Full wwPDB EM Validation Report (i)

Sep 8, 2026 – 07:16 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

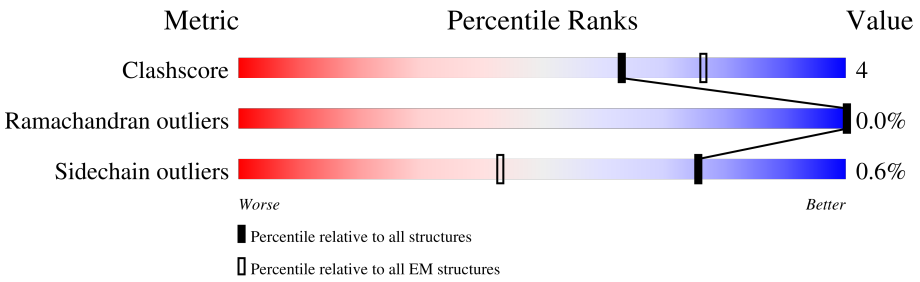
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

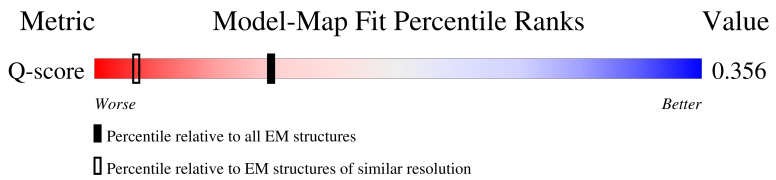
1 Overall quality at a glance (i)

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	83% 16%
31	AU	150	7% 89% 10%
32	AV	138	78% 19%
33	AW	133	71% 26%
34	AX	121	87% 11%
35	AY	116	84% 15%
36	AZ	103	35% 84% 7% 9%
37	B0	94	89% 10%
38	B1	93	9% 95%
39	B2	94	16% 87% 12%
40	B3	83	12% 84% 12%
41	B4	73	19% 95% 5%
42	B5	71	6% 70% 6% 24%
43	B6	59	69% 31%
44	BA	212	17% 85% 9% 6%
45	BB	214	8% 71% 7% 22%
46	BC	207	75% 9% 16%
47	BD	205	6% 68% 28%
48	BE	189	14% 80% 8% 11%
49	BF	188	77% 18% 6%
50	BG	175	6% 84% 7% 9%
51	BH	178	90% 10%
52	BI	172	80% 6% 13%
53	BJ	166	82% 5% 13%
54	BK	144	5% 72% 24%

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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	68% 91% 9%
81	CN	62	71% 85% 15%
82	CC	60	70% 95%
83	CO	46	59% 85% 9% 7%
84	CD	44	77% 95% 5%
85	A	513	6% 82% 12% 6%
85	a	513	37% 81% 13% 6%
86	B	482	22% 82% 13% 5%
86	b	482	26% 85% 10% 5%
87	C	426	15% 85% 15%
87	c	426	87% 13%
88	D	319	83% 9% 8%
88	d	319	21% 82% 10% 8%
89	E	269	33% 82% 9% 9%
89	e	269	60% 77% 14% 9%
90	F	86	13% 88% 12%
90	f	86	56% 90% 9%
91	G	328	33% 87% 12%
91	g	328	12% 87% 13%
92	H	130	22% 84% 15%
92	h	130	85% 15%
93	I	119	8% 87% 12%
93	i	119	34% 95%
94	J	66	74% 100%
94	j	66	76% 100%

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Mol	Chain	Length	Quality of chain
95	K	62	16% 81% 13% 6%
95	k	62	29% 81% 13% 6%
96	L	41	22% 66% 12% 22%
96	l	41	7% 71% 7% 22%
97	DA	688	83% 14%
97	Da	688	81% 16%
98	DB	604	9% 89% 11%
98	Db	604	12% 87% 12%
99	DC	594	7% 86% 12%
99	Dc	594	12% 85% 13%
100	DD	637	76% 11% 12%
100	Dd	637	75% 12% 12%
101	DE	130	88% 9%
101	De	130	83% 14%
102	DF	230	5% 85% 12%
102	Df	230	6% 87% 10%
103	DG	103	6% 82% 13% 5%
103	Dg	103	88% 7% 5%
104	DH	134	84% 16%
104	Dh	134	82% 18%
105	DI	236	77% 9% 13%
105	Di	236	75% 12% 13%
106	DJ	220	88% 11%
106	Dj	220	85% 14%
107	DK	990	12% 87%

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Mol	Chain	Length	Quality of chain
107	Dk	990	12% 87%
108	DM	490	80% 12% 7%
108	Dm	490	78% 14% 7%
109	DN	453	10% 91% 9%
109	Dn	453	13% 88% 12%
110	DO	473	19% 81% 11% 8%
110	Do	473	41% 79% 12% 8%
111	DP	402	7% 65% 7% 28%
111	Dp	402	13% 64% 8% 28%
112	DQ	386	85% 14%
112	Dq	386	87% 12%
113	DR	348	60% 9% 30%
113	Dr	348	59% 10% 30%
114	DS	347	88% 11%
114	Ds	347	85% 14%
115	DT	318	73% 19% 8%
115	Dt	318	76% 16% 8%
116	DU	330	5% 88% 12%
116	Du	330	9% 82% 17%
117	DV	319	89% 11%
117	Dv	319	86% 14%
118	DW	318	13% 88% 7% 5%
118	Dw	318	9% 85% 9% 5%
119	DX	252	9% 88% 11%
119	Dx	252	7% 87% 12%

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

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

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

- Molecule 9 is a protein called ND5a.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called Ymf65.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 20 is a protein called Ymf62.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is a protein called Acyl carrier protein.

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

- Molecule 33 is a protein called Acyl carrier protein.

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

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

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

- Molecule 35 is a protein called Ymf58.

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

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

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

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

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

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

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

- Molecule 39 is a protein called GRAM domain protein.

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 44 is a protein called Transmembrane protein.

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

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

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

- Molecule 46 is a protein called NDUB8.

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

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

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

- Molecule 48 is a protein called NDUPH2.

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

- Molecule 49 is a protein called NDUB10.

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

- Molecule 50 is a protein called NDUA13.

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

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

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

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

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

- Molecule 53 is a protein called Thioredoxin.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 59 is a protein called NDUB6.

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

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

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

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

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

- Molecule 62 is a protein called NDUB4.

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

- Molecule 63 is a protein called NDUTT10.

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

- Molecule 64 is a protein called NDUTT11.

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

- Molecule 65 is a protein called NDUTT12.

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

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

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

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

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

- Molecule 68 is a protein called Ymf57.

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

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

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

- Molecule 70 is a protein called Diphthamide synthesis protein.

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

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

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

- Molecule 72 is a protein called Transposase.

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

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

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

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

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

- Molecule 75 is a protein called succinate dehydrogenase.

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

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

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

- Molecule 77 is a protein called chain 77.

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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called Transmembrane protein.

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

- Molecule 83 is a protein called SDHTT11.

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

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

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

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

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

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

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

- Molecule 87 is a protein called Apocytochrome b.

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

- Molecule 88 is a protein called Cytochrome protein c1.

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

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

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

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

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

- Molecule 91 is a protein called UQCRTT1.

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

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

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

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

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

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

- Molecule 94 is a protein called UQCRTT3.

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

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

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

- Molecule 96 is a protein called UQCRTT2.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 99 is a protein called Ymf68.

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

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

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

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

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

- Molecule 102 is a protein called Structural protein.

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- Molecule 109 is a protein called Ymf67.

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

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

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

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

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

- Molecule 112 is a protein called TraB family protein.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 116 is a protein called Carrier protein.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 119 is a protein called COXTT9.

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

- Molecule 120 is a protein called COXTT10.

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

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

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

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

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

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

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

- Molecule 124 is a protein called COXTT27.

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

- Molecule 125 is a protein called Ymf75.

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

- Molecule 126 is a protein called Mobilization protein.

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

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

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

- Molecule 128 is a protein called COXTT28.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 130 is a protein called Transmembrane protein.

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

- Molecule 131 is a protein called Decapping nuclease.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 135 is a protein called COXTT22.

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

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

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

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

- Molecule 137 is a protein called Phage protein.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 139 is a protein called Lysozyme.

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

- Molecule 140 is a protein called Ymf70.

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

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

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

- Molecule 142 is a protein called ABC transporter.

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

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

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

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

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

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

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

- Molecule 146 is a protein called Annexin.

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

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

- Molecule 147 is a protein called Transposase.

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

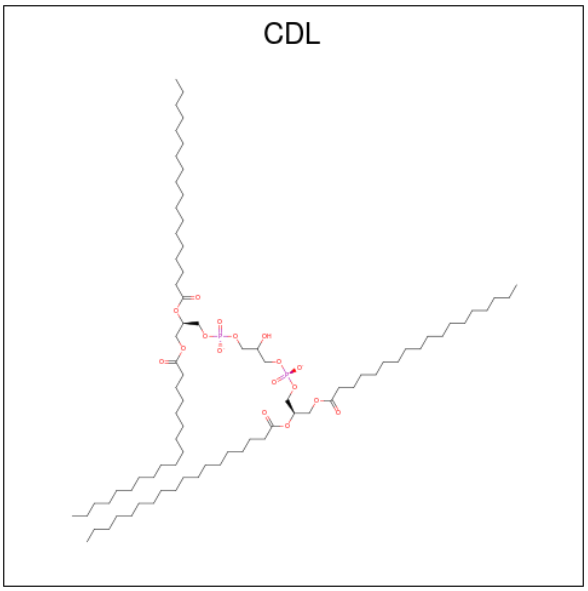
- Molecule 148 is a protein called Tim10/DDP family zinc finger protein.

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

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

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

- Molecule 150 is CARDIOLIPIN (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
			Total	C	H	O	P	
150	BC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BE	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BL	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BT	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BT	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BV	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	BY	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CG	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CJ	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CC	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	CD	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0
			Total	C	H	O	P	
150	C	1	256	81	156	17	2	0

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

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

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

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

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

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

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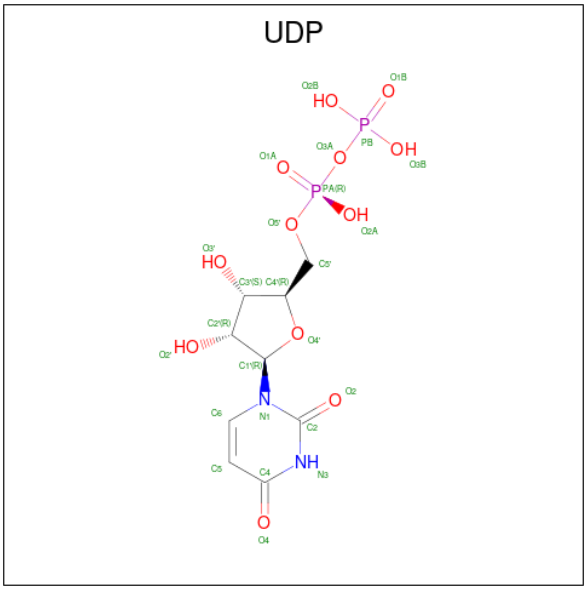
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
150	Eu	1	256	81	156	17	2	0

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

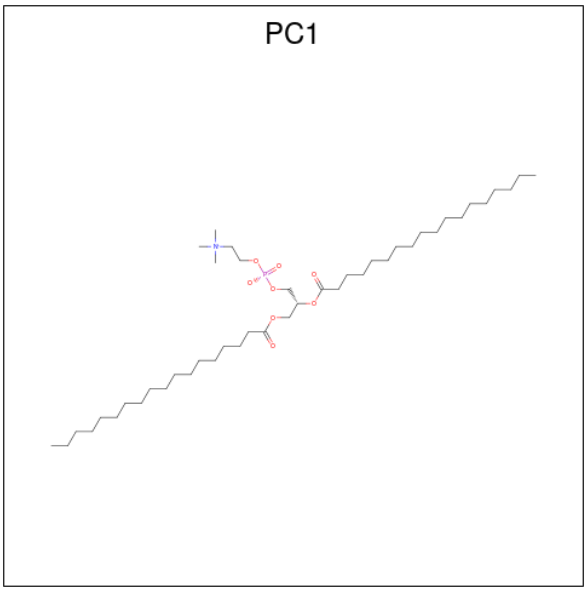


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
151	A0	1	36	9	11	2	12	2	0

- Molecule 152 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 153 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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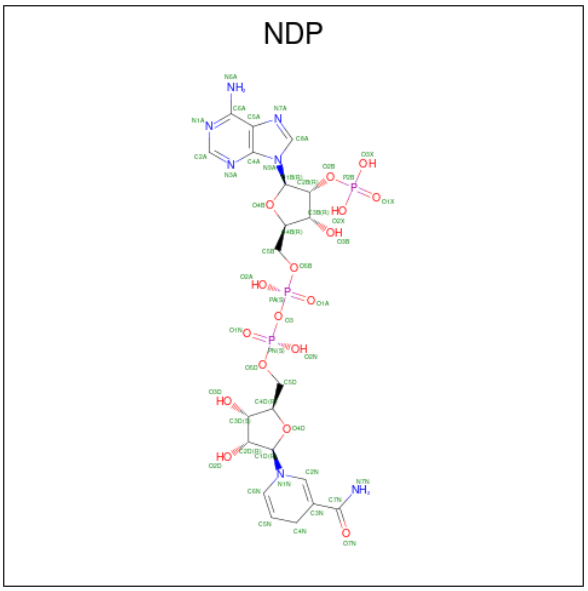
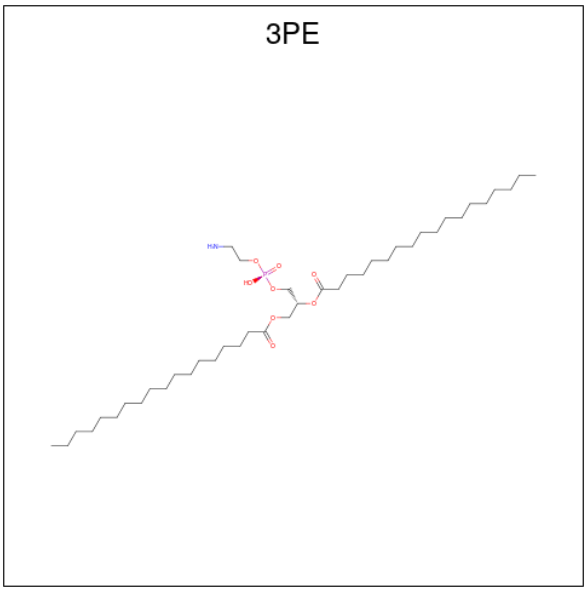
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
153	Dg	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Di	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dj	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dq	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Ds	1	142	44	88	1	8	1	0
			Total	C	H	N	O	P	
153	Dv	1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

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



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

- Molecule 155 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
155	A2	1	133	41	82	1	8	1	0
155	A9	1	133	41	82	1	8	1	0

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

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

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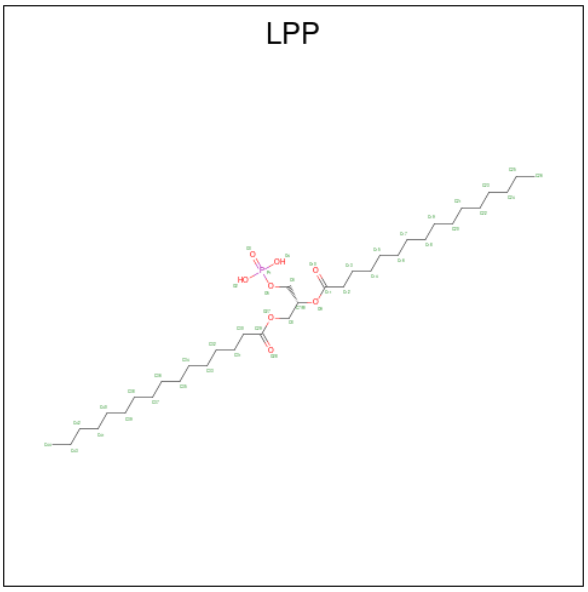
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
155	Eo	1	133	41	82	1	8	1	0

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



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

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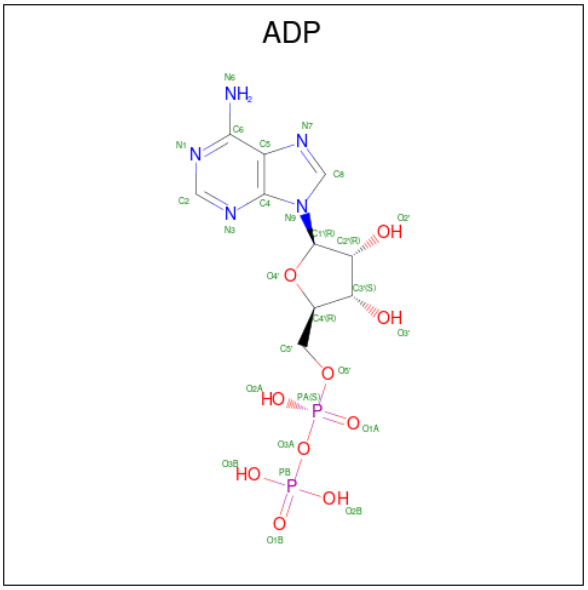
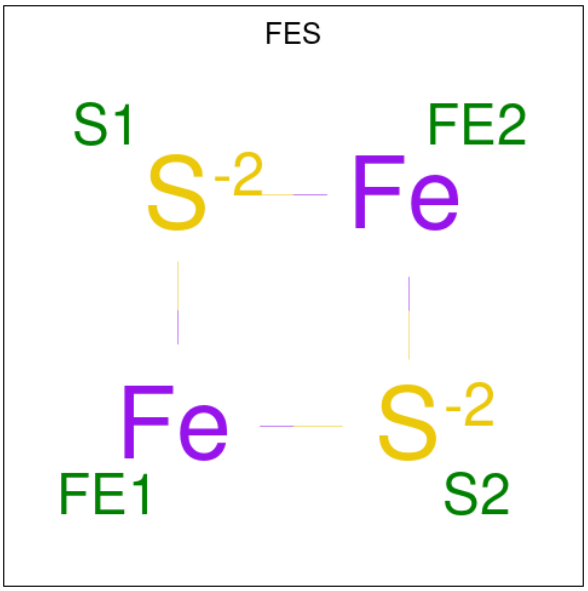
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
156	Dn	1	111	35	67	8	1	0
			Total	C	H	O	P	
156	Ed	1	111	35	67	8	1	0
			Total	C	H	O	P	
156	Dl	1	111	35	67	8	1	0

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



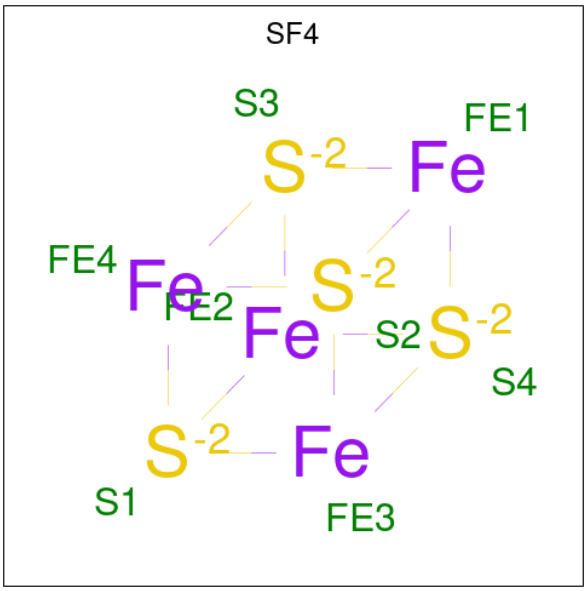
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
157	A8	1	39	10	12	5	10	2	0
			Total	C	H	N	O	P	
157	AQ	1	39	10	12	5	10	2	0

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



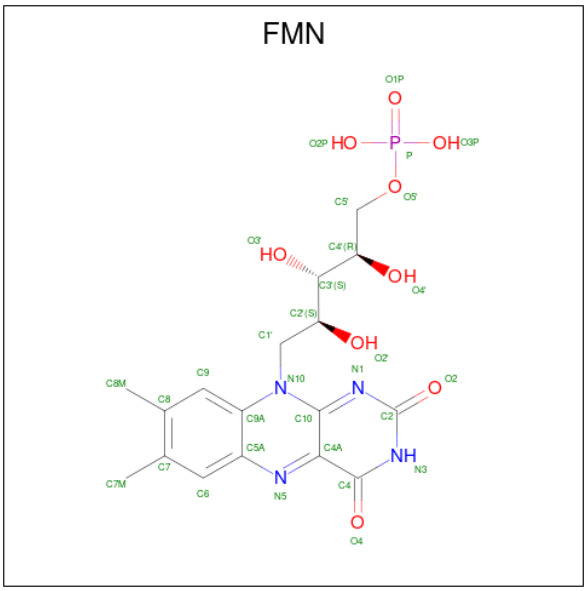
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
158	AB	1	4	2	2	0
158	AI	1	4	2	2	0
158	BI	1	4	2	2	0
158	CB	1	4	2	2	0
158	E	1	4	2	2	0
158	e	1	4	2	2	0
158	EF	1	4	2	2	0
158	EF	1	4	2	2	0
158	Ef	1	4	2	2	0
158	Ef	1	4	2	2	0

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



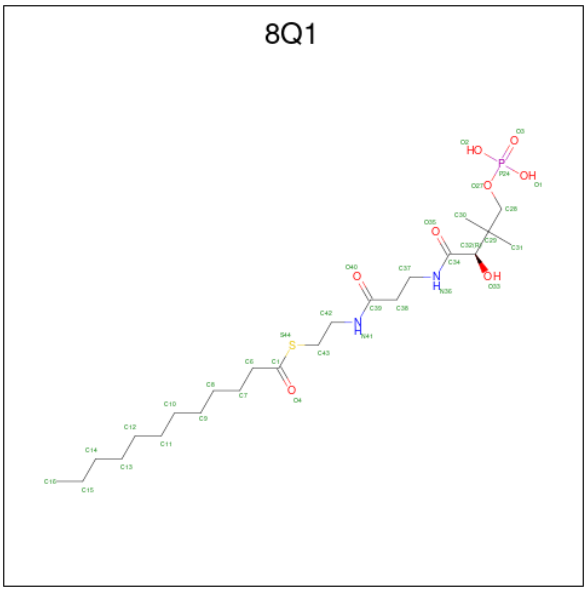
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
159	AB	1	8	4	4	0
159	AB	1	8	4	4	0
159	AD	1	8	4	4	0
159	AL	1	8	4	4	0
159	AL	1	8	4	4	0
159	AT	1	8	4	4	0
159	CB	1	8	4	4	0

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



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

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



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

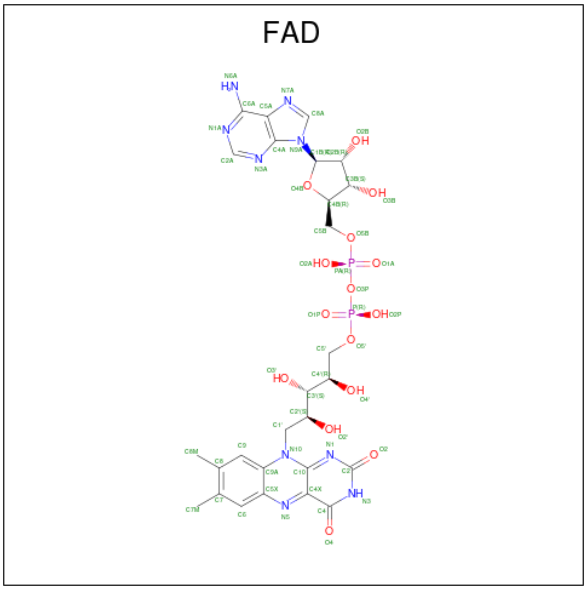
- Molecule 162 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 163 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

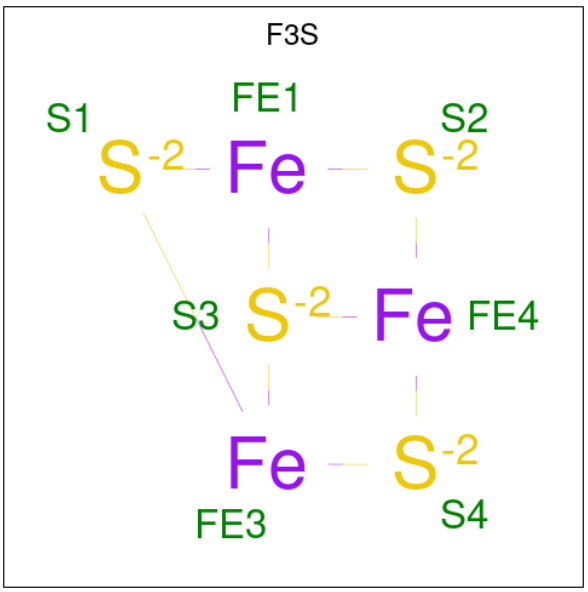
- Molecule 164 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

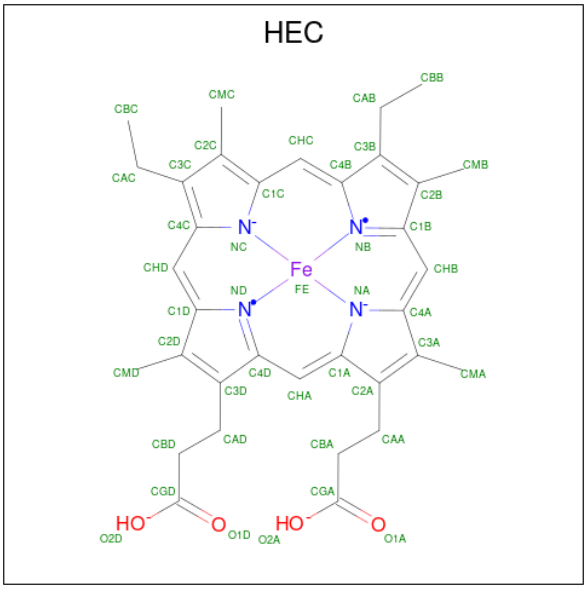
- Molecule 165 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of

Interest" by depositor).



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

- 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
			Total	C	Fe	H	N	O	
166	CE	1	75	34	1	32	4	4	0

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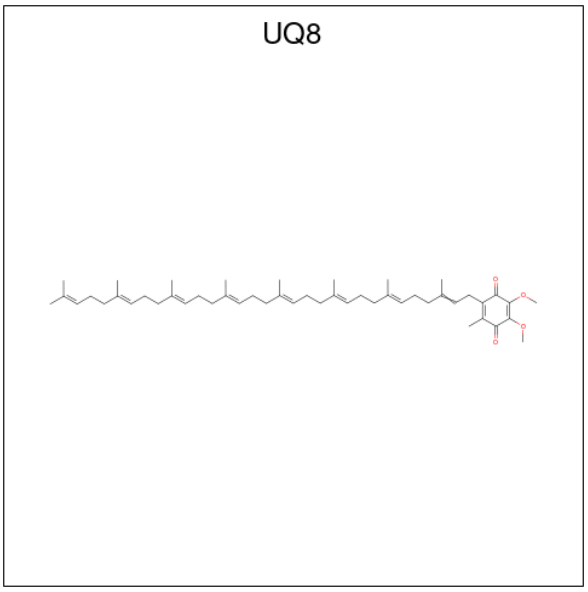
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
166	D	1	73	34	1	30	4	4	0
166	d	1	73	34	1	30	4	4	0

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



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

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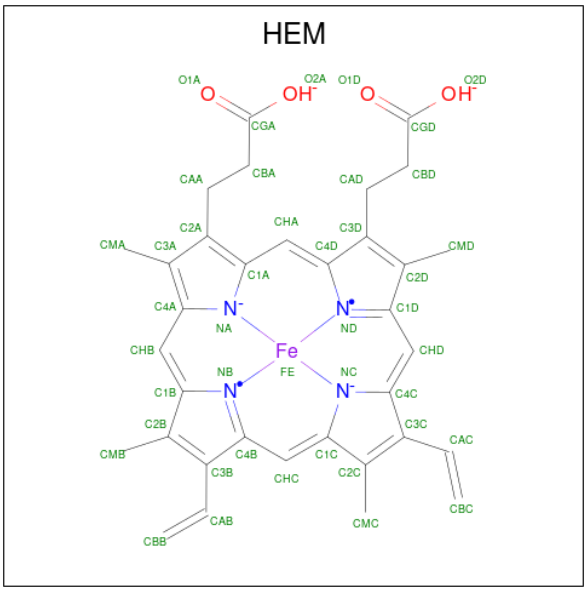
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
167	Ed	1	127	49	74	4	0
			Total	C	H	O	
167	El	1	127	49	74	4	0
			Total	C	H	O	
167	En	1	127	49	74	4	0

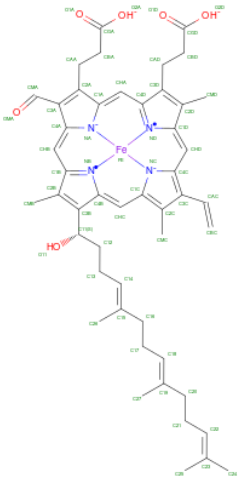
- Molecule 168 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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

HEA

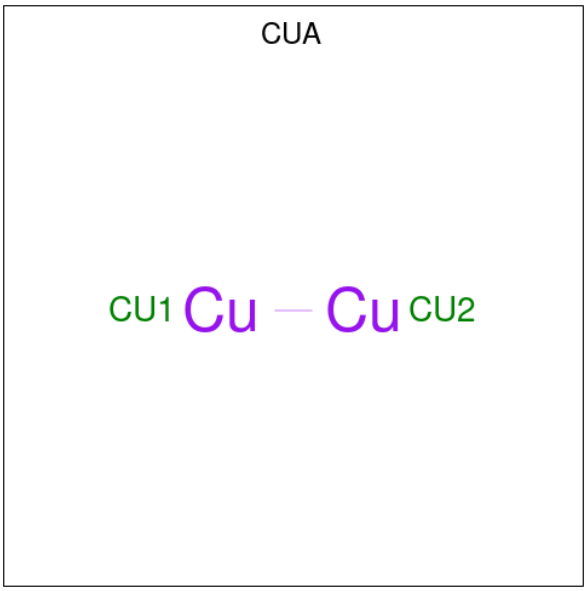


Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
169	DA	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
169	DA	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
169	Da	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
169	Da	1	114	49	1	54	4	6	0

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

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

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

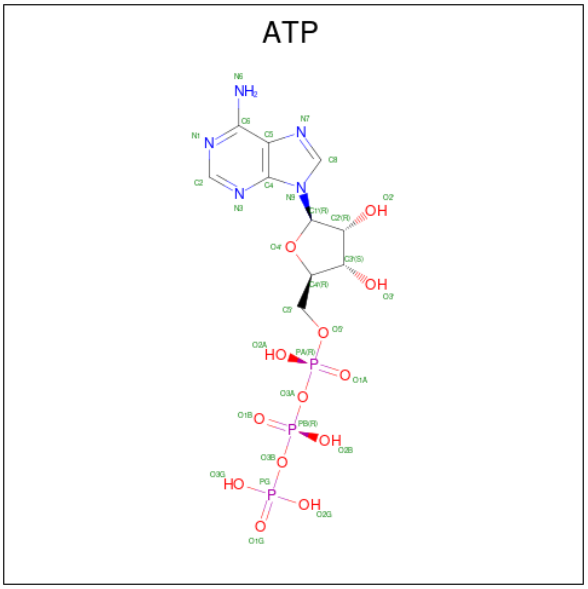


Mol	Chain	Residues	Atoms	AltConf
171	DB	1	Total Cu 2 2	0
171	Db	1	Total Cu 2 2	0

- 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: $C_{10}H_{16}N_5O_{13}P_3$).



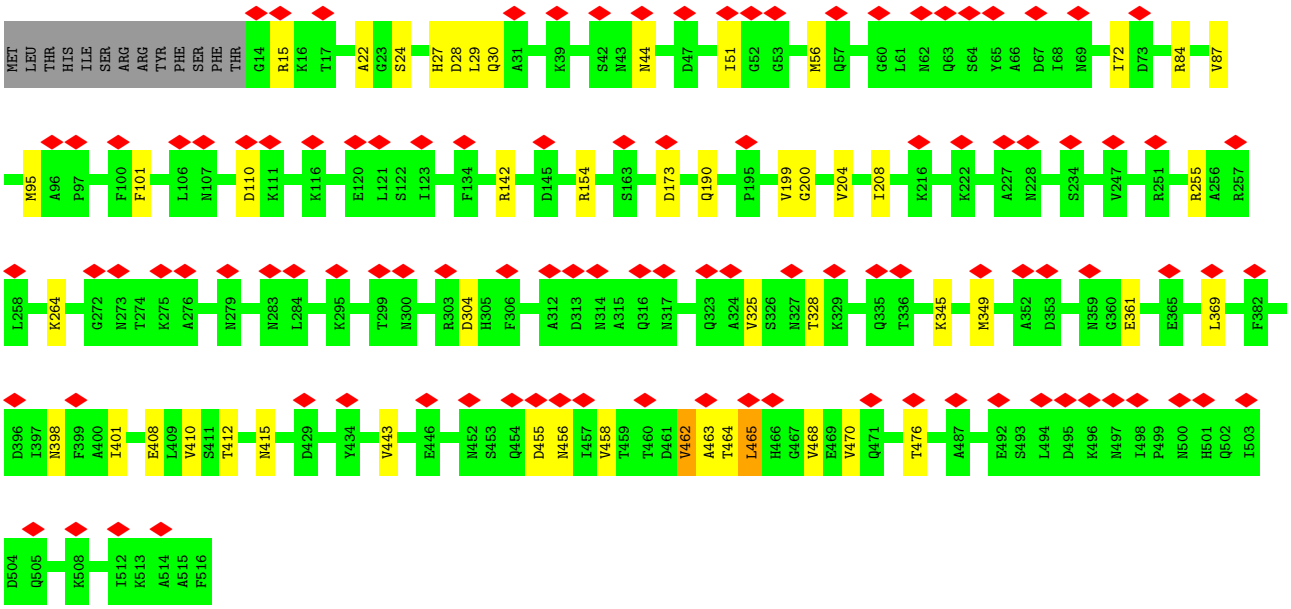
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
173	ER	1	43	10	12	5	13	3	0
			Total	C	H	N	O	P	
173	Er	1	43	10	12	5	13	3	0

3 Residue-property plots (i)

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

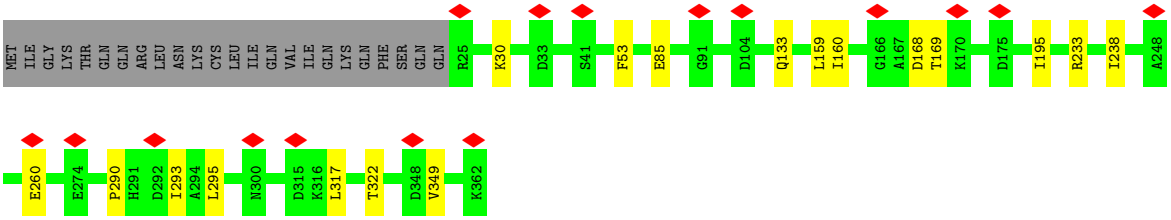
• Molecule 1: Lipid-A-disaccharide synthase

Chain A0:



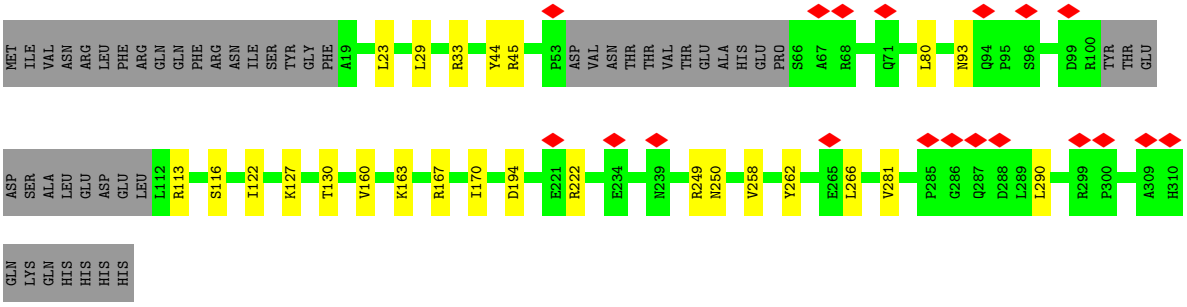
• Molecule 2: NAD-dependent epimerase/dehydratase family protein

Chain A1:



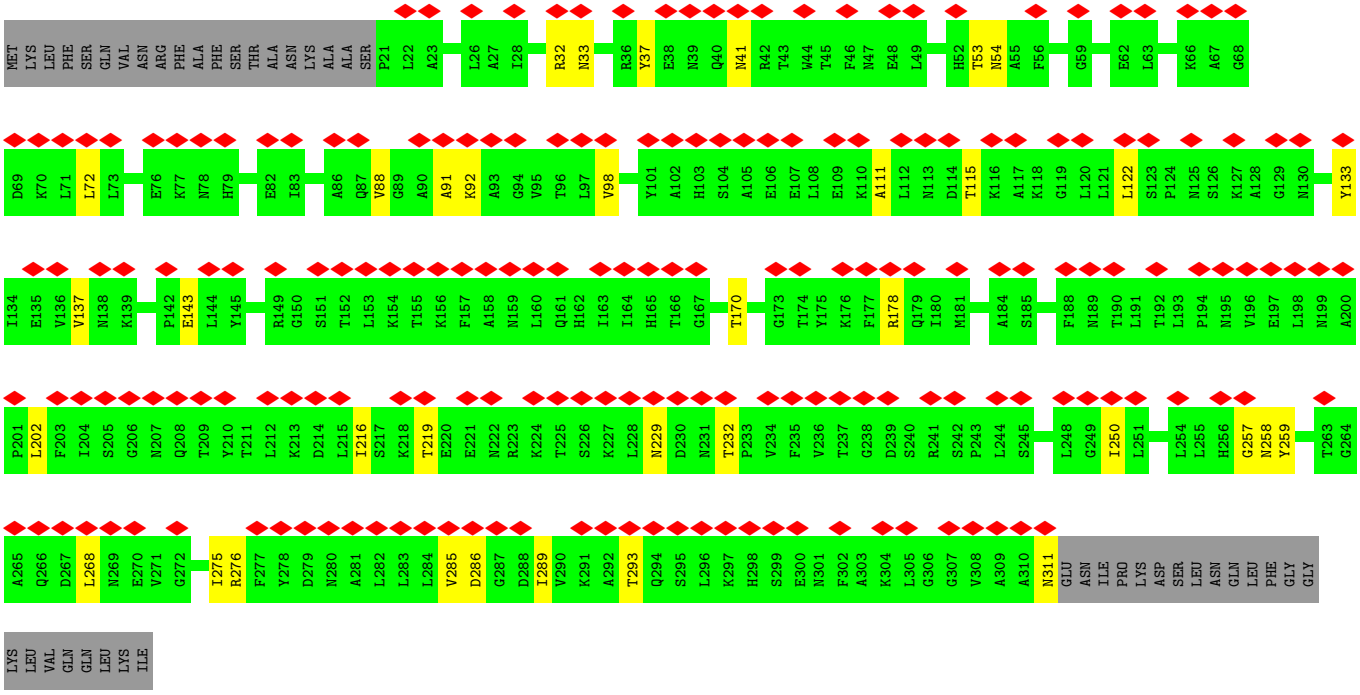
• Molecule 3: DnaJ domain protein

Chain A2:



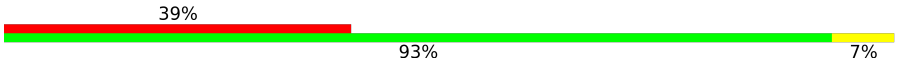
- Molecule 4: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

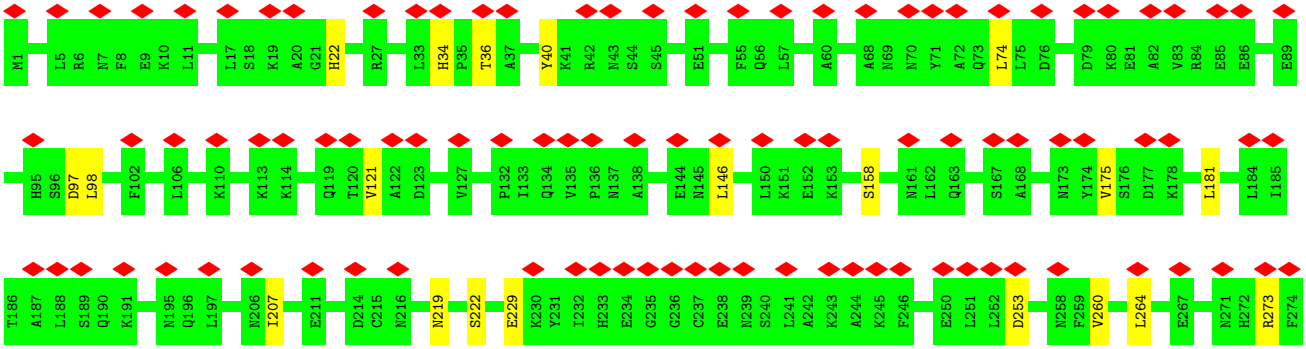
Chain A3:

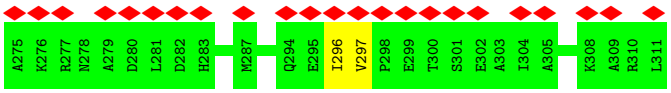


- Molecule 5: RNase III domain-containing protein

Chain A4:

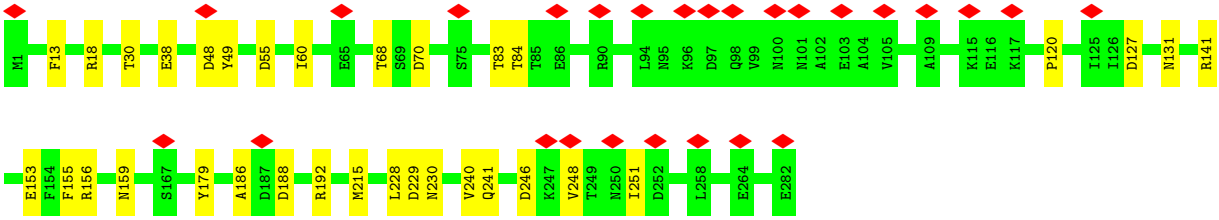






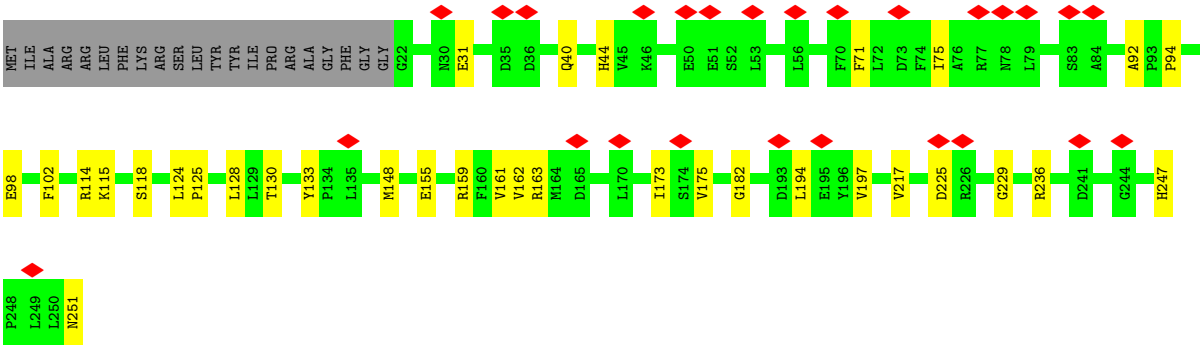
• Molecule 6: 37S ribosomal protein S25, mitochondrial

Chain A5:



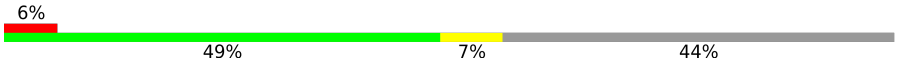
• Molecule 7: Transmembrane protein, putative

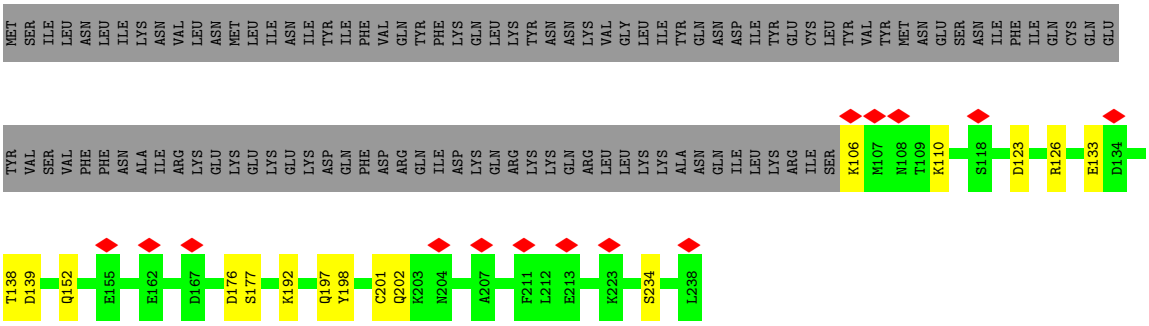
Chain A6:



• Molecule 8: CX9C domain-containing protein

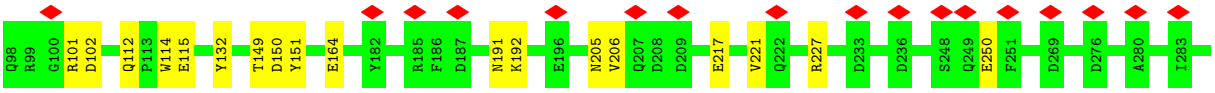
Chain A7:

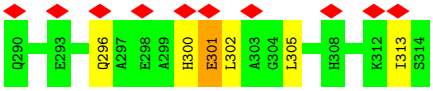




• Molecule 9: ND5a

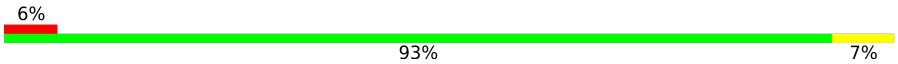
Chain A8:

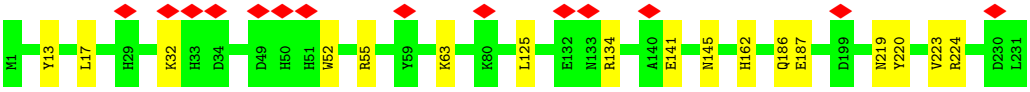




• Molecule 10: Transmembrane protein, putative

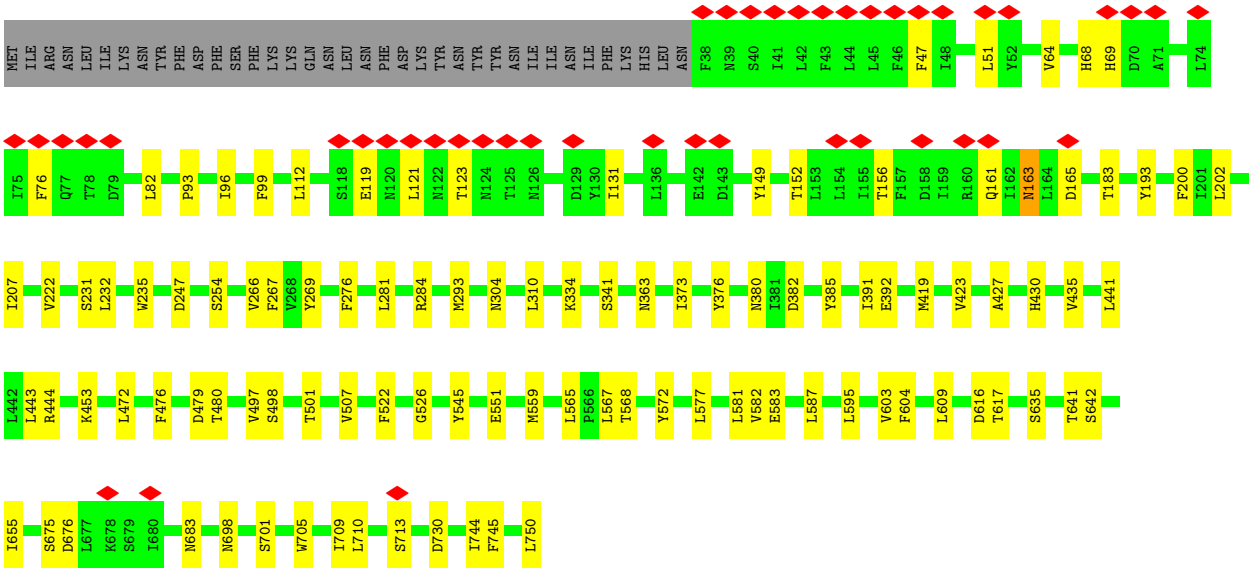
Chain A9:





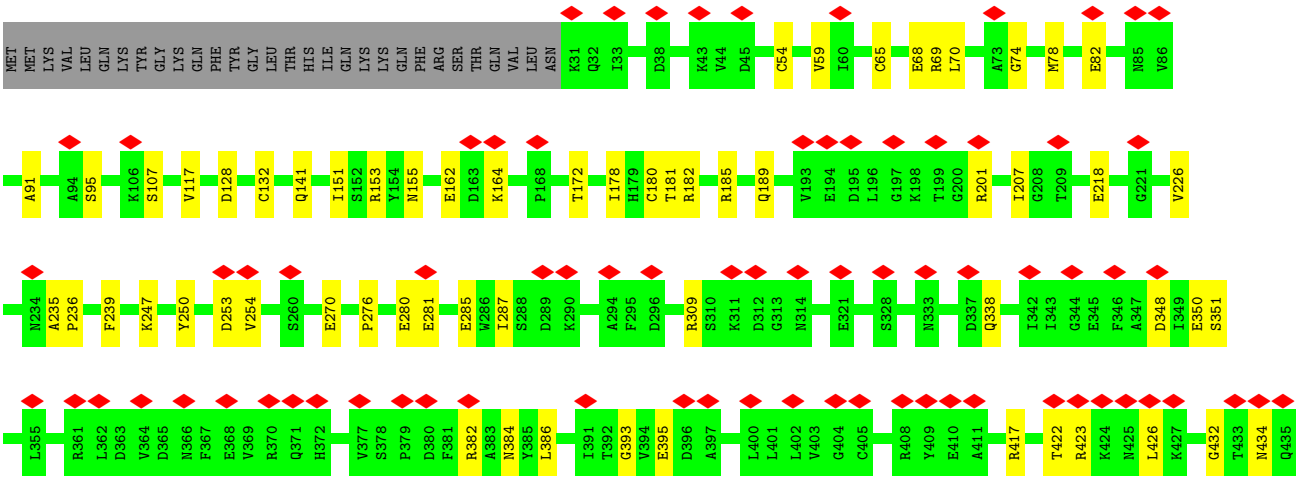
• Molecule 11: NADH dehydrogenase subunit 5

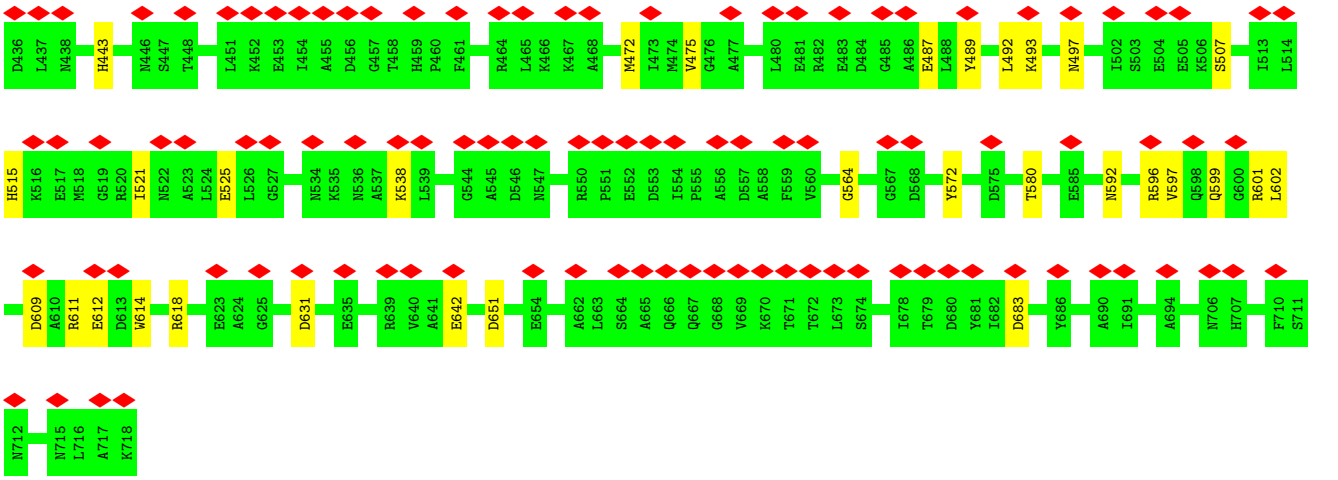
Chain AA:



• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit

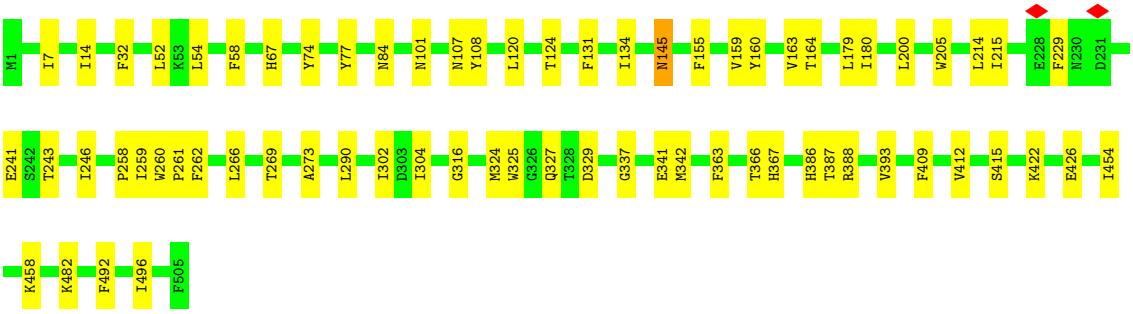
Chain AB:





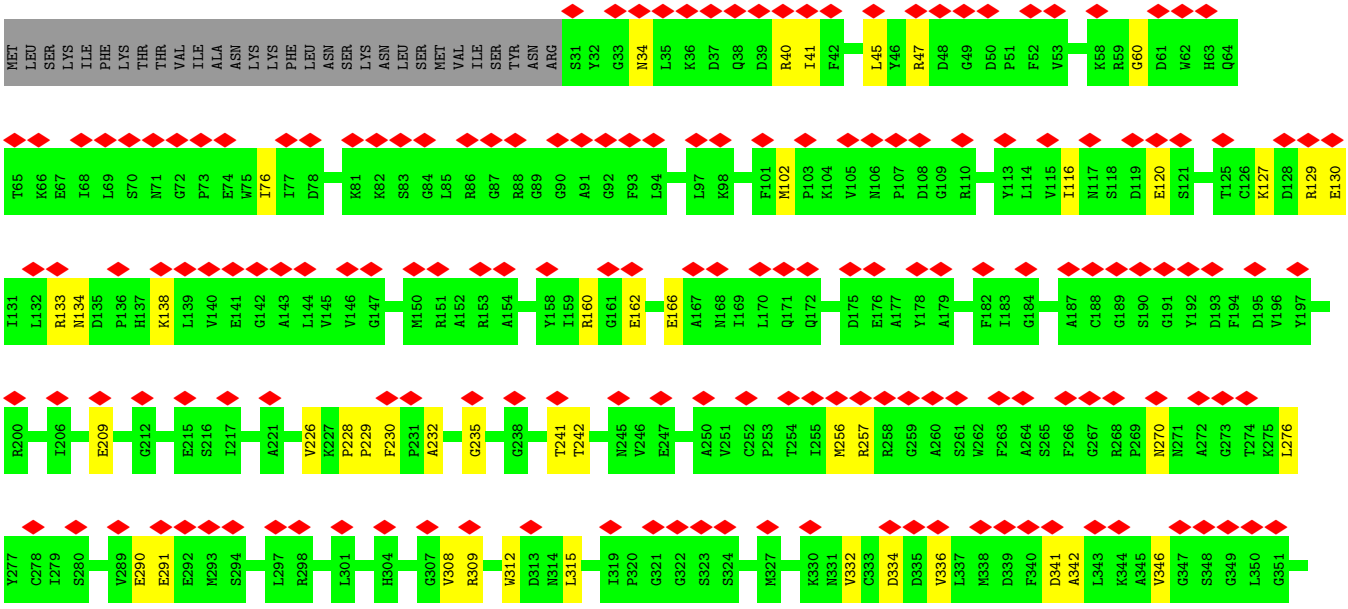
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain AC: 86% 13%



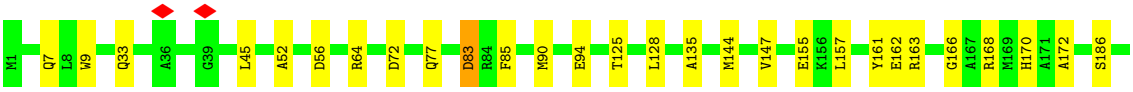
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

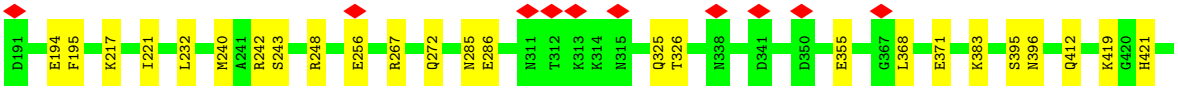
Chain AD: 39% 80% 13% 7%

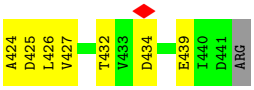


• Molecule 15: NADH dehydrogenase subunit 7

Chain AE:

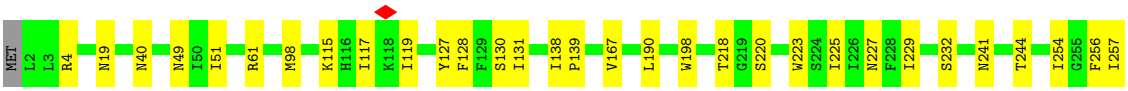






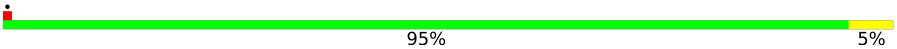
• Molecule 16: Ymf65

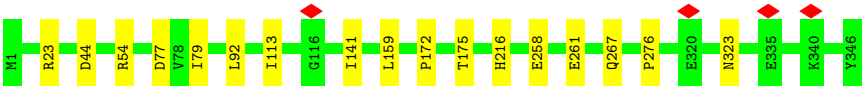
Chain AF:



• Molecule 17: Transcription factor apfi protein, putative

Chain AG:



