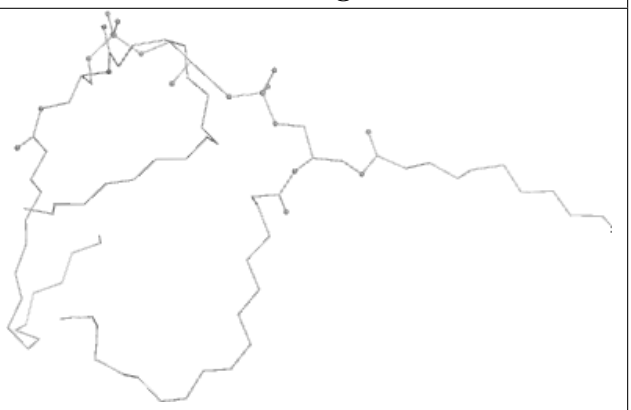
Bond lengths



Bond angles

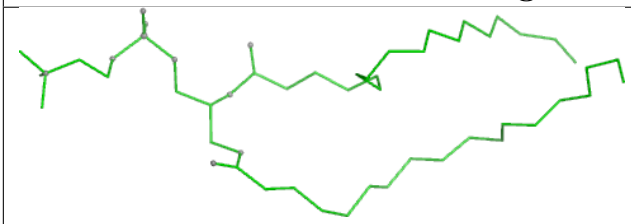


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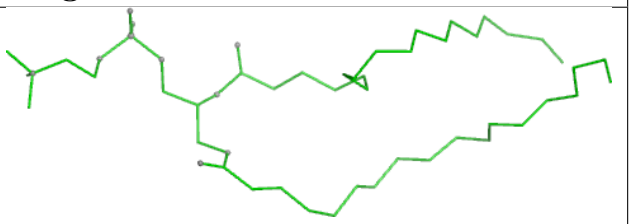


Rings

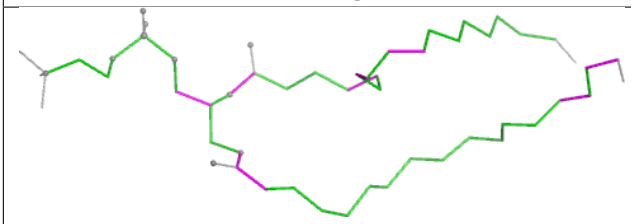
Ligand PC1 Dg 203



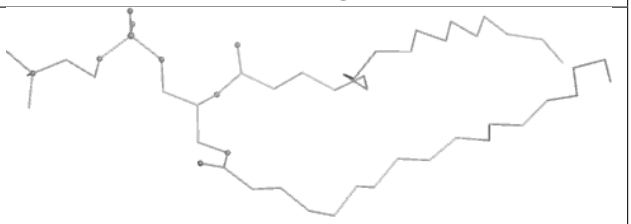
Bond lengths



Bond angles

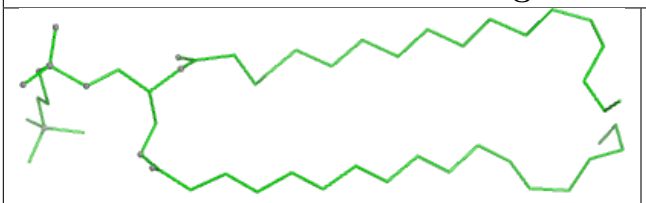


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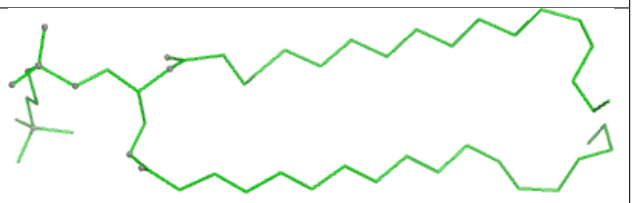


Rings

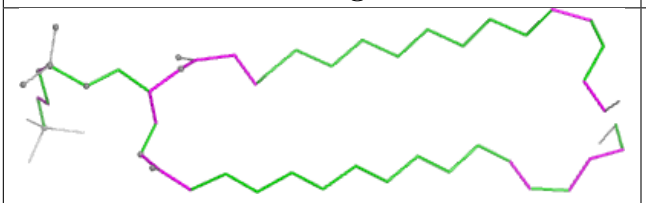
Ligand PC1 AA 906



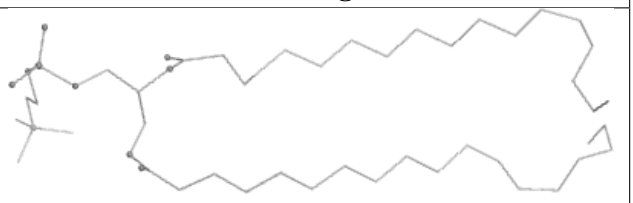
Bond lengths



Bond angles

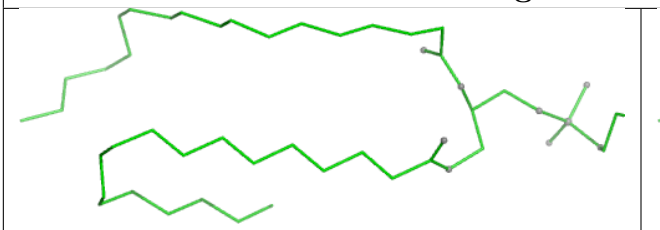


Torsions

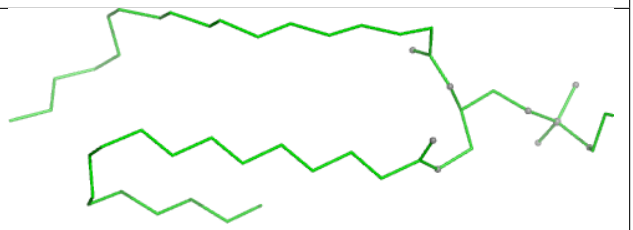


Rings

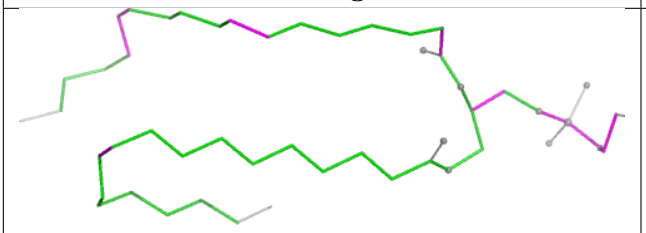
Ligand 3PE DX 302



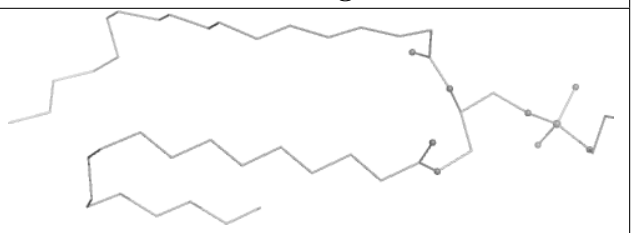
Bond lengths



Bond angles

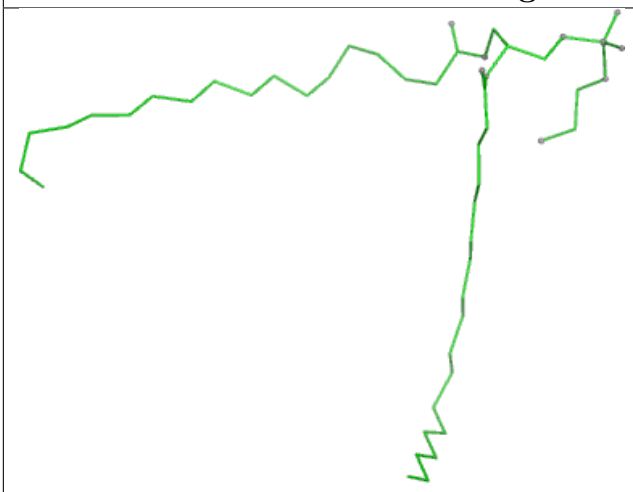


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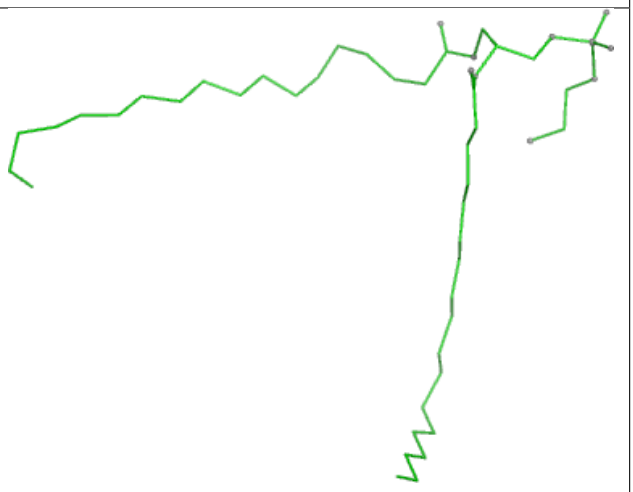


Rings

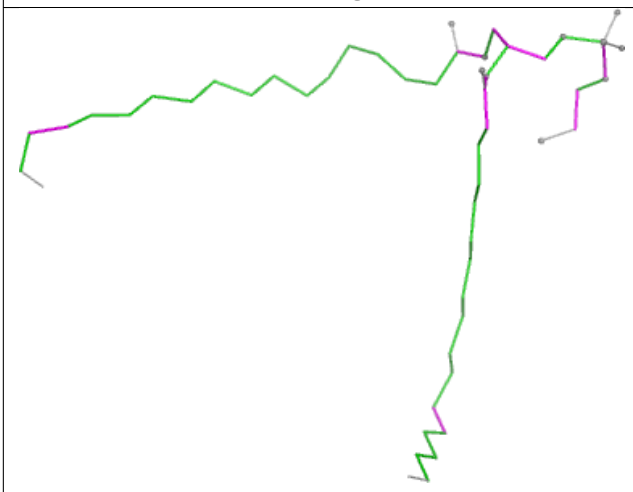
Ligand 3PE AJ 502



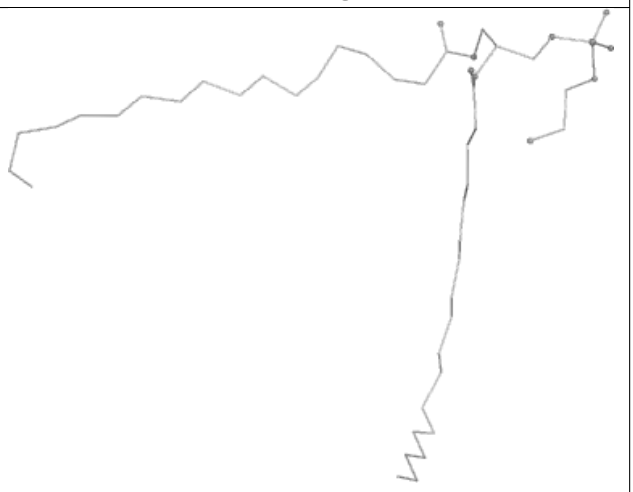
Bond lengths



Bond angles

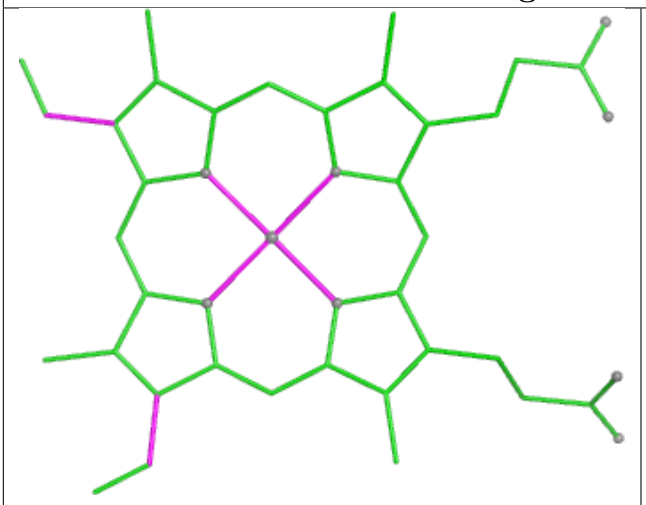


Torsions

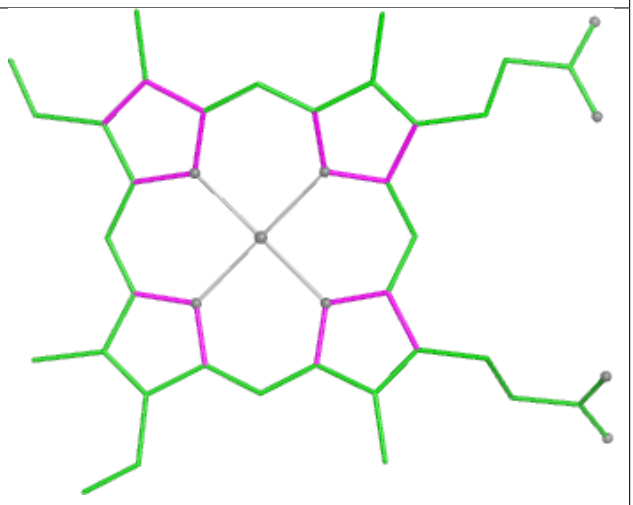


Rings

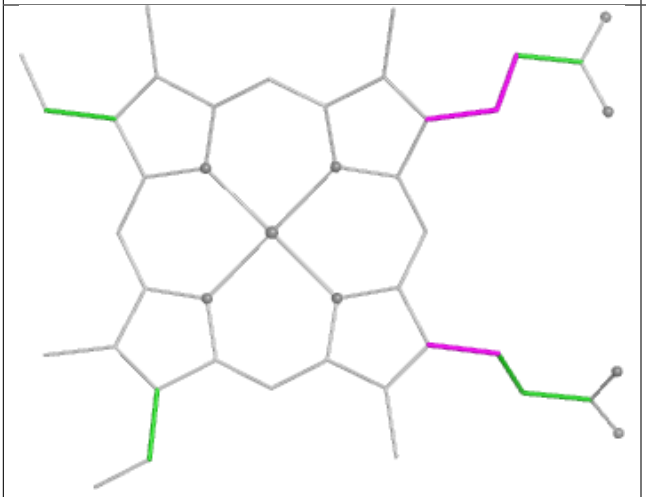
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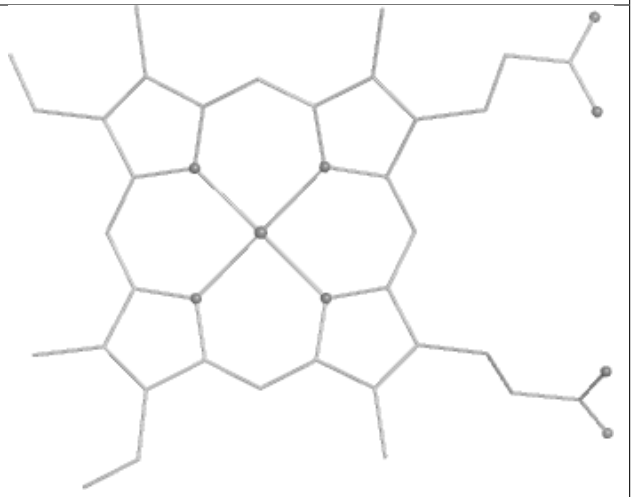
Bond lengths



Bond angles

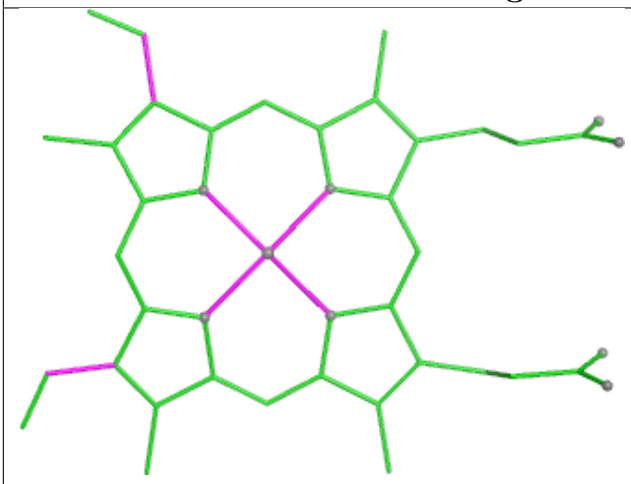


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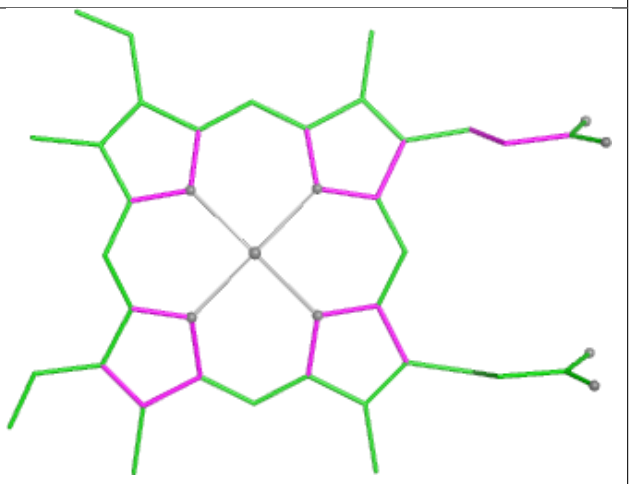


Rings

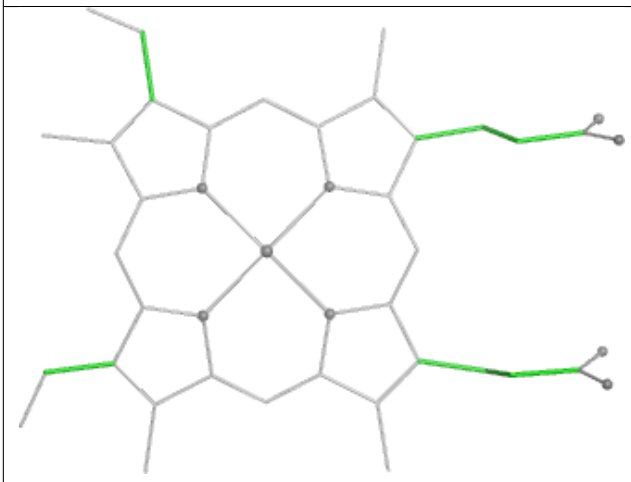
Ligand HEM ED 602



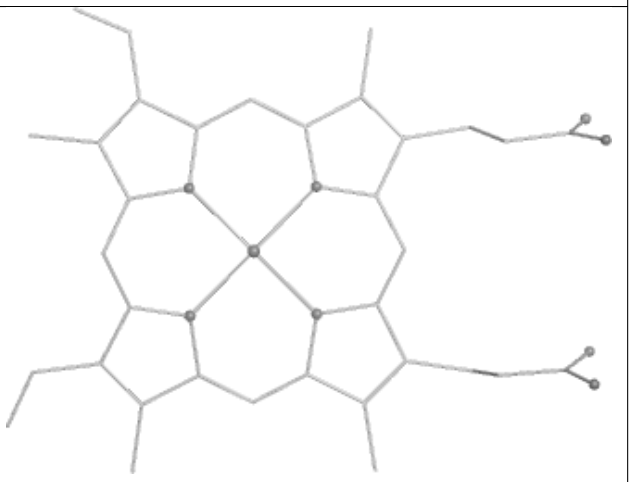
Bond lengths



Bond angles

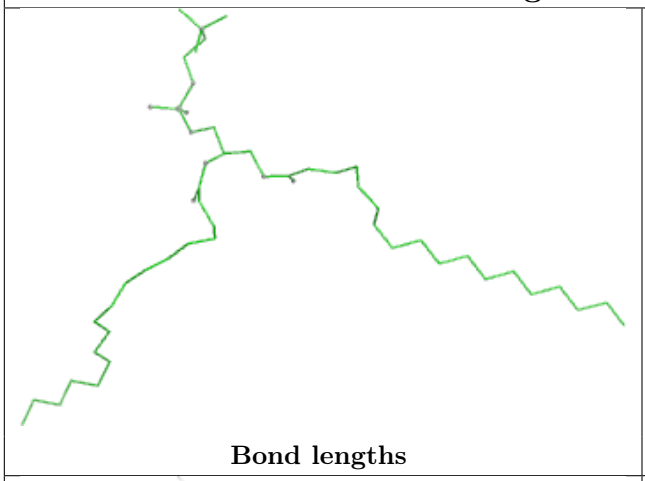


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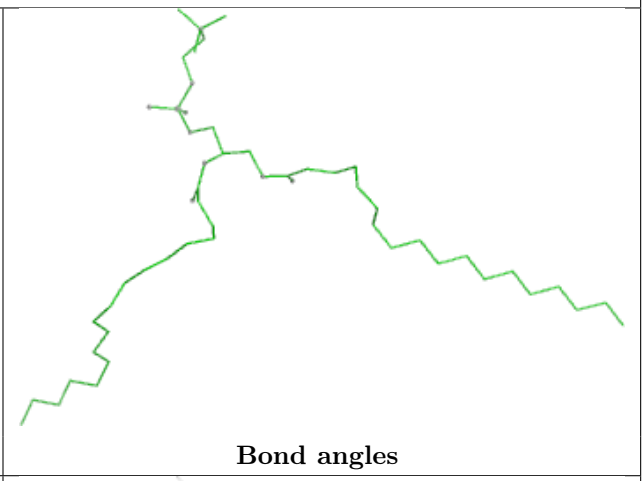


Rings

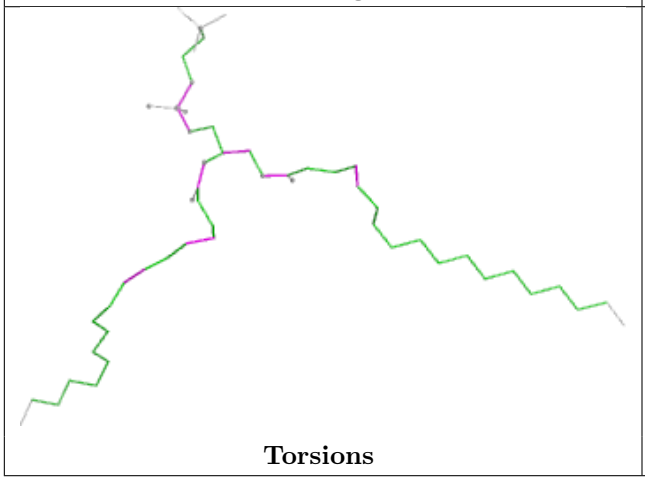
Ligand PC1 Ef 501



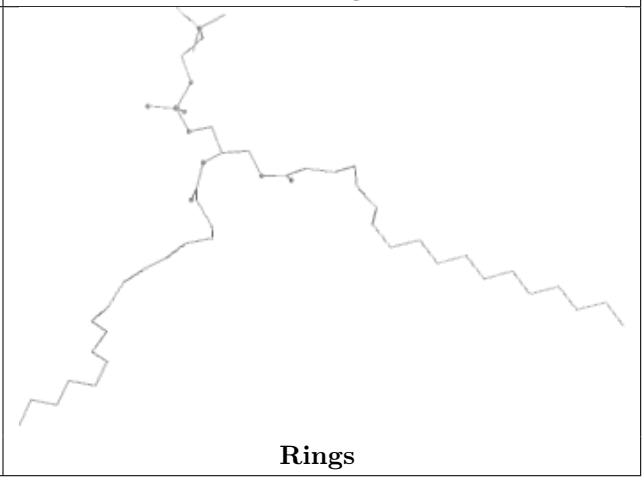
Bond lengths



Bond angles

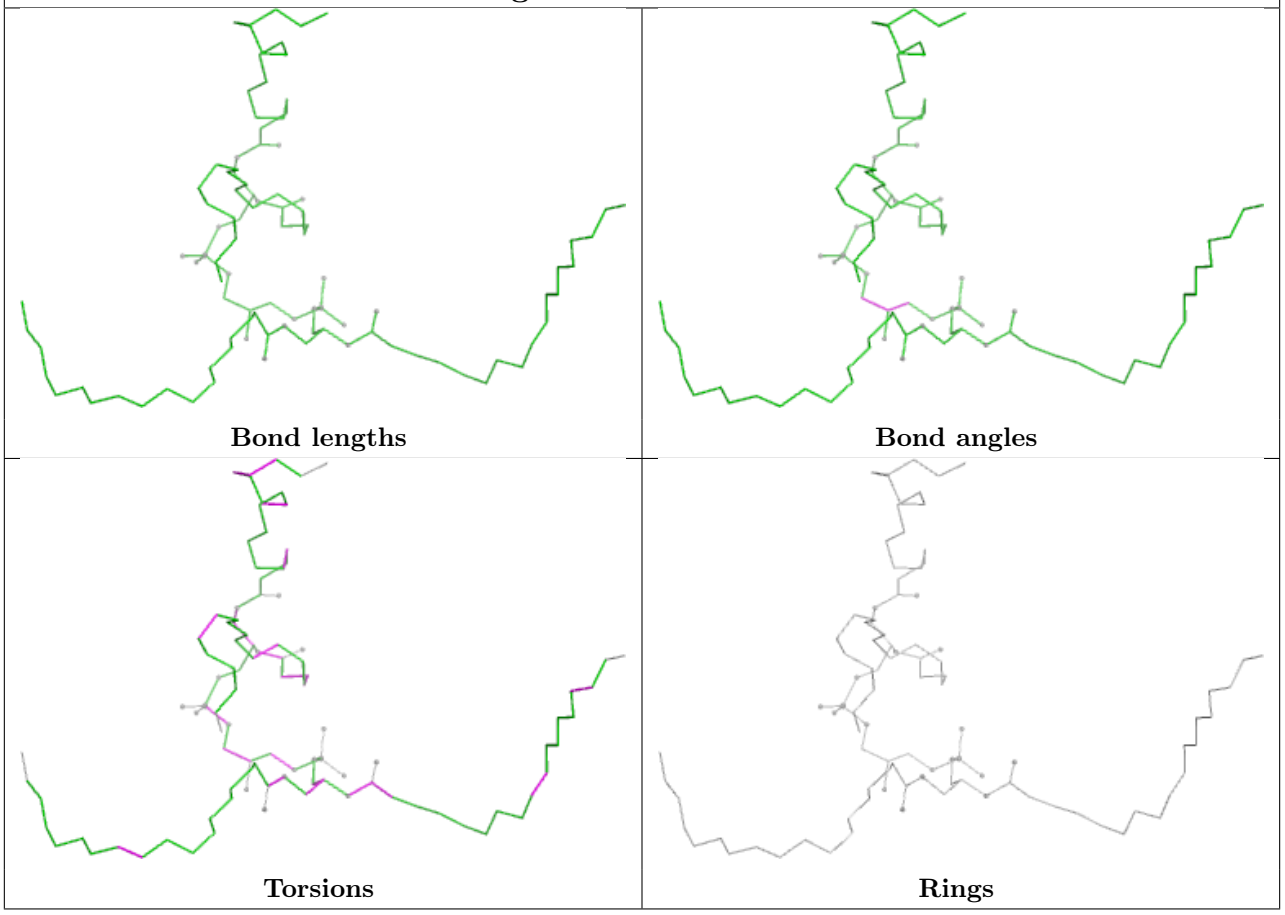


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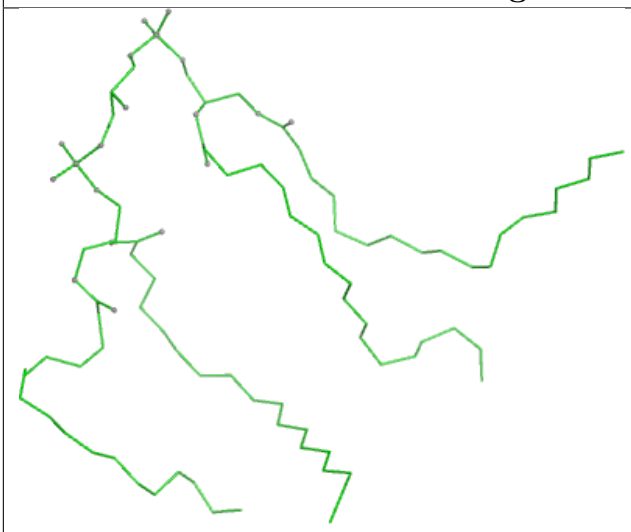


Rings

Ligand CDL DX 307



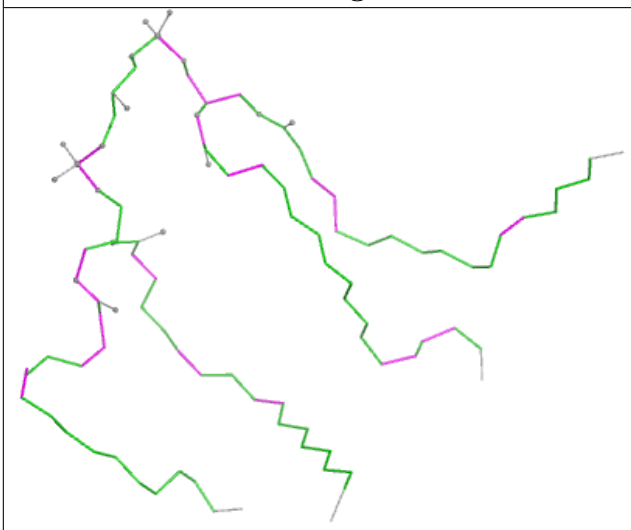
Ligand CDL DG 202



Bond lengths



Bond angles

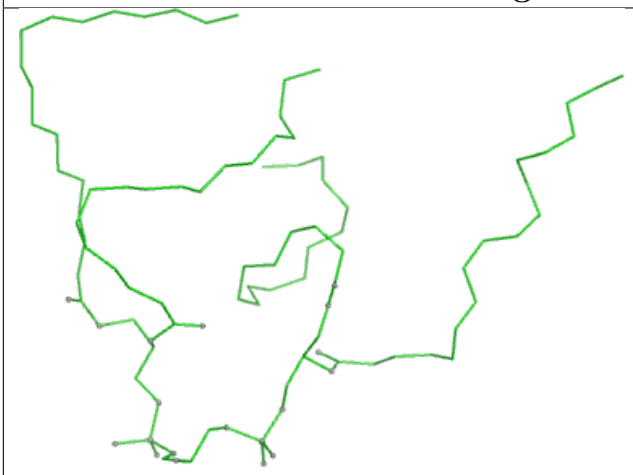


Torsions



Rings

Ligand CDL DS 405



Bond lengths



Bond angles

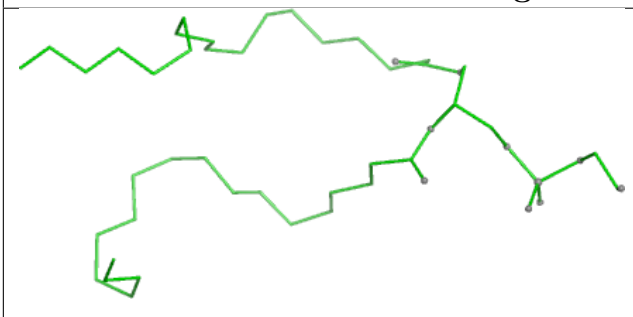


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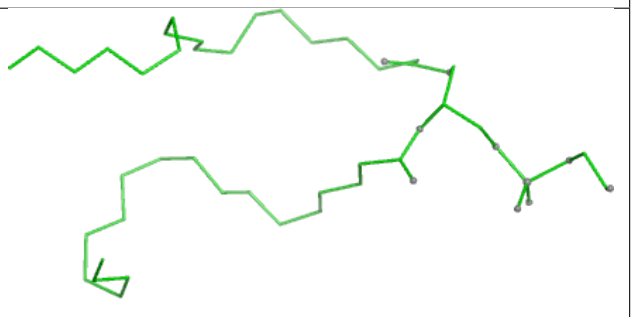


Rings

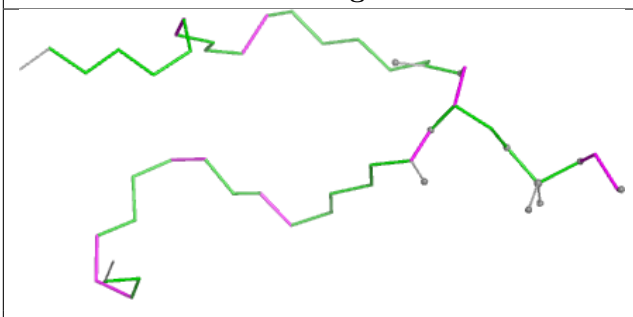
Ligand 3PE DN 501



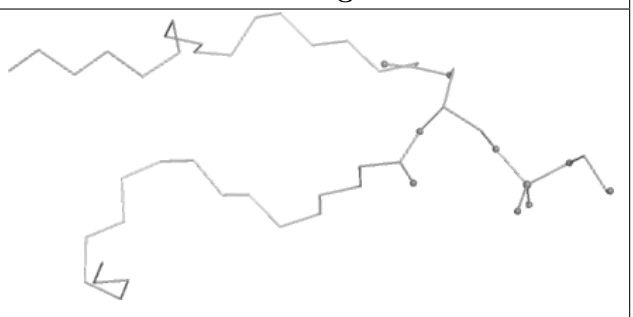
Bond lengths



Bond angles

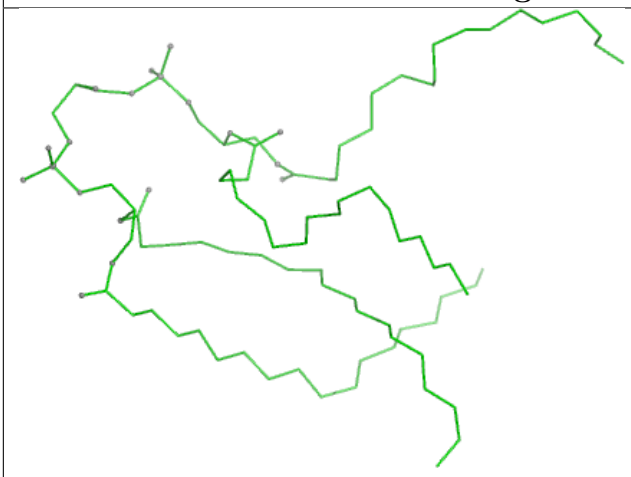


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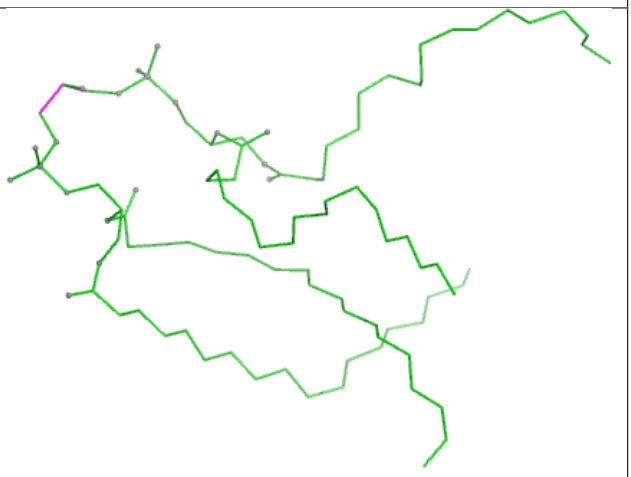


Rings

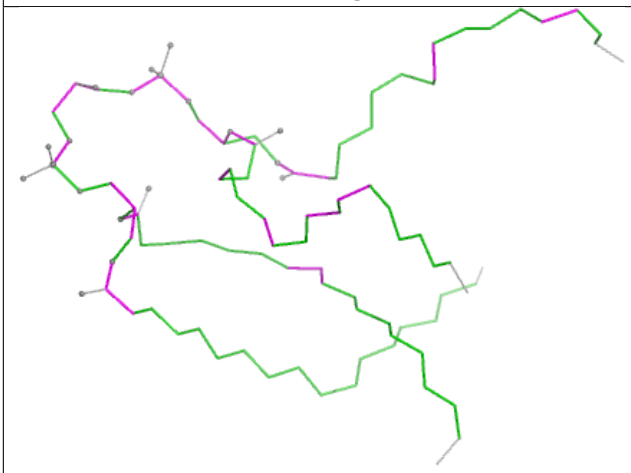
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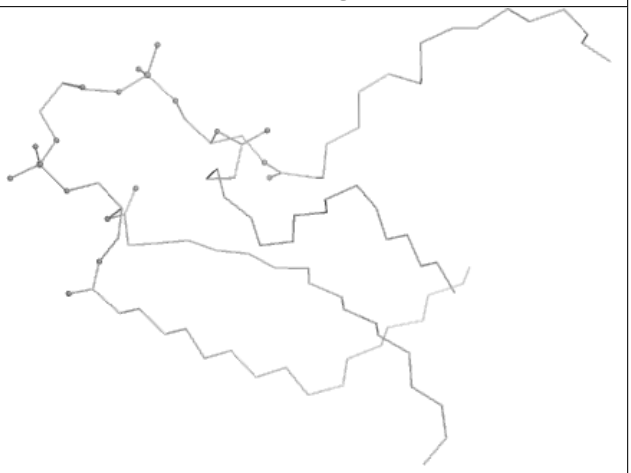
Bond lengths



Bond angles

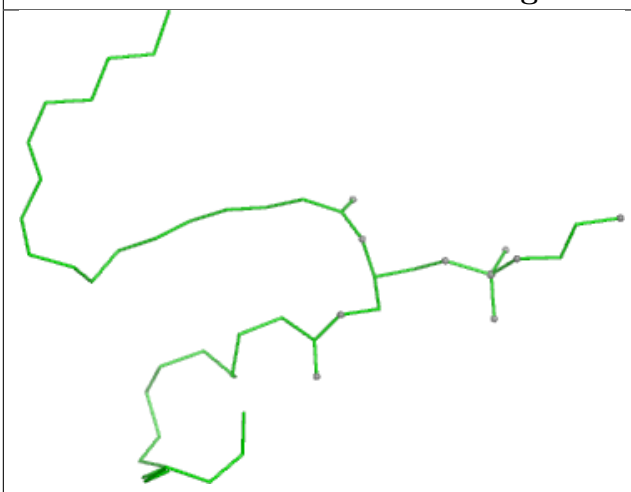


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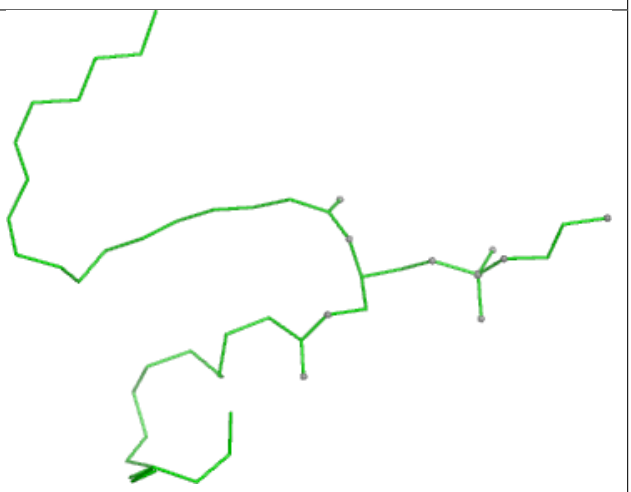


Rings

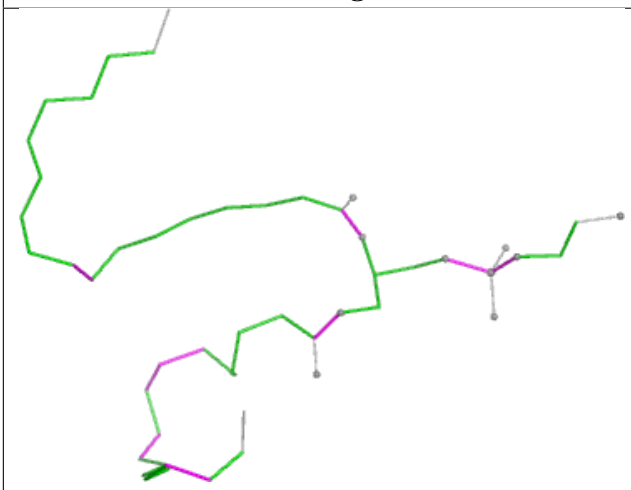
Ligand 3PE Ds 408



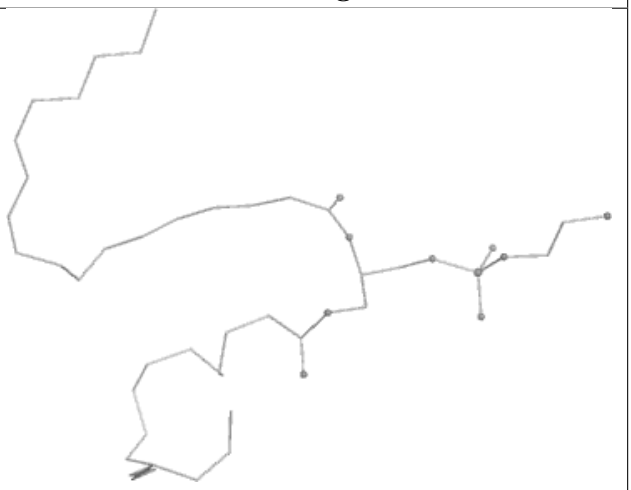
Bond lengths



Bond angles

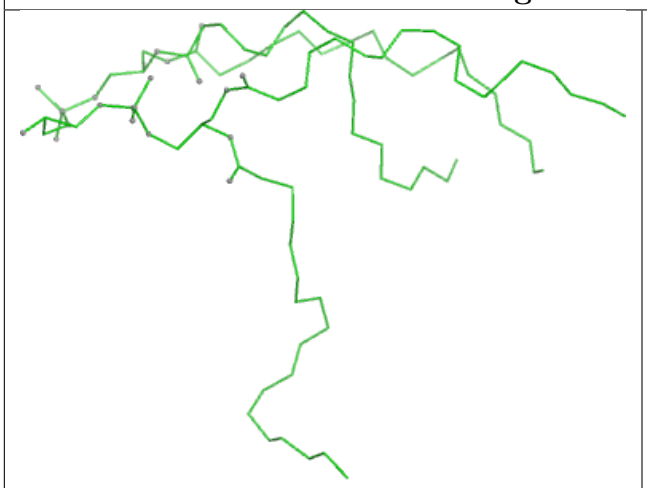


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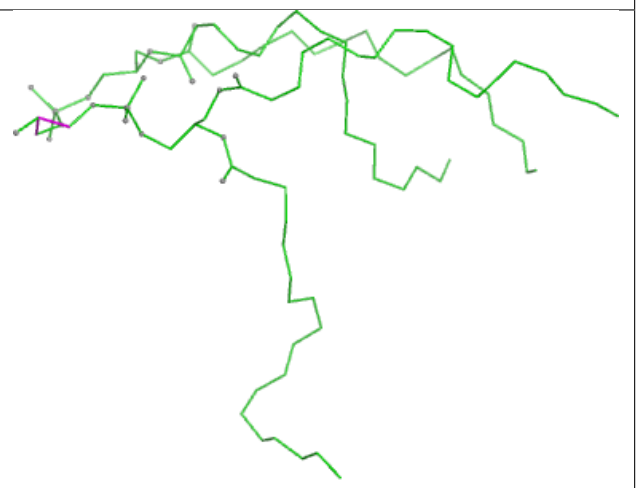


Rings

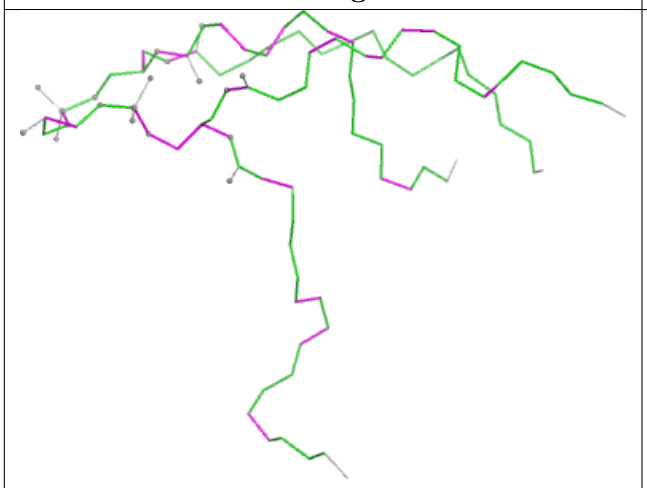
Ligand CDL DS 401



Bond lengths



Bond angles

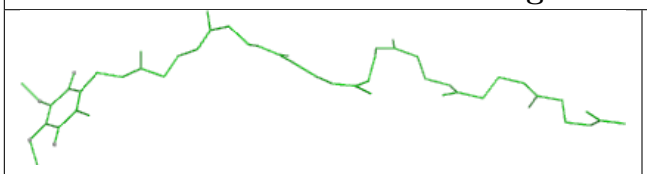


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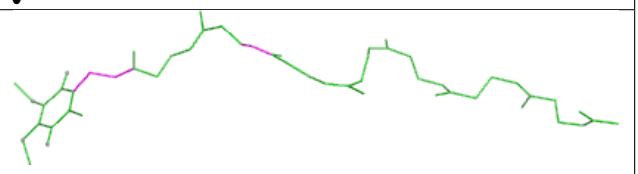


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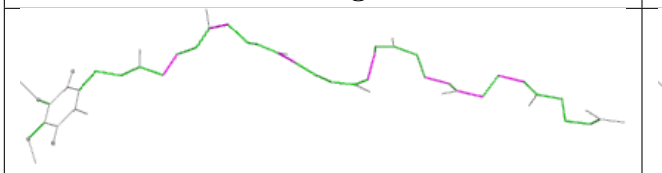
Ligand UQ8 C 512



Bond lengths



Bond angles

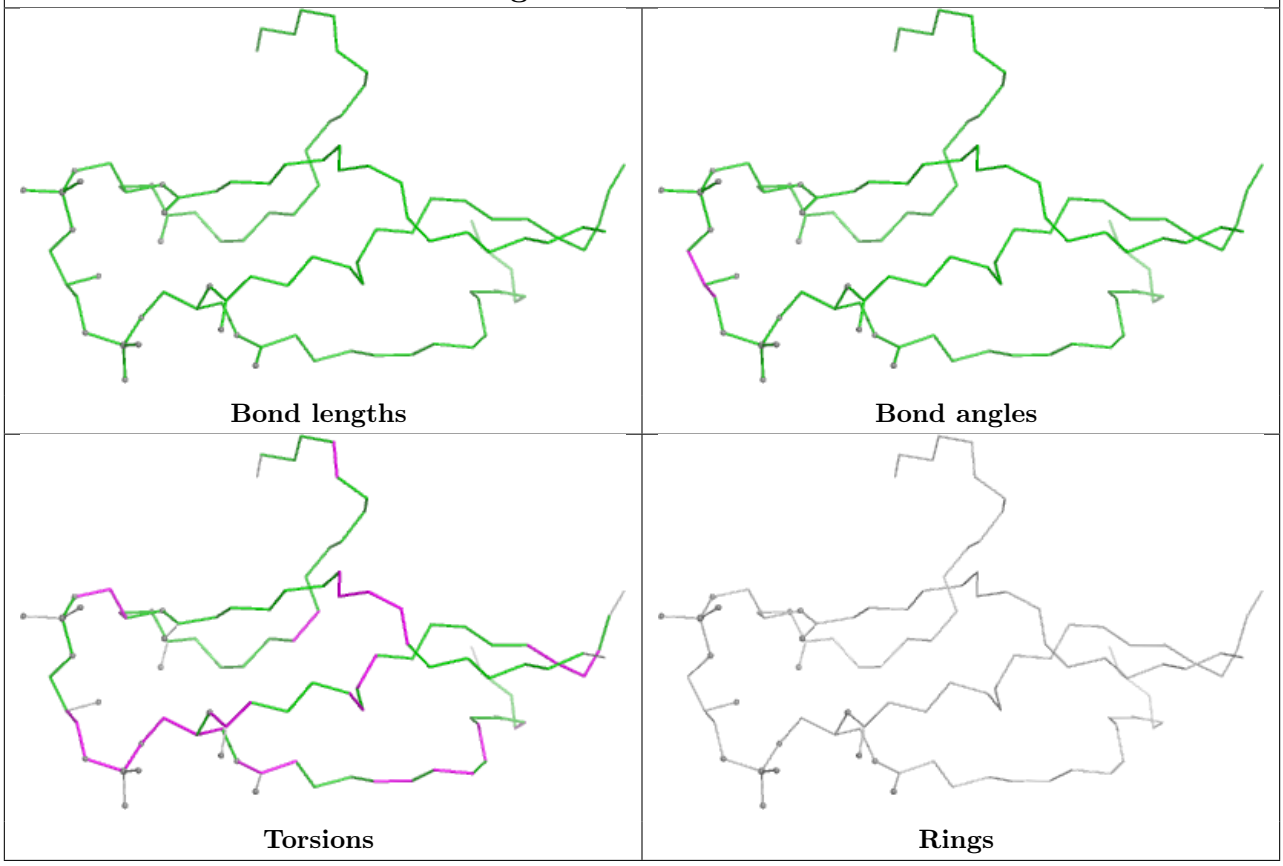


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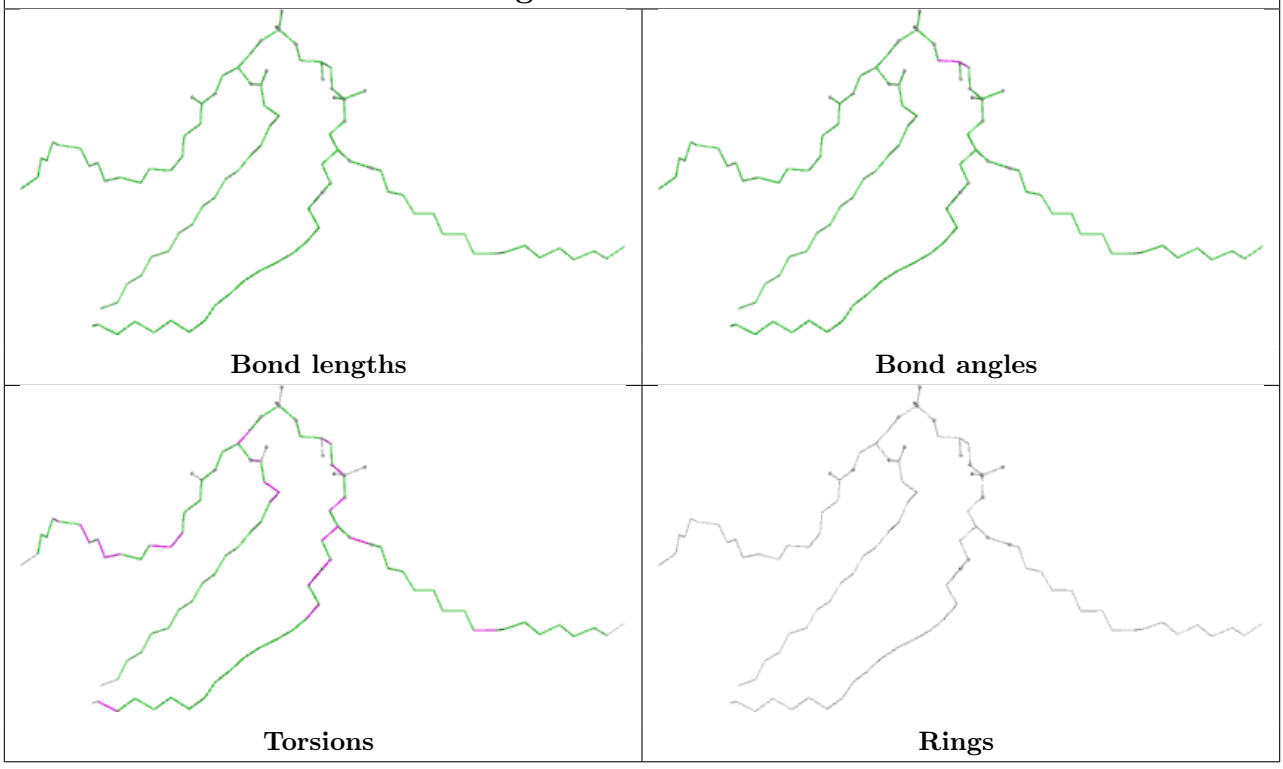