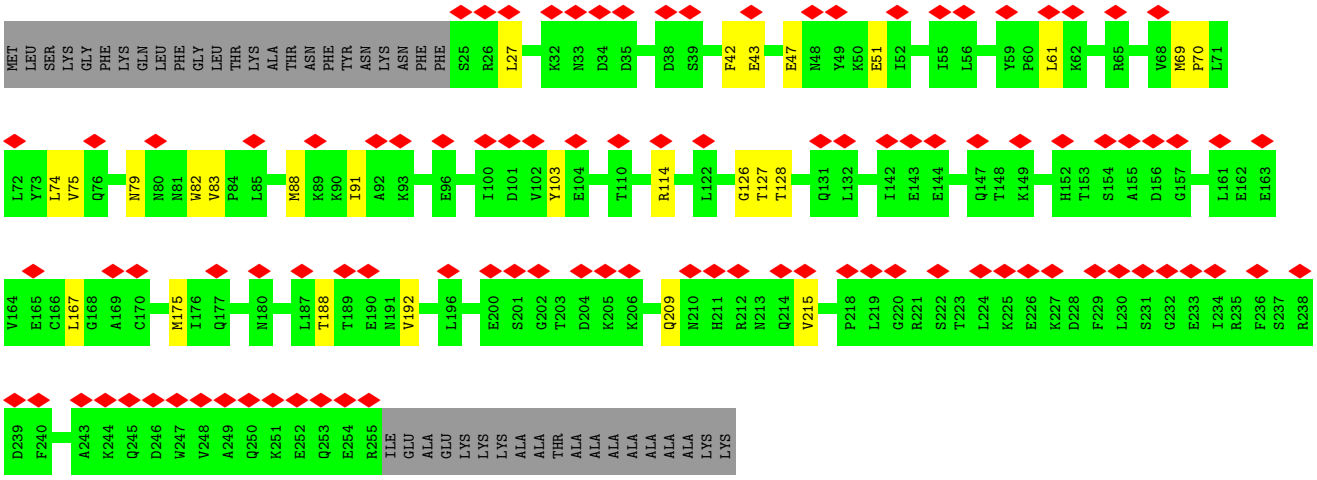


• Molecule 18: NADH-ubiquinone oxidoreductase chain 1

Chain AH:

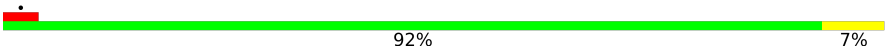
• Molecule 19: NADH-ubiquinone oxidoreductase 24 kDa subunit

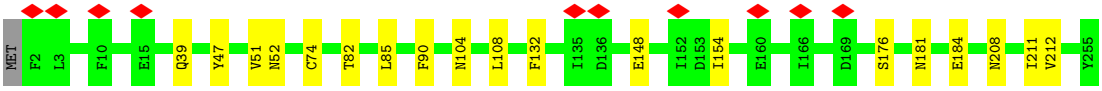
Chain AI:



- Molecule 20: Ymf62

Chain AJ:



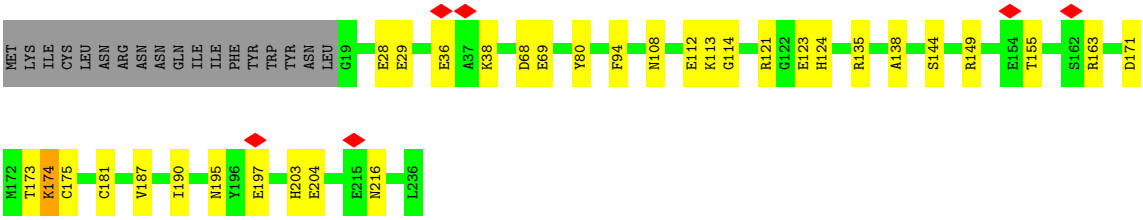


- Molecule 21: Gamma-carbonic anhydrase

Chain AK:

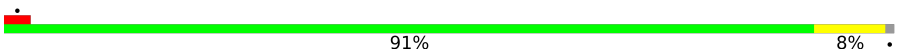
- Molecule 22: NADH-ubiquinone oxidoreductase 1, chain, putative

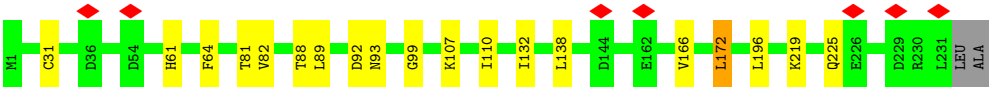
Chain AL:



- Molecule 23: Gamma-carbonic anhydrase

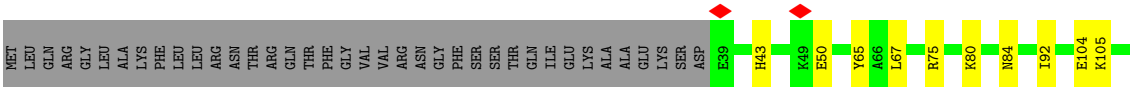
Chain AM:

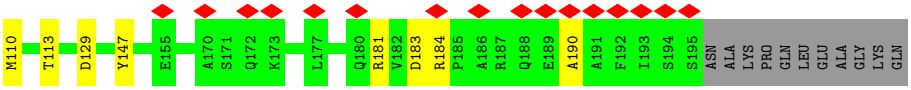




• Molecule 24: ETC complex I subunit motif protein

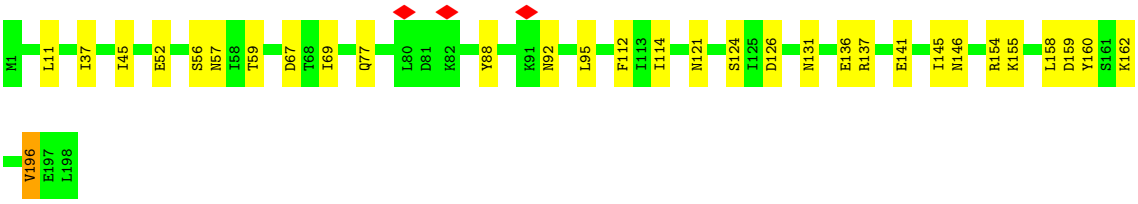
Chain AN:





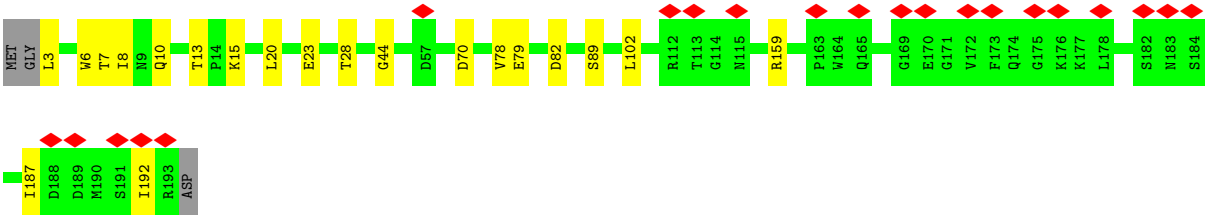
• Molecule 25: NADH dehydrogenase subunit 9

Chain AO:



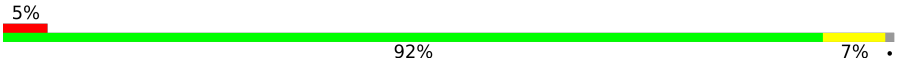
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

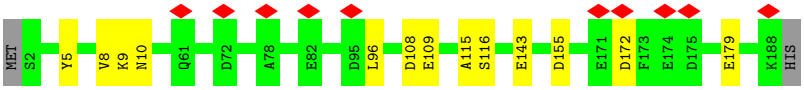
Chain AP:



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

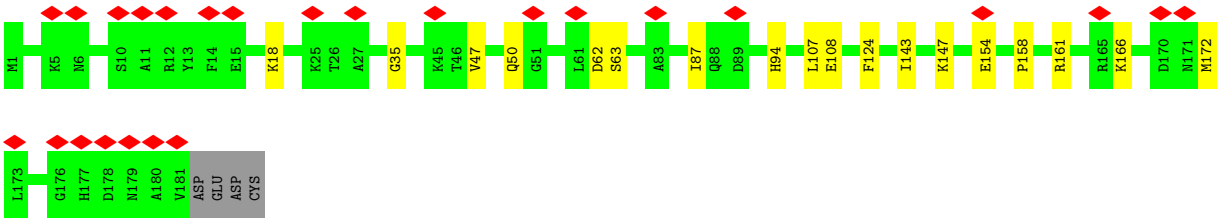
Chain AQ:





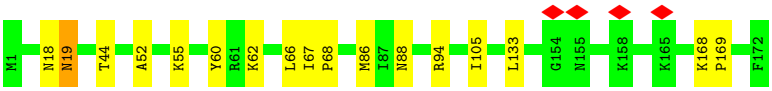
• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain AR:



• Molecule 29: NADH dehydrogenase, putative

Chain AS:

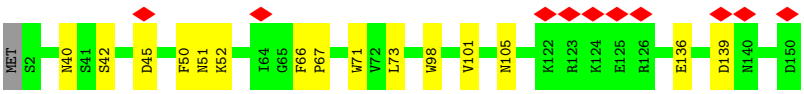


• Molecule 30: NADH dehydrogenase subunit 10

Chain AT:

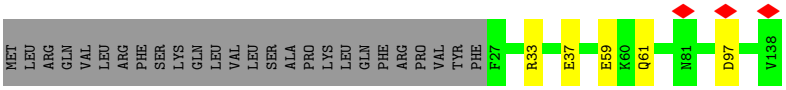
• Molecule 31: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

Chain AU:



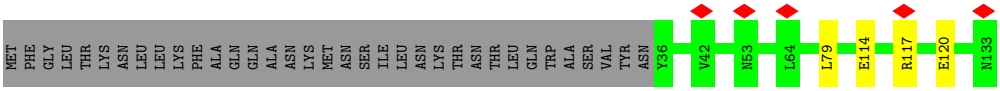
• Molecule 32: Acyl carrier protein

Chain AV:



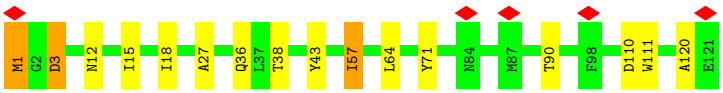
• Molecule 33: Acyl carrier protein

Chain AW:



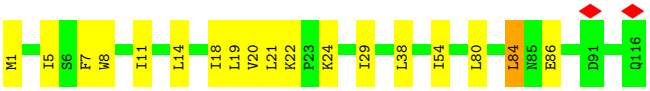
• Molecule 34: NADH-ubiquinone oxidoreductase chain 3

Chain AX:



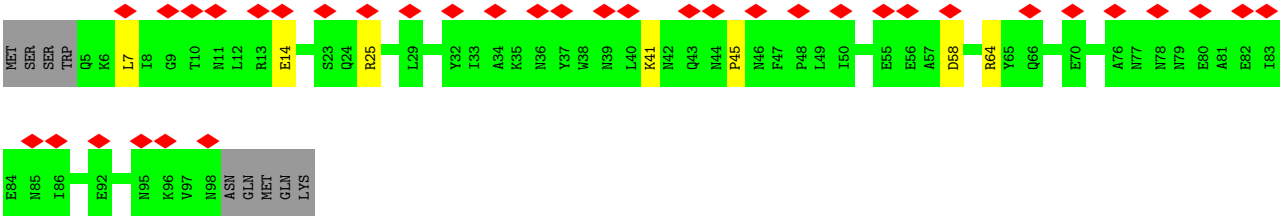
• Molecule 35: Ymf58

Chain AY:



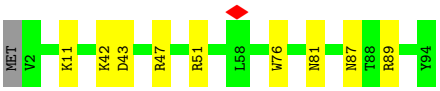
• Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein

Chain AZ:



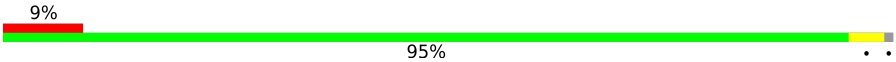
• Molecule 37: Transmembrane protein, putative

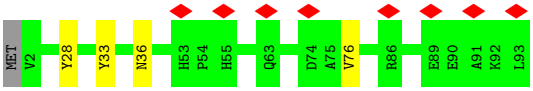
Chain B0:



• Molecule 38: ATP synthase subunit e, mitochondrial

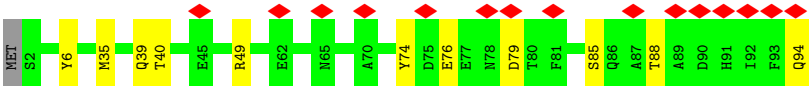
Chain B1:





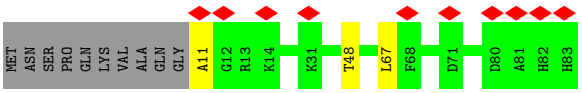
• Molecule 39: GRAM domain protein

Chain B2:



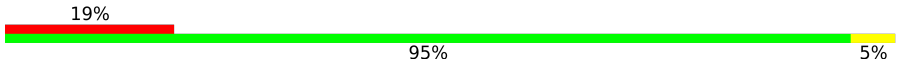
• Molecule 40: Transmembrane protein, putative

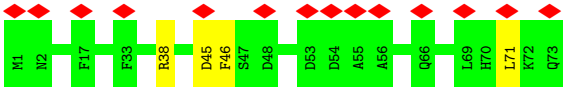
Chain B3:



• Molecule 41: Transmembrane protein, putative

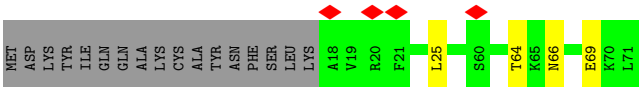
Chain B4:





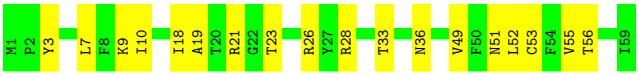
• Molecule 42: Transmembrane protein, putative

Chain B5:



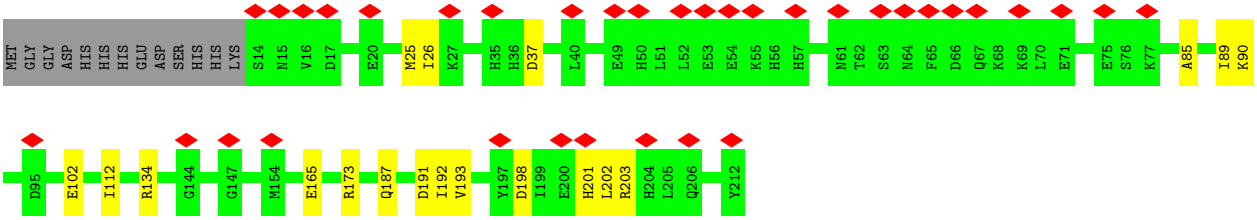
• Molecule 43: NADH dehydrogenase subunit 1

Chain B6:



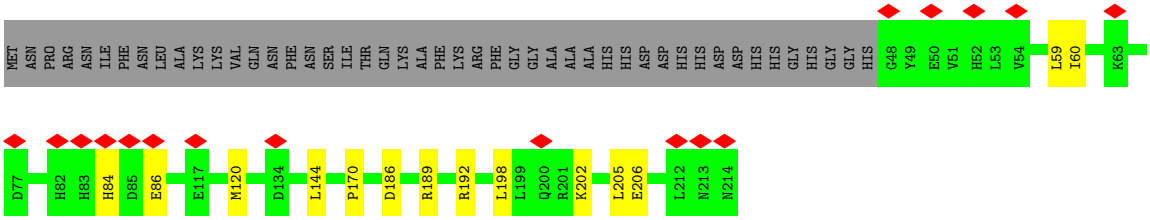
• Molecule 44: Transmembrane protein

Chain BA:



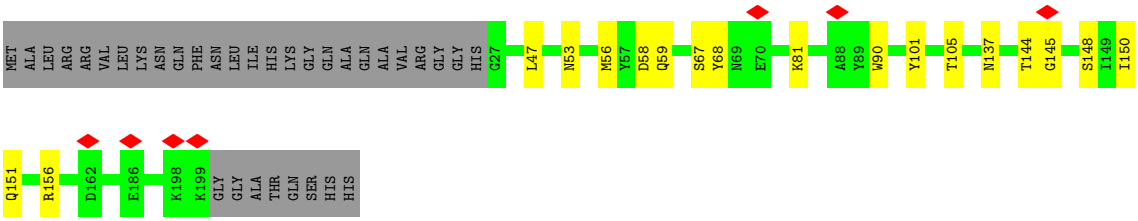
• Molecule 45: Transmembrane protein, putative

Chain BB:



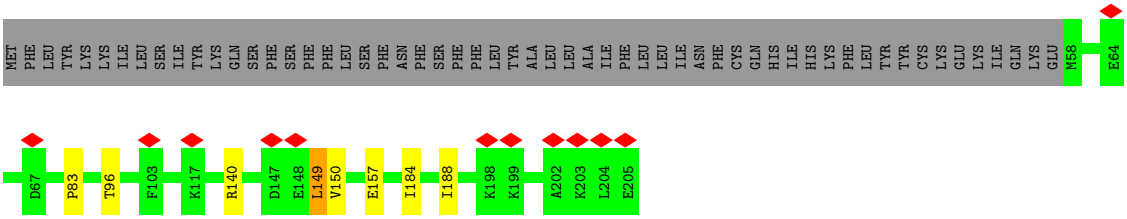
• Molecule 46: NDUB8

Chain BC:



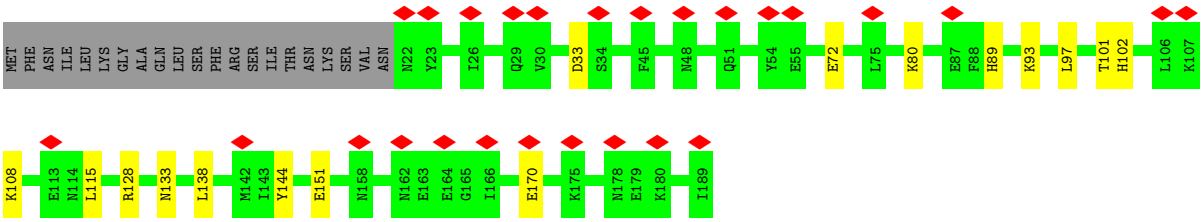
- Molecule 47: Transmembrane protein, putative

Chain BD:



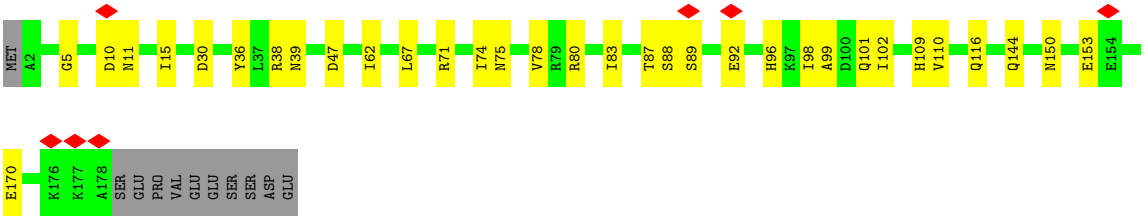
- Molecule 48: NDUPH2

Chain BE:



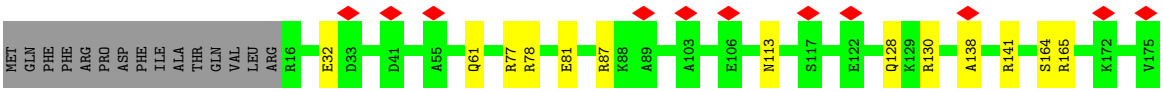
- Molecule 49: NDUB10

Chain BF:



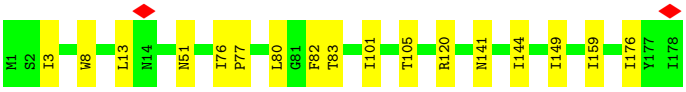
- Molecule 50: NDUA13

Chain BG:



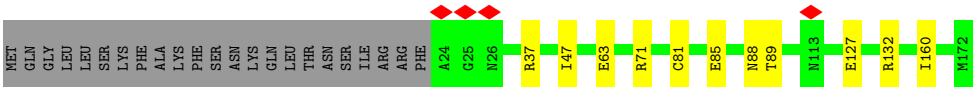
• Molecule 51: NADH dehydrogenase subunit 2

Chain BH:



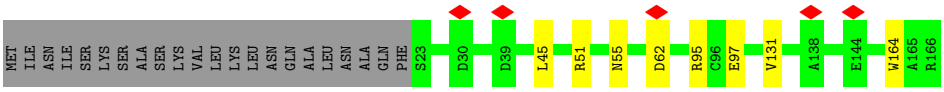
• Molecule 52: 2 iron, 2 sulfur cluster-binding protein

Chain BI:



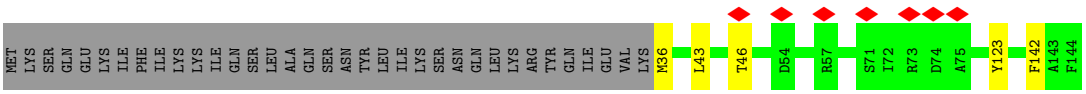
• Molecule 53: Thioredoxin

Chain BJ:



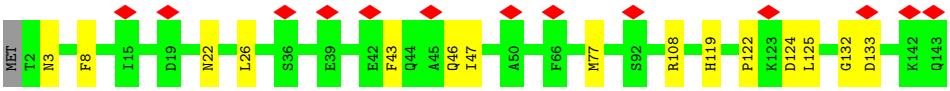
• Molecule 54: COX assembly mitochondrial protein

Chain BK:



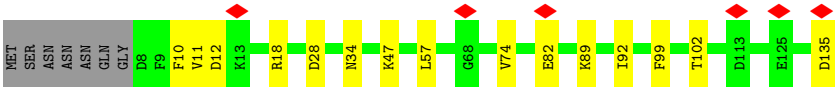
• Molecule 55: Transmembrane protein, putative

Chain BL:



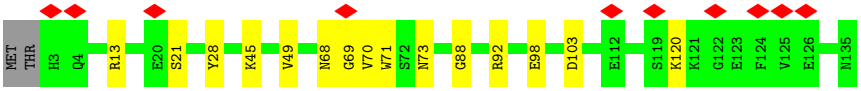
• Molecule 56: Transmembrane protein, putative

Chain BM:



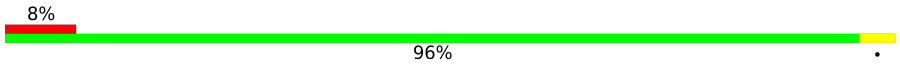
• Molecule 57: PH domain-containing protein

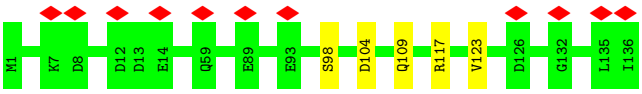
Chain BN:



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

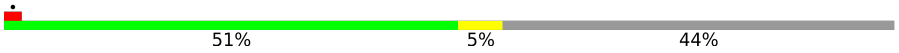
Chain BO:

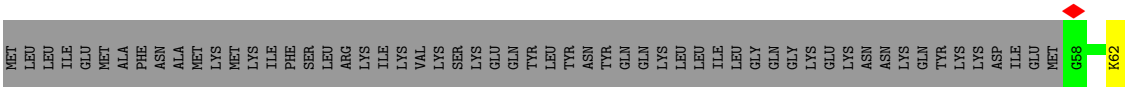


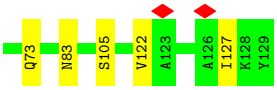


• Molecule 59: NDUB6

Chain BP:

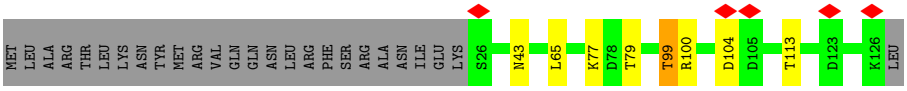






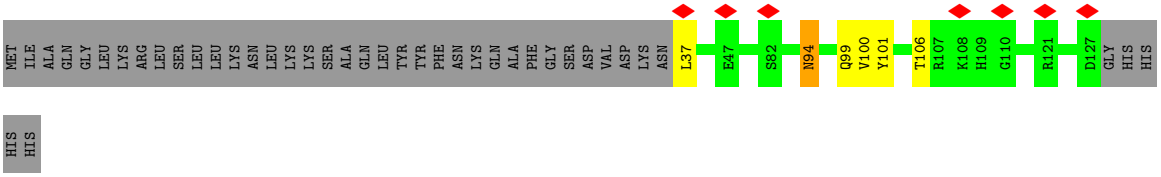
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain BQ:



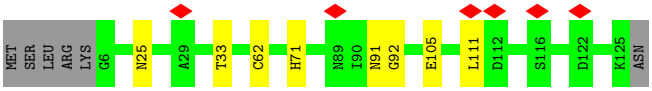
• Molecule 61: Zinc-finger protein

Chain BR:



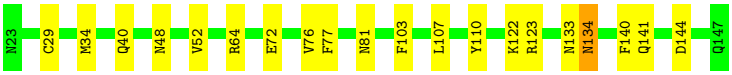
• Molecule 62: NDUB4

Chain BS:



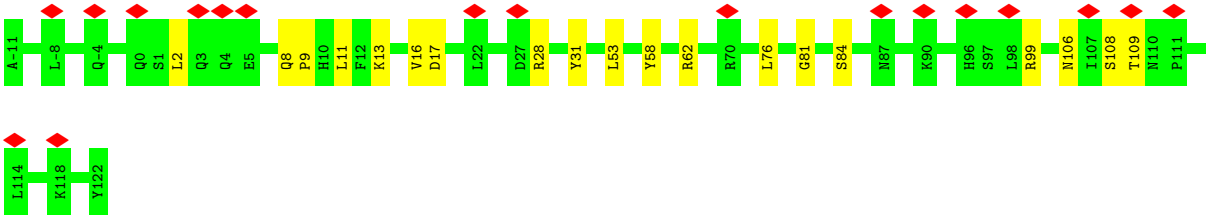
• Molecule 63: NDUTT10

Chain BT:



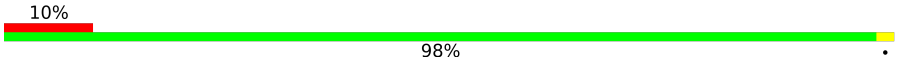
• Molecule 64: NDUTT11

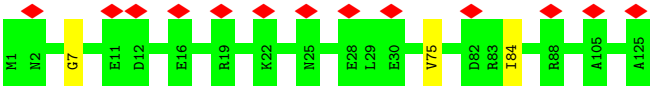
Chain BU:



• Molecule 65: NDUTT12

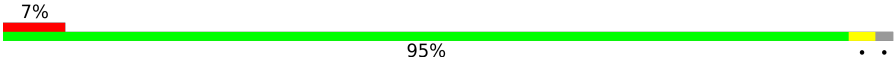
Chain BV:

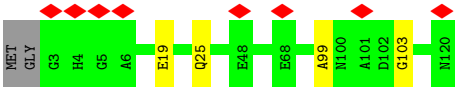




• Molecule 66: CHCH domain-containing protein

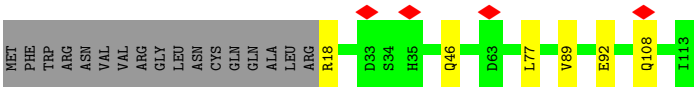
Chain BW:





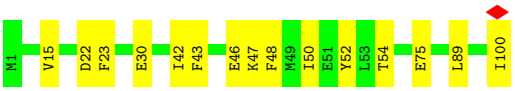
• Molecule 67: Transmembrane protein, putative

Chain BX:



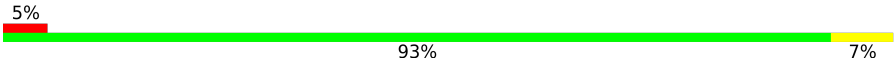
• Molecule 68: Ymf57

Chain BY:



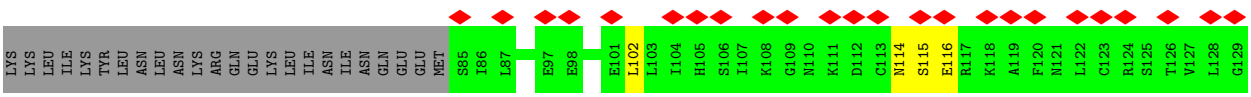
• Molecule 69: Complex I-MNLL

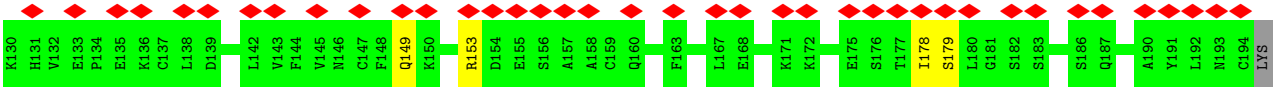
Chain BZ:



- Molecule 70: Diphthamide synthesis protein

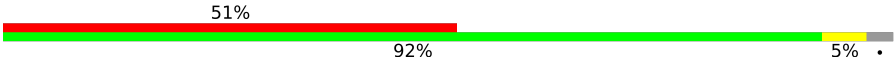
Chain CH:

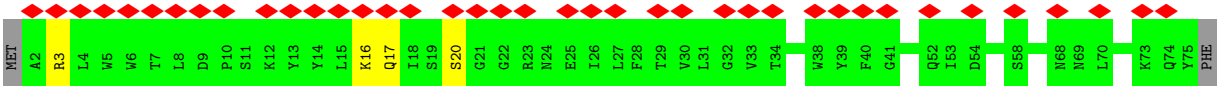




- Molecule 71: Transmembrane protein, putative

Chain CM:



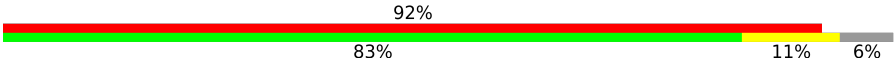


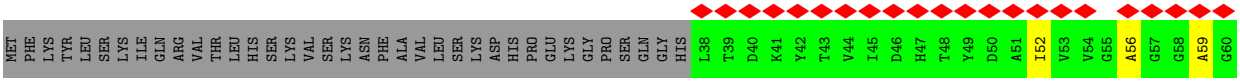
- Molecule 72: Transposase

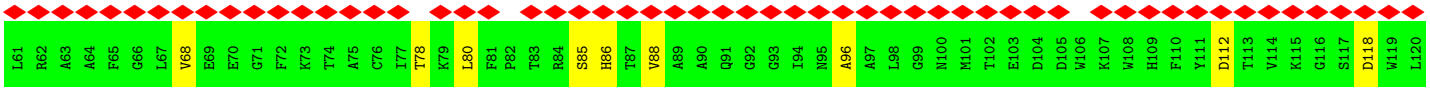
Chain CL:

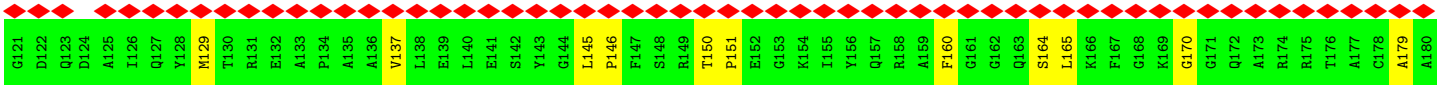
- Molecule 73: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain CA:









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

G301 E302 G303 G304 I305 L306 V307 N308 S309 N310 G311 E312 A313 F314 M315 E316 K317 Y318 A319 P320 T321 A322 K323 D324 L325 A326 S327 R328 D329 V330 V331 S332 R333 A334 M335 T336 I337 E338 I339 L340 E341 G342 R343 G344 V345 G346 P947 K348 K349 D350 H351 I352 F353 L354 Q355 L356 H357 H358 L359 S360

P361 E362 T363 L364 H365 Q366 R367 L368 P369 G370 I371 S372 E373 T374 A375 R376 I377 F378 A379 G380 V381 D382 V383 T384 K385 E386 P387 A388 P389 V390 V391 P392 T393 V394 H395 Y396 M397 M398 G399 G400 V401 P402 T403 N404 W405 K406 T407 E408 V409 I410 T411 Q412 D413 K414 N415 G416 K417 D418 K419 I420

V421 P422 G423 L424 L425 A426 A427 G428 E429 M430 A431 C432 A433 S434 V435 H436 G437 A438 M439 R440 L441 G442 A443 M444 S445 L446 L447 D448 I449 V450 V451 F452 G453 R454 A455 A456 A457 K458 L459 V460 K461 E462 K463 L464 K465 P466 G467 T468 P469 H470 K471 D472 L473 P474 K475 N476 A477 G478 E479 Q480

A481 L482 A483 R484 L485 D486 K487 Y488 R489 F490 A491 M492 G493 E494 Y495 T496 T497 H498 H499 V500 R501 T502 A503 M504 Q505 E506 T507 M508 Q509 R510 H511 A512 A513 V514 F515 R516 I517 E518 K519 L520 M521 A522 E523 G524 V525 Q526 K527 L528 D529 H530 I531 Y532 E533 Q534 S535 K536 S537 L538 K539 T540

F541 D542 R543 G544 L545 V546 W547 N548 T549 D550 L551 I552 E553 T554 L555 E556 L557 E558 N559 L560 L561 L562 C563 S564 K565 Q566 T567 L568 L569 A570 G571 L572 L573 R574 K575 E576 S577 R578 G579 A580 H581 A582 R583 D584 D585 F586 K587 E588 R589 D590 D591 K592 N593 W594 M595 K596 H597 S598 L599 T600

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

- Molecule 74: DUF4885 domain-containing protein

Chain CI: 39% 95% 5%

M1 F2 S3 N6 M7 Y8 E9 A10 L14 V17 A20 F24 R25 L34 A35 R36 Y37 E38 S39 Q40 S41 Q42 S43 G47 S48 T49 S50 G51 A52 I55 D58 R64 N65 F66 K67 A68 L69 K70 K73 Y77 E80 I81 K84 A87

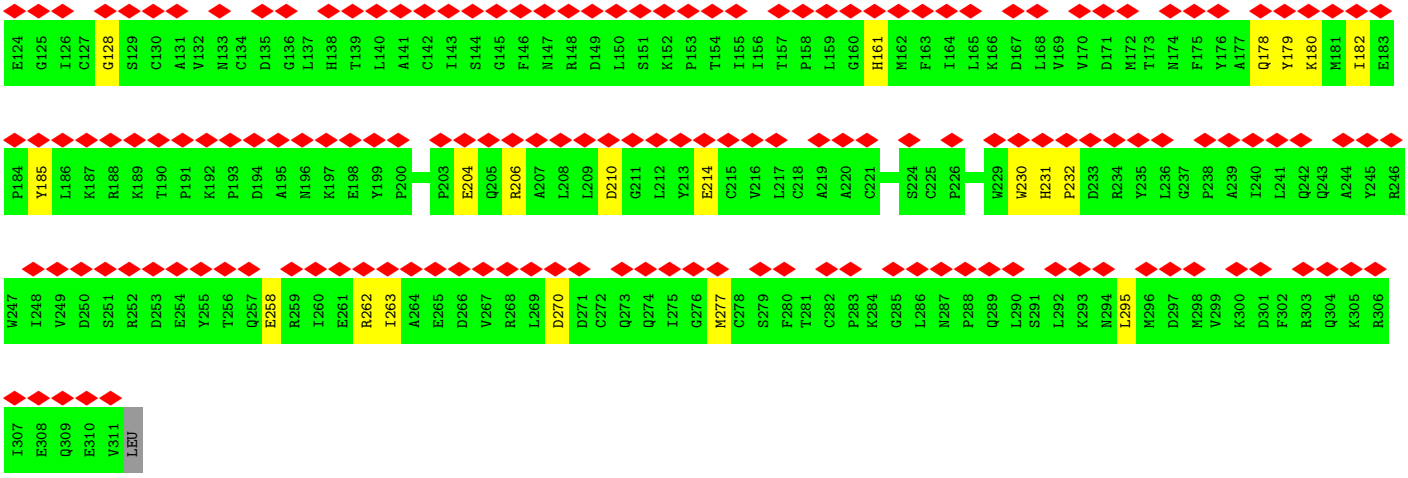
F92 D95 Y96 T97 A98 F102 L103 N104 E105 K108 K109 Q112 D113 A114

- Molecule 75: succinate dehydrogenase

Chain CB: 76% 83% 8% 9%

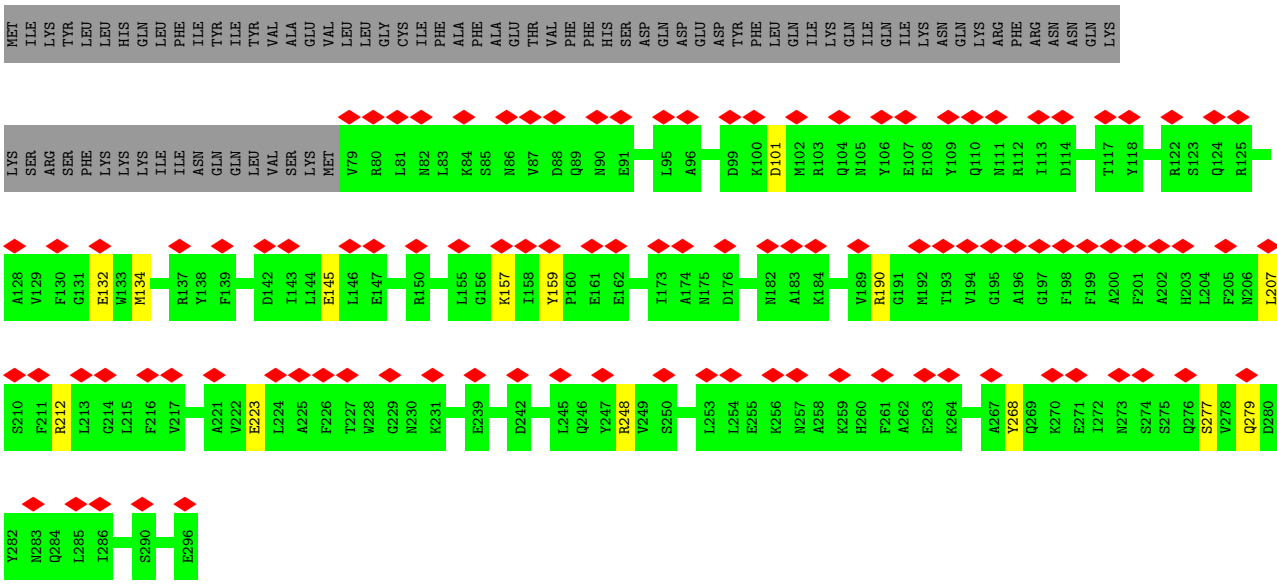
MET LEU ARG THR ILE PHE LYS THR ARG SER LEU PHE ASN ALA SER VAL SER ARG PHE GLY SER GLY PHE ASP ARG ILE A27 E28 S29 N30 D31 A32 T33 S34 I35 C36 L37 I40 S41 G42 T43 I44 L47 Q48 K49 A50 N51 Y52 V53 V54 E55 H56 N57 P58 N59 L60 T61 S62

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



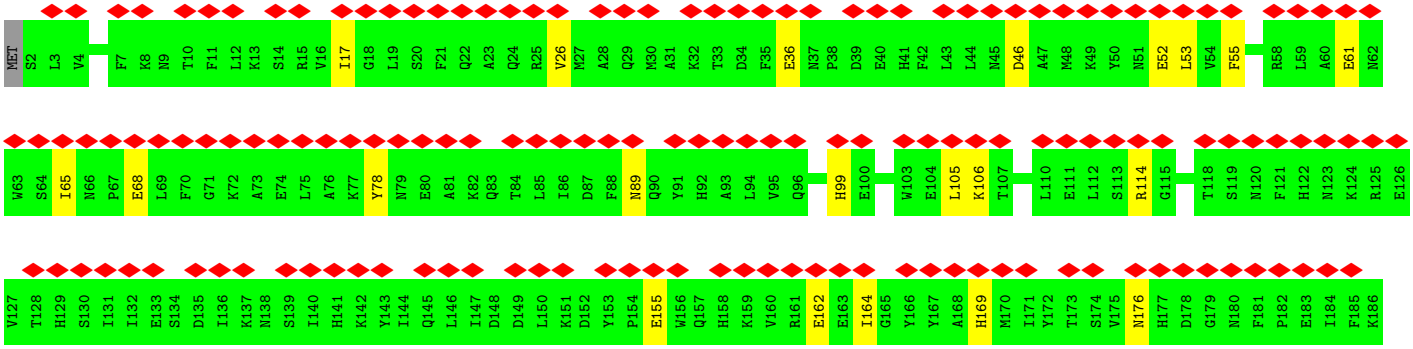
- Molecule 76: Transmembrane protein, putative

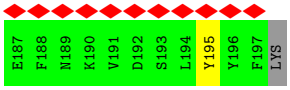
Chain CF:



- Molecule 77: chain 77

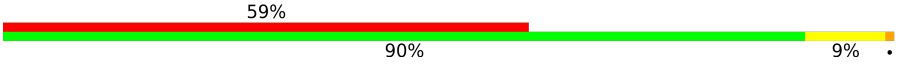
Chain CG:

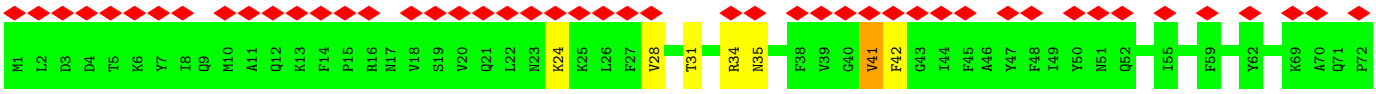


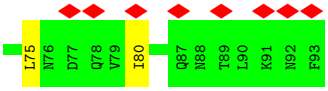


• Molecule 78: Transmembrane protein, putative

Chain CK:

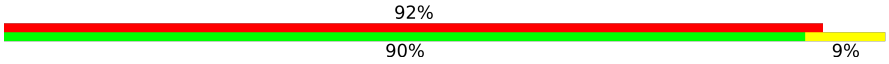


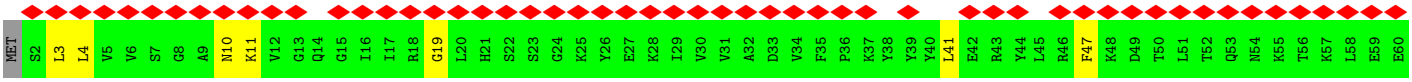


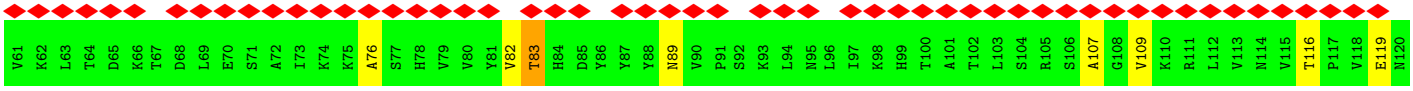


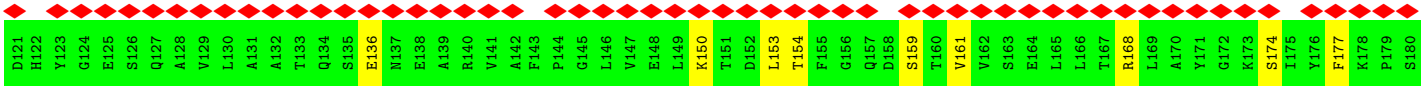
• Molecule 79: NmrA domain-containing protein

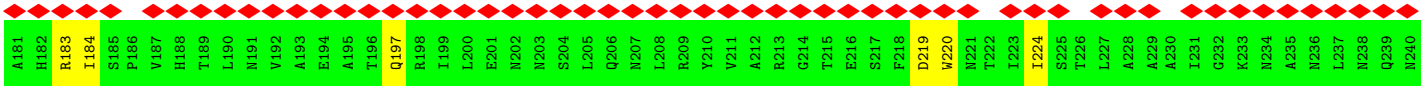
Chain CE:

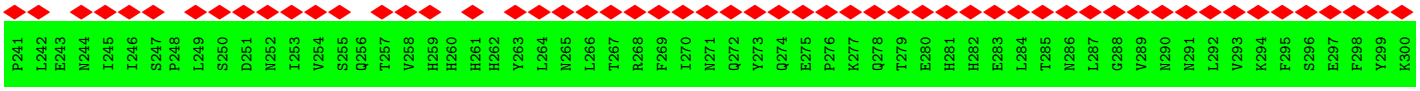


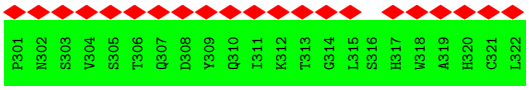






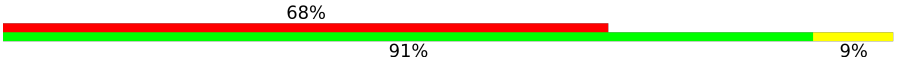


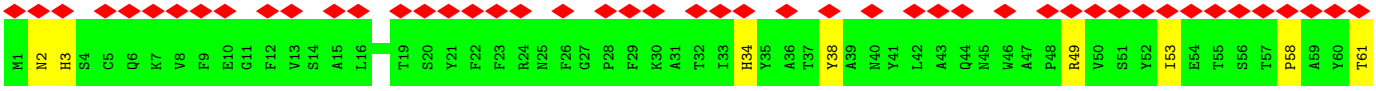


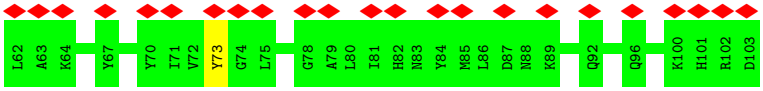


• Molecule 80: Transmembrane protein, putative

Chain CJ:

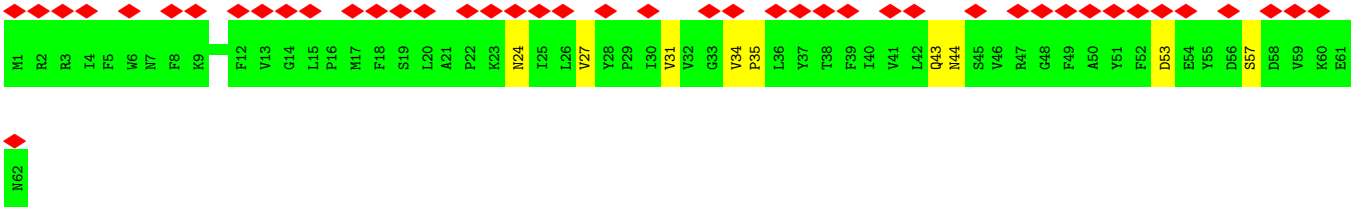






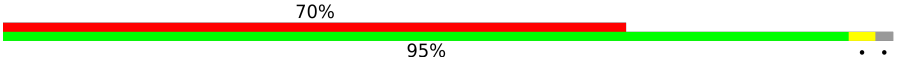
• Molecule 81: Transmembrane protein, putative

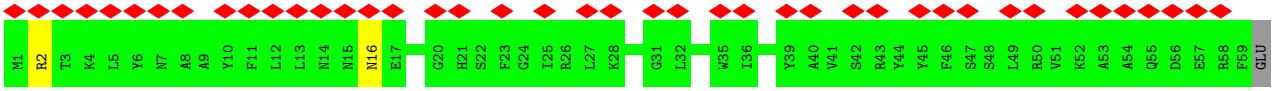
Chain CN:



• Molecule 82: Transmembrane protein

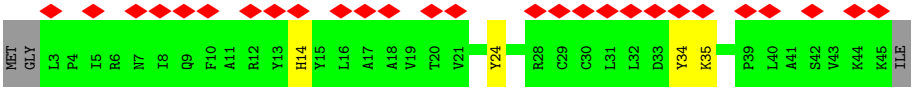
Chain CC:





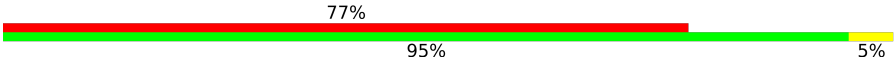
• Molecule 83: SDHTT11

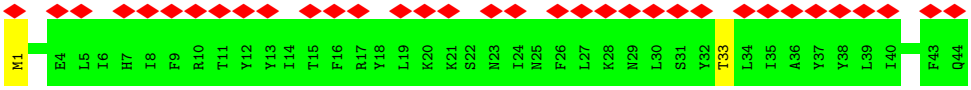
Chain CO:



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

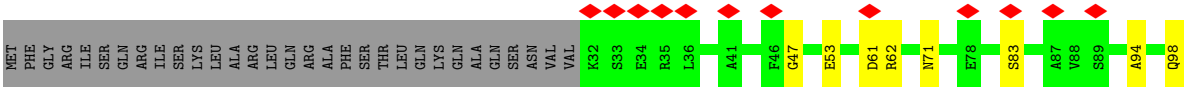
Chain CD:

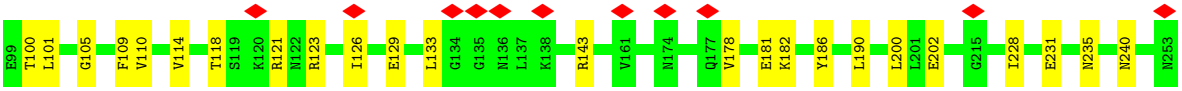


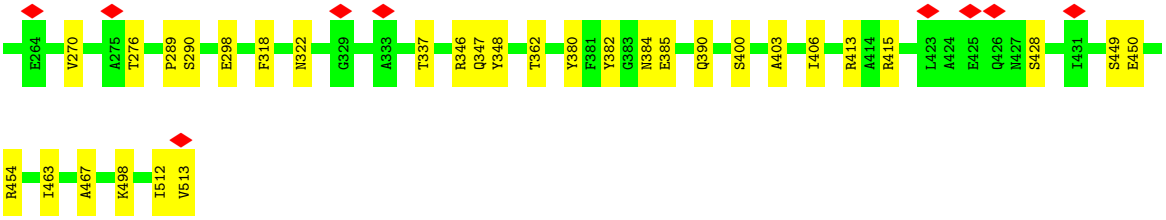


• Molecule 85: Peptidase M16 inactive domain protein

Chain A:

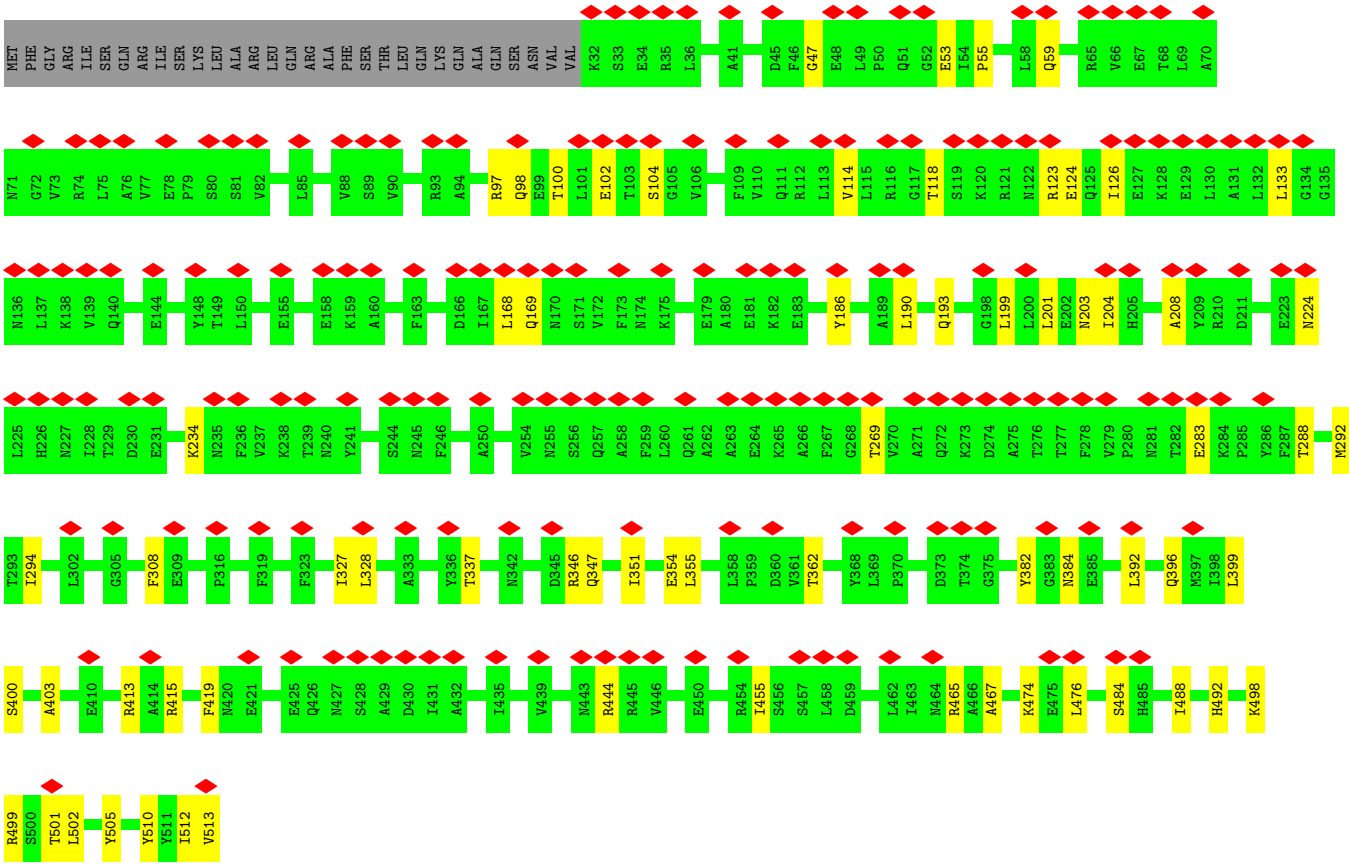






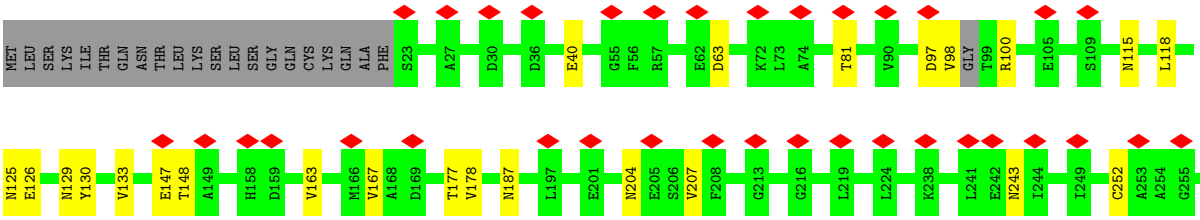
• Molecule 85: Peptidase M16 inactive domain protein

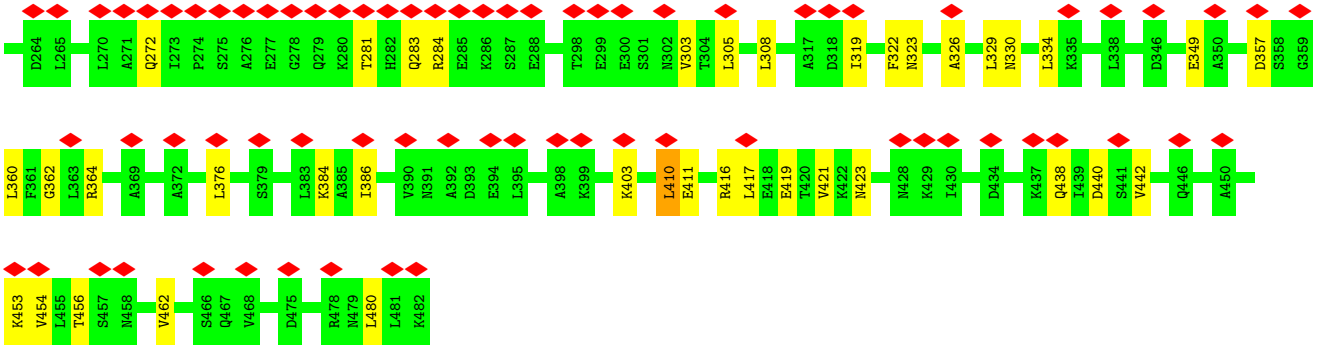
Chain a:



• Molecule 86: M16 family peptidase, putative

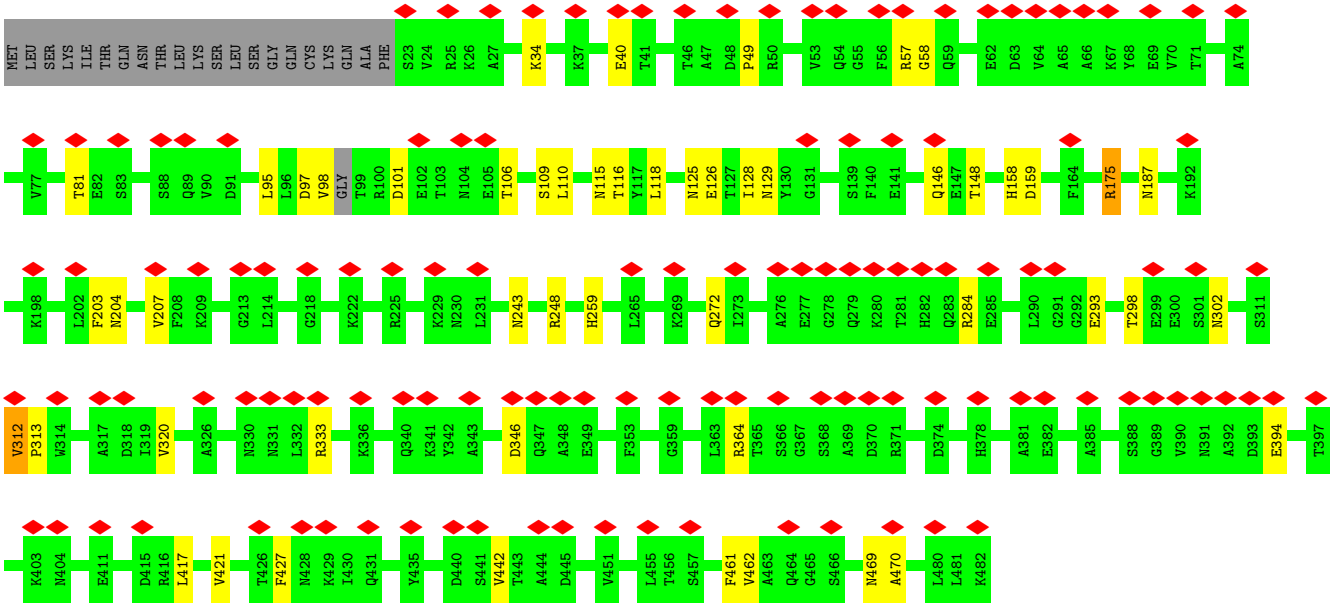
Chain B:





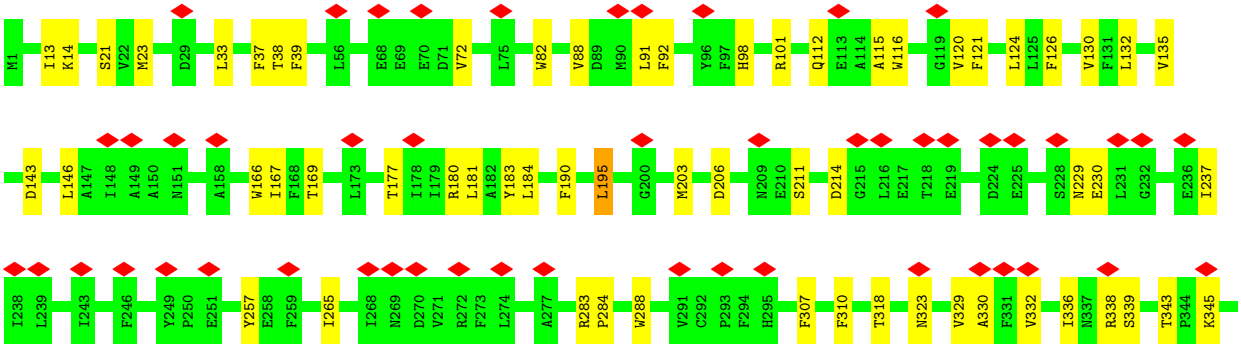
- Molecule 86: M16 family peptidase, putative

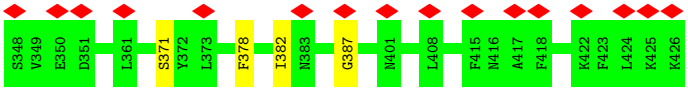
Chain b:



- Molecule 87: Apocytochrome b

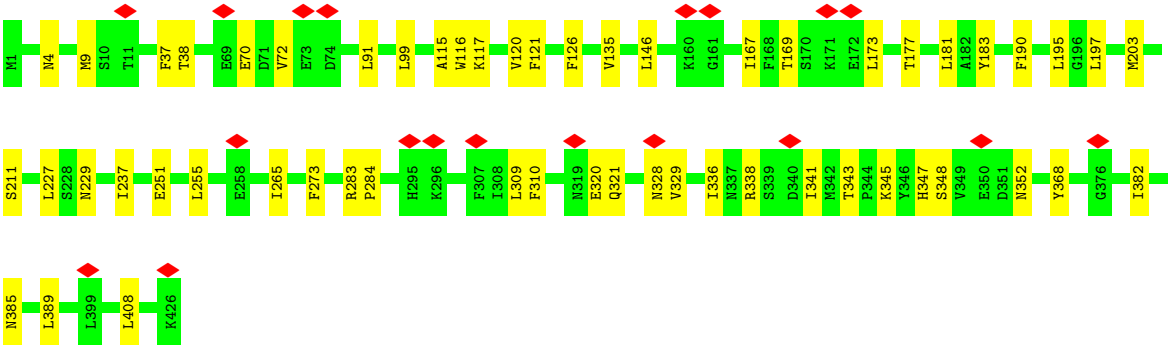
Chain C:





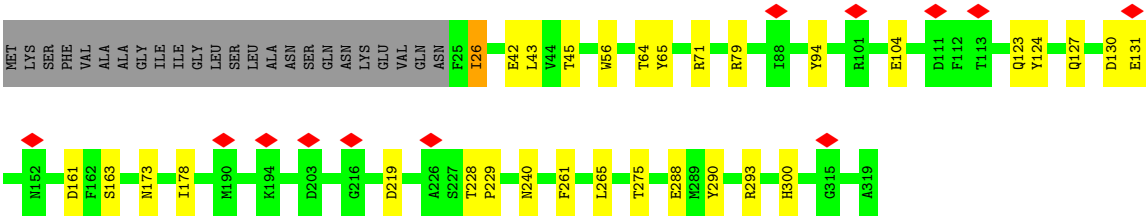
• Molecule 87: Apocytochrome b

Chain c:



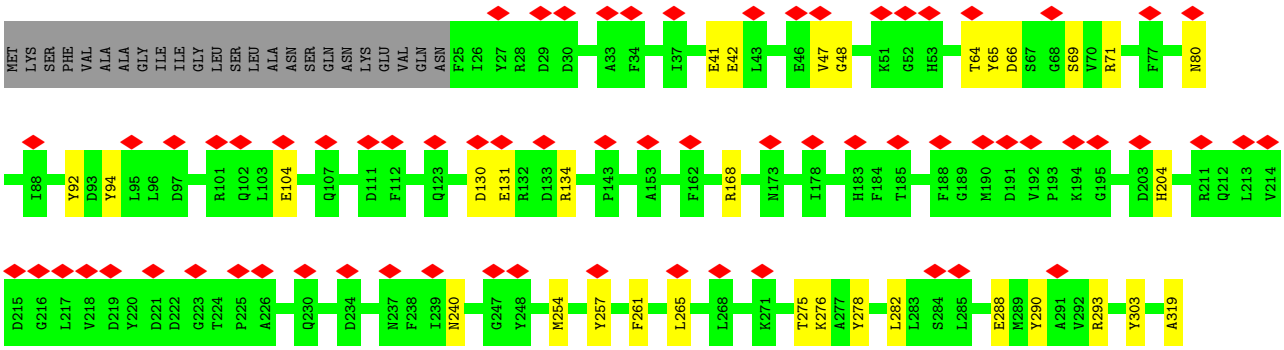
• Molecule 88: Cytochrome protein c1

Chain D:



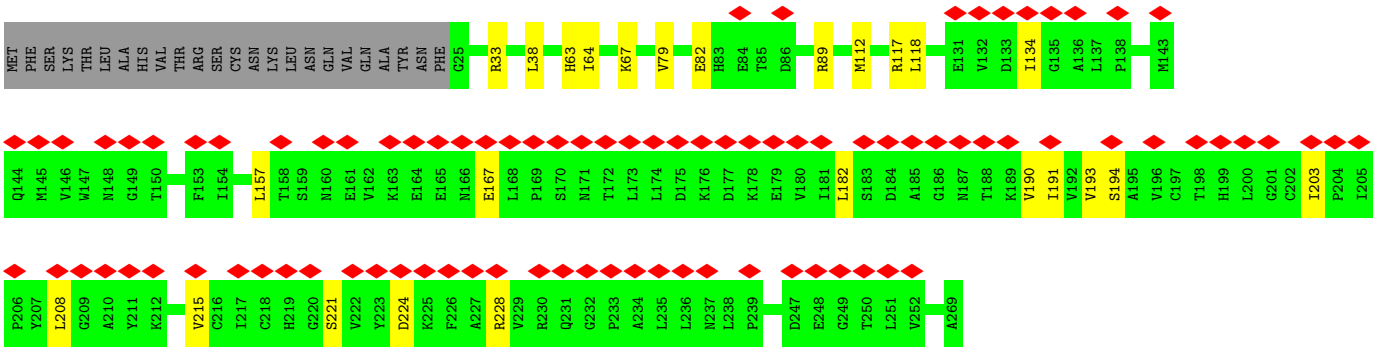
• Molecule 88: Cytochrome protein c1

Chain d:



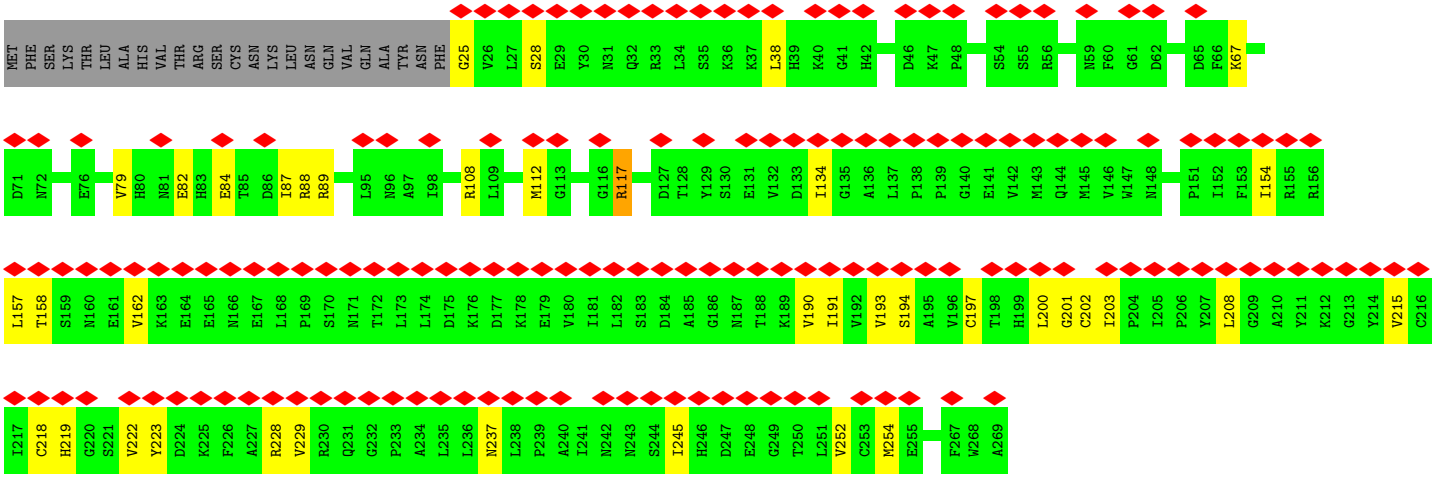
• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain E:



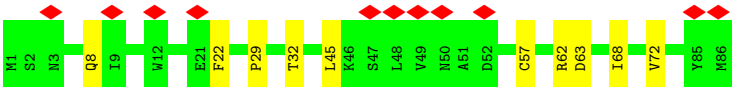
• Molecule 89: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain e:



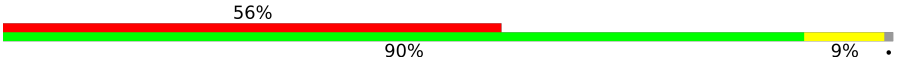
• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

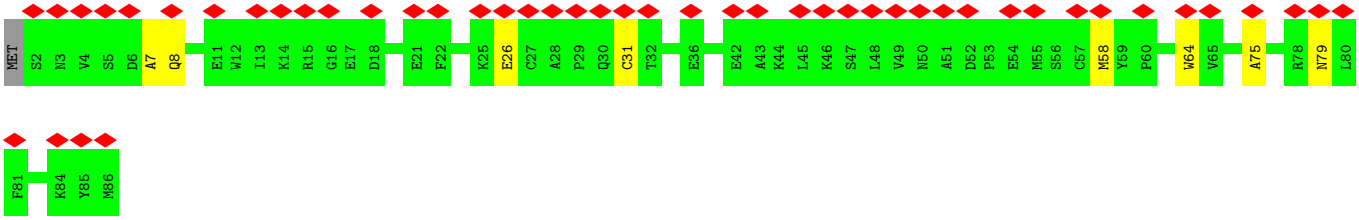
Chain F:



• Molecule 90: Ubiquinol-cytochrome C reductase hinge protein

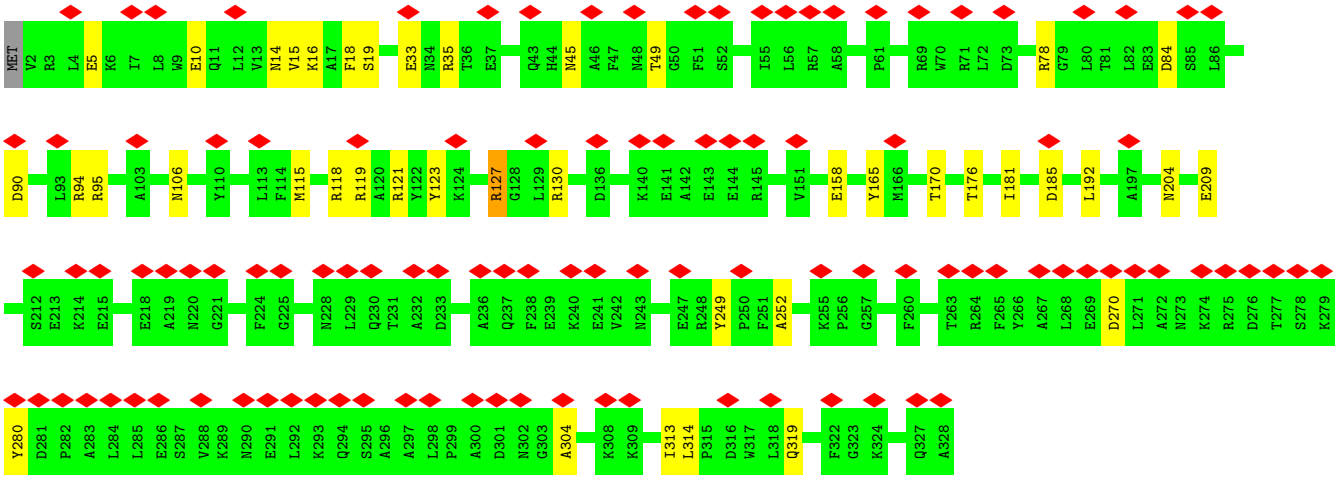
Chain f:





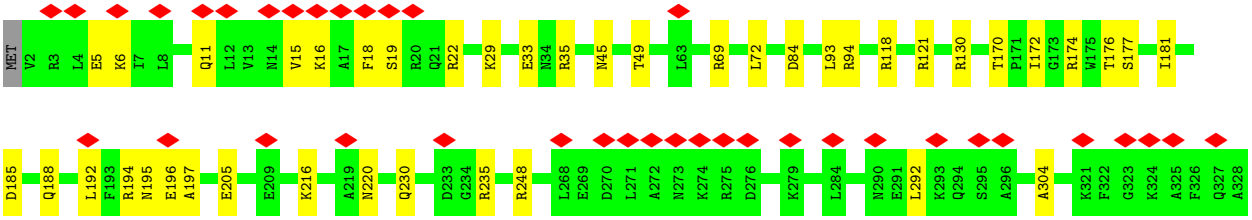
• Molecule 91: UQCRTT1

Chain G: 33% 87% 12%



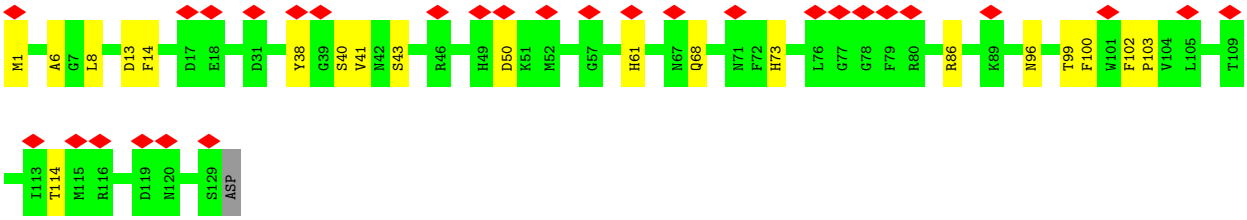
- Molecule 91: UQCRTT1

Chain g: 12% 87% 13%



- Molecule 92: Transmembrane protein, putative

Chain H: 22% 84% 15%

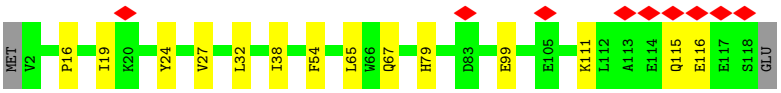


- Molecule 92: Transmembrane protein, putative

Chain h: 85% 15%

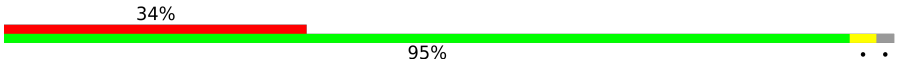
- Molecule 93: Transmembrane protein, putative

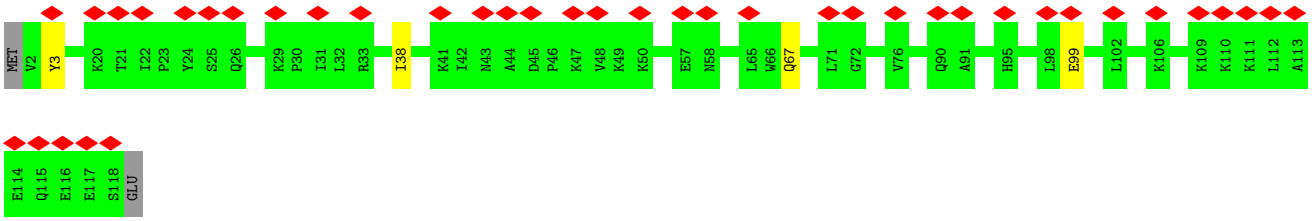
Chain I: 8% 87% 12%



• Molecule 93: Transmembrane protein, putative

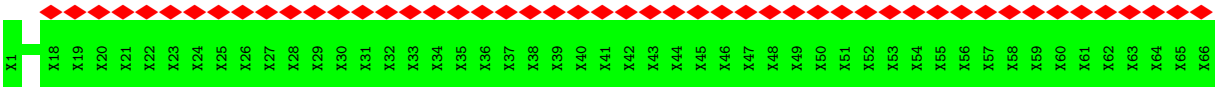
Chain i:





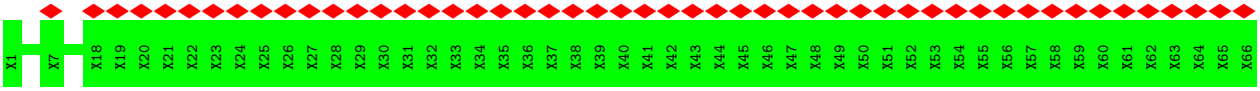
• Molecule 94: UQCRTT3

Chain J:



• Molecule 94: UQCRTT3

Chain j:

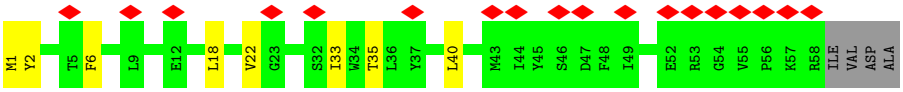


• Molecule 95: Transmembrane protein, putative

Chain K:

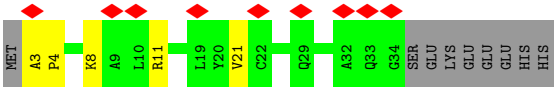
• Molecule 95: Transmembrane protein, putative

Chain k:



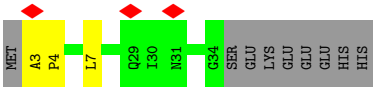
• Molecule 96: UQCRTT2

Chain L:



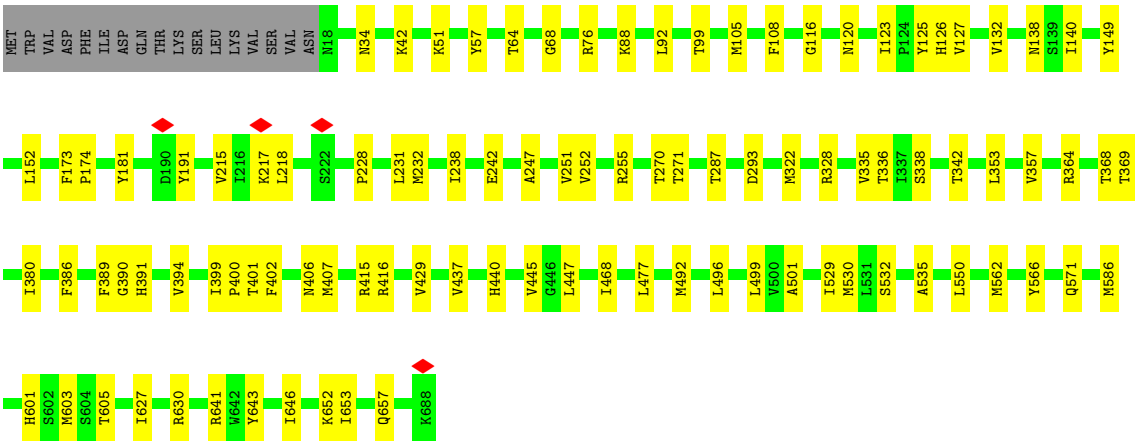
• Molecule 96: UQCRTT2

Chain l:



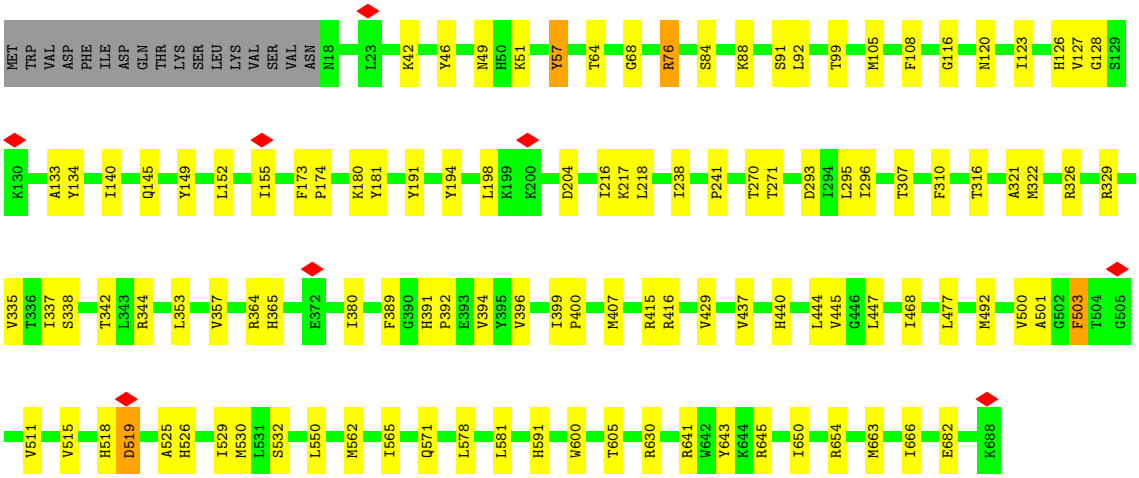
• Molecule 97: Cytochrome c oxidase subunit 1

Chain DA:



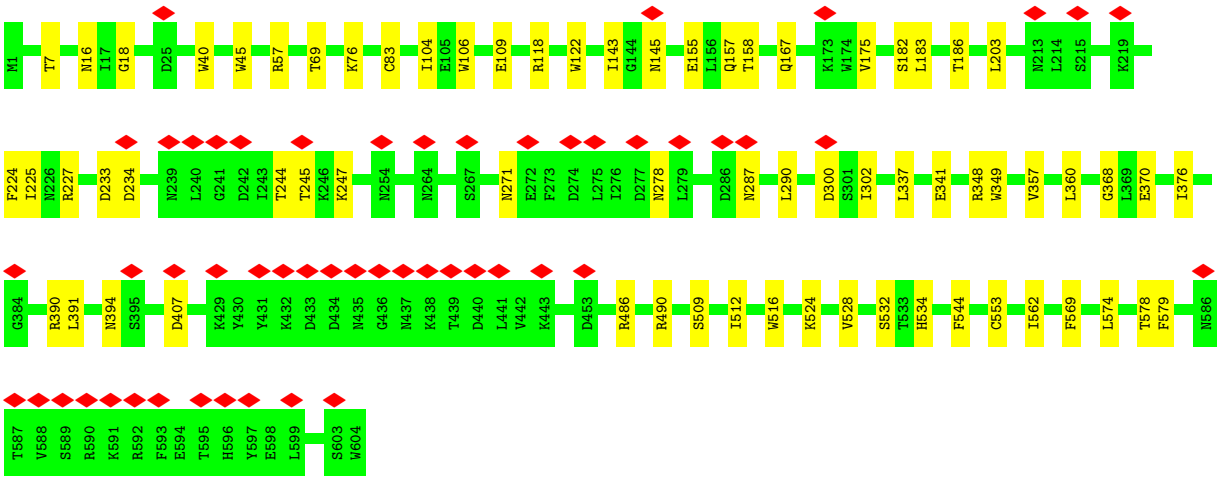
• Molecule 97: Cytochrome c oxidase subunit 1

Chain Da:



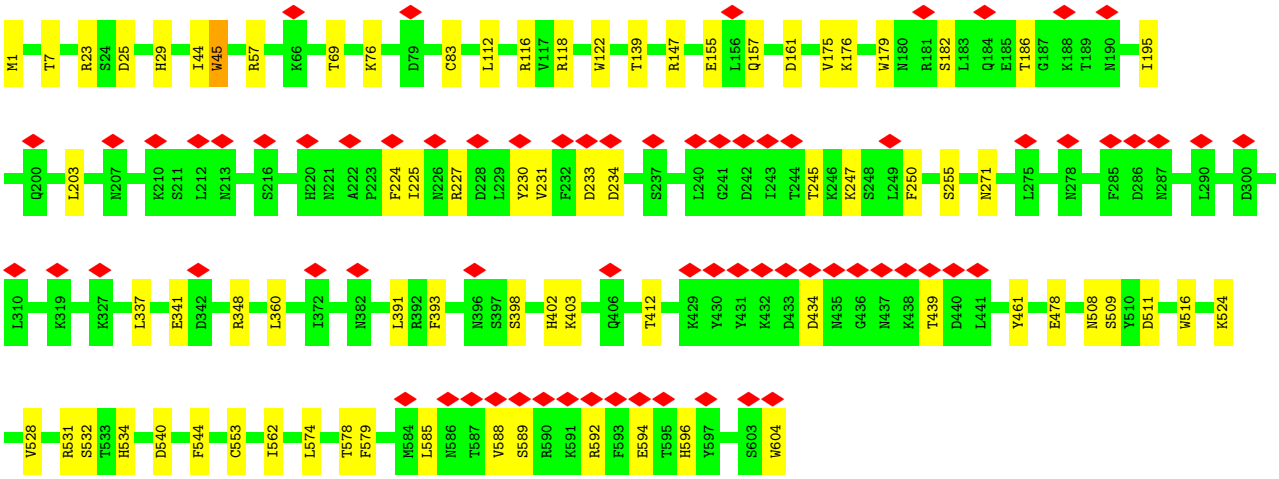
• Molecule 98: Cytochrome c oxidase subunit 2

Chain DB:



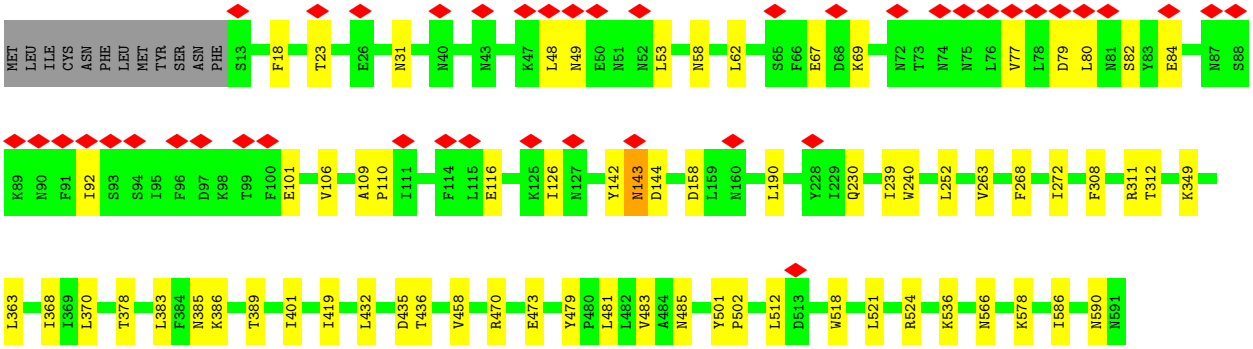
- Molecule 98: Cytochrome c oxidase subunit 2

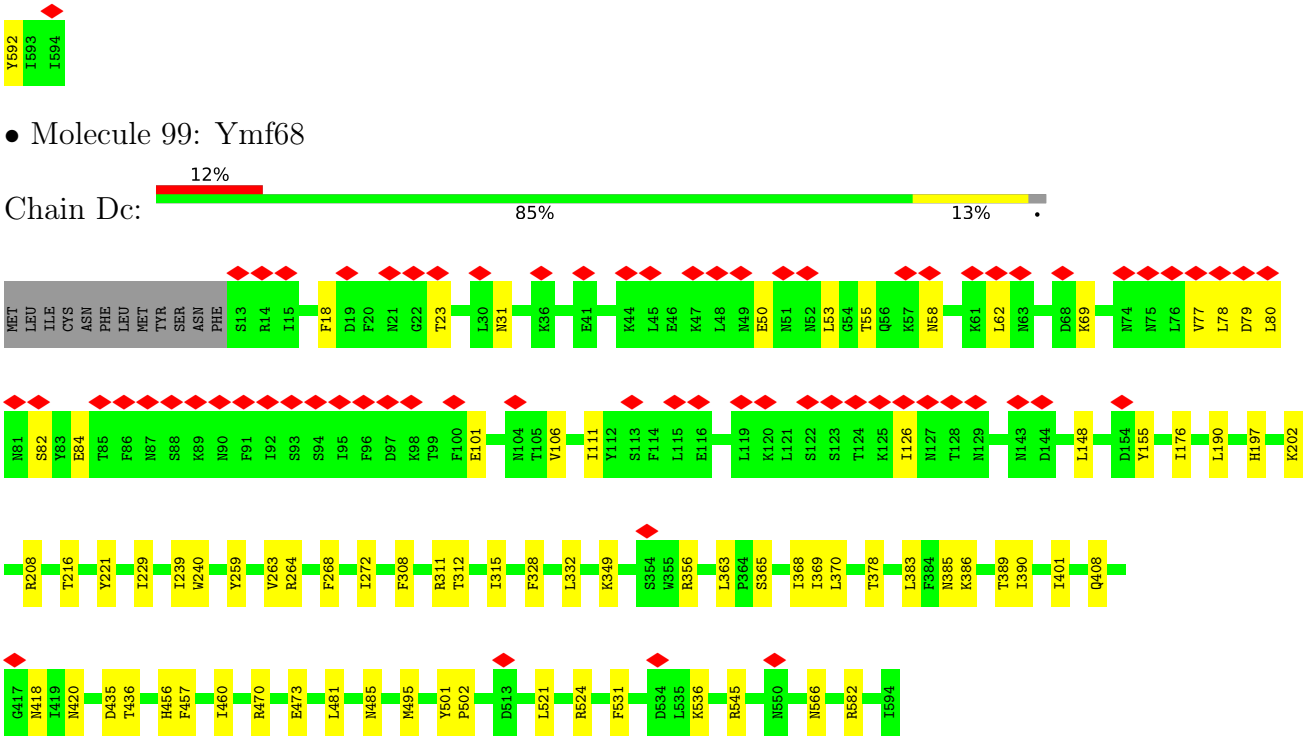
Chain Db:

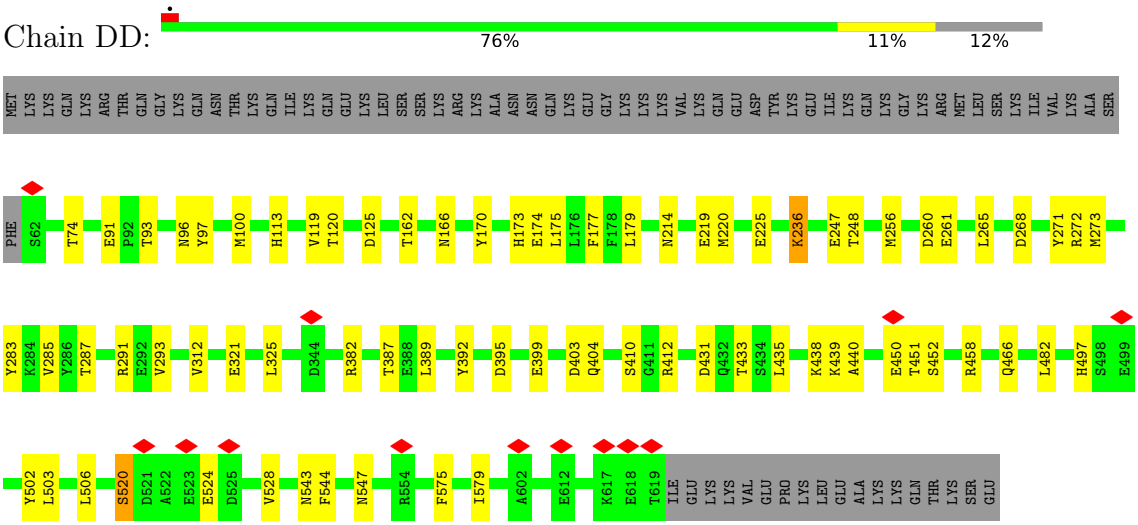


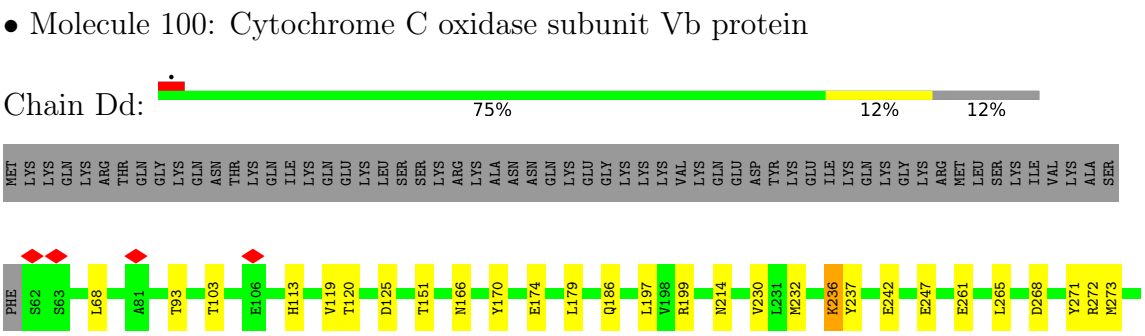
- Molecule 99: Ymf68

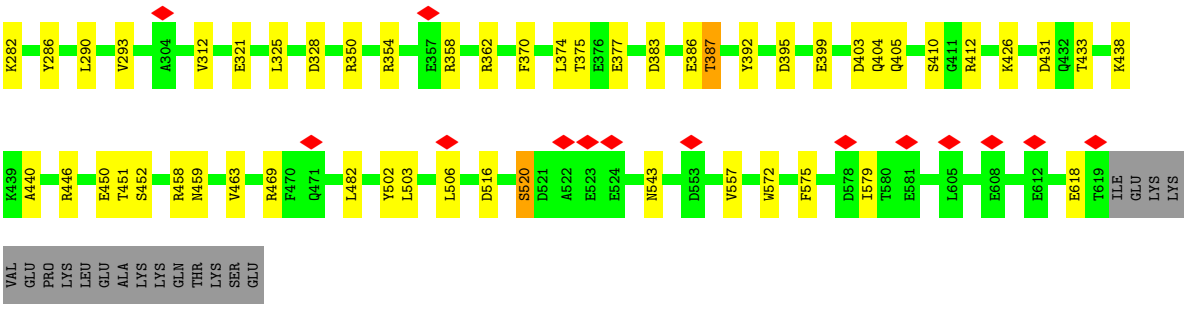
Chain DC:




Y592 I593 I594
• Molecule 99: Ymf68
Chain Dc:
12%
85%
13%
MET LEU ILE CYS ASN PHE LEU MET TYR SER ASN PHE S13 R14 I15 F18 D19 F20 N21 G22 T23 L30 N31 K36 E41 K44 L45 E46 K47 L48 N49 E50 N51 N52 L53 G54 T55 Q56 K57 N58 K61 L62 N63 D68 K69 N74 N75 L76 V77 L78 D79 L80
N81 S82 Y83 E84 T85 F86 N87 S88 K89 N90 F91 I92 S93 S94 I95 F96 D97 K98 T99 F100 E101 N104 T105 V106 I111 Y112 S113 F114 L115 E116 L119 K120 L121 S122 S123 T124 K125 I126 N127 T128 N129 N143 D144 L148 D154 Y155 I176 L190 H197 K202
R208 T216 Y221 I229 I239 W240 Y259 V263 R264 F268 I272 F308 R311 T312 I315 F328 L332 K349 S354 W355 R356 L363 F364 S365 I368 I369 L370 T378 L383 F384 N385 K386 T389 I390 I401 Q408
G417 N418 I419 N420 D435 T436 H456 F457 I460 R470 E473 L481 N485 M495 Y501 P502 D513 L521 R524 F531 D534 L535 K536 R545 N550 N566 R582 I594

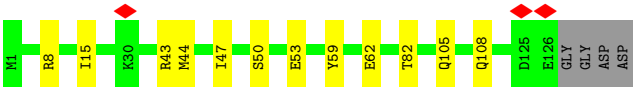

• Molecule 100: Cytochrome C oxidase subunit Vb protein
Chain DD:
76%
11%
12%
MET LYS LYS GLN LYS ARG THR GLN GLY LYS GLN ASN THR LYS GLN ILE LYS GLN GLU LYS LEU SER SER LYS ARG LYS ALA ASN ASN GLN LYS GLU GLY LYS LYS LYS VAL LYS GLN GLU ASP TYR LYS GLU ILE LYS GLN LYS GLY LYS ARG MET LEU SER LYS ILE VAL LYS ALA SER
PHE S62 T74 E91 P92 T93 N96 Y97 M100 H113 V119 T120 D125 T162 N166 Y170 H173 E174 L175 L176 F177 F178 L179 N214 E219 M220 E225 K236 E247 T248 M256 D260 E261 L265 D268 Y271 R272 M273
Y283 K284 V285 Y286 T287 R291 E292 V293 V312 E321 L325 D344 R382 T387 E388 L389 Y392 D395 E399 D403 Q404 S410 G411 R412 D431 Q432 T433 S434 L435 K438 K439 A440 E450 T451 S452 R458 Q466 L482 H497 S498 E499
Y502 L503 L506 S520 D521 A522 E523 E524 D525 V528 N543 F544 N547 R554 F575 I579 A602 E612 K617 E618 T619 ILE GLU LYS LYS VAL GLU PRO LYS LEU GLU ALA LYS LYS GLN THR LYS SER GLU


• Molecule 100: Cytochrome C oxidase subunit Vb protein
Chain Dd:
75%
12%
12%
MET LYS LYS GLN LYS ARG THR GLN GLY LYS GLN ASN THR LYS GLN ILE LYS GLN GLU LYS LEU SER SER LYS ARG LYS ALA ASN ASN GLN LYS GLU GLY LYS LYS LYS VAL LYS GLN GLU ASP TYR LYS GLU ILE LYS GLN LYS GLY LYS ARG MET LEU SER LYS ILE VAL LYS ALA SER
PHE S62 S63 L68 A81 T93 T103 E106 H113 V119 T120 D125 T151 N166 Y170 E174 L179 Q186 L197 V198 R199 N214 V230 L231 M232 K236 Y237 E242 E247 E261 L265 D268 Y271 R272 M273



- Molecule 101: Transmembrane protein, putative

Chain DE:

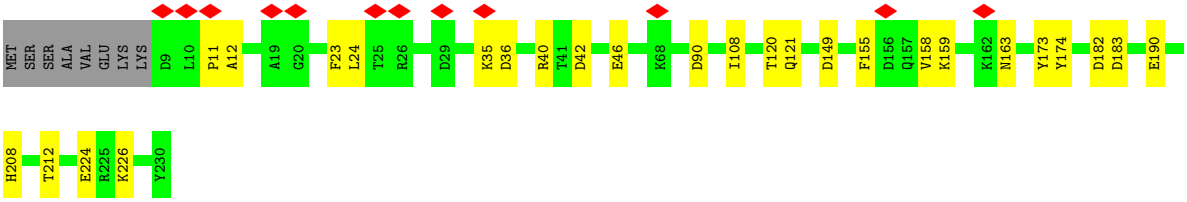


- Molecule 101: Transmembrane protein, putative

Chain De:

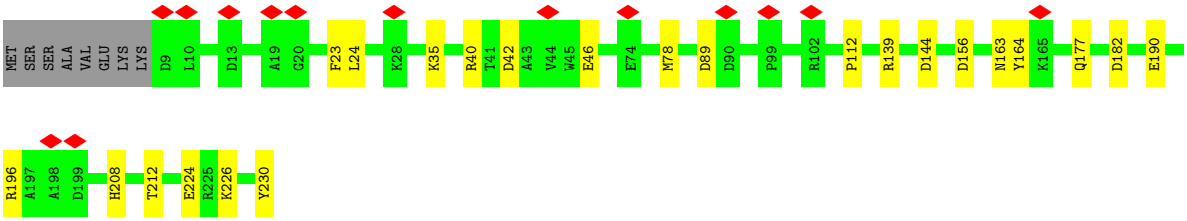
- Molecule 102: Structural protein

Chain DF:



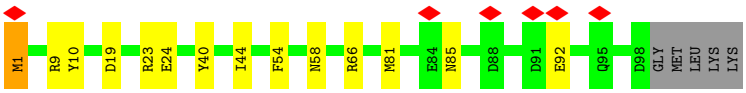
- Molecule 102: Structural protein

Chain Df:



- Molecule 103: Transmembrane protein, putative

Chain DG:

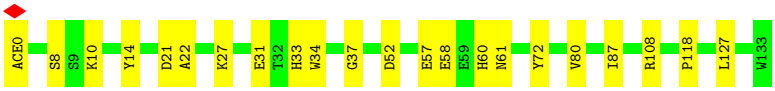


• Molecule 103: Transmembrane protein, putative

Chain Dg:

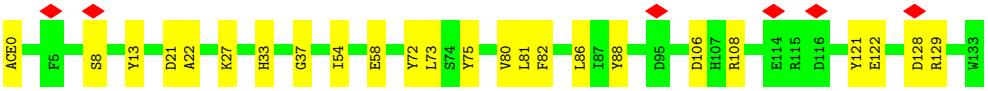
• Molecule 104: Transmembrane protein, putative

Chain DH:



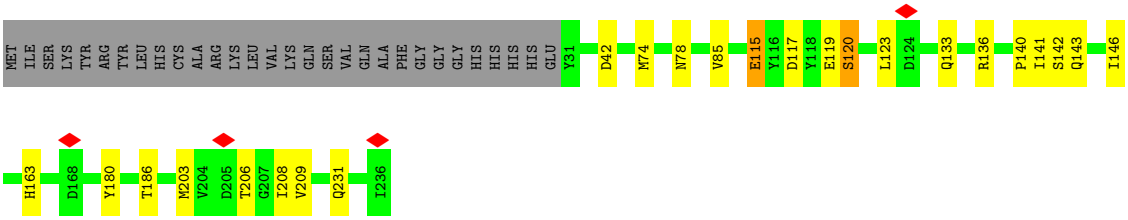
• Molecule 104: Transmembrane protein, putative

Chain Dh:



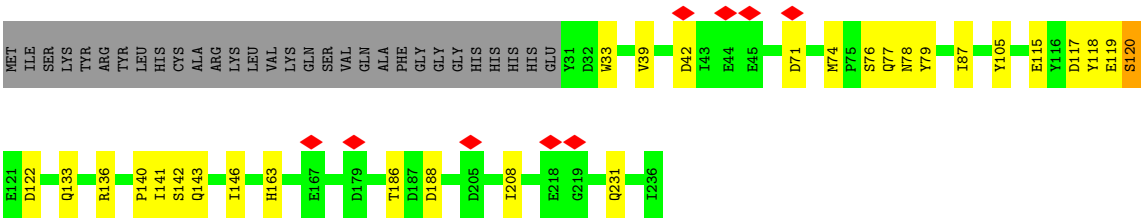
• Molecule 105: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain DI:



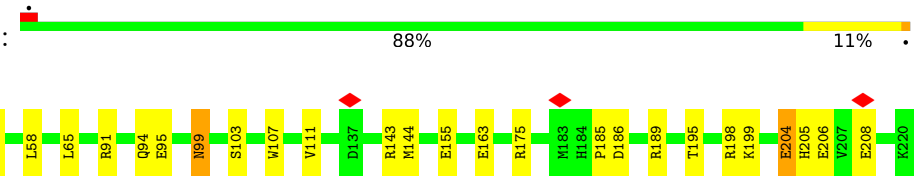
• Molecule 105: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain Di:



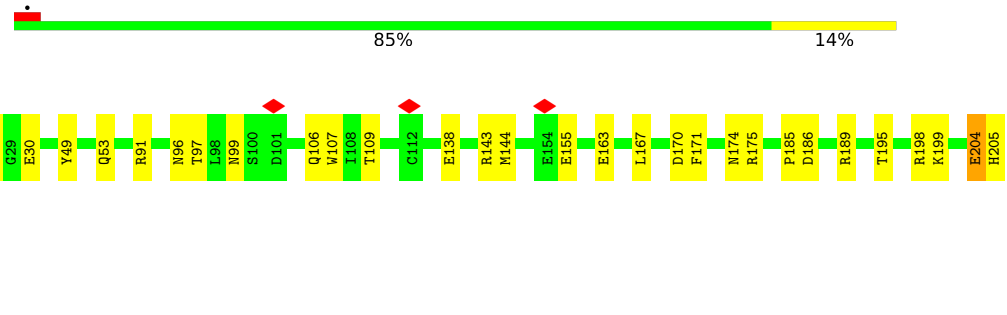
• Molecule 106: Transmembrane protein, putative

Chain DJ:



• Molecule 106: Transmembrane protein, putative

Chain Dj:



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

Chain DK:

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

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

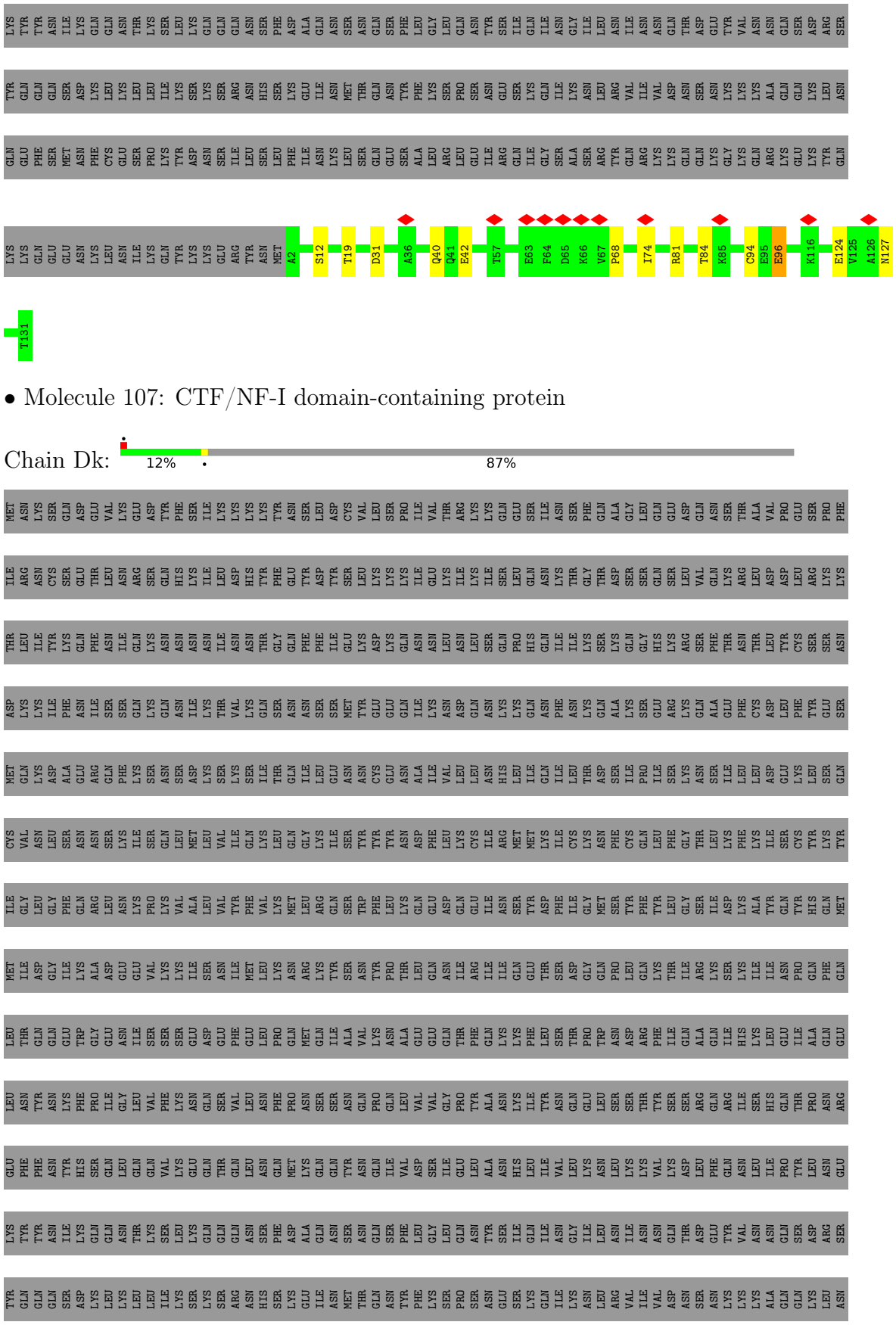
ILE GLY LEU GLY PHE GLN ARG LEU ASN LYS PRO LYS VAL ALA LEU VAL TYR PHE VAL LYS MET LEU ARG GLN SER TRP PHE LEU LYS GLN GLU ASP GLN GLU ILE ASN SER TYR ASP PHE ILE GLY MET SER TYR PHE TYR LEU GLY SER ILE ASP LYS ALA TYR GLN TYR HIS GLN MET

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

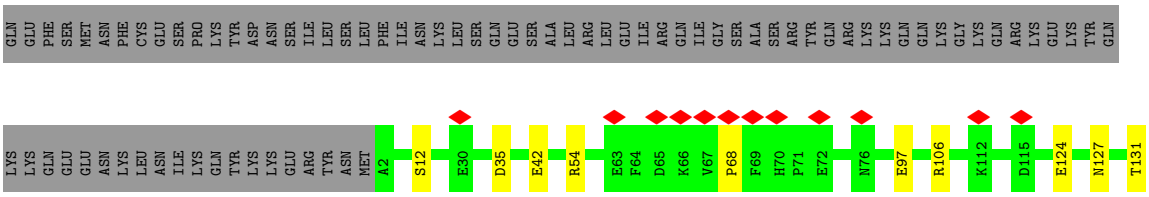
LEU ASN TYR ASN LYS PHE PRO ILE GLY LEU VAL PHE LYS ASN GLN SER VAL LEU ASN PHE PRO ASN SER SER ASN GLN PRO GLN LEU VAL VAL GLY PRO TYR ALA ASN LYS ILE TYR ASN GLN GLU LEU SER SER THR TYR SER SER ARG GLN ARG ILE SER HIS GLN THR PRO ASN ARG

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



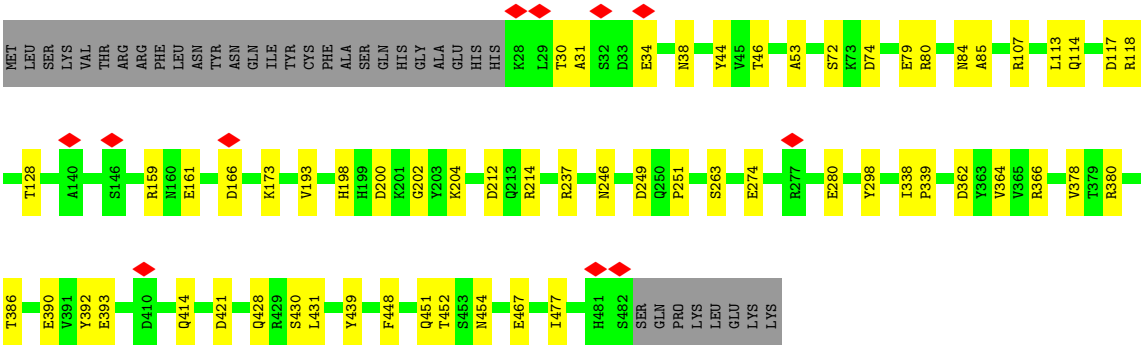
• Molecule 107: CTF/NF-I domain-containing protein

Chain Dk: 12% 87%



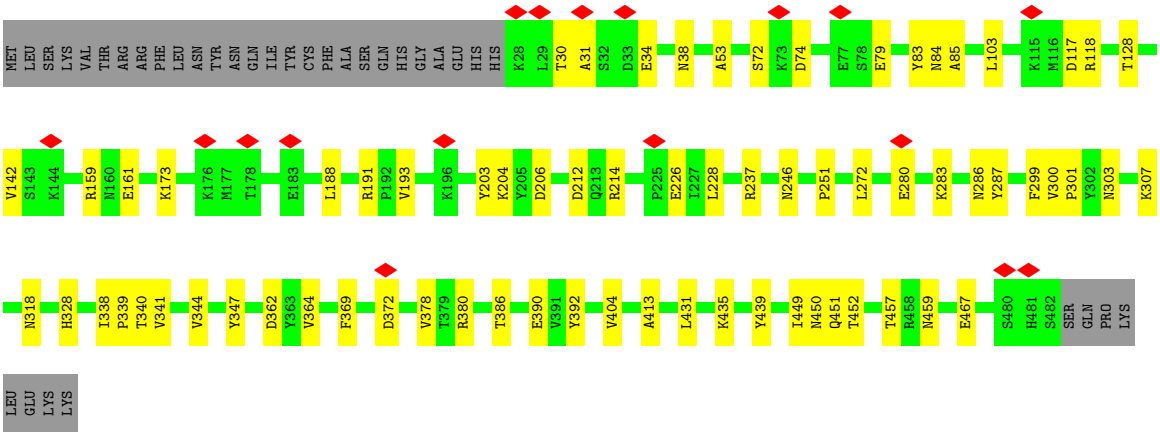
- Molecule 108: Transmembrane protein, putative

Chain DM:



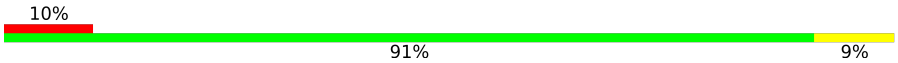
- Molecule 108: Transmembrane protein, putative

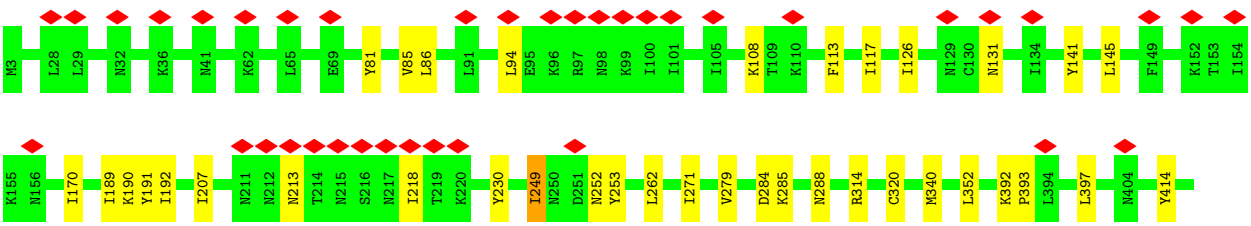
Chain Dm:

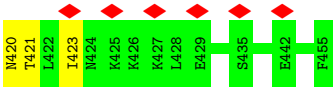


- Molecule 109: Ymf67

Chain DN:

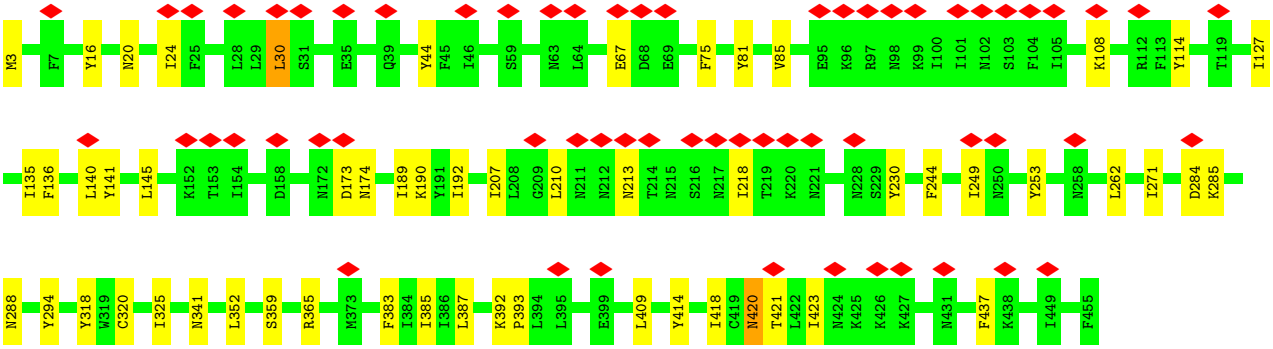






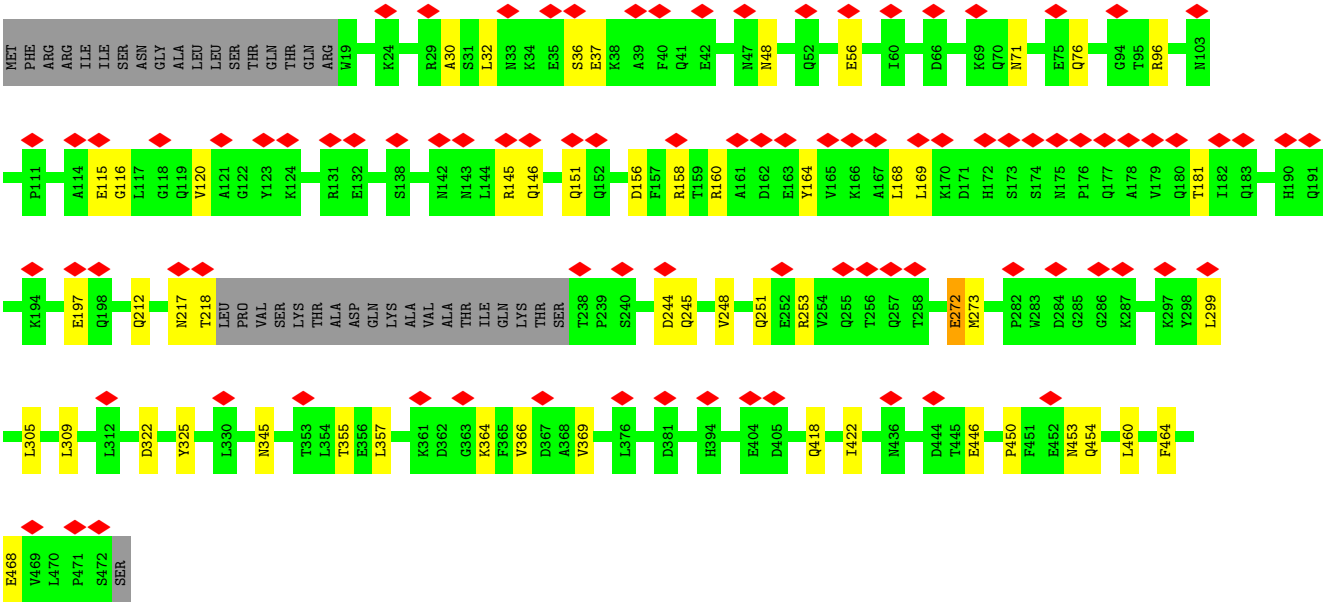
• Molecule 109: Ymf67

Chain Dn:



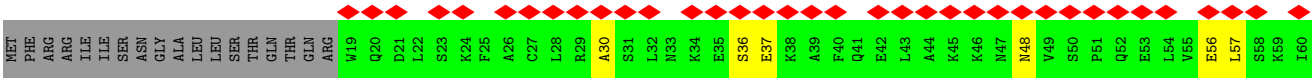
• Molecule 110: Protein phosphatase 2C, putative

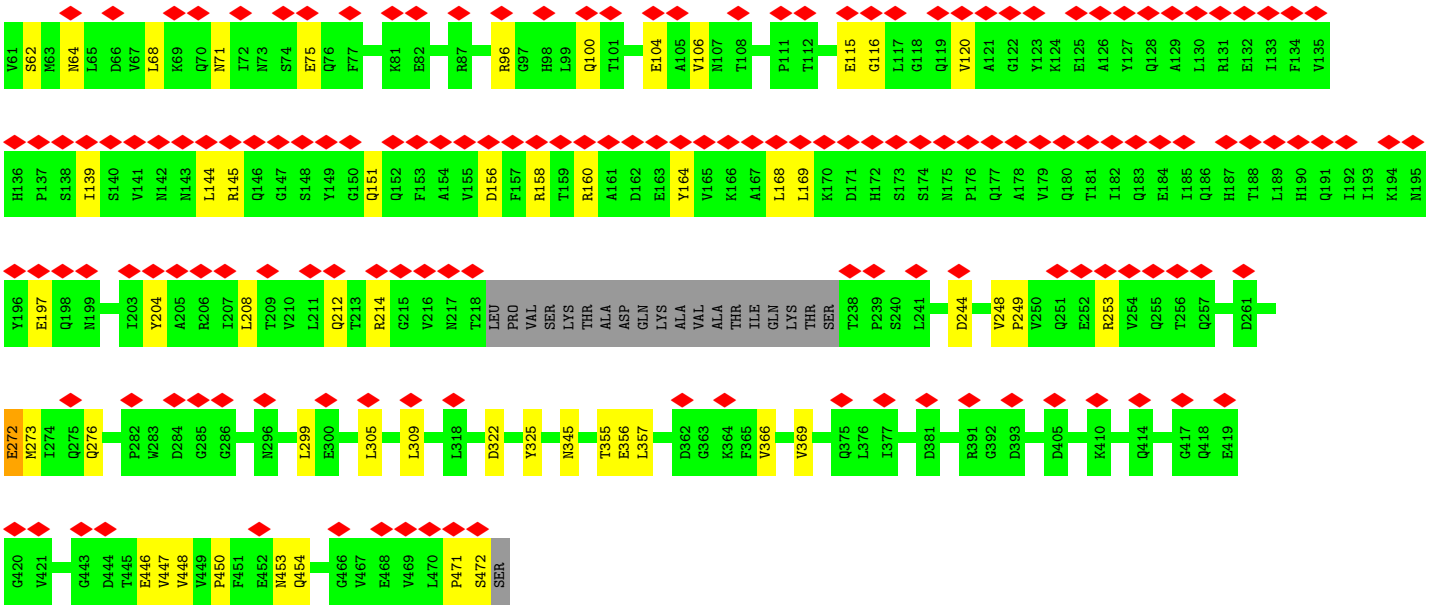
Chain DO:



• Molecule 110: Protein phosphatase 2C, putative

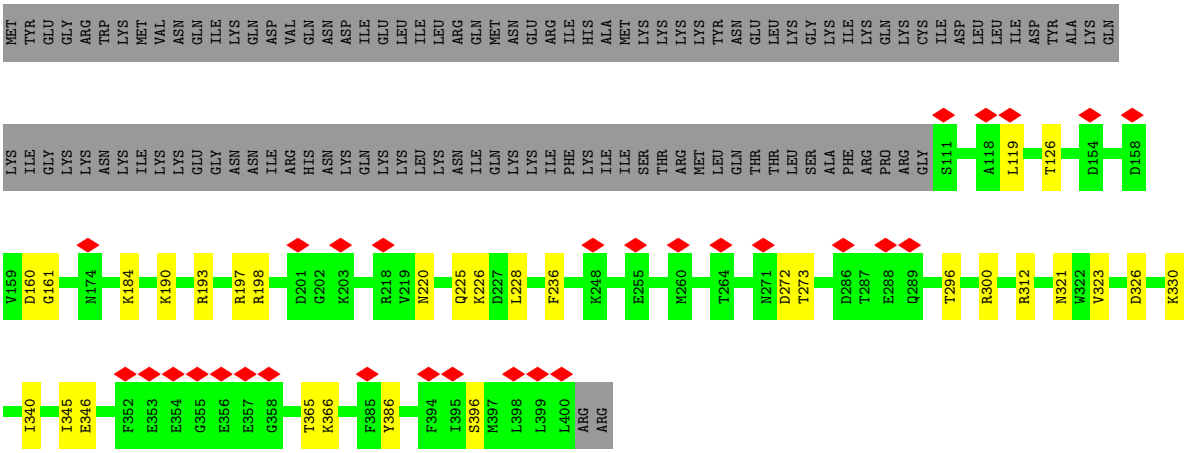
Chain Do:





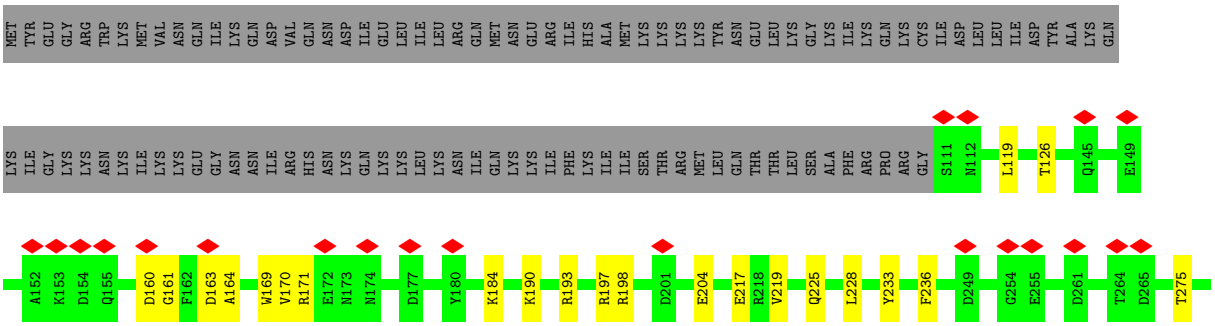
- Molecule 111: SURF1-like protein

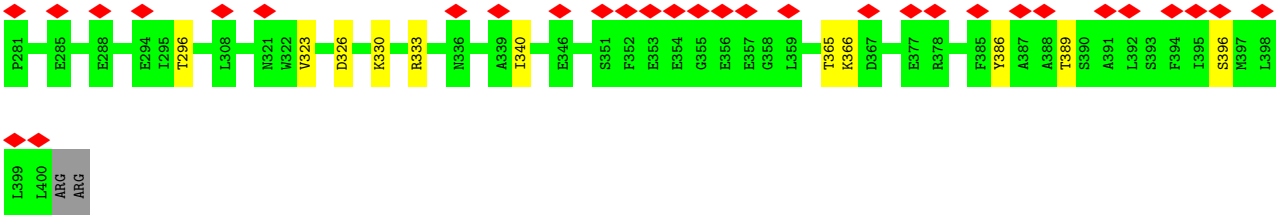
Chain DP:



- Molecule 111: SURF1-like protein

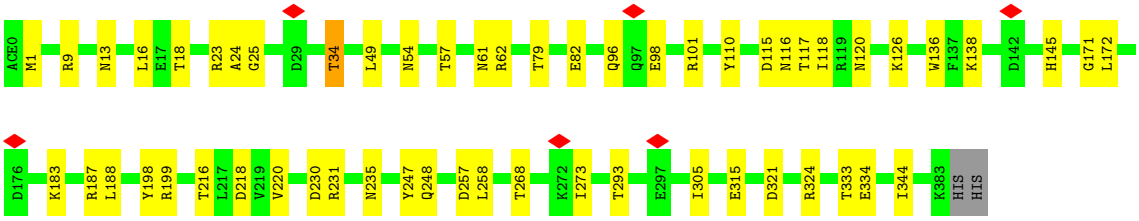
Chain Dp:





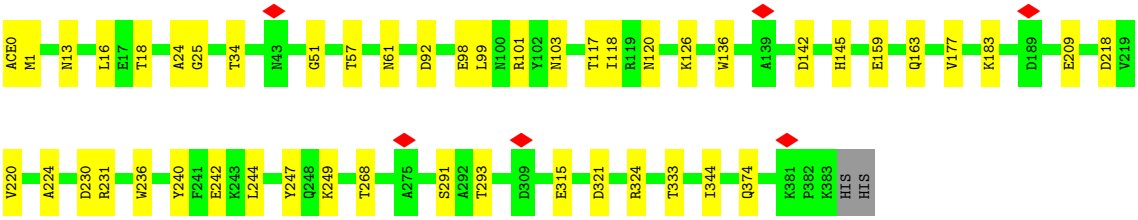
• Molecule 112: TraB family protein

Chain DQ:



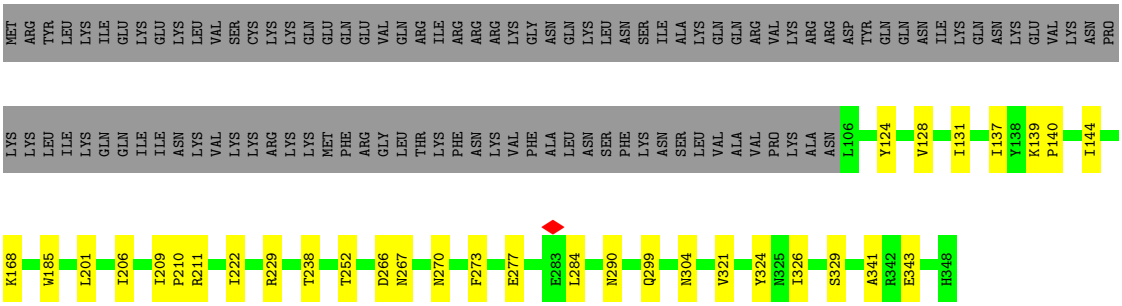
• Molecule 112: TraB family protein

Chain Dq:



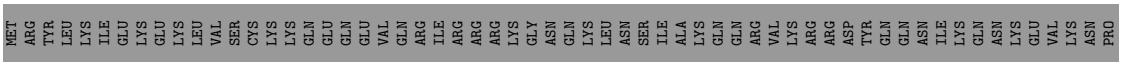
• Molecule 113: Transmembrane protein, putative

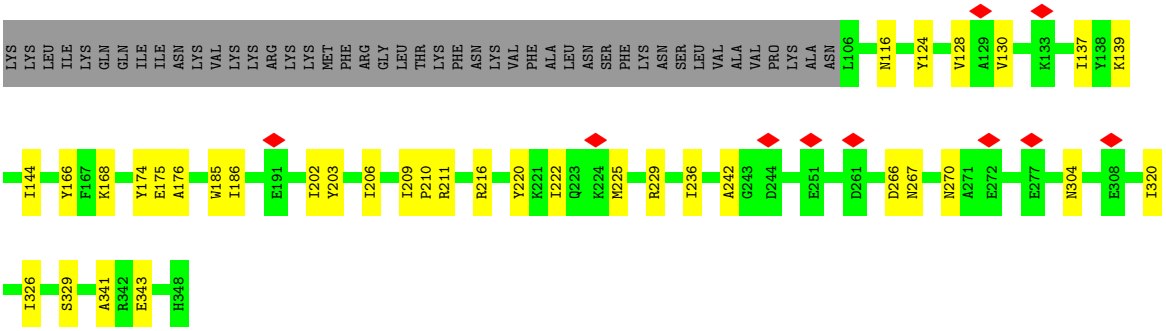
Chain DR:



• Molecule 113: Transmembrane protein, putative

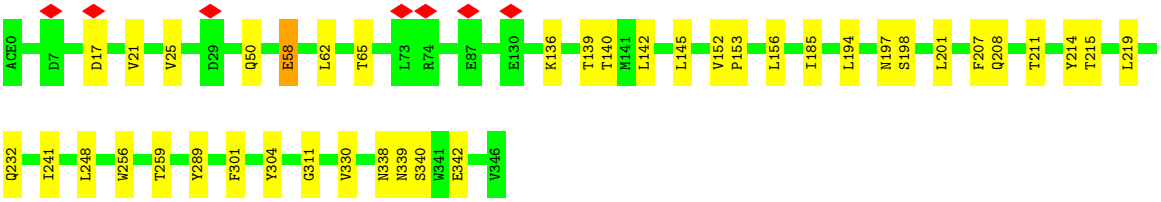
Chain Dr:





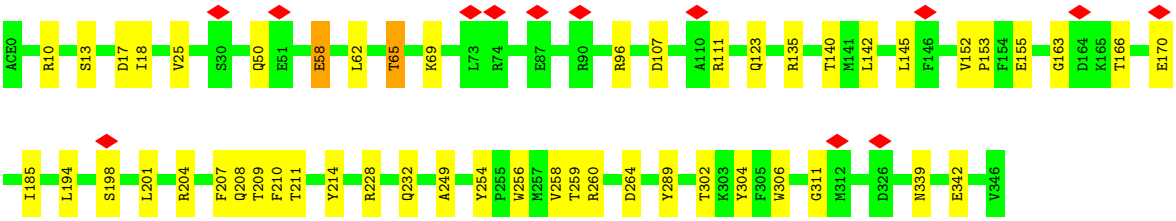
• Molecule 114: Oxoglutarate/malate translocator protein, putative

Chain DS:



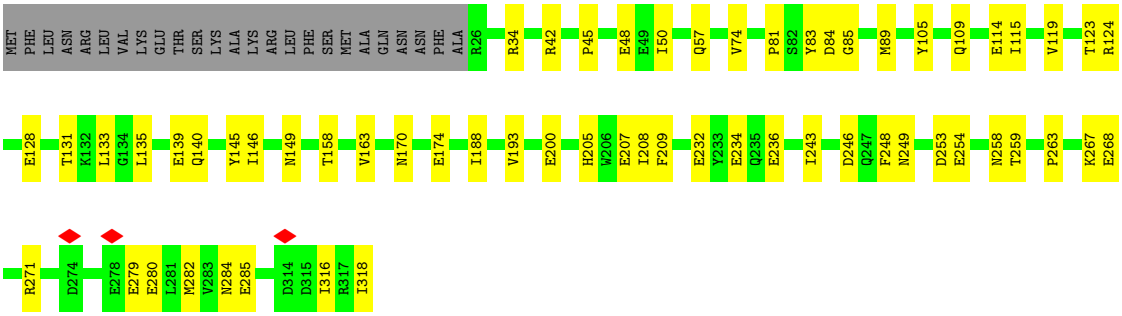
• Molecule 114: Oxoglutarate/malate translocator protein, putative

Chain Ds:



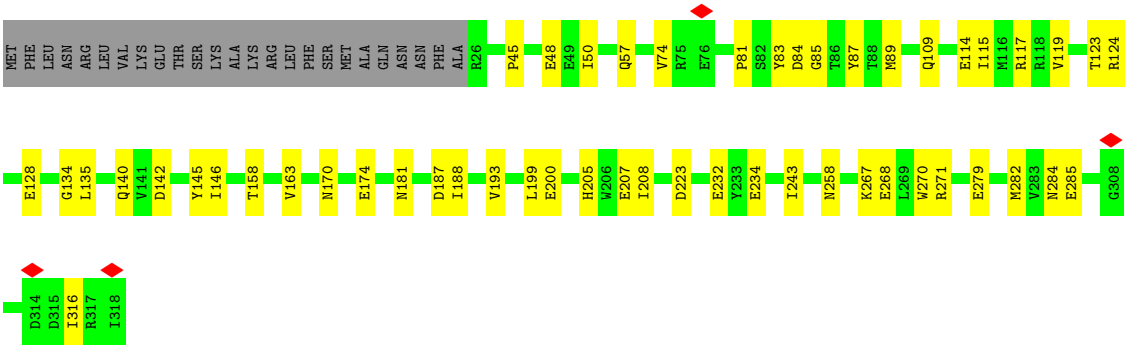
• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain DT:



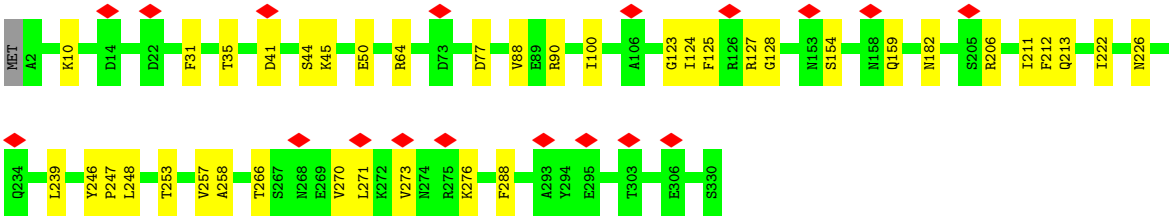
• Molecule 115: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt: 76% 16% 8%



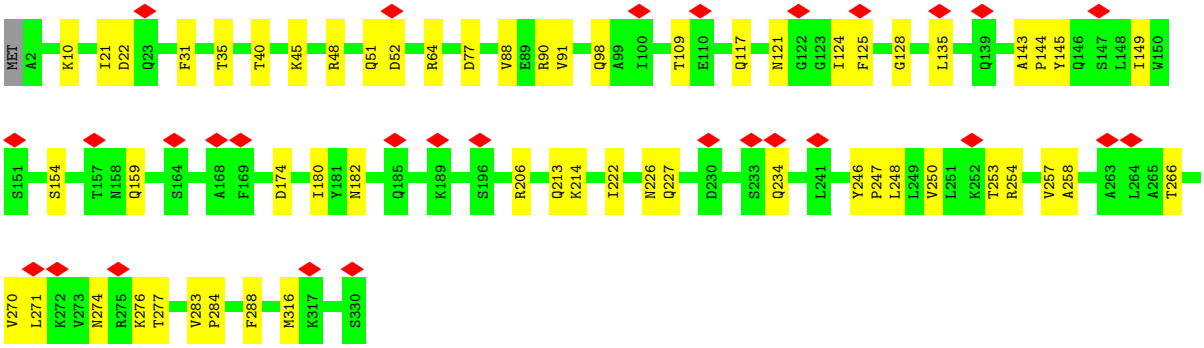
- Molecule 116: Carrier protein

Chain DU: 5% 88% 12%



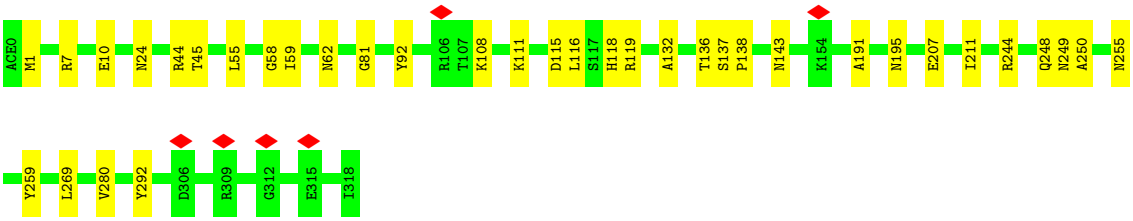
- Molecule 116: Carrier protein

Chain Du: 9% 82% 17%



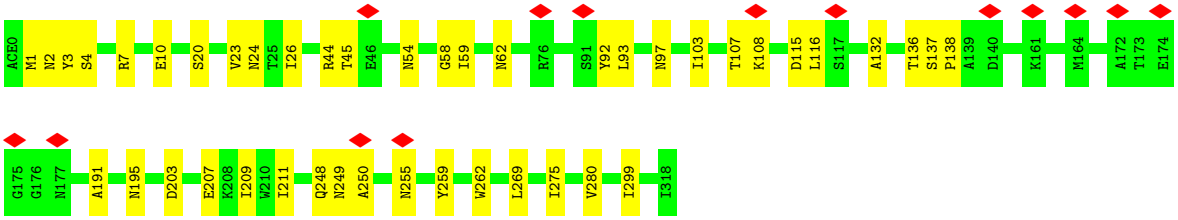
- Molecule 117: 2-oxoglutarate/malate carrier protein

Chain DV: 89% 11%



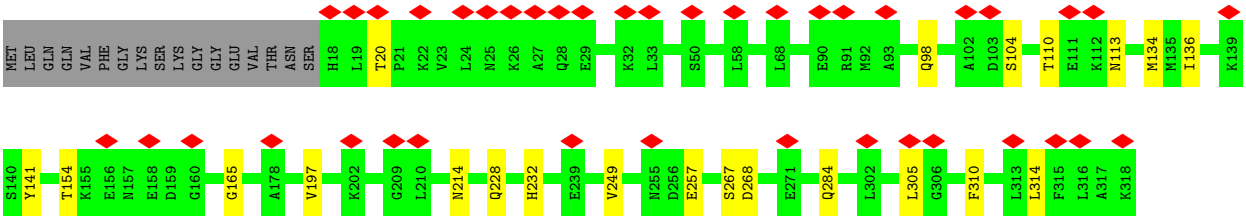
- Molecule 117: 2-oxoglutarate/malate carrier protein

Chain Dv:



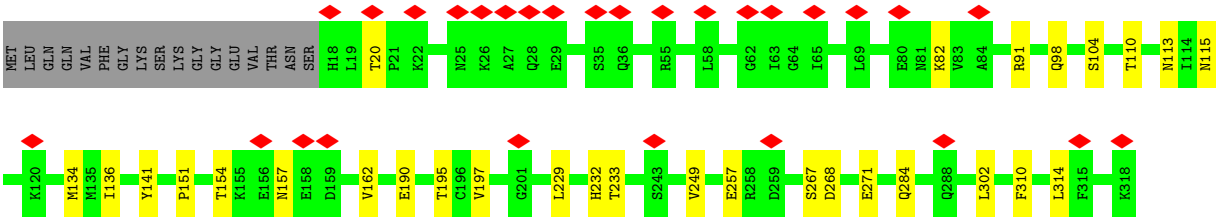
- Molecule 118: SURF1-like protein

Chain DW:



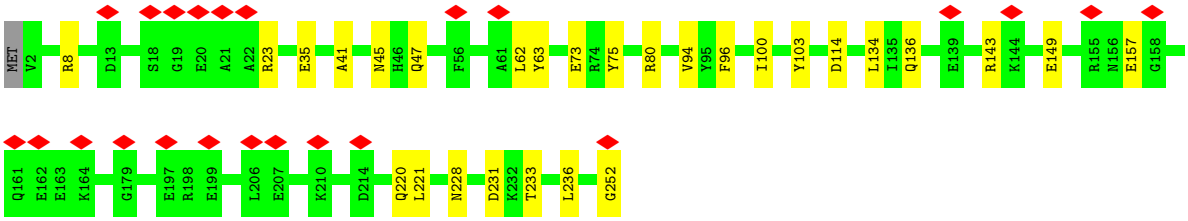
- Molecule 118: SURF1-like protein

Chain Dw:



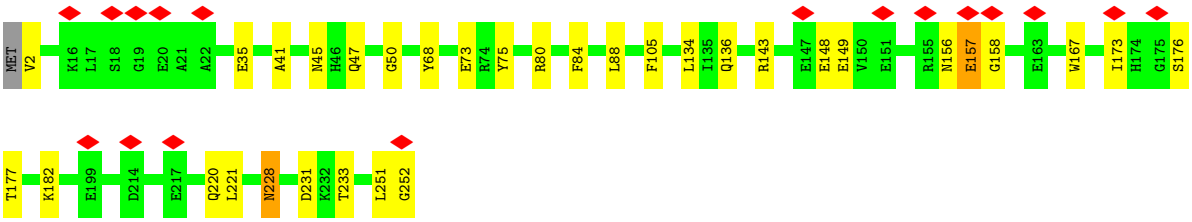
- Molecule 119: COXTT9

Chain DX:



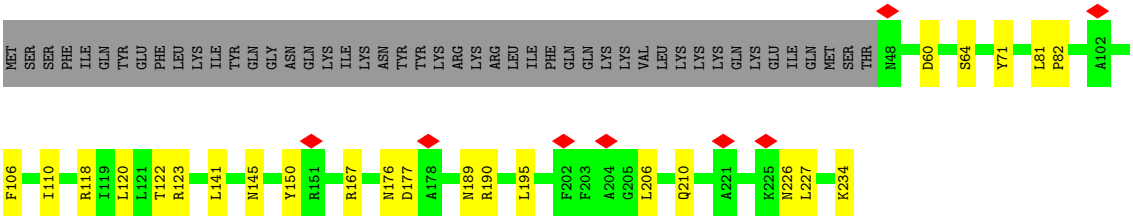
- Molecule 119: COXTT9

Chain Dx:



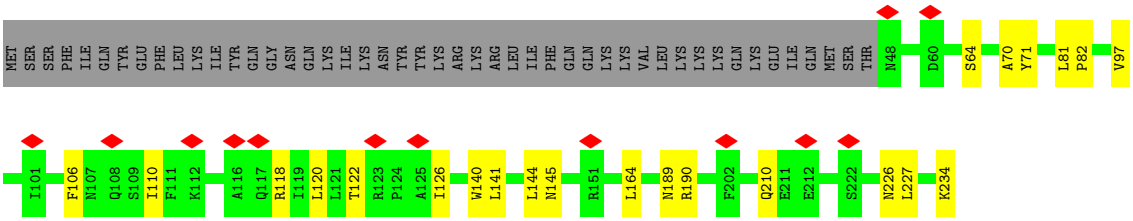
• Molecule 120: COXTT10

Chain DY:



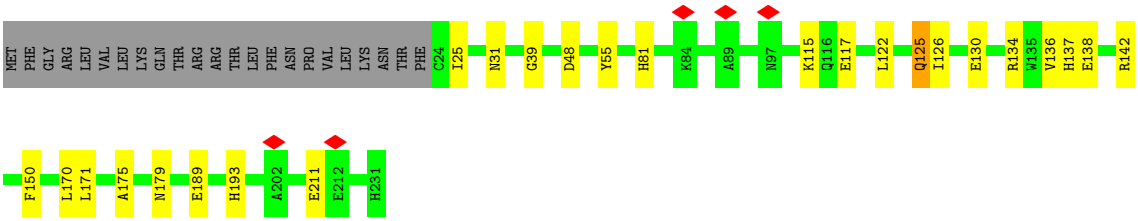
• Molecule 120: COXTT10

Chain Dy:



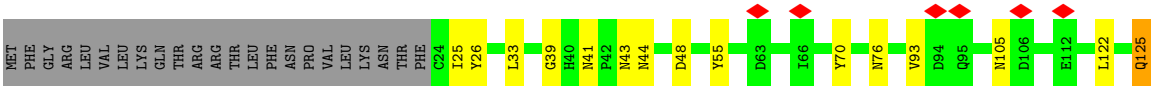
• Molecule 121: 39S ribosomal protein L9, mitochondrial

Chain DZ:



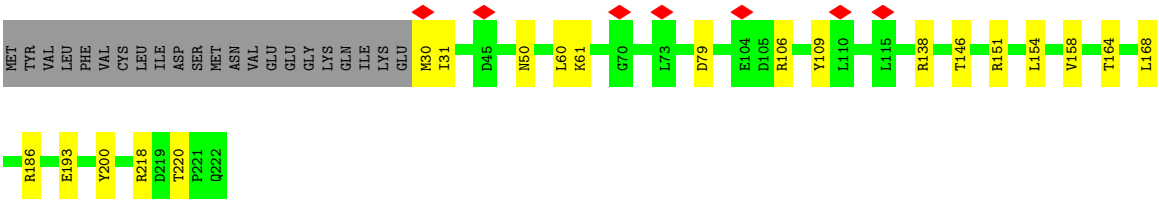
• Molecule 121: 39S ribosomal protein L9, mitochondrial

Chain Dz:



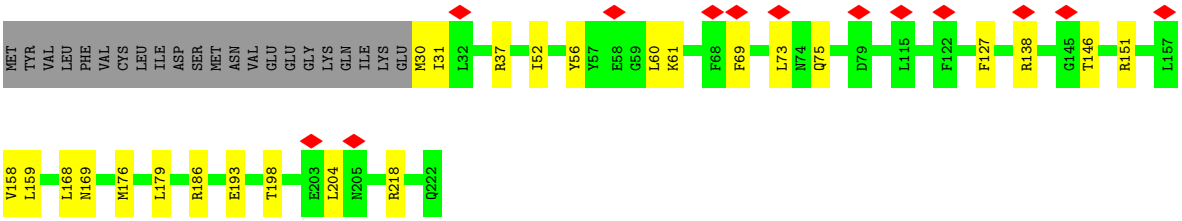
• Molecule 122: COXTT12,Transmembrane protein,Transmembrane protein,Transmembrane protein

Chain EA:



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

Chain Ea:

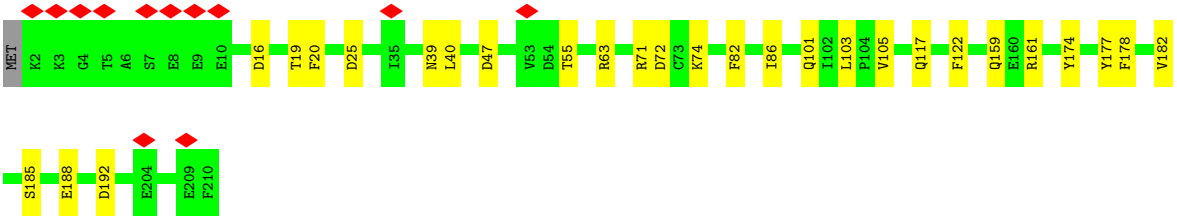


• Molecule 123: Transmembrane protein, putative

Chain EB:

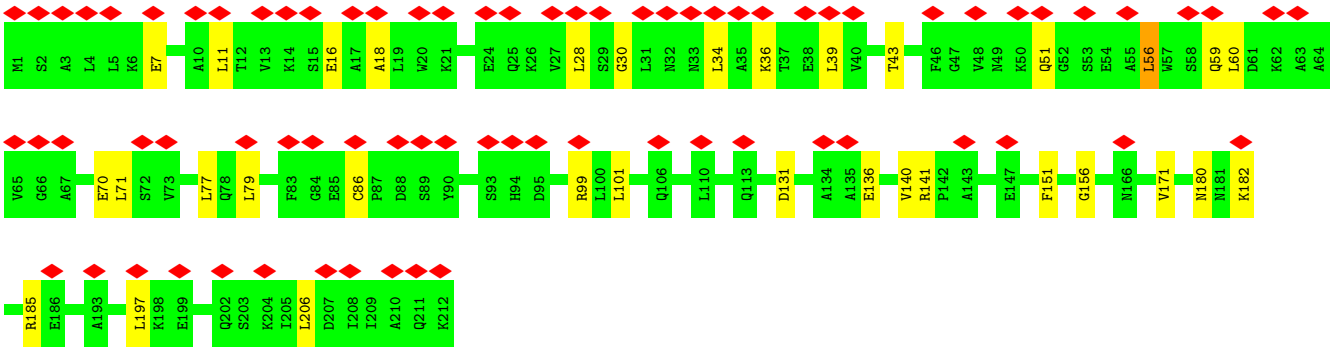
• Molecule 123: Transmembrane protein, putative

Chain Eb:



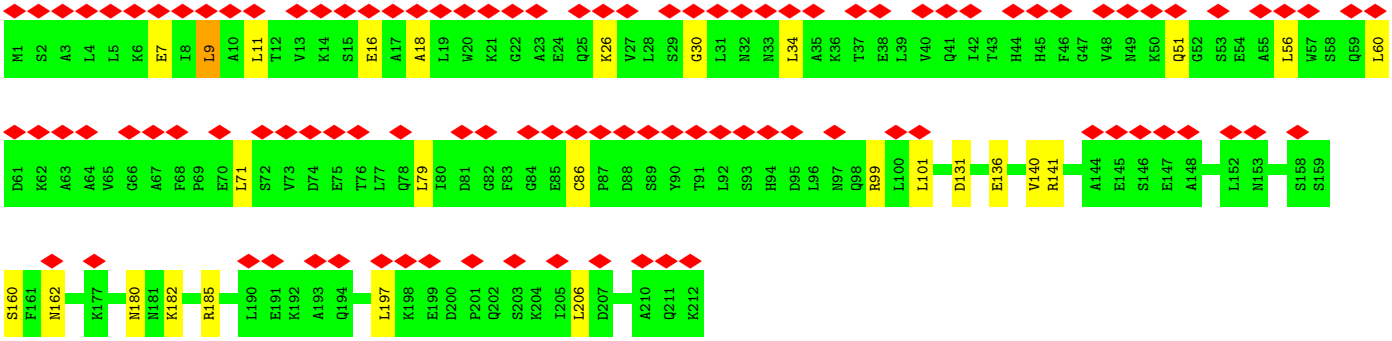
• Molecule 124: COXTT27

Chain EC:



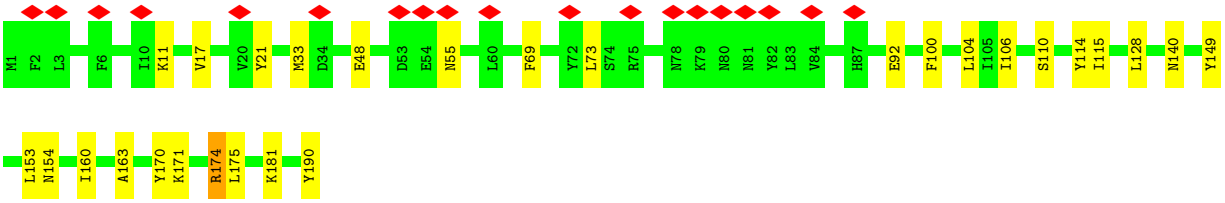
- Molecule 124: COXTT27

Chain Ec:



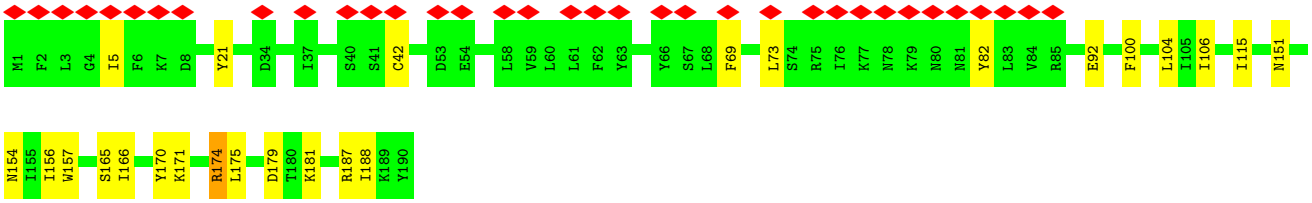
- Molecule 125: Ymf75

Chain ED:



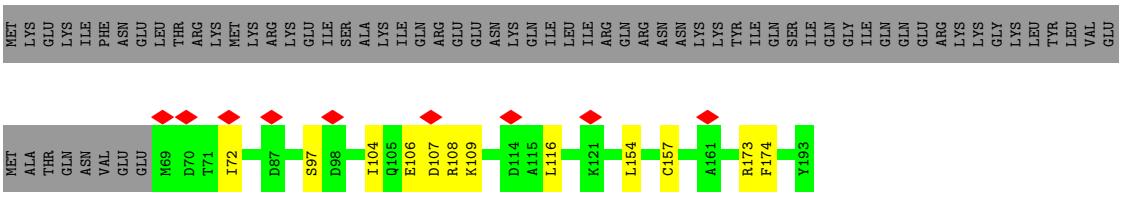
- Molecule 125: Ymf75

Chain Ed:



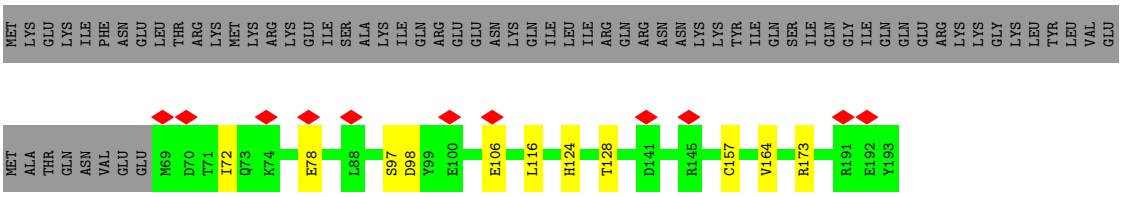
- Molecule 126: Mobilization protein

Chain EE:



• Molecule 126: Mobilization protein

Chain Ee:

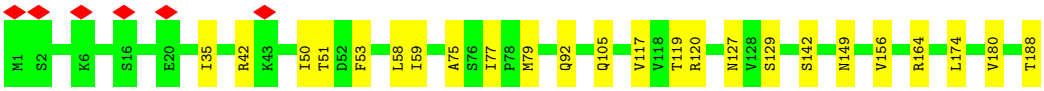


• Molecule 127: Iron-binding zinc finger CDGSH type protein

Chain EF:

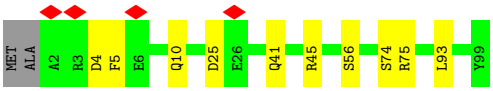
• Molecule 127: Iron-binding zinc finger CDGSH type protein

Chain Ef:



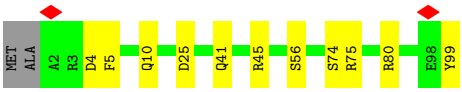
• Molecule 128: COXTT28

Chain EG:



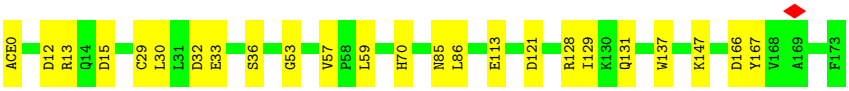
• Molecule 128: COXTT28

Chain Eg:



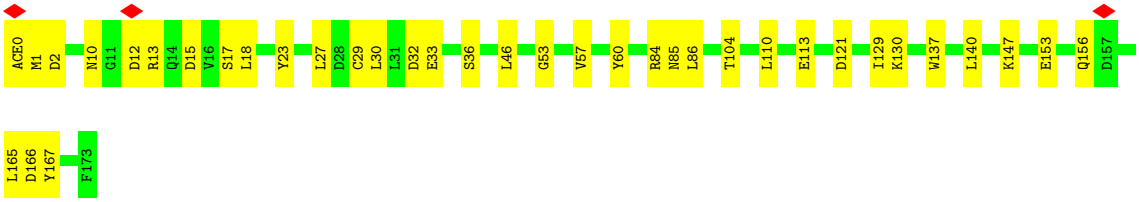
• Molecule 129: Transmembrane protein, putative

Chain EH:



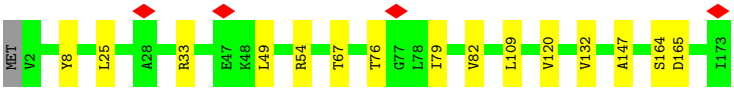
• Molecule 129: Transmembrane protein, putative

Chain Eh:



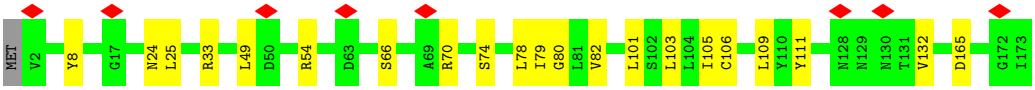
• Molecule 130: Transmembrane protein

Chain EI:



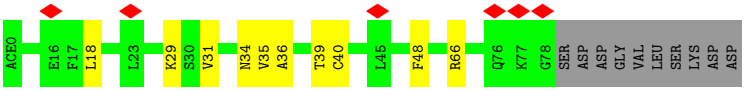
• Molecule 130: Transmembrane protein

Chain Ei:



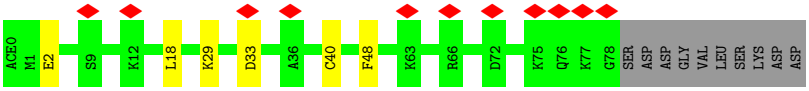
• Molecule 131: Decapping nuclease

Chain EV:



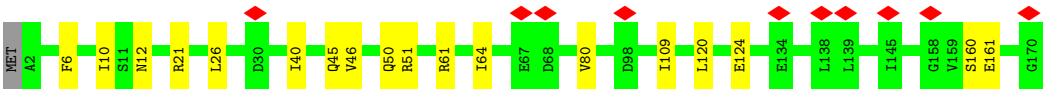
• Molecule 131: Decapping nuclease

Chain Ev:



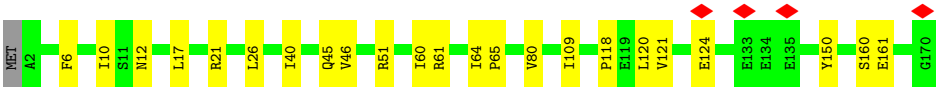
• Molecule 132: Complex III subunit VII

Chain EK:



• Molecule 132: Complex III subunit VII

Chain Ek:

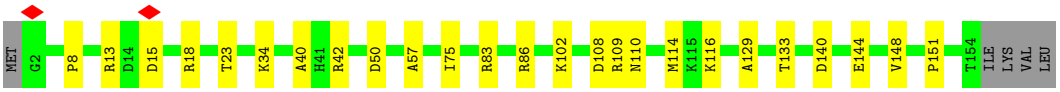


• Molecule 133: Transmembrane protein, putative

Chain EL:

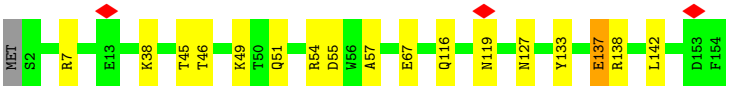
• Molecule 133: Transmembrane protein, putative

Chain El:



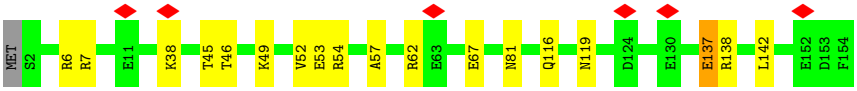
• Molecule 134: Transmembrane protein, putative

Chain EM:



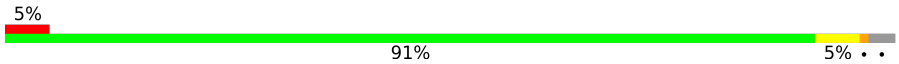
• Molecule 134: Transmembrane protein, putative

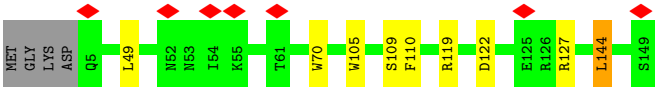
Chain Em:



• Molecule 135: COXTT22

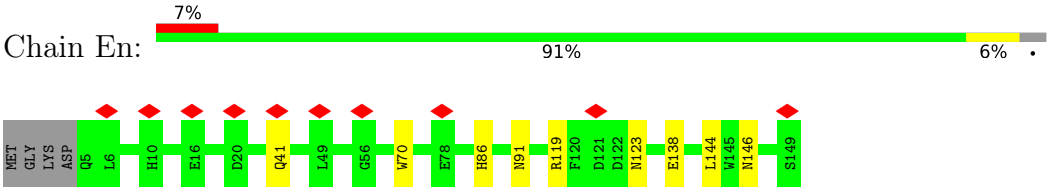
Chain EN:





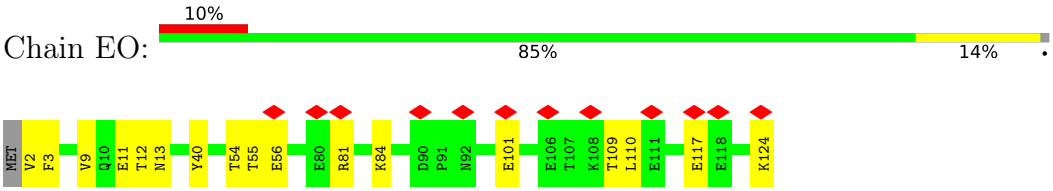
• Molecule 135: COXTT22

Chain En:



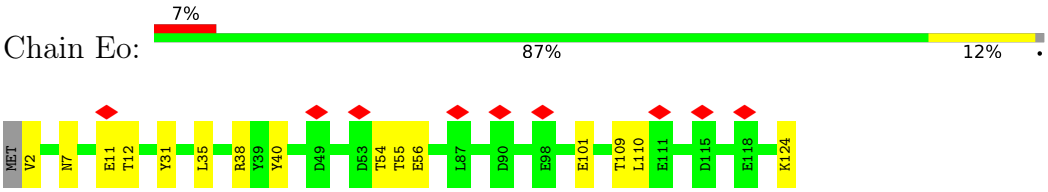
• Molecule 136: Transmembrane protein, putative

Chain EO:



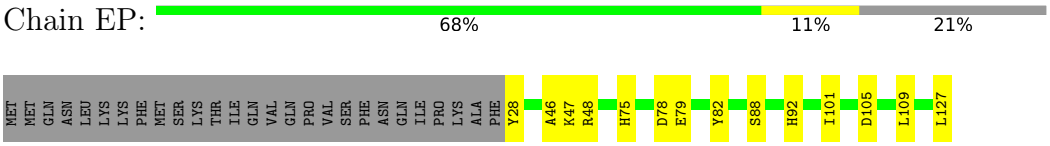
• Molecule 136: Transmembrane protein, putative

Chain Eo:



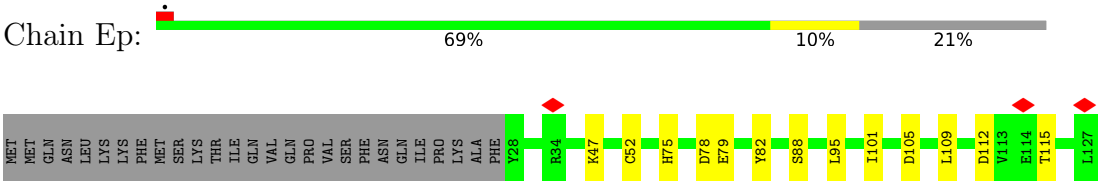
• Molecule 137: Phage protein

Chain EP:



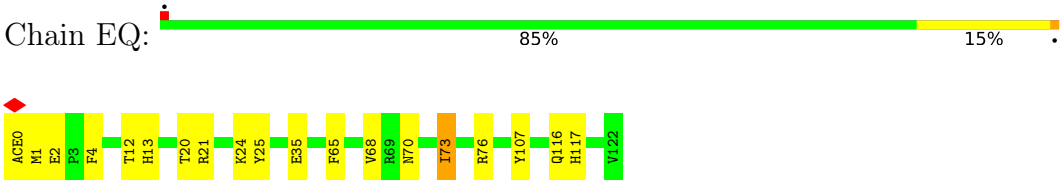
• Molecule 137: Phage protein

Chain Ep:



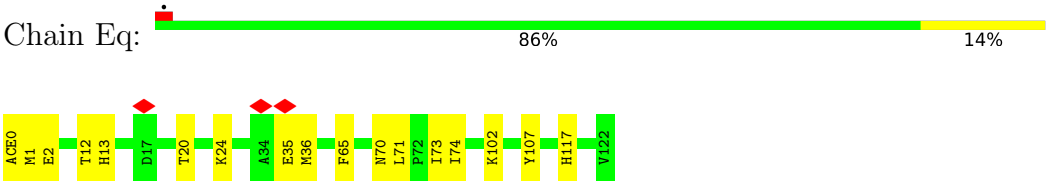
• Molecule 138: Transmembrane protein, putative

Chain EQ:



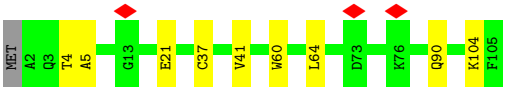
• Molecule 138: Transmembrane protein, putative

Chain Eq:



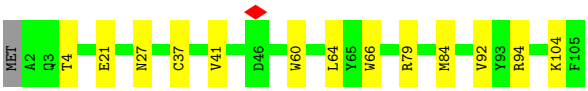
- Molecule 139: Lysozyme

Chain ER:



- Molecule 139: Lysozyme

Chain Er:

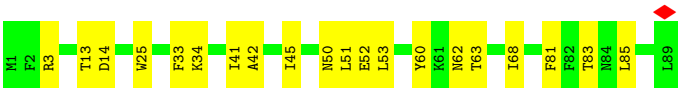


- Molecule 140: Ymf70

Chain ES:

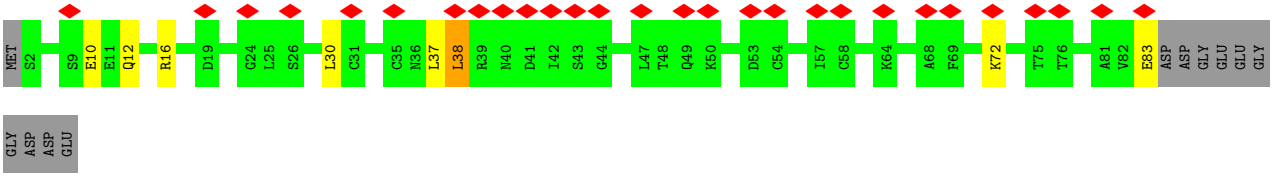
- Molecule 140: Ymf70

Chain Es:



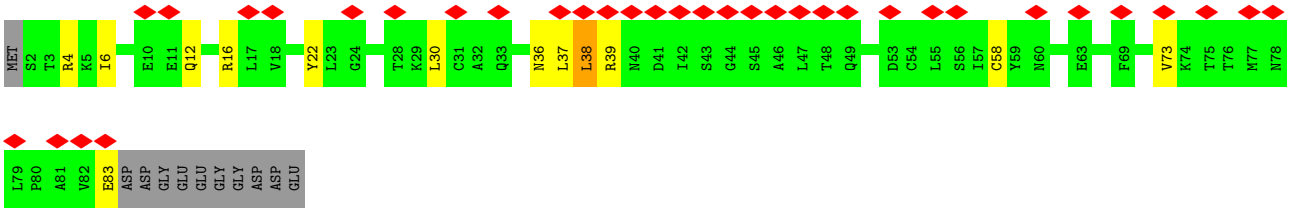
- Molecule 141: Zf-Tim10_DDP domain-containing protein

Chain ET:



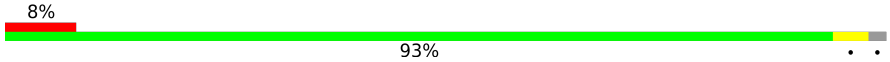
- Molecule 141: Zf-Tim10_DDP domain-containing protein

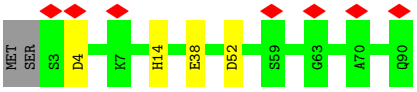
Chain Et:



• Molecule 142: ABC transporter

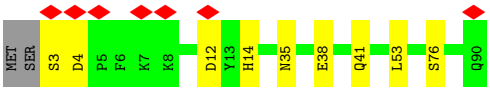
Chain EU:





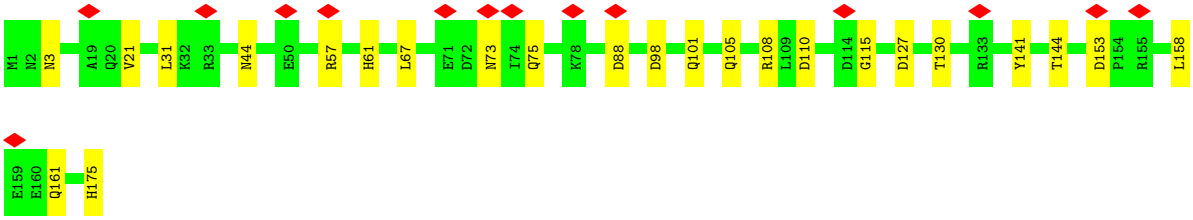
• Molecule 142: ABC transporter

Chain Eu:



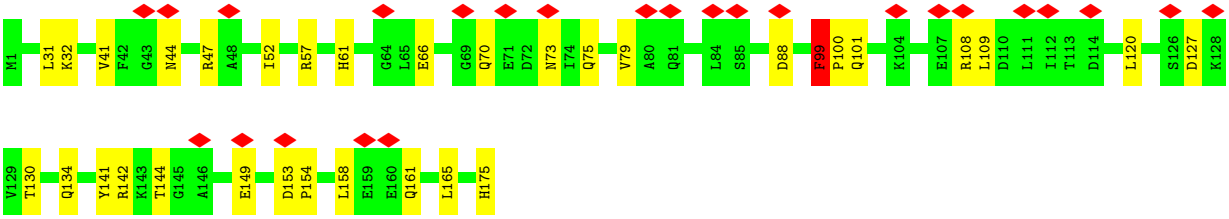
• Molecule 143: YflT domain-containing protein

Chain EJ:



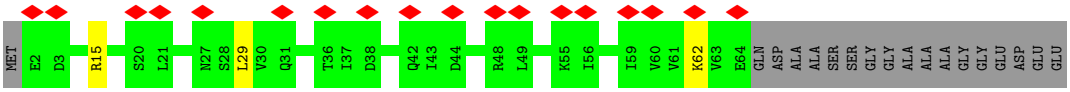
• Molecule 143: YflT domain-containing protein

Chain Ej:



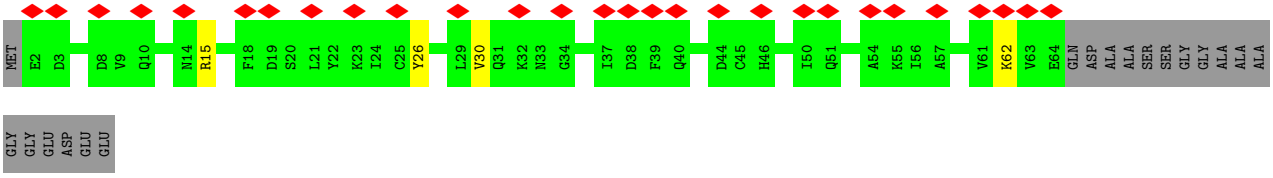
• Molecule 144: Cullin domain-containing protein

Chain EW:



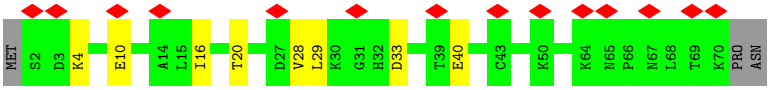
• Molecule 144: Cullin domain-containing protein

Chain Ew:



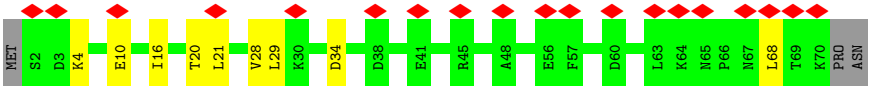
- Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain EX:



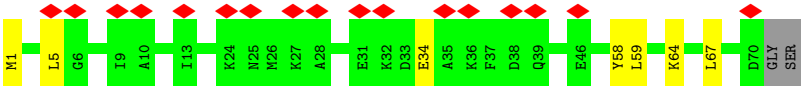
- Molecule 145: Zf-Tim10_DDP domain-containing protein

Chain Ex:



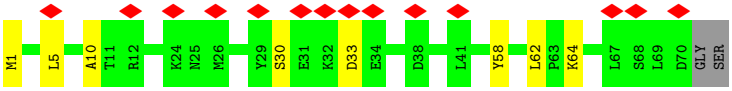
- Molecule 146: Annexin

Chain EY:



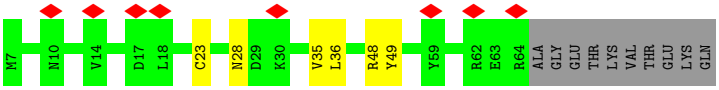
- Molecule 146: Annexin

Chain Ey:



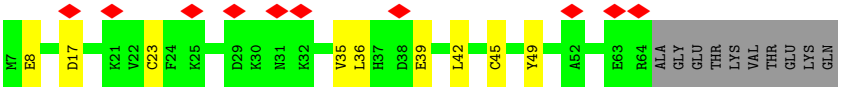
- Molecule 147: Transposase

Chain EZ:



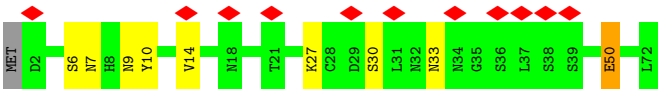
- Molecule 147: Transposase

Chain Ez:



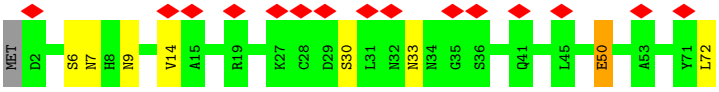
• Molecule 148: Tim10/DDP family zinc finger protein

Chain FA:



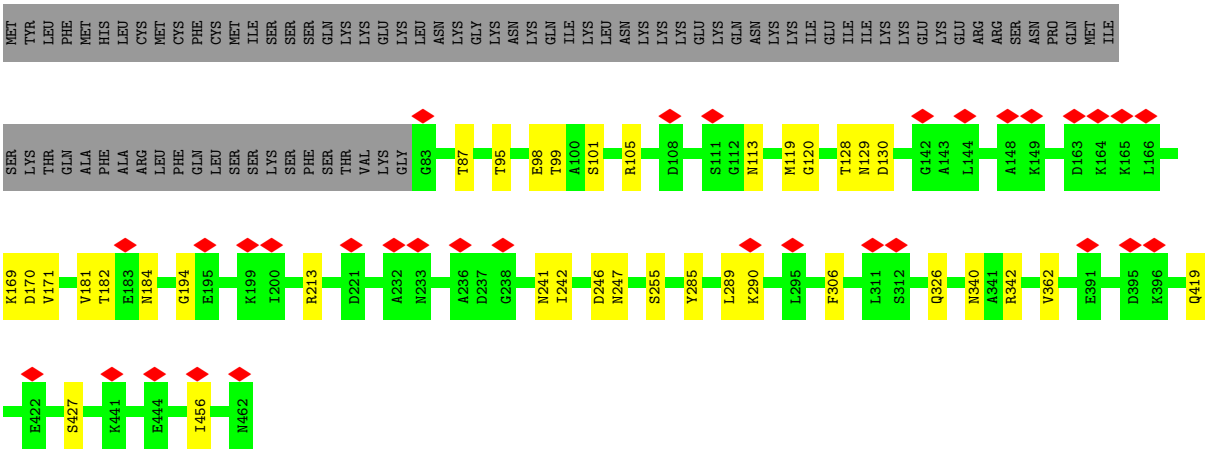
• Molecule 148: Tim10/DDP family zinc finger protein

Chain Fa:



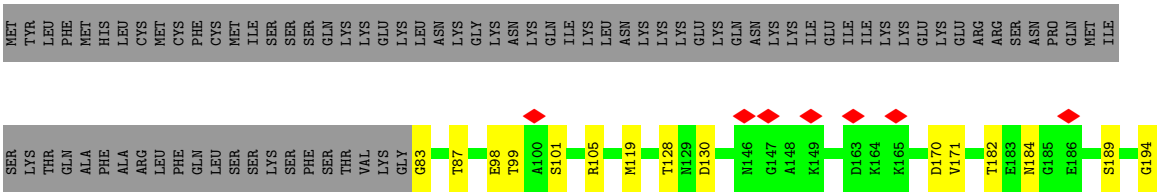
• Molecule 149: Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein,chain 150

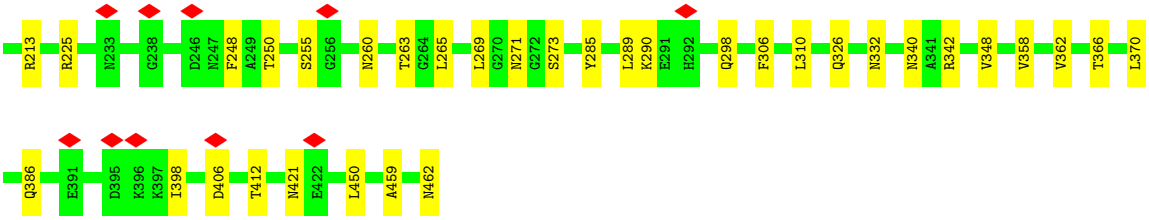
Chain Dl:



• 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
I398
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.