Rings

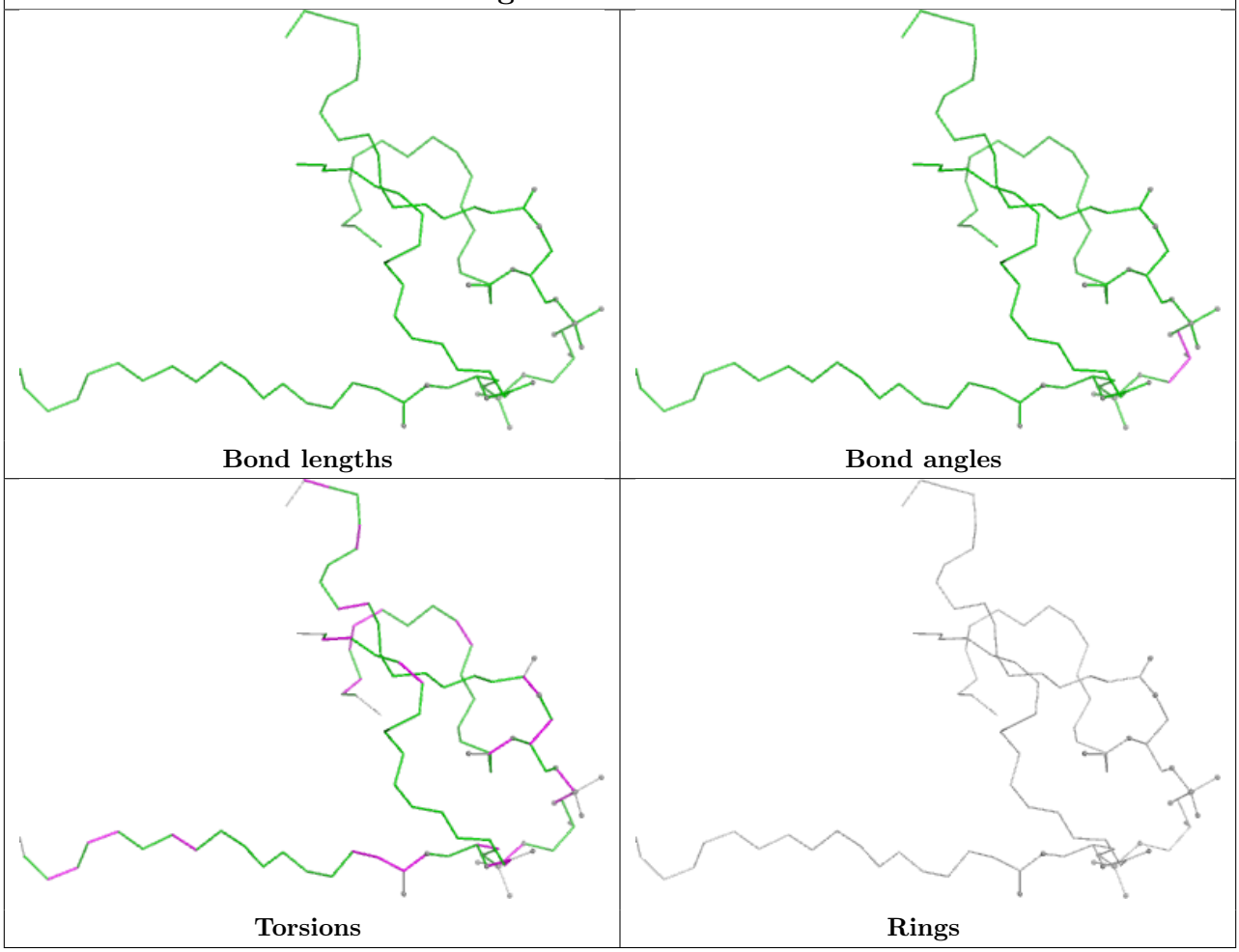
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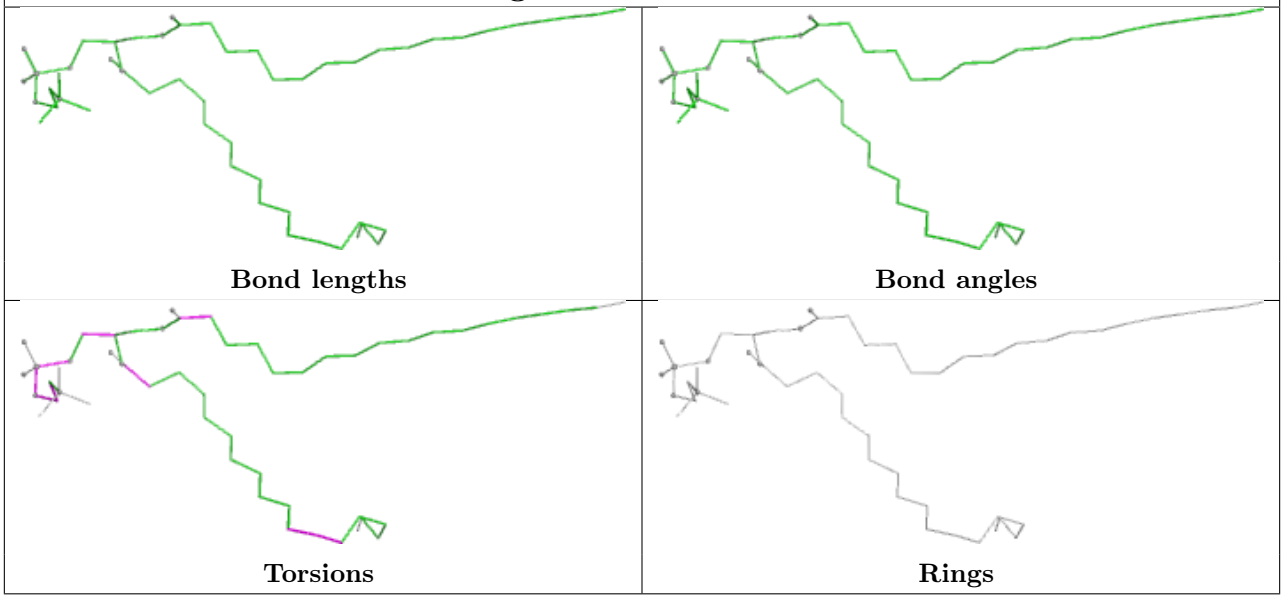
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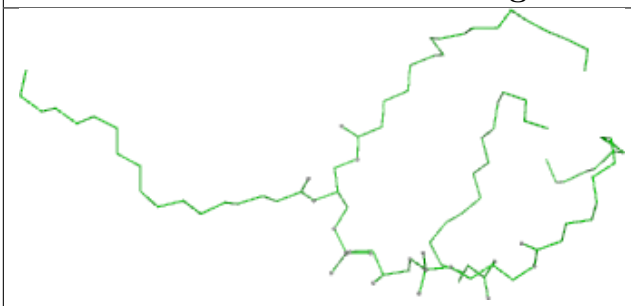
Ligand CDL EL 903



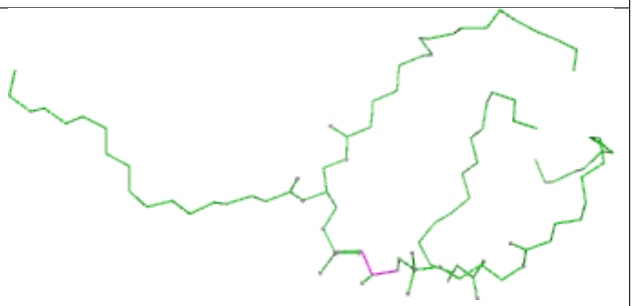
Ligand PC1 Dx 1203



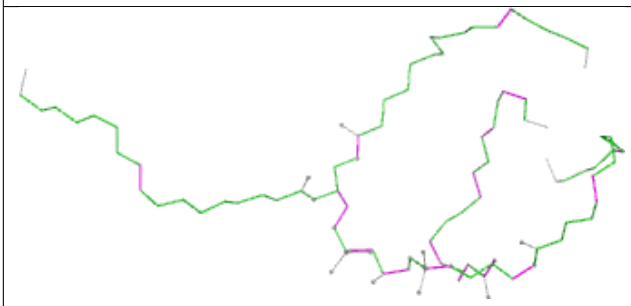
Ligand CDL DU 404



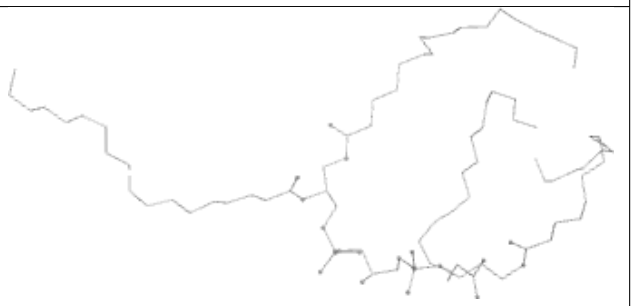
Bond lengths



Bond angles

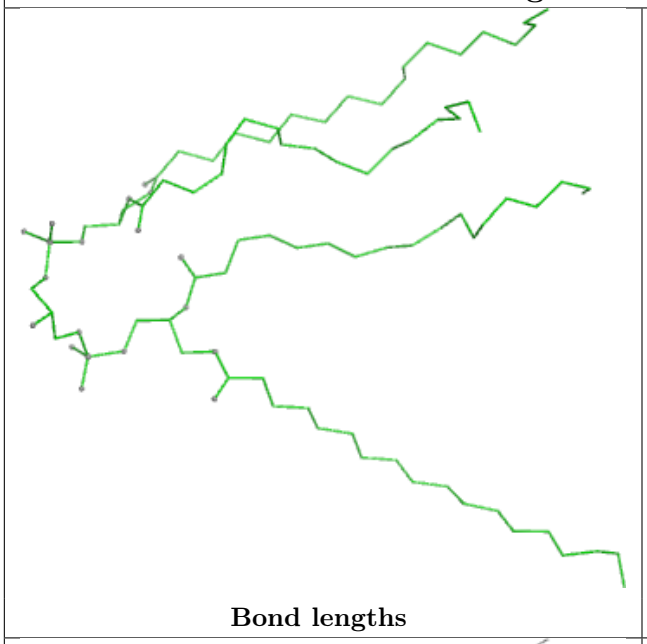


Torsions

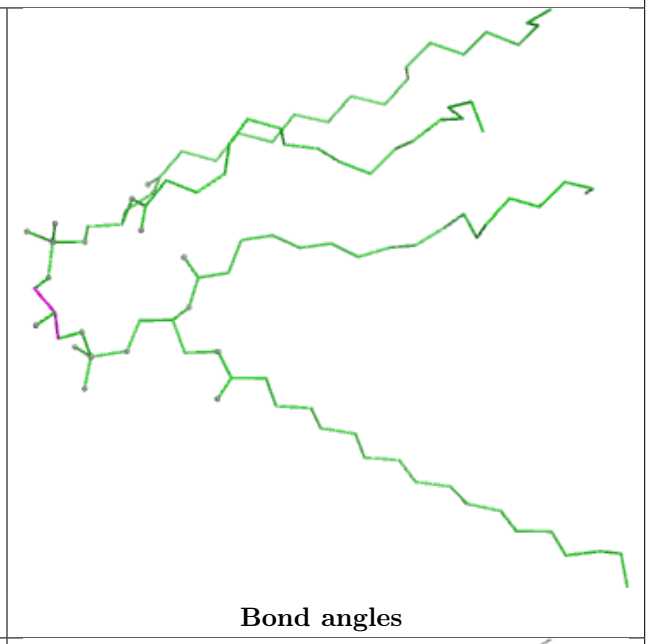


Rings

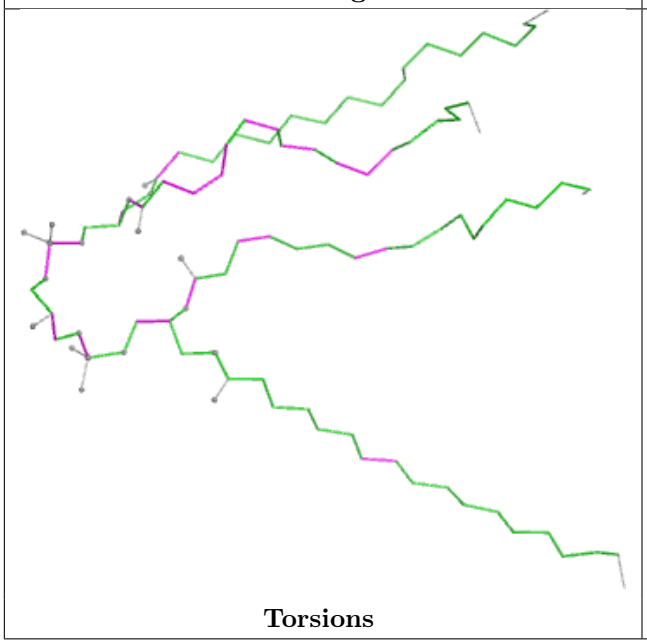
Ligand CDL E 301



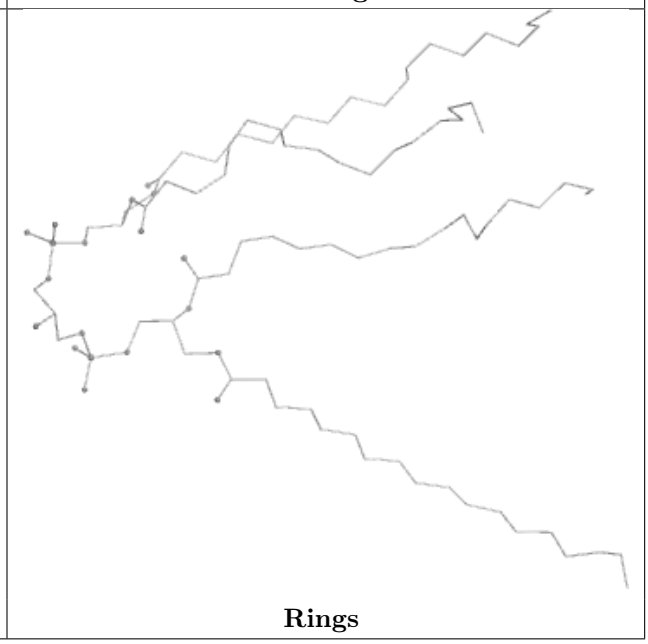
Bond lengths



Bond angles

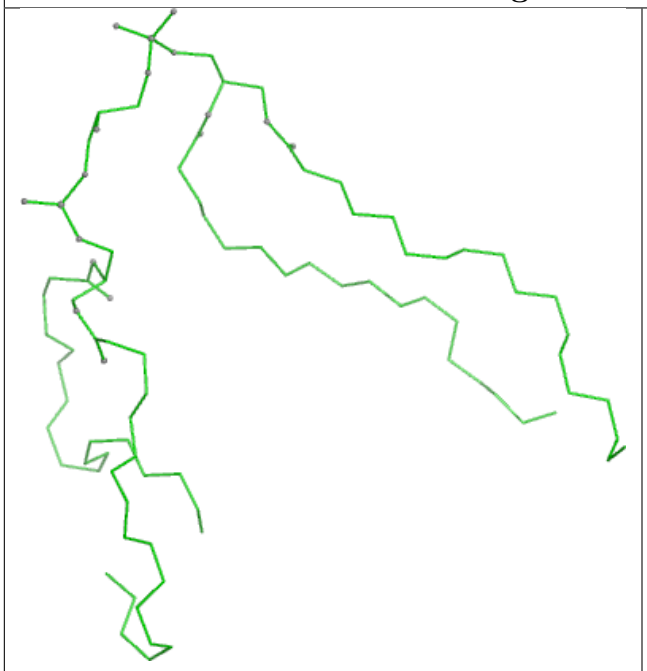


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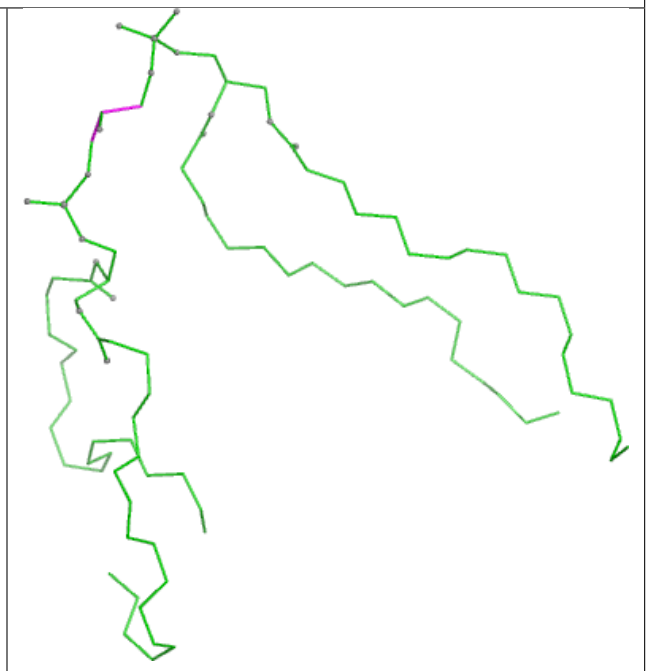


Rings

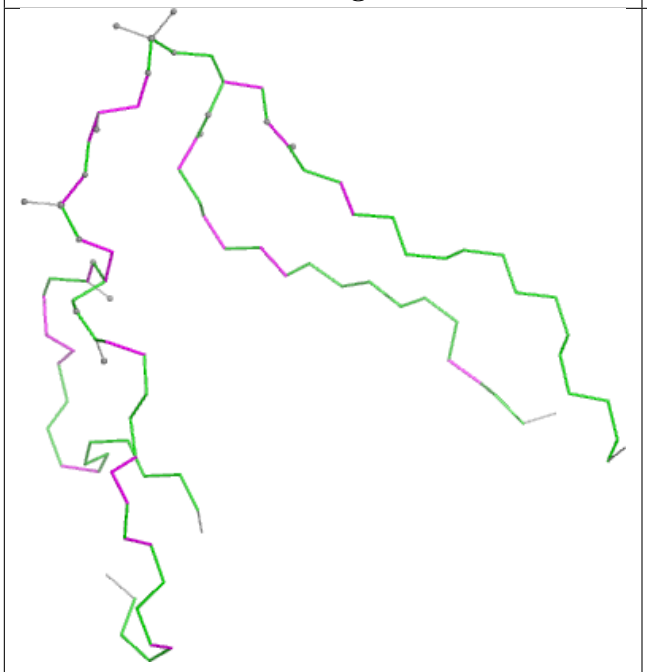
Ligand CDL DR 403



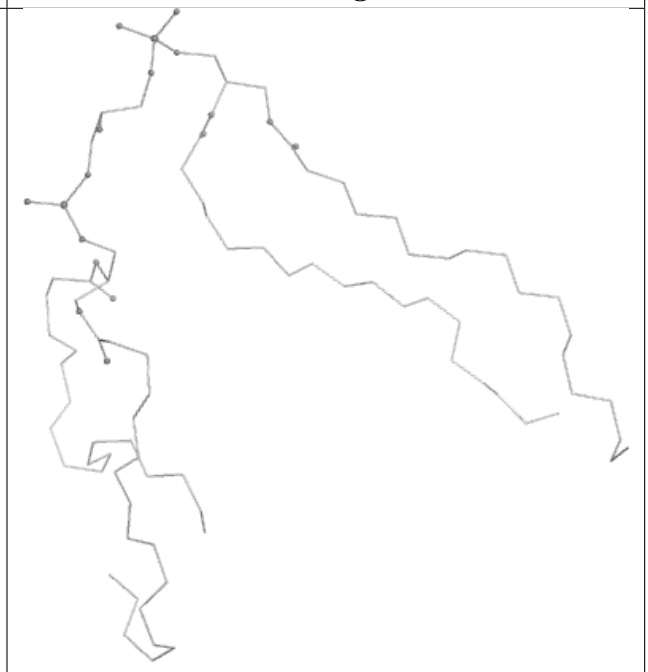
Bond lengths



Bond angles

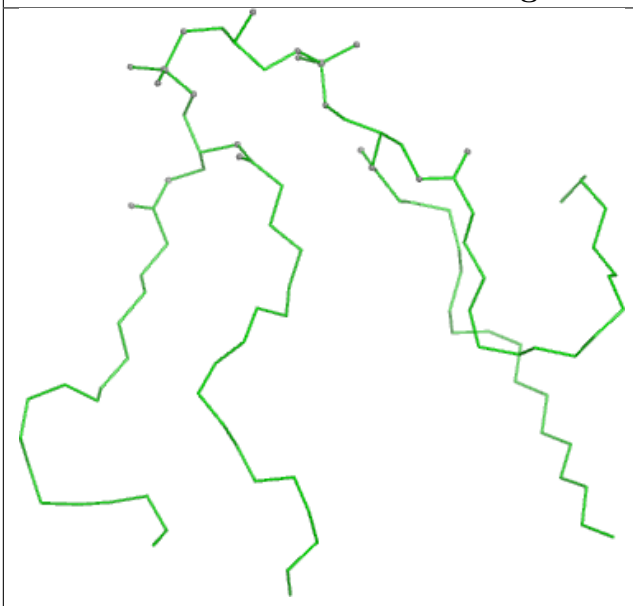


Torsions

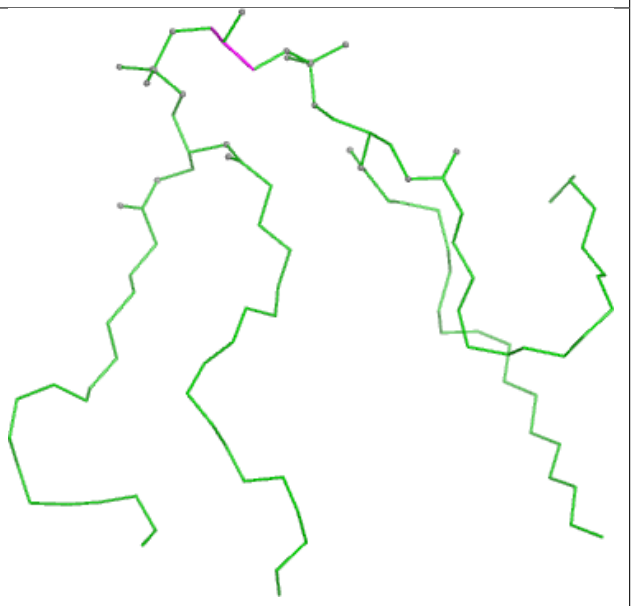


Rings

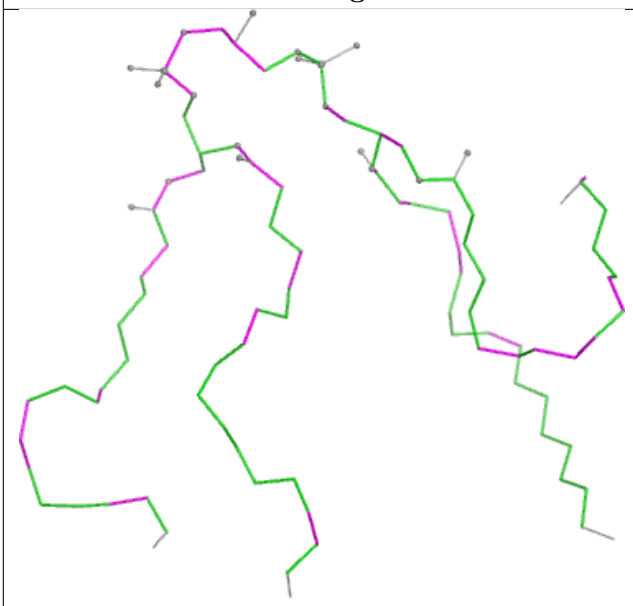
Ligand CDL El 902



Bond lengths



Bond angles

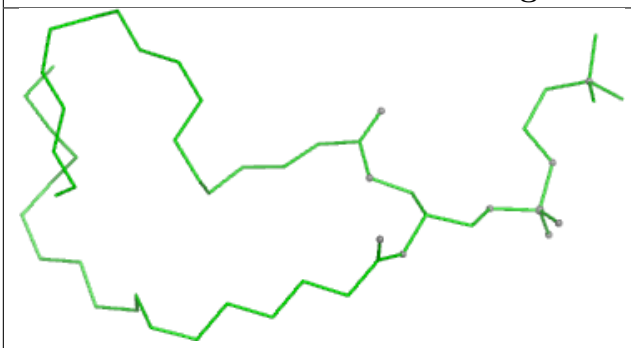


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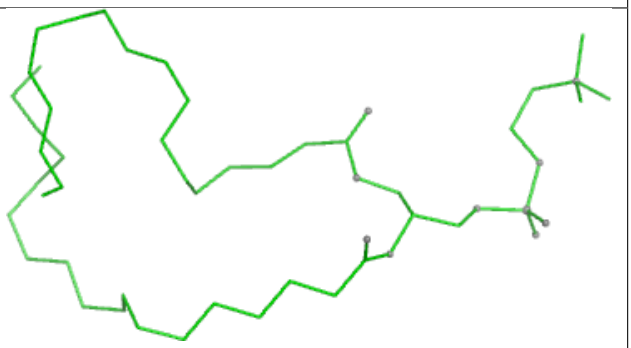


Rings

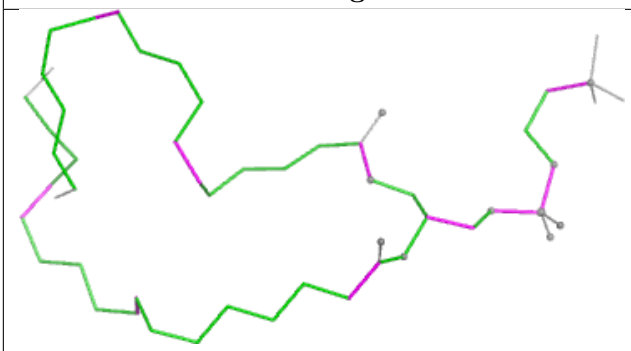
Ligand PC1 DI 303



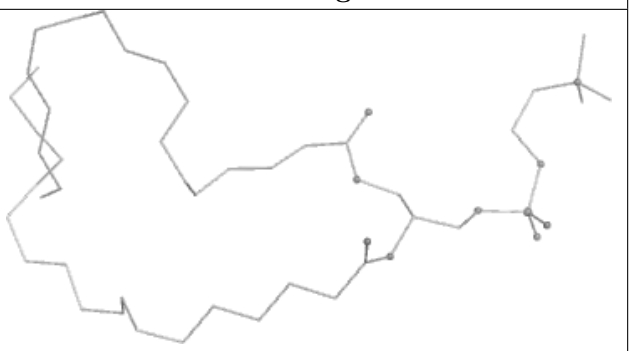
Bond lengths



Bond angles

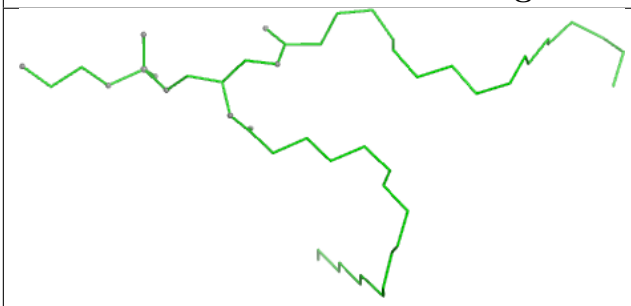


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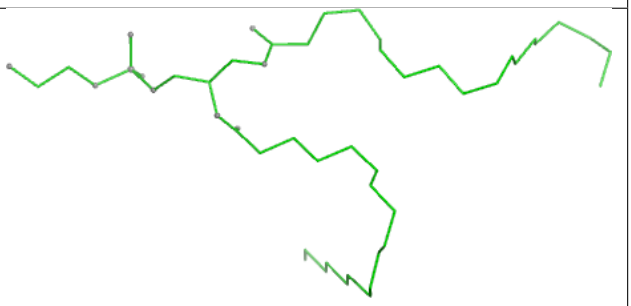


Rings

Ligand 3PE DX 303



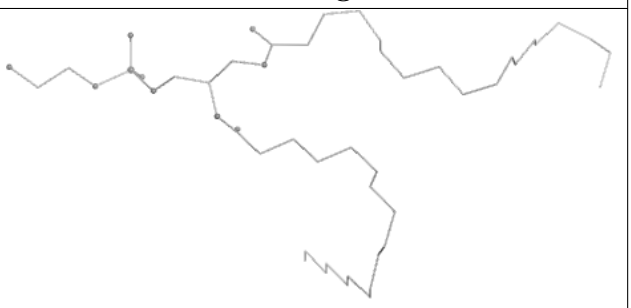
Bond lengths



Bond angles

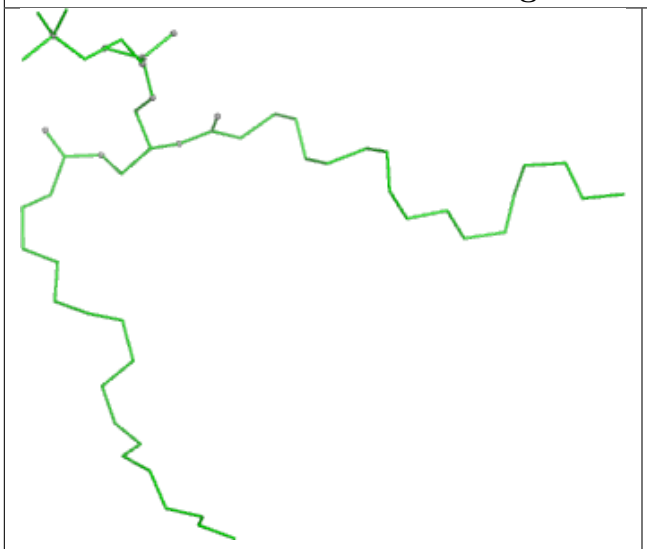


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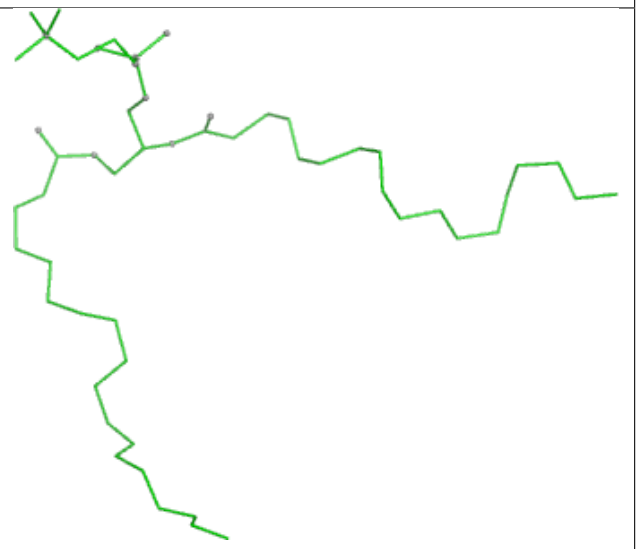


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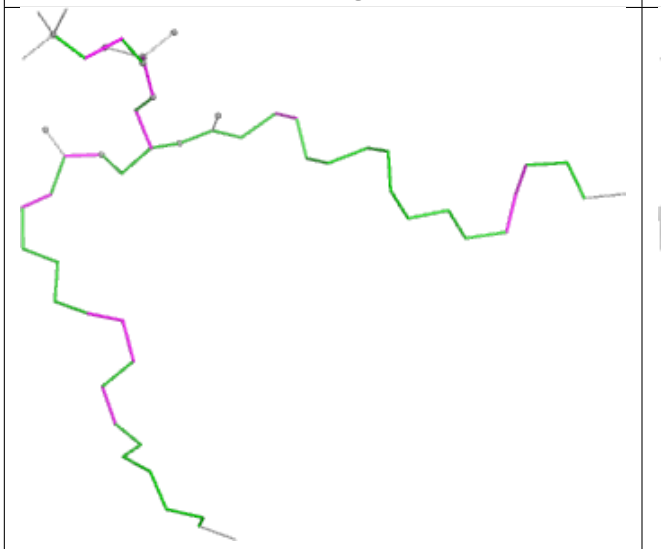
Ligand PC1 B1 403



Bond lengths



Bond angles

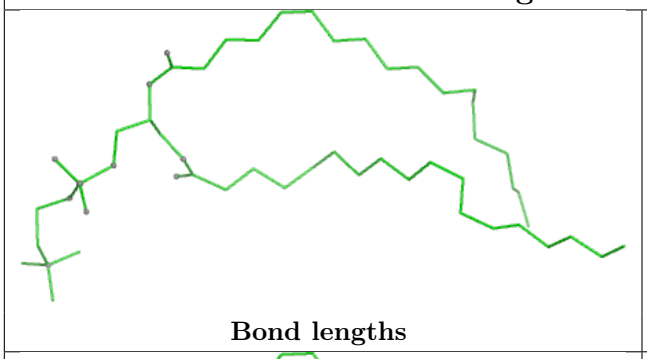


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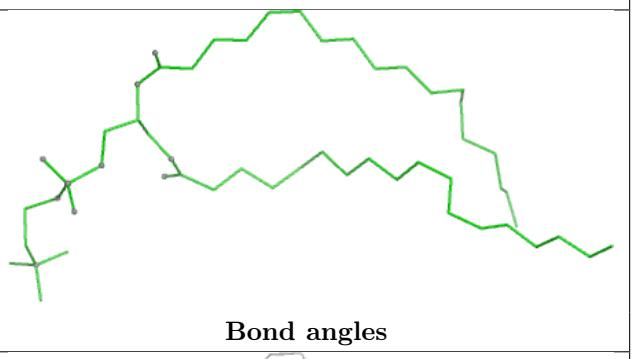


Rings

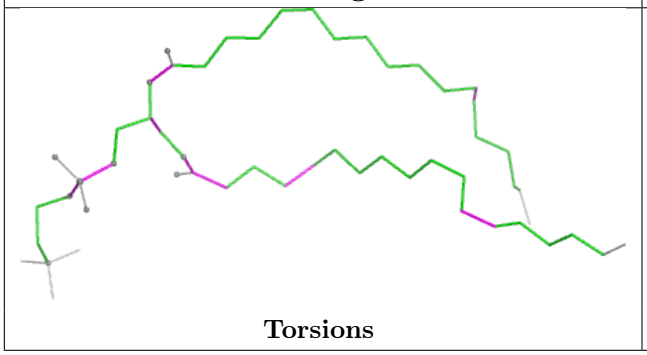
Ligand PC1 BT 203



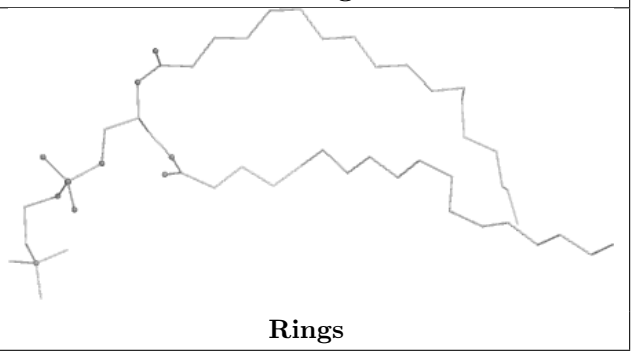
Bond lengths



Bond angles

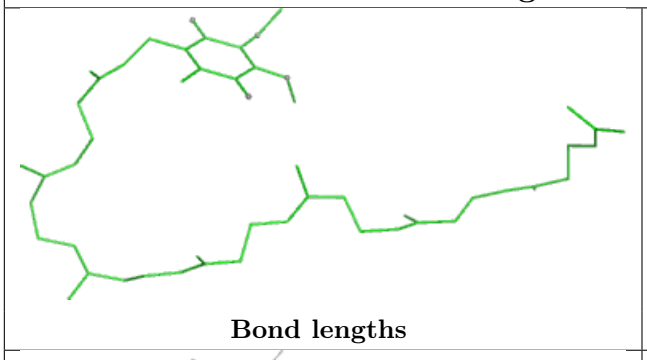


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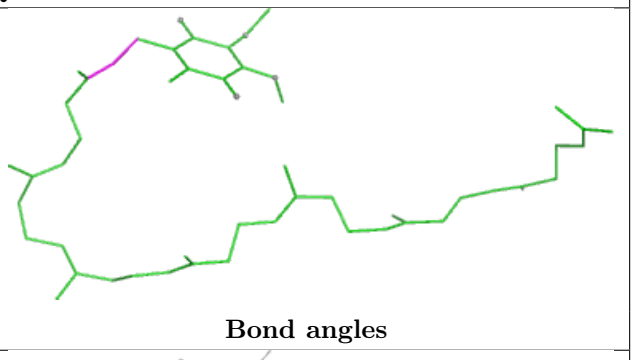


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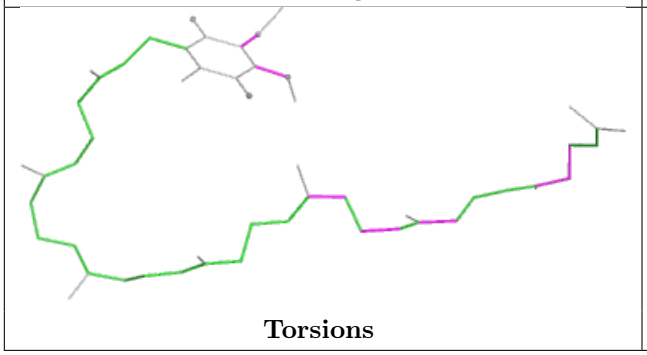
Ligand UQ8 Ds 404



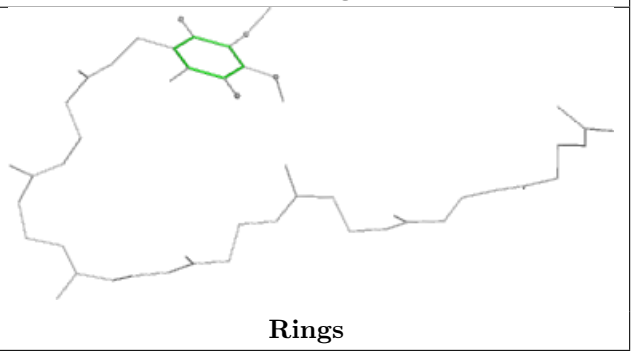
Bond lengths



Bond angles

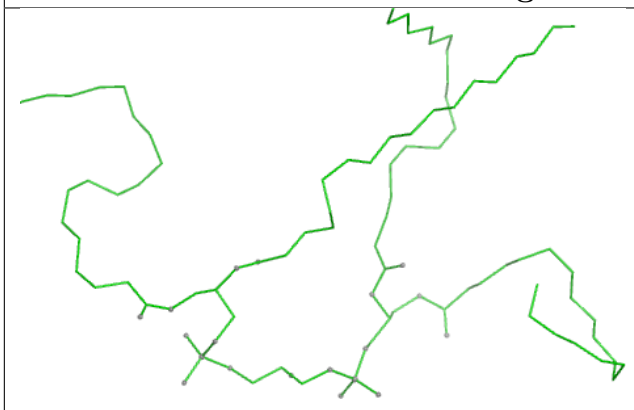


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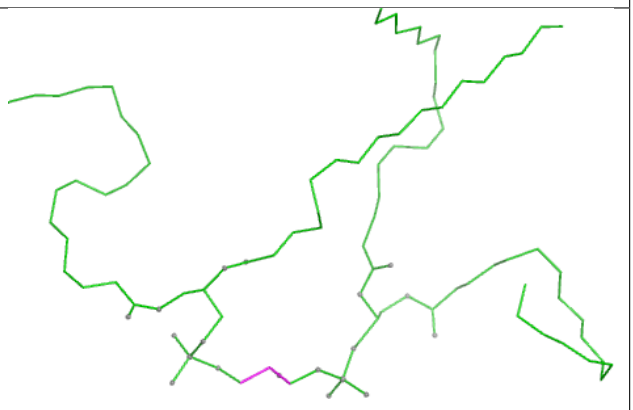


Rings

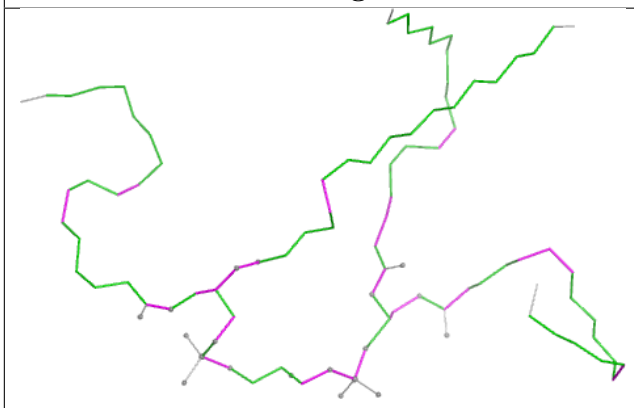
Ligand CDL Ek 201



Bond lengths



Bond angles

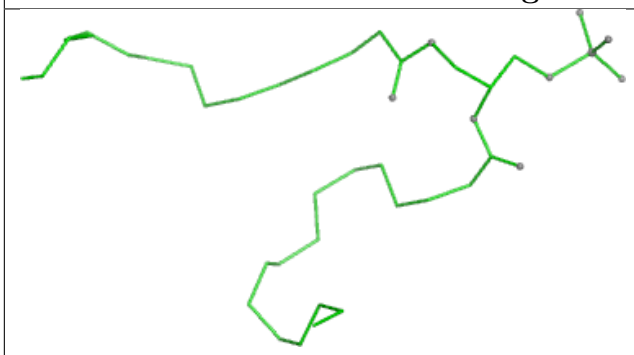


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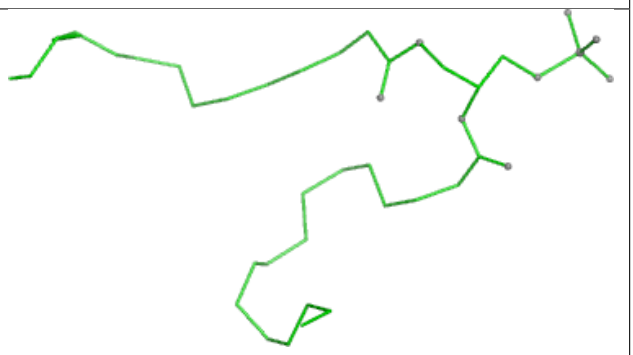


Rings

Ligand LPP EI 402



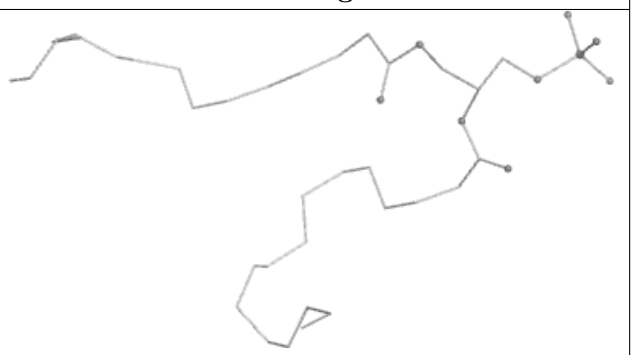
Bond lengths



Bond angles

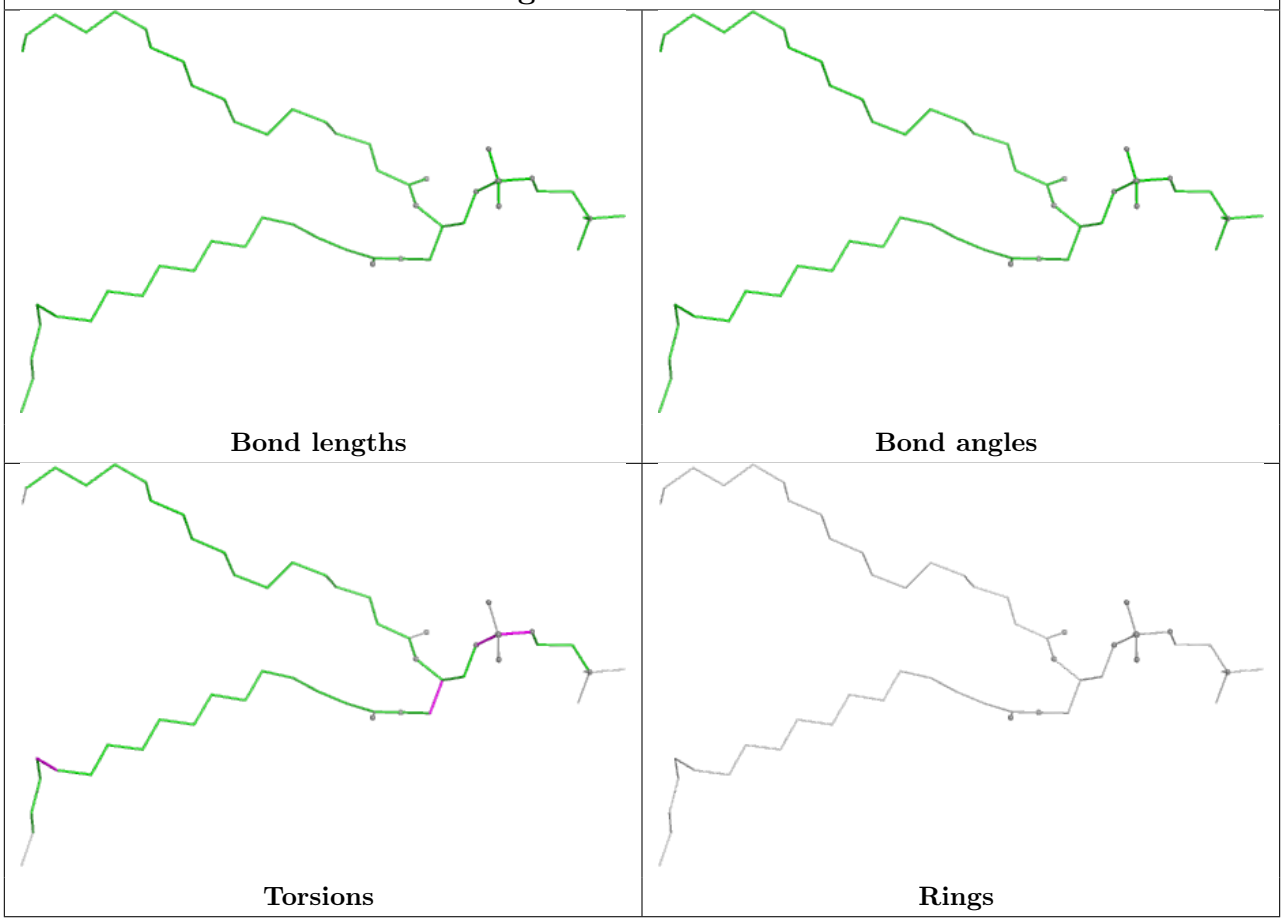


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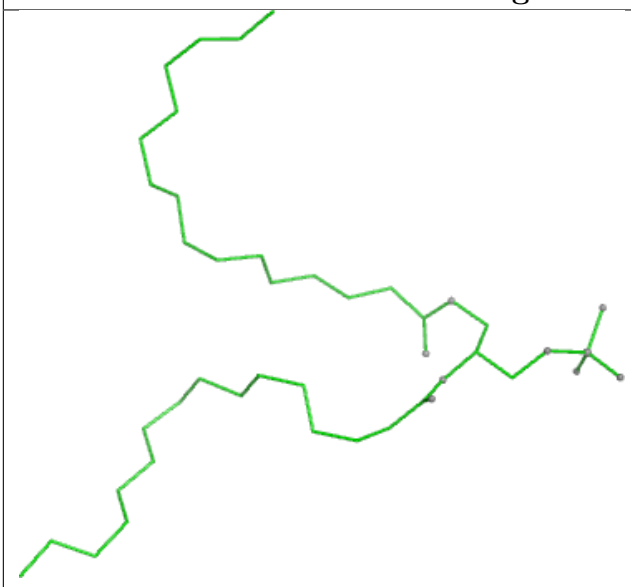


Rings

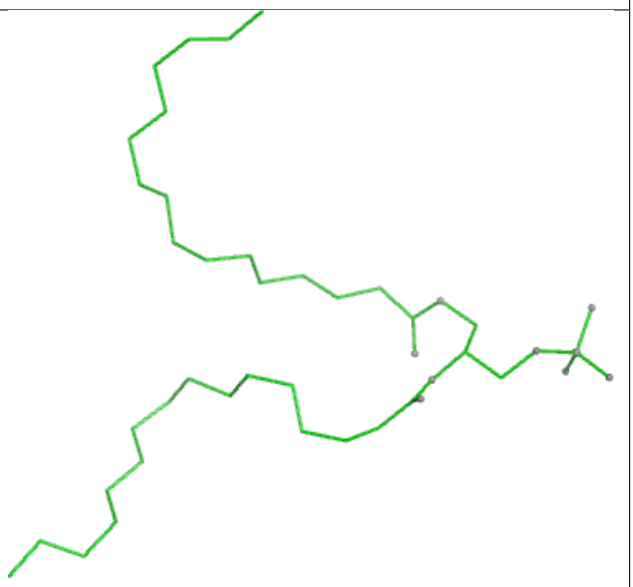
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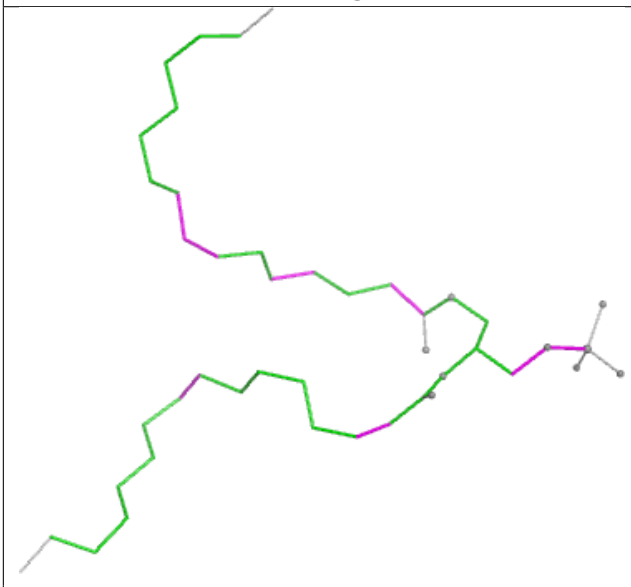
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Bond lengths



Bond angles

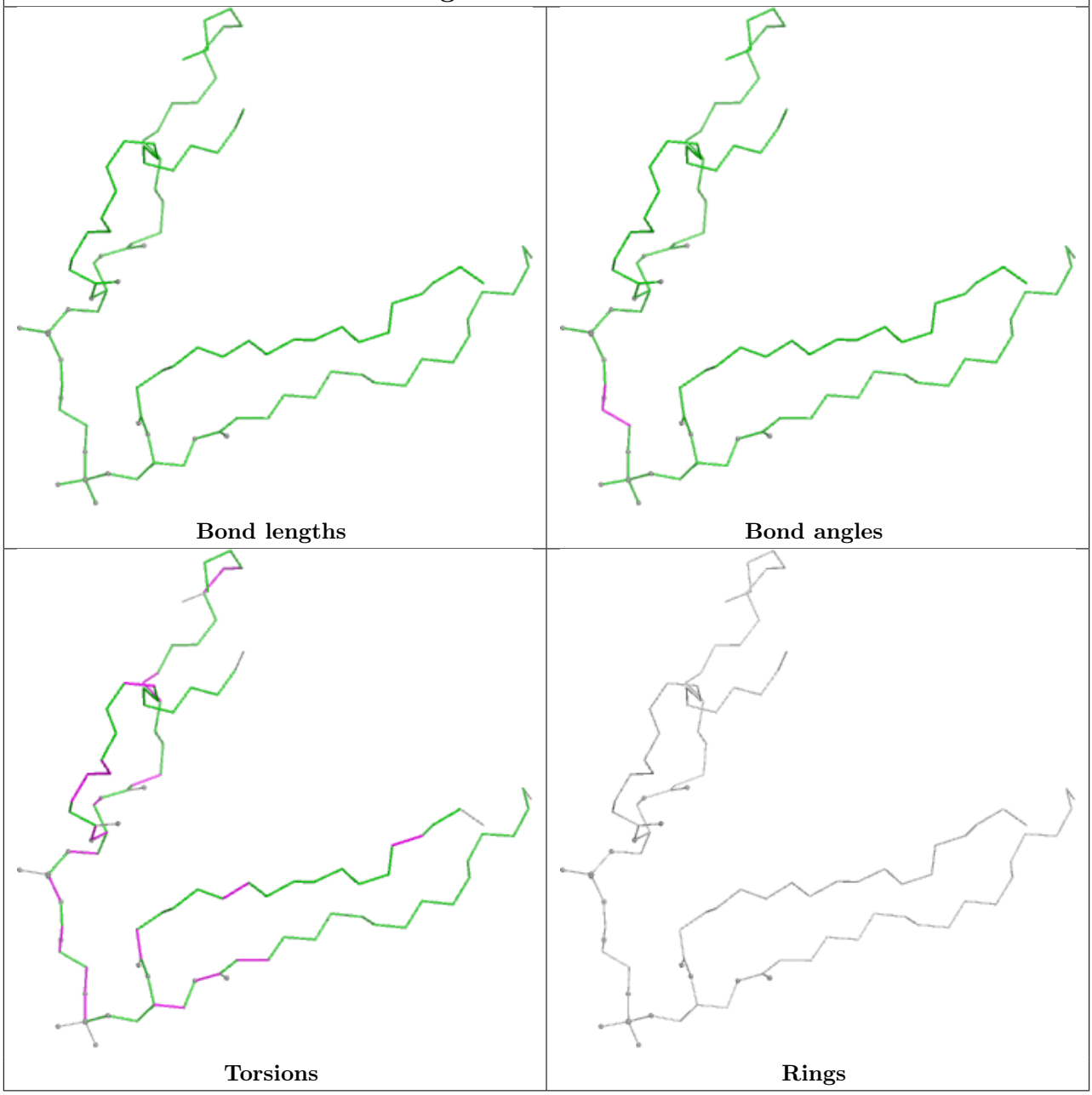


Torsions



Rings

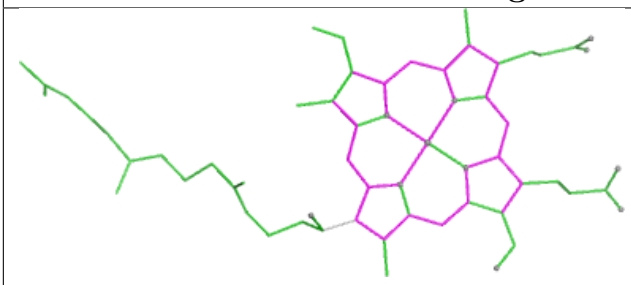
Ligand CDL Dr 403



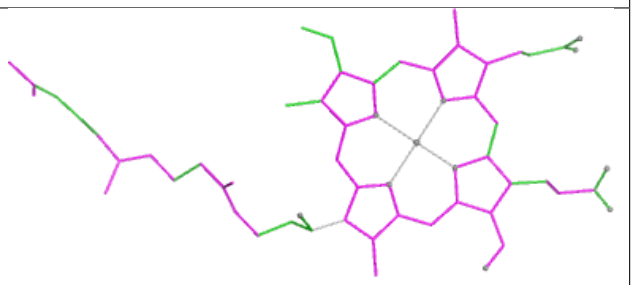
Bond lengths **Bond angles**

Torsions **Rings**

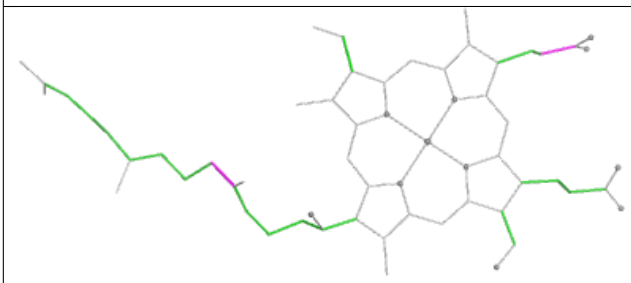
Ligand HEA DA 702



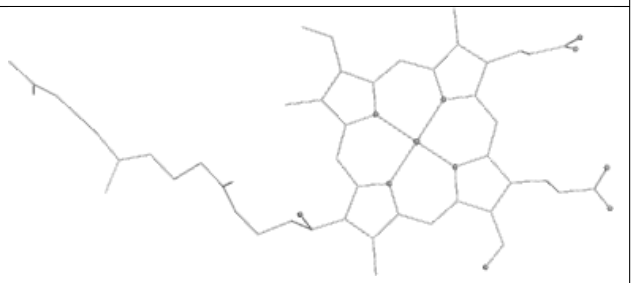
Bond lengths



Bond angles



Torsions



Rings

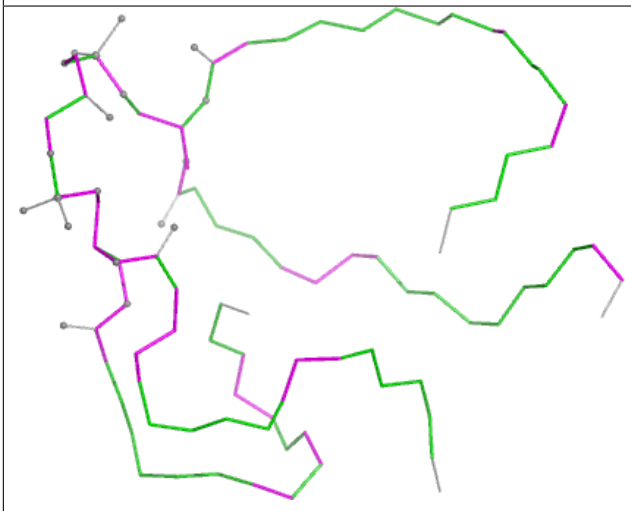
Ligand CDL Dn 502



Bond lengths



Bond angles

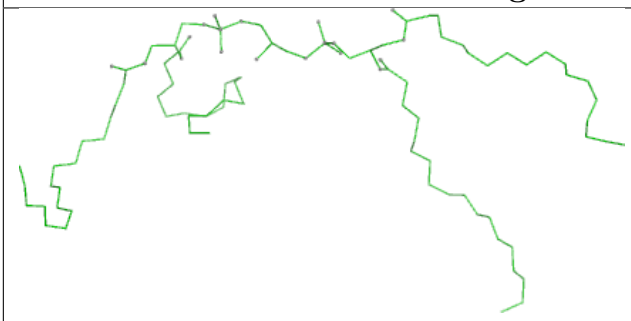


Torsions



Rings

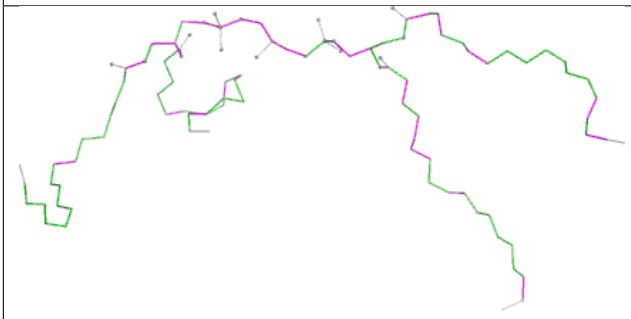
Ligand CDL DG 201



Bond lengths



Bond angles

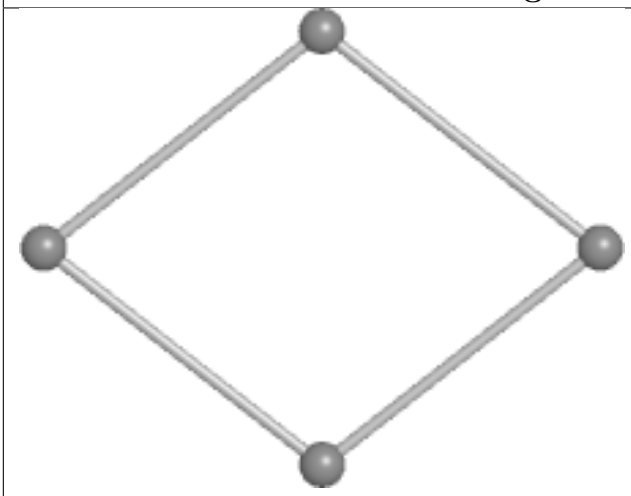


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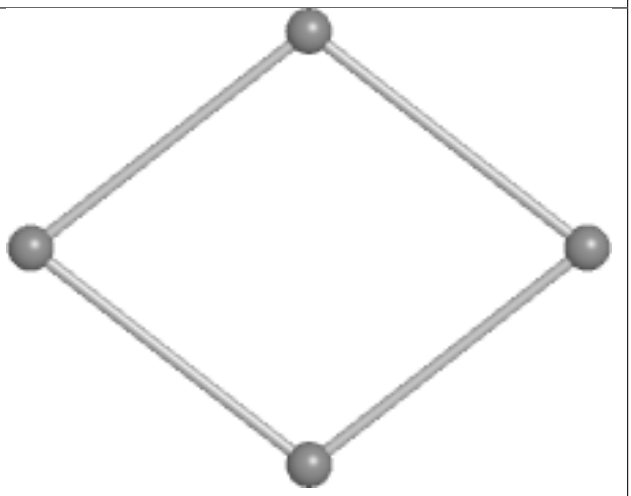


Rings

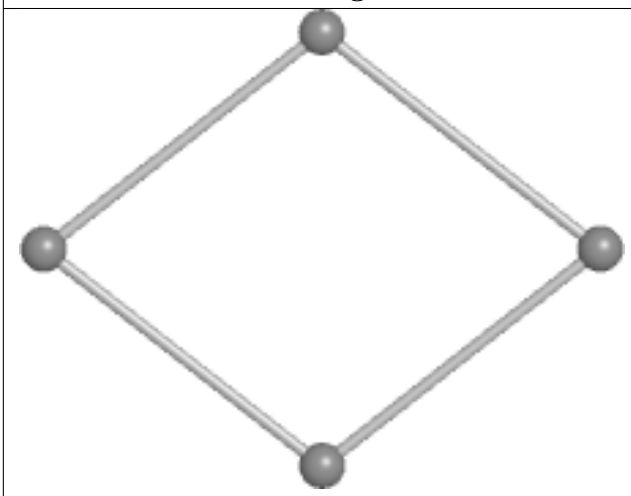
Ligand FES e 1102



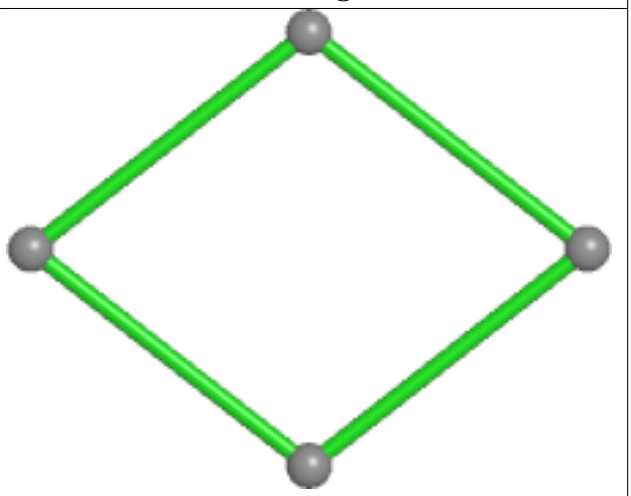
Bond lengths



Bond angles

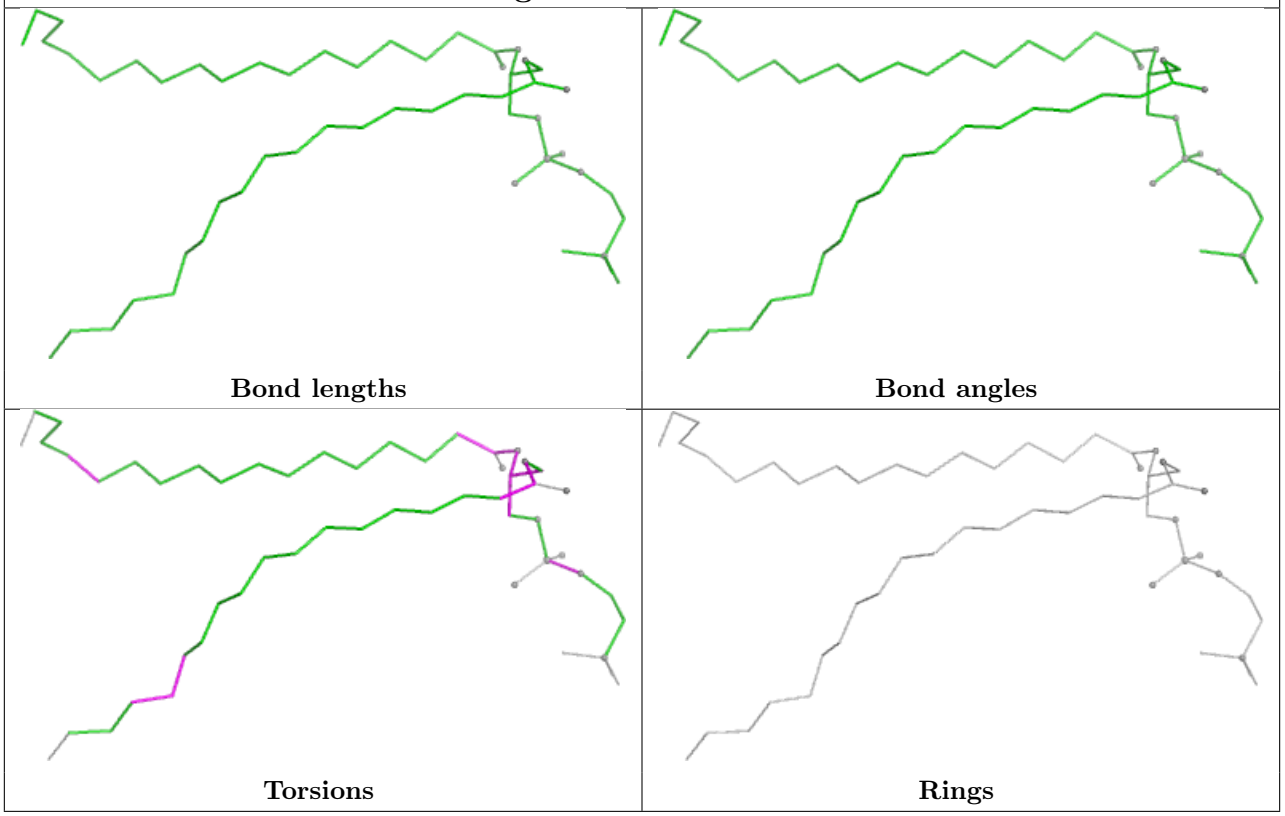


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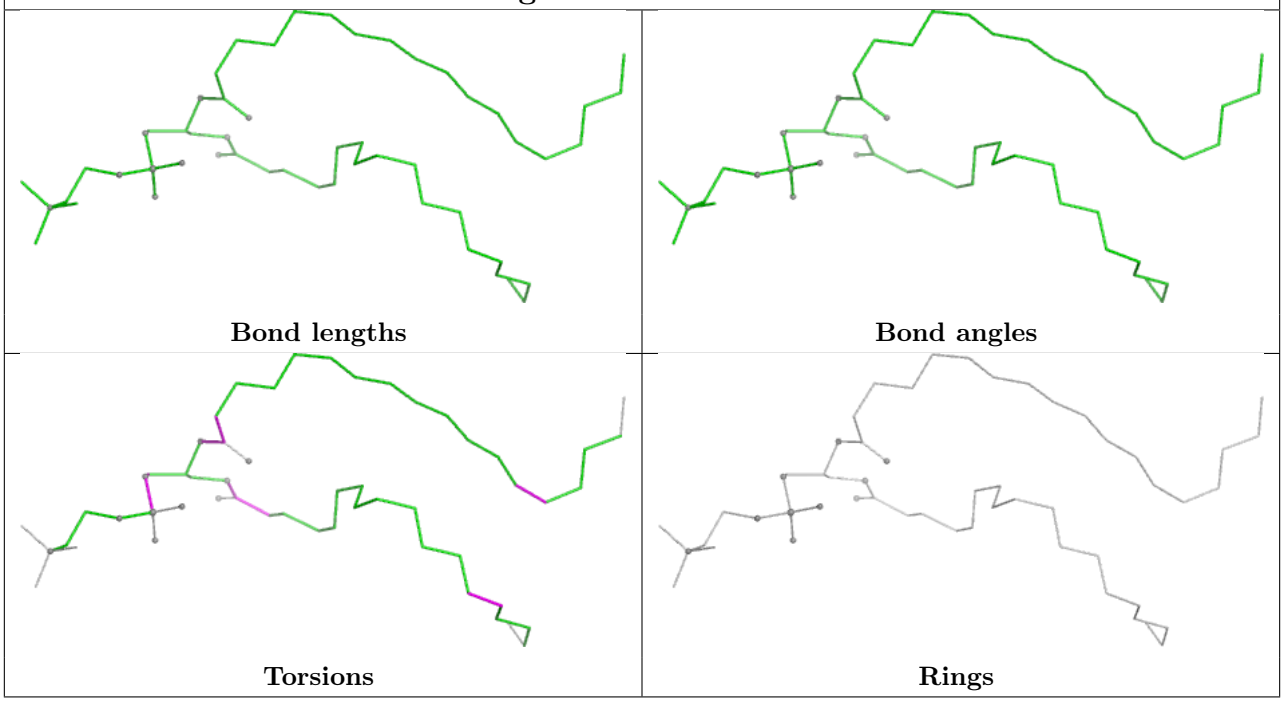


Rings

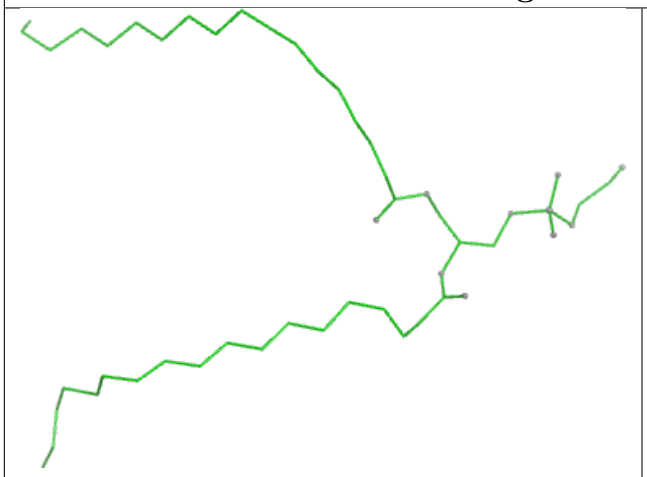
Ligand PC1 DC 608



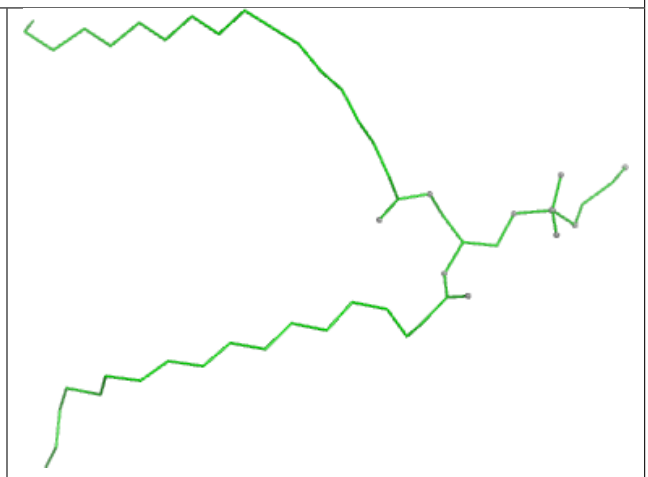
Ligand PC1 A0 605



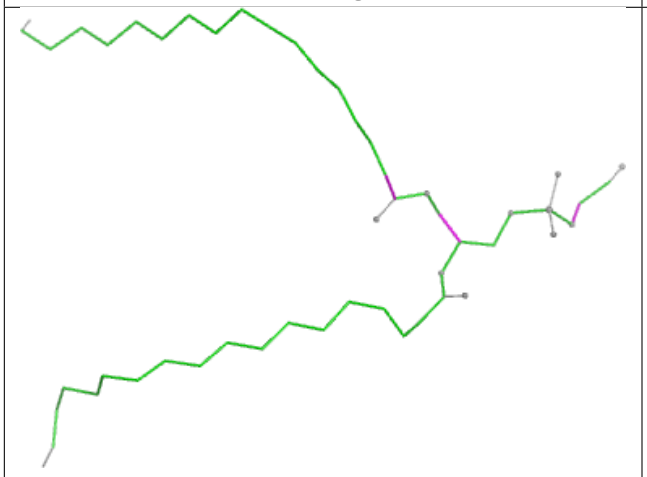
Ligand 3PE CC 301



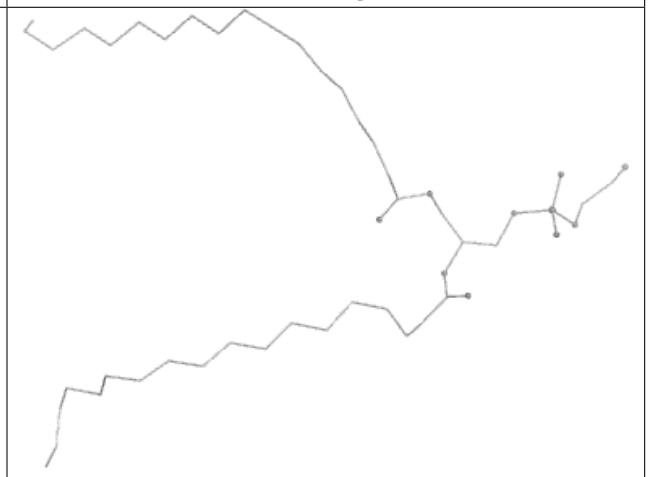
Bond lengths



Bond angles



Torsions



Rings

Ligand CDL DY 301



Bond lengths



Bond angles

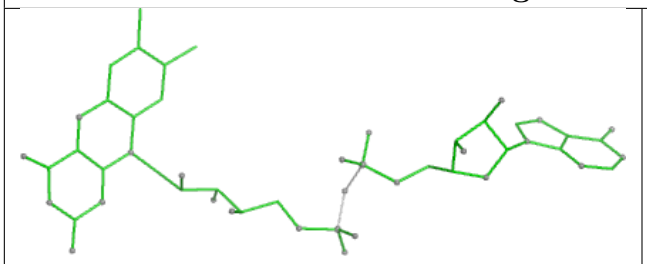


Torsions

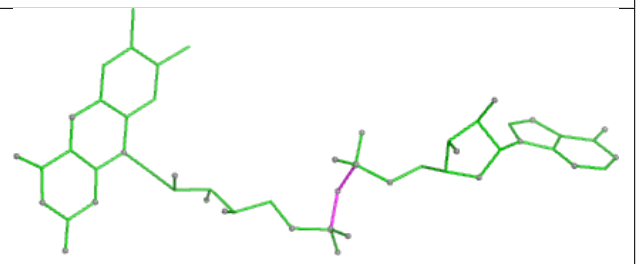


Rings

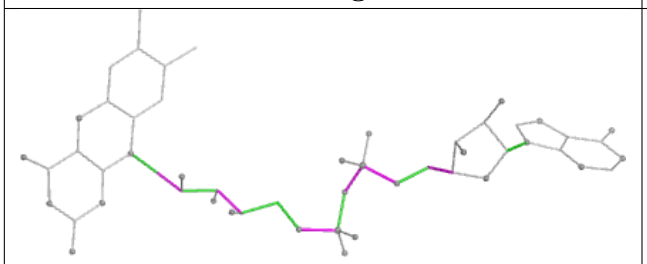
Ligand FAD CA 702



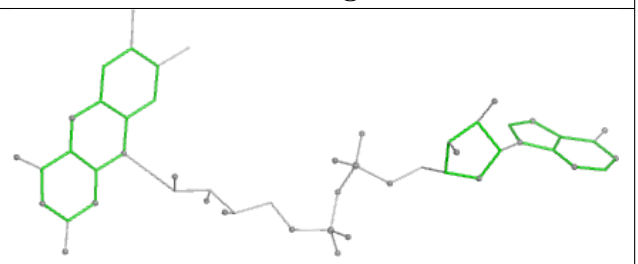
Bond lengths



Bond angles

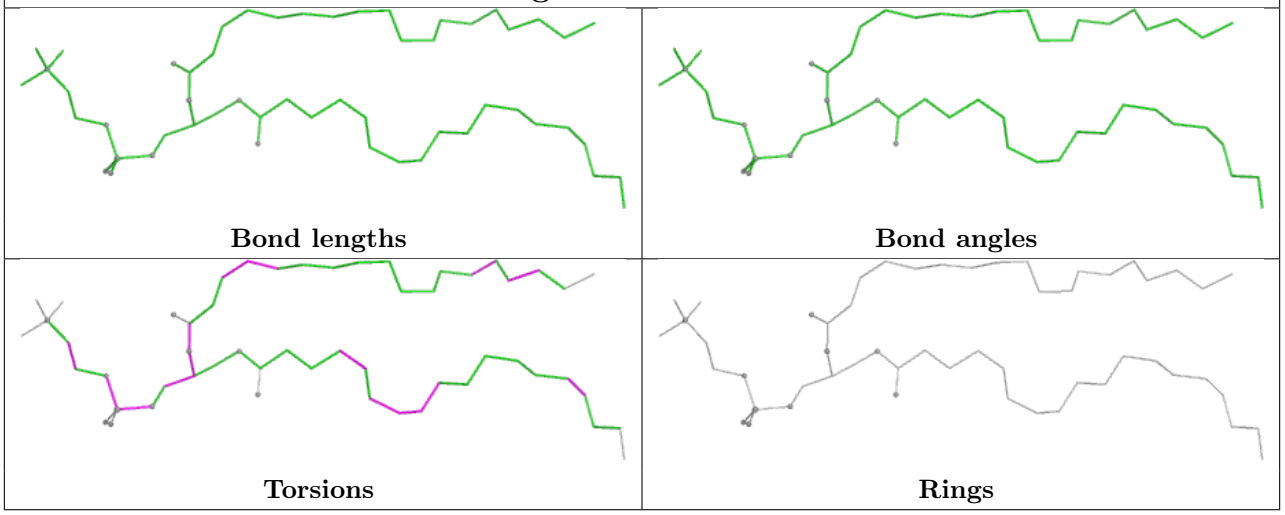


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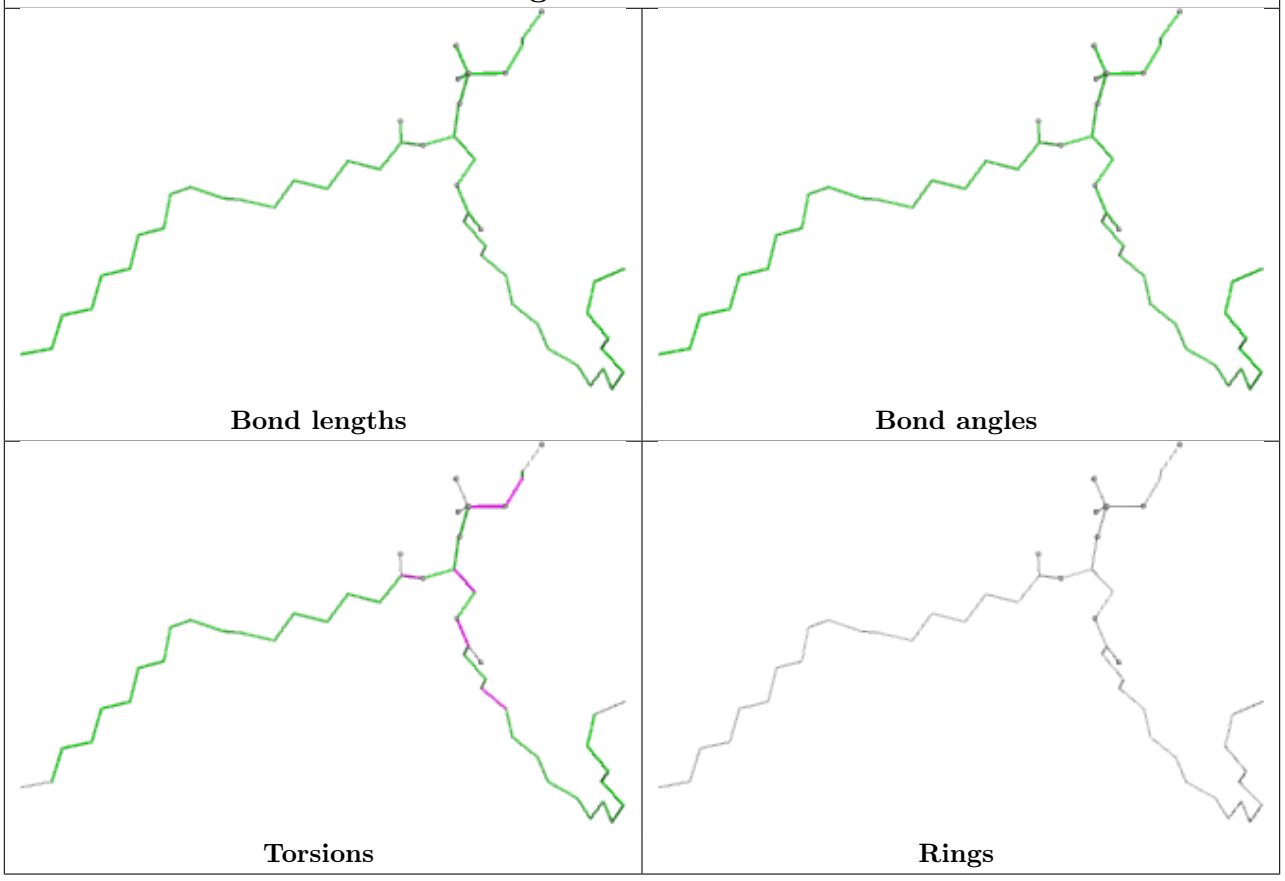


Rings

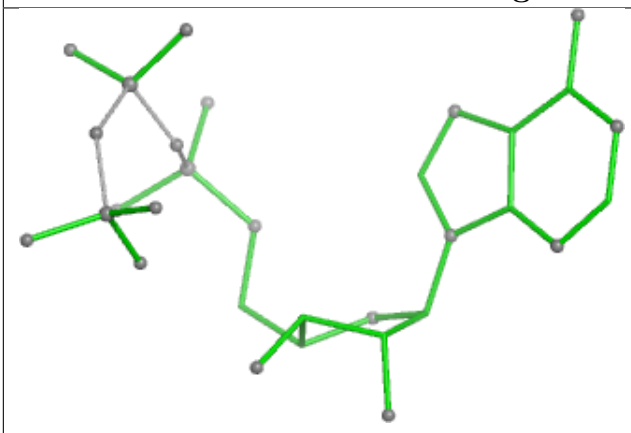
Ligand PC1 k 301



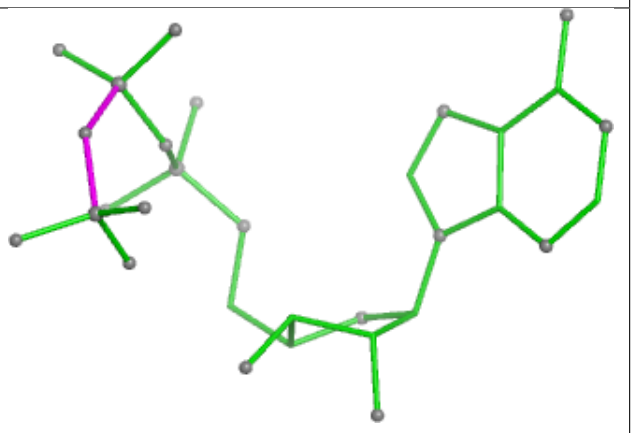
Ligand 3PE C 513



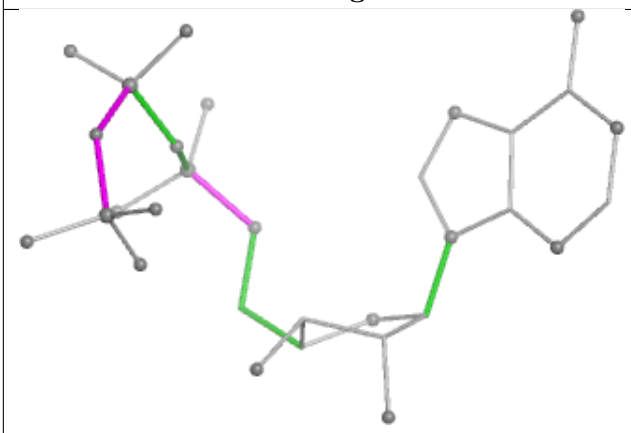
Ligand ATP ER 201



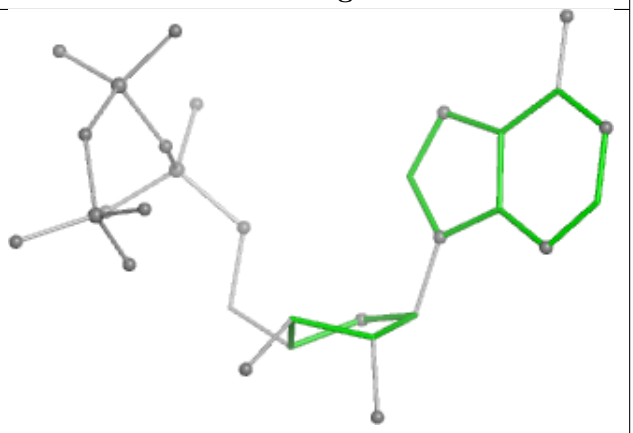
Bond lengths



Bond angles

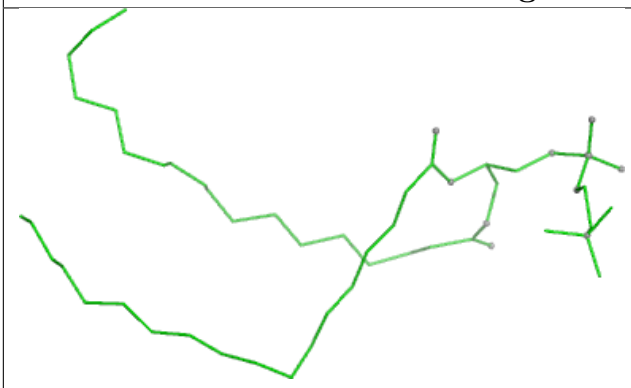


Torsions

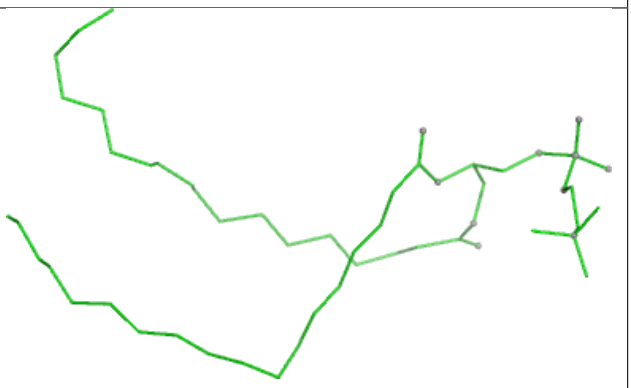


Rings

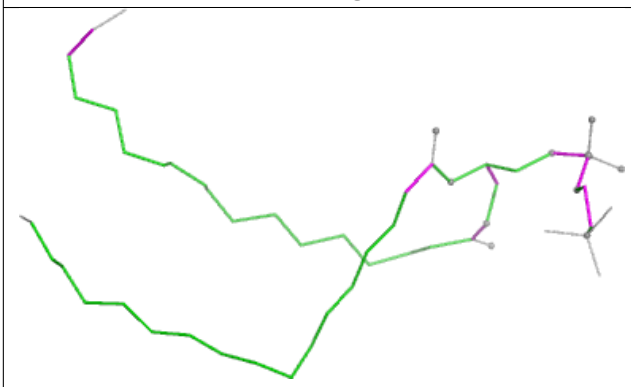
Ligand PC1 Dc 604



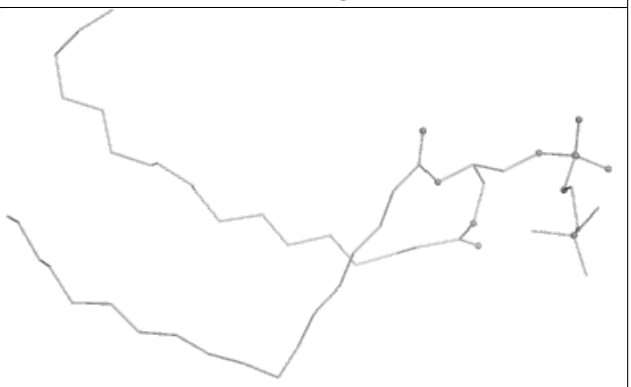
Bond lengths



Bond angles

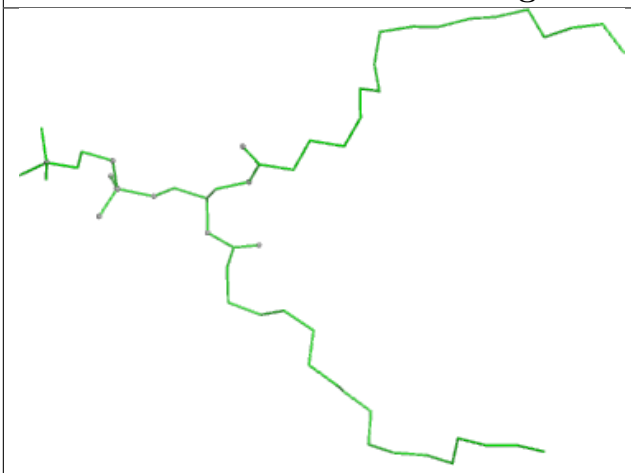


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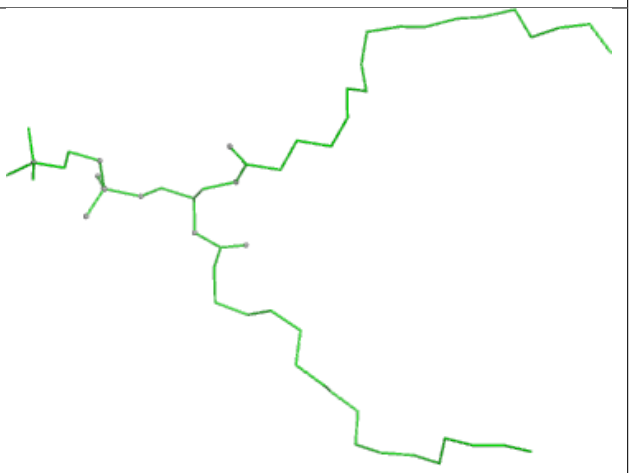