All (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
105:Di:142:SER:OG	150:Di:1103:CDL:OB4	1.92	0.85
148:Fa:30:SER:O	148:Fa:33:ASN:ND2	2.10	0.84
150:DJ:302:CDL:OB3	112:Dq:126:LYS:NZ	2.11	0.83
89:e:134:ILE:HD13	89:e:154:ILE:HG21	1.61	0.83
113:DR:304:ASN:OD1	132:Ek:160:SER:OG	1.96	0.83
12:AB:384:ASN:O	12:AB:489:TYR:OH	1.95	0.83
116:Du:48:ARG:NH1	116:Du:52:ASP:OD2	2.12	0.82
113:Dr:229:ARG:NH1	115:Dt:114:GLU:OE1	2.12	0.82
168:Ed:201:HEM:HBB2	168:Ed:201:HEM:HMB2	1.62	0.82
168:ED:602:HEM:HMB2	168:ED:602:HEM:HBB2	1.61	0.82
99:DC:79:ASP:OD2	99:DC:82:SER:OG	1.99	0.81
114:DS:289:TYR:OH	150:DS:404:CDL:OA9	1.98	0.81
98:DB:509:SER:OG	98:DB:512:ILE:O	1.97	0.81
150:DN:507:CDL:O1	125:ED:92:GLU:OE1	1.98	0.81
112:Dq:13:ASN:ND2	112:Dq:24:ALA:O	2.14	0.81
109:Dn:108:LYS:NZ	124:Ec:86:CYS:SG	2.53	0.81
11:AA:498:SER:O	11:AA:501:THR:OG1	1.98	0.81
87:C:345:LYS:NZ	91:G:158:GLU:OE2	2.14	0.81
86:b:97:ASP:O	86:b:284:ARG:NH2	2.13	0.81
97:DA:238:ILE:O	123:EB:71:ARG:NH2	2.14	0.81
144:EW:15:ARG:NH1	145:EX:10:GLU:OE2	2.14	0.81
87:C:343:THR:O	91:G:35:ARG:NH2	2.13	0.80
113:DR:229:ARG:NH1	115:DT:114:GLU:OE1	2.14	0.80
108:Dm:439:TYR:OH	121:Dz:189:GLU:OE1	1.97	0.80
92:H:86:ARG:NH2	150:H:1301:CDL:OB3	2.13	0.80
116:Du:206:ARG:NH2	116:Du:258:ALA:O	2.14	0.80
17:AG:54:ARG:O	23:AM:225:GLN:NE2	2.14	0.80
92:h:82:TYR:O	92:h:86:ARG:NH1	2.15	0.80
132:EK:160:SER:OG	113:Dr:304:ASN:OD1	1.99	0.80
7:A6:31:GLU:OE2	11:AA:635:SER:OG	1.99	0.79
168:ED:602:HEM:HBC2	168:ED:602:HEM:HMC2	1.64	0.79
18:AH:125:TYR:OH	34:AX:1:MET:O	1.99	0.79
98:DB:145:ASN:O	103:DG:66:ARG:NH2	2.16	0.79
87:c:343:THR:O	91:g:35:ARG:NH2	2.16	0.79
97:DA:181:TYR:OH	123:EB:47:ASP:OD2	1.99	0.79
99:Dc:23:THR:O	99:Dc:69:LYS:NZ	2.15	0.79
125:Ed:92:GLU:OE1	150:Eg:101:CDL:O1	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
168:Ed:201:HEM:HMC2	168:Ed:201:HEM:HBC2	1.65	0.79
99:DC:536:LYS:NZ	129:EH:0:ACE:O	2.16	0.79
24:AN:105:LYS:NZ	25:AO:52:GLU:OE2	2.15	0.79
91:g:84:ASP:OD1	91:g:118:ARG:NH1	2.16	0.79
100:DD:482:LEU:HD11	132:EK:26:LEU:HD22	1.64	0.79
110:DO:56:GLU:OE1	110:DO:96:ARG:NH2	2.14	0.79
110:Do:56:GLU:OE1	110:Do:96:ARG:NH2	2.15	0.79
114:DS:208:GLN:OE1	114:DS:304:TYR:OH	2.01	0.78
118:DW:20:THR:OG1	124:Ec:99:ARG:NH1	2.16	0.78
97:Da:238:ILE:O	123:Eb:71:ARG:NH2	2.16	0.78
101:De:7:GLN:NE2	112:Dq:136:TRP:O	2.17	0.78
102:Df:46:GLU:OE2	107:Dk:127:ASN:ND2	2.15	0.78
125:Ed:187:ARG:NH1	125:Ed:188:ILE:O	2.17	0.78
112:Dq:321:ASP:OD1	112:Dq:324:ARG:NH2	2.16	0.78
99:DC:349:LYS:NZ	101:DE:105:GLN:O	2.16	0.78
97:DA:42:LYS:NZ	105:DI:117:ASP:OD2	2.13	0.78
97:DA:293:ASP:OD1	97:DA:364:ARG:NE	2.16	0.78
97:Da:415:ARG:NH2	103:Dg:19:ASP:OD1	2.16	0.78
14:AD:40:ARG:NH1	14:AD:290:GLU:O	2.17	0.77
10:A9:63:LYS:NZ	68:BY:100:ILE:OXT	2.17	0.77
117:DV:7:ARG:NH1	117:DV:10:GLU:OE2	2.16	0.77
110:Do:30:ALA:O	110:Do:36:SER:OG	2.01	0.77
1:A0:200:GLY:O	1:A0:476:THR:OG1	2.02	0.77
13:AC:341:GLU:OE1	13:AC:367:HIS:ND1	2.17	0.77
106:Dj:195:THR:OG1	139:Er:4:THR:O	2.00	0.77
149:DL:255:SER:O	149:DL:290:LYS:NZ	2.16	0.77
12:AB:201:ARG:NH1	14:AD:377:HIS:O	2.18	0.77
15:AE:33:GLN:OE1	34:AX:43:TYR:OH	2.01	0.77
91:G:176:THR:OG1	91:G:185:ASP:O	1.99	0.77
122:Ea:146:THR:O	122:Ea:151:ARG:NH1	2.16	0.77
150:C:506:CDL:OA4	91:G:130:ARG:NH1	2.17	0.77
46:BC:101:TYR:O	46:BC:105:THR:OG1	2.03	0.77
48:BE:33:ASP:OD1	48:BE:89:HIS:ND1	2.16	0.77
17:AG:141:ILE:HG23	17:AG:159:LEU:HD11	1.65	0.76
122:Ea:138:ARG:O	122:Ea:151:ARG:NH2	2.17	0.76
128:Eg:25:ASP:OD2	128:Eg:74:SER:OG	2.01	0.76
16:AF:49:ASN:ND2	16:AF:51:ILE:O	2.19	0.76
101:DE:62:GLU:OE2	109:DN:285:LYS:NZ	2.16	0.76
106:DJ:195:THR:OG1	139:ER:4:THR:O	2.03	0.76
150:AA:901:CDL:OA3	48:BE:128:ARG:NH1	2.19	0.76
109:Dn:414:TYR:OH	110:Do:446:GLU:OE1	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:CF:101:ASP:OD2	76:CF:159:TYR:OH	2.03	0.76
105:DI:163:HIS:NE2	153:DI:303:PC1:O14	2.17	0.76
98:Db:245:THR:OG1	98:Db:247:LYS:NZ	2.19	0.76
133:El:15:ASP:OD1	133:El:18:ARG:NH2	2.18	0.76
50:BG:77:ARG:NH1	60:BQ:104:ASP:OD1	2.19	0.76
115:DT:232:GLU:OE1	115:DT:232:GLU:N	2.18	0.76
143:EJ:98:ASP:O	143:EJ:101:GLN:NE2	2.17	0.76
97:Da:181:TYR:OH	123:Eb:47:ASP:OD2	2.03	0.76
12:AB:281:GLU:OE1	12:AB:596:ARG:NH2	2.19	0.76
44:BA:203:ARG:NH2	62:BS:105:GLU:OE1	2.19	0.76
88:D:293:ARG:NH1	91:g:304:ALA:O	2.19	0.76
119:Dx:157:GLU:OE1	119:Dx:158:GLY:N	2.19	0.76
17:AG:23:ARG:NH2	56:BM:18:ARG:O	2.19	0.76
91:G:304:ALA:O	88:d:293:ARG:NH1	2.19	0.76
102:DF:46:GLU:OE2	107:DK:127:ASN:ND2	2.19	0.76
18:AH:155:ARG:NH1	18:AH:227:GLU:OE1	2.19	0.76
111:DP:197:ARG:NH1	120:DY:210:GLN:OE1	2.18	0.76
118:Dw:104:SER:O	118:Dw:154:THR:OG1	2.04	0.75
150:c:501:CDL:OA4	91:g:130:ARG:NH1	2.18	0.75
105:Di:163:HIS:NE2	153:Di:1104:PC1:O14	2.19	0.75
107:Dk:12:SER:OG	127:Ef:188:THR:O	2.02	0.75
98:Db:76:LYS:NZ	136:Eo:11:GLU:O	2.19	0.75
100:Dd:321:GLU:OE1	101:De:59:TYR:OH	2.04	0.75
11:AA:380:ASN:OD1	46:BC:156:ARG:NH1	2.19	0.75
25:AO:124:SER:OG	25:AO:136:GLU:OE1	2.03	0.75
126:Ee:157:CYS:SG	126:Ee:173:ARG:NH2	2.59	0.75
9:A8:132:TYR:OH	22:AL:29:GLU:O	2.04	0.75
122:EA:146:THR:O	122:EA:151:ARG:NH1	2.20	0.75
13:AC:422:LYS:NZ	13:AC:426:GLU:OE2	2.19	0.75
97:Da:501:ALA:HB1	97:Da:530:MET:HG2	1.69	0.75
107:Dk:124:GLU:OE1	118:Dw:267:SER:OG	2.05	0.75
110:DO:76:GLN:NE2	110:DO:145:ARG:O	2.20	0.74
26:AP:70:ASP:OD2	37:B0:11:LYS:NZ	2.17	0.74
100:DD:321:GLU:OE1	101:DE:59:TYR:OH	2.04	0.74
11:AA:730:ASP:OD1	44:BA:134:ARG:NH2	2.20	0.74
75:CB:180:LYS:NZ	77:CG:195:TYR:O	2.19	0.74
110:DO:322:ASP:O	120:DY:190:ARG:NH1	2.20	0.74
112:DQ:138:LYS:NZ	150:DQ:1502:CDL:OB3	2.18	0.74
117:Dv:249:ASN:N	117:Dv:255:ASN:OD1	2.20	0.74
104:DH:58:GLU:N	104:DH:58:GLU:OE1	2.19	0.74
110:DO:151:GLN:N	110:DO:151:GLN:OE1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
134:EM:38:LYS:O	142:Eu:14:HIS:NE2	2.21	0.74
54:BK:43:LEU:O	54:BK:46:THR:OG1	2.05	0.74
110:DO:158:ARG:NH2	110:DO:197:GLU:OE2	2.20	0.74
112:DQ:126:LYS:NZ	150:Dj:401:CDL:OB3	2.20	0.74
118:DW:257:GLU:O	118:DW:284:GLN:NE2	2.20	0.74
112:Dq:92:ASP:O	132:Ek:51:ARG:NH1	2.21	0.74
116:Du:90:ARG:NH1	116:Du:128:GLY:O	2.20	0.74
111:Dp:197:ARG:NH1	120:Dy:210:GLN:OE1	2.21	0.74
26:AP:3:LEU:N	150:AP:301:CDL:OA3	2.20	0.74
88:D:71:ARG:NH2	88:D:104:GLU:OE1	2.21	0.74
75:CB:262:ARG:NH2	77:CG:162:GLU:OE2	2.21	0.74
91:G:84:ASP:OD1	91:G:118:ARG:NH1	2.21	0.74
25:AO:88:TYR:O	25:AO:92:ASN:ND2	2.20	0.74
98:DB:7:THR:O	98:DB:544:PHE:N	2.20	0.74
98:DB:167:GLN:OE1	102:DF:174:TYR:OH	2.06	0.74
21:AK:60:SER:OG	21:AK:75:TRP:O	2.05	0.73
116:DU:31:PHE:O	116:DU:45:LYS:NZ	2.21	0.73
128:EG:41:GLN:OE1	128:EG:45:ARG:NH1	2.21	0.73
106:Dj:143:ARG:NH2	106:Dj:186:ASP:OD1	2.21	0.73
7:A6:217:VAL:O	7:A6:236:ARG:NH1	2.20	0.73
109:DN:108:LYS:NZ	124:EC:86:CYS:SG	2.58	0.73
117:Dv:7:ARG:NH1	117:Dv:10:GLU:OE2	2.21	0.73
98:Db:255:SER:OG	147:Ez:17:ASP:OD2	2.07	0.73
86:B:97:ASP:O	86:B:284:ARG:NH2	2.20	0.73
108:DM:390:GLU:OE1	108:DM:392:TYR:OH	2.06	0.73
122:EA:186:ARG:NH2	122:EA:193:GLU:O	2.21	0.73
16:AF:241:ASN:OD1	16:AF:244:THR:OG1	2.01	0.73
125:Ed:171:LYS:NZ	140:Es:33:PHE:O	2.20	0.73
149:DL:340:ASN:OD1	149:DL:342:ARG:NH1	2.21	0.73
87:C:23:MET:CE	167:C:512:UQ8:H3MB	2.19	0.73
103:DG:23:ARG:NH1	115:DT:246:ASP:OD1	2.21	0.73
116:DU:41:ASP:OD1	116:DU:44:SER:OG	2.04	0.73
117:Dv:132:ALA:O	117:Dv:136:THR:HG22	1.89	0.73
124:Ec:16:GLU:OE1	124:Ec:18:ALA:N	2.22	0.73
15:AE:125:THR:OG1	15:AE:161:TYR:OH	2.06	0.73
17:AG:23:ARG:NH1	23:AM:31:CYS:SG	2.62	0.73
85:A:346:ARG:NH1	91:G:170:THR:O	2.21	0.73
89:E:224:ASP:OD1	89:E:228:ARG:N	2.21	0.73
89:e:208:LEU:HD22	89:e:215:VAL:HG21	1.70	0.73
91:g:176:THR:OG1	91:g:185:ASP:O	2.05	0.73
131:EV:29:LYS:NZ	131:EV:40:CYS:SG	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:200:PHE:O	11:AA:269:TYR:OH	2.07	0.73
91:G:115:MET:SD	91:G:118:ARG:NH2	2.62	0.73
85:a:53:GLU:OE1	85:a:53:GLU:N	2.22	0.73
98:DB:368:GLY:O	173:ER:201:ATP:N6	2.22	0.72
116:Du:154:SER:O	116:Du:159:GLN:NE2	2.22	0.72
128:Eg:10:GLN:NE2	129:Eh:113:GLU:OE2	2.22	0.72
12:AB:155:ASN:O	14:AD:468:ASN:ND2	2.22	0.72
137:EP:28:TYR:N	112:Dq:291:SER:HG	1.85	0.72
100:Dd:261:GLU:O	100:Dd:265:LEU:HD22	1.88	0.72
108:DM:274:GLU:OE2	108:DM:366:ARG:NH1	2.22	0.72
121:DZ:130:GLU:OE1	121:DZ:130:GLU:N	2.22	0.72
99:Dc:101:GLU:HG2	116:Du:271:LEU:HD21	1.71	0.72
98:DB:118:ARG:NH1	102:DF:182:ASP:OD1	2.21	0.72
85:a:327:ILE:O	85:a:413:ARG:NH2	2.23	0.72
99:DC:53:LEU:HD23	99:DC:58:ASN:OD1	1.90	0.72
97:Da:501:ALA:HB2	97:Da:529:ILE:HG22	1.71	0.72
3:A2:167:ARG:NH1	21:AK:83:ASP:O	2.23	0.72
63:BT:107:LEU:HB2	150:BT:204:CDL:H411	1.70	0.72
80:CJ:49:ARG:NH1	150:CJ:201:CDL:OB7	2.23	0.72
86:b:106:THR:HG1	86:b:109:SER:HG	1.38	0.72
98:Db:176:LYS:NZ	126:Ee:78:GLU:OE2	2.16	0.72
2:A1:233:ARG:NH2	2:A1:317:LEU:O	2.22	0.72
85:A:390:GLN:NE2	85:A:512:ILE:O	2.23	0.72
150:H:1301:CDL:OA2	88:d:276:LYS:NZ	2.23	0.72
99:Dc:308:PHE:O	99:Dc:312:THR:HG23	1.89	0.72
4:A3:33:ASN:ND2	19:AI:43:GLU:OE1	2.22	0.72
131:Ev:29:LYS:NZ	131:Ev:40:CYS:SG	2.63	0.72
12:AB:609:ASP:OD1	12:AB:611:ARG:NH1	2.23	0.71
110:DO:450:PRO:O	110:DO:453:ASN:ND2	2.22	0.71
114:DS:17:ASP:O	114:DS:339:ASN:ND2	2.23	0.71
100:Dd:377:GLU:N	100:Dd:377:GLU:OE1	2.22	0.71
108:Dm:53:ALA:O	108:Dm:173:LYS:NZ	2.23	0.71
149:DL:128:THR:OG1	149:DL:130:ASP:OD1	2.08	0.71
13:AC:74:TYR:OH	63:BT:140:PHE:O	2.09	0.71
13:AC:325:TRP:O	46:BC:53:ASN:ND2	2.23	0.71
87:c:211:SER:O	91:g:94:ARG:NH2	2.24	0.71
87:c:328:ASN:ND2	150:g:801:CDL:OB3	2.22	0.71
118:Dw:110:THR:OG1	118:Dw:113:ASN:OD1	2.08	0.71
52:BI:63:GLU:OE2	52:BI:71:ARG:NH2	2.24	0.71
11:AA:254:SER:OG	11:AA:444:ARG:NH2	2.24	0.71
15:AE:383:LYS:NZ	15:AE:434:ASP:OD1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AT:82:GLU:OE1	34:AX:38:THR:OG1	2.08	0.71
45:BB:202:LYS:NZ	45:BB:206:GLU:OE2	2.23	0.71
108:DM:34:GLU:O	108:DM:38:ASN:ND2	2.23	0.71
98:Db:118:ARG:NH1	102:Df:182:ASP:OD1	2.24	0.71
140:Es:50:ASN:OD1	140:Es:51:LEU:N	2.24	0.71
149:DL:87:THR:HG23	149:DL:119:MET:HE1	1.72	0.71
4:A3:54:ASN:OD1	4:A3:92:LYS:NZ	2.20	0.71
98:Db:271:ASN:ND2	148:Fa:7:ASN:OD1	2.24	0.71
100:Dd:433:THR:O	100:Dd:438:LYS:NZ	2.24	0.71
7:A6:130:THR:HG21	11:AA:744:ILE:HD13	1.73	0.71
81:CN:43:GLN:NE2	81:CN:44:ASN:OD1	2.23	0.71
88:d:71:ARG:NH2	88:d:104:GLU:OE1	2.22	0.71
91:g:174:ARG:NH1	91:g:177:SER:OG	2.22	0.71
116:DU:90:ARG:NH1	116:DU:128:GLY:O	2.23	0.71
16:AF:263:ALA:HB2	16:AF:349:ILE:HD11	1.72	0.71
91:g:6:LYS:O	91:g:11:GLN:NE2	2.23	0.71
118:DW:257:GLU:N	118:DW:257:GLU:OE1	2.23	0.71
6:A5:38:GLU:OE2	15:AE:163:ARG:NH2	2.24	0.70
93:I:99:GLU:N	93:I:99:GLU:OE1	2.24	0.70
98:Db:122:TRP:CD1	98:Db:553:CYS:HG	2.09	0.70
12:AB:153:ARG:NH1	14:AD:415:GLN:OE1	2.25	0.70
19:AI:167:LEU:N	158:AI:301:FES:S1	2.64	0.70
12:AB:141:GLN:NE2	159:AB:803:SF4:S4	2.65	0.70
18:AH:43:GLU:OE2	43:B6:21:ARG:NH2	2.24	0.70
168:C:501:HEM:HBC2	168:C:501:HEM:HMC1	1.72	0.70
119:DX:143:ARG:NH1	119:DX:221:LEU:O	2.24	0.70
99:Dc:79:ASP:OD2	99:Dc:82:SER:OG	2.10	0.70
114:Ds:50:GLN:OE1	114:Ds:311:GLY:N	2.25	0.70
122:Ea:218:ARG:NH1	146:Ey:58:TYR:OH	2.24	0.70
146:Ey:5:LEU:HD21	148:Fa:14:VAL:HG11	1.72	0.70
128:EG:25:ASP:OD2	128:EG:74:SER:OG	2.05	0.70
120:Dy:234:LYS:NZ	138:Eq:35:GLU:OE2	2.25	0.70
3:A2:167:ARG:NH2	21:AK:65:GLU:OE1	2.24	0.70
32:AV:33:ARG:NH1	52:BI:127:GLU:OE1	2.24	0.70
45:BB:192:ARG:NH2	49:BF:170:GLU:OE1	2.25	0.70
106:DJ:199:LYS:NZ	119:Dx:252:GLY:O	2.25	0.70
127:EF:174:LEU:HD22	153:Dx:1203:PC1:H2I2	1.73	0.70
110:Do:322:ASP:O	120:Dy:190:ARG:NH1	2.25	0.70
121:Dz:55:TYR:O	123:Eb:117:GLN:NE2	2.24	0.70
14:AD:370:ARG:NE	19:AI:126:GLY:O	2.25	0.70
87:C:120:VAL:HG11	87:C:310:PHE:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
125:ED:171:LYS:NZ	140:ES:33:PHE:O	2.25	0.70
147:Ez:39:GLU:N	147:Ez:39:GLU:OE1	2.25	0.70
86:B:204:ASN:OD1	86:B:364:ARG:NH1	2.24	0.69
109:DN:414:TYR:OH	110:DO:446:GLU:OE1	2.10	0.69
112:DQ:120:ASN:OD1	112:DQ:183:LYS:NZ	2.24	0.69
115:DT:83:TYR:OH	127:EF:27:ASP:OD2	2.09	0.69
108:Dm:299:PHE:O	108:Dm:303:ASN:ND2	2.25	0.69
133:EL:15:ASP:OD1	133:EL:18:ARG:NH2	2.25	0.69
7:A6:251:ASN:O	40:B3:11:ALA:N	2.24	0.69
18:AH:70:ASP:OD1	18:AH:71:ALA:N	2.25	0.69
114:Ds:152:VAL:HG21	114:Ds:198:SER:HB2	1.73	0.69
144:Ew:15:ARG:NH1	145:Ex:10:GLU:OE2	2.25	0.69
15:AE:155:GLU:OE1	15:AE:168:ARG:NH2	2.25	0.69
97:Da:241:PRO:O	123:Eb:74:LYS:NZ	2.25	0.69
109:Dn:44:TYR:OH	150:Dn:503:CDL:OB5	2.10	0.69
140:ES:14:ASP:OD2	140:ES:34:LYS:NZ	2.26	0.69
100:Dd:482:LEU:HD11	132:Ek:26:LEU:HD22	1.72	0.69
114:Ds:10:ARG:NH1	117:Dv:4:SER:OG	2.25	0.69
123:Eb:16:ASP:O	123:Eb:19:THR:HG22	1.93	0.69
6:A5:179:TYR:OH	15:AE:285:ASN:OD1	2.09	0.69
11:AA:382:ASP:OD2	63:BT:123:ARG:NE	2.25	0.69
44:BA:26:ILE:HG13	62:BS:111:LEU:HD13	1.74	0.69
109:Dn:3:MET:N	150:Eg:101:CDL:OA4	2.25	0.69
100:DD:431:ASP:OD2	100:DD:433:THR:OG1	2.09	0.69
116:DU:206:ARG:NH2	116:DU:258:ALA:O	2.26	0.69
110:Do:158:ARG:NH2	110:Do:197:GLU:OE2	2.25	0.69
149:Dl:87:THR:HG23	149:Dl:119:MET:HE1	1.73	0.69
44:BA:187:GLN:NE2	44:BA:191:ASP:OD1	2.26	0.69
86:B:419:GLU:O	86:B:423:ASN:ND2	2.26	0.69
99:DC:308:PHE:O	99:DC:312:THR:HG23	1.93	0.69
100:DD:287:THR:HG22	109:DN:279:VAL:CG1	2.23	0.69
112:DQ:18:THR:OG1	137:EP:79:GLU:O	2.06	0.69
114:DS:152:VAL:HG21	114:DS:198:SER:HB2	1.75	0.69
120:DY:234:LYS:NZ	138:EQ:35:GLU:OE2	2.25	0.69
99:Dc:84:GLU:OE1	116:Du:266:THR:OG1	2.10	0.69
141:ET:12:GLN:OE1	141:ET:16:ARG:NH2	2.26	0.69
59:BP:73:GLN:N	59:BP:73:GLN:OE1	2.25	0.69
124:EC:16:GLU:OE1	124:EC:18:ALA:N	2.25	0.69
108:Dm:34:GLU:O	108:Dm:38:ASN:ND2	2.26	0.69
121:Dz:210:LEU:HD23	121:Dz:226:ARG:HA	1.75	0.69
122:Ea:186:ARG:NH2	122:Ea:193:GLU:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AD:130:GLU:O	14:AD:134:ASN:ND2	2.25	0.68
48:BE:170:GLU:OE1	48:BE:170:GLU:N	2.26	0.68
86:B:403:LYS:NZ	86:B:440:ASP:OD1	2.20	0.68
86:b:116:THR:O	86:b:175:ARG:NH2	2.26	0.68
106:DJ:175:ARG:NH2	106:DJ:204:GLU:OE2	2.26	0.68
99:Dc:349:LYS:NZ	101:De:105:GLN:O	2.26	0.68
115:Dt:57:GLN:NE2	140:Es:13:THR:O	2.26	0.68
119:DX:23:ARG:NH1	119:DX:45:ASN:OD1	2.25	0.68
122:EA:218:ARG:NH1	146:EY:58:TYR:OH	2.27	0.68
11:AA:565:LEU:O	11:AA:568:THR:OG1	2.11	0.68
102:DF:40:ARG:NH2	134:EM:127:ASN:O	2.27	0.68
19:AI:27:LEU:O	19:AI:114:ARG:NH2	2.27	0.68
99:DC:263:VAL:O	104:DH:108:ARG:NH1	2.26	0.68
86:b:417:LEU:O	86:b:421:VAL:HG23	1.93	0.68
108:DM:53:ALA:O	108:DM:173:LYS:NZ	2.26	0.68
104:DH:33:HIS:O	104:DH:37:GLY:N	2.26	0.68
98:Db:7:THR:O	98:Db:544:PHE:N	2.26	0.68
14:AD:102:MET:SD	14:AD:242:THR:OG1	2.51	0.68
30:AT:4:ASP:OD2	30:AT:161:THR:OG1	2.12	0.68
145:EX:40:GLU:OE1	147:EZ:48:ARG:NH2	2.27	0.68
99:Dc:435:ASP:OD1	99:Dc:436:THR:N	2.27	0.68
34:AX:64:LEU:HD13	43:B6:33:THR:HG21	1.75	0.68
92:h:40:SER:OG	92:h:43:SER:OG	2.10	0.68
3:A2:249:ARG:NH1	3:A2:250:ASN:OD1	2.27	0.68
22:AL:69:GLU:OE2	56:BM:47:LYS:NZ	2.27	0.68
56:BM:28:ASP:O	56:BM:34:ASN:ND2	2.27	0.68
123:EB:16:ASP:O	123:EB:19:THR:HG22	1.94	0.68
114:Ds:140:THR:HG21	114:Ds:214:TYR:HB2	1.75	0.68
132:Ek:109:ILE:HG21	132:Ek:124:GLU:HG3	1.76	0.68
46:BC:151:GLN:OE1	46:BC:151:GLN:N	2.27	0.67
87:C:338:ARG:NH2	91:G:33:GLU:OE1	2.28	0.67
107:DK:94:CYS:SG	136:EO:84:LYS:NZ	2.67	0.67
150:Dn:503:CDL:O1	150:Dn:503:CDL:OB7	2.10	0.67
101:DE:53:GLU:OE1	125:ED:170:TYR:OH	2.12	0.67
111:DP:326:ASP:OD1	111:DP:330:LYS:NZ	2.26	0.67
115:DT:45:PRO:HG2	115:DT:50:ILE:HD11	1.76	0.67
129:EH:166:ASP:OD1	129:EH:167:TYR:N	2.27	0.67
111:Dp:160:ASP:OD1	111:Dp:161:GLY:N	2.27	0.67
119:Dx:143:ARG:NH1	119:Dx:221:LEU:O	2.27	0.67
86:b:204:ASN:OD1	86:b:364:ARG:NH1	2.26	0.67
102:DF:40:ARG:NH1	102:DF:42:ASP:OD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
102:DF:224:GLU:OE1	102:DF:224:GLU:N	2.27	0.67
3:A2:33:ARG:NH2	3:A2:93:ASN:O	2.27	0.67
66:BW:25:GLN:OE1	66:BW:25:GLN:N	2.27	0.67
93:I:116:GLU:OE1	93:I:116:GLU:N	2.27	0.67
99:DC:23:THR:O	99:DC:69:LYS:NZ	2.25	0.67
102:Df:208:HIS:O	102:Df:212:THR:HG23	1.93	0.67
108:Dm:237:ARG:NH2	121:Dz:48:ASP:OD2	2.27	0.67
116:Du:31:PHE:O	116:Du:45:LYS:NZ	2.26	0.67
136:Eo:101:GLU:N	136:Eo:101:GLU:OE1	2.27	0.67
17:AG:258:GLU:OE1	60:BQ:43:ASN:ND2	2.27	0.67
24:AN:75:ARG:NH1	24:AN:113:THR:O	2.28	0.67
98:DB:245:THR:OG1	98:DB:247:LYS:NZ	2.28	0.67
114:DS:50:GLN:OE1	114:DS:311:GLY:N	2.27	0.67
124:Ec:51:GLN:OE1	124:Ec:51:GLN:N	2.28	0.67
29:AS:18:ASN:O	29:AS:19:ASN:ND2	2.26	0.67
148:FA:30:SER:O	148:FA:33:ASN:ND2	2.26	0.67
150:Eh:1601:CDL:OB4	133:El:116:LYS:NZ	2.22	0.67
16:AF:40:ASN:ND2	22:AL:68:ASP:OD1	2.27	0.67
75:CB:178:GLN:NE2	75:CB:232:PRO:O	2.28	0.67
136:EO:101:GLU:OE1	136:EO:101:GLU:N	2.26	0.67
105:Di:74:MET:SD	115:Dt:109:GLN:NE2	2.68	0.67
128:Eg:41:GLN:OE1	128:Eg:45:ARG:NH1	2.28	0.67
34:AX:90:THR:OG1	56:BM:92:ILE:O	2.12	0.67
87:C:387:GLY:H	92:H:114:THR:HG21	1.59	0.67
100:Dd:503:LEU:HB3	132:Ek:40:ILE:HD11	1.76	0.67
8:A7:176:ASP:OD1	8:A7:177:SER:N	2.28	0.67
104:Dh:80:VAL:HG21	109:Dn:352:LEU:HB2	1.76	0.67
39:B2:49:ARG:NH1	50:BG:141:ARG:O	2.28	0.67
97:DA:501:ALA:HB1	97:DA:530:MET:HG2	1.75	0.67
87:C:132:LEU:HD11	87:C:184:LEU:HD23	1.77	0.66
133:El:102:LYS:NZ	150:El:901:CDL:OB4	2.29	0.66
73:CA:406:LYS:O	73:CA:407:THR:OG1	2.11	0.66
87:C:184:LEU:HD22	167:C:511:UQ8:H30B	1.77	0.66
113:Dr:139:LYS:NZ	113:Dr:329:SER:OG	2.28	0.66
149:DL:170:ASP:OD1	149:DL:171:VAL:N	2.28	0.66
11:AA:559:MET:HE2	11:AA:609:LEU:HD23	1.76	0.66
85:a:498:LYS:O	89:e:89:ARG:NH2	2.29	0.66
120:DY:167:ARG:NH1	123:EB:210:PHE:O	2.28	0.66
110:Do:116:GLY:O	110:Do:120:VAL:HG23	1.96	0.66
135:En:123:ASN:ND2	135:En:138:GLU:O	2.28	0.66
27:AQ:143:GLU:OE1	27:AQ:155:ASP:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:DZ:55:TYR:O	123:EB:117:GLN:NE2	2.28	0.66
99:DC:435:ASP:OD1	99:DC:436:THR:N	2.29	0.66
125:ED:140:ASN:OD1	132:EK:21:ARG:NH2	2.29	0.66
149:Dl:419:GLN:OE1	149:Dl:427:SER:OG	2.14	0.66
128:EG:75:ARG:NH2	142:EU:38:GLU:OE2	2.29	0.66
97:Da:550:LEU:O	105:Di:136:ARG:NH1	2.29	0.66
128:Eg:74:SER:OG	129:Eh:13:ARG:NH2	2.29	0.66
137:EP:78:ASP:OD1	137:EP:82:TYR:N	2.29	0.66
116:Du:117:GLN:NE2	116:Du:121:ASN:OD1	2.28	0.66
44:BA:165:GLU:OE1	44:BA:173:ARG:NH2	2.29	0.66
77:CG:26:VAL:HG21	77:CG:53:LEU:HD12	1.77	0.66
86:B:281:THR:OG1	86:B:283:GLN:OE1	2.14	0.66
100:Dd:458:ARG:NE	100:Dd:520:SEP:O1P	2.29	0.66
89:e:208:LEU:CD2	89:e:215:VAL:HG21	2.25	0.65
99:DC:349:LYS:NZ	101:DE:108:GLN:O	2.19	0.65
102:DF:226:LYS:NZ	173:ER:201:ATP:O2A	2.22	0.65
99:Dc:368:ILE:HD12	99:Dc:401:ILE:HD12	1.78	0.65
85:a:53:GLU:O	85:a:415:ARG:NH2	2.28	0.65
102:Df:226:LYS:NZ	173:Er:201:ATP:O2A	2.28	0.65
112:DQ:13:ASN:ND2	112:DQ:24:ALA:O	2.29	0.65
116:Du:266:THR:O	116:Du:270:VAL:HG23	1.96	0.65
136:Eo:40:TYR:OH	153:Eo:204:PC1:O32	2.07	0.65
137:Ep:78:ASP:OD1	137:Ep:82:TYR:N	2.30	0.65
88:d:41:GLU:N	88:d:41:GLU:OE1	2.29	0.65
99:Dc:356:ARG:NH1	153:Dc:609:PC1:O14	2.30	0.65
110:Do:151:GLN:OE1	110:Do:151:GLN:N	2.29	0.65
36:AZ:41:LYS:NZ	36:AZ:45:PRO:O	2.30	0.65
53:BJ:51:ARG:NH1	53:BJ:62:ASP:OD2	2.29	0.65
150:C:505:CDL:H621	167:C:512:UQ8:H25B	1.78	0.65
117:DV:132:ALA:O	117:DV:136:THR:HG22	1.96	0.65
110:Do:355:THR:OG1	110:Do:369:VAL:O	2.13	0.65
129:Eh:156:GLN:OE1	129:Eh:156:GLN:N	2.29	0.65
8:A7:152:GLN:N	8:A7:152:GLN:OE1	2.29	0.65
105:DI:78:ASN:ND2	115:DT:128:GLU:OE1	2.30	0.65
105:DI:120:SEP:O	108:DM:246:ASN:ND2	2.29	0.65
107:DK:124:GLU:OE1	118:DW:267:SER:OG	2.13	0.65
150:EL:901:CDL:H873	150:ES:1101:CDL:H832	1.77	0.65
130:Ei:25:LEU:O	130:Ei:33:ARG:NH1	2.30	0.65
143:Ej:142:ARG:NH2	143:Ej:149:GLU:OE2	2.29	0.65
5:A4:175:VAL:HG23	5:A4:181:LEU:HD22	1.79	0.65
91:G:45:ASN:O	91:G:49:THR:OG1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
124:EC:51:GLN:OE1	124:EC:51:GLN:N	2.30	0.65
101:De:62:GLU:OE2	109:Dn:285:LYS:NZ	2.24	0.65
114:Ds:58:GLU:OE1	114:Ds:58:GLU:N	2.30	0.65
20:AJ:184:GLU:OE1	20:AJ:184:GLU:N	2.30	0.64
168:c:504:HEM:HBC2	168:c:504:HEM:HMC2	1.77	0.64
150:EH:1601:CDL:H272	150:EH:1601:CDL:H172	1.80	0.64
116:DU:266:THR:O	116:DU:270:VAL:HG23	1.97	0.64
118:DW:104:SER:O	118:DW:154:THR:OG1	2.15	0.64
108:Dm:286:ASN:OD1	108:Dm:287:TYR:N	2.31	0.64
115:Dt:117:ARG:HA	127:Ef:51:THR:HG21	1.79	0.64
81:CN:44:ASN:ND2	83:CO:34:TYR:OH	2.30	0.64
97:DA:643:TYR:O	98:DB:69:THR:HG23	1.98	0.64
114:DS:342:GLU:N	114:DS:342:GLU:OE1	2.30	0.64
149:Dl:182:THR:OG1	149:Dl:184:ASN:OD1	2.13	0.64
149:DL:182:THR:OG1	149:DL:184:ASN:OD1	2.13	0.64
33:AW:114:GLU:O	33:AW:117:ARG:NH1	2.29	0.64
150:EL:901:CDL:H871	150:EL:901:CDL:H671	1.77	0.64
100:Dd:265:LEU:HD12	100:Dd:272:ARG:HA	1.78	0.64
73:CA:112:ASP:OD1	73:CA:164:SER:OG	2.14	0.64
85:A:83:SER:OG	86:B:411:GLU:OE2	2.15	0.64
148:FA:6:SER:OG	148:FA:9:ASN:OD1	2.15	0.64
97:Da:155:ILE:HD13	97:Da:295:LEU:HD11	1.80	0.64
98:Db:69:THR:HG21	115:Dt:234:GLU:O	1.97	0.64
109:Dn:409:LEU:HD11	109:Dn:437:PHE:CD1	2.33	0.64
129:Eh:53:GLY:O	129:Eh:57:VAL:HG23	1.98	0.64
97:DA:496:LEU:HG	167:EN:1205:UQ8:H10A	1.80	0.64
107:Dk:97:GLU:N	107:Dk:97:GLU:OE1	2.30	0.64
112:Dq:98:GLU:OE2	132:Ek:51:ARG:NE	2.30	0.64
47:BD:149:LEU:O	49:BF:80:ARG:NH2	2.31	0.64
73:CA:257:ALA:HB1	75:CB:121:SER:O	1.98	0.64
108:DM:46:THR:HG21	108:DM:107:ARG:HG2	1.79	0.64
117:Dv:249:ASN:OD1	117:Dv:250:ALA:N	2.31	0.64
79:CE:168:ARG:NH2	79:CE:174:SER:O	2.29	0.64
92:h:40:SER:HG	92:h:43:SER:HG	1.40	0.64
79:CE:83:THR:HG23	79:CE:116:THR:HA	1.80	0.64
100:DD:433:THR:O	100:DD:438:LYS:NZ	2.31	0.64
105:DI:42:ASP:OD1	117:DV:44:ARG:NH1	2.31	0.64
104:Dh:21:ASP:OD1	104:Dh:22:ALA:N	2.30	0.64
73:CA:589:ARG:NH2	73:CA:632:ALA:O	2.31	0.63
85:A:348:TYR:O	85:A:413:ARG:NH1	2.31	0.63
99:Dc:268:PHE:O	99:Dc:272:ILE:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
105:Di:120:SEP:O	108:Dm:246:ASN:ND2	2.30	0.63
108:Dm:272:LEU:HD22	108:Dm:369:PHE:CE2	2.33	0.63
121:Dz:130:GLU:OE1	121:Dz:130:GLU:N	2.31	0.63
129:Eh:166:ASP:OD1	129:Eh:167:TYR:N	2.31	0.63
130:Ei:49:LEU:O	130:Ei:54:ARG:NE	2.30	0.63
15:AE:242:ARG:NH2	15:AE:286:GLU:OE2	2.30	0.63
20:AJ:148:GLU:N	20:AJ:148:GLU:OE1	2.31	0.63
134:EM:67:GLU:OE1	134:EM:67:GLU:N	2.31	0.63
145:EX:20:THR:HG22	147:EZ:49:TYR:HE1	1.62	0.63
97:Da:344:ARG:NH1	150:Da:709:CDL:OA4	2.31	0.63
12:AB:507:SER:OG	24:AN:190:ALA:O	2.13	0.63
115:DT:128:GLU:O	115:DT:131:THR:OG1	2.15	0.63
123:EB:63:ARG:NH1	123:EB:67:ASP:OD2	2.30	0.63
100:Dd:618:GLU:OE1	100:Dd:618:GLU:N	2.31	0.63
106:Dj:170:ASP:OD1	106:Dj:174:ASN:ND2	2.31	0.63
1:A0:264:LYS:NZ	1:A0:304:ASP:O	2.27	0.63
110:DO:30:ALA:O	110:DO:36:SER:OG	2.16	0.63
11:AA:616:ASP:OD1	11:AA:617:THR:N	2.31	0.63
87:C:387:GLY:N	92:H:114:THR:HG21	2.12	0.63
108:DM:166:ASP:OD1	125:ED:190:TYR:OH	2.13	0.63
118:DW:98:GLN:N	118:DW:98:GLN:OE1	2.32	0.63
117:Dv:92:TYR:HB2	117:Dv:136:THR:HG21	1.80	0.63
129:Eh:15:ASP:O	129:Eh:147:LYS:NZ	2.32	0.63
117:DV:191:ALA:O	117:DV:195:ASN:ND2	2.32	0.63
145:EX:20:THR:HG22	147:EZ:49:TYR:CE1	2.33	0.63
110:Do:244:ASP:O	110:Do:248:VAL:HG13	1.99	0.63
4:A3:32:ARG:NH1	4:A3:257:GLY:O	2.31	0.63
87:c:120:VAL:HG11	87:c:310:PHE:HA	1.79	0.63
97:DA:550:LEU:O	105:DI:136:ARG:NH1	2.31	0.63
99:Dc:176:ILE:O	121:Dz:141:GLN:NE2	2.32	0.63
117:Dv:20:SER:O	117:Dv:24:ASN:ND2	2.32	0.63
16:AF:232:SER:CB	39:B2:40:THR:HG21	2.29	0.63
54:BK:123:TYR:OH	57:BN:98:GLU:OE1	2.09	0.63
85:A:298:GLU:OE1	88:D:300:HIS:ND1	2.31	0.63
126:EE:106:GLU:OE1	126:EE:106:GLU:N	2.32	0.63
153:Da:707:PC1:H2E1	153:Da:707:PC1:H2I3	1.80	0.63
100:Dd:575:PHE:CE2	100:Dd:579:ILE:HD11	2.34	0.63
6:A5:215:MET:SD	15:AE:325:GLN:NE2	2.71	0.63
6:A5:241:GLN:NE2	6:A5:246:ASP:OD2	2.32	0.63
76:CF:134:MET:SD	83:CO:24:TYR:OH	2.53	0.63
100:DD:261:GLU:O	100:DD:265:LEU:HD22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:398:ASN:ND2	1:A0:408:GLU:OE2	2.32	0.62
22:AL:80:TYR:OH	153:AL:303:PC1:O32	2.17	0.62
89:E:157:LEU:HD13	89:E:191:ILE:HD13	1.80	0.62
97:Da:116:GLY:O	97:Da:120:ASN:ND2	2.31	0.62
116:Du:254:ARG:NH2	116:Du:277:THR:O	2.32	0.62
11:AA:161:GLN:O	11:AA:163:ASN:ND2	2.32	0.62
73:CA:145:LEU:HD12	73:CA:146:PRO:HD2	1.81	0.62
86:b:81:THR:OG1	86:b:259:HIS:ND1	2.20	0.62
105:DI:115:GLU:OE1	105:DI:115:GLU:N	2.32	0.62
98:Db:478:GLU:OE2	114:Ds:228:ARG:NE	2.30	0.62
104:Dh:54:ILE:O	104:Dh:54:ILE:HG22	1.99	0.62
109:Dn:253:TYR:N	109:Dn:284:ASP:OD2	2.32	0.62
143:Ej:99:PHE:O	143:Ej:134:GLN:NE2	2.32	0.62
4:A3:216:ILE:O	4:A3:219:THR:OG1	2.16	0.62
9:A8:191:ASN:OD1	9:A8:192:LYS:N	2.31	0.62
51:BH:120:ARG:NH2	52:BI:88:ASN:OD1	2.33	0.62
73:CA:86:HIS:HD1	73:CA:257:ALA:HB2	1.64	0.62
75:CB:258:GLU:N	75:CB:258:GLU:OE1	2.32	0.62
150:C:506:CDL:OB7	92:H:96:ASN:ND2	2.32	0.62
110:DO:37:GLU:OE1	110:DO:37:GLU:N	2.33	0.62
132:EK:109:ILE:HG21	132:EK:124:GLU:HG3	1.80	0.62
148:Fa:50:GLU:OE1	148:Fa:50:GLU:N	2.32	0.62
15:AE:125:THR:HG1	15:AE:161:TYR:HH	1.41	0.62
21:AK:197:ASP:OD2	67:BX:18:ARG:N	2.31	0.62
49:BF:71:ARG:NH1	49:BF:75:ASN:OD1	2.31	0.62
89:e:108:ARG:NH1	89:e:112:MET:SD	2.72	0.62
99:DC:101:GLU:HG2	116:DU:271:LEU:HD21	1.81	0.62
100:Dd:403:ASP:OD1	100:Dd:404:GLN:N	2.31	0.62
106:Dj:167:LEU:O	106:Dj:171:PHE:N	2.28	0.62
14:AD:162:GLU:OE1	14:AD:162:GLU:N	2.32	0.62
36:AZ:14:GLU:OE1	36:AZ:64:ARG:NH2	2.31	0.62
79:CE:154:THR:O	79:CE:159:SER:OG	2.15	0.62
91:G:95:ARG:NH1	92:H:50:ASP:OD1	2.33	0.62
108:DM:79:GLU:N	108:DM:79:GLU:OE1	2.31	0.62
111:DP:160:ASP:OD1	111:DP:161:GLY:N	2.33	0.62
142:EU:14:HIS:NE2	134:Em:38:LYS:O	2.31	0.62
111:Dp:190:LYS:O	111:Dp:193:ARG:NH1	2.31	0.62
91:g:5:GLU:OE1	91:g:5:GLU:N	2.32	0.62
109:DN:253:TYR:N	109:DN:284:ASP:OD2	2.29	0.62
150:Ds:405:CDL:OB9	117:Dv:62:ASN:ND2	2.33	0.62
86:B:329:LEU:HD21	86:B:386:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:E:67:LYS:O	91:g:121:ARG:NE	2.32	0.62
89:e:25:GLY:N	89:e:28:SER:HG	1.98	0.62
115:Dt:81:PRO:HG2	115:Dt:89:MET:HE3	1.81	0.62
1:A0:345:LYS:NZ	151:A0:603:UDP:O2'	2.31	0.62
14:AD:45:LEU:O	14:AD:134:ASN:ND2	2.33	0.62
89:e:82:GLU:OE1	89:e:82:GLU:N	2.33	0.62
97:DA:51:LYS:NZ	115:DT:205:HIS:O	2.27	0.62
99:DC:521:LEU:HD21	106:DJ:144:MET:HE1	1.82	0.62
112:DQ:199:ARG:NH1	150:DQ:1501:CDL:O1	2.33	0.62
113:DR:124:TYR:O	113:DR:128:VAL:HG22	2.00	0.62
100:Dd:503:LEU:CB	132:Ek:40:ILE:HD11	2.29	0.62
118:Dw:98:GLN:OE1	118:Dw:98:GLN:N	2.33	0.62
124:Ec:56:LEU:O	124:Ec:60:LEU:HG	1.99	0.62
44:BA:134:ARG:NE	155:BA:301:3PE:O12	2.30	0.62
89:E:82:GLU:OE1	89:E:82:GLU:N	2.32	0.62
114:DS:156:LEU:HD12	114:DS:194:LEU:C	2.25	0.62
100:Dd:431:ASP:OD2	100:Dd:433:THR:OG1	2.16	0.62
168:Ed:201:HEM:HBC2	168:Ed:201:HEM:CMC	2.29	0.62
128:Eg:75:ARG:NH2	142:Eu:38:GLU:OE2	2.32	0.62
133:El:13:ARG:NH2	139:Er:104:LYS:O	2.33	0.62
18:AH:25:ASN:OD1	34:AX:12:ASN:ND2	2.33	0.62
87:C:211:SER:O	91:G:94:ARG:NH2	2.33	0.62
98:DB:69:THR:HG21	115:DT:234:GLU:O	2.00	0.62
105:DI:74:MET:SD	115:DT:109:GLN:NE2	2.73	0.62
119:Dx:220:GLN:OE1	119:Dx:220:GLN:N	2.33	0.62
145:Ex:20:THR:HG22	147:Ez:49:TYR:CE1	2.35	0.62
17:AG:323:ASN:OD1	28:AR:63:SER:OG	2.16	0.61
87:C:167:ILE:HG21	167:C:511:UQ8:H30A	1.80	0.61
86:b:57:ARG:NH1	86:b:58:GLY:O	2.33	0.61
111:DP:190:LYS:O	111:DP:193:ARG:NH1	2.32	0.61
168:Ed:201:HEM:HBB2	168:Ed:201:HEM:CMB	2.29	0.61
7:A6:71:PHE:CE2	7:A6:75:ILE:HD11	2.36	0.61
18:AH:264:PHE:O	43:B6:9:LYS:NZ	2.29	0.61
88:D:79:ARG:NH1	88:D:219:ASP:O	2.32	0.61
97:Da:682:GLU:OE1	114:Ds:96:ARG:NH2	2.33	0.61
114:Ds:152:VAL:HG21	114:Ds:198:SER:CB	2.29	0.61
121:Dz:122:LEU:O	121:Dz:126:ILE:HG22	2.00	0.61
14:AD:60:GLY:O	14:AD:257:ARG:NH1	2.33	0.61
14:AD:76:ILE:HG23	14:AD:256:MET:HE3	1.81	0.61
98:DB:122:TRP:CD1	98:DB:553:CYS:HG	2.17	0.61
100:DD:119:VAL:HG23	100:DD:120:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:Db:112:LEU:HD11	98:Db:139:THR:HG22	1.81	0.61
16:AF:257:ILE:HD13	16:AF:262:ILE:HD12	1.83	0.61
77:CG:17:ILE:HG21	79:CE:41:LEU:HD21	1.80	0.61
97:DA:415:ARG:NH1	97:DA:416:ARG:O	2.34	0.61
98:Db:155:GLU:OE1	98:Db:157:GLN:N	2.32	0.61
100:Dd:293:VAL:HG13	109:Dn:271:ILE:HD13	1.82	0.61
115:Dt:48:GLU:OE1	115:Dt:48:GLU:N	2.32	0.61
11:AA:604:PHE:HZ	11:AA:710:LEU:HD22	1.64	0.61
24:AN:65:TYR:OH	24:AN:129:ASP:OD2	2.18	0.61
87:C:169:THR:OG1	87:C:177:THR:OG1	2.19	0.61
89:E:118:LEU:HD11	167:c:510:UQ8:H45A	1.81	0.61
99:Dc:536:LYS:NZ	129:Eh:0:ACE:O	2.33	0.61
114:Ds:208:GLN:OE1	114:Ds:304:TYR:OH	2.14	0.61
45:BB:84:HIS:NE2	45:BB:86:GLU:OE2	2.33	0.61
121:DZ:115:LYS:NZ	121:DZ:150:PHE:O	2.21	0.61
26:AP:6:TRP:NE1	26:AP:28:THR:O	2.32	0.61
90:f:31:CYS:HG	90:f:64:TRP:CD1	2.18	0.61
113:Dr:242:ALA:O	127:Ef:164:ARG:NH1	2.33	0.61
117:Dv:262:TRP:N	150:Dv:402:CDL:OB3	2.34	0.61
13:AC:14:ILE:O	13:AC:160:TYR:OH	2.18	0.61
22:AL:124:HIS:CE1	159:AL:302:SF4:S1	2.94	0.61
97:DA:586:MET:SD	97:DA:601:HIS:NE2	2.73	0.61
112:DQ:230:ASP:OD1	112:DQ:231:ARG:N	2.32	0.61
115:Dt:45:PRO:HG2	115:Dt:50:ILE:HD11	1.83	0.61
16:AF:115:LYS:NZ	21:AK:248:GLU:OE2	2.29	0.61
100:DD:403:ASP:OD1	100:DD:404:GLN:N	2.34	0.61
136:EO:9:VAL:O	136:EO:13:ASN:ND2	2.34	0.61
98:Db:508:ASN:OD1	98:Db:509:SER:N	2.33	0.61
129:Eh:36:SER:OG	129:Eh:121:ASP:OD2	2.12	0.61
31:AU:51:ASN:OD1	31:AU:52:LYS:N	2.33	0.61
63:BT:103:PHE:CZ	150:BT:204:CDL:H451	2.35	0.61
134:EM:133:TYR:OH	142:Eu:12:ASP:OD1	2.19	0.61
101:De:8:ARG:NH1	112:Dq:218:ASP:OD1	2.34	0.61
114:Ds:289:TYR:OH	150:Ds:405:CDL:OA9	2.08	0.61
12:AB:350:GLU:N	12:AB:350:GLU:OE1	2.34	0.60
114:DS:140:THR:HG21	114:DS:214:TYR:HB2	1.83	0.60
113:Dr:174:TYR:O	113:Dr:203:TYR:OH	2.14	0.60
68:BY:50:ILE:O	68:BY:54:THR:OG1	2.16	0.60
86:B:40:GLU:OE1	86:B:40:GLU:N	2.33	0.60
87:C:135:VAL:HG11	87:C:181:LEU:HD23	1.83	0.60
87:C:183:TYR:HB3	167:C:511:UQ8:H21A	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:e:157:LEU:HD13	89:e:191:ILE:HD13	1.83	0.60
108:DM:237:ARG:NH2	121:DZ:48:ASP:OD2	2.34	0.60
112:DQ:116:ASN:ND2	150:DX:301:CDL:OB3	2.34	0.60
134:EM:49:LYS:O	134:EM:54:ARG:NH1	2.34	0.60
118:Dw:134:MET:HE3	118:Dw:232:HIS:HD2	1.65	0.60
149:DL:406:ASP:O	149:DL:421:ASN:ND2	2.33	0.60
23:AM:166:VAL:HG23	23:AM:196:LEU:HD11	1.81	0.60
3:A2:127:LYS:O	3:A2:130:THR:OG1	2.11	0.60
35:AY:20:VAL:O	35:AY:24:LYS:NZ	2.30	0.60
79:CE:183:ARG:NE	79:CE:219:ASP:OD1	2.34	0.60
98:DB:574:LEU:O	98:DB:578:THR:HG22	2.01	0.60
114:DS:152:VAL:HG21	114:DS:198:SER:CB	2.31	0.60
127:Ef:180:VAL:HG21	153:Ef:501:PC1:H282	1.83	0.60
149:Dl:98:GLU:OE1	149:Dl:98:GLU:N	2.34	0.60
71:CM:17:GLN:NE2	80:CJ:53:ILE:O	2.33	0.60
88:D:288:GLU:OE1	88:D:290:TYR:OH	2.16	0.60
92:H:38:TYR:OH	85:a:384:ASN:ND2	2.34	0.60
98:DB:233:ASP:OD1	98:DB:234:ASP:N	2.34	0.60
100:DD:575:PHE:CE2	100:DD:579:ILE:HD11	2.36	0.60
114:DS:207:PHE:O	114:DS:211:THR:HG22	2.02	0.60
168:ED:602:HEM:HBB2	168:ED:602:HEM:CMB	2.29	0.60
168:ED:602:HEM:HBC2	168:ED:602:HEM:CMC	2.29	0.60
112:Dq:1:MET:N	112:Dq:1:MET:SD	2.75	0.60
19:AI:75:VAL:HG21	19:AI:91:ILE:HD11	1.84	0.60
91:g:5:GLU:OE2	95:k:2:TYR:OH	2.19	0.60
137:EP:92:HIS:ND1	137:EP:105:ASP:OD1	2.33	0.60
112:Dq:101:ARG:NH1	132:Ek:45:GLN:OE1	2.35	0.60
119:Dx:41:ALA:O	119:Dx:45:ASN:ND2	2.34	0.60
55:BL:124:ASP:OD1	55:BL:125:LEU:N	2.35	0.60
77:CG:114:ARG:NH1	150:CD:301:CDL:OB4	2.35	0.60
88:D:65:TYR:OH	88:D:240:ASN:OD1	2.12	0.60
153:DG:203:PC1:O12	127:EF:86:TYR:OH	2.15	0.60
124:EC:56:LEU:O	124:EC:60:LEU:HG	2.00	0.60
11:AA:545:TYR:CZ	40:B3:48:THR:HG22	2.36	0.60
20:AJ:208:ASN:O	20:AJ:212:VAL:HG23	2.00	0.60
56:BM:11:VAL:HG12	56:BM:12:ASP:H	1.66	0.60
167:c:510:UQ8:H40A	167:c:510:UQ8:H43	1.83	0.60
153:DA:708:PC1:H2I3	153:DA:708:PC1:H2E1	1.83	0.60
98:DB:155:GLU:OE1	98:DB:157:GLN:N	2.33	0.60
147:EZ:28:ASN:O	148:FA:27:LYS:NZ	2.34	0.60
108:Dm:79:GLU:OE1	108:Dm:79:GLU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
143:Ej:79:VAL:HG11	143:Ej:99:PHE:CZ	2.37	0.60
11:AA:572:TYR:HH	62:BS:62:CYS:HG	1.49	0.60
108:DM:280:GLU:OE2	138:EQ:70:ASN:ND2	2.33	0.60
119:DX:220:GLN:N	119:DX:220:GLN:OE1	2.35	0.60
114:Ds:207:PHE:O	114:Ds:211:THR:HG22	2.01	0.60
19:AI:79:ASN:OD1	19:AI:82:TRP:NE1	2.34	0.60
22:AL:171:ASP:OD2	22:AL:174:LYS:NZ	2.35	0.60
98:DB:145:ASN:ND2	107:DK:31:ASP:OD2	2.35	0.60
130:EI:49:LEU:O	130:EI:54:ARG:NE	2.35	0.60
115:Dt:135:LEU:O	115:Dt:140:GLN:NE2	2.34	0.60
23:AM:89:LEU:HD22	23:AM:110:ILE:HD12	1.83	0.59
49:BF:101:GLN:NE2	59:BP:127:ILE:O	2.35	0.59
155:EL:904:3PE:H2E2	155:EL:904:3PE:H2I2	1.84	0.59
109:Dn:67:GLU:OE1	109:Dn:67:GLU:N	2.35	0.59
110:Do:450:PRO:O	110:Do:453:ASN:ND2	2.34	0.59
12:AB:68:GLU:OE1	12:AB:68:GLU:N	2.34	0.59
38:B1:76:VAL:HG11	39:B2:35:MET:CE	2.32	0.59
86:B:118:LEU:O	86:B:129:ASN:ND2	2.36	0.59
150:DG:201:CDL:H222	127:EF:177:LEU:HD11	1.83	0.59
150:DN:507:CDL:OA3	128:EG:56:SER:OG	2.20	0.59
113:DR:139:LYS:NZ	113:DR:329:SER:OG	2.34	0.59
115:DT:200:GLU:N	115:DT:200:GLU:OE1	2.35	0.59
113:Dr:124:TYR:O	113:Dr:128:VAL:HG22	2.02	0.59
150:Ds:401:CDL:OA3	135:En:70:TRP:N	2.34	0.59
149:Dl:170:ASP:OD1	149:Dl:171:VAL:N	2.33	0.59
10:A9:186:GLN:OE1	10:A9:186:GLN:N	2.36	0.59
16:AF:218:THR:HG22	16:AF:229:ILE:HG21	1.83	0.59
50:BG:32:GLU:OE1	50:BG:32:GLU:N	2.36	0.59
67:BX:46:GLN:OE1	67:BX:46:GLN:N	2.35	0.59
92:H:40:SER:OG	92:H:43:SER:OG	2.20	0.59
112:DQ:16:LEU:O	137:EP:75:HIS:NE2	2.35	0.59
112:DQ:98:GLU:OE2	132:EK:51:ARG:NE	2.35	0.59
115:DT:145:TYR:O	115:DT:149:ASN:ND2	2.33	0.59
97:Da:296:ILE:HG23	97:Da:357:VAL:CG1	2.32	0.59
143:Ej:73:ASN:OD1	143:Ej:108:ARG:NH2	2.34	0.59
5:A4:253:ASP:OD2	5:A4:273:ARG:NE	2.34	0.59
77:CG:52:GLU:OE1	77:CG:52:GLU:N	2.35	0.59
97:DA:532:SER:OG	97:DA:571:GLN:NE2	2.32	0.59
155:DC:607:3PE:H2E2	155:DC:607:3PE:H2I3	1.85	0.59
104:DH:72:TYR:OH	121:DZ:39:GLY:O	2.14	0.59
112:DQ:101:ARG:NH1	132:EK:45:GLN:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:Db:574:LEU:O	98:Db:578:THR:HG22	2.02	0.59
85:A:61:ASP:OD2	85:A:449:SER:OG	2.20	0.59
103:DG:81:MET:O	103:DG:85:ASN:ND2	2.35	0.59
97:Da:643:TYR:O	98:Db:69:THR:HG23	2.03	0.59
108:Dm:449:ILE:HD12	108:Dm:450:ASN:N	2.16	0.59
64:BU:106:ASN:O	64:BU:106:ASN:ND2	2.36	0.59
75:CB:214:GLU:N	75:CB:214:GLU:OE1	2.35	0.59
87:C:339:SER:OG	91:G:209:GLU:OE1	2.17	0.59
97:DA:252:VAL:O	97:DA:255:ARG:NH1	2.35	0.59
129:EH:36:SER:OG	129:EH:121:ASP:OD2	2.18	0.59
99:Dc:80:LEU:HD13	110:Do:273:MET:SD	2.43	0.59
86:B:272:GLN:OE1	86:B:272:GLN:N	2.35	0.59
85:a:47:GLY:O	95:k:1:MET:N	2.33	0.59
85:a:382:TYR:OH	92:h:1:MET:O	2.16	0.59
97:DA:116:GLY:O	97:DA:120:ASN:ND2	2.36	0.59
104:DH:34:TRP:O	108:DM:428:GLN:NE2	2.35	0.59
136:EO:56:GLU:N	136:EO:56:GLU:OE1	2.35	0.59
102:Df:224:GLU:OE1	102:Df:224:GLU:N	2.34	0.59
107:Dk:42:GLU:N	107:Dk:42:GLU:OE1	2.34	0.59
128:Eg:80:ARG:CZ	129:Eh:1:MET:HE3	2.32	0.59
8:A7:110:LYS:NZ	42:B5:64:THR:O	2.35	0.59
48:BE:72:GLU:OE1	48:BE:80:LYS:NZ	2.35	0.59
168:C:501:HEM:HBB2	168:C:501:HEM:HMB2	1.84	0.59
168:C:502:HEM:HMC1	168:C:502:HEM:HBC2	1.83	0.59
86:b:40:GLU:OE1	86:b:40:GLU:N	2.35	0.59
97:DA:468:ILE:HD11	98:DB:83:CYS:SG	2.43	0.59
100:Dd:312:VAL:HG21	101:De:15:ILE:HD11	1.84	0.59
86:b:118:LEU:O	86:b:129:ASN:ND2	2.35	0.59
99:DC:566:ASN:ND2	122:EA:30:MET:SD	2.74	0.59
100:DD:497:HIS:ND1	109:DN:191:TYR:OH	2.34	0.59
100:DD:502:TYR:CE1	100:DD:506:LEU:HD21	2.37	0.59
115:DT:267:LYS:NZ	115:DT:268:GLU:OE2	2.26	0.59
137:EP:88:SER:OG	137:EP:109:LEU:HD11	2.03	0.59
99:Dc:263:VAL:O	104:Dh:108:ARG:NH1	2.35	0.59
145:Ex:20:THR:HG22	147:Ez:49:TYR:HE1	1.66	0.59
87:c:135:VAL:HG11	87:c:181:LEU:HD23	1.85	0.58
102:DF:36:ASP:OD2	136:EO:81:ARG:NH2	2.35	0.58
98:Db:182:SER:O	98:Db:186:THR:HG22	2.02	0.58
150:Dx:1204:CDL:H872	150:Dx:1204:CDL:H831	1.84	0.58
116:DU:88:VAL:HG11	116:DU:288:PHE:CD1	2.38	0.58
126:EE:157:CYS:SG	126:EE:173:ARG:NH2	2.75	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
129:EH:59:LEU:HD22	150:EH:1601:CDL:H271	1.85	0.58
97:Da:296:ILE:HG23	97:Da:357:VAL:HG13	1.84	0.58
149:Dl:340:ASN:OD1	149:Dl:342:ARG:NH1	2.36	0.58
1:A0:15:ARG:NH1	1:A0:44:ASN:OD1	2.36	0.58
37:B0:43:ASP:OD1	41:B4:38:ARG:NH1	2.37	0.58
85:A:513:VAL:O	92:h:35:ASN:ND2	2.36	0.58
97:Da:353:LEU:HD22	97:Da:389:PHE:CE2	2.38	0.58
101:De:23:LYS:NZ	125:Ed:151:ASN:OD1	2.36	0.58
109:Dn:385:ILE:HD11	120:Dy:126:ILE:CD1	2.32	0.58
110:Do:75:GLU:OE1	110:Do:145:ARG:NH2	2.35	0.58
117:Dv:2:ASN:ND2	123:Eb:25:ASP:OD1	2.37	0.58
25:AO:159:ASP:OD1	25:AO:160:TYR:N	2.36	0.58
86:B:319:ILE:O	86:B:323:ASN:ND2	2.35	0.58
114:DS:152:VAL:HG23	114:DS:201:LEU:HD22	1.85	0.58
116:DU:50:GLU:OE1	138:EQ:25:TYR:OH	2.21	0.58
100:Dd:469:ARG:NH1	100:Dd:516:ASP:OD2	2.37	0.58
106:Dj:91:ARG:NH1	136:Eo:7:ASN:OD1	2.36	0.58
120:Dy:226:ASN:C	120:Dy:227:LEU:HD12	2.28	0.58
124:Ec:136:GLU:O	124:Ec:140:VAL:HG23	2.03	0.58
133:El:57:ALA:O	140:Es:83:THR:HG21	2.04	0.58
134:Em:67:GLU:OE1	134:Em:67:GLU:N	2.37	0.58
118:Dw:271:GLU:OE1	118:Dw:271:GLU:N	2.35	0.58
134:Em:116:GLN:O	134:Em:119:ASN:ND2	2.36	0.58
29:AS:44:THR:O	29:AS:55:LYS:NZ	2.35	0.58
91:G:121:ARG:NE	89:e:67:LYS:O	2.36	0.58
100:DD:74:THR:OG1	150:DD:703:CDL:OA3	2.15	0.58
115:DT:170:ASN:ND2	115:DT:174:GLU:O	2.37	0.58
133:EL:57:ALA:O	140:ES:83:THR:HG21	2.02	0.58
99:Dc:470:ARG:NH1	99:Dc:473:GLU:OE2	2.36	0.58
103:Dg:81:MET:O	103:Dg:85:ASN:ND2	2.37	0.58
104:Dh:72:TYR:OH	121:Dz:39:GLY:O	2.12	0.58
111:Dp:326:ASP:OD1	111:Dp:330:LYS:NZ	2.35	0.58
118:Dw:134:MET:HE3	118:Dw:232:HIS:CD2	2.39	0.58
133:El:108:ASP:OD1	133:El:109:ARG:N	2.37	0.58
149:DL:189:SER:OG	149:DL:225:ARG:NH1	2.36	0.58
11:AA:501:THR:O	11:AA:683:ASN:ND2	2.37	0.58
86:B:115:ASN:ND2	86:B:187:ASN:OD1	2.37	0.58
168:c:504:HEM:HMB2	168:c:504:HEM:HBB2	1.85	0.58
115:DT:271:ARG:NH1	115:DT:279:GLU:OE1	2.36	0.58
100:Dd:119:VAL:HG23	100:Dd:120:THR:HG23	1.85	0.58
114:Ds:342:GLU:OE1	114:Ds:342:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
124:Ec:7:GLU:OE2	124:Ec:26:LYS:NZ	2.36	0.58
137:Ep:79:GLU:OE1	137:Ep:79:GLU:N	2.35	0.58
7:A6:155:GLU:OE2	7:A6:159:ARG:NE	2.37	0.58
87:C:135:VAL:HG11	87:C:181:LEU:CD2	2.34	0.58
2:A1:30:LYS:NZ	12:AB:609:ASP:OD2	2.36	0.58
3:A2:29:LEU:HD12	3:A2:80:LEU:HD12	1.84	0.58
6:A5:141:ARG:NH1	24:AN:104:GLU:OE2	2.36	0.58
9:A8:300:HIS:ND1	9:A8:301:GLU:OE1	2.37	0.58
61:BR:99:GLN:OE1	61:BR:101:TYR:OH	2.08	0.58
97:Da:565:ILE:HD11	150:En:1201:CDL:H342	1.86	0.58
3:A2:113:ARG:NH1	3:A2:122:ILE:O	2.37	0.58
15:AE:368:LEU:HD12	15:AE:368:LEU:O	2.04	0.58
17:AG:44:ASP:O	21:AK:222:GLN:NE2	2.36	0.58
100:DD:439:LYS:NZ	100:DD:524:GLU:OE1	2.35	0.58
99:Dc:524:ARG:NH2	133:El:140:ASP:O	2.36	0.58
112:Dq:34:THR:OG1	112:Dq:51:GLY:O	2.22	0.58
16:AF:223:TRP:O	16:AF:227:ASN:ND2	2.34	0.57
18:AH:183:PHE:HB3	18:AH:261:ILE:HG21	1.85	0.57
34:AX:111:TRP:CE2	56:BM:57:LEU:HD21	2.39	0.57
73:CA:623:ASP:OD1	73:CA:624:SER:N	2.34	0.57
112:DQ:1:MET:N	112:DQ:1:MET:SD	2.77	0.57
104:Dh:128:ASP:OD1	104:Dh:129:ARG:N	2.37	0.57
150:Dh:201:CDL:H671	150:Dn:506:CDL:H822	1.85	0.57
29:AS:88:ASN:ND2	29:AS:133:LEU:O	2.37	0.57
73:CA:573:LEU:HD12	73:CA:612:VAL:HG21	1.86	0.57
86:B:81:THR:OG1	86:B:259:HIS:ND1	2.20	0.57
100:DD:410:SER:OG	100:DD:412:ARG:NH1	2.36	0.57
98:Db:578:THR:HG23	98:Db:579:PHE:CD2	2.39	0.57
136:Eo:12:THR:O	136:Eo:12:THR:HG22	2.04	0.57
88:D:94:TYR:CZ	87:c:72:VAL:HG21	2.40	0.57
86:b:469:ASN:OD1	86:b:470:ALA:N	2.37	0.57
168:c:505:HEM:HBC2	168:c:505:HEM:HMC1	1.86	0.57
108:DM:362:ASP:O	108:DM:380:ARG:NH2	2.38	0.57
114:DS:58:GLU:N	114:DS:58:GLU:OE1	2.36	0.57
119:Dx:228:ASN:ND2	119:Dx:228:ASN:O	2.37	0.57
11:AA:82:LEU:O	118:Dw:302:LEU:HD11	2.04	0.57
24:AN:50:GLU:OE1	24:AN:50:GLU:N	2.35	0.57
25:AO:155:LYS:NZ	25:AO:162:LYS:O	2.36	0.57
76:CF:190:ARG:NH2	76:CF:223:GLU:OE2	2.37	0.57
76:CF:277:SER:HB3	78:CK:80:ILE:HD11	1.86	0.57
76:CF:279:GLN:N	76:CF:279:GLN:OE1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B:326:ALA:O	86:B:330:ASN:ND2	2.37	0.57
89:E:190:VAL:C	89:E:191:ILE:HD12	2.30	0.57
85:a:124:GLU:N	85:a:124:GLU:OE1	2.38	0.57
86:b:101:ASP:OD2	86:b:248:ARG:NH2	2.37	0.57
99:DC:481:LEU:O	99:DC:485:ASN:ND2	2.37	0.57
100:DD:466:GLN:OE1	100:DD:547:ASN:ND2	2.36	0.57
108:DM:439:TYR:OH	121:DZ:189:GLU:OE1	2.15	0.57
105:Di:115:GLU:OE1	105:Di:115:GLU:N	2.36	0.57
116:Du:145:TYR:CE2	116:Du:149:ILE:HD11	2.39	0.57
119:Dx:35:GLU:OE1	119:Dx:35:GLU:N	2.36	0.57
121:Dz:186:ILE:O	143:Ej:32:LYS:NZ	2.37	0.57
149:Dl:113:ASN:O	149:Dl:129:ASN:N	2.37	0.57
6:A5:186:ALA:O	6:A5:192:ARG:NH1	2.38	0.57
150:C:505:CDL:C62	167:C:512:UQ8:H25B	2.34	0.57
88:d:65:TYR:OH	88:d:240:ASN:OD1	2.18	0.57
89:e:218:CYS:SG	89:e:219:HIS:N	2.77	0.57
111:DP:197:ARG:O	111:DP:198:ARG:NH1	2.37	0.57
104:Dh:27:LYS:NZ	109:Dn:288:ASN:O	2.37	0.57
17:AG:261:GLU:OE2	60:BQ:43:ASN:ND2	2.36	0.57
89:e:134:ILE:HD12	89:e:252:VAL:HG21	1.86	0.57
89:e:245:ILE:HD12	89:e:252:VAL:HG22	1.86	0.57
97:DA:242:GLU:OE2	123:EB:74:LYS:NZ	2.35	0.57
104:DH:80:VAL:HG21	109:DN:352:LEU:HB2	1.86	0.57
117:DV:249:ASN:N	117:DV:255:ASN:OD1	2.36	0.57
120:DY:64:SER:OG	120:DY:189:ASN:OD1	2.16	0.57
135:EN:70:TRP:N	150:EN:1202:CDL:OA3	2.38	0.57
137:EP:79:GLU:OE1	137:EP:79:GLU:N	2.37	0.57
110:Do:454:GLN:OE1	110:Do:454:GLN:N	2.38	0.57
123:Eb:82:PHE:CE2	123:Eb:86:ILE:HD11	2.39	0.57
5:A4:175:VAL:HG21	5:A4:296:ILE:HG21	1.87	0.57
11:AA:501:THR:HG22	11:AA:581:LEU:HA	1.86	0.57
13:AC:145:ASN:OD1	13:AC:145:ASN:N	2.34	0.57
25:AO:77:GLN:N	25:AO:77:GLN:OE1	2.37	0.57
37:B0:47:ARG:NH1	37:B0:51:ARG:O	2.38	0.57
97:DA:380:ILE:HD12	97:DA:445:VAL:CG1	2.35	0.57
99:DC:80:LEU:HD13	110:DO:273:MET:SD	2.45	0.57
99:DC:368:ILE:HD12	99:DC:401:ILE:HD12	1.87	0.57
137:Ep:88:SER:OG	137:Ep:109:LEU:HD11	2.04	0.57
14:AD:120:GLU:O	14:AD:160:ARG:NH1	2.36	0.57
89:e:190:VAL:C	89:e:191:ILE:HD12	2.29	0.57
105:DI:203:MET:O	105:DI:206:THR:OG1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:DZ:122:LEU:O	121:DZ:126:ILE:HG22	2.04	0.57
128:EG:10:GLN:NE2	129:EH:113:GLU:OE2	2.38	0.57
74:CI:95:ASP:OD1	74:CI:96:TYR:N	2.38	0.57
86:b:128:ILE:HD12	91:g:29:LYS:HA	1.87	0.57
93:i:99:GLU:OE1	93:i:99:GLU:N	2.37	0.57
100:Dd:242:GLU:N	100:Dd:242:GLU:OE1	2.38	0.57
100:Dd:426:LYS:O	140:Es:60:TYR:OH	2.14	0.57
15:AE:77:GLN:O	30:AT:102:TYR:OH	2.22	0.57
49:BF:88:SER:O	49:BF:89:SER:OG	2.17	0.57
155:DS:402:3PE:H3I3	155:DS:402:3PE:H3E2	1.87	0.57
125:ED:115:ILE:HG12	167:ED:603:UQ8:H4MB	1.86	0.57
98:Db:592:ARG:O	98:Db:596:HIS:ND1	2.38	0.57
73:CA:246:GLY:O	73:CA:262:GLY:N	2.37	0.56
110:Do:62:SER:OG	110:Do:214:ARG:NH2	2.38	0.56
120:Dy:118:ARG:O	120:Dy:122:THR:HG22	2.05	0.56
135:EN:105:TRP:O	135:EN:109:SER:OG	2.14	0.56
97:Da:42:LYS:NZ	105:Di:117:ASP:OD2	2.29	0.56
100:Dd:440:ALA:O	100:Dd:543:ASN:ND2	2.37	0.56
113:Dr:343:GLU:HA	127:Ef:77:ILE:HD11	1.86	0.56
1:A0:458:VAL:HG13	1:A0:470:VAL:HG23	1.86	0.56
13:AC:215:ILE:CD1	51:BH:105:THR:HG21	2.32	0.56
18:AH:37:ALA:O	18:AH:40:THR:OG1	2.22	0.56
21:AK:103:THR:HG22	21:AK:115:VAL:HG23	1.86	0.56
85:a:354:GLU:OE1	85:a:510:TYR:OH	2.21	0.56
87:c:38:THR:HG23	87:c:91:LEU:HD12	1.88	0.56
100:DD:435:LEU:HD22	100:DD:528:VAL:HG11	1.85	0.56
106:DJ:143:ARG:NH2	106:DJ:186:ASP:OD1	2.38	0.56
110:DO:253:ARG:NH2	143:EJ:88:ASP:O	2.37	0.56
118:DW:141:TYR:O	134:EM:7:ARG:NH1	2.36	0.56
138:EQ:0:ACE:H1	138:EQ:4:PHE:HZ	1.70	0.56
138:EQ:1:MET:HB3	138:EQ:107:TYR:OH	2.05	0.56
117:Dv:115:ASP:OD1	117:Dv:116:LEU:N	2.38	0.56
134:Em:49:LYS:O	134:Em:54:ARG:NH1	2.38	0.56
10:A9:219:ASN:O	10:A9:224:ARG:NH2	2.37	0.56
168:c:505:HEM:HMB2	168:c:505:HEM:HBB2	1.86	0.56
146:EY:5:LEU:HD21	148:FA:14:VAL:HG11	1.86	0.56
125:Ed:170:TYR:O	125:Ed:174:ARG:NH1	2.38	0.56
18:AH:43:GLU:HA	43:B6:18:ILE:HD13	1.87	0.56
63:BT:107:LEU:HB2	150:BT:204:CDL:C41	2.36	0.56
155:C:513:3PE:H3I1	96:L:21:VAL:HG11	1.87	0.56
103:DG:40:TYR:CE2	103:DG:44:ILE:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:DP:312:ARG:O	111:DP:321:ASN:ND2	2.38	0.56
129:Eh:85:ASN:OD1	129:Eh:86:LEU:N	2.39	0.56
133:El:42:ARG:NE	139:Er:21:GLU:OE2	2.31	0.56
62:BS:71:HIS:NE2	153:BS:1301:PC1:O14	2.30	0.56
124:EC:99:ARG:NH1	118:Dw:20:THR:OG1	2.38	0.56
100:Dd:265:LEU:HD13	100:Dd:271:TYR:CD2	2.41	0.56
101:De:34:ASP:OD1	101:De:38:LYS:NZ	2.33	0.56
105:Di:87:ILE:HG23	113:Dr:130:VAL:HG12	1.88	0.56
112:Dq:220:VAL:HG22	112:Dq:224:ALA:CB	2.36	0.56
113:Dr:166:TYR:O	113:Dr:211:ARG:NH2	2.39	0.56
141:Et:12:GLN:OE1	141:Et:16:ARG:NH2	2.39	0.56
12:AB:642:GLU:OE2	28:AR:35:GLY:N	2.38	0.56
13:AC:261:PRO:CG	153:AC:804:PC1:H2H1	2.36	0.56
16:AF:119:ILE:CD1	51:BH:144:ILE:HD12	2.36	0.56
16:AF:198:TRP:CH2	35:AY:29:ILE:HG22	2.41	0.56
21:AK:227:GLU:OE1	21:AK:227:GLU:N	2.38	0.56
168:C:502:HEM:HBB2	168:C:502:HEM:HMB1	1.87	0.56
86:b:125:ASN:OD1	86:b:126:GLU:N	2.38	0.56
97:DA:353:LEU:HD22	97:DA:389:PHE:CE2	2.41	0.56
97:DA:501:ALA:HB2	97:DA:529:ILE:HG22	1.88	0.56
106:DJ:49:TYR:OH	137:EP:105:ASP:O	2.22	0.56
119:DX:41:ALA:O	119:DX:45:ASN:ND2	2.39	0.56
122:EA:60:LEU:HD23	122:EA:61:LYS:N	2.21	0.56
109:Dn:213:ASN:OD1	124:Ec:182:LYS:NZ	2.39	0.56
112:Dq:16:LEU:O	137:Ep:75:HIS:NE2	2.38	0.56
115:Dt:83:TYR:N	127:Ef:59:ILE:O	2.37	0.56
115:Dt:170:ASN:ND2	115:Dt:174:GLU:O	2.39	0.56
128:Eg:4:ASP:OD1	128:Eg:5:PHE:N	2.39	0.56
14:AD:226:VAL:HG12	14:AD:228:PRO:HD3	1.88	0.56
19:AI:209:GLN:OE1	19:AI:209:GLN:N	2.39	0.56
85:A:428:SER:OG	86:B:411:GLU:OE2	2.15	0.56
88:D:261:PHE:CE2	88:D:265:LEU:HD11	2.41	0.56
100:DD:220:MET:HE3	100:DD:248:THR:HG21	1.88	0.56
118:DW:197:VAL:HG23	118:DW:249:VAL:HG11	1.87	0.56
108:Dm:203:TYR:N	108:Dm:206:ASP:OD1	2.37	0.56
114:Ds:306:TRP:NE1	150:Ds:401:CDL:OB7	2.37	0.56
133:El:23:THR:HG22	133:El:151:PRO:HG2	1.87	0.56
6:A5:229:ASP:OD1	6:A5:230:ASN:N	2.36	0.56
35:AY:80:LEU:HG	35:AY:84:LEU:HD12	1.87	0.56
46:BC:58:ASP:OD1	46:BC:59:GLN:N	2.38	0.56
109:DN:192:ILE:HD11	132:EK:46:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:Dp:197:ARG:NE	111:Dp:204:GLU:OE2	2.39	0.56
7:A6:115:LYS:O	7:A6:118:SER:OG	2.23	0.56
12:AB:487:GLU:OE1	12:AB:487:GLU:N	2.37	0.56
13:AC:54:LEU:HD12	13:AC:58:PHE:CD2	2.40	0.56
85:A:71:ASN:ND2	85:A:270:VAL:O	2.39	0.56
89:e:117:ARG:NE	89:e:117:ARG:O	2.37	0.56
120:DY:226:ASN:C	120:DY:227:LEU:HD12	2.30	0.56
124:EC:180:ASN:O	124:EC:185:ARG:NH1	2.38	0.56
148:FA:50:GLU:OE1	148:FA:50:GLU:N	2.39	0.56
87:c:251:GLU:OE1	87:c:251:GLU:N	2.37	0.55
110:DO:116:GLY:O	110:DO:120:VAL:HG23	2.06	0.55
112:DQ:110:TYR:CE2	112:DQ:172:LEU:HD23	2.41	0.55
150:DS:404:CDL:OB9	117:DV:62:ASN:ND2	2.40	0.55
115:DT:253:ASP:OD1	115:DT:254:GLU:N	2.38	0.55
99:Dc:69:LYS:NZ	143:Ej:66:GLU:OE2	2.32	0.55
123:Eb:39:ASN:C	123:Eb:40:LEU:HD12	2.31	0.55
2:A1:133:GLN:OE1	2:A1:133:GLN:N	2.39	0.55
49:BF:92:GLU:OE1	49:BF:92:GLU:N	2.37	0.55
85:a:419:PHE:CE1	85:a:455:ILE:HD11	2.41	0.55
98:Db:461:TYR:OH	118:Dw:190:GLU:OE2	2.19	0.55
129:Eh:2:ASP:OD2	129:Eh:10:ASN:ND2	2.38	0.55
3:A2:222:ARG:O	53:BJ:95:ARG:NH2	2.40	0.55
100:DD:120:THR:HG22	140:ES:25:TRP:CD2	2.41	0.55
100:DD:293:VAL:HG13	109:DN:271:ILE:HD13	1.88	0.55
120:DY:118:ARG:O	120:DY:122:THR:HG22	2.06	0.55
97:Da:128:GLY:HA3	97:Da:322:MET:HE2	1.88	0.55
119:Dx:47:GLN:NE2	130:Ei:165:ASP:OD1	2.39	0.55
120:Dy:141:LEU:O	120:Dy:145:ASN:ND2	2.39	0.55
13:AC:67:HIS:NE2	13:AC:124:THR:OG1	2.35	0.55
13:AC:458:LYS:NZ	46:BC:56:MET:SD	2.80	0.55
60:BQ:100:ARG:NH1	60:BQ:104:ASP:OD2	2.39	0.55
150:CG:301:CDL:OB3	80:CJ:38:TYR:OH	2.22	0.55
87:c:117:LYS:NZ	91:g:188:GLN:OE1	2.37	0.55
91:g:216:LYS:O	91:g:220:ASN:ND2	2.39	0.55
133:EL:23:THR:HG22	133:EL:151:PRO:HG2	1.87	0.55
98:Db:398:SER:OG	126:Ee:98:ASP:OD2	2.16	0.55
106:Dj:49:TYR:OH	137:Ep:105:ASP:O	2.25	0.55
6:A5:153:GLU:OE1	6:A5:156:ARG:NH2	2.39	0.55
11:AA:427:ALA:HB2	11:AA:522:PHE:HB3	1.89	0.55
86:b:146:GLN:OE1	86:b:146:GLN:N	2.38	0.55
86:b:272:GLN:OE1	86:b:272:GLN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:229:ASN:ND2	4:A3:232:THR:OG1	2.40	0.55
58:BO:104:ASP:OD2	58:BO:109:GLN:NE2	2.39	0.55
73:CA:118:ASP:OD1	73:CA:589:ARG:NH1	2.38	0.55
87:c:203:MET:HE3	167:c:510:UQ8:H4MA	1.89	0.55
168:c:504:HEM:HBC2	168:c:504:HEM:CMC	2.37	0.55
98:DB:360:LEU:HD23	126:EE:154:LEU:HD23	1.87	0.55
102:DF:23:PHE:C	102:DF:24:LEU:HD12	2.31	0.55
98:Db:116:ARG:NH2	102:Df:177:GLN:O	2.37	0.55
116:Du:182:ASN:ND2	116:Du:257:VAL:HG21	2.22	0.55
153:Eo:204:PC1:H2E2	153:Eo:204:PC1:H2I3	1.89	0.55
7:A6:130:THR:HG21	11:AA:744:ILE:CD1	2.36	0.55
77:CG:155:GLU:N	77:CG:155:GLU:OE1	2.37	0.55
85:A:101:LEU:HD11	93:I:32:LEU:HD12	1.89	0.55
108:DM:44:TYR:OH	112:DQ:315:GLU:OE2	2.22	0.55
126:EE:107:ASP:OD2	126:EE:108:ARG:NH1	2.40	0.55
97:Da:84:SER:HG	97:Da:591:HIS:HD1	1.51	0.55
98:Db:233:ASP:OD1	98:Db:234:ASP:N	2.39	0.55
99:Dc:566:ASN:ND2	122:Ea:30:MET:SD	2.80	0.55
110:Do:37:GLU:OE1	110:Do:37:GLU:N	2.39	0.55
150:Dr:402:CDL:H472	127:Ef:174:LEU:HD12	1.89	0.55
114:Ds:142:LEU:HD23	150:Ds:406:CDL:H851	1.89	0.55
122:Ea:60:LEU:HD23	122:Ea:61:LYS:N	2.22	0.55
132:Ek:6:PHE:CE2	132:Ek:10:ILE:HD11	2.42	0.55
149:DL:248:PHE:HB2	149:DL:269:LEU:HD21	1.87	0.55
19:AI:88:MET:HE2	19:AI:103:TYR:HD1	1.71	0.55
87:C:190:PHE:CE2	167:C:511:UQ8:H10B	2.42	0.55
99:DC:586:ILE:O	99:DC:590:ASN:ND2	2.40	0.55
100:DD:506:LEU:HD22	100:DD:544:PHE:CZ	2.42	0.55
143:EJ:67:LEU:O	143:EJ:75:GLN:NE2	2.39	0.55
14:AD:312:TRP:NE1	14:AD:334:ASP:OD1	2.38	0.55
48:BE:108:LYS:NZ	48:BE:151:GLU:OE1	2.39	0.55
73:CA:413:ASP:OD1	73:CA:414:LYS:N	2.38	0.55
100:DD:392:TYR:OH	100:DD:399:GLU:OE2	2.20	0.55
127:EF:174:LEU:HD23	127:EF:177:LEU:HD12	1.89	0.55
128:EG:4:ASP:OD1	128:EG:5:PHE:N	2.38	0.55
125:Ed:42:CYS:SG	168:Ed:201:HEM:C1A	2.99	0.55
1:A0:255:ARG:NH2	1:A0:264:LYS:O	2.40	0.55
11:AA:341:SER:HA	13:AC:454:ILE:HD11	1.88	0.55
13:AC:412:VAL:O	13:AC:415:SER:OG	2.21	0.55
15:AE:90:MET:SD	15:AE:170:HIS:N	2.79	0.55
47:BD:140:ARG:NH1	67:BX:92:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:b:333:ARG:NH2	86:b:394:GLU:OE1	2.39	0.55
125:ED:21:TYR:HE2	130:EI:79:ILE:HD11	1.72	0.55
17:AG:216:HIS:NE2	21:AK:83:ASP:OD2	2.37	0.54
22:AL:123:GLU:OE1	22:AL:195:ASN:ND2	2.40	0.54
72:CL:35:GLN:O	72:CL:69:LYS:NZ	2.28	0.54
89:E:112:MET:HG2	95:K:35:THR:HG23	1.88	0.54
115:DT:84:ASP:OD1	115:DT:85:GLY:N	2.40	0.54
119:DX:114:ASP:OD2	150:DX:307:CDL:O1	2.25	0.54
120:DY:141:LEU:O	120:DY:145:ASN:ND2	2.40	0.54
98:Db:391:LEU:HG	126:Ee:116:LEU:HD22	1.89	0.54
99:Dc:202:LYS:NZ	149:Dl:427:SER:O	2.32	0.54
108:Dm:84:ASN:OD1	108:Dm:85:ALA:N	2.40	0.54
113:Dr:222:ILE:HD12	113:Dr:236:ILE:HB	1.87	0.54
114:Ds:62:LEU:O	114:Ds:65:THR:HG22	2.06	0.54
140:Es:42:ALA:HB1	140:Es:53:LEU:HD11	1.89	0.54
9:A8:205:ASN:ND2	9:A8:205:ASN:O	2.40	0.54
16:AF:190:LEU:HB2	35:AY:84:LEU:HD13	1.89	0.54
77:CG:36:GLU:OE2	77:CG:106:LYS:NZ	2.41	0.54
104:DH:27:LYS:NZ	109:DN:288:ASN:O	2.40	0.54
99:Dc:386:LYS:O	99:Dc:389:THR:HG22	2.08	0.54
99:Dc:531:PHE:O	129:Eh:60:TYR:OH	2.23	0.54
111:Dp:333:ARG:HB3	116:Du:40:THR:HG21	1.89	0.54
116:Du:143:ALA:HB3	116:Du:144:PRO:HD3	1.89	0.54
8:A7:192:LYS:NZ	55:BL:8:PHE:O	2.26	0.54
86:b:115:ASN:ND2	86:b:187:ASN:OD1	2.38	0.54
99:DC:31:ASN:ND2	143:EJ:61:HIS:O	2.41	0.54
112:DQ:9:ARG:O	112:DQ:235:ASN:ND2	2.36	0.54
129:EH:12:ASP:OD1	129:EH:13:ARG:N	2.38	0.54
139:ER:60:TRP:CE2	139:ER:64:LEU:HD11	2.42	0.54
97:Da:123:ILE:O	97:Da:127:VAL:HG22	2.06	0.54
97:Da:180:LYS:NZ	97:Da:204:ASP:O	2.38	0.54
97:Da:342:THR:HG21	97:Da:400:PRO:HD3	1.88	0.54
109:Dn:359:SER:OG	150:Dn:501:CDL:OB4	2.19	0.54
126:Ee:106:GLU:N	126:Ee:106:GLU:OE1	2.41	0.54
143:Ej:101:GLN:OE1	143:Ej:101:GLN:N	2.40	0.54
148:Fa:6:SER:OG	148:Fa:9:ASN:OD1	2.26	0.54
13:AC:302:ILE:HG22	13:AC:304:ILE:HG22	1.88	0.54
150:AP:301:CDL:OA4	150:AP:301:CDL:O1	2.23	0.54
68:BY:22:ASP:OD1	68:BY:23:PHE:N	2.41	0.54
69:BZ:16:ARG:NH2	69:BZ:29:THR:O	2.40	0.54
108:DM:249:ASP:O	115:DT:34:ARG:NH2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
116:DU:182:ASN:ND2	116:DU:257:VAL:HG21	2.23	0.54
143:EJ:73:ASN:OD1	143:EJ:108:ARG:NH2	2.41	0.54
110:Do:253:ARG:NH2	143:Ej:88:ASP:O	2.40	0.54
115:Dt:232:GLU:OE1	115:Dt:232:GLU:N	2.36	0.54
134:Em:137:GLU:N	134:Em:137:GLU:OE1	2.41	0.54
5:A4:219:ASN:ND2	5:A4:222:SER:O	2.40	0.54
100:DD:166:ASN:O	100:DD:170:TYR:N	2.36	0.54
100:DD:219:GLU:OE1	100:DD:220:MET:N	2.41	0.54
104:DH:61:ASN:ND2	150:DH:201:CDL:OB2	2.41	0.54
150:DH:201:CDL:H671	150:DN:506:CDL:H822	1.88	0.54
112:DQ:57:THR:O	112:DQ:61:ASN:ND2	2.40	0.54
132:EK:6:PHE:CE2	132:EK:10:ILE:HD11	2.43	0.54
99:Dc:190:LEU:HD11	121:Dz:170:LEU:HD11	1.88	0.54
99:Dc:582:ARG:HD2	138:Eq:1:MET:HG3	1.89	0.54
108:Dm:280:GLU:OE2	138:Eq:70:ASN:ND2	2.40	0.54
109:Dn:414:TYR:CE2	109:Dn:418:ILE:HD11	2.42	0.54
139:Er:60:TRP:NE1	139:Er:64:LEU:HD11	2.22	0.54
149:Dl:194:GLY:O	149:Dl:213:ARG:NH1	2.40	0.54
13:AC:258:PRO:HG3	13:AC:266:LEU:HD22	1.89	0.54
97:DA:641:ARG:NE	100:DD:174:GLU:OE2	2.41	0.54
108:DM:451:GLN:O	108:DM:454:ASN:ND2	2.40	0.54
113:DR:290:ASN:OD1	113:DR:299:GLN:NE2	2.39	0.54
115:DT:57:GLN:NE2	140:ES:13:THR:O	2.40	0.54
97:Da:532:SER:OG	97:Da:571:GLN:NE2	2.35	0.54
116:Du:98:GLN:NE2	116:Du:109:THR:O	2.41	0.54
146:Ey:1:MET:HG3	146:Ey:5:LEU:HD23	1.88	0.54
15:AE:425:ASP:OD1	43:B6:28:ARG:NH1	2.41	0.54
85:A:512:ILE:HG22	85:A:513:VAL:HG23	1.87	0.54
110:DO:71:ASN:ND2	110:DO:212:GLN:OE1	2.40	0.54
112:DQ:248:GLN:N	112:DQ:248:GLN:OE1	2.39	0.54
113:DR:343:GLU:HA	127:EF:77:ILE:HD11	1.90	0.54
113:Dr:341:ALA:O	127:Ef:77:ILE:HD12	2.07	0.54
114:Ds:17:ASP:O	114:Ds:339:ASN:ND2	2.40	0.54
149:Dl:101:SER:OG	149:Dl:105:ARG:NE	2.40	0.54
22:AL:36:GLU:OE1	22:AL:36:GLU:N	2.39	0.54
23:AM:92:ASP:OD1	23:AM:93:ASN:N	2.41	0.54
66:BW:99:ALA:O	66:BW:103:GLY:HA2	2.08	0.54
133:EL:108:ASP:OD1	133:EL:109:ARG:N	2.41	0.54
97:Da:437:VAL:O	97:Da:440:HIS:ND1	2.41	0.54
105:Di:78:ASN:ND2	115:Dt:128:GLU:OE1	2.41	0.54
113:Dr:124:TYR:CZ	113:Dr:128:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
113:Dr:216:ARG:NH2	113:Dr:220:TYR:OH	2.40	0.54
119:Dx:75:TYR:OH	153:Dx:1203:PC1:O12	2.20	0.54
149:DL:98:GLU:N	149:DL:98:GLU:OE1	2.41	0.54
39:B2:88:THR:O	39:B2:94:GLN:NE2	2.41	0.54
64:BU:13:LYS:NZ	64:BU:17:ASP:OD1	2.41	0.54
85:A:362:THR:HG22	92:H:8:LEU:HD12	1.90	0.54
85:a:444:ARG:NH2	86:b:49:PRO:O	2.36	0.54
97:DA:657:GLN:OE1	115:DT:105:TYR:OH	2.26	0.54
104:DH:0:ACE:H3	108:DM:467:GLU:HB2	1.90	0.54
104:DH:118:PRO:HD3	104:DH:127:LEU:HD22	1.90	0.54
110:DO:454:GLN:OE1	110:DO:454:GLN:N	2.41	0.54
97:Da:562:MET:HE1	167:Ds:404:UQ8:H30	1.90	0.54
108:Dm:283:LYS:NZ	150:Dm:502:CDL:OA4	2.39	0.54
136:Eo:56:GLU:OE1	136:Eo:56:GLU:N	2.40	0.54
8:A7:123:ASP:OD1	8:A7:126:ARG:NH2	2.41	0.54
12:AB:612:GLU:OE1	12:AB:614:TRP:NE1	2.37	0.54
16:AF:127:TYR:O	16:AF:130:SER:OG	2.22	0.54
61:BR:94:ASN:O	61:BR:94:ASN:ND2	2.39	0.54
89:e:112:MET:HG2	95:k:35:THR:HG23	1.89	0.54
121:DZ:175:ALA:O	121:DZ:179:ASN:ND2	2.41	0.54
137:EP:48:ARG:NH2	137:EP:127:LEU:OXT	2.40	0.54
98:Db:540:ASP:OD2	103:Dg:57:ARG:NH1	2.40	0.54
100:Dd:166:ASN:O	100:Dd:170:TYR:N	2.40	0.54
116:Du:222:ILE:O	116:Du:226:ASN:ND2	2.40	0.54
31:AU:42:SER:N	31:AU:45:ASP:OD2	2.38	0.53
87:C:33:LEU:HD22	87:C:230:GLU:HG2	1.89	0.53
89:e:197:CYS:O	89:e:201:GLY:N	2.40	0.53
97:DA:437:VAL:O	97:DA:440:HIS:ND1	2.40	0.53
146:EY:59:LEU:O	146:EY:64:LYS:NZ	2.41	0.53
115:Dt:271:ARG:NH1	115:Dt:279:GLU:OE1	2.41	0.53
1:A0:95:MET:HE2	1:A0:95:MET:HA	1.90	0.53
12:AB:253:ASP:OD1	12:AB:254:VAL:N	2.41	0.53
12:AB:285:GLU:OE1	28:AR:161:ARG:NH1	2.40	0.53
20:AJ:39:GLN:OE1	38:B1:28:TYR:OH	2.18	0.53
34:AX:3:ASP:N	34:AX:3:ASP:OD1	2.40	0.53
44:BA:25:MET:HB3	62:BS:111:LEU:HD11	1.90	0.53
51:BH:149:ILE:HD12	69:BZ:19:ALA:HA	1.90	0.53
5:A4:260:VAL:O	5:A4:264:LEU:N	2.35	0.53
6:A5:13:PHE:O	6:A5:18:ARG:NH2	2.41	0.53
16:AF:98:MET:HA	16:AF:98:MET:HE2	1.90	0.53
89:E:221:SER:OG	158:E:302:FES:S2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:a:98:GLN:OE1	85:a:98:GLN:N	2.41	0.53
123:EB:39:ASN:C	123:EB:40:LEU:HD12	2.33	0.53
108:Dm:72:SER:OG	108:Dm:74:ASP:OD1	2.26	0.53
4:A3:111:ALA:O	4:A3:115:THR:HG22	2.08	0.53
13:AC:180:ILE:HD11	51:BH:76:ILE:HG21	1.91	0.53
87:C:72:VAL:HG21	88:d:94:TYR:CZ	2.43	0.53
87:c:116:TRP:O	87:c:120:VAL:HG23	2.08	0.53
99:DC:385:ASN:ND2	108:DM:362:ASP:OD1	2.39	0.53
104:DH:21:ASP:OD1	104:DH:22:ALA:N	2.42	0.53
134:EM:116:GLN:O	134:EM:119:ASN:ND2	2.40	0.53
134:EM:137:GLU:OE1	134:EM:137:GLU:N	2.42	0.53
99:Dc:363:LEU:C	99:Dc:363:LEU:HD23	2.33	0.53
155:Dc:606:3PE:H3E2	155:Dc:606:3PE:H3I3	1.91	0.53
11:AA:698:ASN:O	11:AA:701:SER:OG	2.16	0.53
45:BB:120:MET:SD	59:BP:62:LYS:NZ	2.81	0.53
79:CE:82:VAL:O	79:CE:83:THR:C	2.52	0.53
97:DA:126:HIS:ND1	97:DA:336:THR:OG1	2.41	0.53
97:Da:84:SER:OG	97:Da:591:HIS:ND1	2.36	0.53
110:Do:299:LEU:O	110:Do:345:ASN:ND2	2.39	0.53
145:Ex:28:VAL:HG23	145:Ex:29:LEU:HD12	1.90	0.53
116:DU:125:PHE:O	116:DU:128:GLY:N	2.36	0.53
125:ED:69:PHE:CE2	125:ED:73:LEU:HD11	2.44	0.53
114:Ds:256:TRP:O	114:Ds:259:THR:HG22	2.08	0.53
129:Eh:46:LEU:HA	129:Eh:110:LEU:HD13	1.89	0.53
143:Ej:141:TYR:HA	143:Ej:144:THR:HG22	1.90	0.53
20:AJ:132:PHE:CE1	68:BY:100:ILE:HD11	2.43	0.53
63:BT:110:TYR:OH	153:BT:203:PC1:O14	2.27	0.53
67:BX:108:GLN:OE1	67:BX:108:GLN:N	2.42	0.53
85:A:318:PHE:O	85:A:322:ASN:ND2	2.40	0.53
97:DA:562:MET:HE1	167:DS:403:UQ8:H30	1.89	0.53
119:DX:252:GLY:O	106:Dj:199:LYS:NZ	2.41	0.53
155:Ds:403:3PE:H3E2	155:Ds:403:3PE:H3I3	1.90	0.53
12:AB:393:GLY:C	12:AB:472:MET:HE1	2.34	0.53
51:BH:13:LEU:N	57:BN:88:GLY:O	2.38	0.53
64:BU:9:PRO:O	64:BU:31:TYR:OH	2.27	0.53
87:c:341:ILE:HD13	87:c:408:LEU:HD22	1.91	0.53
123:EB:82:PHE:CE2	123:EB:86:ILE:HD11	2.43	0.53
97:Da:650:ILE:HG21	115:Dt:163:VAL:HG22	1.91	0.53
98:Db:147:ARG:NH1	107:Dk:35:ASP:OD1	2.40	0.53
99:Dc:418:ASN:OD1	99:Dc:420:ASN:ND2	2.42	0.53
104:Dh:106:ASP:O	104:Dh:129:ARG:NH2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:Dn:173:ASP:OD1	109:Dn:174:ASN:N	2.41	0.53
35:AY:8:TRP:CE3	35:AY:11:ILE:HD11	2.44	0.53
76:CF:145:GLU:OE1	83:CO:35:LYS:NZ	2.42	0.53
85:A:289:PRO:O	85:A:290:SER:OG	2.26	0.53
86:B:453:LYS:O	86:B:456:THR:OG1	2.26	0.53
92:H:96:ASN:O	92:H:99:THR:OG1	2.21	0.53
92:h:101:TRP:NE1	150:h:501:CDL:OA7	2.42	0.53
97:DA:380:ILE:HD11	98:DB:528:VAL:HG11	1.90	0.53
115:Dt:282:MET:O	137:Ep:47:LYS:NZ	2.31	0.53
123:Eb:159:GLN:OE1	123:Eb:161:ARG:NH2	2.42	0.53
86:B:349:GLU:OE2	86:B:364:ARG:NH2	2.39	0.53
87:C:38:THR:HG23	87:C:91:LEU:HD12	1.91	0.53
89:e:134:ILE:CD1	89:e:154:ILE:HG21	2.35	0.53
100:DD:312:VAL:HG21	101:DE:15:ILE:HD11	1.91	0.53
111:DP:119:LEU:HD21	111:DP:396:SER:HB2	1.91	0.53
113:DR:270:ASN:O	113:DR:270:ASN:ND2	2.42	0.53
117:DV:244:ARG:NH2	117:DV:259:TYR:OH	2.42	0.53
118:DW:134:MET:N	118:DW:134:MET:SD	2.82	0.53
125:ED:154:ASN:OD1	133:EL:86:ARG:NH1	2.42	0.53
97:Da:307:THR:HA	97:Da:310:PHE:CE2	2.44	0.53
108:Dm:457:THR:OG1	108:Dm:459:ASN:OD1	2.25	0.53
112:Dq:230:ASP:OD1	112:Dq:231:ARG:N	2.41	0.53
127:Ef:42:ARG:NH2	127:Ef:50:ILE:O	2.42	0.53
149:Dl:169:LYS:N	149:Dl:181:VAL:O	2.41	0.53
102:DF:163:ASN:ND2	102:DF:163:ASN:O	2.42	0.52
104:DH:52:ASP:O	105:DI:123:LEU:HD12	2.09	0.52
107:DK:74:ILE:O	107:DK:81:ARG:NH1	2.42	0.52
119:DX:143:ARG:NH2	119:DX:149:GLU:OE2	2.40	0.52
155:EO:203:3PE:H2I3	155:EO:203:3PE:H2E2	1.91	0.52
143:EJ:75:GLN:OE1	143:EJ:105:GLN:NE2	2.42	0.52
143:EJ:153:ASP:OD1	143:EJ:161:GLN:NE2	2.42	0.52
97:Da:663:MET:HG3	97:Da:666:ILE:HD11	1.92	0.52
112:Dq:220:VAL:HG22	112:Dq:224:ALA:HB3	1.91	0.52
118:Dw:134:MET:N	118:Dw:134:MET:SD	2.82	0.52
121:Dz:105:ASN:OD1	121:Dz:156:GLN:NE2	2.41	0.52
1:A0:412:THR:O	1:A0:415:ASN:ND2	2.39	0.52
9:A8:250:GLU:OE1	9:A8:250:GLU:N	2.40	0.52
11:AA:476:PHE:CD1	68:BY:15:VAL:HG11	2.45	0.52
14:AD:270:ASN:ND2	14:AD:341:ASP:OD2	2.42	0.52
78:CK:34:ARG:NH1	78:CK:35:ASN:OD1	2.43	0.52
87:C:116:TRP:O	87:C:120:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
99:DC:67:GLU:OE1	99:DC:67:GLU:N	2.40	0.52
111:DP:300:ARG:NH1	111:DP:346:GLU:OE1	2.42	0.52
114:DS:197:ASN:N	150:DS:405:CDL:OA3	2.42	0.52
105:Di:77:GLN:OE1	105:Di:79:TYR:OH	2.11	0.52
121:Dz:41:ASN:O	121:Dz:43:ASN:ND2	2.43	0.52
133:El:114:MET:CE	140:Es:68:ILE:HD12	2.39	0.52
149:Dl:246:ASP:OD1	149:Dl:247:ASN:N	2.42	0.52
3:A2:262:TYR:CE2	3:A2:266:LEU:HD11	2.44	0.52
9:A8:206:VAL:O	9:A8:206:VAL:HG23	2.08	0.52
15:AE:371:GLU:OE1	15:AE:371:GLU:N	2.40	0.52
73:CA:500:VAL:HG21	73:CA:538:LEU:HD21	1.92	0.52
78:CK:31:THR:O	78:CK:34:ARG:NH1	2.41	0.52
87:C:39:PHE:CE2	167:C:512:UQ8:H1MA	2.44	0.52
97:DA:287:THR:O	97:DA:364:ARG:NH2	2.40	0.52
99:DC:18:PHE:HD2	99:DC:62:LEU:HD11	1.74	0.52
97:Da:108:PHE:CE2	97:Da:152:LEU:HD12	2.44	0.52
118:Dw:157:ASN:ND2	118:Dw:162:VAL:O	2.42	0.52
145:Ex:16:ILE:O	145:Ex:20:THR:HG23	2.09	0.52
3:A2:45:ARG:NE	3:A2:45:ARG:HA	2.25	0.52
22:AL:138:ALA:O	22:AL:163:ARG:NH2	2.40	0.52
65:BV:75:VAL:HG11	65:BV:84:ILE:HD13	1.92	0.52
85:a:199:LEU:O	85:a:203:ASN:ND2	2.41	0.52
99:DC:239:ILE:HD11	123:EB:122:PHE:CE1	2.45	0.52
106:DJ:107:TRP:O	106:DJ:111:VAL:HG23	2.10	0.52
117:DV:248:GLN:NE2	117:DV:259:TYR:O	2.41	0.52
99:Dc:148:LEU:O	143:Ej:57:ARG:NH2	2.41	0.52
150:Dh:201:CDL:H673	150:Dh:202:CDL:CB5	2.39	0.52
109:Dn:383:PHE:CE2	109:Dn:387:LEU:HD11	2.45	0.52
49:BF:5:GLY:N	49:BF:30:ASP:OD2	2.42	0.52
100:DD:503:LEU:HB3	132:EK:40:ILE:HD11	1.92	0.52
103:DG:1:MET:CE	150:Dx:1201:CDL:H472	2.40	0.52
120:DY:71:TYR:CD2	120:DY:195:LEU:HD23	2.44	0.52
120:DY:106:PHE:CD1	120:DY:110:ILE:HD12	2.44	0.52
1:A0:72:ILE:HD11	1:A0:101:PHE:CD2	2.45	0.52
11:AA:497:VAL:O	11:AA:501:THR:HG23	2.09	0.52
13:AC:363:PHE:HA	13:AC:366:THR:HG22	1.91	0.52
19:AI:127:THR:HG22	19:AI:128:THR:H	1.73	0.52
21:AK:147:LEU:HD12	21:AK:166:PRO:HD3	1.90	0.52
64:BU:16:VAL:HG13	64:BU:28:ARG:HG3	1.91	0.52
64:BU:58:TYR:OH	64:BU:62:ARG:NH1	2.38	0.52
87:c:368:TYR:OH	87:c:385:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:d:80:ASN:OD1	166:d:802:HEC:HAB	2.10	0.52
97:DA:652:LYS:NZ	115:DT:139:GLU:OE1	2.38	0.52
98:DB:182:SER:O	98:DB:186:THR:HG22	2.10	0.52
100:DD:395:ASP:N	109:DN:230:TYR:OH	2.41	0.52
110:DO:156:ASP:OD1	110:DO:160:ARG:NE	2.42	0.52
114:DS:142:LEU:HD23	150:DS:405:CDL:H851	1.90	0.52
129:EH:128:ARG:NH1	129:EH:131:GLN:OE1	2.42	0.52
12:AB:247:LYS:NZ	28:AR:108:GLU:OE2	2.43	0.52
12:AB:597:VAL:O	12:AB:651:ASP:N	2.40	0.52
30:AT:144:LEU:C	30:AT:144:LEU:HD23	2.34	0.52
87:c:227:LEU:HD13	167:c:510:UQ8:H15	1.92	0.52
112:DQ:187:ARG:O	112:DQ:248:GLN:NE2	2.41	0.52
97:Da:335:VAL:HG21	97:Da:407:MET:HE2	1.91	0.52
97:Da:645:ARG:NE	115:Dt:146:ILE:HD11	2.25	0.52
115:Dt:267:LYS:NZ	115:Dt:268:GLU:OE2	2.38	0.52
116:Du:174:ASP:OD2	116:Du:214:LYS:NZ	2.41	0.52
149:Dl:255:SER:O	149:Dl:290:LYS:NZ	2.39	0.52
11:AA:112:LEU:HD22	67:BX:89:VAL:HG21	1.92	0.52
22:AL:28:GLU:N	22:AL:28:GLU:OE1	2.42	0.52
31:AU:101:VAL:O	31:AU:105:ASN:ND2	2.41	0.52
55:BL:122:PRO:HD2	55:BL:125:LEU:HD12	1.91	0.52
57:BN:68:ASN:OD1	57:BN:69:GLY:N	2.40	0.52
63:BT:72:GLU:O	63:BT:76:VAL:HG23	2.09	0.52
73:CA:585:ASP:OD1	73:CA:586:PHE:N	2.43	0.52
79:CE:177:PHE:CE1	79:CE:224:ILE:HD12	2.45	0.52
87:C:91:LEU:HD23	87:C:126:PHE:CE1	2.45	0.52
105:DI:208:ILE:HG23	105:DI:209:VAL:HG23	1.90	0.52
133:EL:110:ASN:ND2	140:ES:62:ASN:O	2.43	0.52
6:A5:83:THR:HG22	6:A5:84:THR:H	1.75	0.52
6:A5:251:ILE:O	6:A5:251:ILE:HG22	2.09	0.52
29:AS:52:ALA:HB1	29:AS:105:ILE:HG21	1.91	0.52
70:CH:153:ARG:NH1	72:CL:19:LYS:O	2.43	0.52
90:F:62:ARG:NH1	90:F:63:ASP:OD1	2.43	0.52
87:c:99:LEU:HD11	87:c:309:LEU:HD11	1.91	0.52
112:DQ:344:ILE:O	112:DQ:344:ILE:HG22	2.10	0.52
109:Dn:136:PHE:CZ	109:Dn:140:LEU:HD11	2.45	0.52
115:Dt:258:ASN:ND2	115:Dt:258:ASN:O	2.43	0.52
149:Dl:87:THR:HG21	149:Dl:95:THR:HA	1.91	0.52
9:A8:101:ARG:NH2	9:A8:115:GLU:O	2.43	0.52
12:AB:178:ILE:O	14:AD:387:ARG:NH2	2.43	0.52
12:AB:218:GLU:OE1	12:AB:218:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:G:78:ARG:NH1	91:G:123:TYR:OH	2.43	0.52
97:DA:99:THR:HG21	97:DA:271:THR:HG21	1.92	0.52
99:DC:370:LEU:HD13	101:DE:82:THR:HG23	1.92	0.52
100:DD:291:ARG:NH1	109:DN:252:ASN:OD1	2.43	0.52
113:DR:185:TRP:O	135:EN:119:ARG:NH2	2.39	0.52
141:ET:72:LYS:NZ	146:EY:34:GLU:OE2	2.42	0.52
97:Da:217:LYS:O	97:Da:218:LEU:HD12	2.10	0.52
98:Db:341:GLU:OE1	126:Ee:97:SER:N	2.38	0.52
100:Dd:232:MET:N	150:Dd:706:CDL:OB4	2.41	0.52
113:Dr:266:ASP:OD1	113:Dr:267:ASN:N	2.43	0.52
149:DL:285:TYR:CE2	149:DL:289:LEU:HD11	2.45	0.52
1:A0:199:VAL:O	1:A0:199:VAL:HG23	2.10	0.51
7:A6:161:VAL:HG13	7:A6:175:VAL:HG13	1.92	0.51
9:A8:217:GLU:O	9:A8:221:VAL:HG12	2.10	0.51
34:AX:71:TYR:OH	34:AX:110:ASP:OD2	2.28	0.51
87:C:166:TRP:O	87:C:180:ARG:NH1	2.43	0.51
87:c:135:VAL:HG13	87:c:173:LEU:HD21	1.92	0.51
87:c:321:GLN:NE2	91:g:196:GLU:OE2	2.40	0.51
106:DJ:185:PRO:HG3	139:ER:64:LEU:HD13	1.92	0.51
109:DN:420:ASN:OD1	109:DN:421:THR:N	2.43	0.51
116:DU:222:ILE:O	116:DU:226:ASN:ND2	2.40	0.51
108:Dm:390:GLU:OE1	108:Dm:392:TYR:OH	2.21	0.51
115:Dt:200:GLU:OE1	115:Dt:200:GLU:N	2.38	0.51
120:Dy:64:SER:OG	120:Dy:189:ASN:OD1	2.18	0.51
124:Ec:180:ASN:O	124:Ec:185:ARG:NH1	2.43	0.51
16:AF:61:ARG:NH1	31:AU:71:TRP:O	2.43	0.51
17:AG:276:PRO:O	24:AN:147:TYR:OH	2.18	0.51
85:A:450:GLU:OE2	85:A:454:ARG:NH1	2.37	0.51
130:EI:25:LEU:O	130:EI:33:ARG:NH1	2.43	0.51
132:EK:161:GLU:OE1	113:Dr:168:LYS:NZ	2.43	0.51
99:Dc:208:ARG:NH2	123:Eb:101:GLN:O	2.42	0.51
108:Dm:117:ASP:OD1	108:Dm:118:ARG:N	2.43	0.51
110:Do:115:GLU:OE1	110:Do:115:GLU:N	2.40	0.51