Rings

Ligand PC1 Dc 605



Bond lengths



Bond angles

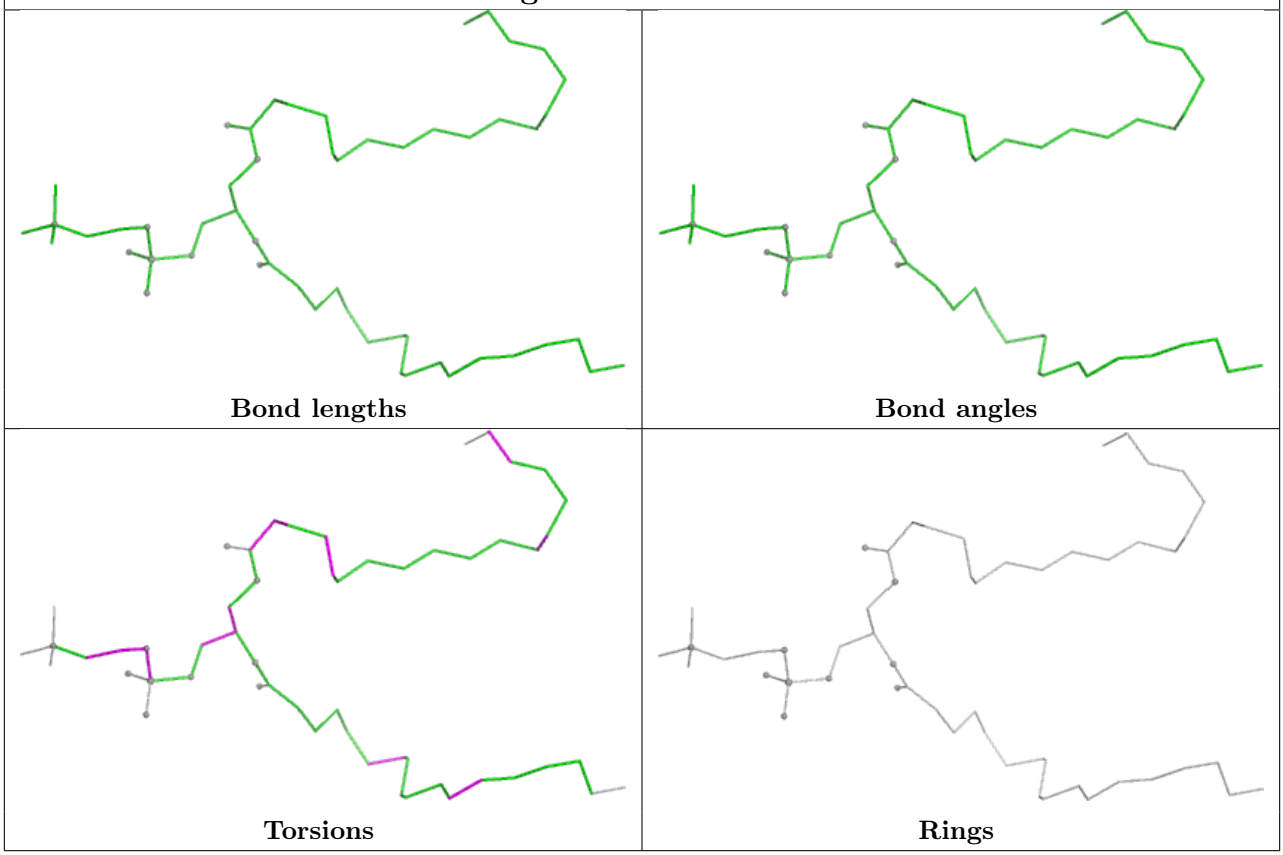


Torsions

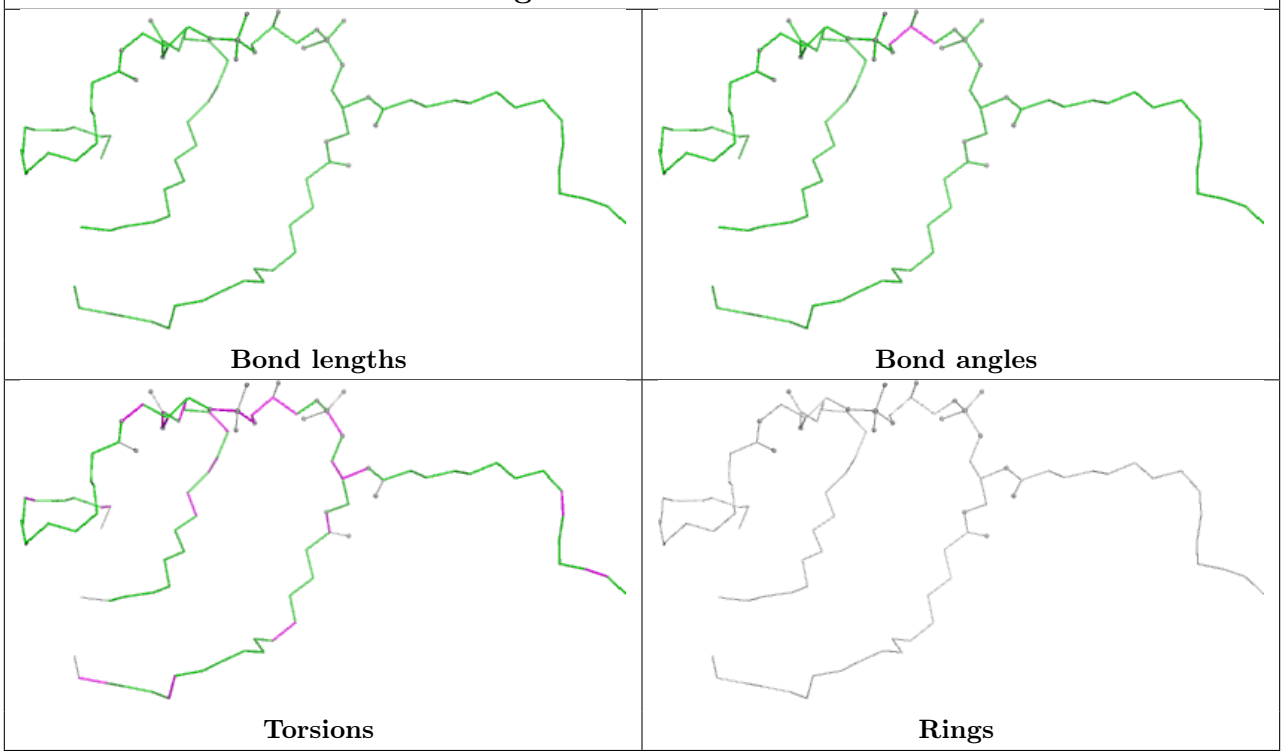


Rings

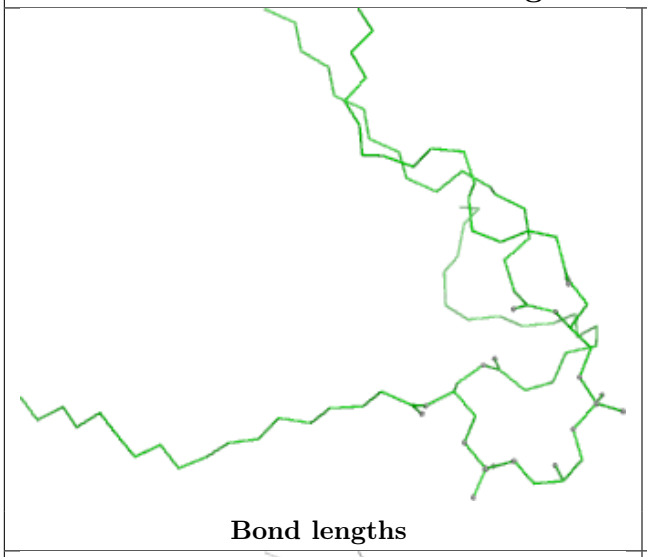
Ligand PC1 Eo 201



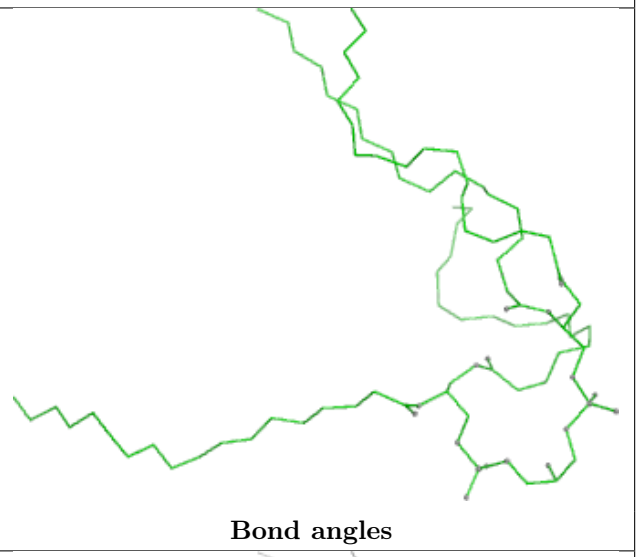
Ligand CDL Du 403



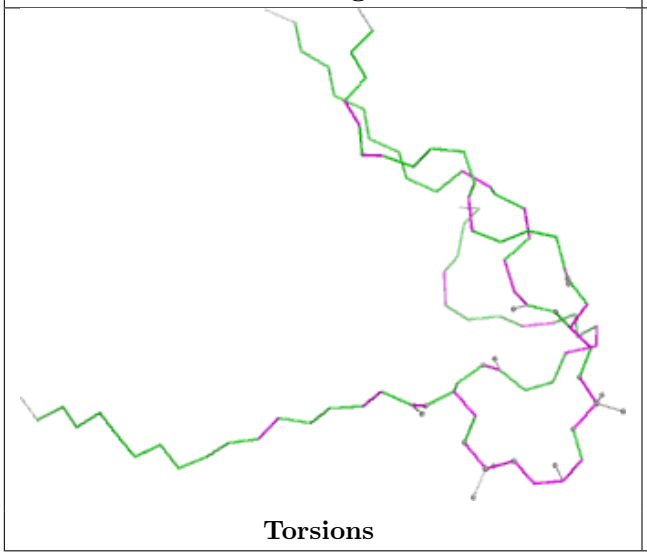
Ligand CDL C 503



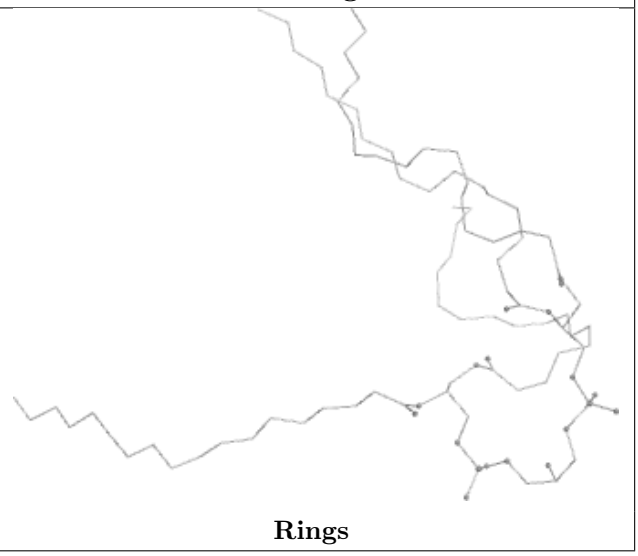
Bond lengths



Bond angles

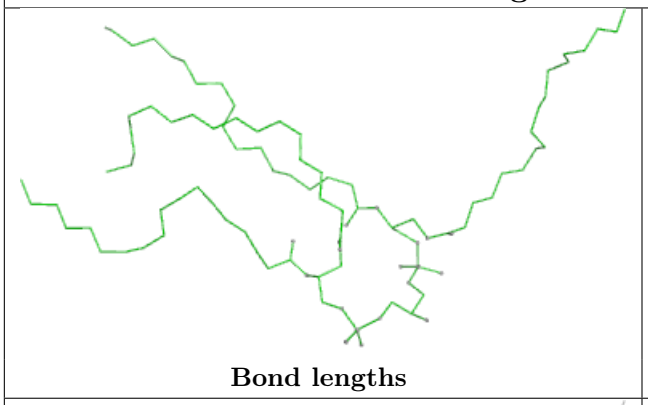


Torsions

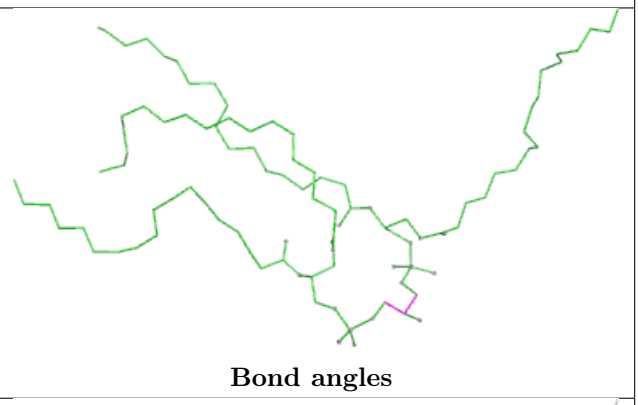


Rings

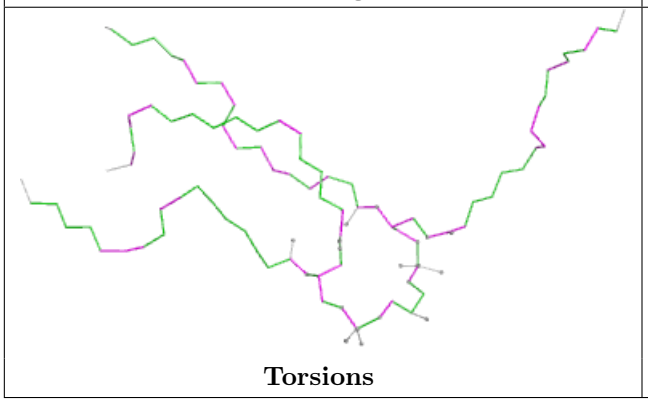
Ligand CDL DN 506



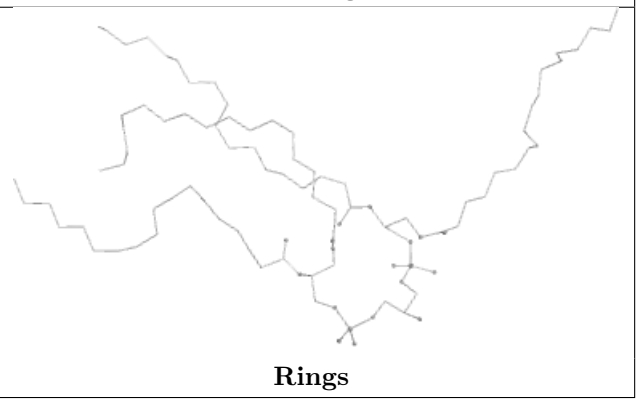
Bond lengths



Bond angles

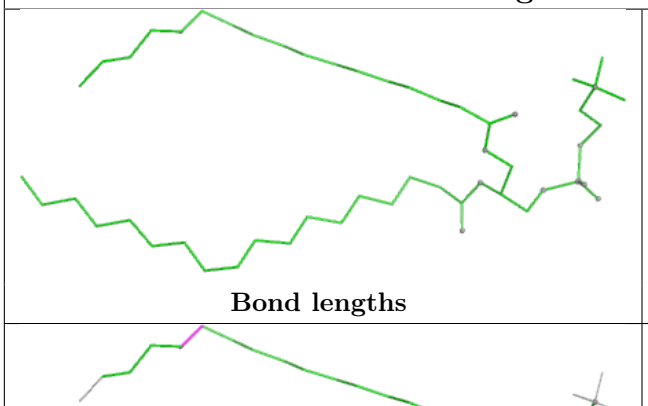


Torsions

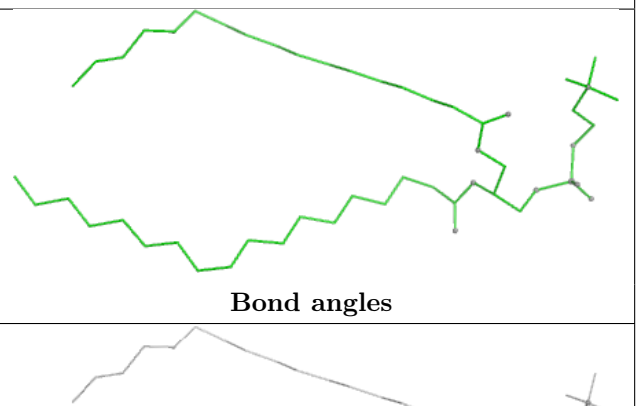


Rings

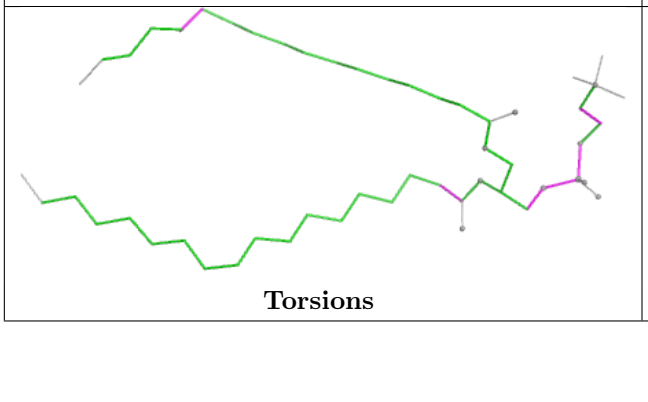
Ligand PC1 EO 204



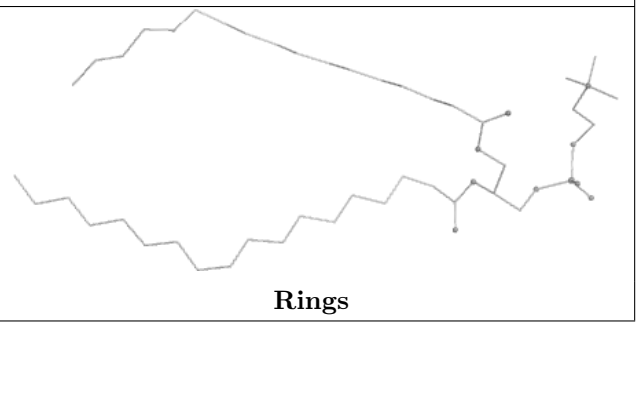
Bond lengths



Bond angles

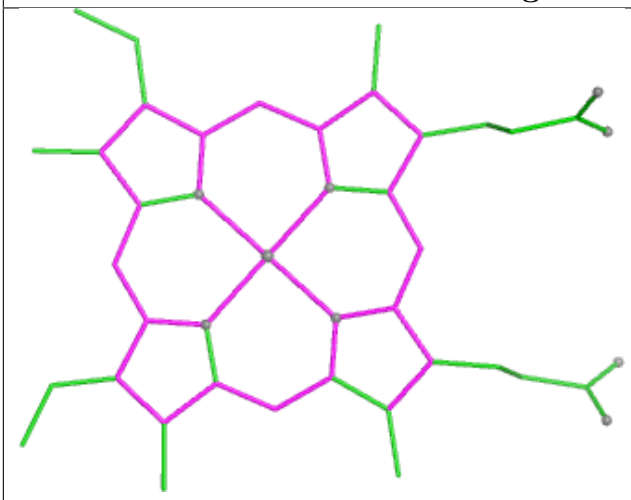


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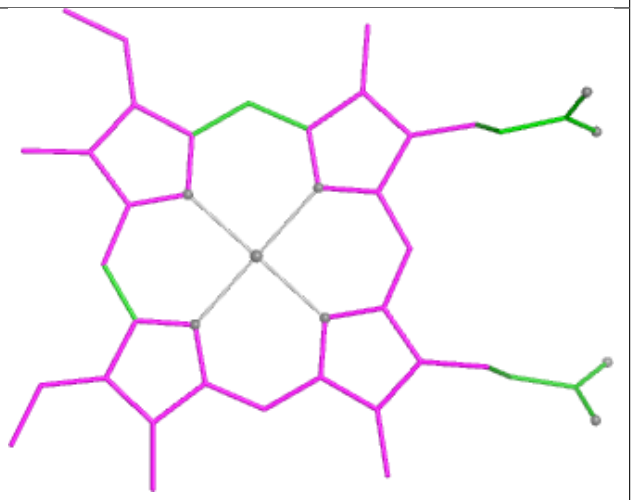


Rings

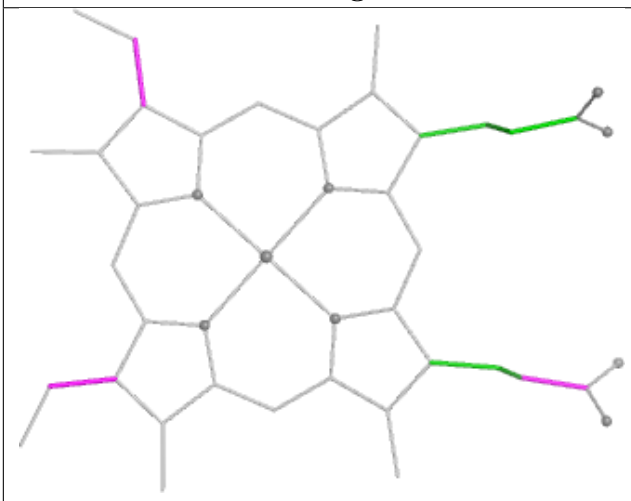
Ligand HEC D 401



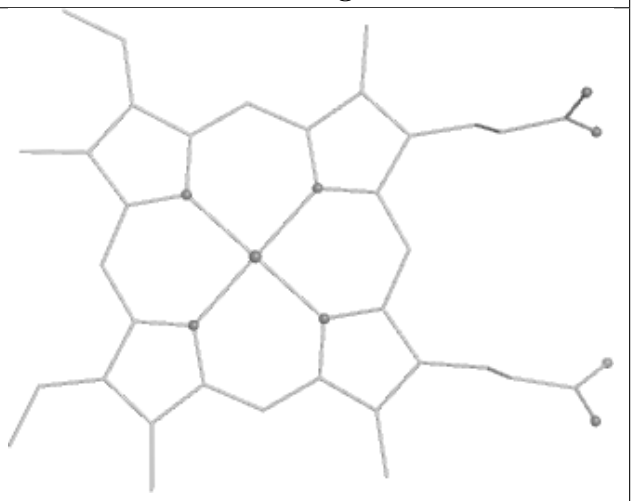
Bond lengths



Bond angles



Torsions



Rings

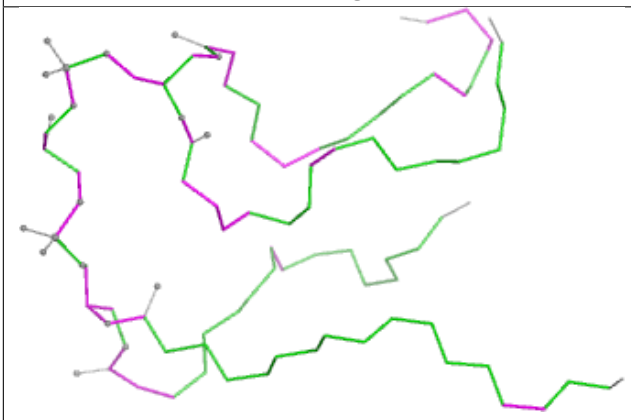
Ligand CDL Ea 501



Bond lengths



Bond angles

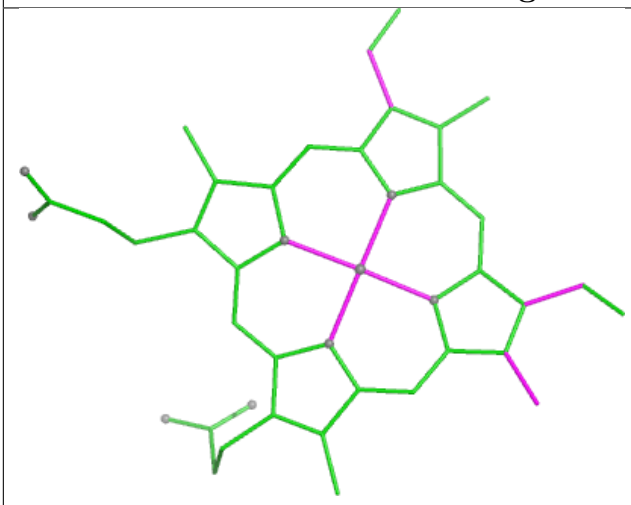


Torsions

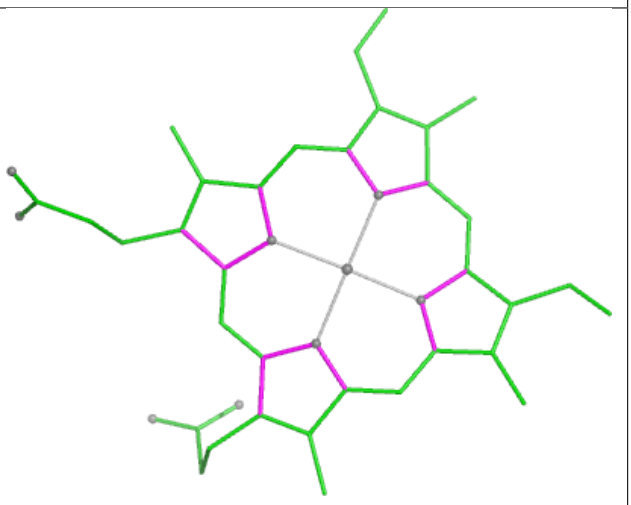


Rings

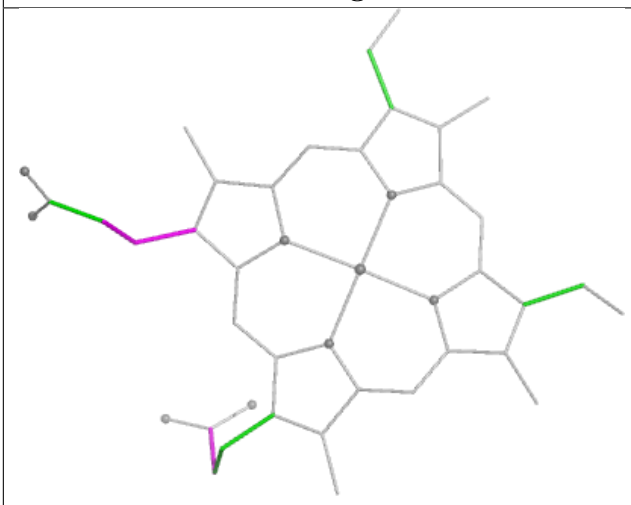
Ligand HEM C 502



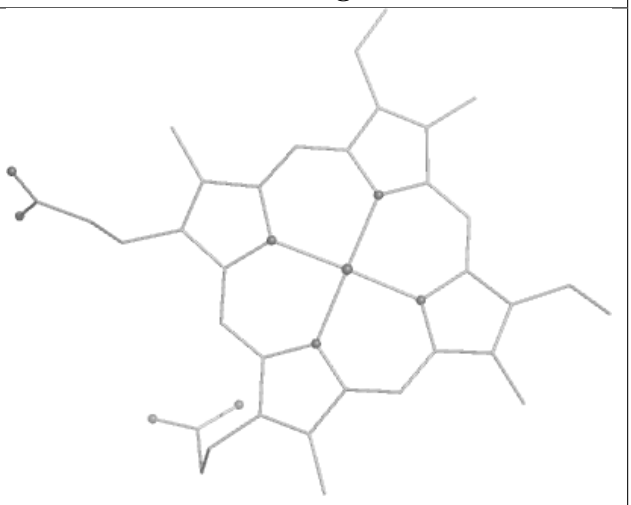
Bond lengths



Bond angles



Torsions

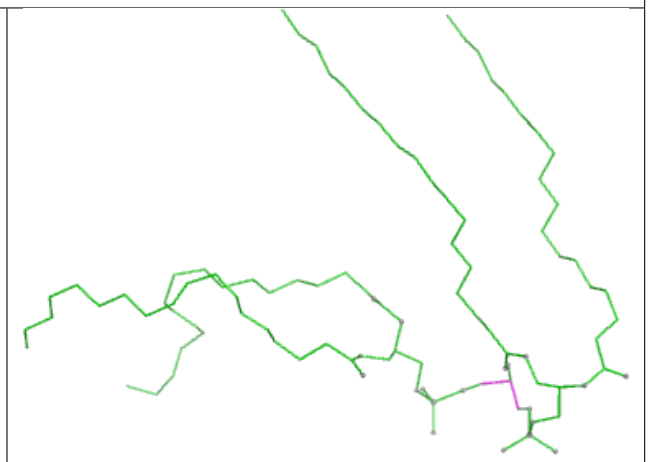


Rings

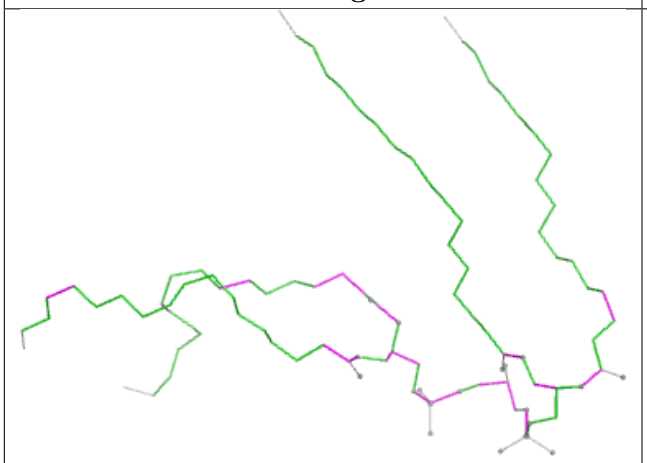
Ligand CDL BE 201



Bond lengths



Bond angles

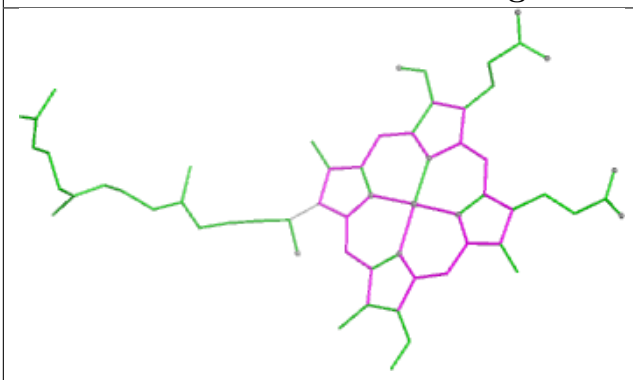


Torsions

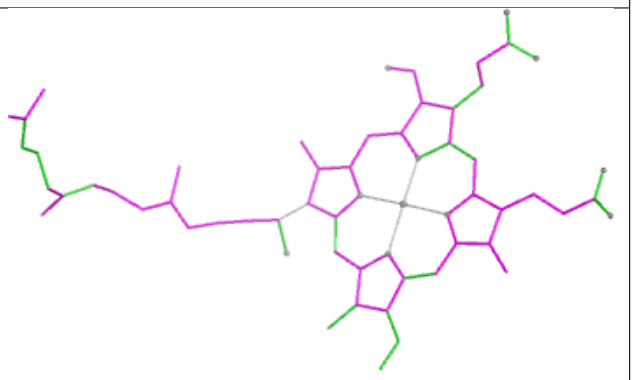


Rings

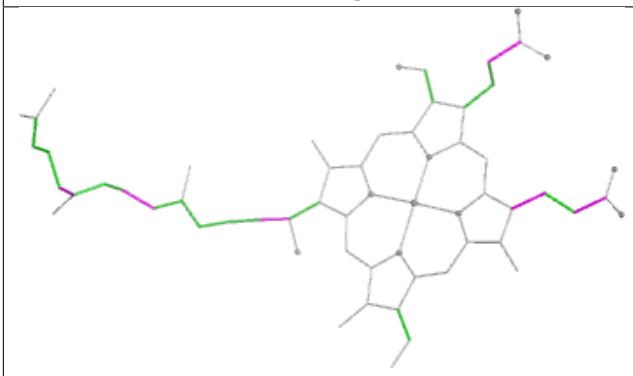
Ligand HEA DA 703



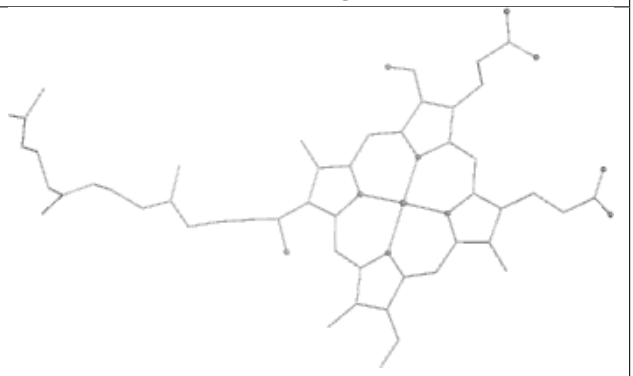
Bond lengths



Bond angles

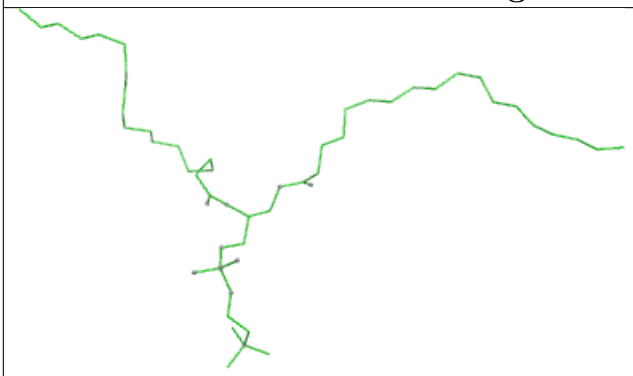


Torsions



Rings

Ligand PC1 Dx 1205



Bond lengths



Bond angles

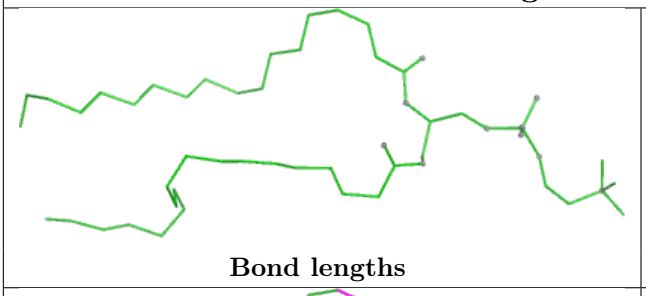


Torsions

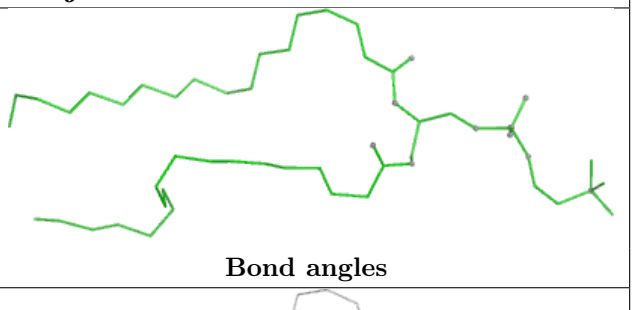


Rings

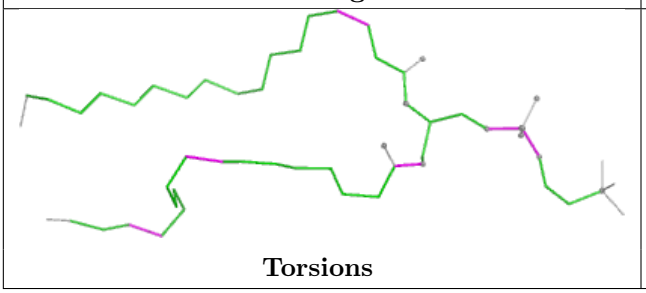
Ligand PC1 Dj 406



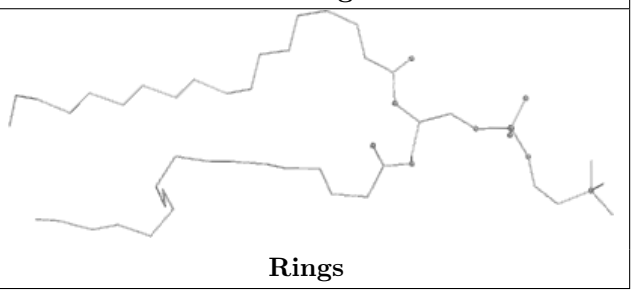
Bond lengths



Bond angles

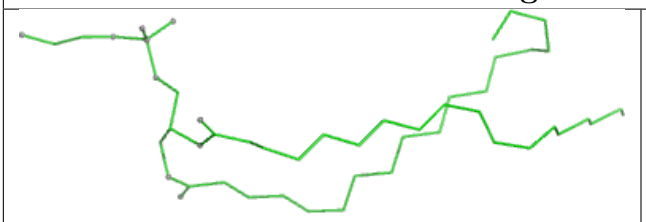


Torsions

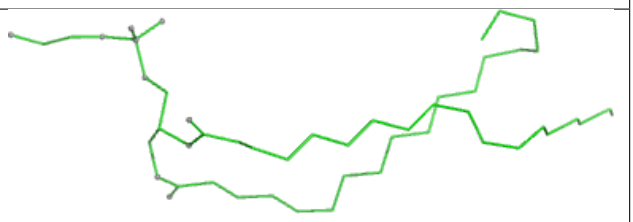


Rings

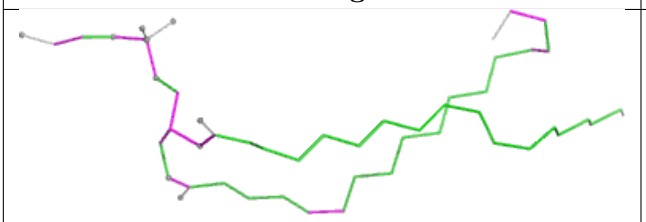
Ligand 3PE Dr 401



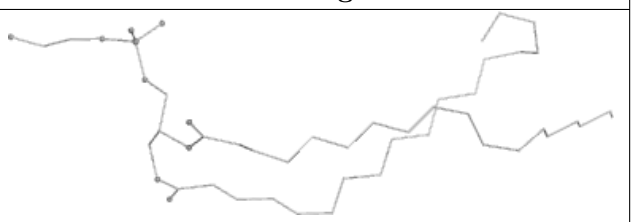
Bond lengths



Bond angles

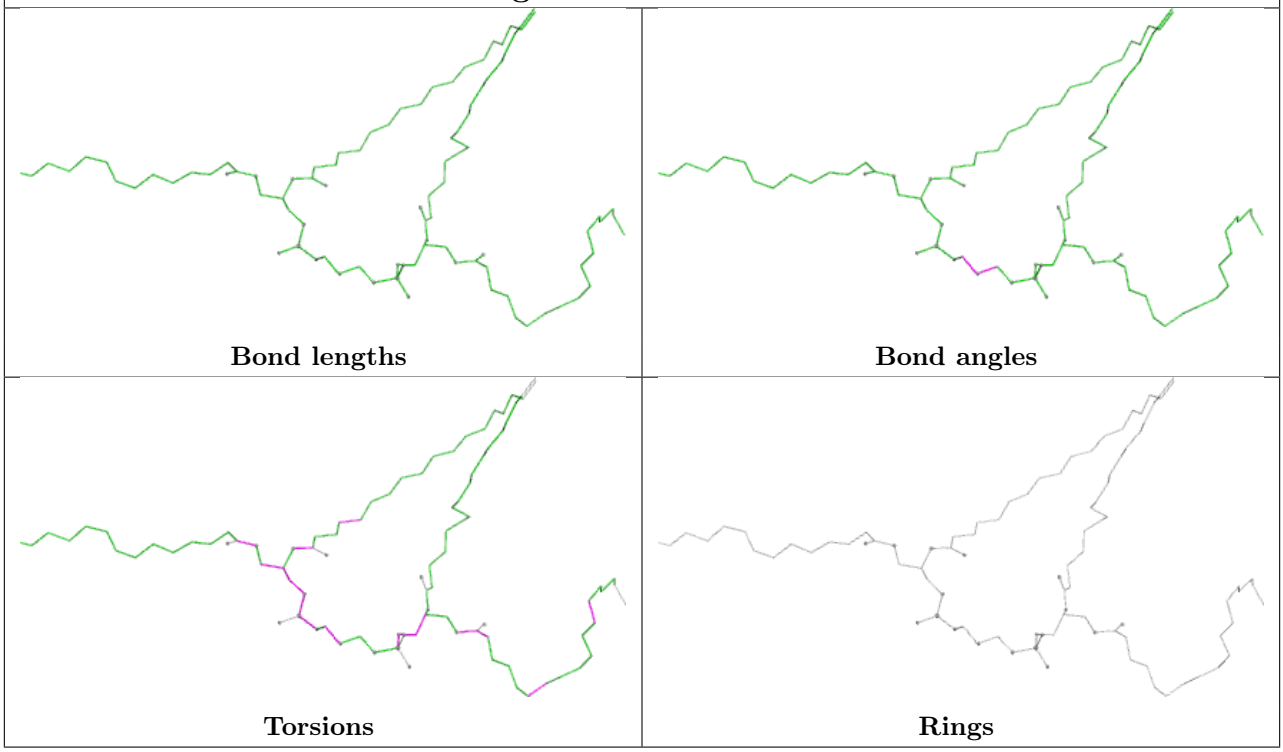


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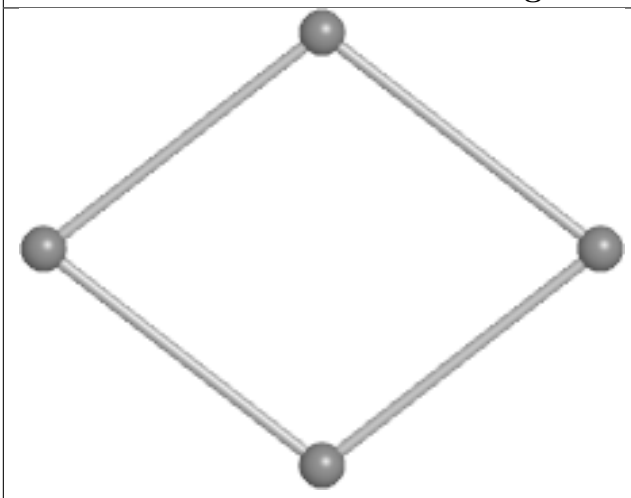


Rings

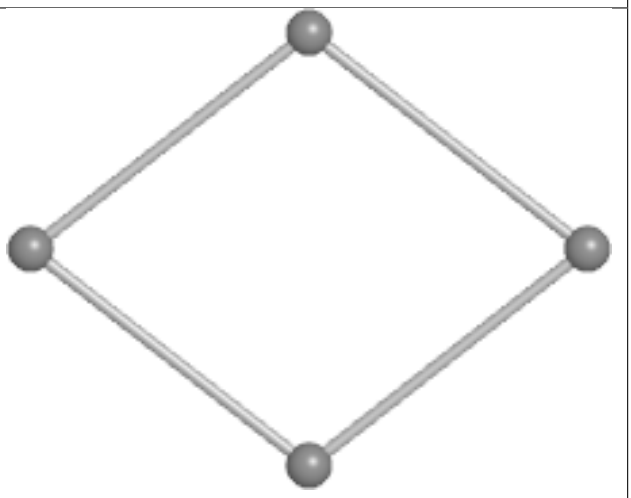
Ligand CDL ED 604



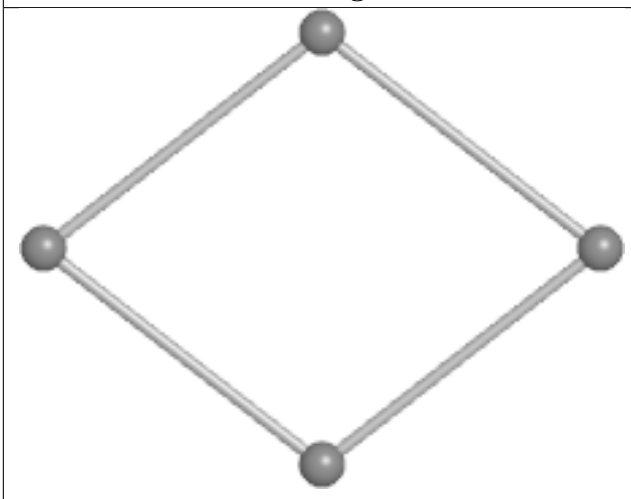
Ligand FES Ef 503



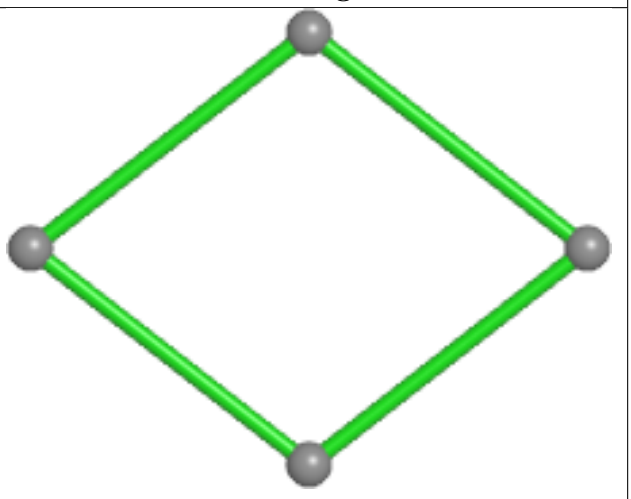
Bond lengths



Bond angles

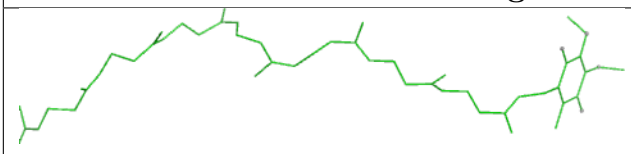


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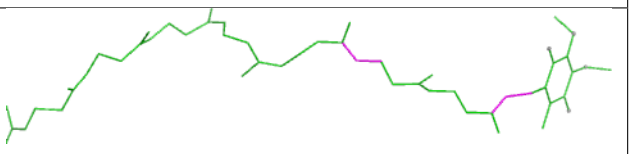


Rings

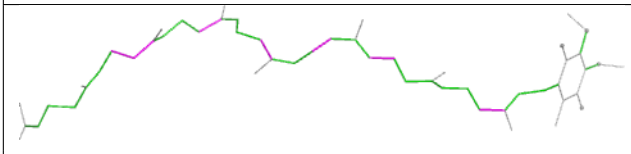
Ligand UQ8 En 1202



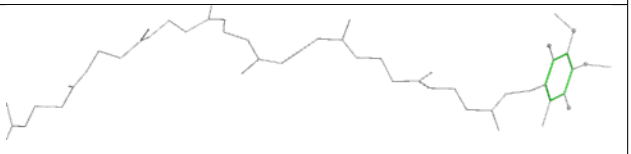
Bond lengths



Bond angles

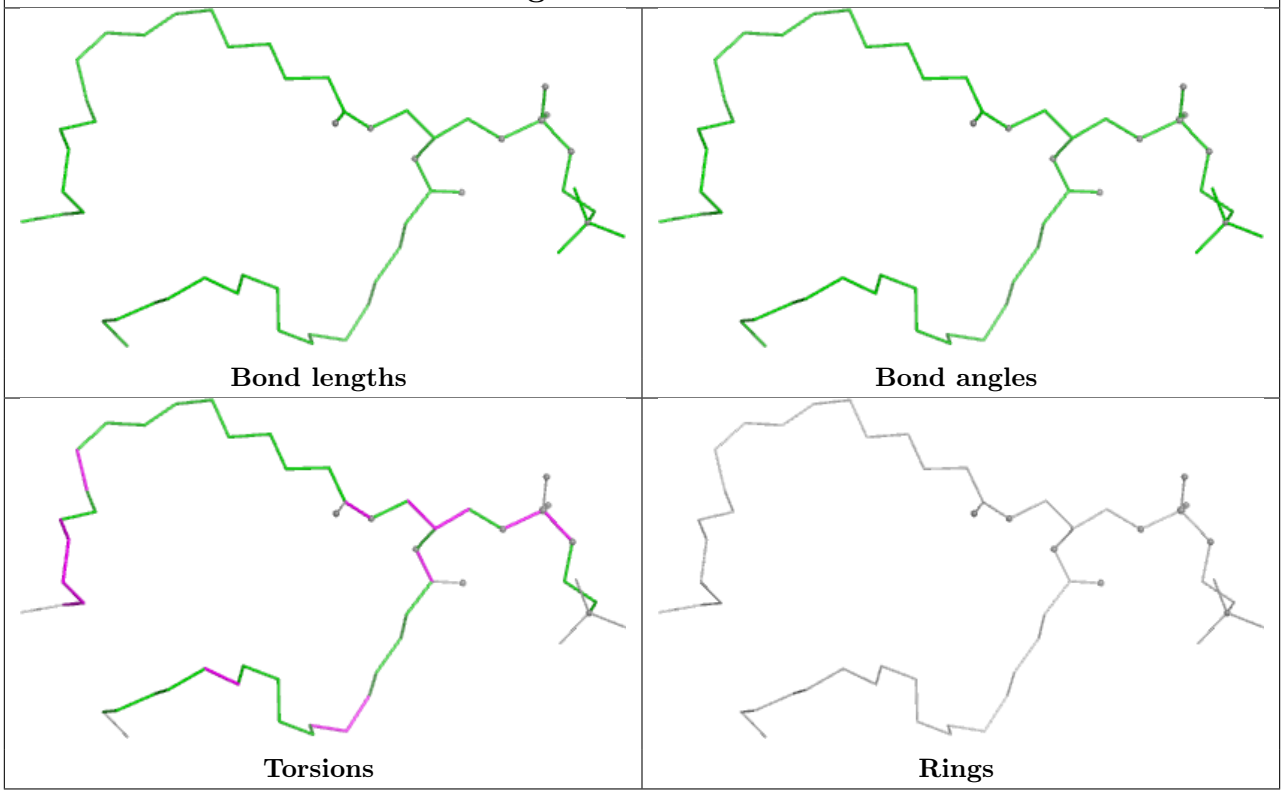


Torsions

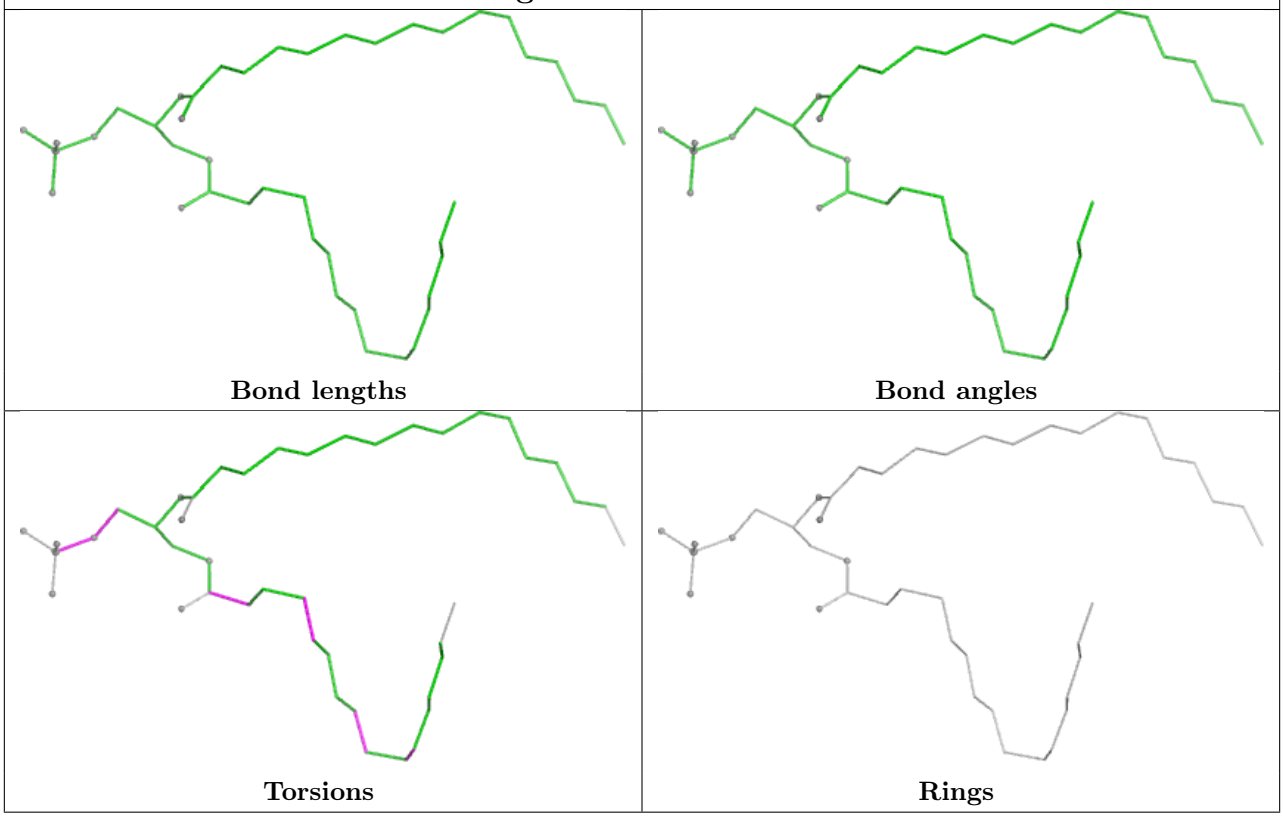


Rings

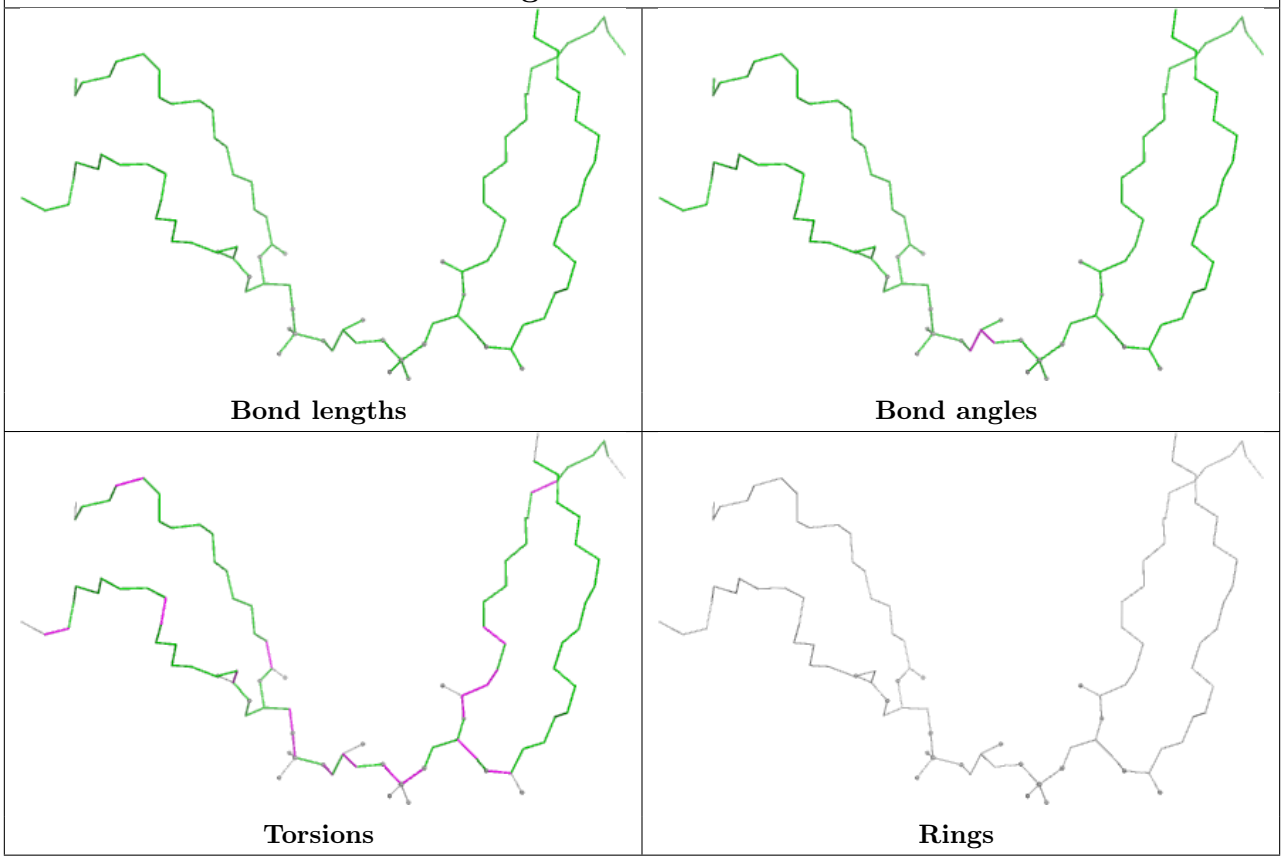
Ligand PC1 D 402



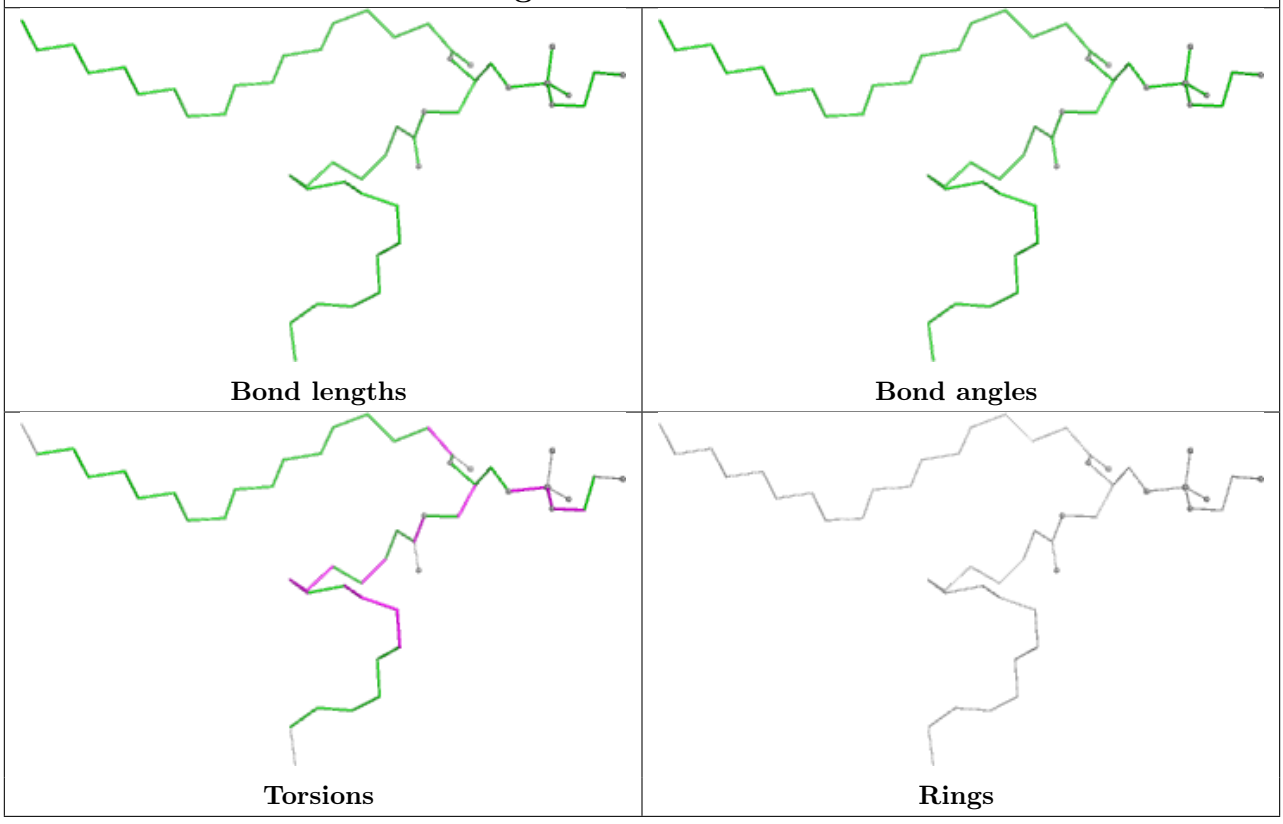
Ligand LPP Dn 504



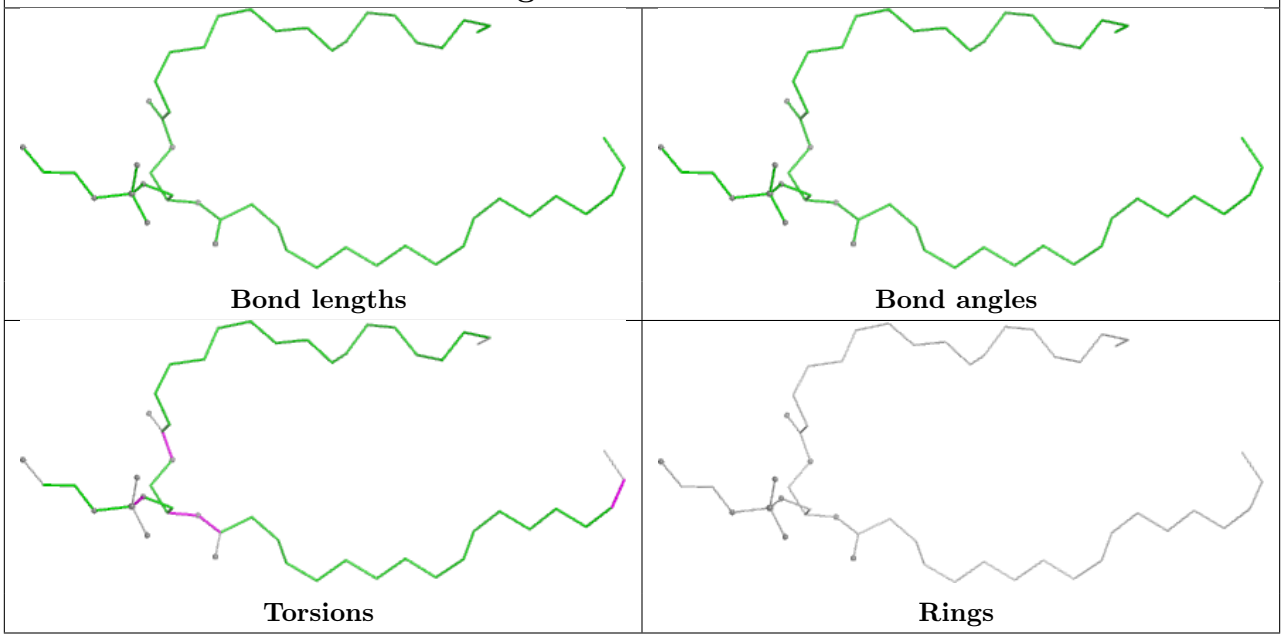
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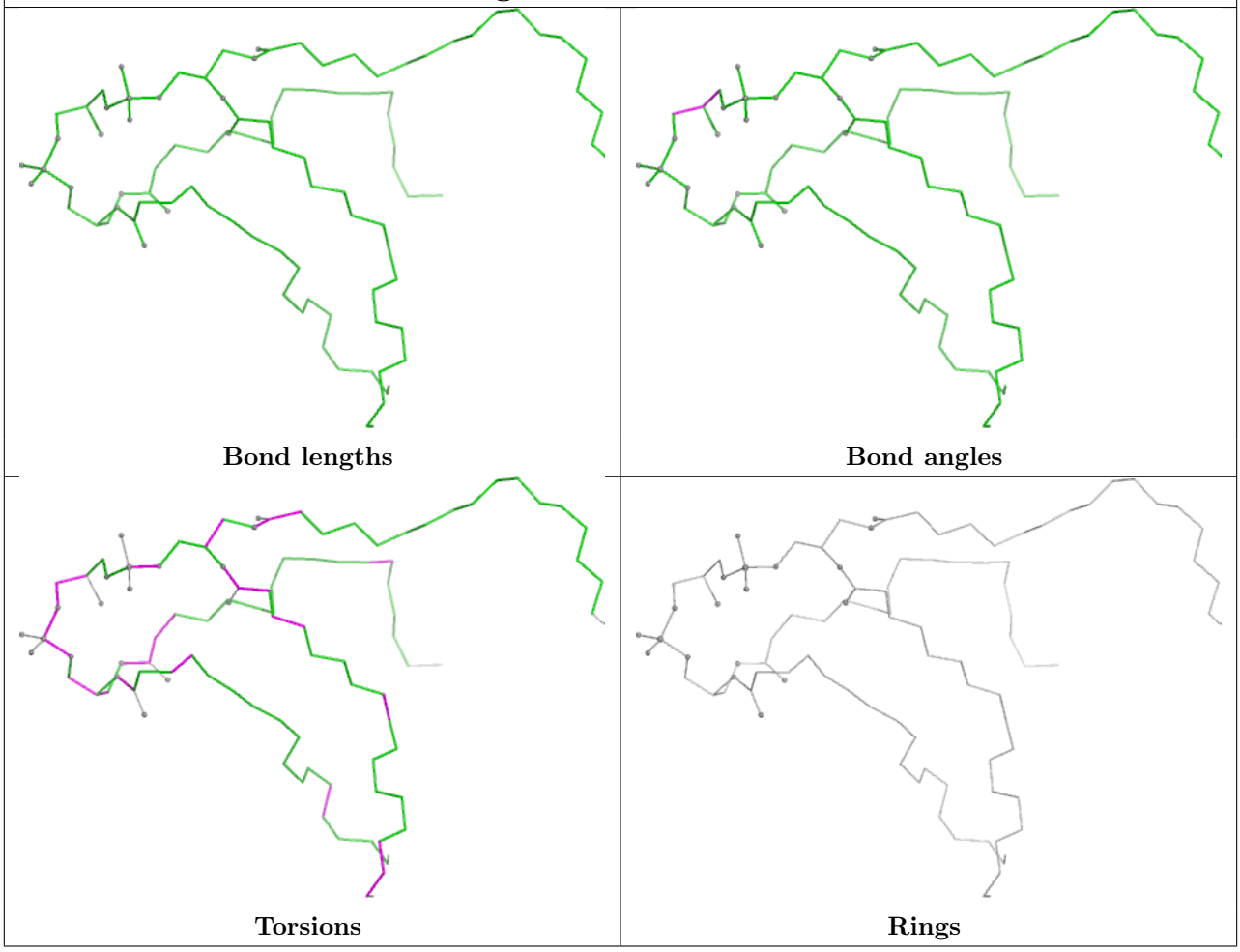
Ligand 3PE Di 1102



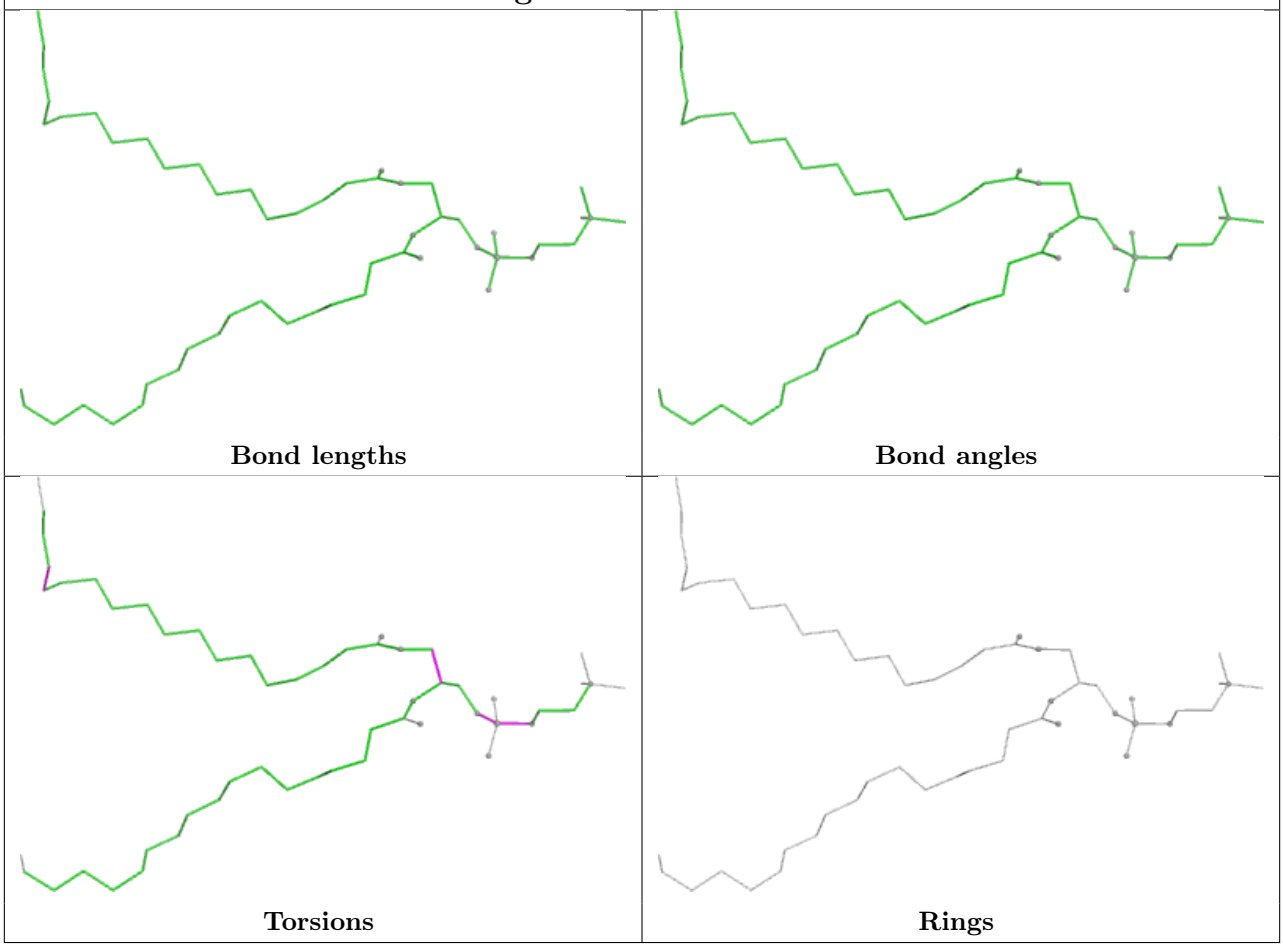
Ligand 3PE EO 203



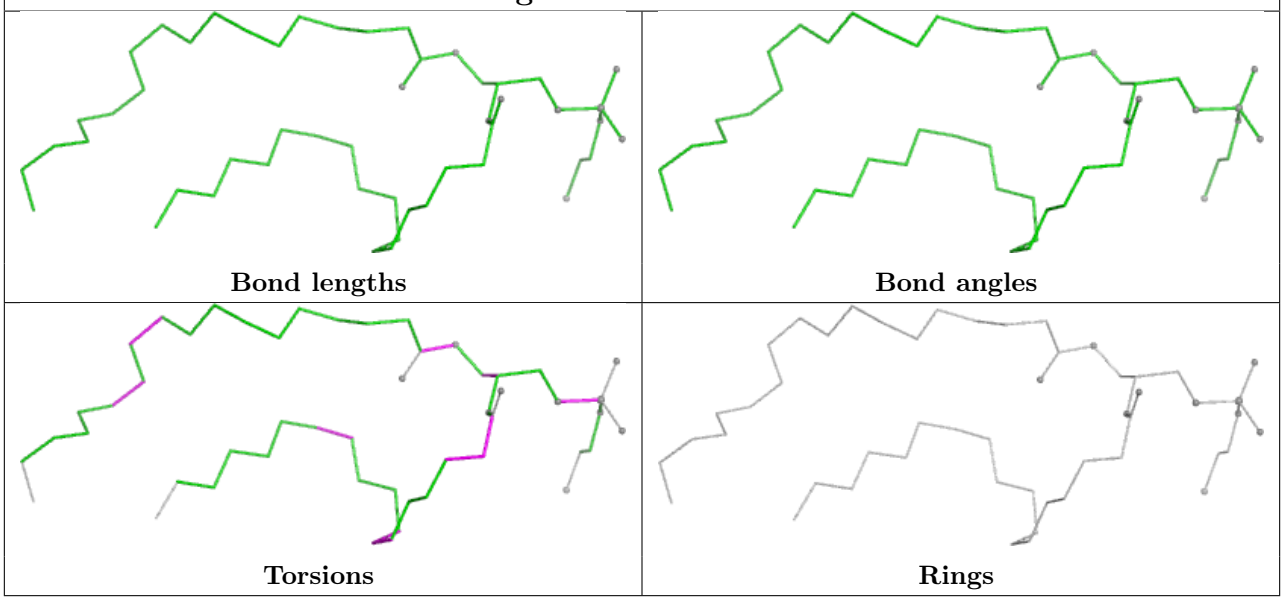
Ligand CDL ED 605



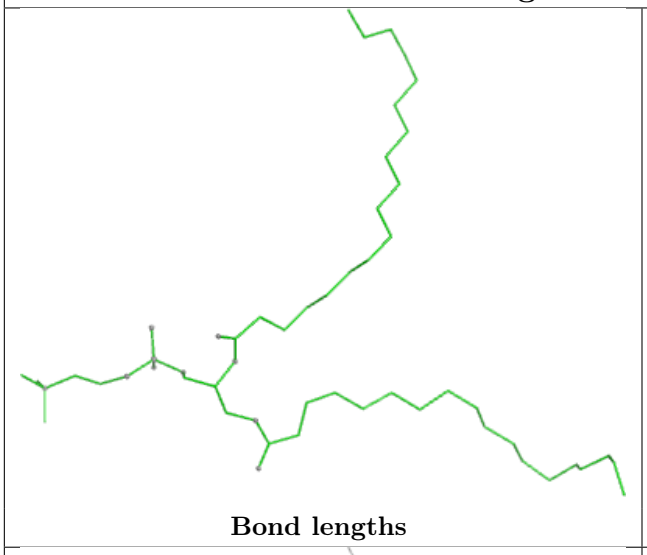
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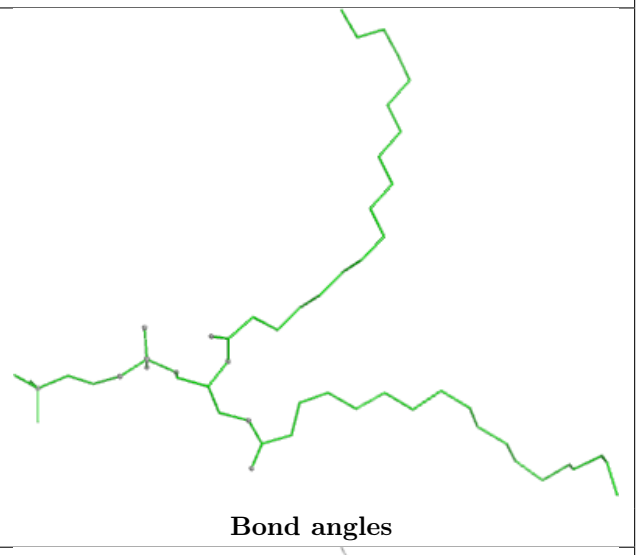
Ligand 3PE Em 901



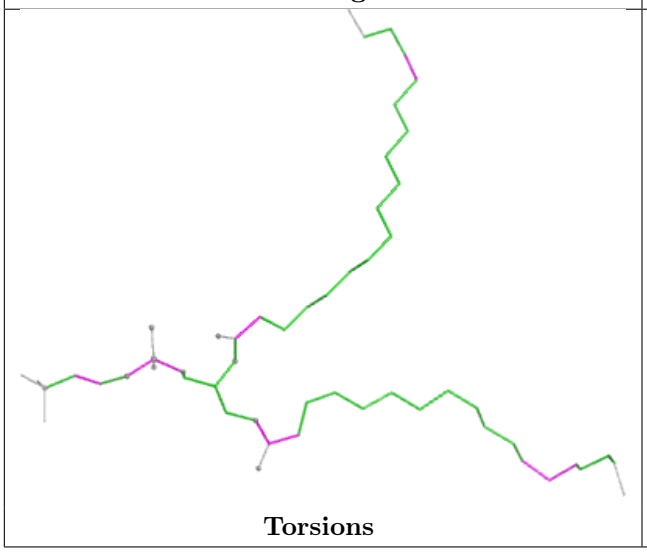
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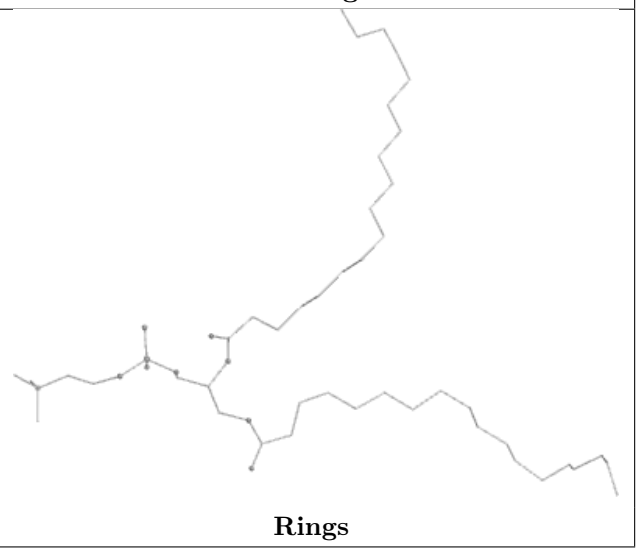
Bond lengths



Bond angles

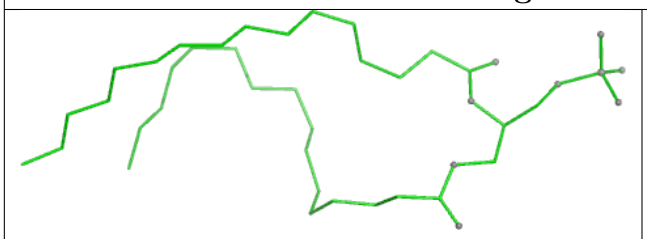


Torsions

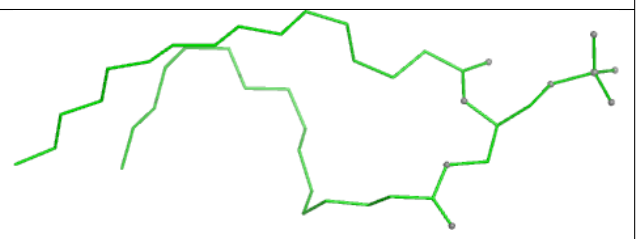


Rings

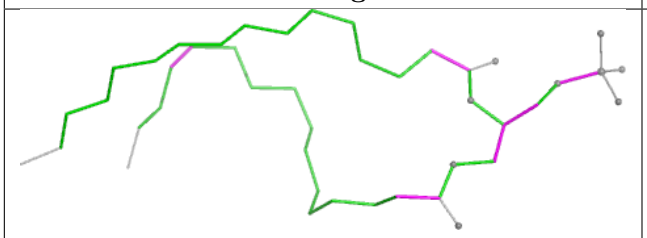
Ligand LPP AC 803



Bond lengths



Bond angles

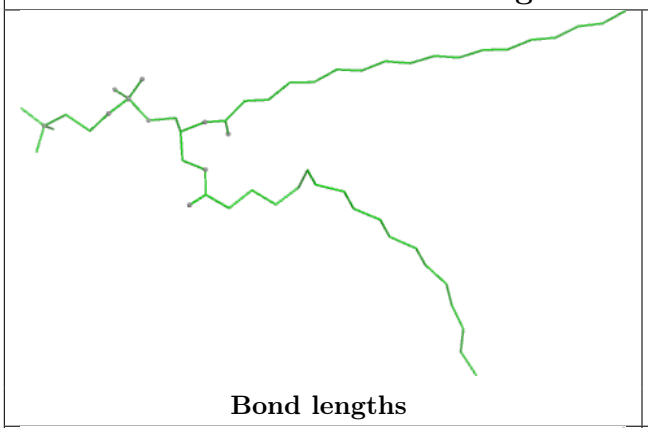


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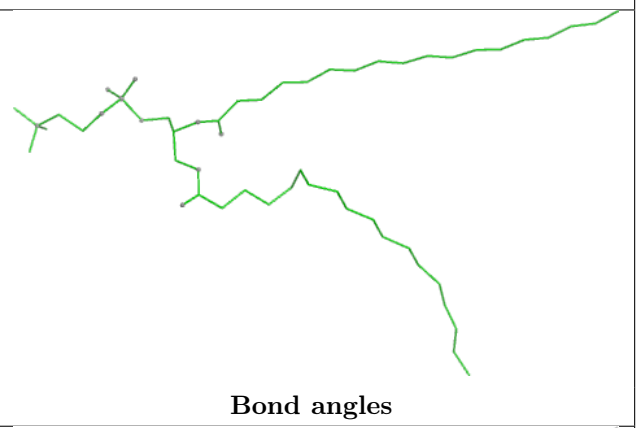


Rings

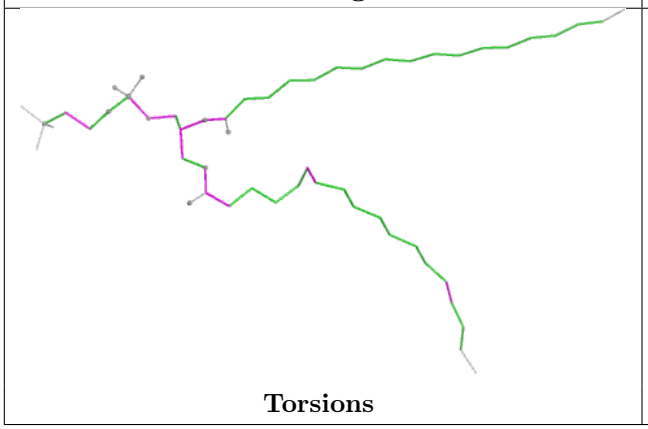
Ligand PC1 CC 302



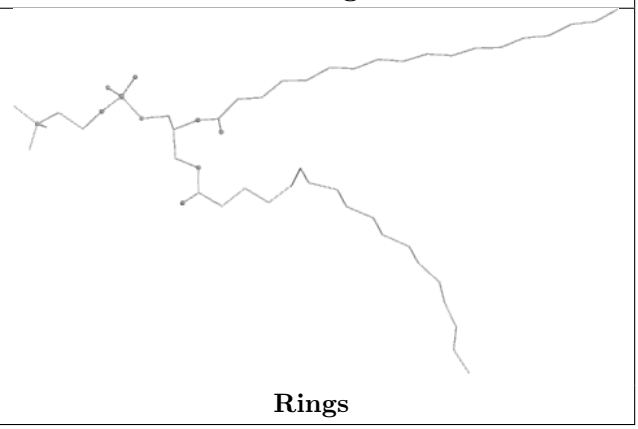
Bond lengths



Bond angles



Torsions



Rings

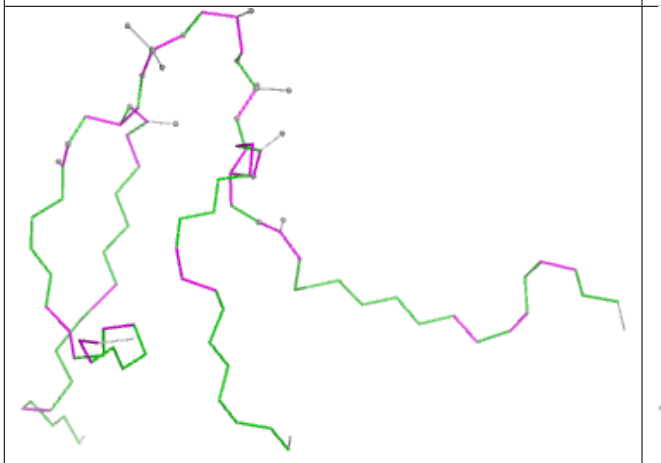
Ligand CDL Dy 301



Bond lengths



Bond angles

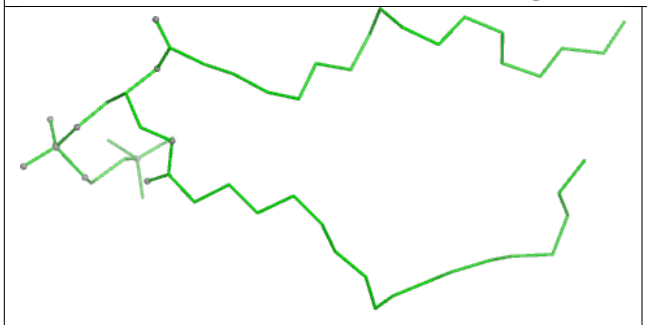


Torsions

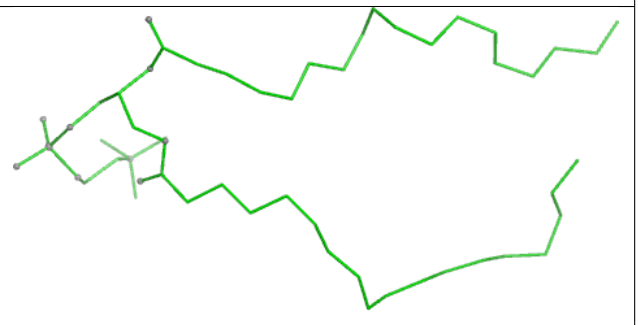


Rings

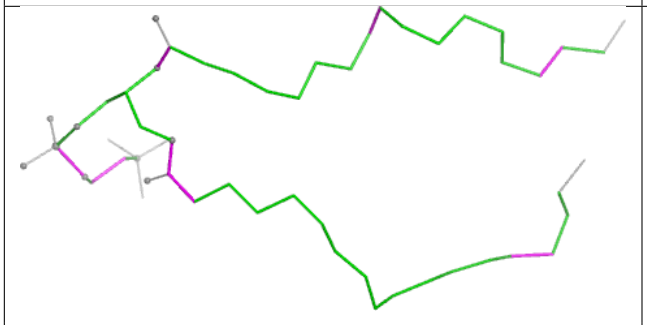
Ligand PC1 K 502



Bond lengths



Bond angles

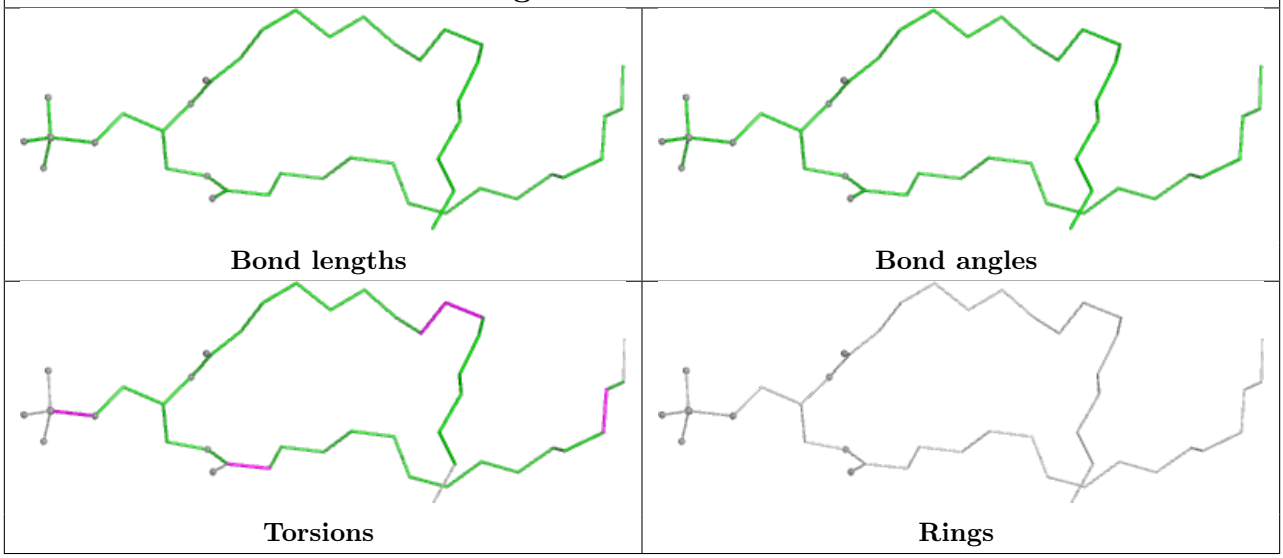


Torsions

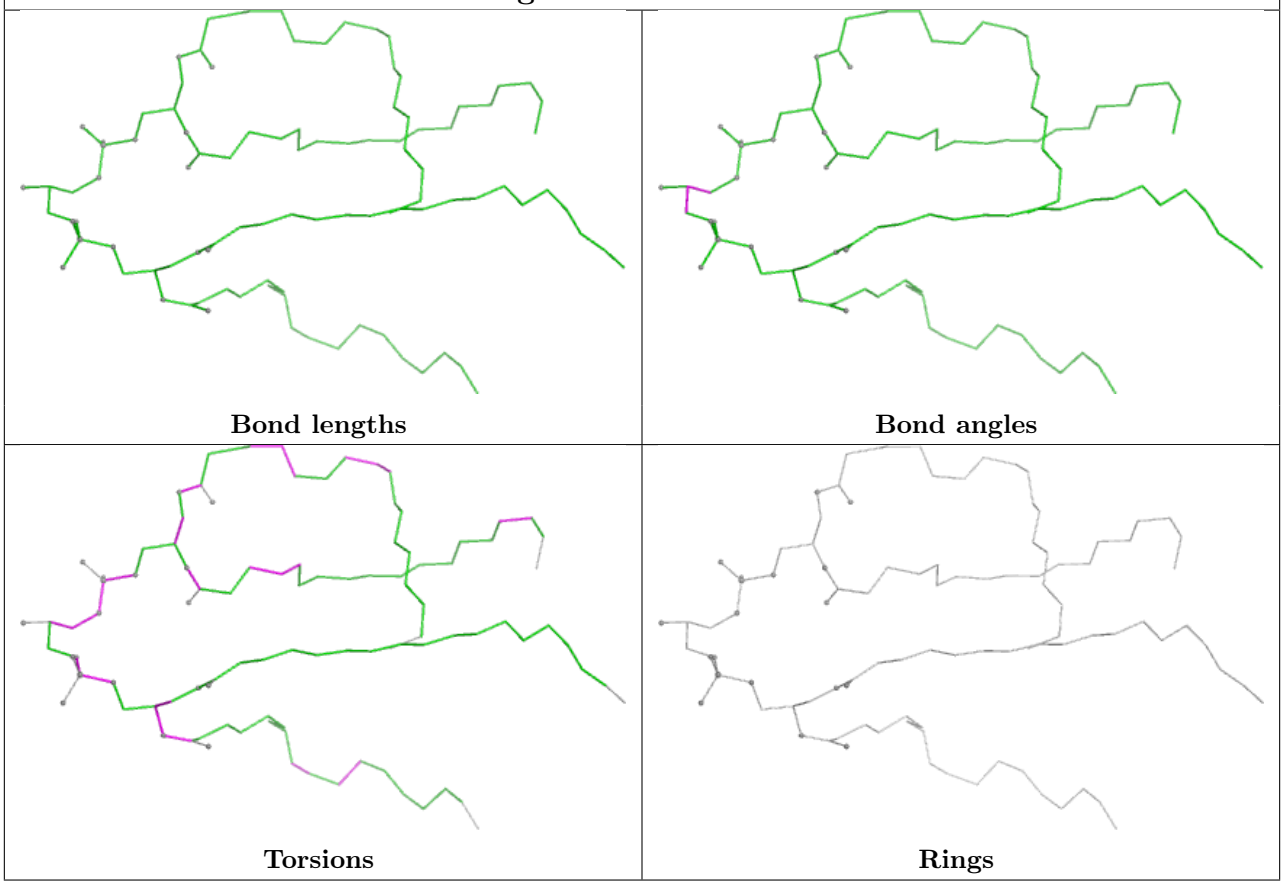


Rings

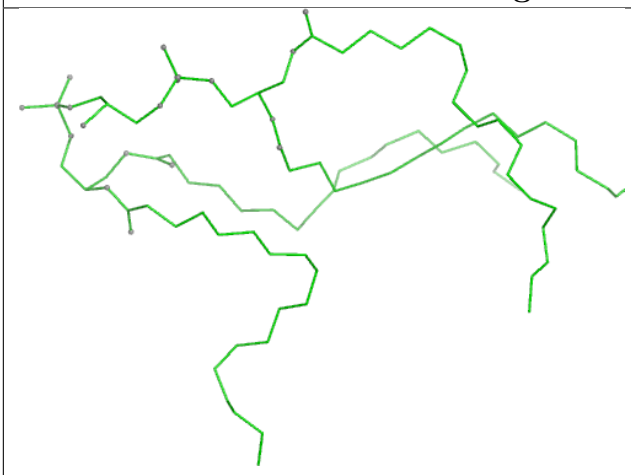
Ligand LPP DA 710



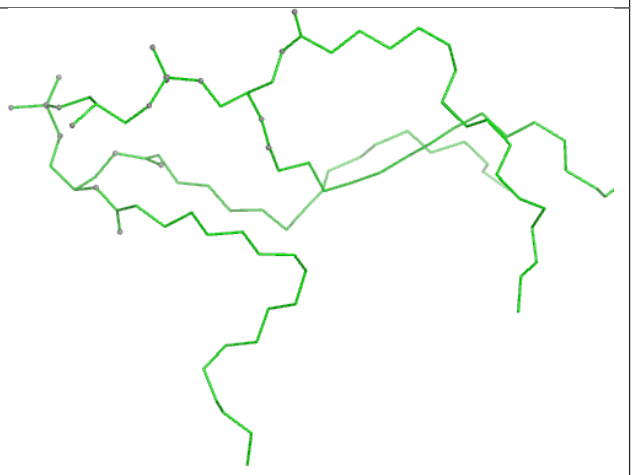
Ligand CDL Ds 401



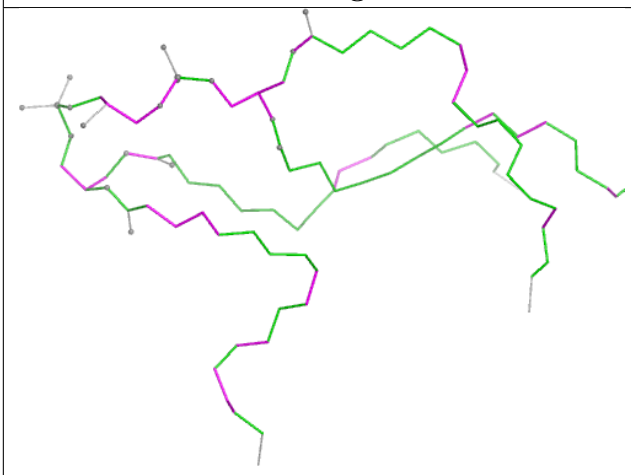
Ligand CDL Dd 704



Bond lengths



Bond angles

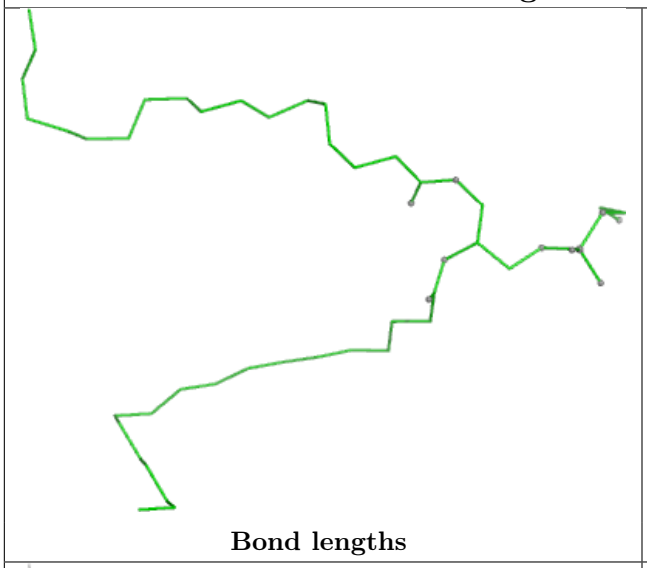


Torsions

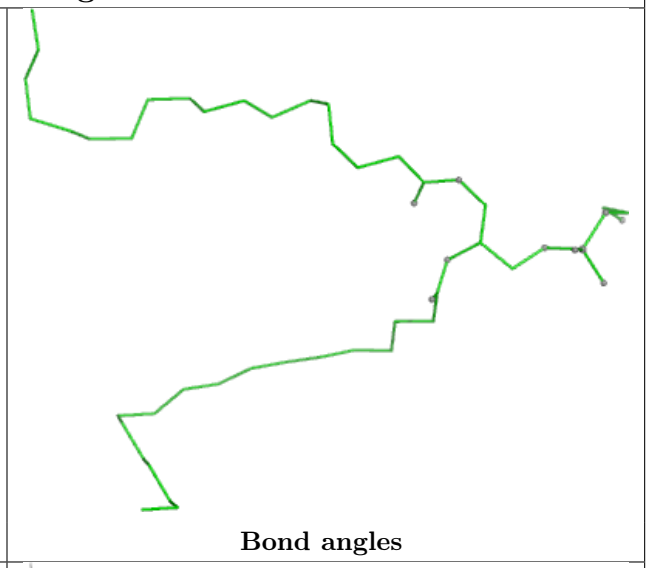


Rings

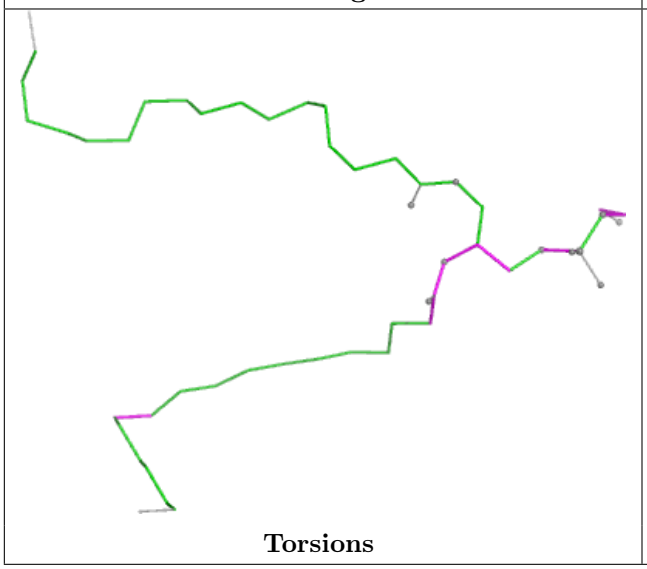
Ligand 3PE Dg 204



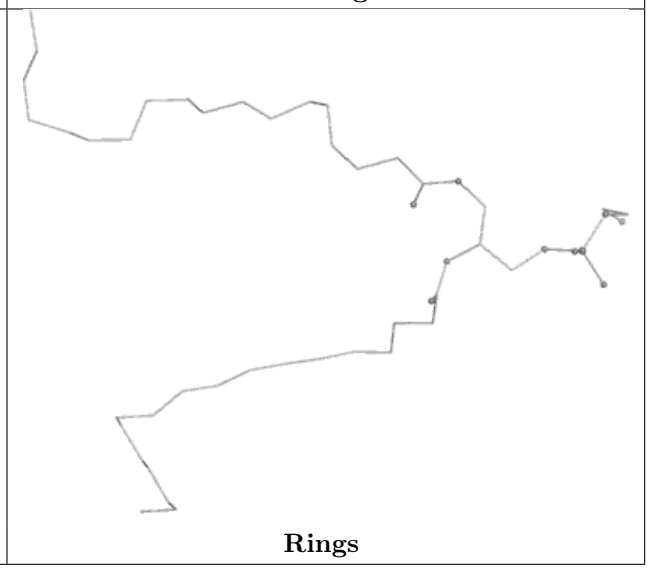
Bond lengths



Bond angles

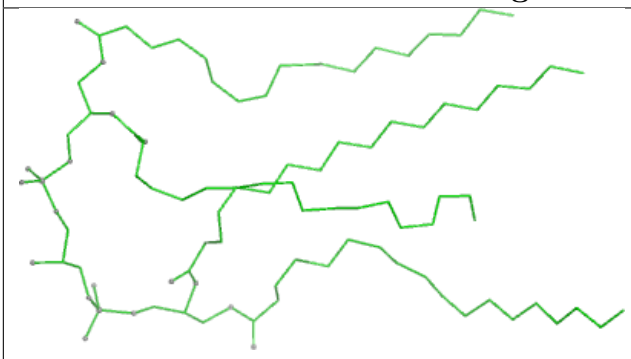


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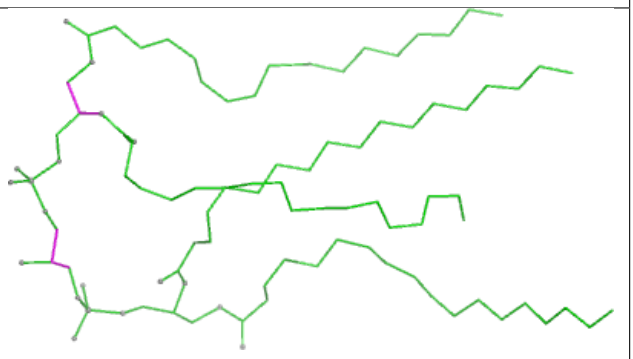