129:Eh:18:LEU:HD11	129:Eh:140:LEU:HD13	1.91	0.51
130:Ei:66:SER:OG	130:Ei:70:ARG:NH1	2.42	0.51
1:A0:30:GLN:NE2	1:A0:361:GLU:OE2	2.41	0.51
1:A0:154:ARG:NH2	1:A0:173:ASP:O	2.43	0.51
22:AL:204:GLU:OE1	22:AL:204:GLU:N	2.41	0.51
49:BF:78:VAL:CG2	49:BF:102:ILE:HD11	2.41	0.51
63:BT:134:ASN:N	63:BT:134:ASN:OD1	2.43	0.51
168:c:504:HEM:HBB2	168:c:504:HEM:CMB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:DB:357:VAL:O	98:DB:394:ASN:ND2	2.41	0.51
85:a:392:LEU:O	85:a:396:GLN:NE2	2.40	0.51
97:DA:492:MET:HE2	150:EN:1201:CDL:H821	1.90	0.51
107:DK:12:SER:OG	127:EF:188:THR:O	2.13	0.51
108:DM:421:ASP:OD1	108:DM:430:SER:OG	2.28	0.51
136:EO:12:THR:HG22	136:EO:12:THR:O	2.09	0.51
100:Dd:354:ARG:NH2	100:Dd:387:TPO:O1P	2.39	0.51
99:DC:126:ILE:HD12	121:DZ:211:GLU:O	2.10	0.51
97:Da:88:LYS:HG3	114:Ds:18:ILE:HD12	1.92	0.51
99:Dc:408:GLN:OE1	108:Dm:318:ASN:ND2	2.40	0.51
100:Dd:68:LEU:HD12	122:Ea:127:PHE:CE2	2.45	0.51
8:A7:106:LYS:N	39:B2:76:GLU:OE2	2.43	0.51
68:BY:48:PHE:O	68:BY:52:TYR:HB3	2.10	0.51
98:DB:271:ASN:ND2	148:FA:7:ASN:OD1	2.43	0.51
101:DE:53:GLU:OE2	125:ED:181:LYS:NZ	2.40	0.51
153:DG:203:PC1:H3H1	150:Dx:1201:CDL:H473	1.93	0.51
110:DO:364:LYS:NZ	110:DO:468:GLU:OE1	2.41	0.51
113:DR:206:ILE:HG13	113:DR:209:ILE:HD12	1.92	0.51
98:Db:45:TRP:CE2	167:En:1202:UQ8:H3MA	2.46	0.51
100:Dd:395:ASP:N	109:Dn:230:TYR:OH	2.41	0.51
101:De:53:GLU:OE1	125:Ed:170:TYR:OH	2.24	0.51
109:Dn:420:ASN:OD1	109:Dn:421:THR:N	2.44	0.51
11:AA:156:THR:HG23	47:BD:96:THR:HG23	1.92	0.51
43:B6:19:ALA:O	43:B6:23:THR:HG23	2.11	0.51
89:E:63:HIS:ND1	89:E:64:ILE:O	2.40	0.51
87:c:37:PHE:CE2	87:c:237:ILE:HD12	2.46	0.51
100:DD:97:TYR:OH	100:DD:225:GLU:OE1	2.17	0.51
100:DD:236:LYS:NZ	150:DD:704:CDL:OB4	2.44	0.51
110:DO:299:LEU:O	110:DO:345:ASN:ND2	2.40	0.51
115:DT:246:ASP:O	127:EF:164:ARG:NH2	2.44	0.51
117:DV:58:GLY:C	117:DV:59:ILE:HD12	2.36	0.51
117:DV:115:ASP:OD1	117:DV:116:LEU:N	2.43	0.51
100:Dd:230:VAL:O	129:Eh:84:ARG:NH2	2.43	0.51
115:Dt:134:GLY:C	115:Dt:135:LEU:HD12	2.36	0.51
123:Eb:55:THR:HG22	123:Eb:55:THR:O	2.11	0.51
74:CI:3:SER:OG	74:CI:6:ASN:OD1	2.29	0.51
85:a:362:THR:CG2	92:h:8:LEU:HD11	2.41	0.51
88:d:42:GLU:N	88:d:42:GLU:OE1	2.44	0.51
91:g:69:ARG:NH1	91:g:248:ARG:O	2.43	0.51
110:DO:115:GLU:N	110:DO:115:GLU:OE1	2.42	0.51
113:DR:277:GLU:OE1	113:DR:277:GLU:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
100:Dd:450:GLU:OE1	100:Dd:450:GLU:N	2.44	0.51
110:Do:100:GLN:NE2	110:Do:104:GLU:OE2	2.42	0.51
135:En:146:ASN:HB2	167:En:1202:UQ8:H4M	1.92	0.51
71:CM:3:ARG:NH2	75:CB:270:ASP:O	2.44	0.51
85:A:98:GLN:OE1	85:A:98:GLN:N	2.44	0.51
86:B:252:CYS:HB3	86:B:421:VAL:HG22	1.92	0.51
97:DA:353:LEU:O	97:DA:357:VAL:HG23	2.11	0.51
115:DT:284:ASN:OD1	115:DT:285:GLU:N	2.43	0.51
119:DX:73:GLU:OE1	119:DX:80:ARG:NE	2.43	0.51
97:Da:76:ARG:NH1	97:Da:605:THR:OG1	2.44	0.51
131:Ev:18:LEU:HD13	131:Ev:48:PHE:HA	1.92	0.51
143:Ej:79:VAL:HG11	143:Ej:99:PHE:CE2	2.46	0.51
35:AY:7:PHE:O	35:AY:11:ILE:HG23	2.11	0.51
73:CA:404:ASN:O	73:CA:405:TRP:HB3	2.11	0.51
85:A:94:ALA:HB2	85:A:240:ASN:HB3	1.93	0.51
129:EH:53:GLY:O	129:EH:57:VAL:HG23	2.11	0.51
155:EM:901:3PE:H2I2	155:Dx:1206:3PE:H2E1	1.93	0.51
99:Dc:31:ASN:ND2	143:Ej:61:HIS:O	2.44	0.51
150:Dg:201:CDL:H272	150:Dg:201:CDL:C46	2.41	0.51
143:Ej:70:GLN:O	143:Ej:75:GLN:NE2	2.44	0.51
1:A0:28:ASP:OD1	1:A0:29:LEU:N	2.44	0.50
41:B4:45:ASP:OD1	41:B4:46:PHE:N	2.40	0.50
73:CA:52:ILE:HD11	73:CA:235:ILE:HG22	1.92	0.50
85:a:362:THR:HG21	92:h:6:ALA:HB3	1.93	0.50
150:DD:704:CDL:H273	150:DJ:303:CDL:CB7	2.42	0.50
105:DI:180:TYR:O	105:DI:186:THR:OG1	2.28	0.50
116:DU:64:ARG:NE	116:DU:77:ASP:OD2	2.45	0.50
109:Dn:141:TYR:CE2	109:Dn:145:LEU:HD11	2.47	0.50
115:Dt:115:ILE:O	115:Dt:119:VAL:HG22	2.10	0.50
141:Et:4:ARG:N	146:Ey:1:MET:O	2.40	0.50
4:A3:178:ARG:NE	12:AB:434:ASN:O	2.43	0.50
30:AT:144:LEU:HD23	30:AT:145:TYR:N	2.26	0.50
168:C:501:HEM:HBB2	168:C:501:HEM:CMB	2.41	0.50
127:EF:117:VAL:HG13	127:EF:119:THR:HG22	1.93	0.50
147:EZ:35:VAL:HG22	147:EZ:36:LEU:H	1.77	0.50
99:Dc:78:LEU:HD23	99:Dc:79:ASP:N	2.25	0.50
104:Dh:73:LEU:HD23	104:Dh:73:LEU:C	2.35	0.50
7:A6:148:MET:HE2	11:AA:713:SER:HB3	1.93	0.50
18:AH:76:ILE:HD13	30:AT:14:VAL:HG13	1.94	0.50
45:BB:186:ASP:OD1	45:BB:189:ARG:NH1	2.44	0.50
73:CA:578:ARG:NH2	73:CA:591:ASP:OD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:A:231:GLU:OE2	85:A:235:ASN:ND2	2.44	0.50
87:C:112:GLN:NE2	87:C:206:ASP:OD2	2.45	0.50
85:a:193:GLN:HA	85:a:199:LEU:HD22	1.93	0.50
117:DV:249:ASN:OD1	117:DV:250:ALA:N	2.44	0.50
99:Dc:370:LEU:HD13	101:De:82:THR:HG23	1.93	0.50
121:Dz:210:LEU:HD23	121:Dz:226:ARG:CA	2.41	0.50
122:Ea:37:ARG:NH2	122:Ea:204:LEU:O	2.44	0.50
4:A3:143:GLU:OE1	4:A3:143:GLU:N	2.42	0.50
8:A7:234:SER:O	50:BG:78:ARG:NH2	2.45	0.50
12:AB:65:CYS:O	12:AB:185:ARG:NH2	2.42	0.50
13:AC:329:ASP:OD2	13:AC:388:ARG:NH1	2.45	0.50
26:AP:15:LYS:NZ	26:AP:44:GLY:O	2.44	0.50
27:AQ:179:GLU:OE2	57:BN:28:TYR:OH	2.18	0.50
57:BN:13:ARG:NH1	57:BN:21:SER:OG	2.43	0.50
85:A:403:ALA:HA	85:A:467:ALA:HB3	1.93	0.50
106:DJ:163:GLU:OE2	106:DJ:198:ARG:NH1	2.42	0.50
99:Dc:481:LEU:O	99:Dc:485:ASN:ND2	2.38	0.50
106:Dj:107:TRP:NE1	153:Eo:201:PC1:O12	2.41	0.50
108:Dm:214:ARG:NH1	108:Dm:251:PRO:O	2.41	0.50
108:Dm:449:ILE:HA	108:Dm:452:THR:HG22	1.94	0.50
111:Dp:197:ARG:O	111:Dp:198:ARG:NH1	2.44	0.50
125:Ed:154:ASN:OD1	133:El:86:ARG:NH1	2.44	0.50
149:DL:250:THR:OG1	149:DL:260:ASN:ND2	2.44	0.50
5:A4:175:VAL:HG22	5:A4:175:VAL:O	2.11	0.50
13:AC:412:VAL:HB	150:AC:801:CDL:H271	1.93	0.50
14:AD:228:PRO:N	14:AD:229:PRO:CD	2.74	0.50
49:BF:78:VAL:HG21	49:BF:102:ILE:HD11	1.92	0.50
85:A:118:THR:HG23	85:A:121:ARG:H	1.77	0.50
85:A:143:ARG:NH1	85:A:202:GLU:OE1	2.41	0.50
88:D:45:THR:HG21	87:c:255:LEU:HD21	1.94	0.50
87:c:135:VAL:HG11	87:c:181:LEU:CD2	2.41	0.50
106:DJ:111:VAL:HG21	153:EO:201:PC1:H2A1	1.93	0.50
115:DT:248:PHE:CD1	127:EF:162:THR:HG21	2.46	0.50
98:Db:23:ARG:NH2	131:Ev:2:GLU:OE2	2.44	0.50
108:Dm:226:GLU:OE1	108:Dm:226:GLU:N	2.42	0.50
109:Dn:136:PHE:CE2	109:Dn:140:LEU:HD11	2.47	0.50
139:Er:60:TRP:CE2	139:Er:64:LEU:HD11	2.46	0.50
7:A6:197:VAL:O	7:A6:197:VAL:HG13	2.12	0.50
12:AB:493:LYS:O	12:AB:497:ASN:ND2	2.40	0.50
16:AF:276:LEU:O	16:AF:337:LYS:NZ	2.44	0.50
21:AK:238:VAL:O	21:AK:238:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AO:121:ASN:OD1	25:AO:146:ASN:ND2	2.44	0.50
68:BY:75:GLU:OE1	68:BY:75:GLU:N	2.41	0.50
87:C:307:PHE:CB	153:K:502:PC1:H2I3	2.42	0.50
91:G:18:PHE:O	91:G:19:SER:OG	2.20	0.50
113:DR:273:PHE:CD1	113:DR:284:LEU:HD22	2.47	0.50
104:Dh:58:GLU:OE2	104:Dh:75:TYR:OH	2.30	0.50
107:Dk:131:THR:O	134:Em:6:ARG:NH2	2.45	0.50
109:Dn:218:ILE:O	109:Dn:218:ILE:HG22	2.12	0.50
115:Dt:119:VAL:HG11	115:Dt:145:TYR:HA	1.94	0.50
118:Dw:197:VAL:HG23	118:Dw:249:VAL:HG21	1.92	0.50
9:A8:112:GLN:OE1	9:A8:114:TRP:NE1	2.44	0.50
12:AB:309:ARG:NH1	12:AB:572:TYR:O	2.44	0.50
13:AC:77:TYR:OH	63:BT:144:ASP:OD2	2.21	0.50
150:B0:102:CDL:OA3	41:B4:38:ARG:NH2	2.45	0.50
85:a:328:LEU:HD11	85:a:399:LEU:HD21	1.93	0.50
106:DJ:208:GLU:OE1	106:DJ:208:GLU:N	2.44	0.50
108:DM:72:SER:OG	108:DM:74:ASP:OD1	2.26	0.50
108:DM:84:ASN:OD1	108:DM:85:ALA:N	2.44	0.50
110:DO:244:ASP:O	110:DO:248:VAL:HG13	2.11	0.50
150:Da:709:CDL:C16	106:Dj:109:THR:HG21	2.41	0.50
116:Du:257:VAL:O	116:Du:257:VAL:HG12	2.11	0.50
118:Dw:141:TYR:O	134:Em:7:ARG:NH1	2.43	0.50
127:Ef:92:GLN:NE2	127:Ef:129:SER:O	2.44	0.50
3:A2:44:TYR:CE2	3:A2:45:ARG:NH2	2.80	0.50
14:AD:230:PHE:O	14:AD:232:ALA:N	2.45	0.50
44:BA:89:ILE:HD11	44:BA:192:ILE:HD13	1.94	0.50
55:BL:119:HIS:HB3	60:BQ:113:THR:HG23	1.94	0.50
99:DC:383:LEU:HD13	100:DD:93:THR:HG21	1.92	0.50
99:DC:592:TYR:OH	138:EQ:21:ARG:NH2	2.45	0.50
105:DI:140:PRO:O	105:DI:143:GLN:NE2	2.43	0.50
119:DX:75:TYR:OH	153:DX:308:PC1:O12	2.22	0.50
125:ED:114:TYR:CD2	167:ED:603:UQ8:H4M	2.47	0.50
141:ET:38:LEU:N	141:ET:38:LEU:HD23	2.27	0.50
99:Dc:365:SER:O	99:Dc:369:ILE:HG23	2.12	0.50
121:Dz:175:ALA:O	121:Dz:179:ASN:ND2	2.43	0.50
124:Ec:7:GLU:O	124:Ec:11:LEU:HD13	2.11	0.50
138:Eq:0:ACE:H3	138:Eq:117:HIS:CD2	2.47	0.50
149:DL:271:ASN:ND2	149:DL:273:SER:OG	2.44	0.50
2:A1:159:LEU:HD23	2:A1:160:ILE:N	2.27	0.50
4:A3:72:LEU:HD23	4:A3:98:VAL:HB	1.94	0.50
13:AC:7:ILE:HG23	13:AC:77:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AC:241:GLU:OE2	49:BF:38:ARG:NH2	2.44	0.50
150:AF:402:CDL:OB4	69:BZ:37:TYR:OH	2.29	0.50
56:BM:82:GLU:O	56:BM:89:LYS:NZ	2.45	0.50
56:BM:99:PHE:HA	56:BM:102:THR:HG22	1.94	0.50
153:DC:608:PC1:H2I1	150:EH:1601:CDL:H361	1.94	0.50
100:DD:220:MET:HE1	125:ED:163:ALA:O	2.11	0.50
101:DE:50:SER:O	125:ED:174:ARG:NH2	2.45	0.50
108:DM:117:ASP:OD1	108:DM:118:ARG:N	2.44	0.50
153:DQ:1503:PC1:O12	119:DX:63:TYR:OH	2.28	0.50
116:DU:253:THR:O	116:DU:257:VAL:HG23	2.12	0.50
97:Da:155:ILE:HG21	97:Da:295:LEU:HD11	1.93	0.50
115:Dt:284:ASN:OD1	115:Dt:285:GLU:N	2.45	0.50
15:AE:56:ASP:OD1	25:AO:154:ARG:NH2	2.45	0.49
31:AU:139:ASP:OD1	122:EA:50:ASN:ND2	2.45	0.49
87:c:345:LYS:O	87:c:347:HIS:ND1	2.42	0.49
143:EJ:127:ASP:OD2	143:EJ:130:THR:OG1	2.25	0.49
117:Dv:1:MET:HE3	117:Dv:207:GLU:HG3	1.93	0.49
17:AG:77:ASP:OD1	17:AG:79:ILE:HD11	2.11	0.49
85:A:362:THR:HG21	92:H:6:ALA:HB3	1.93	0.49
87:C:371:SER:O	153:C:509:PC1:H133	2.12	0.49
97:DA:217:LYS:O	97:DA:218:LEU:HD12	2.12	0.49
106:DJ:204:GLU:OE1	106:DJ:206:GLU:N	2.44	0.49
114:DS:62:LEU:O	114:DS:65:THR:HG22	2.11	0.49
97:Da:64:THR:HG22	97:Da:149:TYR:CD1	2.47	0.49
99:Dc:126:ILE:HD12	121:Dz:211:GLU:O	2.12	0.49
150:Dd:705:CDL:O1	150:Ea:502:CDL:OA3	2.23	0.49
106:Dj:155:GLU:O	106:Dj:189:ARG:NH2	2.39	0.49
118:Dw:91:ARG:NH2	118:Dw:115:ASN:O	2.43	0.49
124:Ec:131:ASP:OD2	124:Ec:141:ARG:NH2	2.41	0.49
134:Em:45:THR:HG23	134:Em:57:ALA:HB3	1.95	0.49
149:Dl:285:TYR:CE2	149:Dl:289:LEU:HD11	2.47	0.49
1:A0:72:ILE:HD12	1:A0:72:ILE:H	1.77	0.49
2:A1:168:ASP:OD1	2:A1:169:THR:N	2.45	0.49
14:AD:410:ILE:HG23	14:AD:440:ILE:HD12	1.94	0.49
16:AF:302:TYR:CG	51:BH:176:ILE:HD11	2.47	0.49
55:BL:22:ASN:ND2	55:BL:132:GLY:O	2.42	0.49
86:B:329:LEU:CD2	86:B:386:ILE:HD11	2.43	0.49
153:E:303:PC1:H152	153:E:303:PC1:O13	2.12	0.49
117:DV:81:GLY:O	117:DV:143:ASN:ND2	2.45	0.49
126:EE:154:LEU:HD22	126:EE:174:PHE:CG	2.48	0.49
98:Db:57:ARG:NH2	150:Dr:402:CDL:OA4	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
99:Dc:239:ILE:HD11	123:Eb:122:PHE:CE1	2.47	0.49
106:Dj:11:ASN:ND2	106:Dj:30:GLU:OE1	2.45	0.49
114:Ds:152:VAL:HG23	114:Ds:201:LEU:HD22	1.94	0.49
122:Ea:69:PHE:CE2	122:Ea:73:LEU:HD11	2.47	0.49
133:El:140:ASP:OD2	133:El:144:GLU:N	2.45	0.49
138:Eq:1:MET:HB3	138:Eq:107:TYR:OH	2.13	0.49
149:DL:194:GLY:O	149:DL:213:ARG:NH1	2.45	0.49
44:BA:89:ILE:HG12	44:BA:202:LEU:HD11	1.95	0.49
86:B:147:GLU:O	86:B:148:THR:OG1	2.30	0.49
167:C:511:UQ8:H20	87:c:190:PHE:CE2	2.48	0.49
99:DC:84:GLU:OE1	116:DU:266:THR:OG1	2.30	0.49
97:Da:134:TYR:OH	99:Dc:312:THR:HG22	2.11	0.49
14:AD:332:VAL:O	14:AD:336:VAL:HG23	2.11	0.49
15:AE:272:GLN:OE1	15:AE:272:GLN:N	2.46	0.49
38:B1:76:VAL:HG11	39:B2:35:MET:HE2	1.95	0.49
72:CL:1:MET:N	76:CF:132:GLU:O	2.46	0.49
75:CB:83:ASP:OD1	75:CB:84:GLN:N	2.45	0.49
87:C:288:TRP:CH2	155:C:513:3PE:H3I3	2.48	0.49
89:E:112:MET:CG	95:K:35:THR:HG23	2.42	0.49
91:G:84:ASP:O	91:G:119:ARG:NH2	2.42	0.49
98:DB:341:GLU:OE1	126:EE:97:SER:N	2.42	0.49
110:DO:272:GLU:OE1	110:DO:272:GLU:N	2.46	0.49
111:DP:126:THR:HG23	111:DP:386:TYR:HD1	1.77	0.49
119:DX:96:PHE:CE2	119:DX:100:ILE:HD11	2.47	0.49
97:Da:380:ILE:HD12	97:Da:445:VAL:CG1	2.42	0.49
102:Df:40:ARG:NH1	102:Df:42:ASP:OD2	2.40	0.49
107:Dk:68:PRO:HG3	126:Ee:72:ILE:HD13	1.94	0.49
114:Ds:260:ARG:NH1	114:Ds:264:ASP:OD2	2.45	0.49
5:A4:207:ILE:HD13	7:A6:162:VAL:HG13	1.94	0.49
87:c:336:ILE:O	87:c:336:ILE:HG22	2.11	0.49
87:c:338:ARG:NH2	91:g:33:GLU:OE1	2.45	0.49
100:DD:450:GLU:OE1	100:DD:450:GLU:N	2.45	0.49
105:DI:231:GLN:OE1	105:DI:231:GLN:N	2.45	0.49
98:Db:231:VAL:HG21	145:Ex:68:LEU:HD12	1.94	0.49
113:Dr:144:ILE:HD12	113:Dr:144:ILE:N	2.28	0.49
116:Du:35:THR:O	116:Du:35:THR:HG22	2.12	0.49
124:Ec:30:GLY:O	124:Ec:34:LEU:HD22	2.13	0.49
143:Ej:47:ARG:NH2	143:Ej:154:PRO:O	2.46	0.49
8:A7:197:GLN:NE2	55:BL:133:ASP:OD2	2.45	0.49
28:AR:18:LYS:O	28:AR:147:LYS:NZ	2.43	0.49
51:BH:76:ILE:HG22	51:BH:77:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:C:184:LEU:HD22	167:C:511:UQ8:C30	2.43	0.49
116:DU:270:VAL:O	116:DU:273:VAL:HG23	2.13	0.49
119:DX:47:GLN:NE2	130:EI:165:ASP:OD1	2.45	0.49
139:ER:60:TRP:NE1	139:ER:64:LEU:HD11	2.27	0.49
97:Da:140:ILE:HA	109:Dn:320:CYS:SG	2.53	0.49
99:Dc:18:PHE:HD2	99:Dc:62:LEU:HD11	1.77	0.49
99:Dc:501:TYR:N	99:Dc:502:PRO:CD	2.76	0.49
114:Ds:107:ASP:OD1	114:Ds:111:ARG:NE	2.46	0.49
149:DL:260:ASN:HB3	149:DL:269:LEU:HD22	1.95	0.49
2:A1:349:VAL:HG23	2:A1:349:VAL:O	2.13	0.49
4:A3:170:THR:HG22	12:AB:683:ASP:OD2	2.13	0.49
10:A9:52:TRP:CZ2	153:c:503:PC1:H2C1	2.48	0.49
15:AE:157:LEU:HD21	15:AE:195:PHE:CE2	2.47	0.49
22:AL:123:GLU:OE2	22:AL:216:ASN:ND2	2.45	0.49
93:I:16:PRO:HD2	93:I:19:ILE:HD12	1.94	0.49
90:f:75:ALA:O	90:f:79:ASN:ND2	2.41	0.49
98:DB:225:ILE:O	98:DB:227:ARG:NH1	2.46	0.49
98:DB:244:THR:OG1	141:ET:10:GLU:OE1	2.29	0.49
102:DF:182:ASP:OD1	102:DF:183:ASP:N	2.45	0.49
125:ED:48:GLU:O	125:ED:55:ASN:ND2	2.46	0.49
97:Da:293:ASP:OD2	97:Da:365:HIS:NE2	2.46	0.49
100:Dd:392:TYR:OH	100:Dd:399:GLU:OE2	2.22	0.49
121:Dz:70:TYR:HB3	121:Dz:126:ILE:HD11	1.94	0.49
11:AA:267:PHE:CZ	11:AA:655:ILE:HD12	2.47	0.49
12:AB:164:LYS:O	12:AB:172:THR:OG1	2.29	0.49
34:AX:15:ILE:HD13	34:AX:18:ILE:HD12	1.94	0.49
81:CN:27:VAL:O	81:CN:31:VAL:HG22	2.12	0.49
99:DC:501:TYR:N	99:DC:502:PRO:CD	2.76	0.49
112:DQ:54:ASN:O	112:DQ:96:GLN:NE2	2.45	0.49
129:EH:85:ASN:OD1	129:EH:86:LEU:N	2.46	0.49
134:EM:45:THR:HG23	134:EM:57:ALA:HB3	1.93	0.49
97:Da:338:SER:HB2	97:Da:399:ILE:HG22	1.93	0.49
98:Db:225:ILE:O	98:Db:227:ARG:NH1	2.46	0.49
102:Df:163:ASN:O	102:Df:163:ASN:ND2	2.46	0.49
116:Du:124:ILE:HD12	116:Du:124:ILE:N	2.28	0.49
15:AE:94:GLU:OE2	15:AE:172:ALA:N	2.45	0.49
16:AF:227:ASN:ND2	16:AF:303:TYR:O	2.42	0.49
17:AG:267:GLN:HG2	24:AN:67:LEU:HD13	1.94	0.49
54:BK:142:PHE:O	58:BO:117:ARG:NH1	2.42	0.49
75:CB:128:GLY:N	158:CB:1000:FES:S2	2.79	0.49
85:A:384:ASN:OD1	85:A:385:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
168:c:505:HEM:HBC2	168:c:505:HEM:CMC	2.42	0.49
100:DD:435:LEU:HD21	100:DD:439:LYS:HE2	1.94	0.49
109:DN:218:ILE:O	109:DN:218:ILE:HG22	2.13	0.49
110:DO:48:ASN:ND2	110:DO:48:ASN:O	2.46	0.49
130:EI:76:THR:HA	130:EI:79:ILE:HD12	1.95	0.49
137:EP:48:ARG:NH1	137:EP:127:LEU:OXT	2.45	0.49
97:Da:477:LEU:HD11	97:Da:492:MET:HE1	1.95	0.49
100:Dd:282:LYS:NZ	115:Dt:45:PRO:O	2.41	0.49
101:De:13:ASN:OD1	133:El:83:ARG:NH2	2.42	0.49
109:Dn:423:ILE:O	109:Dn:423:ILE:HG22	2.13	0.49
112:Dq:145:HIS:ND1	112:Dq:145:HIS:O	2.46	0.49
130:Ei:79:ILE:O	130:Ei:82:VAL:HG12	2.12	0.49
11:AA:99:PHE:CE1	11:AA:131:ILE:HD11	2.48	0.48
18:AH:115:SER:O	50:BG:165:ARG:NH2	2.44	0.48
27:AQ:115:ALA:O	27:AQ:116:SER:OG	2.18	0.48
85:a:104:SER:O	85:a:224:ASN:ND2	2.46	0.48
150:c:501:CDL:H271	150:c:502:CDL:C19	2.43	0.48
168:c:505:HEM:HBB2	168:c:505:HEM:CMB	2.43	0.48
113:DR:266:ASP:OD1	113:DR:267:ASN:N	2.46	0.48
134:EM:46:THR:O	119:Dx:136:GLN:NE2	2.45	0.48
134:EM:138:ARG:NH1	134:EM:142:LEU:HD22	2.27	0.48
138:EQ:0:ACE:H1	138:EQ:4:PHE:CZ	2.47	0.48
99:Dc:385:ASN:ND2	108:Dm:362:ASP:OD1	2.37	0.48
99:Dc:545:ARG:NH1	129:Eh:104:THR:OG1	2.41	0.48
150:Dg:201:CDL:H272	150:Dg:201:CDL:H472	1.95	0.48
124:Ec:71:LEU:HD13	124:Ec:79:LEU:HD12	1.95	0.48
10:A9:125:LEU:HD12	150:c:501:CDL:H273	1.95	0.48
15:AE:424:ALA:HA	15:AE:427:VAL:HG22	1.94	0.48
23:AM:81:THR:OG1	23:AM:99:GLY:O	2.31	0.48
25:AO:67:ASP:OD1	25:AO:69:ILE:HG22	2.13	0.48
26:AP:10:GLN:O	26:AP:13:THR:OG1	2.25	0.48
56:BM:11:VAL:O	56:BM:12:ASP:C	2.56	0.48
86:B:329:LEU:HD22	86:B:334:LEU:HD13	1.96	0.48
97:Da:415:ARG:NH1	97:Da:416:ARG:O	2.46	0.48
103:Dg:40:TYR:CE2	103:Dg:44:ILE:HD11	2.47	0.48
106:Dj:175:ARG:NH2	106:Dj:204:GLU:OE2	2.40	0.48
150:Dj:404:CDL:OA4	136:Eo:38:ARG:NH2	2.42	0.48
114:Ds:185:ILE:HG21	114:Ds:194:LEU:HD21	1.95	0.48
117:Dv:93:LEU:O	117:Dv:97:ASN:ND2	2.42	0.48
146:Ey:62:LEU:O	146:Ey:64:LYS:NZ	2.46	0.48
6:A5:30:THR:HG22	15:AE:194:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AL:124:HIS:CE1	159:AL:302:SF4:S2	3.06	0.48
86:B:98:VAL:HG22	86:B:243:ASN:HB3	1.95	0.48
168:C:501:HEM:HBC2	168:C:501:HEM:CMC	2.42	0.48
100:DD:260:ASP:OD2	115:DT:42:ARG:NH2	2.46	0.48
117:DV:92:TYR:HB2	117:DV:136:THR:HG21	1.94	0.48
121:DZ:31:ASN:OD1	149:DL:332:ASN:ND2	2.46	0.48
121:DZ:138:GLU:OE1	121:DZ:142:ARG:NH2	2.46	0.48
125:ED:100:PHE:CE2	125:ED:104:LEU:HD11	2.49	0.48
150:Dd:705:CDL:HA61	109:Dn:30:LEU:HD11	1.95	0.48
109:Dn:218:ILE:HD12	109:Dn:218:ILE:N	2.28	0.48
112:Dq:118:ILE:HD11	150:Dx:1204:CDL:H732	1.96	0.48
114:Ds:10:ARG:NH2	117:Dv:203:ASP:OD2	2.42	0.48
115:Dt:223:ASP:OD1	136:Eo:2:VAL:HG23	2.13	0.48
124:Ec:197:LEU:HD11	124:Ec:206:LEU:HG	1.95	0.48
125:Ed:21:TYR:HE1	130:Ei:79:ILE:HD11	1.79	0.48
139:Er:27:ASN:ND2	139:Er:84:MET:O	2.43	0.48
11:AA:551:GLU:OE1	11:AA:551:GLU:N	2.45	0.48
15:AE:77:GLN:NE2	22:AL:144:SER:O	2.46	0.48
77:CG:55:PHE:HA	80:CJ:34:HIS:NE2	2.29	0.48
77:CG:68:GLU:OE1	77:CG:68:GLU:N	2.41	0.48
86:B:129:ASN:OD1	86:B:130:TYR:N	2.47	0.48
98:DB:578:THR:HG23	98:DB:579:PHE:CD2	2.48	0.48
110:DO:164:TYR:CE2	110:DO:168:LEU:HD11	2.49	0.48
116:DU:239:LEU:O	116:DU:239:LEU:HD23	2.12	0.48
116:DU:257:VAL:O	116:DU:257:VAL:HG12	2.13	0.48
97:Da:525:ALA:HB2	97:Da:578:LEU:HB2	1.95	0.48
108:Dm:118:ARG:NH1	112:Dq:315:GLU:OE2	2.43	0.48
114:Ds:69:LYS:NZ	150:Ds:401:CDL:OA4	2.47	0.48
2:A1:85:GLU:OE2	34:AX:36:GLN:NE2	2.46	0.48
11:AA:745:PHE:O	11:AA:750:LEU:N	2.45	0.48
91:g:230:GLN:O	91:g:235:ARG:NH1	2.46	0.48
112:DQ:247:TYR:CD1	115:DT:316:ILE:HD11	2.49	0.48
116:DU:123:GLY:C	116:DU:124:ILE:HD12	2.39	0.48
122:EA:218:ARG:HH12	146:EY:58:TYR:HH	1.60	0.48
141:ET:38:LEU:HD23	141:ET:38:LEU:H	1.78	0.48
117:Dv:26:ILE:HD11	117:Dv:299:ILE:HD12	1.95	0.48
117:Dv:249:ASN:O	117:Dv:255:ASN:ND2	2.42	0.48
129:Eh:153:GLU:OE1	129:Eh:153:GLU:N	2.45	0.48
133:El:110:ASN:ND2	140:Es:62:ASN:O	2.46	0.48
143:Ej:153:ASP:OD1	143:Ej:161:GLN:NE2	2.46	0.48
18:AH:176:PHE:CE1	43:B6:52:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AK:209:HIS:NE2	23:AM:92:ASP:OD2	2.39	0.48
70:CH:178:ILE:HG22	70:CH:179:SER:N	2.28	0.48
168:C:502:HEM:HBB2	168:C:502:HEM:CMB	2.43	0.48
100:DD:575:PHE:CZ	100:DD:579:ILE:HD11	2.48	0.48
106:DJ:94:GLN:OE1	106:DJ:94:GLN:N	2.47	0.48
99:Dc:197:HIS:CE1	99:Dc:229:ILE:HG21	2.49	0.48
100:Dd:273:MET:HE2	100:Dd:273:MET:HA	1.95	0.48
102:Df:23:PHE:C	102:Df:24:LEU:HD12	2.39	0.48
11:AA:183:THR:HG23	11:AA:202:LEU:HG	1.96	0.48
73:CA:96:ALA:HB2	73:CA:137:VAL:HG21	1.94	0.48
85:A:178:VAL:HA	85:A:181:GLU:HG2	1.96	0.48
87:C:229:ASN:HA	88:d:275:THR:HG21	1.96	0.48
167:C:511:UQ8:H11	87:c:183:TYR:HB3	1.95	0.48
99:DC:230:GLN:NE2	143:EJ:3:ASN:OD1	2.47	0.48
153:DC:608:PC1:H2I1	150:EH:1601:CDL:C36	2.44	0.48
112:DQ:145:HIS:ND1	112:DQ:145:HIS:O	2.46	0.48
122:EA:31:ILE:HD13	122:EA:200:TYR:CE2	2.49	0.48
133:EL:42:ARG:NE	139:ER:21:GLU:OE2	2.42	0.48
100:Dd:405:GLN:NE2	109:Dn:244:PHE:O	2.46	0.48
112:Dq:344:ILE:HB	136:Eo:2:VAL:HG21	1.96	0.48
127:Ef:117:VAL:HG13	127:Ef:119:THR:HG22	1.95	0.48
149:DL:99:THR:O	149:DL:105:ARG:NH2	2.46	0.48
18:AH:226:SER:OG	43:B6:26:ARG:NH2	2.47	0.48
25:AO:137:ARG:NE	25:AO:154:ARG:O	2.44	0.48
75:CB:230:TRP:NE1	167:CC:303:UQ8:O5	2.45	0.48
98:DB:278:ASN:O	148:FA:10:TYR:OH	2.32	0.48
106:DJ:58:LEU:HD11	106:DJ:65:LEU:HD23	1.94	0.48
107:DK:42:GLU:OE1	107:DK:42:GLU:N	2.43	0.48
122:EA:109:TYR:HB3	122:EA:164:THR:HG23	1.96	0.48
143:EJ:141:TYR:HA	143:EJ:144:THR:HG22	1.95	0.48
98:Db:250:PHE:O	141:Et:22:TYR:OH	2.30	0.48
113:Dr:185:TRP:O	135:En:119:ARG:NH2	2.43	0.48
26:AP:23:GLU:OE1	26:AP:23:GLU:N	2.47	0.48
150:DH:201:CDL:H673	150:DH:202:CDL:OB7	2.13	0.48
105:Di:133:GLN:NE2	115:Dt:207:GLU:O	2.42	0.48
109:Dn:192:ILE:HD11	132:Ek:46:VAL:HG11	1.95	0.48
111:Dp:126:THR:HG22	111:Dp:386:TYR:O	2.12	0.48
115:Dt:84:ASP:OD1	115:Dt:85:GLY:N	2.47	0.48
139:Er:79:ARG:O	139:Er:94:ARG:NH2	2.41	0.48
15:AE:83:ASP:N	15:AE:83:ASP:OD1	2.45	0.48
35:AY:21:LEU:HD23	35:AY:21:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:CJ:73:TYR:OH	83:CO:14:HIS:NE2	2.33	0.48
103:DG:54:PHE:O	103:DG:58:ASN:ND2	2.43	0.48
109:DN:141:TYR:CE2	109:DN:145:LEU:HD11	2.48	0.48
143:EJ:31:LEU:O	143:EJ:175:HIS:NE2	2.45	0.48
100:Dd:502:TYR:CE1	100:Dd:506:LEU:HD21	2.48	0.48
110:Do:204:TYR:CE2	110:Do:208:LEU:HD11	2.49	0.48
113:Dr:176:ALA:O	134:Em:81:ASN:ND2	2.42	0.48
121:Dz:125:GLN:OE1	121:Dz:125:GLN:N	2.47	0.48
1:A0:24:SER:OG	1:A0:27:HIS:ND1	2.37	0.47
11:AA:419:MET:SD	11:AA:430:HIS:NE2	2.87	0.47
43:B6:3:TYR:O	43:B6:7:LEU:HD23	2.13	0.47
67:BX:77:LEU:HD23	67:BX:77:LEU:O	2.13	0.47
87:C:101:ARG:NH1	150:C:506:CDL:OB3	2.43	0.47
87:C:132:LEU:CD1	87:C:184:LEU:HD23	2.44	0.47
113:DR:284:LEU:HD21	113:DR:321:VAL:HG11	1.95	0.47
115:Dt:243:ILE:HG21	127:Ef:79:MET:SD	2.54	0.47
153:Eb:303:PC1:H2E1	153:Eb:303:PC1:H2I2	1.95	0.47
149:DL:83:GLY:N	149:DL:462:ASN:OD1	2.47	0.47
76:CF:268:TYR:CD2	78:CK:75:LEU:HD13	2.50	0.47
89:E:79:VAL:HG23	89:E:79:VAL:O	2.13	0.47
89:E:134:ILE:HG22	89:E:134:ILE:O	2.14	0.47
93:I:111:LYS:NZ	93:I:115:GLN:OE1	2.40	0.47
97:DA:342:THR:HG21	97:DA:400:PRO:HD3	1.96	0.47
111:DP:225:GLN:OE1	111:DP:225:GLN:N	2.46	0.47
133:EL:34:LYS:NZ	133:EL:50:ASP:OD1	2.46	0.47
97:Da:518:HIS:NE2	97:Da:519:ASP:OD1	2.47	0.47
105:Di:231:GLN:N	105:Di:231:GLN:OE1	2.47	0.47
108:Dm:347:TYR:CE2	150:Du:401:CDL:H873	2.49	0.47
123:Eb:182:VAL:HG23	123:Eb:185:SER:HB2	1.97	0.47
156:Ed:203:LPP:H261	130:Ei:103:LEU:HD21	1.97	0.47
147:Ez:35:VAL:HG22	147:Ez:36:LEU:H	1.78	0.47
4:A3:285:VAL:O	4:A3:311:ASN:ND2	2.47	0.47
6:A5:83:THR:HG22	6:A5:84:THR:N	2.28	0.47
14:AD:47:ARG:NH2	14:AD:133:ARG:O	2.47	0.47
48:BE:89:HIS:O	48:BE:93:LYS:N	2.47	0.47
92:h:13:ASP:OD1	92:h:14:PHE:N	2.47	0.47
98:DB:69:THR:HG22	98:DB:69:THR:O	2.14	0.47
99:DC:512:LEU:HD21	155:DC:606:3PE:H272	1.96	0.47
111:DP:272:ASP:OD1	111:DP:273:THR:N	2.47	0.47
113:DR:252:THR:HG21	113:DR:324:TYR:O	2.14	0.47
114:DS:156:LEU:HD12	114:DS:194:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:DZ:134:ARG:NE	143:EJ:175:HIS:O	2.47	0.47
99:Dc:268:PHE:CZ	99:Dc:272:ILE:HG21	2.49	0.47
112:Dq:57:THR:O	112:Dq:61:ASN:ND2	2.48	0.47
139:Er:64:LEU:HD12	139:Er:92:VAL:HG11	1.96	0.47
4:A3:122:LEU:HD22	4:A3:137:VAL:HG21	1.96	0.47
20:AJ:74:CYS:SG	20:AJ:82:THR:HG21	2.55	0.47
49:BF:36:TYR:O	49:BF:39:ASN:ND2	2.47	0.47
85:A:200:LEU:HD23	85:A:380:TYR:HD1	1.79	0.47
86:B:308:LEU:HD23	86:B:362:GLY:HA3	1.95	0.47
86:B:410:LEU:O	86:B:416:ARG:NH1	2.45	0.47
91:G:5:GLU:OE1	91:G:5:GLU:N	2.38	0.47
99:DC:116:GLU:OE1	116:DU:276:LYS:NZ	2.34	0.47
106:DJ:91:ARG:NH2	106:DJ:95:GLU:OE2	2.47	0.47
139:ER:5:ALA:HB1	119:Dx:251:LEU:HD22	1.97	0.47
97:Da:51:LYS:NZ	115:Dt:205:HIS:O	2.32	0.47
101:De:125:ASP:OD1	101:De:126:GLU:N	2.47	0.47
155:Dr:401:3PE:H3I1	150:Dr:402:CDL:H251	1.97	0.47
167:Ed:202:UQ8:H45B	132:Ek:65:PRO:HG3	1.95	0.47
137:Ep:112:ASP:OD1	137:Ep:115:THR:OG1	2.20	0.47
11:AA:479:ASP:OD1	11:AA:480:THR:N	2.47	0.47
13:AC:482:LYS:HA	45:BB:144:LEU:HD12	1.95	0.47
16:AF:19:ASN:OD1	31:AU:98:TRP:NE1	2.45	0.47
30:AT:18:ARG:HG3	30:AT:144:LEU:HD21	1.97	0.47
43:B6:53:CYS:HB3	56:BM:74:VAL:HG11	1.96	0.47
52:BI:85:GLU:O	52:BI:89:THR:HG22	2.14	0.47
79:CE:136:GLU:OE2	79:CE:150:LYS:NZ	2.46	0.47
86:B:376:LEU:C	86:B:376:LEU:HD23	2.40	0.47
87:c:173:LEU:HD12	87:c:265:ILE:CD1	2.45	0.47
100:DD:179:LEU:HD11	115:DT:193:VAL:HG13	1.95	0.47
112:DQ:268:THR:HG21	112:DQ:273:ILE:HD11	1.96	0.47
98:Db:161:ASP:OD1	102:Df:164:TYR:OH	2.32	0.47
99:Dc:521:LEU:HD21	106:Dj:144:MET:HE1	1.96	0.47
10:A9:162:HIS:NE2	155:BT:201:3PE:O14	2.45	0.47
15:AE:186:SER:OG	15:AE:326:THR:HG21	2.14	0.47
88:D:56:TRP:NE1	88:D:173:ASN:OD1	2.45	0.47
86:b:158:HIS:ND1	86:b:159:ASP:OD1	2.43	0.47
86:b:320:VAL:HG12	86:b:442:VAL:HG21	1.95	0.47
89:e:134:ILE:HD12	89:e:252:VAL:CG2	2.44	0.47
108:DM:159:ARG:NE	108:DM:161:GLU:OE2	2.42	0.47
122:EA:146:THR:OG1	150:EA:301:CDL:OB4	2.20	0.47
153:EB:303:PC1:H2I2	153:EB:303:PC1:H2E1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
131:EV:31:VAL:O	131:EV:34:ASN:ND2	2.48	0.47
133:EL:13:ARG:NH2	139:ER:104:LYS:O	2.47	0.47
138:EQ:0:ACE:H3	138:EQ:117:HIS:CD2	2.49	0.47
106:Dj:53:GLN:HA	140:Es:41:ILE:HD11	1.96	0.47
110:Do:139:ILE:CG2	110:Do:144:LEU:HD11	2.44	0.47
113:Dr:206:ILE:HG13	113:Dr:209:ILE:HD12	1.97	0.47
117:Dv:58:GLY:C	117:Dv:59:ILE:HD12	2.40	0.47
119:Dx:73:GLU:OE1	119:Dx:80:ARG:NH2	2.47	0.47
155:Dx:1207:3PE:H3E2	155:Dx:1207:3PE:H3I3	1.96	0.47
140:Es:14:ASP:OD2	140:Es:34:LYS:NZ	2.48	0.47
2:A1:290:PRO:HB2	2:A1:293:ILE:HG22	1.96	0.47
3:A2:249:ARG:HH12	42:B5:25:LEU:HD13	1.79	0.47
5:A4:121:VAL:HG13	5:A4:146:LEU:HB3	1.97	0.47
10:A9:52:TRP:HB3	10:A9:55:ARG:HB3	1.97	0.47
11:AA:193:TYR:O	59:BP:83:ASN:ND2	2.46	0.47
11:AA:641:THR:OG1	11:AA:642:SER:N	2.48	0.47
12:AB:54:CYS:HB3	12:AB:59:VAL:HG13	1.96	0.47
12:AB:270:GLU:OE2	26:AP:159:ARG:NH1	2.48	0.47
12:AB:618:ARG:NH2	12:AB:631:ASP:OD1	2.45	0.47
15:AE:395:SER:OG	15:AE:396:ASN:N	2.47	0.47
23:AM:61:HIS:O	23:AM:219:LYS:NZ	2.48	0.47
27:AQ:10:ASN:ND2	27:AQ:10:ASN:O	2.48	0.47
35:AY:5:ILE:HD12	35:AY:5:ILE:H	1.80	0.47
46:BC:137:ASN:OD1	49:BF:109:HIS:ND1	2.46	0.47
51:BH:101:ILE:O	51:BH:105:THR:HG23	2.14	0.47
55:BL:43:PHE:HA	55:BL:46:GLN:HG2	1.96	0.47
74:CI:41:SER:OG	78:CK:75:LEU:HD11	2.15	0.47
87:C:329:VAL:HG12	87:C:330:ALA:N	2.30	0.47
87:c:329:VAL:HG11	87:c:341:ILE:HD12	1.97	0.47
89:e:134:ILE:HG22	89:e:134:ILE:O	2.15	0.47
100:DD:100:MET:SD	100:DD:248:THR:HG23	2.55	0.47
108:DM:364:VAL:HG13	108:DM:378:VAL:HG13	1.96	0.47
109:DN:423:ILE:O	109:DN:423:ILE:HG22	2.14	0.47
113:DR:326:ILE:N	113:DR:326:ILE:HD12	2.30	0.47
115:DT:249:ASN:ND2	127:EF:77:ILE:HD13	2.30	0.47
117:DV:59:ILE:HD13	117:DV:280:VAL:HG13	1.96	0.47
155:DX:303:3PE:H3I3	155:DX:303:3PE:H3E2	1.96	0.47
120:DY:122:THR:HG23	120:DY:123:ARG:HG3	1.97	0.47
143:EJ:110:ASP:O	143:EJ:115:GLY:N	2.46	0.47
97:Da:99:THR:HG21	97:Da:271:THR:HG21	1.97	0.47
98:Db:516:TRP:CD1	98:Db:562:ILE:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
99:Dc:55:THR:HG23	99:Dc:58:ASN:H	1.78	0.47
100:Dd:236:LYS:NZ	150:Dd:704:CDL:OB4	2.47	0.47
100:Dd:237:TYR:OH	155:Dd:703:3PE:O14	2.25	0.47
111:Dp:126:THR:HG21	111:Dp:389:THR:HB	1.95	0.47
112:Dq:103:ASN:ND2	112:Dq:142:ASP:OD1	2.46	0.47
113:Dr:186:ILE:O	135:En:119:ARG:NH2	2.48	0.47
115:Dt:87:TYR:OH	115:Dt:142:ASP:OD1	2.25	0.47
120:Dy:120:LEU:HD23	120:Dy:120:LEU:O	2.15	0.47
11:AA:423:VAL:HG11	11:AA:526:GLY:HA3	1.97	0.47
86:B:322:PHE:CE1	86:B:454:VAL:HG21	2.50	0.47
87:C:23:MET:HE2	167:C:512:UQ8:H3MB	1.96	0.47
97:DA:123:ILE:O	97:DA:127:VAL:HG22	2.15	0.47
110:DO:32:LEU:HD21	110:DO:181:THR:OG1	2.14	0.47
112:DQ:79:THR:O	112:DQ:171:GLY:N	2.38	0.47
116:DU:35:THR:HG22	116:DU:35:THR:O	2.15	0.47
126:EE:72:ILE:N	126:EE:72:ILE:HD12	2.30	0.47
100:Dd:451:THR:HG22	100:Dd:452:SER:H	1.78	0.47
112:Dq:374:GLN:OE1	112:Dq:374:GLN:N	2.47	0.47
126:Ee:164:VAL:HG22	145:Ex:34:ASP:OD1	2.15	0.47
12:AB:91:ALA:O	12:AB:95:SER:OG	2.28	0.47
30:AT:152:GLU:OE1	30:AT:152:GLU:N	2.44	0.47
77:CG:17:ILE:HG21	79:CE:41:LEU:CD2	2.45	0.47
85:A:513:VAL:HG21	92:h:46:ARG:HD2	1.96	0.47
87:c:348:SER:O	87:c:352:ASN:ND2	2.48	0.47
91:g:45:ASN:O	91:g:49:THR:OG1	2.32	0.47
100:DD:113:HIS:NE2	100:DD:125:ASP:OD1	2.45	0.47
104:DH:10:LYS:NZ	108:DM:263:SER:OG	2.48	0.47
135:EN:110:PHE:CD2	135:EN:144:LEU:HD13	2.50	0.47
149:DL:101:SER:OG	149:DL:105:ARG:NE	2.48	0.47
1:A0:22:ALA:HB2	1:A0:56:MET:HE1	1.96	0.47
12:AB:475:VAL:HG21	12:AB:492:LEU:HD13	1.96	0.47
31:AU:66:PHE:HB3	31:AU:67:PRO:HD3	1.97	0.47
73:CA:197:ALA:HB2	75:CB:185:TYR:CG	2.50	0.47
85:A:101:LEU:HD12	85:A:101:LEU:H	1.80	0.47
89:e:84:GLU:CG	89:e:87:ILE:HD12	2.45	0.47
97:DA:76:ARG:NH1	97:DA:605:THR:OG1	2.47	0.47
97:DA:228:PRO:HG2	97:DA:231:LEU:HD12	1.97	0.47
97:DA:391:HIS:O	97:DA:394:VAL:HG22	2.15	0.47
100:DD:273:MET:HE2	100:DD:273:MET:HA	1.97	0.47
101:DE:8:ARG:NH1	112:DQ:218:ASP:OD1	2.48	0.47
124:EC:101:LEU:HD23	124:EC:101:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
138:EQ:1:MET:HG2	138:EQ:1:MET:O	2.15	0.47
99:Dc:80:LEU:HD12	110:Do:276:GLN:CD	2.41	0.47
103:Dg:77:GLU:OE2	107:Dk:106:ARG:NE	2.48	0.47
110:Do:48:ASN:O	110:Do:48:ASN:ND2	2.48	0.47
126:Ee:72:ILE:HD12	126:Ee:72:ILE:N	2.29	0.47
4:A3:178:ARG:NH2	12:AB:434:ASN:O	2.46	0.46
6:A5:68:THR:OG1	6:A5:70:ASP:OD1	2.29	0.46
11:AA:235:TRP:CH2	11:AA:310:LEU:HD22	2.50	0.46
11:AA:604:PHE:CZ	11:AA:710:LEU:HD22	2.48	0.46
12:AB:235:ALA:HB3	12:AB:236:PRO:HD3	1.97	0.46
22:AL:113:LYS:NZ	22:AL:197:GLU:OE2	2.48	0.46
69:BZ:49:ASP:HA	69:BZ:52:ARG:HG2	1.97	0.46
77:CG:61:GLU:OE2	77:CG:89:ASN:ND2	2.47	0.46
80:CJ:58:PRO:HA	80:CJ:61:THR:HG22	1.97	0.46
108:DM:128:THR:O	108:DM:128:THR:HG22	2.15	0.46
112:DQ:268:THR:HG23	112:DQ:268:THR:O	2.15	0.46
113:DR:144:ILE:HD12	113:DR:144:ILE:N	2.30	0.46
113:DR:341:ALA:O	127:EF:77:ILE:HD12	2.15	0.46
123:EB:182:VAL:HG23	123:EB:185:SER:HB2	1.96	0.46
97:Da:380:ILE:HD11	98:Db:528:VAL:HG11	1.97	0.46
100:Dd:186:GLN:OE1	115:Dt:181:ASN:ND2	2.45	0.46
150:Dg:201:CDL:H321	127:Ef:156:VAL:HG13	1.97	0.46
104:Dh:88:TYR:OH	109:Dn:341:ASN:O	2.31	0.46
110:Do:356:GLU:HB2	110:Do:369:VAL:HG22	1.96	0.46
110:Do:357:LEU:HD21	110:Do:366:VAL:HG13	1.97	0.46
141:Et:38:LEU:HD23	141:Et:38:LEU:H	1.81	0.46
147:Ez:35:VAL:HG22	147:Ez:36:LEU:N	2.30	0.46
11:AA:267:PHE:HZ	11:AA:655:ILE:HD12	1.79	0.46
11:AA:443:LEU:HD11	11:AA:507:VAL:HG11	1.97	0.46
14:AD:34:ASN:N	14:AD:291:GLU:OE2	2.48	0.46
23:AM:132:ILE:HD13	23:AM:138:LEU:HD11	1.97	0.46
49:BF:144:GLN:OE1	49:BF:144:GLN:N	2.42	0.46
91:G:106:ASN:ND2	91:G:165:TYR:OH	2.48	0.46
85:a:346:ARG:NH1	91:g:170:THR:O	2.48	0.46
91:g:172:ILE:HG22	95:k:6:PHE:HB2	1.96	0.46
97:DA:415:ARG:NH2	103:DG:19:ASP:OD1	2.48	0.46
109:DN:207:ILE:N	109:DN:207:ILE:HD12	2.30	0.46
150:EI:401:CDL:OA4	150:EI:401:CDL:O1	2.30	0.46
155:EM:901:3PE:H2I2	155:Dx:1206:3PE:C2E	2.45	0.46
97:Da:46:TYR:HH	109:Dn:318:TYR:HH	1.59	0.46
97:Da:321:ALA:O	97:Da:326:ARG:NH1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:Db:69:THR:O	98:Db:69:THR:HG22	2.15	0.46
98:Db:508:ASN:ND2	98:Db:531:ARG:O	2.47	0.46
155:Dg:204:3PE:O12	134:Em:62:ARG:NH1	2.41	0.46
106:Dj:163:GLU:OE2	106:Dj:198:ARG:NH1	2.45	0.46
116:Du:125:PHE:O	116:Du:128:GLY:N	2.38	0.46
126:Ee:164:VAL:HG22	145:Ex:34:ASP:CG	2.40	0.46
129:Eh:129:ILE:HG22	129:Eh:137:TRP:HB2	1.97	0.46
141:Et:36:ASN:O	141:Et:39:ARG:NH1	2.47	0.46
141:Et:38:LEU:HD23	141:Et:38:LEU:N	2.29	0.46
26:AP:78:VAL:CG2	26:AP:102:LEU:HD11	2.46	0.46
73:CA:197:ALA:HB2	75:CB:185:TYR:CD1	2.50	0.46
73:CA:449:ILE:HD11	164:CA:702:FAD:H4'	1.96	0.46
85:A:498:LYS:O	89:E:89:ARG:NH2	2.48	0.46
88:D:124:TYR:O	88:D:127:GLN:NE2	2.40	0.46
95:k:18:LEU:O	95:k:22:VAL:HG23	2.15	0.46
124:EC:28:LEU:HD11	124:EC:59:GLN:OE1	2.15	0.46
109:Dn:207:ILE:HD12	109:Dn:207:ILE:N	2.30	0.46
110:Do:71:ASN:ND2	110:Do:212:GLN:OE1	2.48	0.46
125:Ed:69:PHE:CE2	125:Ed:73:LEU:HD11	2.50	0.46
11:AA:207:ILE:HG12	11:AA:266:VAL:HG22	1.97	0.46
13:AC:74:TYR:CD2	13:AC:120:LEU:HD12	2.51	0.46
87:C:146:LEU:O	87:C:146:LEU:HD13	2.16	0.46
90:F:29:PRO:O	90:F:32:THR:OG1	2.28	0.46
88:d:92:TYR:OH	88:d:134:ARG:NH1	2.48	0.46
109:DN:189:ILE:HB	132:EK:46:VAL:HG13	1.97	0.46
124:EC:197:LEU:HD11	124:EC:206:LEU:HG	1.96	0.46
100:Dd:120:THR:HG22	140:Es:25:TRP:CD2	2.51	0.46
104:Dh:33:HIS:O	104:Dh:37:GLY:N	2.49	0.46
106:Dj:185:PRO:HG3	139:Er:64:LEU:HD13	1.98	0.46
111:Dp:126:THR:HG23	111:Dp:386:TYR:HD1	1.81	0.46
115:Dt:188:ILE:HG21	115:Dt:208:ILE:HD11	1.97	0.46
125:Ed:115:ILE:HG12	167:Ed:202:UQ8:H4MB	1.98	0.46
15:AE:144:MET:O	15:AE:147:VAL:HG12	2.15	0.46
21:AK:210:ARG:NH2	21:AK:253:ASN:OD1	2.49	0.46
70:CH:149:GLN:NE2	72:CL:21:LEU:O	2.44	0.46
75:CB:277:MET:SD	82:CC:16:ASN:ND2	2.83	0.46
85:A:110:VAL:O	85:A:114:VAL:HG23	2.16	0.46
91:g:18:PHE:O	91:g:19:SER:OG	2.27	0.46
98:DB:157:GLN:NE2	98:DB:370:GLU:OE2	2.48	0.46
112:DQ:321:ASP:OD1	112:DQ:324:ARG:NH2	2.46	0.46
115:DT:115:ILE:O	115:DT:119:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:DZ:81:HIS:NE2	121:DZ:117:GLU:OE1	2.44	0.46
146:EY:1:MET:HG3	146:EY:5:LEU:HD23	1.98	0.46