Rings

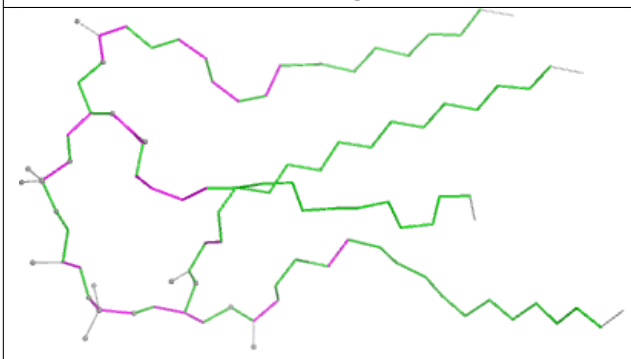
Ligand CDL BC 302



Bond lengths



Bond angles

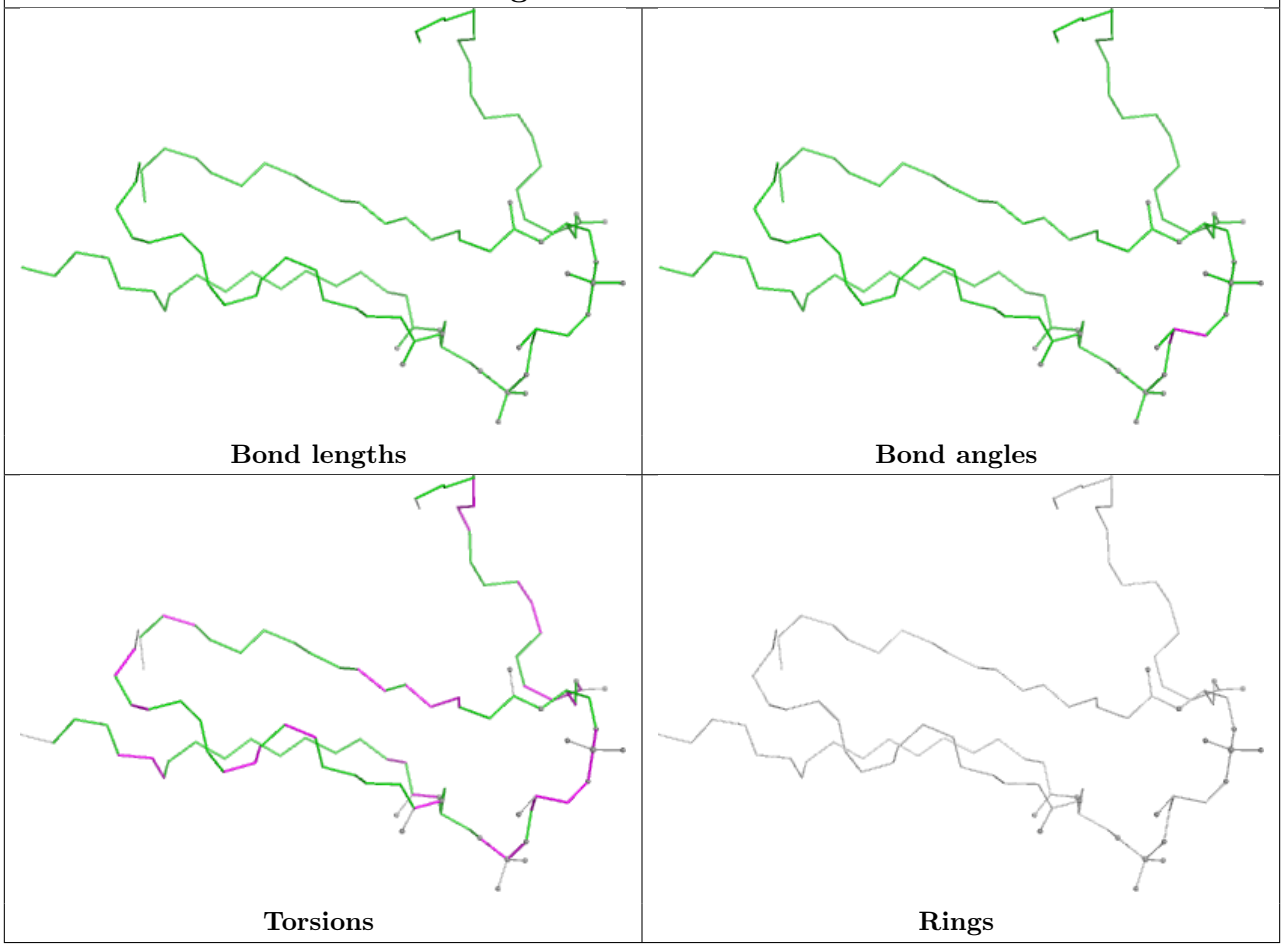


Torsions



Rings

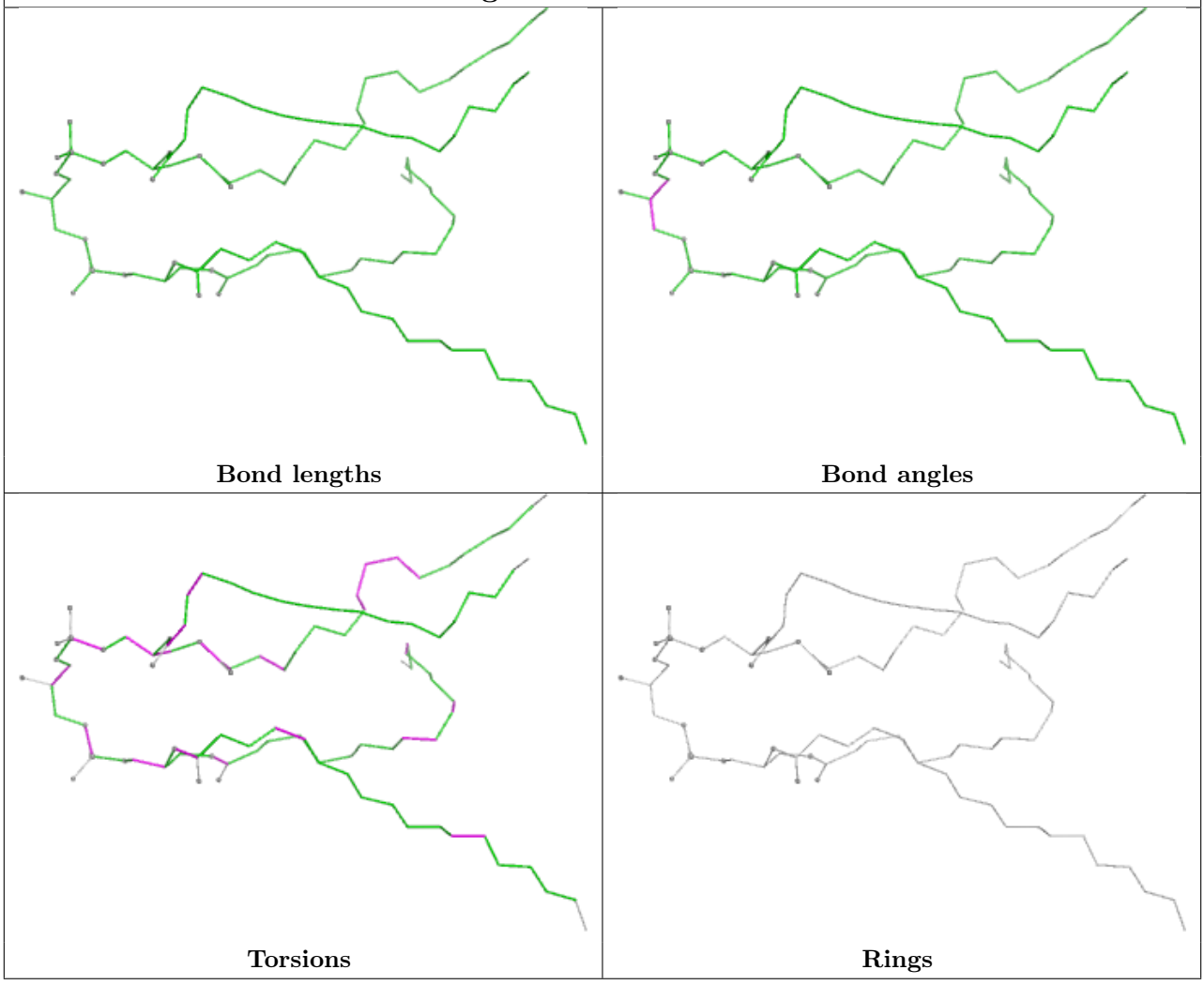
Ligand CDL DH 202



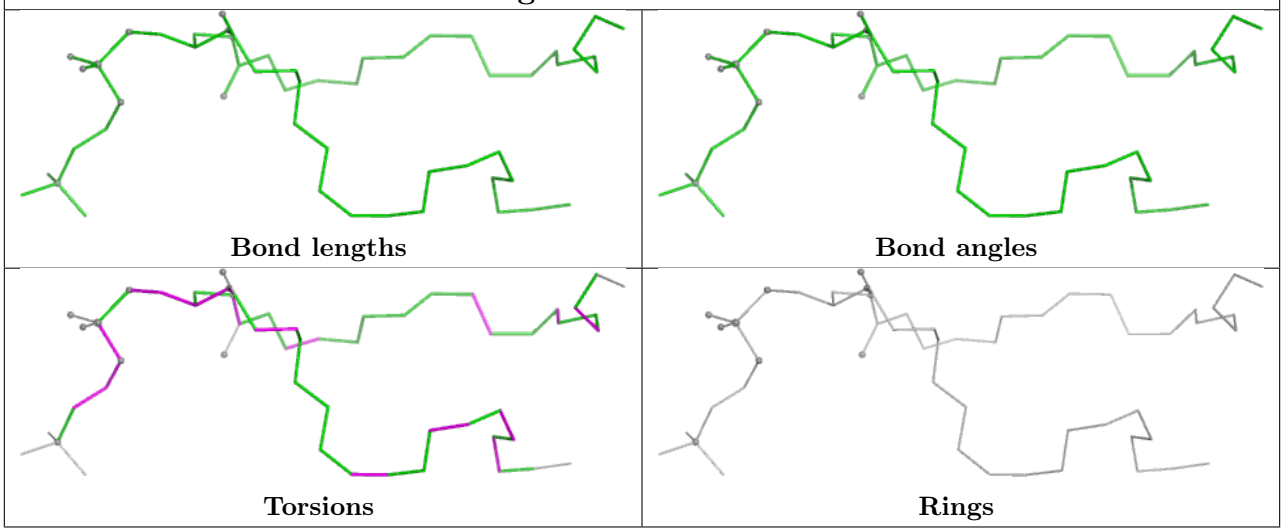
Ligand PC1 AL 303



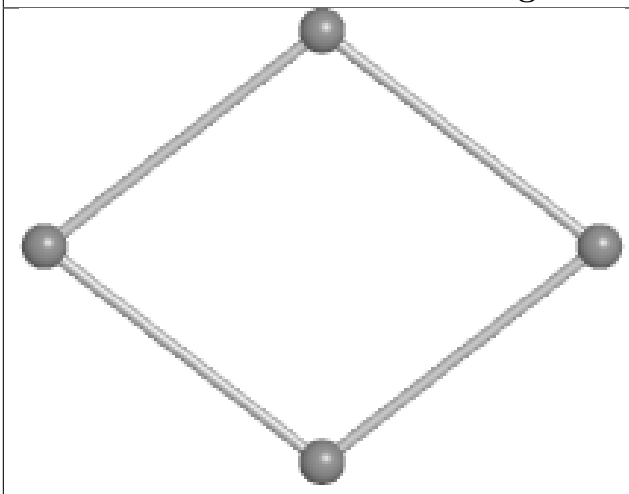
Ligand CDL AF 402



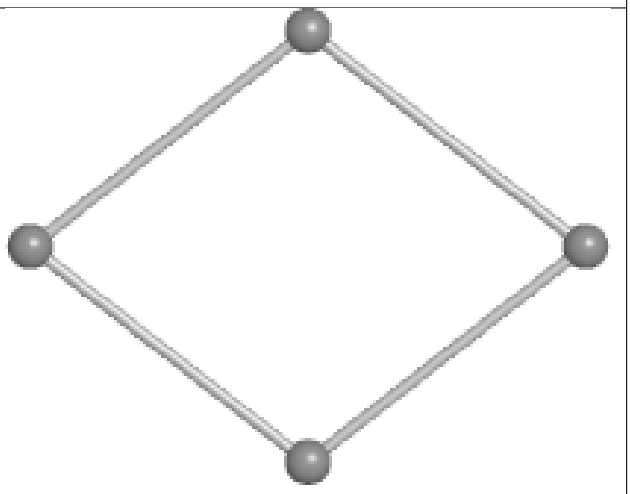
Ligand PC1 Db 702



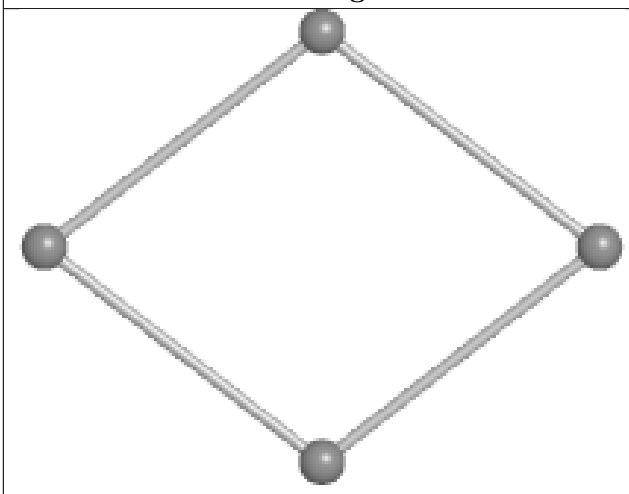
Ligand FES EF 202



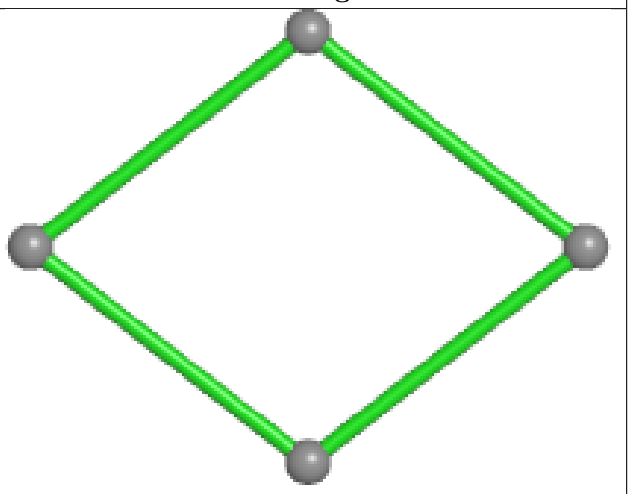
Bond lengths



Bond angles

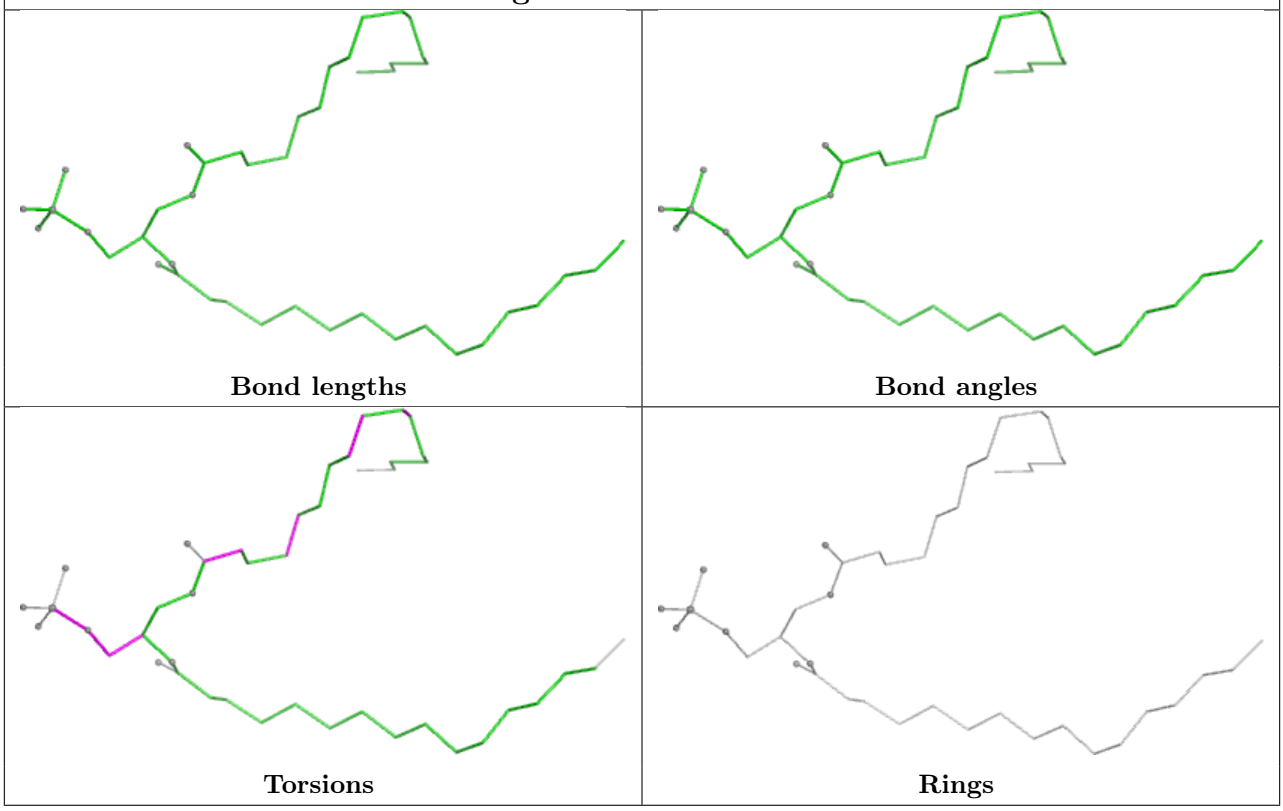


Torsions

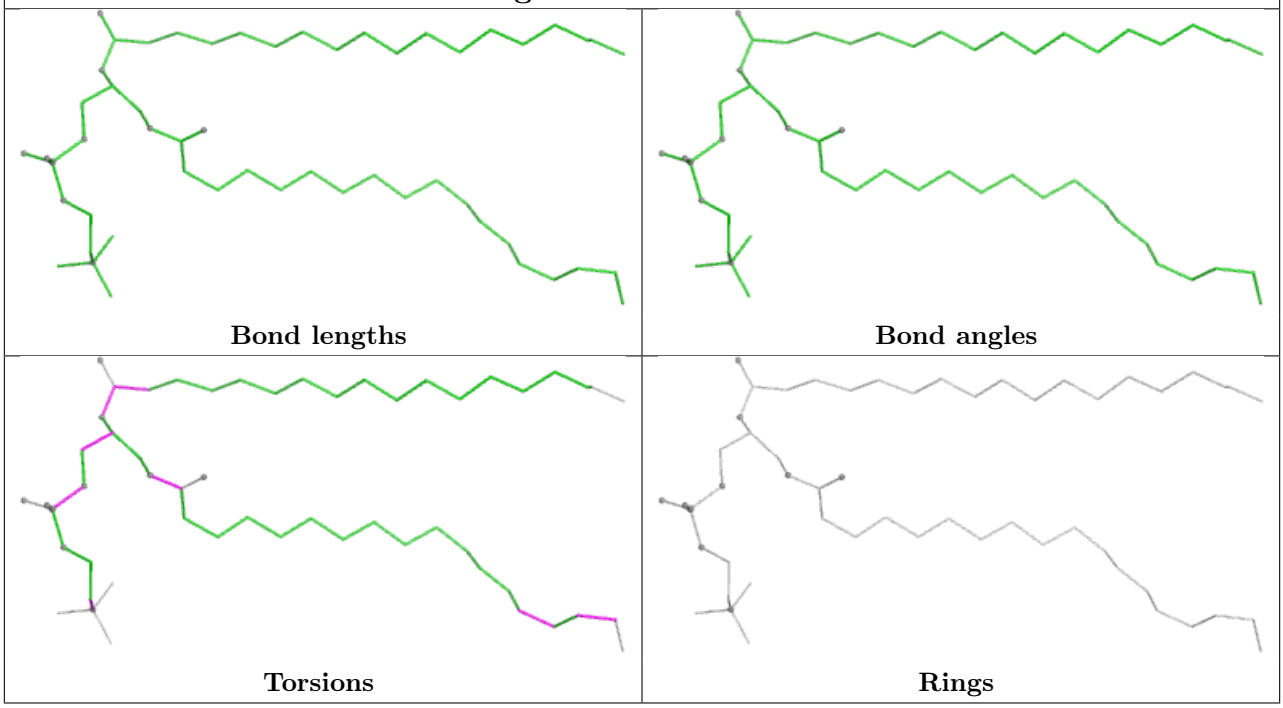


Rings

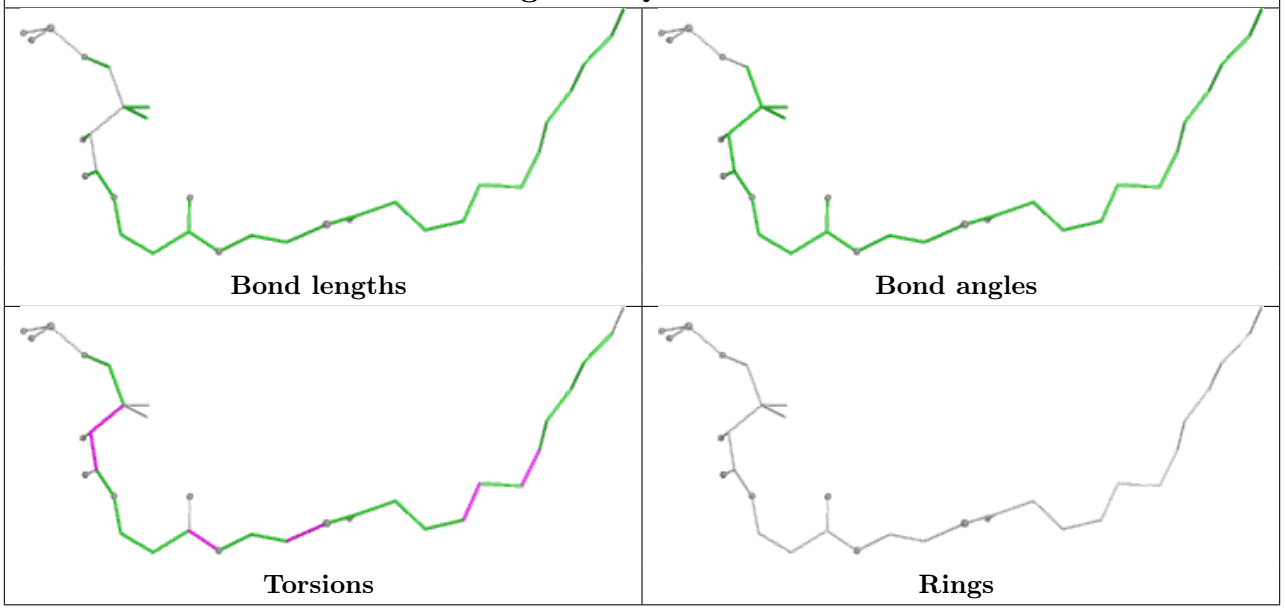
Ligand LPP DN 504



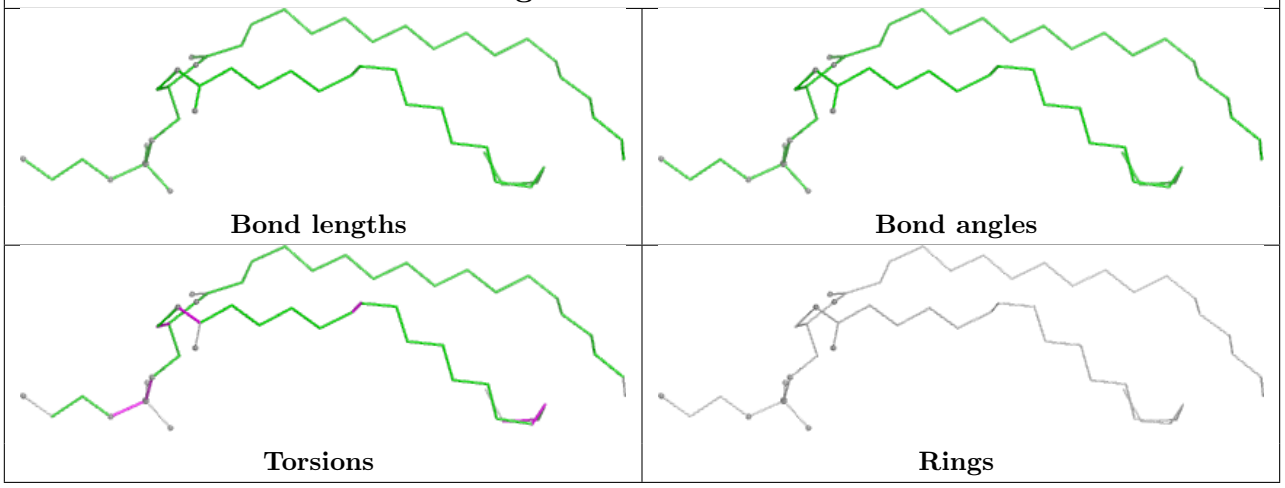
Ligand PC1 AA 904



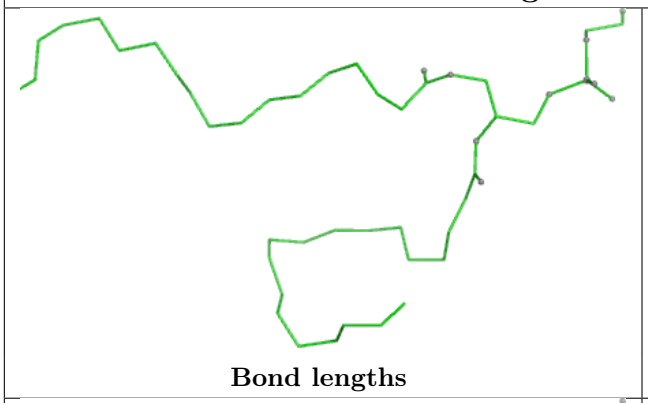
Ligand 8Q1 AS 200



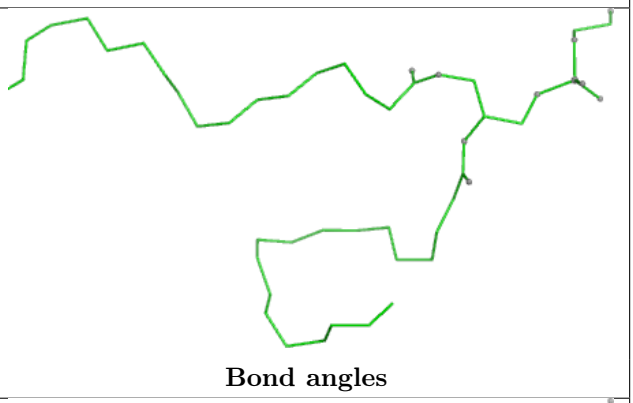
Ligand 3PE DR 401



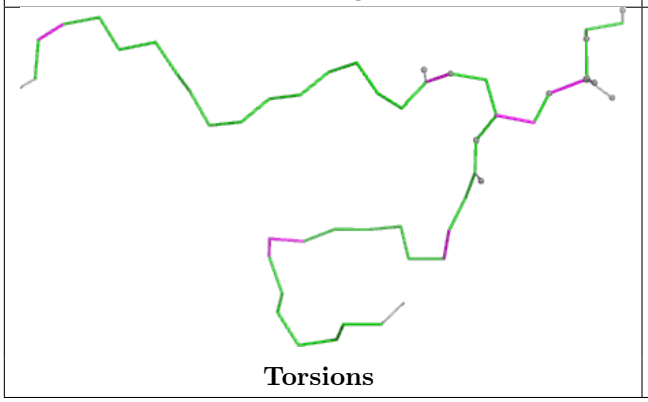
Ligand 3PE Dr 404



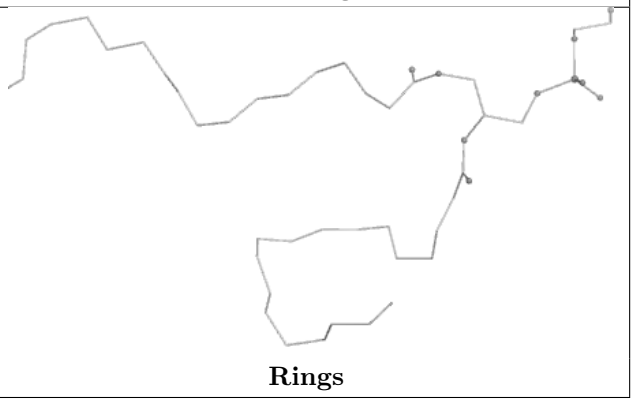
Bond lengths



Bond angles

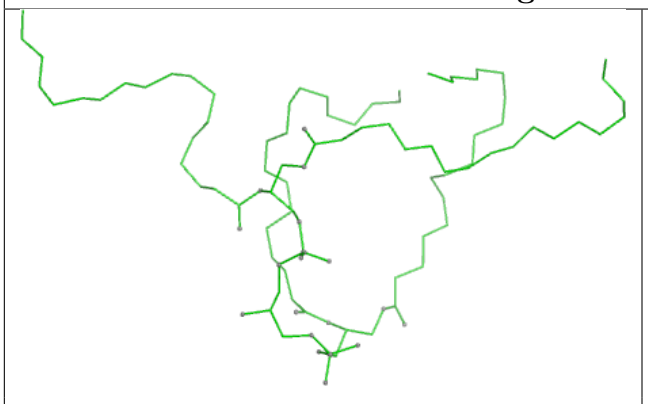


Torsions



Rings

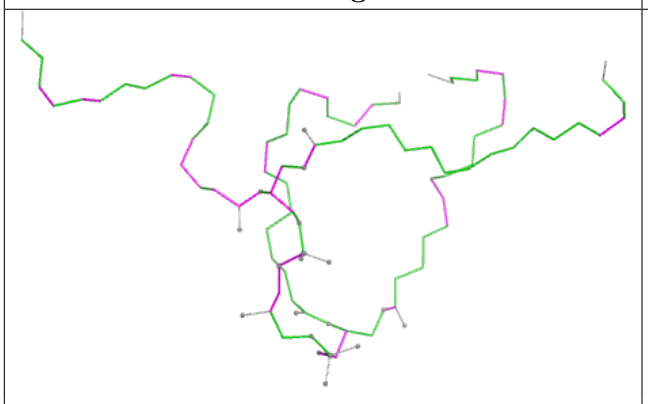
Ligand CDL Eg 101



Bond lengths



Bond angles



Torsions

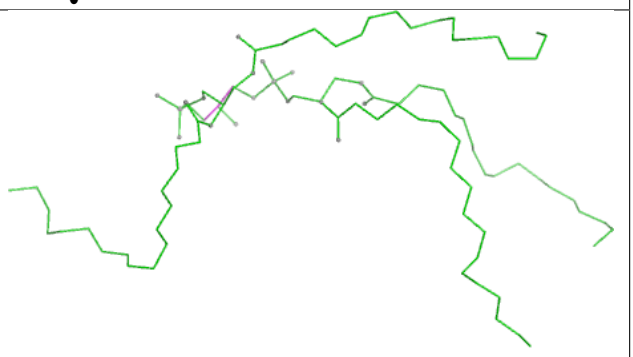


Rings

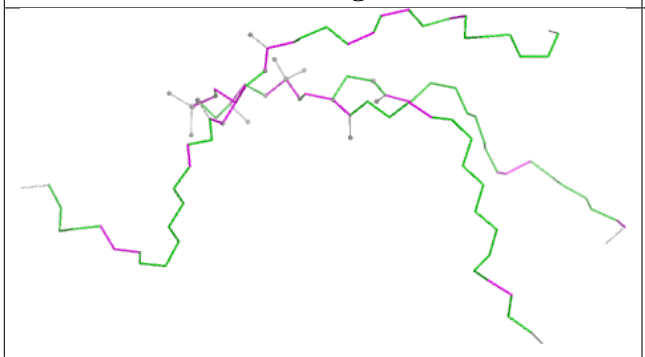
Ligand CDL DQ 1502



Bond lengths



Bond angles

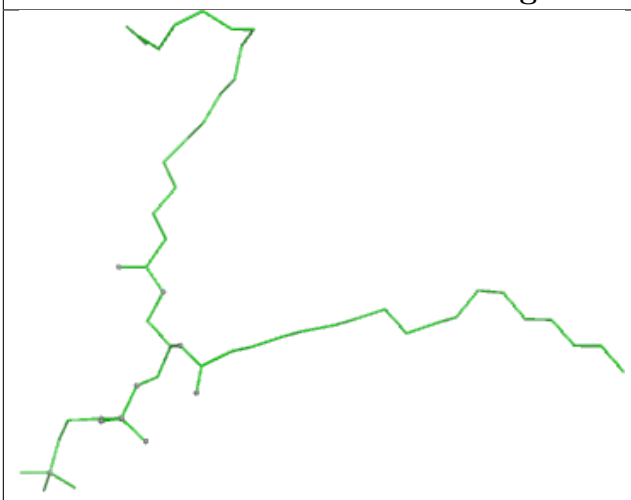


Torsions



Rings

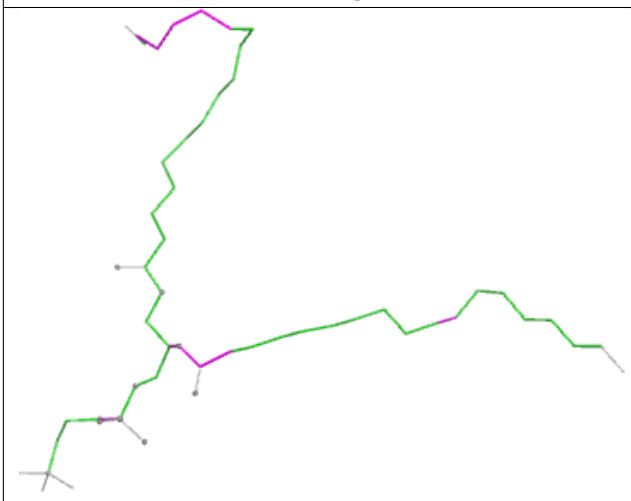
Ligand PC1 Eo 205



Bond lengths



Bond angles

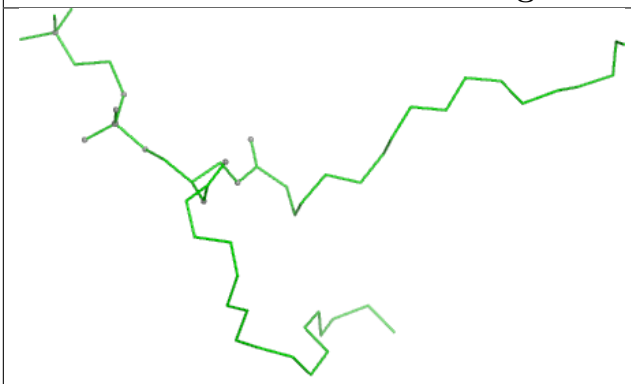


Torsions

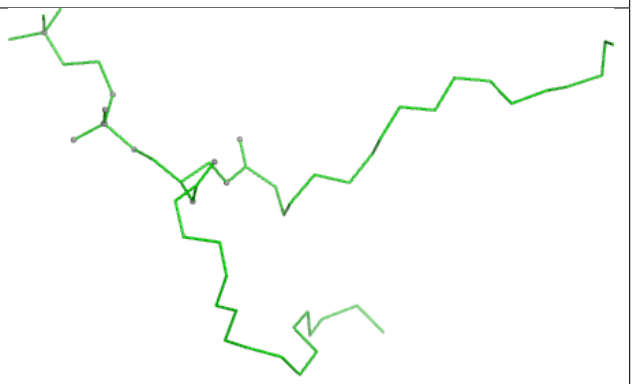


Rings

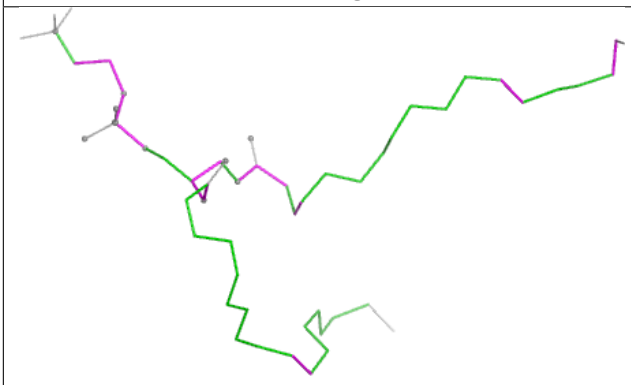
Ligand PC1 Dv 405



Bond lengths



Bond angles

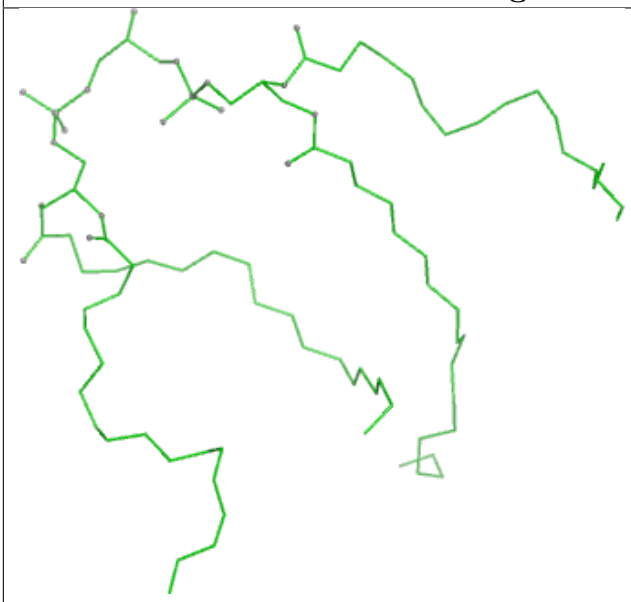


Torsions

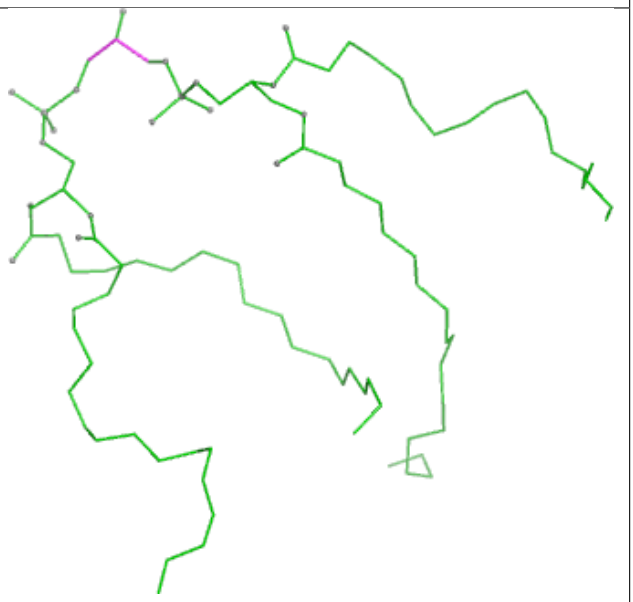


Rings

Ligand CDL DH 201



Bond lengths



Bond angles

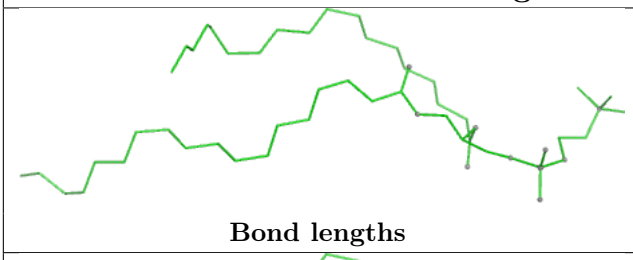


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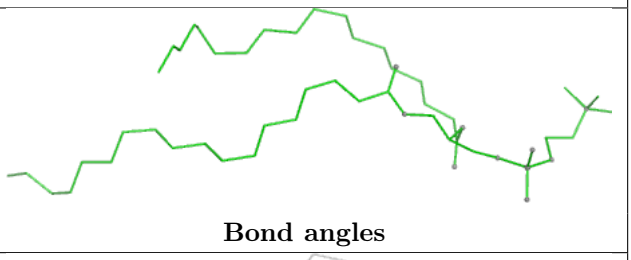


Rings

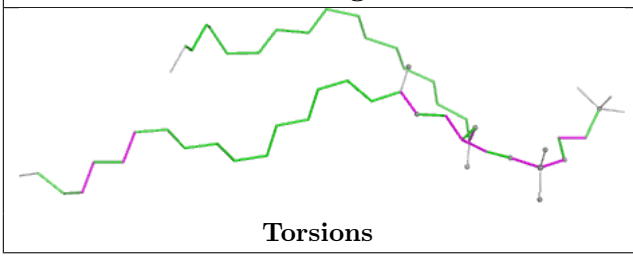
Ligand PC1 AA 905



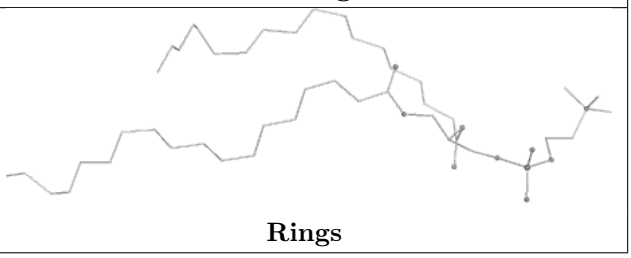
Bond lengths



Bond angles

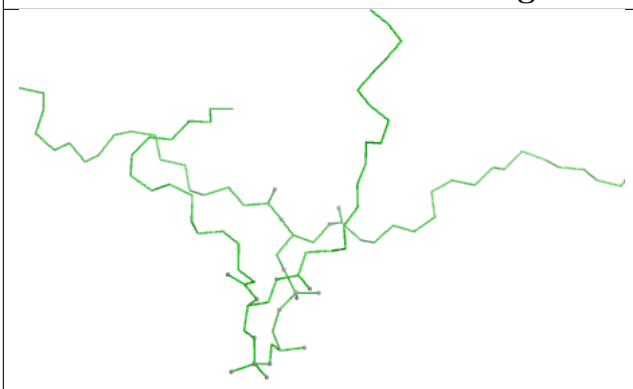


Torsions



Rings

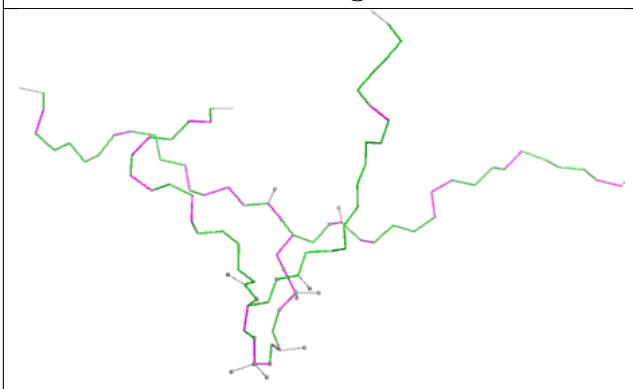
Ligand CDL Dj 403



Bond lengths



Bond angles

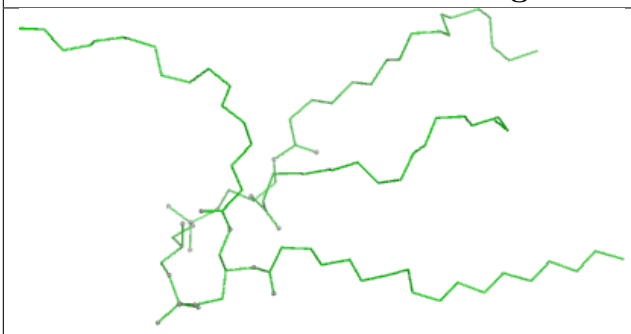


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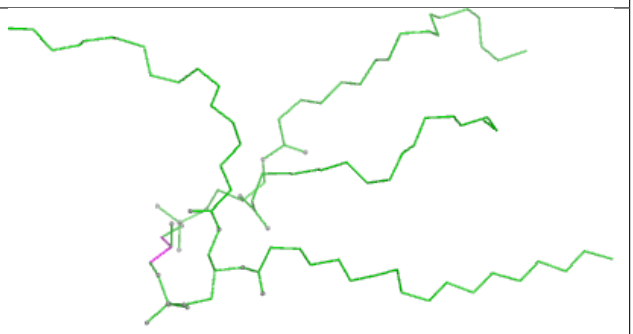


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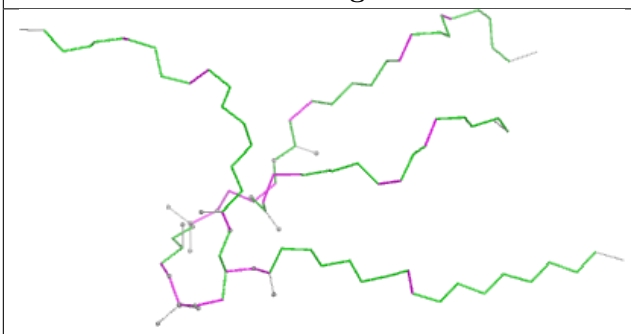
Ligand CDL BY 201



Bond lengths



Bond angles

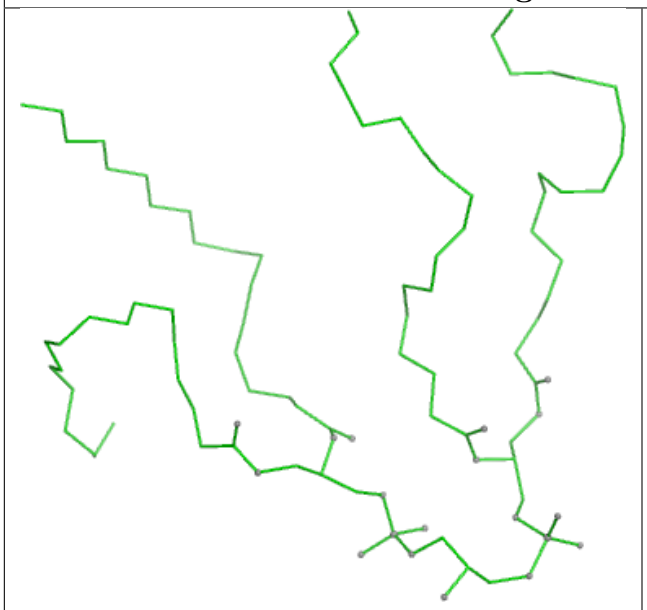


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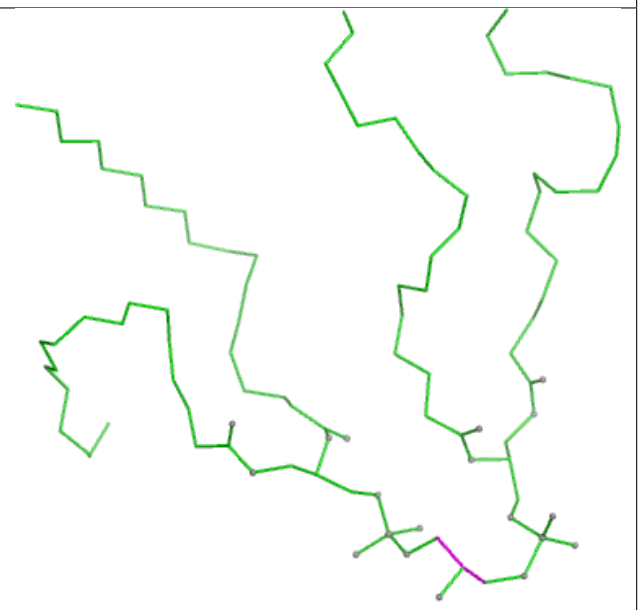


Rings

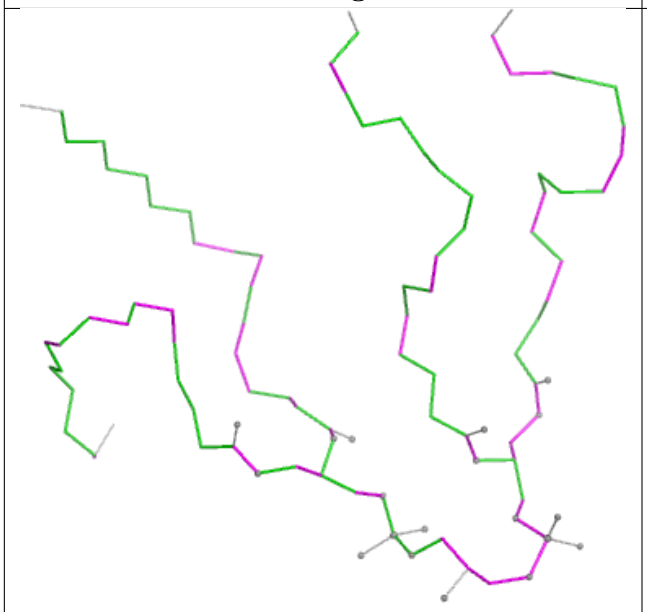
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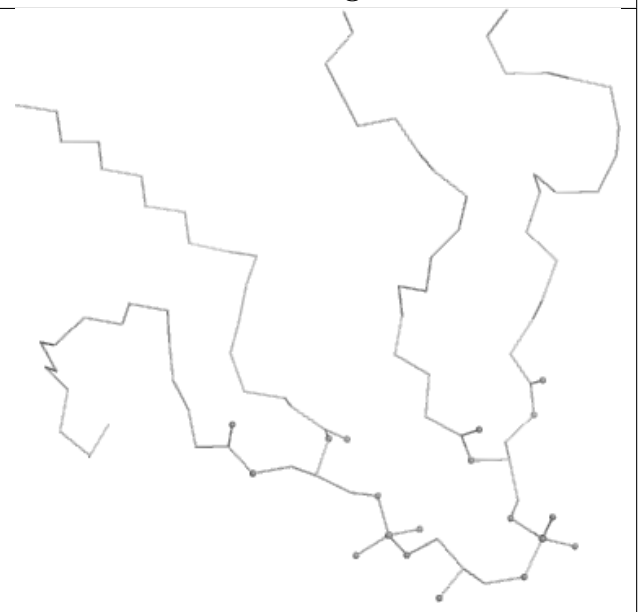
Bond lengths



Bond angles

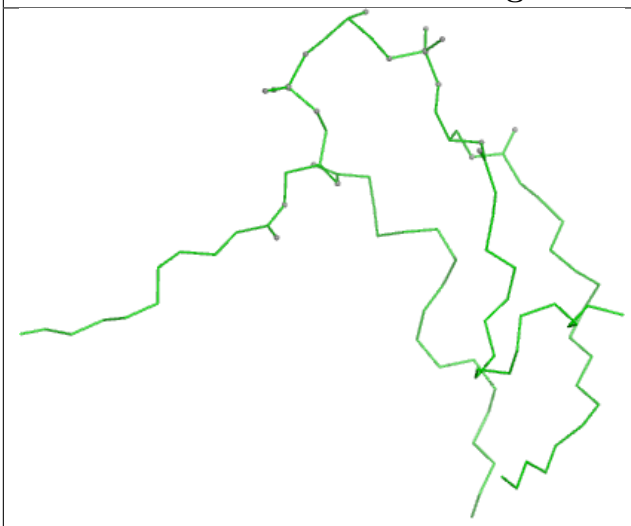


Torsions



Rings

Ligand CDL Eh 1601



Bond lengths



Bond angles

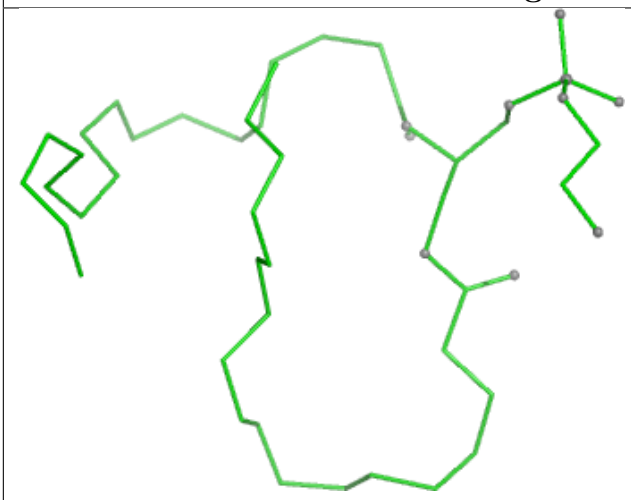


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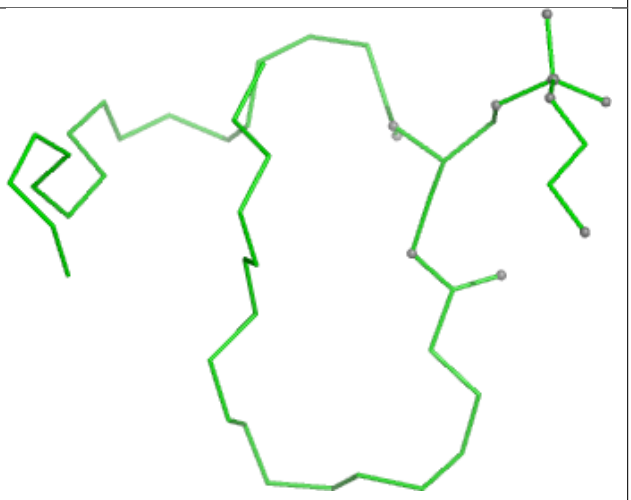


Rings

Ligand 3PE El 905



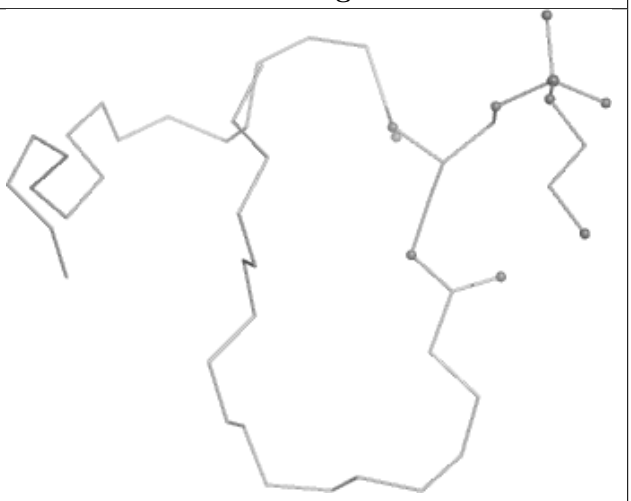
Bond lengths



Bond angles

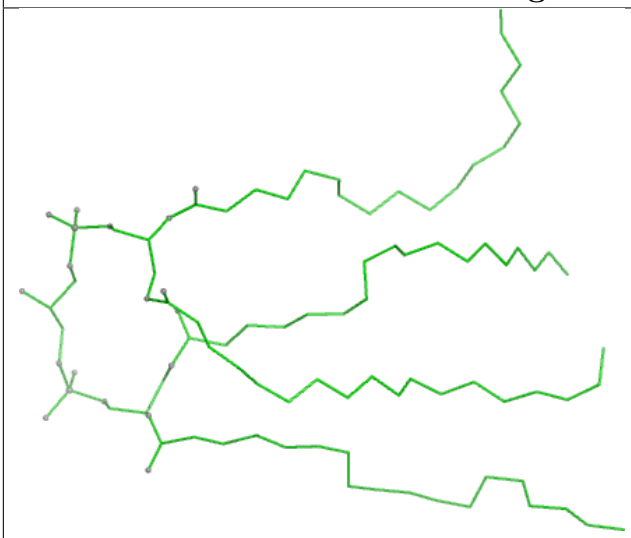


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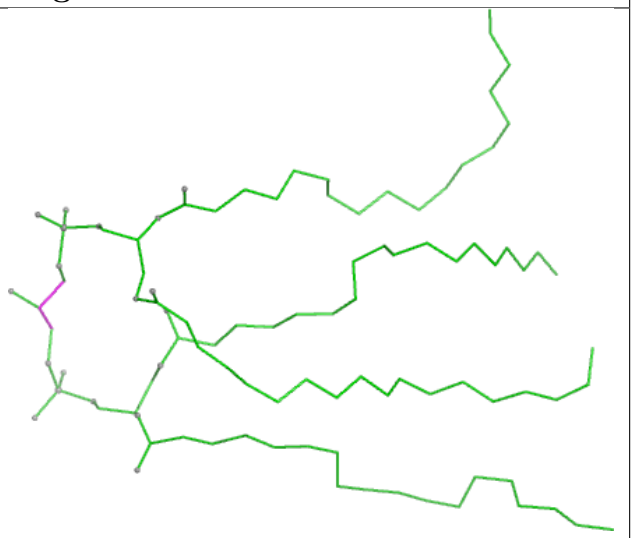


Rings

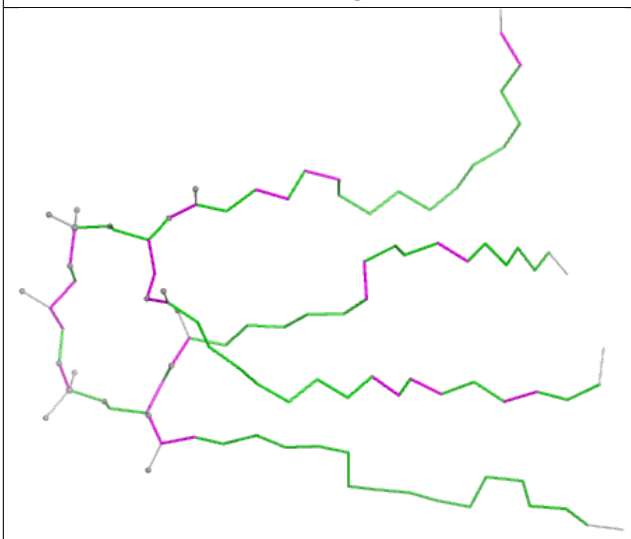
Ligand CDL g 801



Bond lengths



Bond angles

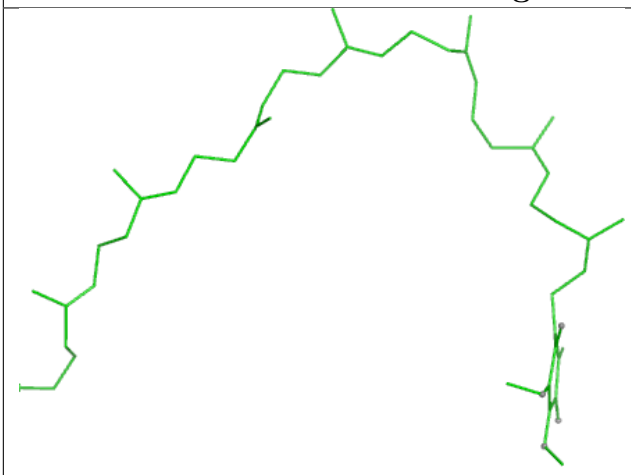


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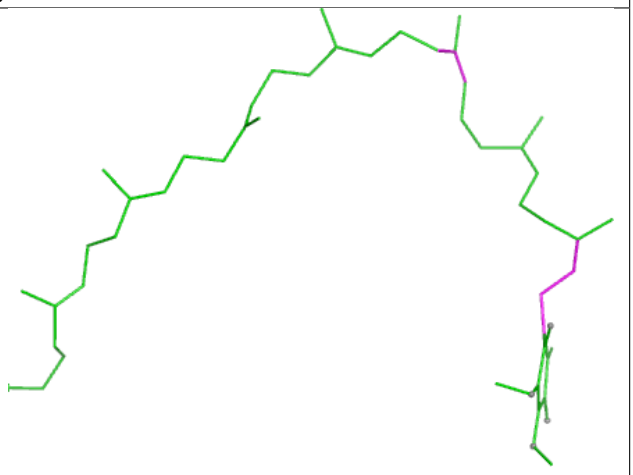


Rings

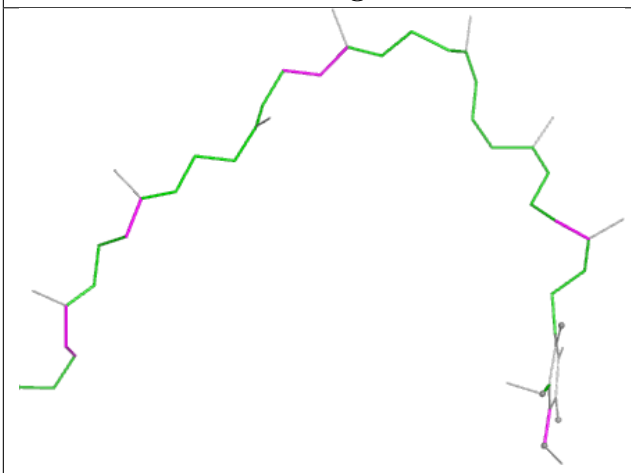
Ligand UQ8 ED 603



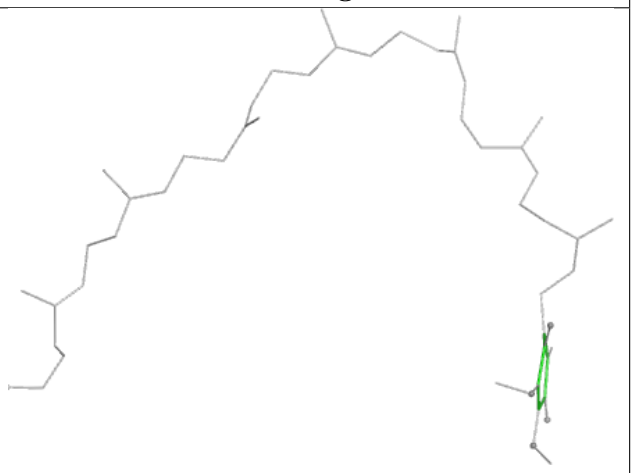
Bond lengths



Bond angles

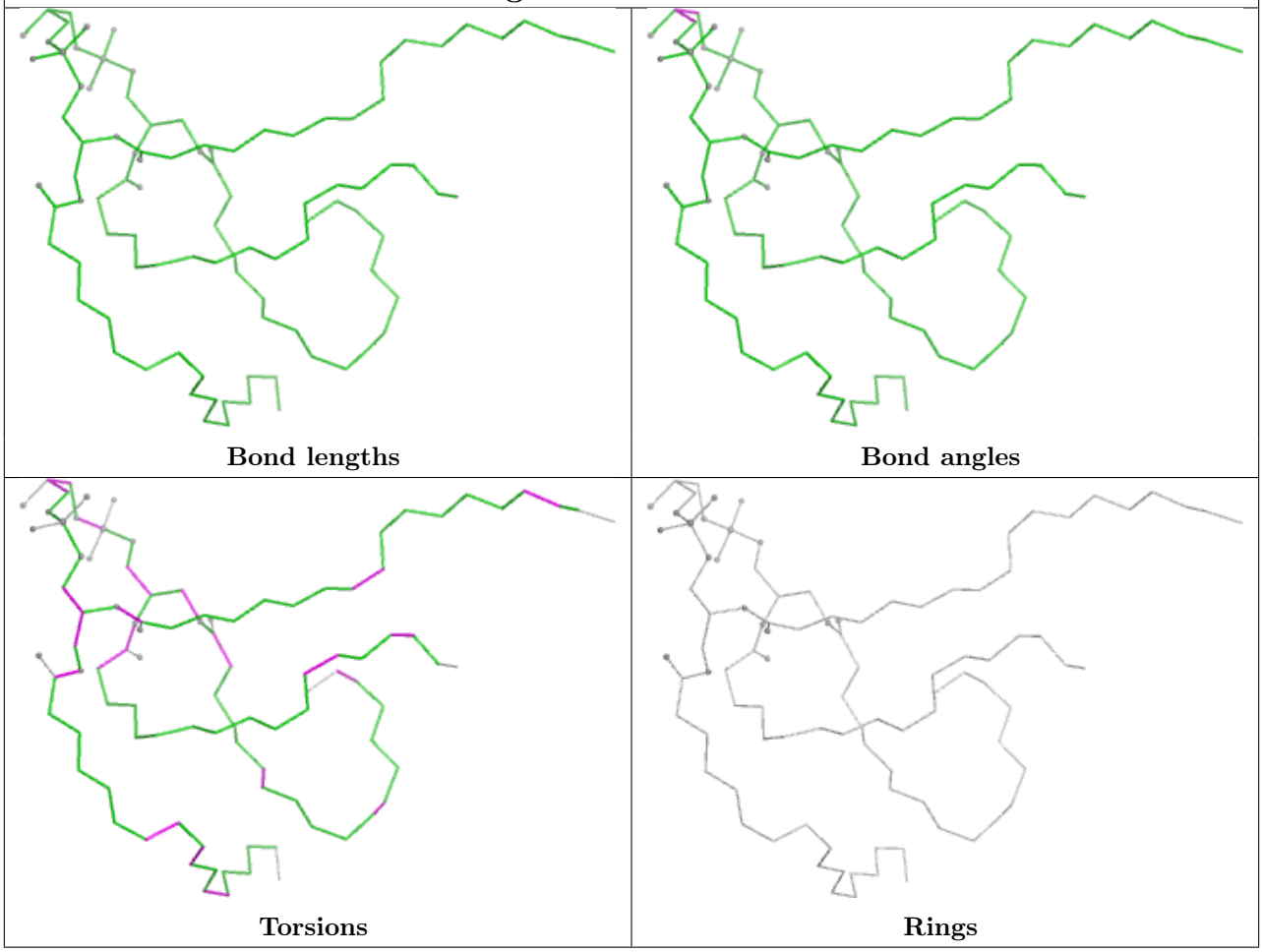


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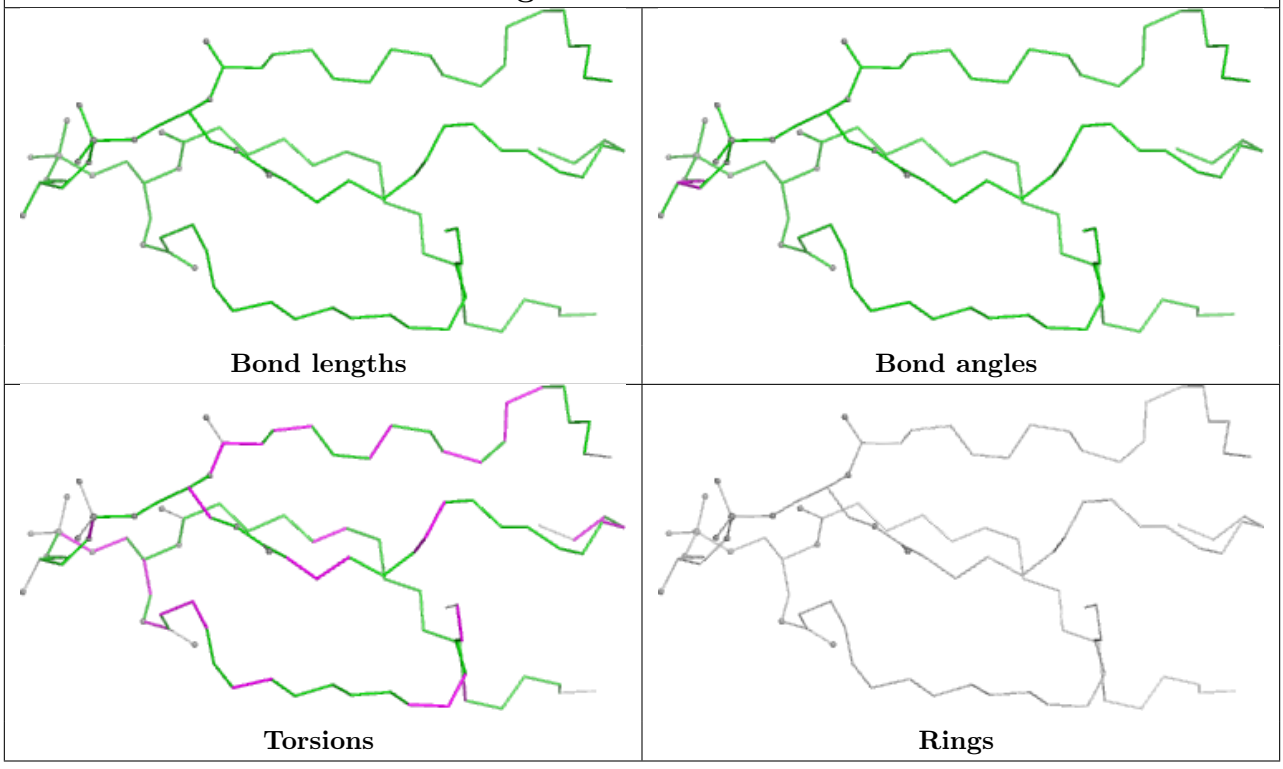


Rings

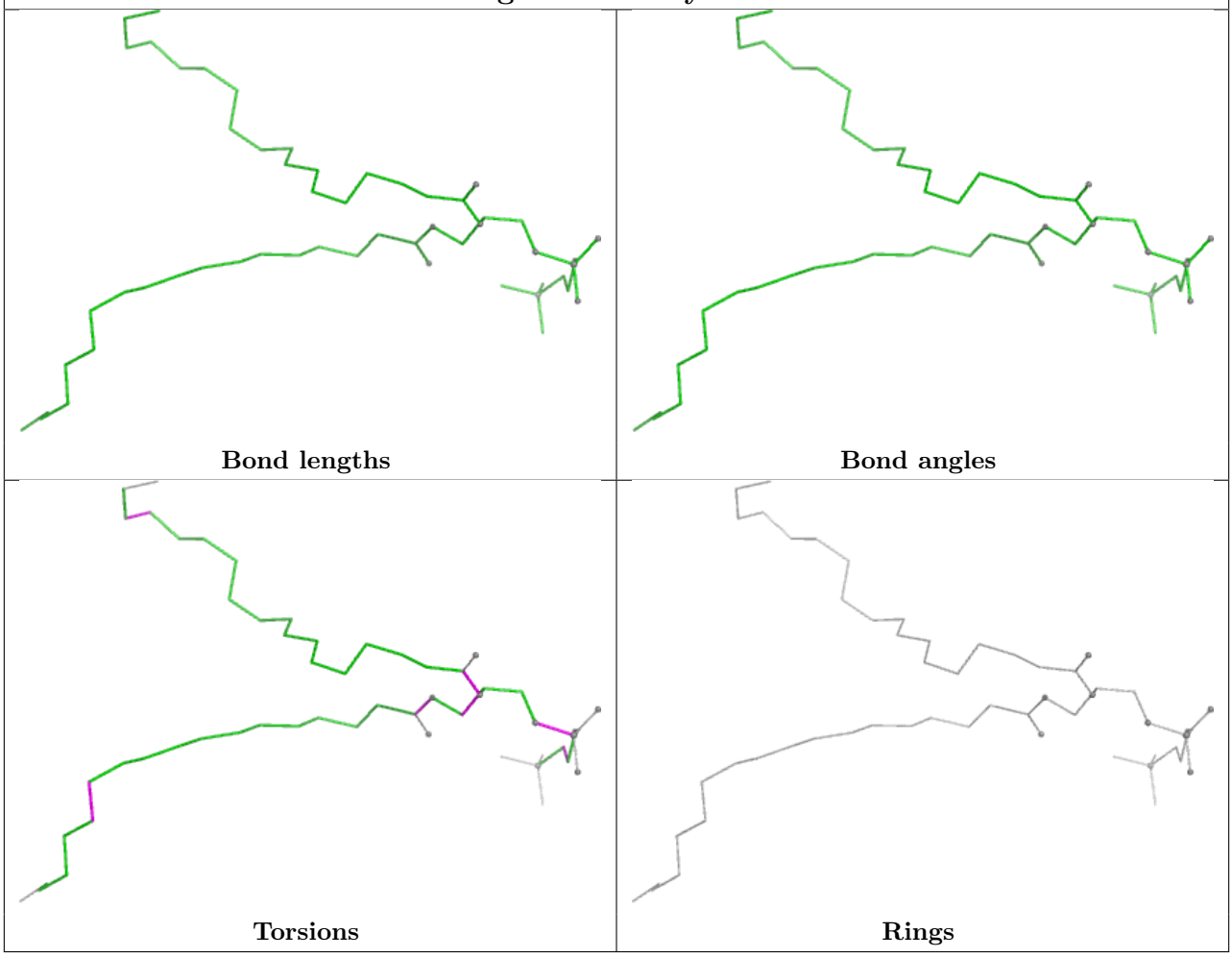
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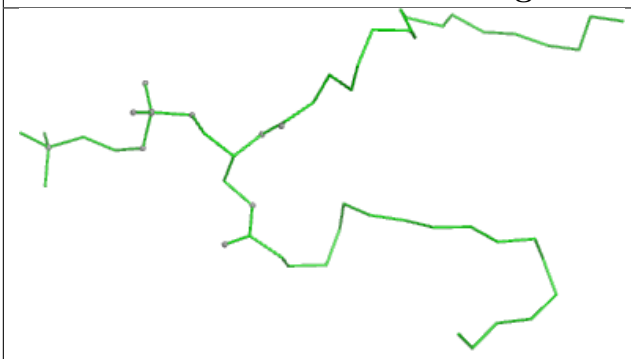
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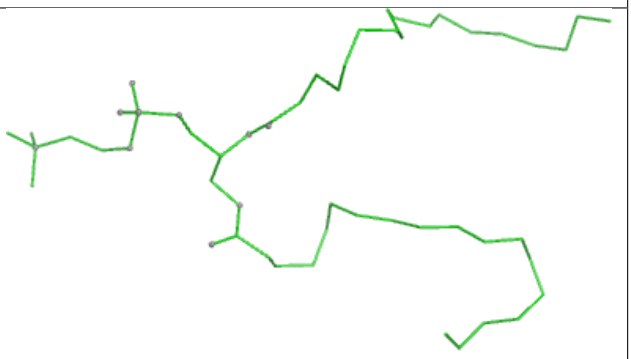
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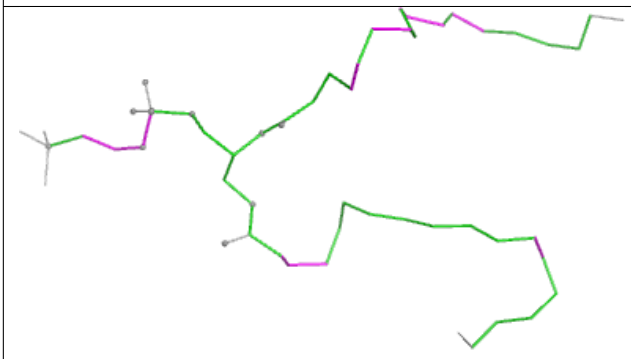
Ligand PC1 EO 201



Bond lengths



Bond angles

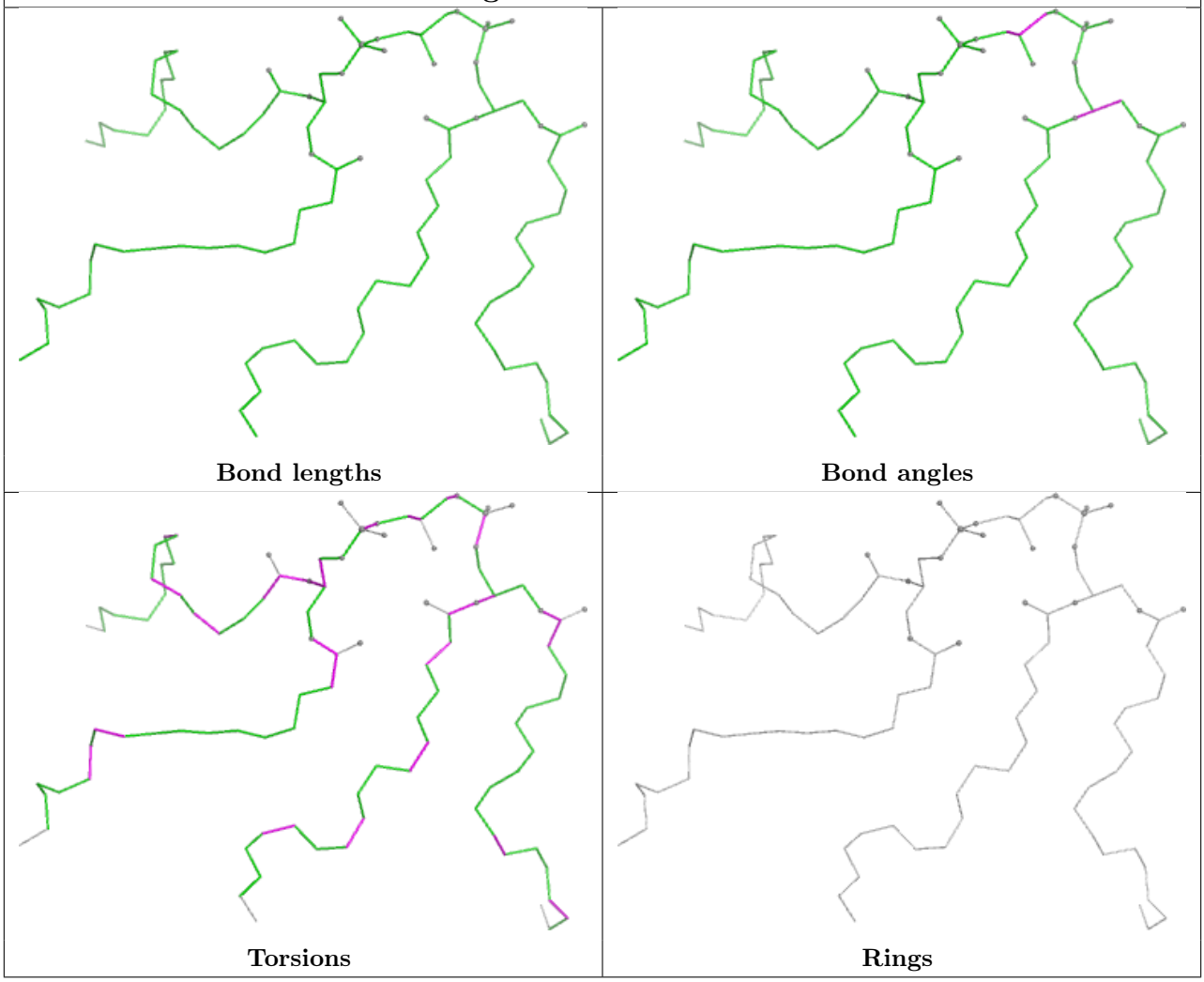


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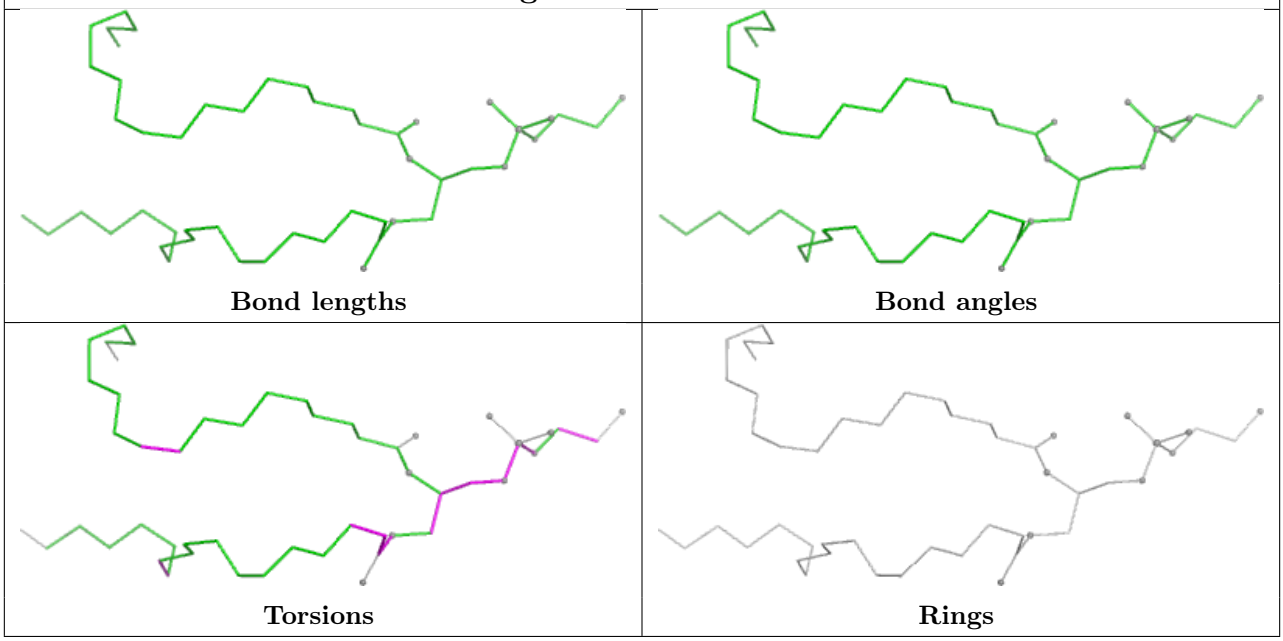


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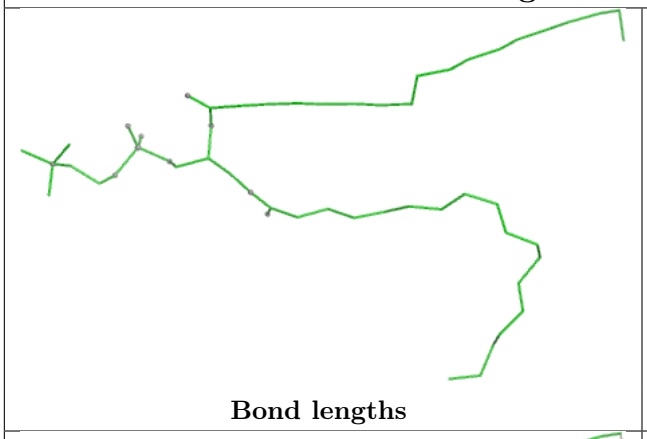
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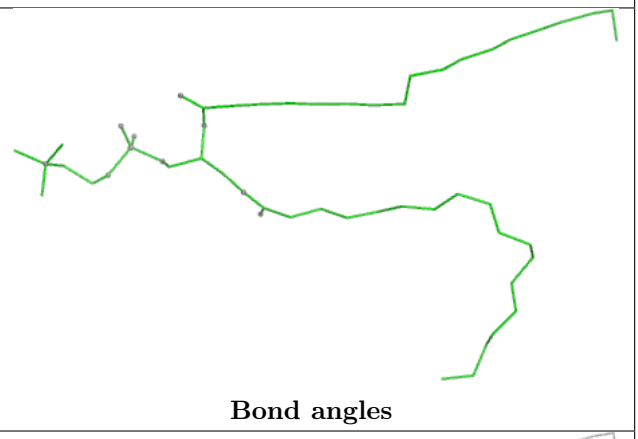
Ligand 3PE Da 708



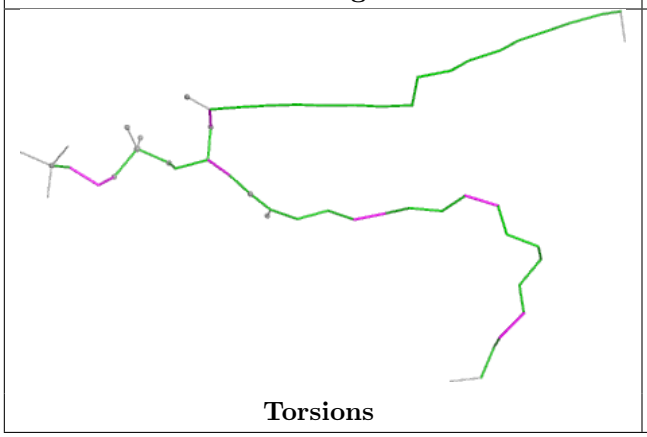
Ligand PC1 A2 402



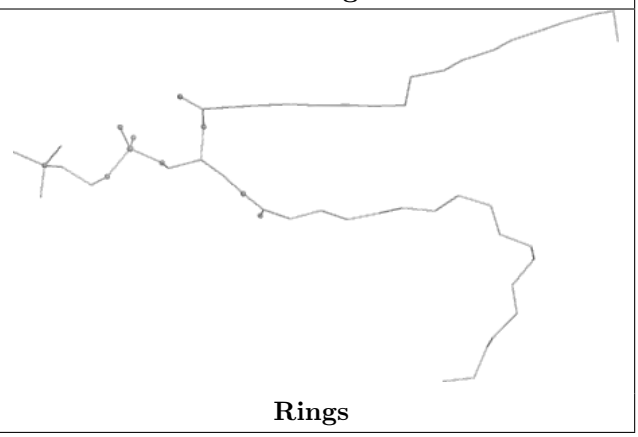
Bond lengths



Bond angles

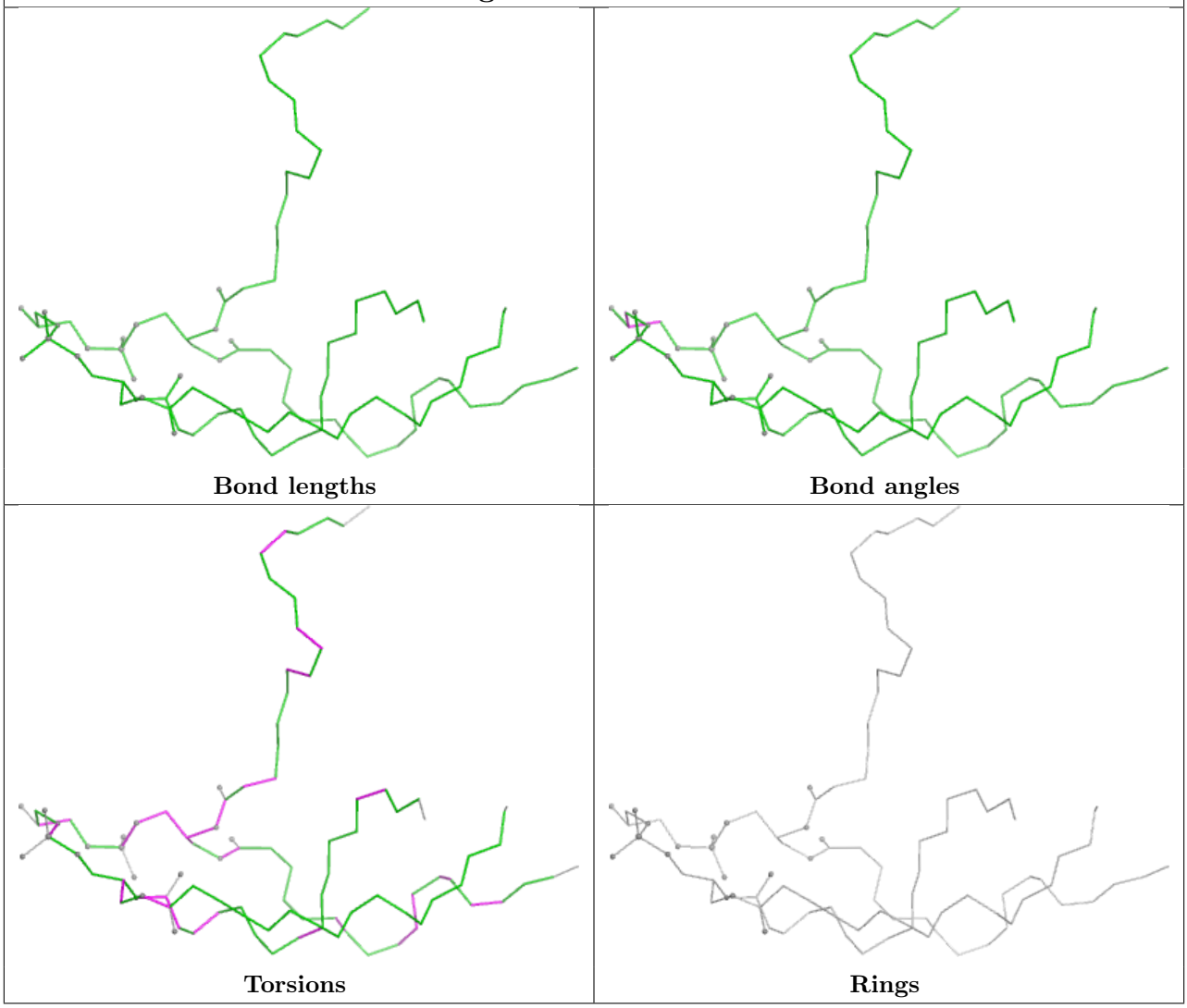


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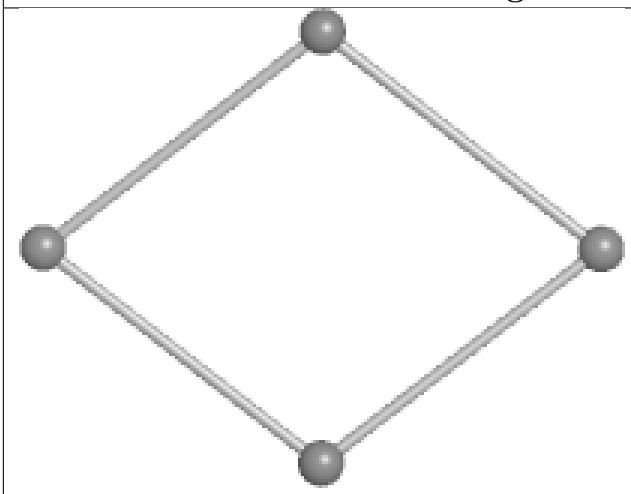


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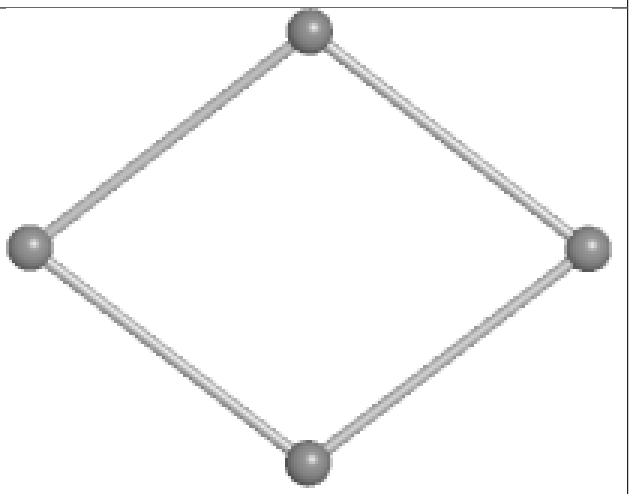
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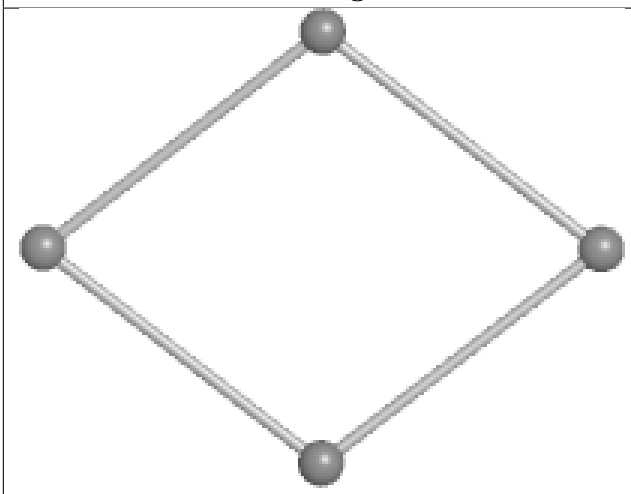
Ligand FES CB 1000



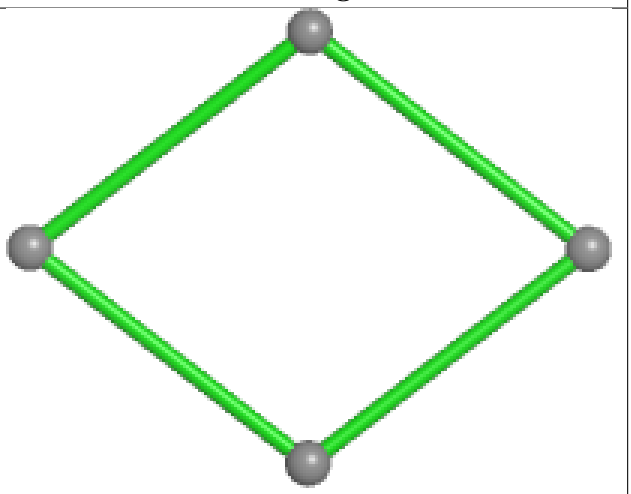
Bond lengths



Bond angles

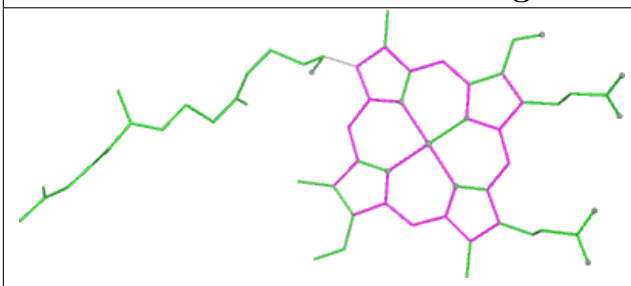


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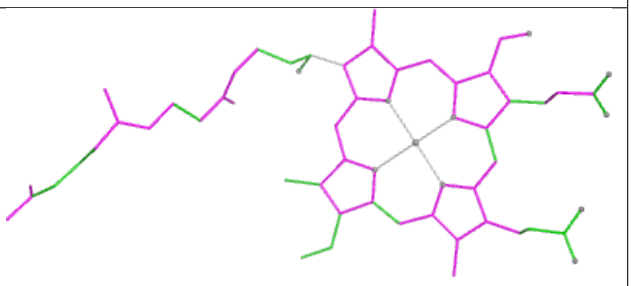


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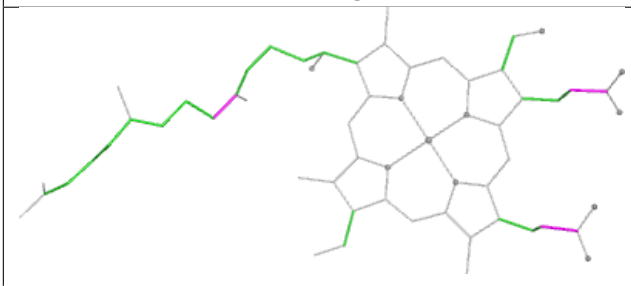
Ligand HEA Da 702



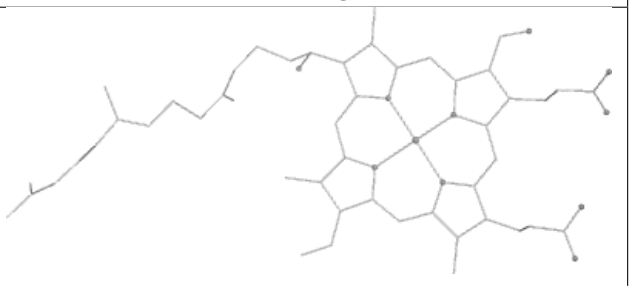
Bond lengths



Bond angles

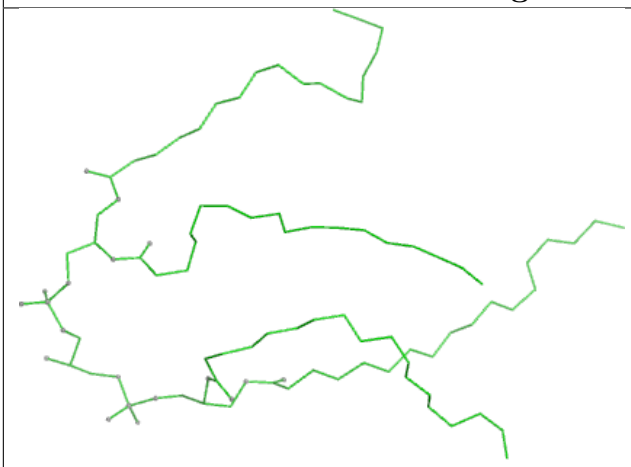


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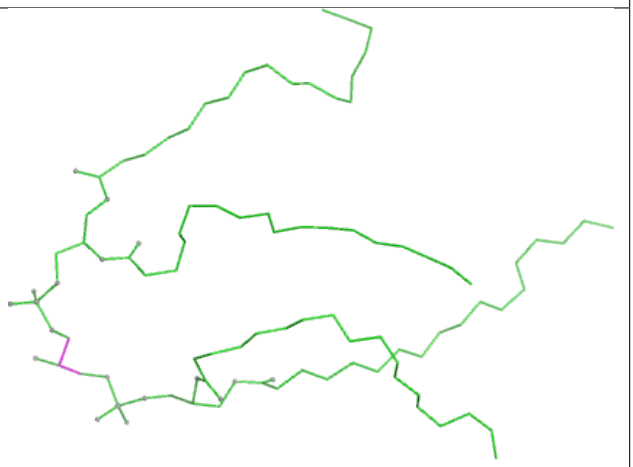


Rings

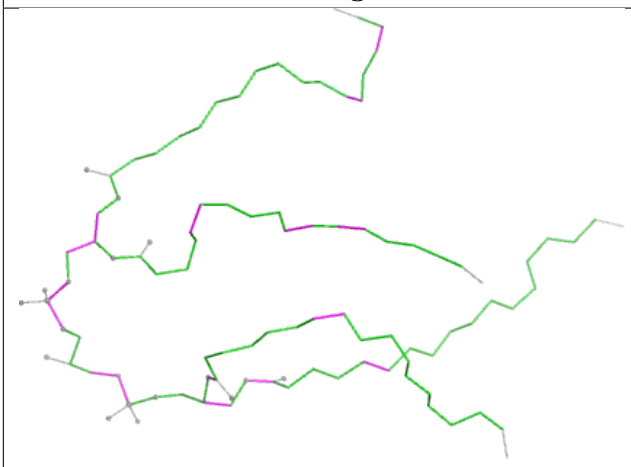
Ligand CDL CC 304



Bond lengths



Bond angles

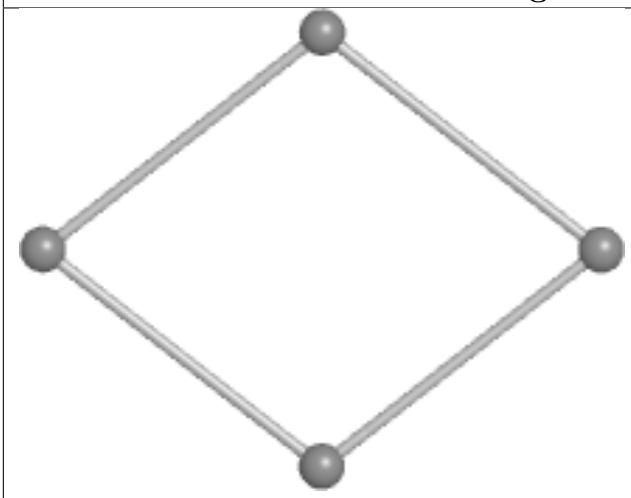


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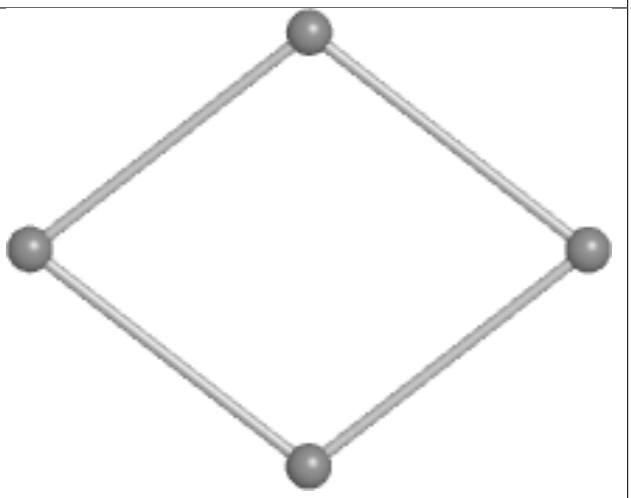


Rings

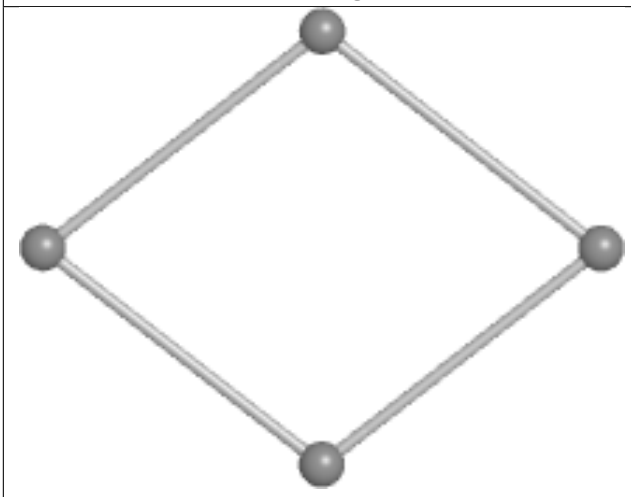
Ligand FES E 302



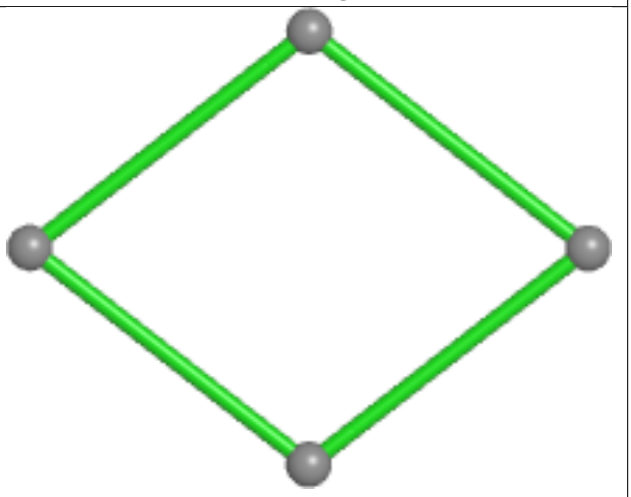
Bond lengths



Bond angles

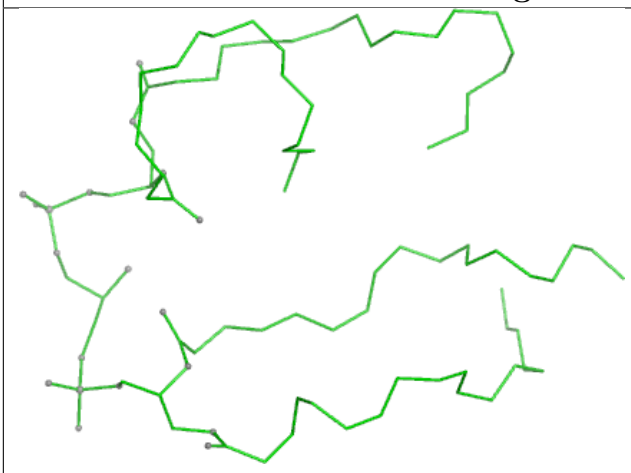


Torsions



Rings

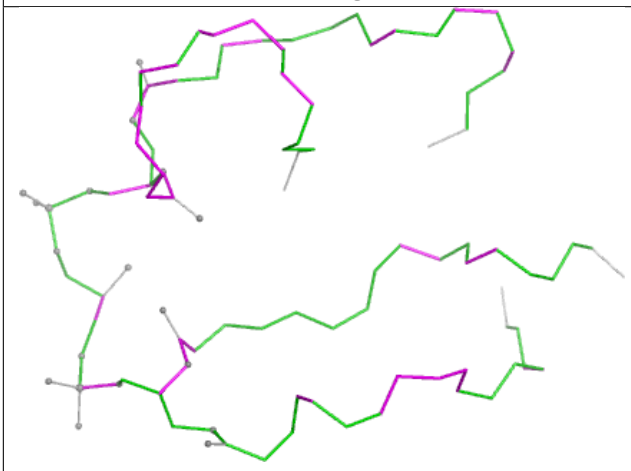
Ligand CDL DS 404



Bond lengths



Bond angles

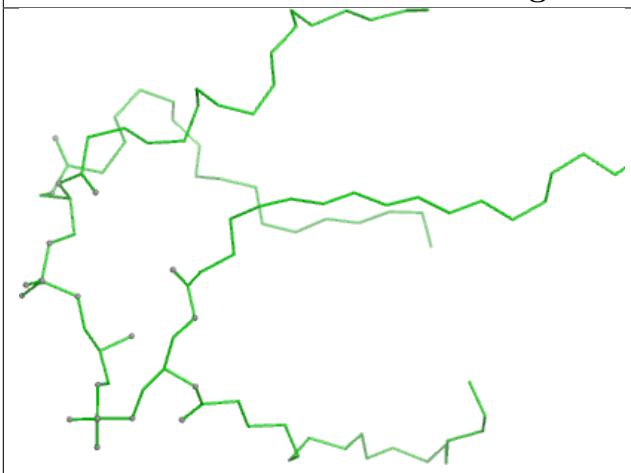


Torsions



Rings

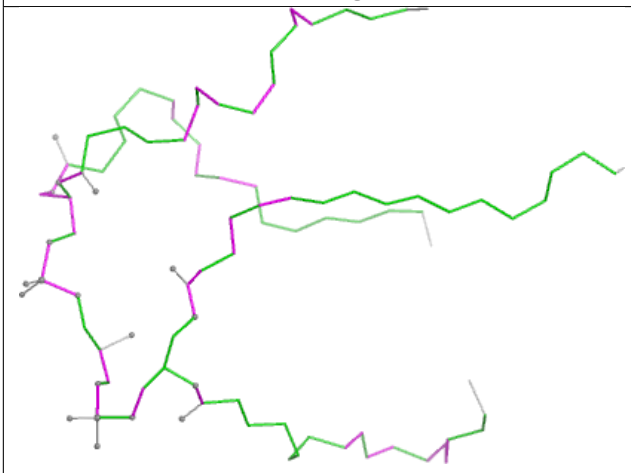
Ligand CDL c 506



Bond lengths



Bond angles

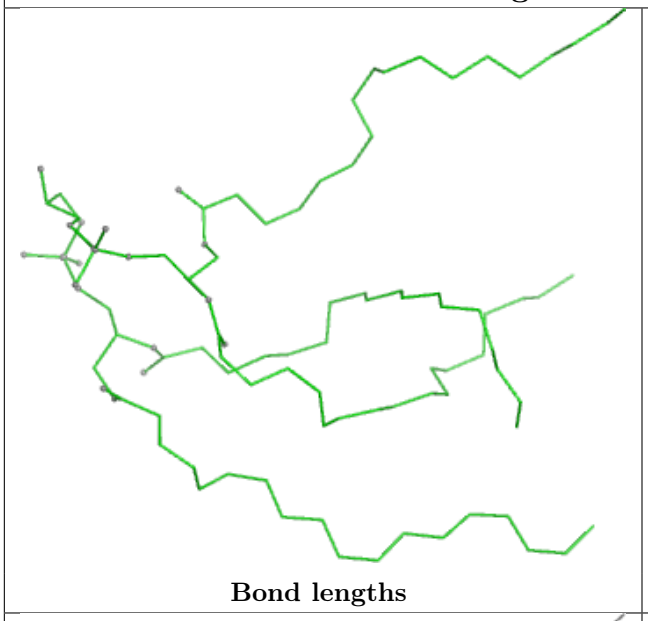


Torsions

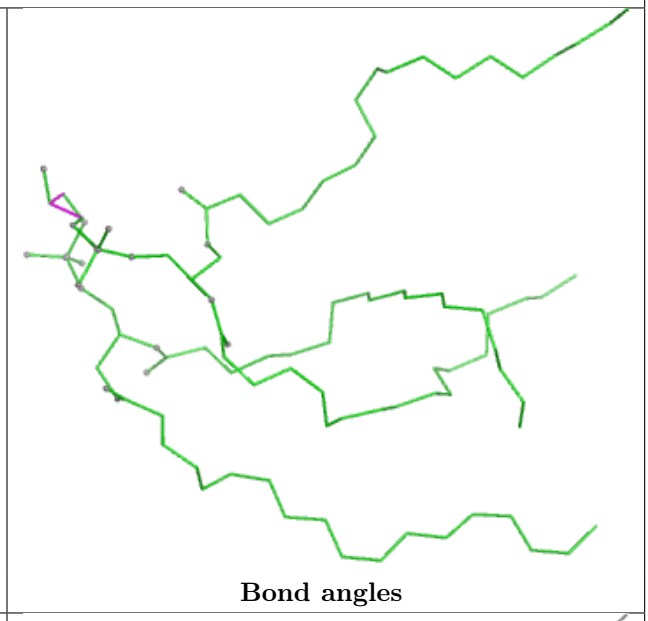


Rings

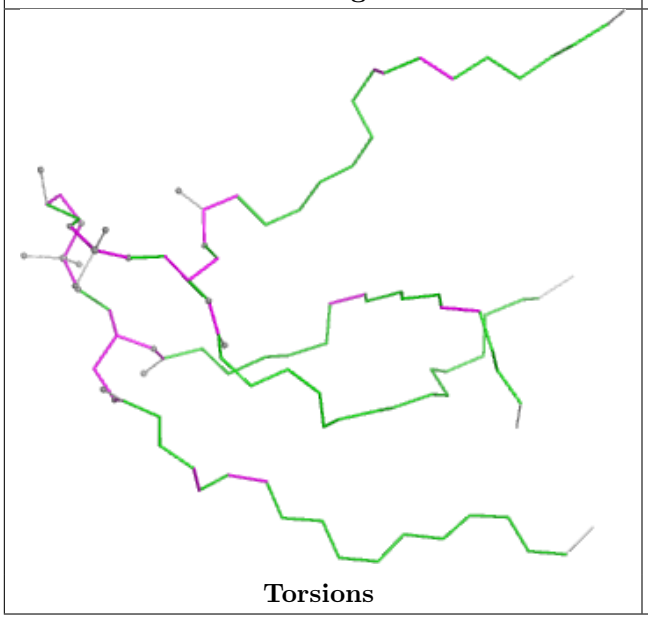
Ligand CDL CD 301



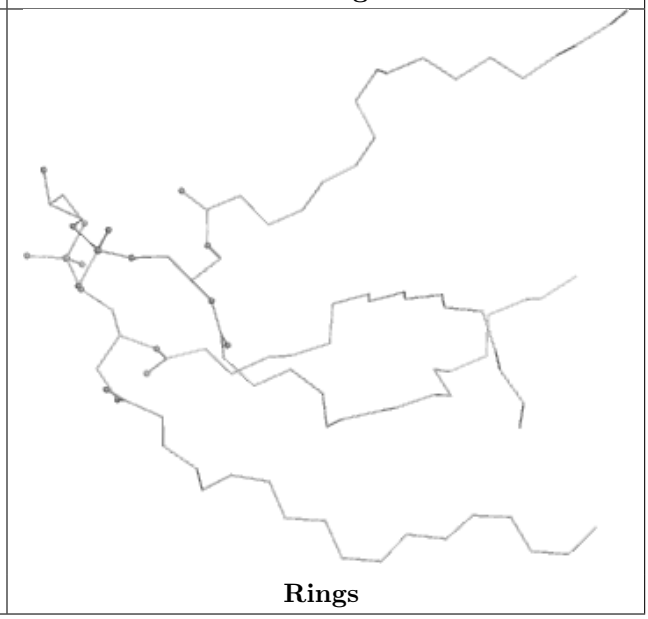
Bond lengths



Bond angles



Torsions

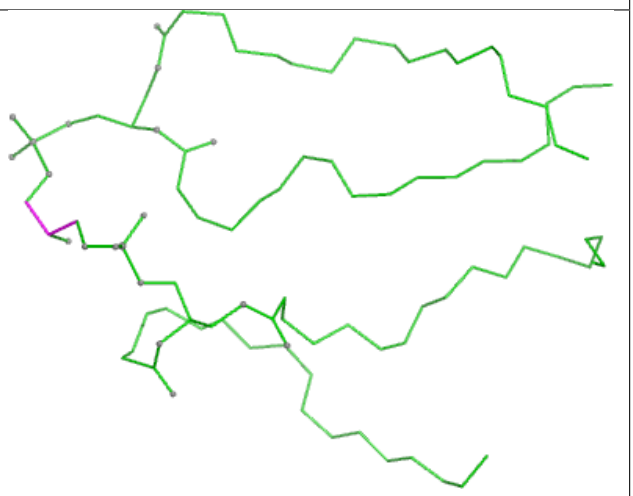


Rings

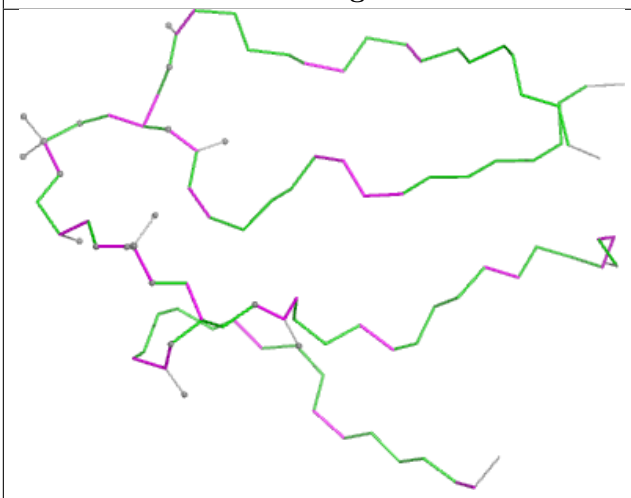
Ligand CDL BT 202



Bond lengths



Bond angles

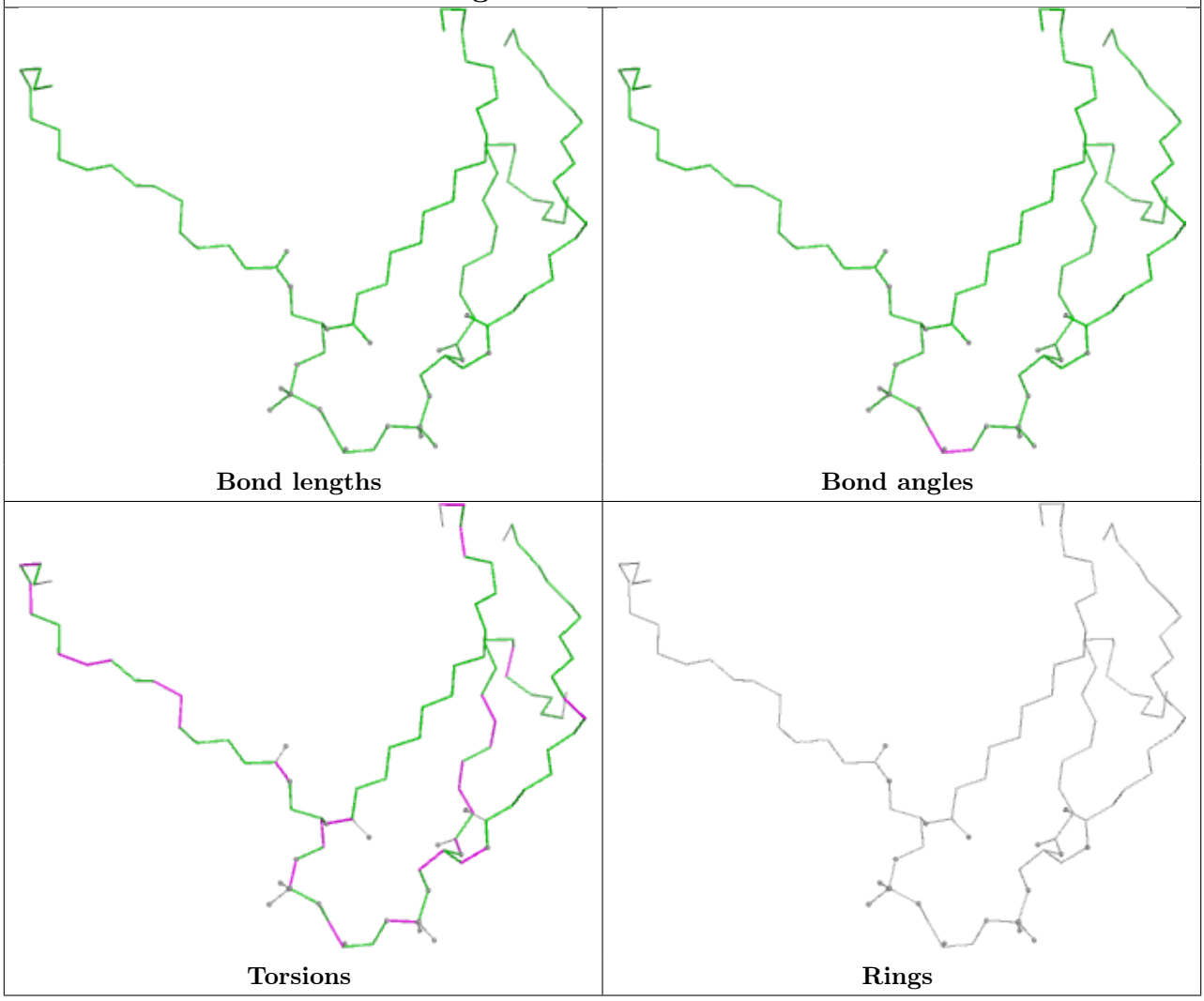


Torsions



Rings

Ligand CDL EH 1601



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.

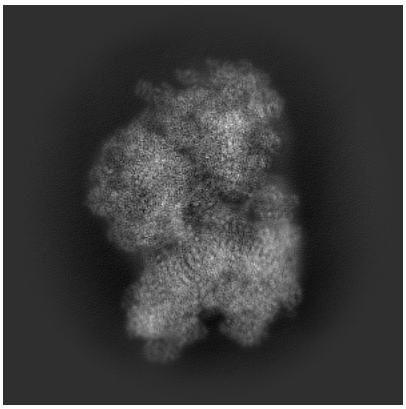
6 Map visualisation

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.

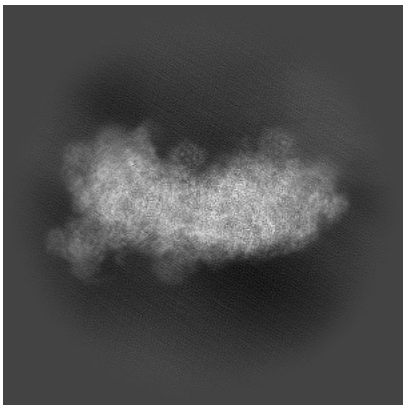
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

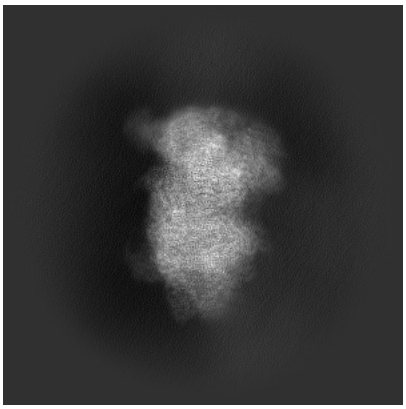
6.1.1 Primary map



X

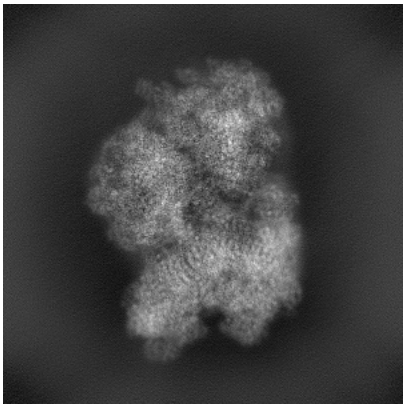


Y

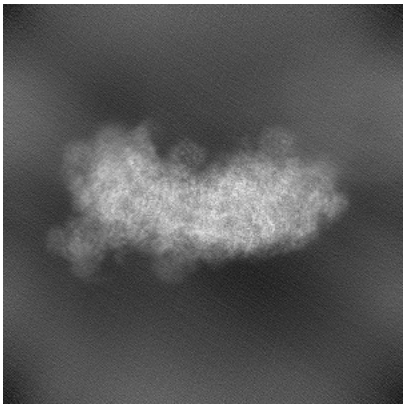


Z

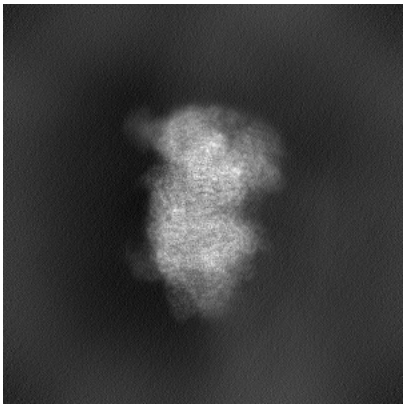
6.1.2 Raw map



X



Y

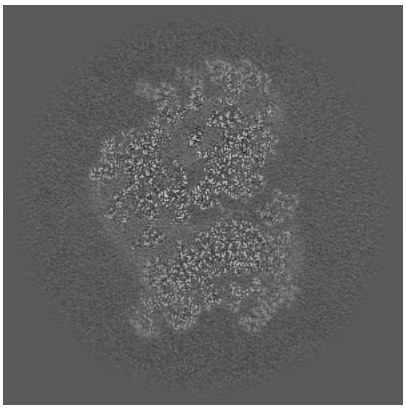


Z

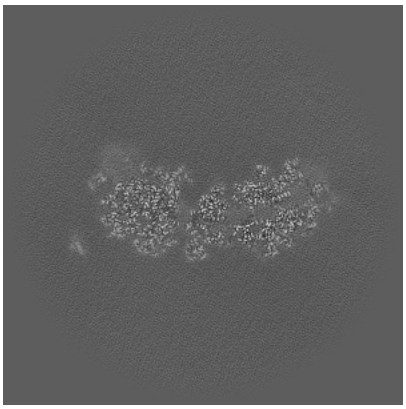
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 240

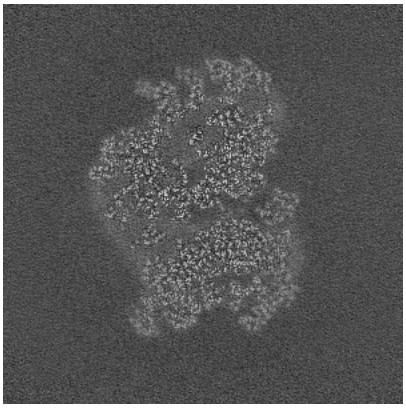


Y Index: 240

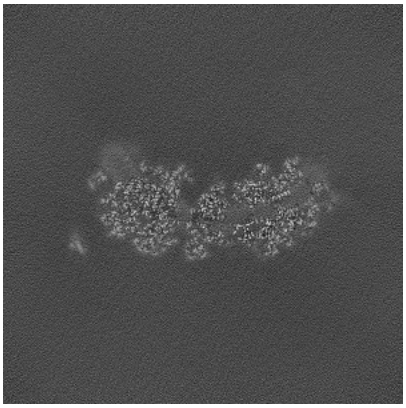


Z Index: 240

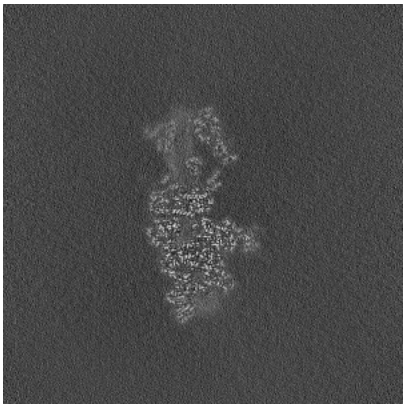
6.2.2 Raw map



X Index: 240



Y Index: 240

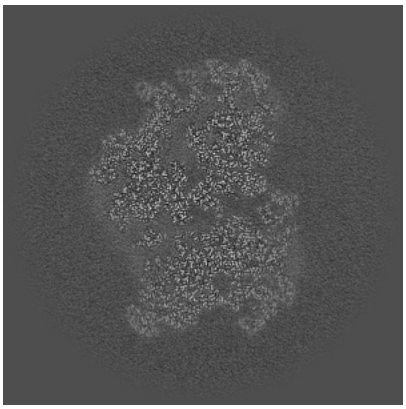


Z Index: 240

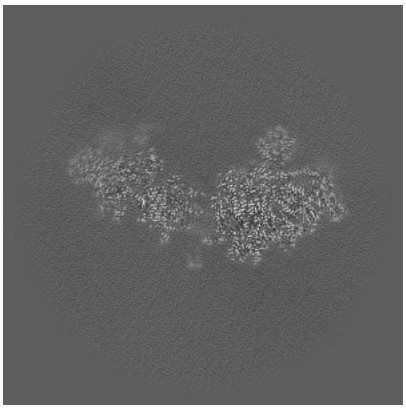
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

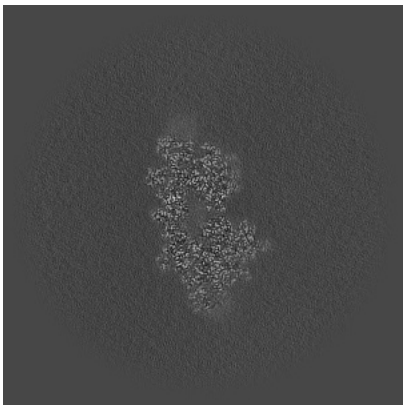
6.3.1 Primary map



X Index: 243

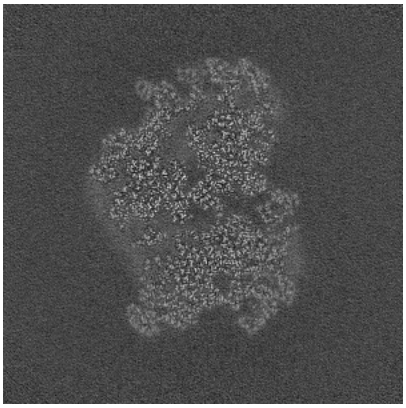


Y Index: 272

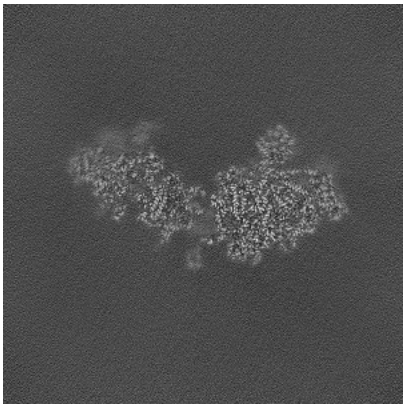


Z Index: 287

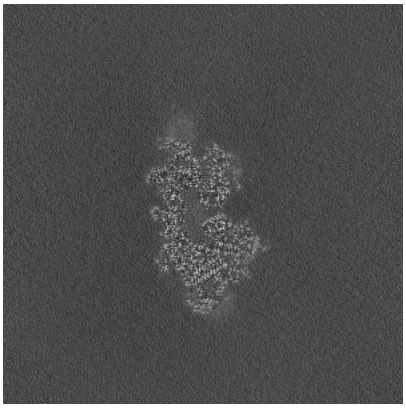
6.3.2 Raw map



X Index: 243



Y Index: 271

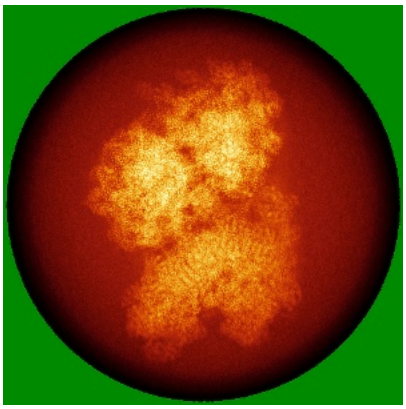


Z Index: 284

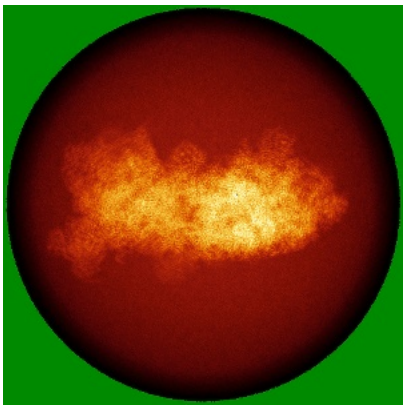
The images above show the largest variance slices of the map in three orthogonal directions.

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

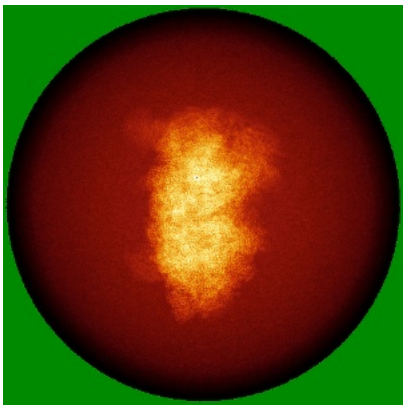
6.4.1 Primary map



X

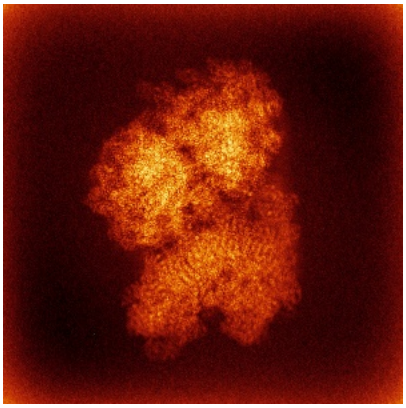


Y

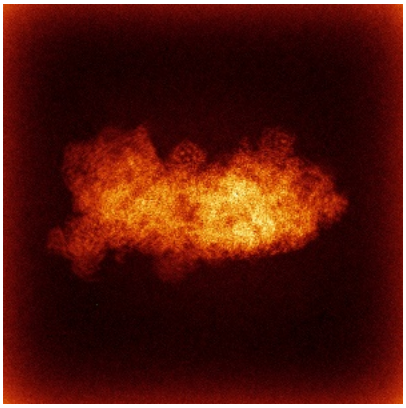


Z

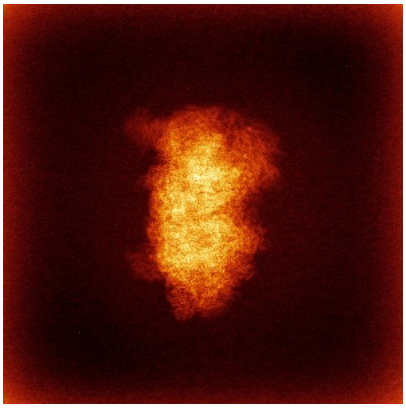
6.4.2 Raw map



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.

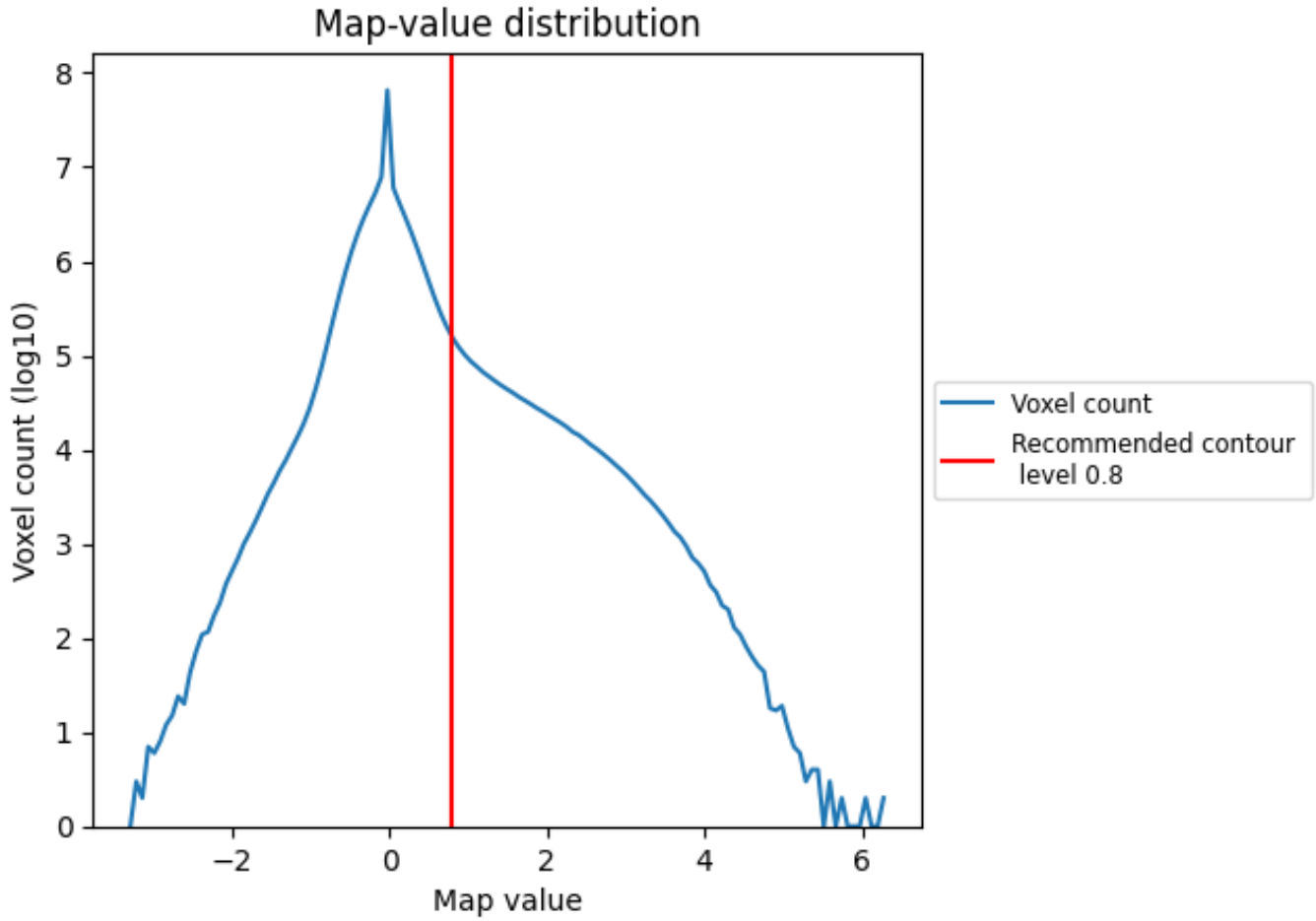
6.6 Mask visualisation (i)

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

7 Map analysis

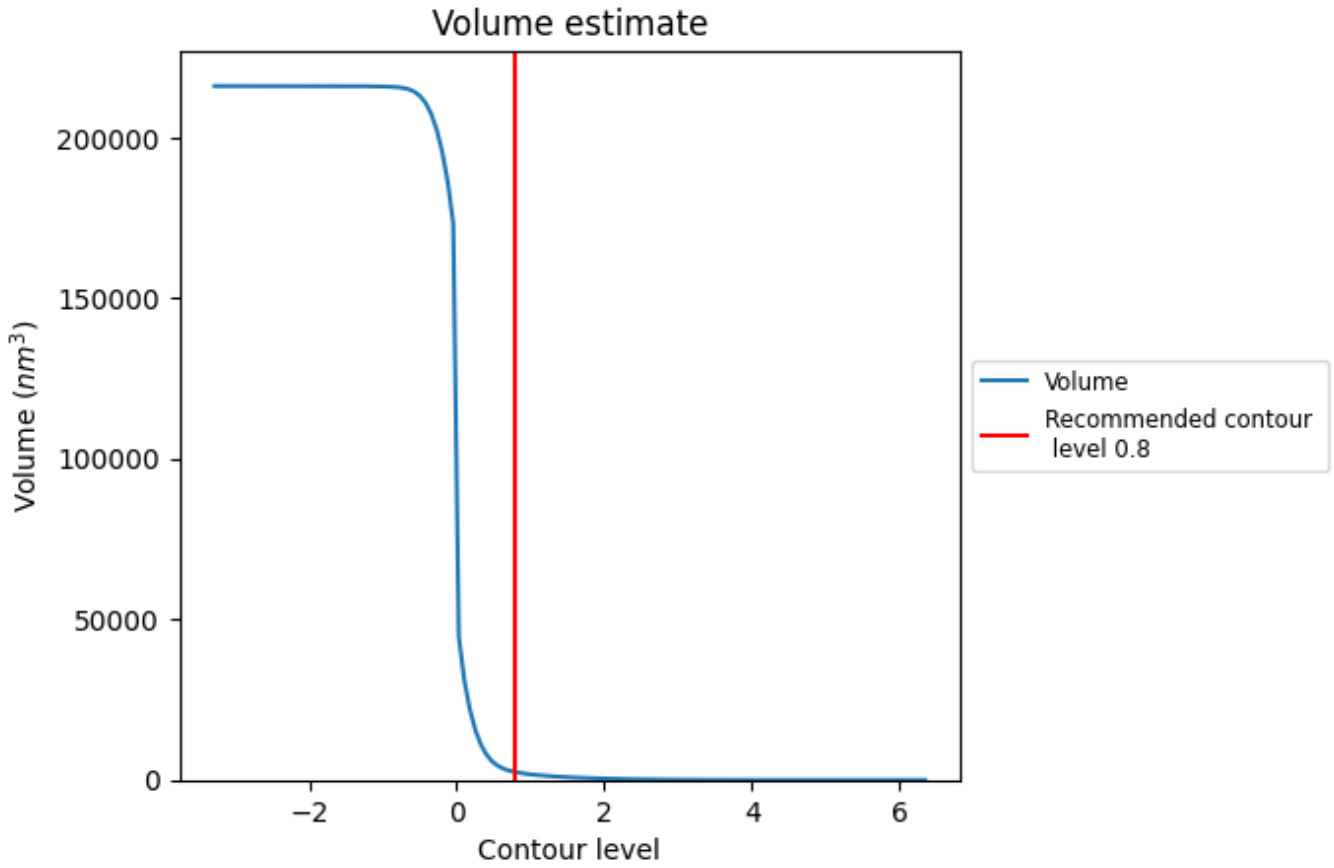
This section contains the results of statistical analysis of the map.

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.

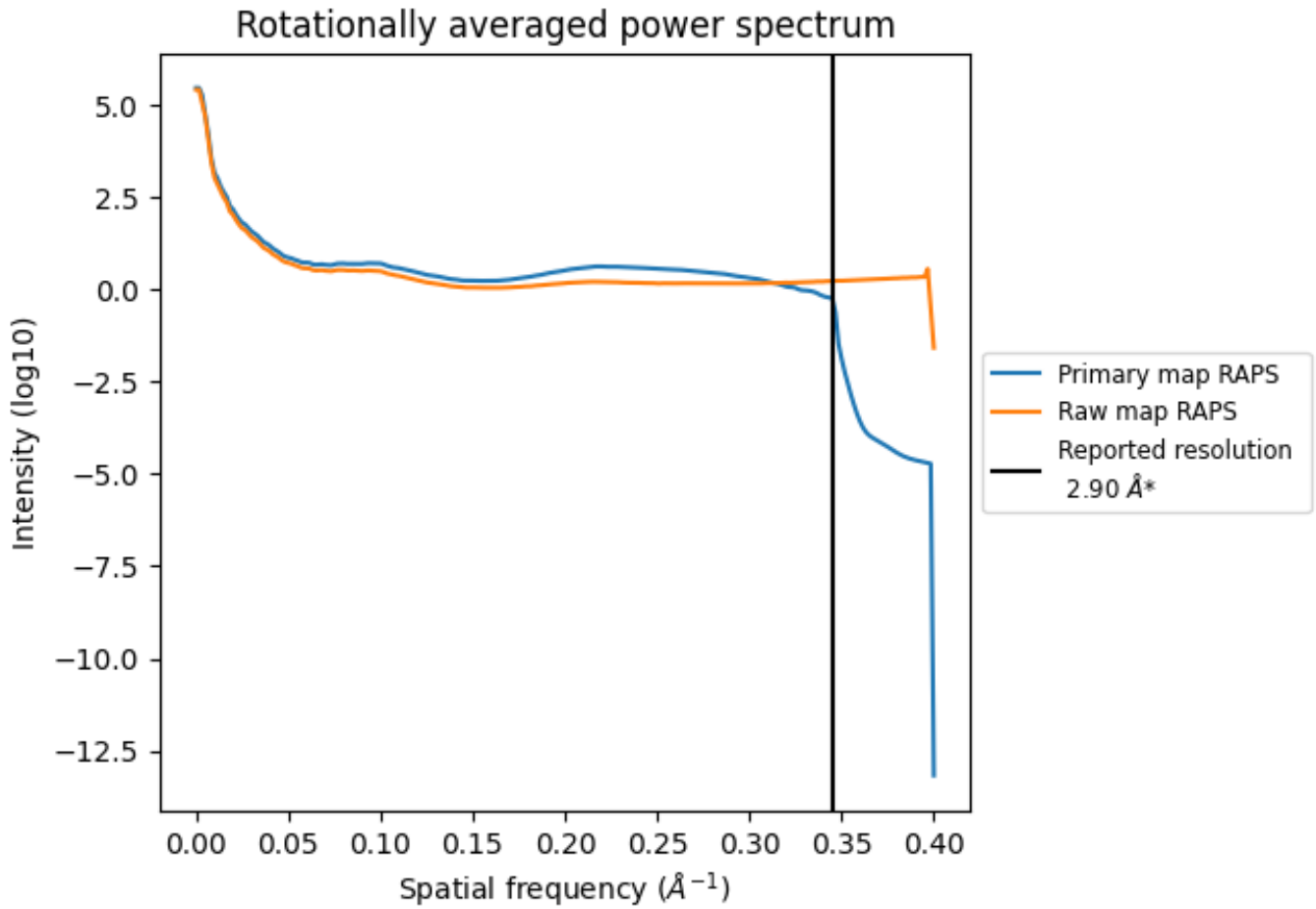
7.2 Volume estimate (i)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

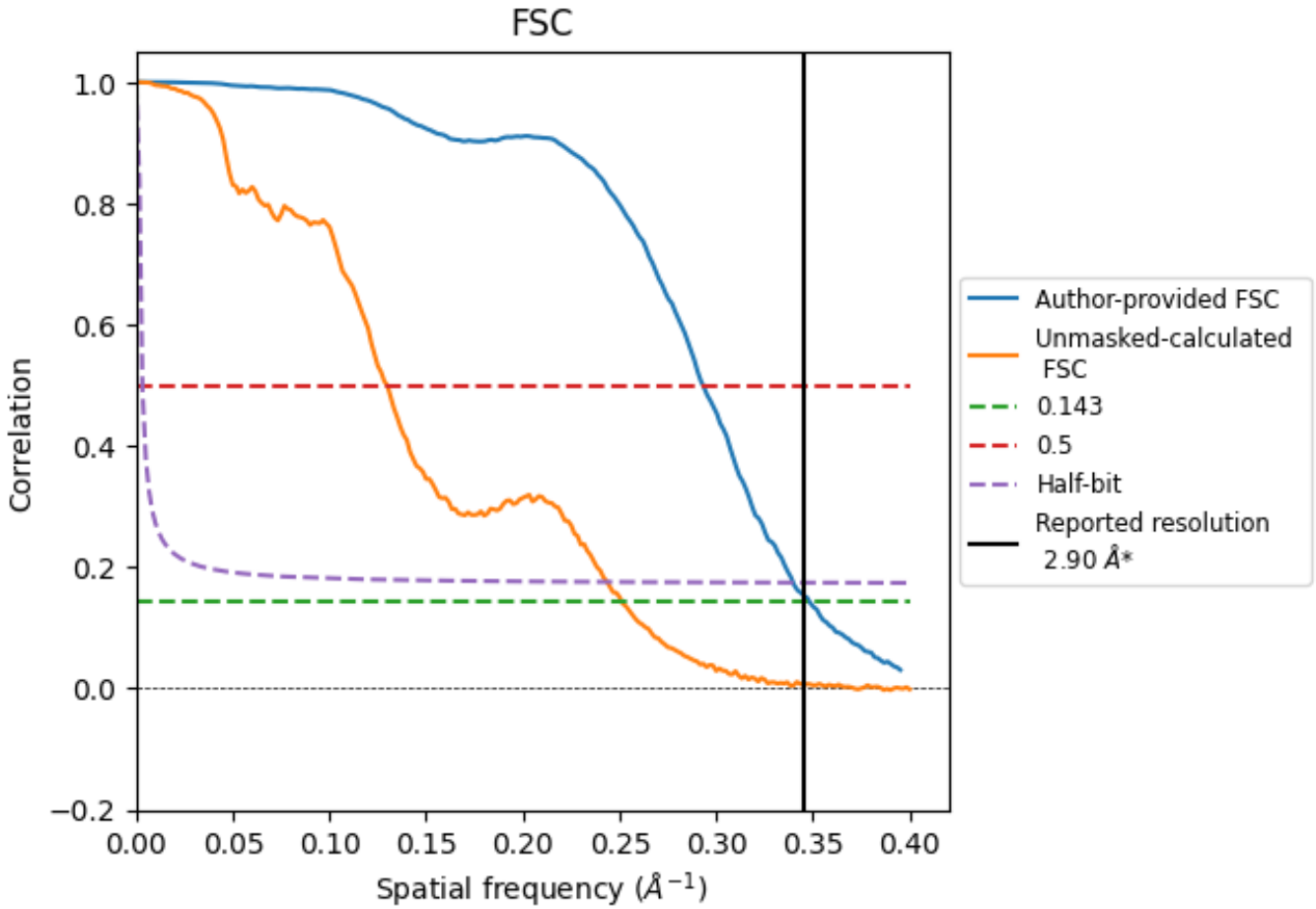


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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)

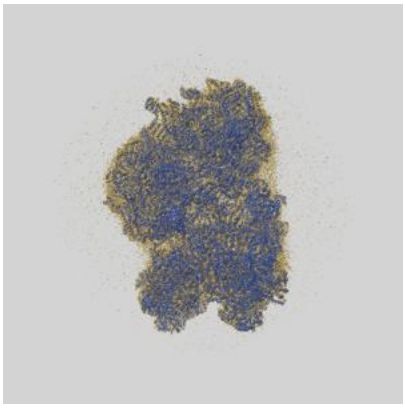
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.41	2.94
Unmasked-calculated*	3.98	7.70	4.11

*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 %

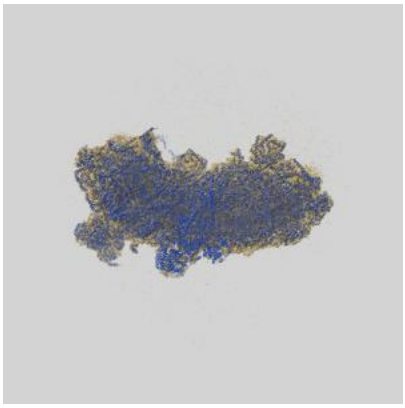
9 Map-model fit

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 67.

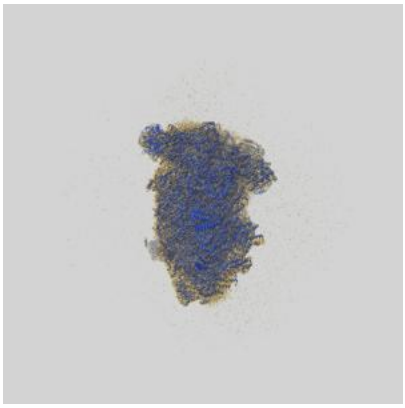
9.1 Map-model overlay



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.

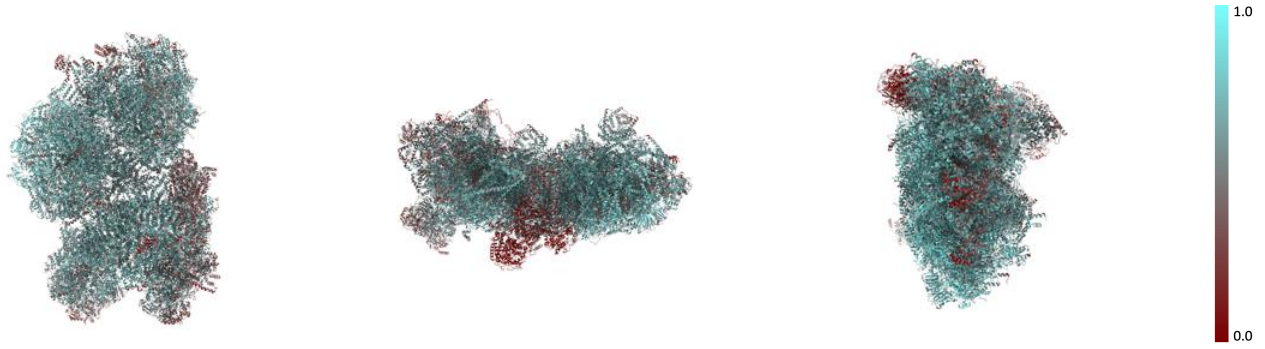
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

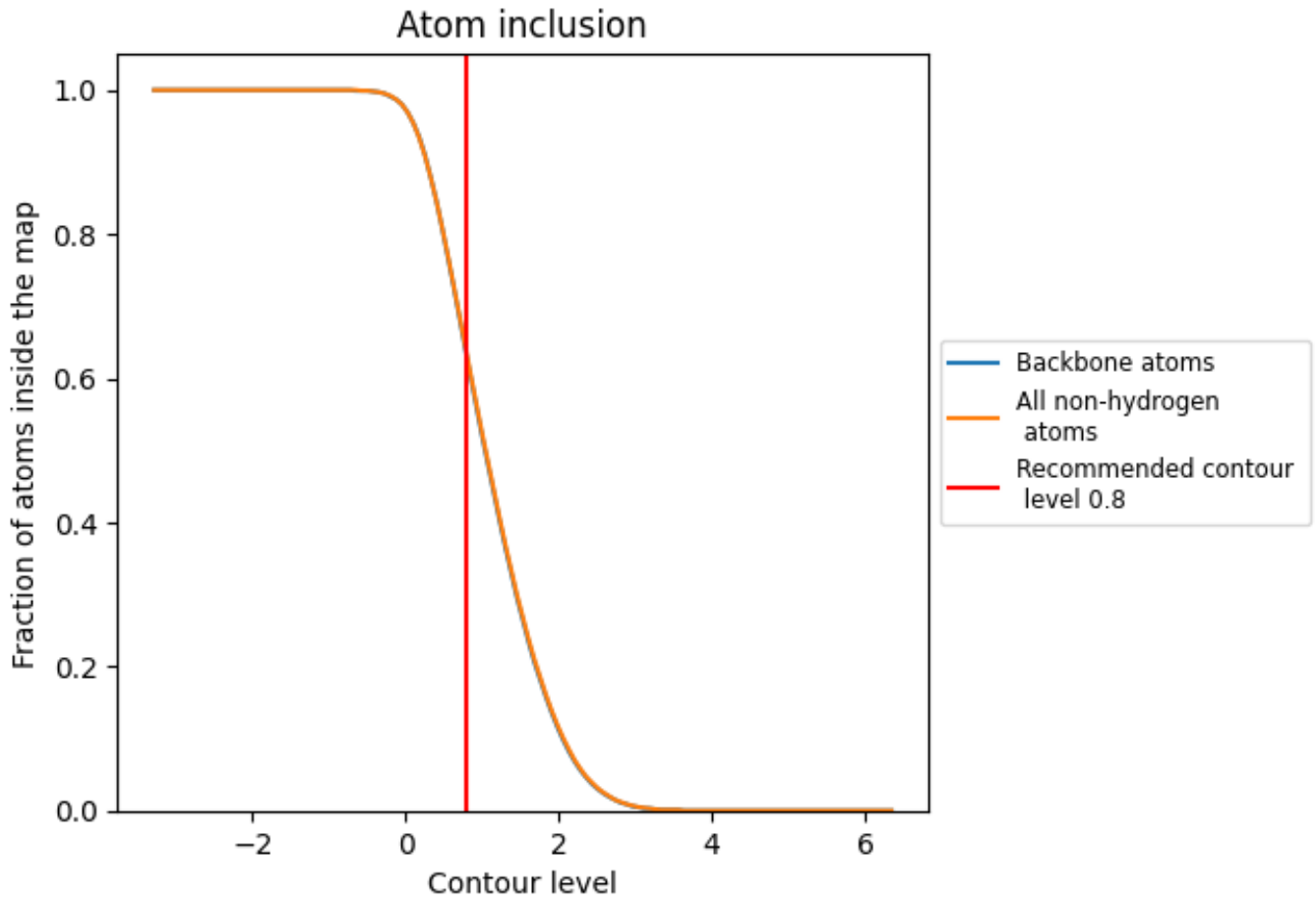
9.3 Atom inclusion mapped to coordinate model (i)



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



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

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

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

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

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