108:Dm:30:THR:HG22	108:Dm:31:ALA:N	2.31	0.46
117:Dv:103:ILE:O	117:Dv:107:THR:HG22	2.15	0.46
129:Eh:23:TYR:CZ	129:Eh:27:LEU:HD11	2.50	0.46
132:Ek:120:LEU:O	132:Ek:120:LEU:HD23	2.15	0.46
7:A6:133:TYR:OH	44:BA:37:ASP:OD2	2.31	0.46
8:A7:201:CYS:SG	8:A7:202:GLN:N	2.89	0.46
53:BJ:45:LEU:HD21	53:BJ:131:VAL:HG21	1.97	0.46
64:BU:53:LEU:HD11	64:BU:76:LEU:HD11	1.98	0.46
88:D:42:GLU:C	88:D:43:LEU:HD12	2.41	0.46
85:a:208:ALA:O	85:a:288:THR:N	2.44	0.46
115:DT:119:VAL:HG11	115:DT:145:TYR:HA	1.97	0.46
120:DY:60:ASP:OD2	120:DY:150:TYR:OH	2.34	0.46
122:Ea:31:ILE:HD11	122:Ea:198:THR:O	2.15	0.46
11:AA:472:LEU:HD12	46:BC:90:TRP:CH2	2.51	0.46
12:AB:599:GLN:NE2	28:AR:154:GLU:OE1	2.49	0.46
27:AQ:172:ASP:OD1	64:BU:62:ARG:NH2	2.47	0.46
32:AV:59:GLU:OE1	32:AV:61:GLN:NE2	2.41	0.46
45:BB:59:LEU:C	45:BB:60:ILE:HD12	2.41	0.46
56:BM:12:ASP:OD1	110:DO:146:GLN:NE2	2.46	0.46
73:CA:449:ILE:HD11	164:CA:702:FAD:C4'	2.45	0.46
87:C:121:PHE:CD2	87:C:195:LEU:HD21	2.51	0.46
112:DQ:23:ARG:NH1	112:DQ:25:GLY:O	2.48	0.46
150:Dg:201:CDL:H272	150:Dg:201:CDL:H461	1.97	0.46
110:Do:164:TYR:CE2	110:Do:168:LEU:HD11	2.50	0.46
121:Dz:171:LEU:HD23	121:Dz:171:LEU:C	2.41	0.46
132:Ek:150:TYR:N	150:Ek:201:CDL:OA4	2.40	0.46
147:Ez:8:GLU:N	147:Ez:8:GLU:OE1	2.46	0.46
10:A9:141:GLU:O	10:A9:145:ASN:ND2	2.49	0.46
16:AF:119:ILE:HD11	51:BH:141:ASN:CB	2.45	0.46
31:AU:136:GLU:OE1	31:AU:136:GLU:N	2.43	0.46
85:A:337:THR:OG1	85:A:347:GLN:OE1	2.33	0.46
88:d:261:PHE:CE2	88:d:265:LEU:HD11	2.49	0.46
107:DK:68:PRO:HG3	126:EE:72:ILE:HD13	1.97	0.46
109:DN:170:ILE:HG21	124:EC:171:VAL:HG11	1.98	0.46
121:DZ:171:LEU:C	121:DZ:171:LEU:HD23	2.41	0.46
97:Da:353:LEU:O	97:Da:357:VAL:HG23	2.16	0.46
97:Da:565:ILE:HD11	150:En:1201:CDL:C34	2.45	0.46
118:Dw:151:PRO:HG3	118:Dw:233:THR:HG22	1.98	0.46
118:Dw:229:LEU:O	118:Dw:233:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
136:Eo:31:TYR:CE2	136:Eo:35:LEU:HD11	2.51	0.46
139:Er:37:CYS:O	139:Er:41:VAL:HG23	2.16	0.46
1:A0:462:VAL:HG12	1:A0:463:ALA:H	1.81	0.46
13:AC:200:LEU:HD11	51:BH:120:ARG:HB2	1.97	0.46
15:AE:72:ASP:OD2	22:AL:149:ARG:NH2	2.46	0.46
22:AL:135:ARG:O	22:AL:187:VAL:HG21	2.16	0.46
62:BS:25:ASN:O	62:BS:33:THR:OG1	2.28	0.46
86:B:308:LEU:HD13	86:B:360:LEU:HD23	1.98	0.46
150:C:504:CDL:OA4	91:g:181:ILE:N	2.43	0.46
89:E:117:ARG:NH1	87:c:70:GLU:OE2	2.46	0.46
86:b:203:PHE:O	86:b:207:VAL:HG23	2.16	0.46
99:DC:77:VAL:HG22	99:DC:77:VAL:O	2.16	0.46
100:DD:175:LEU:HD21	100:DD:177:PHE:CE2	2.51	0.46
98:Db:360:LEU:HD13	98:Db:393:PHE:CZ	2.51	0.46
108:Dm:128:THR:O	108:Dm:128:THR:HG22	2.16	0.46
125:Ed:100:PHE:CE2	125:Ed:104:LEU:HD11	2.51	0.46
127:Ef:51:THR:HG22	127:Ef:53:PHE:H	1.81	0.46
132:Ek:118:PRO:HA	132:Ek:121:VAL:HG22	1.98	0.46
155:El:905:3PE:H2E2	155:El:905:3PE:H2I2	1.97	0.46
12:AB:592:ASN:OD1	12:AB:596:ARG:N	2.48	0.46
16:AF:138:ILE:N	16:AF:139:PRO:HD2	2.31	0.46
25:AO:196:VAL:HG22	28:AR:124:PHE:CZ	2.51	0.46
37:B0:87:ASN:O	37:B0:89:ARG:NH1	2.49	0.46
49:BF:71:ARG:O	49:BF:74:ILE:HG22	2.16	0.46
85:A:47:GLY:O	95:K:1:MET:N	2.36	0.46
88:D:43:LEU:HD12	88:D:43:LEU:N	2.30	0.46
87:c:120:VAL:HG11	87:c:310:PHE:CA	2.46	0.46
98:DB:348:ARG:NH1	102:DF:190:GLU:OE2	2.43	0.46
117:DV:1:MET:HE3	117:DV:207:GLU:HG3	1.97	0.46
133:EL:140:ASP:OD2	133:EL:144:GLU:N	2.49	0.46
97:Da:444:LEU:HD21	97:Da:515:VAL:HG22	1.98	0.46
153:Dc:609:PC1:H2I1	150:Eh:1601:CDL:H361	1.98	0.46
119:Dx:231:ASP:OD1	119:Dx:233:THR:OG1	2.34	0.46
49:BF:15:ILE:HG21	90:F:22:PHE:CE2	2.51	0.45
57:BN:45:LYS:O	57:BN:49:VAL:HG23	2.16	0.45
150:CJ:201:CDL:H801	84:CD:33:THR:HG21	1.96	0.45
85:a:512:ILE:HG22	85:a:513:VAL:HG23	1.97	0.45
87:c:120:VAL:HG22	168:c:505:HEM:CBC	2.46	0.45
87:c:146:LEU:HD13	87:c:146:LEU:C	2.41	0.45
88:d:66:ASP:OD2	88:d:69:SER:N	2.46	0.45
90:f:7:ALA:O	90:f:8:GLN:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:DB:244:THR:N	141:ET:10:GLU:OE2	2.48	0.45
102:DF:121:GLN:NE2	106:DJ:186:ASP:O	2.47	0.45
112:DQ:333:THR:OG1	112:DQ:334:GLU:N	2.48	0.45
129:EH:15:ASP:O	129:EH:147:LYS:NZ	2.49	0.45
145:EX:28:VAL:HG23	145:EX:29:LEU:HD12	1.98	0.45
97:Da:562:MET:SD	167:Ds:404:UQ8:H25A	2.57	0.45
100:Dd:120:THR:HG22	140:Es:25:TRP:CE3	2.51	0.45
135:En:86:HIS:NE2	135:En:91:ASN:OD1	2.44	0.45
9:A8:164:GLU:OE1	22:AL:38:LYS:NZ	2.36	0.45
10:A9:187:GLU:OE1	10:A9:187:GLU:N	2.49	0.45
25:AO:11:LEU:HD22	25:AO:45:ILE:HG23	1.98	0.45
26:AP:7:THR:HG22	26:AP:8:ILE:H	1.80	0.45
57:BN:70:VAL:HG13	57:BN:71:TRP:N	2.30	0.45
73:CA:604:ASP:O	73:CA:607:THR:N	2.49	0.45
85:A:178:VAL:O	85:A:182:LYS:HG3	2.16	0.45
87:C:88:VAL:HG21	168:C:501:HEM:HMA3	1.98	0.45
87:C:146:LEU:HD13	87:C:146:LEU:C	2.41	0.45
91:G:314:LEU:O	91:G:319:GLN:NE2	2.50	0.45
97:DA:338:SER:HB2	97:DA:399:ILE:HG22	1.97	0.45
103:DG:1:MET:HE1	150:Dx:1201:CDL:H472	1.97	0.45
124:EC:43:THR:HG22	124:EC:60:LEU:HD13	1.98	0.45
133:EL:114:MET:CE	140:ES:68:ILE:HD12	2.47	0.45
99:Dc:383:LEU:HD13	100:Dd:93:THR:HG21	1.97	0.45
100:Dd:68:LEU:C	100:Dd:68:LEU:HD13	2.42	0.45
102:Df:144:ASP:OD2	102:Df:196:ARG:NH2	2.42	0.45
105:Di:140:PRO:O	105:Di:143:GLN:NE2	2.49	0.45
106:Dj:204:GLU:OE1	106:Dj:206:GLU:N	2.49	0.45
129:Eh:32:ASP:OD1	129:Eh:33:GLU:N	2.49	0.45
149:DL:358:VAL:N	149:DL:370:LEU:O	2.45	0.45
13:AC:54:LEU:HD12	13:AC:58:PHE:CE2	2.50	0.45
13:AC:163:VAL:HG23	13:AC:164:THR:HG23	1.98	0.45
34:AX:111:TRP:NE1	56:BM:57:LEU:HD21	2.32	0.45
39:B2:39:GLN:OE1	39:B2:39:GLN:N	2.48	0.45
50:BG:130:ARG:NH2	50:BG:138:ALA:O	2.49	0.45
73:CA:583:ARG:NH2	73:CA:585:ASP:OD2	2.50	0.45
168:C:502:HEM:HBC2	168:C:502:HEM:CMC	2.46	0.45
150:DN:507:CDL:H562	130:EI:109:LEU:HD22	1.98	0.45
112:DQ:216:THR:O	112:DQ:220:VAL:HG22	2.16	0.45
99:Dc:389:THR:HG23	99:Dc:390:ILE:N	2.31	0.45
109:Dn:190:LYS:NZ	132:Ek:80:VAL:O	2.49	0.45
113:Dr:326:ILE:HD12	113:Dr:326:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A7:192:LYS:NZ	50:BG:81:GLU:OE1	2.49	0.45
11:AA:68:HIS:O	11:AA:69:HIS:C	2.60	0.45
18:AH:117:PHE:HB2	18:AH:119:LEU:HD13	1.98	0.45
44:BA:90:LYS:NZ	44:BA:102:GLU:O	2.49	0.45
49:BF:47:ASP:N	49:BF:47:ASP:OD1	2.49	0.45
73:CA:78:THR:O	73:CA:206:TYR:N	2.45	0.45
73:CA:85:SER:O	73:CA:88:VAL:HG12	2.16	0.45
75:CB:263:ILE:CD1	75:CB:295:LEU:HD22	2.47	0.45
91:G:204:ASN:OD1	95:K:3:LEU:HD12	2.17	0.45
110:DO:355:THR:OG1	110:DO:369:VAL:O	2.32	0.45
117:DV:45:THR:O	117:DV:45:THR:HG22	2.16	0.45
117:DV:111:LYS:NZ	123:EB:22:GLU:OE2	2.49	0.45
150:EB:302:CDL:CA5	150:EB:302:CDL:OA8	2.65	0.45
134:EM:138:ARG:HH12	134:EM:142:LEU:HD22	1.80	0.45
99:Dc:80:LEU:HD11	110:Do:272:GLU:HB3	1.99	0.45
99:Dc:240:TRP:NE1	150:Dc:601:CDL:OA4	2.46	0.45
101:De:43:ARG:NE	101:De:62:GLU:OE1	2.47	0.45
109:Dn:75:PHE:HD1	124:Ec:140:VAL:HG21	1.81	0.45
114:Ds:25:VAL:O	114:Ds:25:VAL:HG23	2.16	0.45
114:Ds:123:GLN:O	114:Ds:135:ARG:NH2	2.50	0.45
121:Dz:76:ASN:HA	121:Dz:93:VAL:HG22	1.98	0.45
8:A7:126:ARG:NH2	56:BM:135:ASP:OD2	2.46	0.45
14:AD:228:PRO:N	14:AD:229:PRO:HD2	2.31	0.45
15:AE:412:GLN:NE2	25:AO:131:ASN:O	2.46	0.45
18:AH:131:ILE:HG21	20:AJ:90:PHE:HB3	1.98	0.45
18:AH:150:PHE:O	18:AH:153:SER:OG	2.25	0.45
33:AW:79:LEU:O	33:AW:120:GLU:N	2.49	0.45
86:b:312:VAL:HG22	86:b:313:PRO:HD2	1.99	0.45
87:c:203:MET:HE1	167:c:510:UQ8:H3MB	1.97	0.45
97:DA:566:TYR:OH	167:DS:403:UQ8:O2	2.32	0.45
99:DC:106:VAL:HG21	116:DU:248:LEU:CD2	2.47	0.45
100:DD:325:LEU:HD13	100:DD:403:ASP:HB2	1.99	0.45
106:DJ:204:GLU:OE1	106:DJ:205:HIS:N	2.50	0.45
124:EC:30:GLY:O	124:EC:34:LEU:HD22	2.16	0.45
100:Dd:268:ASP:OD1	104:Dh:13:TYR:OH	2.16	0.45
112:Dq:99:LEU:O	112:Dq:99:LEU:HD23	2.17	0.45
112:Dq:117:THR:HG22	112:Dq:118:ILE:N	2.31	0.45
113:Dr:202:ILE:HG23	150:Dr:403:CDL:H201	1.98	0.45
119:Dx:156:ASN:ND2	128:Eg:99:TYR:OH	2.45	0.45
127:Ef:50:ILE:HG22	127:Ef:51:THR:N	2.31	0.45
6:A5:84:THR:HG23	6:A5:120:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
95:k:33:ILE:HD12	95:k:40:LEU:HD22	1.97	0.45
98:DB:287:ASN:O	98:DB:290:LEU:N	2.50	0.45
115:DT:48:GLU:OE1	115:DT:48:GLU:N	2.48	0.45
115:DT:258:ASN:O	115:DT:258:ASN:ND2	2.50	0.45
98:Db:45:TRP:NE1	167:En:1202:UQ8:H3MA	2.31	0.45
99:Dc:268:PHE:CE2	99:Dc:272:ILE:HD13	2.51	0.45
108:Dm:364:VAL:HG13	108:Dm:378:VAL:HG13	1.98	0.45
111:Dp:236:PHE:HD2	111:Dp:340:ILE:HG23	1.82	0.45
130:Ei:24:ASN:OD1	142:Eu:76:SER:OG	2.34	0.45
11:AA:281:LEU:HD13	11:AA:284:ARG:CZ	2.45	0.45
13:AC:290:LEU:HD11	13:AC:342:MET:HE1	1.97	0.45
15:AE:240:MET:O	15:AE:243:SER:OG	2.26	0.45
16:AF:254:ILE:HD11	68:BY:89:LEU:HD22	1.98	0.45
70:CH:116:GLU:OE1	70:CH:116:GLU:N	2.46	0.45
81:CN:53:ASP:OD2	81:CN:57:SER:OG	2.27	0.45
93:i:38:ILE:N	93:i:38:ILE:HD12	2.32	0.45
104:DH:60:HIS:NE2	150:DH:201:CDL:OA3	2.50	0.45
106:DJ:103:SER:OG	153:EO:201:PC1:O12	2.35	0.45
110:DO:217:ASN:OD1	110:DO:218:THR:N	2.50	0.45
110:DO:357:LEU:HD21	110:DO:366:VAL:HG13	1.97	0.45
110:DO:357:LEU:HD23	110:DO:357:LEU:C	2.42	0.45
115:DT:208:ILE:HG23	115:DT:209:PHE:CD2	2.52	0.45
115:DT:263:PRO:HB3	112:Dq:177:VAL:HG22	1.98	0.45
120:DY:120:LEU:O	120:DY:120:LEU:HD23	2.16	0.45
124:EC:39:LEU:O	124:EC:43:THR:HG23	2.17	0.45
98:Db:122:TRP:HD1	98:Db:553:CYS:HG	1.60	0.45
99:Dc:190:LEU:HD11	121:Dz:170:LEU:CD1	2.47	0.45
100:Dd:179:LEU:HD11	115:Dt:193:VAL:HG13	1.99	0.45
100:Dd:374:LEU:HD23	100:Dd:375:THR:N	2.32	0.45
150:Dd:702:CDL:OA4	138:Eq:74:ILE:HG21	2.17	0.45
116:Du:283:VAL:HB	116:Du:284:PRO:HD3	1.99	0.45
167:En:1202:UQ8:H42A	167:En:1202:UQ8:H46	1.84	0.45
12:AB:432:GLY:O	12:AB:443:HIS:NE2	2.49	0.45
14:AD:342:ALA:O	14:AD:346:VAL:HG23	2.17	0.45
15:AE:421:HIS:HB3	15:AE:425:ASP:HB2	1.99	0.45
76:CF:157:LYS:O	76:CF:248:ARG:NH2	2.43	0.45
92:H:73:HIS:O	92:H:73:HIS:ND1	2.45	0.45
95:K:18:LEU:O	95:K:22:VAL:HG23	2.16	0.45
98:DB:109:GLU:OE2	102:DF:120:THR:OG1	2.34	0.45
99:DC:158:ASP:OD2	143:EJ:57:ARG:NH1	2.50	0.45
100:DD:458:ARG:NE	100:DD:520:SEP:O3P	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
107:DK:84:THR:OG1	136:EO:117:GLU:OE1	2.24	0.45
108:DM:193:VAL:HG13	108:DM:204:LYS:HG2	1.99	0.45
109:DN:126:ILE:HD12	109:DN:126:ILE:N	2.32	0.45
112:DQ:305:ILE:HD11	137:EP:46:ALA:CB	2.47	0.45
113:DR:124:TYR:CZ	113:DR:128:VAL:HG21	2.52	0.45
123:EB:55:THR:O	123:EB:55:THR:HG22	2.16	0.45
129:EH:29:CYS:O	129:EH:30:LEU:HD12	2.16	0.45
147:EZ:35:VAL:HG22	147:EZ:36:LEU:N	2.32	0.45
102:Df:112:PRO:O	139:Er:66:TRP:NE1	2.50	0.45
105:Di:71:ASP:OD1	105:Di:76:SER:OG	2.35	0.45
109:Dn:249:ILE:HD12	109:Dn:249:ILE:O	2.16	0.45
112:Dq:344:ILE:HG22	112:Dq:344:ILE:O	2.17	0.45
143:Ej:99:PHE:CE2	143:Ej:109:LEU:HD22	2.51	0.45
1:A0:410:VAL:HG23	1:A0:410:VAL:O	2.16	0.45
4:A3:91:ALA:HA	4:A3:202:LEU:HD13	1.97	0.45
5:A4:181:LEU:HD23	5:A4:297:VAL:HG21	1.99	0.45
12:AB:151:ILE:N	15:AE:355:GLU:OE1	2.50	0.45
13:AC:387:THR:HG23	13:AC:393:VAL:CG2	2.46	0.45
15:AE:135:ALA:HB1	15:AE:147:VAL:HA	1.99	0.45
19:AI:167:LEU:HB2	19:AI:175:MET:HE2	1.99	0.45
26:AP:7:THR:HG22	26:AP:8:ILE:N	2.32	0.45
35:AY:1:MET:O	38:B1:36:ASN:ND2	2.49	0.45
51:BH:77:PRO:HA	51:BH:82:PHE:CG	2.52	0.45
91:G:270:ASP:OD2	91:G:280:TYR:OH	2.26	0.45
86:b:207:VAL:HG22	86:b:462:VAL:HG21	1.99	0.45
89:e:38:LEU:HD23	89:e:38:LEU:H	1.82	0.45
100:DD:96:ASN:N	104:DH:31:GLU:O	2.49	0.45
108:DM:214:ARG:NH1	108:DM:251:PRO:O	2.39	0.45
98:Db:348:ARG:NH1	102:Df:190:GLU:OE2	2.47	0.45
98:Db:434:ASP:OD2	98:Db:439:THR:OG1	2.21	0.45
108:Dm:193:VAL:HG13	108:Dm:204:LYS:HG2	1.97	0.45
109:Dn:81:TYR:O	109:Dn:85:VAL:HG23	2.17	0.45
2:A1:260:GLU:OE1	2:A1:322:THR:N	2.44	0.45
5:A4:158:SER:OG	7:A6:98:GLU:OE2	2.31	0.45
18:AH:123:LEU:HD13	18:AH:171:VAL:HG13	1.99	0.45
34:AX:64:LEU:CD1	43:B6:33:THR:HG21	2.46	0.45
44:BA:25:MET:CB	62:BS:111:LEU:HD11	2.47	0.45
46:BC:47:LEU:N	46:BC:47:LEU:HD12	2.32	0.45
73:CA:261:THR:HA	73:CA:560:LEU:HD21	1.98	0.45
86:b:298:THR:HG22	86:b:298:THR:O	2.16	0.45
89:e:112:MET:CG	95:k:35:THR:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
97:DA:173:PHE:N	97:DA:174:PRO:HD2	2.32	0.45
97:DA:353:LEU:HD22	97:DA:389:PHE:CZ	2.52	0.45
98:DB:391:LEU:HG	126:EE:116:LEU:HD22	1.99	0.45
99:DC:252:LEU:HD23	108:DM:298:TYR:CZ	2.52	0.45
145:EX:16:ILE:O	145:EX:20:THR:HG23	2.17	0.45
101:De:56:ASN:O	101:De:60:VAL:N	2.49	0.45
108:Dm:380:ARG:NH1	108:Dm:392:TYR:OH	2.49	0.45
110:Do:156:ASP:OD1	110:Do:160:ARG:NE	2.49	0.45
113:Dr:116:ASN:ND2	135:En:41:GLN:O	2.49	0.45
133:El:34:LYS:NZ	133:El:50:ASP:OD1	2.49	0.45
12:AB:239:PHE:O	22:AL:155:THR:HG23	2.17	0.44
18:AH:258:VAL:O	18:AH:262:VAL:HG22	2.17	0.44
20:AJ:85:LEU:CD1	35:AY:38:LEU:HD22	2.47	0.44
20:AJ:176:SER:O	20:AJ:181:ASN:N	2.47	0.44
29:AS:60:TYR:OH	29:AS:86:MET:O	2.35	0.44
63:BT:77:PHE:O	63:BT:81:ASN:ND2	2.44	0.44
73:CA:59:ALA:N	73:CA:449:ILE:HG23	2.31	0.44
85:a:55:PRO:O	85:a:59:GLN:HG3	2.18	0.44
87:c:146:LEU:HD13	87:c:146:LEU:O	2.17	0.44
87:c:382:ILE:HD11	92:h:125:TYR:HB2	2.00	0.44
100:DD:440:ALA:O	100:DD:543:ASN:ND2	2.50	0.44
106:DJ:206:GLU:N	106:DJ:206:GLU:OE1	2.51	0.44
117:DV:119:ARG:NH2	150:EB:302:CDL:O1	2.50	0.44
118:DW:305:LEU:HD23	118:DW:305:LEU:C	2.42	0.44
155:DX:304:3PE:N	130:EI:164:SER:O	2.34	0.44
121:DZ:125:GLN:OE1	121:DZ:125:GLN:N	2.50	0.44
97:Da:194:TYR:CE2	97:Da:198:LEU:HD11	2.52	0.44
150:Da:709:CDL:H162	106:Dj:109:THR:HG21	1.99	0.44
98:Db:227:ARG:NE	145:Ex:10:GLU:OE1	2.50	0.44
108:Dm:142:VAL:HG21	112:Dq:25:GLY:HA2	1.99	0.44
112:Dq:120:ASN:OD1	112:Dq:183:LYS:NZ	2.48	0.44
122:Ea:52:ILE:HG22	122:Ea:56:TYR:CE2	2.52	0.44
147:Ez:42:LEU:O	147:Ez:45:CYS:SG	2.75	0.44
12:AB:395:GLU:OE2	12:AB:417:ARG:NH1	2.50	0.44
16:AF:4:ARG:NH2	31:AU:40:ASN:O	2.51	0.44
20:AJ:211:ILE:O	20:AJ:211:ILE:HG22	2.17	0.44
21:AK:83:ASP:OD1	21:AK:84:VAL:N	2.50	0.44
21:AK:98:ASN:ND2	23:AM:107:LYS:O	2.50	0.44
32:AV:37:GLU:OE1	32:AV:37:GLU:N	2.47	0.44
75:CB:204:GLU:OE1	75:CB:204:GLU:N	2.45	0.44
87:C:336:ILE:O	87:C:336:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:DB:390:ARG:NH2	102:DF:149:ASP:OD2	2.47	0.44
99:DC:109:ALA:HB3	99:DC:110:PRO:HD3	2.00	0.44
111:DP:323:VAL:HG23	111:DP:323:VAL:O	2.16	0.44
97:Da:126:HIS:NE2	115:Dt:187:ASP:OD1	2.44	0.44
98:Db:139:THR:OG1	98:Db:604:TRP:NE1	2.50	0.44
100:Dd:325:LEU:HD13	100:Dd:403:ASP:HB2	1.99	0.44
102:Df:139:ARG:NH2	106:Dj:138:GLU:OE1	2.49	0.44
119:Dx:143:ARG:NH2	119:Dx:149:GLU:OE2	2.50	0.44
122:Ea:176:MET:HE3	122:Ea:179:LEU:HD12	1.99	0.44
130:Ei:105:ILE:HG23	130:Ei:106:CYS:N	2.32	0.44
13:AC:54:LEU:HD12	13:AC:58:PHE:HD2	1.82	0.44
18:AH:76:ILE:HA	34:AX:27:ALA:HB1	1.98	0.44
156:AL:304:LPP:O4	60:BQ:79:THR:OG1	2.33	0.44
25:AO:124:SER:OG	25:AO:126:ASP:OD1	2.34	0.44
28:AR:50:GLN:OE1	28:AR:50:GLN:N	2.50	0.44
47:BD:83:PRO:HD3	59:BP:122:VAL:HG21	1.99	0.44
73:CA:368:LEU:HB3	73:CA:371:ILE:CG2	2.48	0.44
79:CE:10:ASN:OD1	79:CE:11:LYS:N	2.50	0.44
85:A:186:TYR:CE2	85:A:190:LEU:HD11	2.53	0.44
87:C:283:ARG:N	87:C:284:PRO:HD2	2.32	0.44
87:C:378:PHE:CD1	87:C:382:ILE:HD12	2.52	0.44
91:G:15:VAL:HG22	91:G:16:LYS:N	2.33	0.44
87:c:283:ARG:N	87:c:284:PRO:HD2	2.32	0.44
89:e:197:CYS:N	89:e:202:CYS:O	2.44	0.44
98:DB:569:PHE:CD2	102:DF:108:ILE:HG21	2.51	0.44
100:DD:268:ASP:OD2	100:DD:271:TYR:N	2.44	0.44
101:DE:44:MET:CE	125:ED:160:ILE:HD11	2.47	0.44
124:EC:36:LYS:NZ	124:EC:70:GLU:O	2.45	0.44
97:Da:91:SER:OG	97:Da:591:HIS:NE2	2.47	0.44
97:Da:173:PHE:N	97:Da:174:PRO:HD2	2.32	0.44
97:Da:391:HIS:O	97:Da:394:VAL:HG22	2.17	0.44
100:Dd:451:THR:HG22	100:Dd:452:SER:N	2.32	0.44
100:Dd:459:ASN:O	100:Dd:463:VAL:HG23	2.17	0.44
150:Dd:705:CDL:H231	150:Dd:705:CDL:H271	1.99	0.44
101:De:52:HIS:O	101:De:56:ASN:ND2	2.51	0.44
150:Dj:404:CDL:OA9	136:Eo:31:TYR:OH	2.36	0.44
127:Ef:35:ILE:N	127:Ef:35:ILE:HD12	2.33	0.44
16:AF:232:SER:HB2	39:B2:40:THR:HG21	1.98	0.44
18:AH:74:LEU:HD13	18:AH:242:ALA:HB2	2.00	0.44
24:AN:92:ILE:N	24:AN:92:ILE:HD12	2.32	0.44
30:AT:51:VAL:HG23	30:AT:51:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:CD:1:MET:HE3	155:CD:303:3PE:H321	1.99	0.44
88:D:26:ILE:HG21	92:h:112:CYS:SG	2.57	0.44
93:I:38:ILE:N	93:I:38:ILE:HD12	2.32	0.44
86:b:293:GLU:HA	86:b:461:PHE:O	2.18	0.44
86:b:302:ASN:ND2	86:b:346:ASP:OD2	2.50	0.44
97:DA:402:PHE:O	97:DA:406:ASN:ND2	2.51	0.44
99:DC:524:ARG:NH2	133:EL:140:ASP:O	2.51	0.44
131:EV:39:THR:O	131:EV:39:THR:HG22	2.16	0.44
98:Db:532:SER:O	98:Db:534:HIS:ND1	2.48	0.44
100:Dd:362:ARG:NH1	100:Dd:383:ASP:OD2	2.49	0.44
106:Dj:206:GLU:N	106:Dj:206:GLU:OE1	2.51	0.44
108:Dm:159:ARG:NH2	108:Dm:161:GLU:OE2	2.47	0.44
112:Dq:117:THR:HG22	112:Dq:118:ILE:H	1.82	0.44
123:Eb:177:TYR:O	123:Eb:185:SER:OG	2.36	0.44
129:Eh:29:CYS:O	129:Eh:30:LEU:HD12	2.18	0.44
149:Dl:128:THR:OG1	149:Dl:130:ASP:OD1	2.21	0.44
6:A5:155:PHE:O	6:A5:159:ASN:ND2	2.44	0.44
12:AB:189:GLN:O	12:AB:423:ARG:NH2	2.47	0.44
12:AB:250:TYR:O	12:AB:601:ARG:NH1	2.49	0.44
13:AC:84:ASN:OD1	49:BF:150:ASN:ND2	2.50	0.44
16:AF:127:TYR:HA	16:AF:167:VAL:HG21	2.00	0.44
150:AF:401:CDL:H861	43:B6:49:VAL:HG21	1.99	0.44
18:AH:101:CYS:HB2	18:AH:247:GLY:HA2	2.00	0.44
18:AH:252:LEU:C	18:AH:252:LEU:HD23	2.42	0.44
18:AH:253:PHE:CE1	43:B6:10:ILE:HG21	2.53	0.44
87:C:120:VAL:HG11	87:C:310:PHE:CA	2.45	0.44
87:C:214:ASP:OD2	91:G:127:ARG:NH1	2.51	0.44
91:G:10:GLU:OE1	91:G:14:ASN:ND2	2.50	0.44
87:c:91:LEU:HD23	87:c:126:PHE:CE1	2.52	0.44
89:e:134:ILE:HD11	89:e:154:ILE:HD13	2.00	0.44
97:DA:92:LEU:HD22	97:DA:270:THR:HB	1.98	0.44
102:DF:159:LYS:NZ	122:EA:220:THR:O	2.49	0.44
105:DI:142:SER:OG	150:DI:302:CDL:OB4	2.35	0.44
136:EO:54:THR:HG22	136:EO:55:THR:N	2.32	0.44
138:EQ:20:THR:OG1	138:EQ:24:LYS:NZ	2.51	0.44
97:Da:641:ARG:NE	100:Dd:174:GLU:OE2	2.50	0.44
106:Dj:204:GLU:OE1	106:Dj:205:HIS:N	2.50	0.44
112:Dq:268:THR:HG23	112:Dq:268:THR:O	2.18	0.44
116:Du:274:ASN:O	116:Du:277:THR:HG22	2.18	0.44
119:Dx:176:SER:OG	119:Dx:177:THR:N	2.49	0.44
6:A5:188:ASP:OD2	15:AE:267:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AJ:154:ILE:HD12	20:AJ:154:ILE:N	2.33	0.44
21:AK:97:GLU:OE1	23:AM:88:THR:OG1	2.35	0.44
44:BA:85:ALA:HB2	44:BA:193:VAL:HG23	2.00	0.44
53:BJ:55:ASN:ND2	53:BJ:97:GLU:O	2.47	0.44
73:CA:146:PRO:O	73:CA:179:ALA:HB1	2.17	0.44
87:C:14:LYS:NZ	87:c:4:ASN:O	2.42	0.44
85:a:400:SER:OG	85:a:502:LEU:O	2.28	0.44
92:h:96:ASN:O	92:h:100:PHE:CD2	2.71	0.44
101:DE:43:ARG:NE	101:DE:62:GLU:OE1	2.44	0.44
104:DH:57:GLU:OE2	109:DN:314:ARG:N	2.40	0.44
112:DQ:82:GLU:OE1	112:DQ:82:GLU:N	2.45	0.44
114:DS:219:LEU:HB3	114:DS:241:ILE:HD12	1.98	0.44
119:DX:103:TYR:OH	153:Ef:501:PC1:O14	2.31	0.44
97:Da:92:LEU:HD22	97:Da:270:THR:HB	1.99	0.44
97:Da:293:ASP:OD1	97:Da:364:ARG:NH2	2.50	0.44
97:Da:468:ILE:HD11	98:Db:83:CYS:SG	2.58	0.44
104:Dh:81:LEU:HB2	109:Dn:325:ILE:HD13	1.99	0.44
125:Ed:179:ASP:OD2	140:Es:3:ARG:NH1	2.51	0.44
127:Ef:75:ALA:O	127:Ef:120:ARG:NH1	2.50	0.44
3:A2:116:SER:O	52:BI:37:ARG:NH2	2.50	0.44
5:A4:22:HIS:NE2	7:A6:92:ALA:O	2.34	0.44
15:AE:64:ARG:HD3	30:AT:68:THR:HG21	2.00	0.44
20:AJ:104:ASN:ND2	20:AJ:108:LEU:O	2.49	0.44
91:G:90:ASP:OD1	91:G:90:ASP:N	2.50	0.44
85:a:294:ILE:HD12	85:a:294:ILE:N	2.33	0.44
87:c:341:ILE:HG21	87:c:408:LEU:HD22	2.00	0.44
100:DD:435:LEU:HD23	100:DD:435:LEU:C	2.43	0.44
109:DN:81:TYR:O	109:DN:85:VAL:HG23	2.18	0.44
109:DN:249:ILE:HD12	109:DN:249:ILE:O	2.18	0.44
110:DO:309:LEU:HD23	110:DO:309:LEU:O	2.18	0.44
111:DP:220:ASN:ND2	111:DP:226:LYS:O	2.50	0.44
115:DT:243:ILE:HG21	127:EF:79:MET:SD	2.58	0.44
100:Dd:358:ARG:NH2	100:Dd:386:GLU:OE1	2.49	0.44
112:Dq:247:TYR:CE1	115:Dt:316:ILE:HD11	2.53	0.44
116:Du:64:ARG:NE	116:Du:77:ASP:OD2	2.51	0.44
117:Dv:211:ILE:HG23	123:Eb:174:TYR:O	2.17	0.44
150:El:903:CDL:H872	150:El:903:CDL:H831	1.99	0.44
149:DL:348:VAL:HG11	149:DL:386:GLN:NE2	2.32	0.44
4:A3:88:VAL:HG23	4:A3:250:ILE:HD12	2.00	0.44
10:A9:220:TYR:HB2	10:A9:223:VAL:HG22	2.00	0.44
47:BD:157:GLU:OE1	47:BD:157:GLU:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:CA:68:VAL:HG11	73:CA:198:TYR:HB3	1.99	0.44
85:A:133:LEU:C	85:A:133:LEU:HD12	2.43	0.44
85:A:346:ARG:NH1	88:d:319:ALA:OXT	2.51	0.44
86:B:125:ASN:OD1	86:B:126:GLU:N	2.51	0.44
87:C:98:HIS:NE2	168:C:502:HEM:ND	2.65	0.44
87:C:115:ALA:HB2	87:C:203:MET:HA	1.99	0.44
85:a:133:LEU:C	85:a:133:LEU:HD12	2.42	0.44
89:e:215:VAL:HG22	89:e:222:VAL:HG13	2.00	0.44
97:DA:627:ILE:HG23	117:DV:55:LEU:HD11	2.00	0.44
106:DJ:51:ARG:NH2	150:DJ:304:CDL:OB7	2.51	0.44
107:DK:96:GLU:OE1	107:DK:96:GLU:N	2.50	0.44
109:DN:94:LEU:HD21	125:ED:11:LYS:O	2.18	0.44
109:DN:397:LEU:HD23	109:DN:397:LEU:O	2.18	0.44
110:DO:460:LEU:HD11	110:DO:464:PHE:CZ	2.52	0.44
117:DV:24:ASN:ND2	117:DV:292:TYR:OH	2.51	0.44
118:DW:310:PHE:CE2	118:DW:314:LEU:HD11	2.52	0.44
124:EC:136:GLU:O	124:EC:140:VAL:HG23	2.18	0.44
132:EK:120:LEU:HD23	132:EK:120:LEU:O	2.17	0.44
135:EN:49:LEU:HD23	135:EN:49:LEU:C	2.43	0.44
97:Da:353:LEU:HD22	97:Da:389:PHE:CZ	2.53	0.44
169:Da:702:HEA:HBC1	169:Da:702:HEA:HMC3	2.00	0.44
150:Dc:608:CDL:OB3	108:Dm:307:LYS:NZ	2.38	0.44
108:Dm:338:ILE:HB	108:Dm:339:PRO:HD3	2.00	0.44
110:Do:325:TYR:N	150:Do:501:CDL:OA3	2.47	0.44
137:Ep:101:ILE:C	137:Ep:101:ILE:HD12	2.42	0.44
3:A2:170:ILE:HD12	3:A2:170:ILE:N	2.33	0.44
11:AA:207:ILE:HD11	11:AA:293:MET:HE1	1.99	0.44
13:AC:260:TRP:HB2	13:AC:316:GLY:HA2	2.00	0.44
16:AF:254:ILE:HD11	68:BY:89:LEU:CD2	2.48	0.44
30:AT:156:ASN:ND2	30:AT:160:LEU:O	2.46	0.44
73:CA:165:LEU:O	73:CA:170:GLY:N	2.45	0.44
86:b:95:LEU:HD11	86:b:148:THR:CG2	2.48	0.44
98:DB:516:TRP:CD1	98:DB:562:ILE:HD13	2.52	0.44
99:DC:386:LYS:O	99:DC:389:THR:HG22	2.18	0.44
100:DD:451:THR:HG22	100:DD:452:SER:N	2.33	0.44
106:DJ:99:ASN:OD1	106:DJ:99:ASN:N	2.51	0.44
114:DS:136:LYS:O	114:DS:139:THR:OG1	2.35	0.44
119:DX:35:GLU:OE1	119:DX:35:GLU:N	2.47	0.44
129:EH:129:ILE:HG22	129:EH:137:TRP:HB2	1.99	0.44
131:EV:18:LEU:HD13	131:EV:48:PHE:HA	2.00	0.44
136:EO:109:THR:HG22	136:EO:110:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
97:Da:310:PHE:CD1	97:Da:310:PHE:C	2.96	0.44
99:Dc:126:ILE:O	99:Dc:126:ILE:HG22	2.18	0.44
99:Dc:216:THR:HG23	121:Dz:33:LEU:HD22	1.99	0.44
99:Dc:221:TYR:CE1	108:Dm:228:LEU:HD23	2.53	0.44
114:Ds:170:GLU:OE1	114:Ds:170:GLU:N	2.46	0.44
120:Dy:106:PHE:CD1	120:Dy:110:ILE:HD12	2.52	0.44
128:Eg:56:SER:OG	150:Eg:101:CDL:OA8	2.36	0.44
132:Ek:61:ARG:O	132:Ek:64:ILE:HG22	2.17	0.44
136:Eo:109:THR:HG22	136:Eo:110:LEU:N	2.33	0.44
6:A5:48:ASP:OD1	6:A5:49:TYR:N	2.51	0.43
21:AK:247:GLU:OE1	21:AK:247:GLU:N	2.42	0.43
22:AL:114:GLY:N	30:AT:131:GLU:OE2	2.39	0.43
26:AP:20:LEU:O	26:AP:20:LEU:HD23	2.18	0.43
28:AR:62:ASP:OD1	28:AR:63:SER:N	2.39	0.43
46:BC:68:TYR:OH	68:BY:30:GLU:OE1	2.17	0.43
55:BL:77:MET:O	60:BQ:77:LYS:NZ	2.37	0.43
77:CG:105:LEU:HD12	77:CG:164:ILE:CG2	2.48	0.43
85:a:337:THR:OG1	85:a:347:GLN:NE2	2.50	0.43
85:a:403:ALA:HA	85:a:467:ALA:HB3	2.00	0.43
97:DA:492:MET:N	97:DA:492:MET:SD	2.90	0.43
98:DB:76:LYS:NZ	136:EO:11:GLU:O	2.48	0.43
114:DS:256:TRP:O	114:DS:259:THR:HG22	2.18	0.43
124:EC:151:PHE:O	124:EC:156:GLY:N	2.47	0.43
97:Da:49:ASN:OD1	97:Da:51:LYS:N	2.52	0.43
98:Db:337:LEU:HD22	98:Db:337:LEU:N	2.33	0.43
112:Dq:18:THR:OG1	137:Ep:79:GLU:O	2.23	0.43
113:Dr:175:GLU:OE1	113:Dr:211:ARG:NH1	2.51	0.43
113:Dr:225:MET:HE2	113:Dr:320:ILE:HG21	1.99	0.43
116:Du:253:THR:O	116:Du:257:VAL:HG23	2.18	0.43
12:AB:564:GLY:C	12:AB:580:THR:HG22	2.43	0.43
16:AF:227:ASN:ND2	54:BK:36:MET:SD	2.91	0.43
17:AG:92:LEU:HD22	17:AG:113:ILE:HD12	1.99	0.43
17:AG:172:PRO:O	17:AG:175:THR:OG1	2.32	0.43
88:d:254:MET:HE2	88:d:257:TYR:CD2	2.53	0.43
97:DA:64:THR:HG22	97:DA:149:TYR:CD1	2.54	0.43
100:DD:265:LEU:HD12	100:DD:272:ARG:HA	1.99	0.43
155:DG:204:3PE:H3I3	113:DR:201:LEU:HB3	1.98	0.43
109:DN:94:LEU:HD11	125:ED:17:VAL:HG13	1.98	0.43
119:DX:62:LEU:HD11	119:DX:94:VAL:CG2	2.49	0.43
133:EL:75:ILE:N	133:EL:75:ILE:HD12	2.33	0.43
98:Db:594:GLU:OE1	126:Ee:72:ILE:HD11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:Do:305:LEU:HD23	110:Do:305:LEU:O	2.18	0.43
113:Dr:270:ASN:ND2	113:Dr:270:ASN:O	2.51	0.43
119:Dx:50:GLY:HA3	119:Dx:105:PHE:HB2	2.00	0.43
127:Ef:142:SER:OG	127:Ef:149:ASN:OD1	2.32	0.43
146:Ey:30:SER:N	146:Ey:33:ASP:OD2	2.50	0.43
3:A2:23:LEU:HD23	3:A2:23:LEU:H	1.82	0.43
7:A6:247:HIS:O	7:A6:251:ASN:ND2	2.42	0.43
11:AA:392:GLU:OE2	11:AA:453:LYS:N	2.43	0.43
15:AE:232:LEU:HD21	25:AO:57:ASN:HA	1.99	0.43
16:AF:127:TYR:CE2	16:AF:131:ILE:HD11	2.54	0.43
18:AH:150:PHE:CE2	34:AX:57:ILE:HG23	2.52	0.43
26:AP:78:VAL:HG12	26:AP:79:GLU:N	2.33	0.43
64:BU:2:LEU:HD23	64:BU:11:LEU:HD13	2.00	0.43
73:CA:212:ILE:O	73:CA:220:ARG:N	2.52	0.43
85:a:186:TYR:CE2	85:a:190:LEU:HD11	2.53	0.43
87:c:169:THR:OG1	87:c:177:THR:OG1	2.34	0.43
97:DA:68:GLY:C	97:DA:105:MET:HE2	2.42	0.43
99:DC:143:ASN:N	110:DO:251:GLN:O	2.50	0.43
100:DD:162:THR:O	100:DD:173:HIS:N	2.42	0.43
102:DF:11:PRO:O	102:DF:12:ALA:HB3	2.19	0.43
110:DO:418:GLN:HB2	110:DO:422:ILE:HG22	1.99	0.43
115:DT:188:ILE:HG21	115:DT:208:ILE:HD11	1.98	0.43
117:DV:211:ILE:HG23	123:EB:174:TYR:O	2.18	0.43
117:DV:269:LEU:HD23	117:DV:269:LEU:C	2.43	0.43
118:DW:136:ILE:HD12	118:DW:136:ILE:N	2.32	0.43
127:EF:35:ILE:HD12	127:EF:35:ILE:N	2.33	0.43
155:Dc:606:3PE:H3I3	155:Dc:606:3PE:C3E	2.48	0.43
150:Dc:608:CDL:H271	108:Dm:341:VAL:HG21	2.00	0.43
100:Dd:103:THR:HG22	109:Dn:294:TYR:O	2.18	0.43
101:De:53:GLU:OE2	125:Ed:181:LYS:NZ	2.39	0.43
111:Dp:163:ASP:OD1	111:Dp:171:ARG:NH2	2.42	0.43
118:Dw:136:ILE:N	118:Dw:136:ILE:HD12	2.33	0.43
134:Em:138:ARG:NH1	134:Em:142:LEU:HD22	2.33	0.43
143:Ej:99:PHE:CG	143:Ej:100:PRO:HD3	2.53	0.43
11:AA:247:ASP:OD1	11:AA:304:ASN:ND2	2.51	0.43
13:AC:259:ILE:O	13:AC:262:PHE:N	2.51	0.43
13:AC:324:MET:HE2	13:AC:337:GLY:HA2	1.98	0.43
14:AD:235:GLY:HA3	14:AD:241:THR:HG22	2.00	0.43
46:BC:137:ASN:CG	49:BF:109:HIS:HD1	2.25	0.43
47:BD:150:VAL:HG21	49:BF:83:ILE:HD12	2.01	0.43
85:A:62:ARG:NH1	86:B:63:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:a:308:PHE:CE2	85:a:476:LEU:HD21	2.54	0.43
113:DR:137:ILE:N	113:DR:137:ILE:HD12	2.32	0.43
118:DW:110:THR:OG1	118:DW:113:ASN:OD1	2.35	0.43
97:Da:133:ALA:H	97:Da:316:THR:HG1	1.67	0.43
97:Da:217:LYS:C	97:Da:218:LEU:HD12	2.43	0.43
100:Dd:113:HIS:NE2	100:Dd:125:ASP:OD1	2.45	0.43
109:Dn:189:ILE:HB	132:Ek:46:VAL:HG13	2.00	0.43
112:Dq:209:GLU:OE1	112:Dq:236:TRP:NE1	2.49	0.43
143:Ej:99:PHE:CG	143:Ej:100:PRO:CD	3.01	0.43
2:A1:195:ILE:HD12	2:A1:195:ILE:N	2.33	0.43
5:A4:34:HIS:ND1	5:A4:36:THR:HG23	2.33	0.43
7:A6:128:LEU:HD22	153:A6:303:PC1:C3B	2.48	0.43
11:AA:47:PHE:CE2	11:AA:51:LEU:HD11	2.53	0.43
11:AA:376:TYR:OH	49:BF:71:ARG:NH2	2.51	0.43
11:AA:497:VAL:HG21	11:AA:595:LEU:HD21	2.01	0.43
16:AF:190:LEU:HD23	35:AY:86:GLU:HG3	1.99	0.43
18:AH:100:ILE:HG22	18:AH:104:PHE:CE1	2.54	0.43
18:AH:149:ALA:HB2	18:AH:234:VAL:HG12	1.99	0.43
20:AJ:85:LEU:HD11	35:AY:38:LEU:HD22	2.00	0.43
51:BH:80:LEU:O	51:BH:83:THR:OG1	2.25	0.43
64:BU:16:VAL:HG13	64:BU:28:ARG:CG	2.49	0.43
79:CE:184:ILE:HD11	79:CE:220:TRP:CD1	2.53	0.43
167:C:511:UQ8:C33	167:C:511:UQ8:H40	2.49	0.43
89:e:79:VAL:HG23	89:e:79:VAL:O	2.18	0.43
98:DB:57:ARG:NH2	150:DR:402:CDL:OA4	2.51	0.43
99:DC:48:LEU:O	99:DC:49:ASN:CB	2.66	0.43
99:DC:268:PHE:CZ	99:DC:272:ILE:HG21	2.54	0.43
99:DC:578:LYS:O	138:EQ:116:GLN:NE2	2.44	0.43
108:DM:338:ILE:HB	108:DM:339:PRO:HD3	2.00	0.43
108:DM:431:LEU:HD12	108:DM:431:LEU:N	2.34	0.43
155:DR:401:3PE:H3I3	155:DR:401:3PE:H3C2	2.01	0.43
119:DX:134:LEU:HD23	119:DX:134:LEU:C	2.44	0.43
126:EE:104:ILE:O	126:EE:109:LYS:NZ	2.49	0.43
138:EQ:12:THR:HG22	138:EQ:13:HIS:N	2.33	0.43
138:EQ:68:VAL:HG12	138:EQ:76:ARG:HG3	2.01	0.43
150:Da:709:CDL:H161	106:Dj:109:THR:HG21	2.00	0.43
104:Dh:82:PHE:CE2	104:Dh:86:LEU:HD11	2.53	0.43
107:Dk:54:ARG:NH2	131:Ev:33:ASP:O	2.50	0.43
108:Dm:188:LEU:O	108:Dm:191:ARG:NE	2.52	0.43
116:Du:21:ILE:HG22	116:Du:22:ASP:N	2.34	0.43
117:Dv:23:VAL:O	117:Dv:26:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
117:Dv:191:ALA:O	117:Dv:195:ASN:ND2	2.44	0.43
125:Ed:106:ILE:HD13	132:Ek:60:ILE:CD1	2.48	0.43
167:Ed:202:UQ8:H10B	167:Ed:202:UQ8:H13	2.00	0.43
127:Ef:58:LEU:HD23	127:Ef:58:LEU:C	2.44	0.43
136:Eo:54:THR:HG22	136:Eo:55:THR:N	2.34	0.43
1:A0:51:ILE:HD12	1:A0:51:ILE:N	2.34	0.43
1:A0:325:VAL:O	1:A0:328:THR:OG1	2.35	0.43
7:A6:128:LEU:HD22	153:A6:303:PC1:H3B1	2.00	0.43
11:AA:545:TYR:CE2	40:B3:48:THR:HG22	2.54	0.43
12:AB:348:ASP:OD1	12:AB:351:SER:OG	2.36	0.43
150:AP:301:CDL:H1O1	150:AP:301:CDL:PA1	2.39	0.43
85:a:102:GLU:OE1	85:a:102:GLU:N	2.46	0.43
97:DA:499:LEU:HD22	169:DA:703:HEA:H202	2.00	0.43
169:DA:702:HEA:HBC1	169:DA:702:HEA:HMC3	2.01	0.43
103:DG:10:TYR:OH	115:DT:236:GLU:OE1	2.34	0.43
119:DX:136:GLN:NE2	134:Em:46:THR:O	2.43	0.43
98:Db:25:ASP:OD1	98:Db:29:HIS:NE2	2.52	0.43
99:Dc:53:LEU:N	99:Dc:53:LEU:HD22	2.34	0.43
100:Dd:370:PHE:CD2	100:Dd:557:VAL:HG22	2.54	0.43
104:Dh:0:ACE:H3	108:Dm:467:GLU:HB2	2.00	0.43
106:Dj:96:ASN:OD1	106:Dj:106:GLN:NE2	2.52	0.43
110:Do:169:LEU:C	110:Do:169:LEU:HD12	2.43	0.43
111:Dp:184:LYS:HG2	111:Dp:296:THR:HG22	2.00	0.43
116:Du:88:VAL:HG11	116:Du:288:PHE:CD1	2.53	0.43
116:Du:135:LEU:CD2	116:Du:180:ILE:HD12	2.48	0.43
124:Ec:101:LEU:HD23	124:Ec:101:LEU:C	2.43	0.43
167:El:906:UQ8:C8	167:El:906:UQ8:C1M	2.97	0.43
3:A2:23:LEU:HD23	3:A2:23:LEU:N	2.33	0.43
3:A2:258:VAL:HG11	155:A2:401:3PE:H2H1	2.01	0.43
11:AA:705:TRP:O	11:AA:709:ILE:HG12	2.19	0.43
13:AC:386:HIS:NE2	63:BT:64:ARG:O	2.52	0.43
48:BE:97:LEU:HD12	48:BE:97:LEU:N	2.34	0.43
75:CB:53:VAL:HG22	75:CB:87:TYR:HB2	2.01	0.43
78:CK:24:LYS:O	78:CK:28:VAL:HG23	2.19	0.43
85:A:400:SER:O	85:A:403:ALA:HB3	2.18	0.43
87:C:82:TRP:NE1	153:C:510:PC1:O14	2.44	0.43
87:C:329:VAL:O	96:L:8:LYS:NZ	2.43	0.43
92:H:68:GLN:O	89:e:88:ARG:NH1	2.52	0.43
85:a:351:ILE:O	85:a:355:LEU:HG	2.19	0.43
97:DA:88:LYS:NZ	114:DS:17:ASP:OD1	2.37	0.43
97:DA:127:VAL:O	97:DA:322:MET:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:DB:300:ASP:CG	98:DB:302:ILE:HG22	2.44	0.43
99:DC:268:PHE:O	99:DC:272:ILE:HG23	2.19	0.43
113:DR:168:LYS:NZ	132:Ek:161:GLU:OE1	2.48	0.43
114:DS:185:ILE:HG21	114:DS:194:LEU:HD21	2.00	0.43
119:DX:62:LEU:HD11	119:DX:94:VAL:HG23	2.00	0.43
124:EC:71:LEU:HD13	124:EC:79:LEU:HD12	2.00	0.43
135:EN:122:ASP:OD2	135:EN:127:ARG:NH2	2.51	0.43
99:Dc:111:ILE:N	99:Dc:111:ILE:HD12	2.33	0.43
100:Dd:410:SER:OG	100:Dd:412:ARG:NH1	2.51	0.43
111:Dp:217:GLU:OE1	111:Dp:233:TYR:OH	2.31	0.43
119:Dx:68:TYR:OH	150:Dx:1204:CDL:OA3	2.31	0.43
120:Dy:81:LEU:N	120:Dy:82:PRO:CD	2.82	0.43
120:Dy:140:TRP:CD1	120:Dy:144:LEU:HD13	2.54	0.43
129:Eh:17:SER:O	129:Eh:18:LEU:HD12	2.19	0.43
141:Et:73:VAL:HG11	146:Ey:10:ALA:HA	2.01	0.43
7:A6:173:ILE:HD12	7:A6:194:LEU:HD11	2.01	0.43
11:AA:121:LEU:HD12	11:AA:121:LEU:H	1.84	0.43
12:AB:395:GLU:OE1	24:AN:184:ARG:NH2	2.51	0.43
15:AE:85:PHE:O	15:AE:439:GLU:N	2.51	0.43
16:AF:119:ILE:HD11	51:BH:144:ILE:HD12	2.01	0.43
39:B2:74:TYR:OH	39:B2:79:ASP:OD1	2.32	0.43
86:B:438:GLN:O	86:B:442:VAL:HG23	2.19	0.43
87:C:332:VAL:O	87:C:332:VAL:HG12	2.19	0.43
89:E:33:ARG:NH1	92:h:74:PHE:O	2.50	0.43
89:E:193:VAL:HG22	89:E:194:SER:N	2.34	0.43
91:G:249:TYR:HB3	91:G:252:ALA:HB2	2.01	0.43
85:a:100:THR:O	85:a:104:SER:N	2.51	0.43
87:c:197:LEU:HD23	87:c:197:LEU:C	2.44	0.43
89:e:229:VAL:N	89:e:237:ASN:OD1	2.52	0.43
98:DB:40:TRP:CH2	127:EF:182:MET:HE1	2.54	0.43
100:DD:285:VAL:HG22	108:DM:477:ILE:HD11	2.00	0.43
117:DV:137:SER:N	117:DV:138:PRO:HD2	2.33	0.43
118:DW:134:MET:HE3	118:DW:232:HIS:HD2	1.84	0.43
97:Da:155:ILE:HG21	97:Da:295:LEU:CD1	2.48	0.43
97:Da:511:VAL:O	97:Da:515:VAL:HG23	2.18	0.43
97:Da:645:ARG:HE	115:Dt:146:ILE:HD11	1.82	0.43
99:Dc:456:HIS:ND1	99:Dc:495:MET:SD	2.91	0.43
109:Dn:127:ILE:HD12	109:Dn:135:ILE:HG23	2.00	0.43
119:Dx:167:TRP:O	119:Dx:182:LYS:NZ	2.51	0.43
121:Dz:136:VAL:HG23	121:Dz:137:HIS:N	2.34	0.43
123:Eb:103:LEU:O	123:Eb:105:VAL:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
125:Ed:165:SER:OG	125:Ed:166:ILE:N	2.52	0.43
11:AA:222:VAL:O	11:AA:675:SER:OG	2.35	0.43
12:AB:82:GLU:OE1	12:AB:107:SER:OG	2.24	0.43
13:AC:155:PHE:O	13:AC:159:VAL:HG23	2.18	0.43
15:AE:162:GLU:O	15:AE:166:GLY:N	2.44	0.43
24:AN:80:LYS:O	24:AN:84:ASN:ND2	2.45	0.43
26:AP:78:VAL:HG21	26:AP:102:LEU:HD11	2.00	0.43
37:B0:76:TRP:NE1	37:B0:81:ASN:OD1	2.40	0.43
150:BC:302:CDL:H512	93:I:54:PHE:CZ	2.53	0.43
49:BF:10:ASP:OD1	49:BF:11:ASN:N	2.52	0.43
73:CA:80:LEU:HD11	73:CA:259:THR:HG21	2.00	0.43
79:CE:4:LEU:HB2	79:CE:76:ALA:HB2	2.01	0.43
79:CE:119:GLU:HB2	79:CE:161:VAL:HG23	2.01	0.43
85:A:228:ILE:HD12	85:A:228:ILE:N	2.34	0.43
92:H:13:ASP:OD1	92:H:14:PHE:N	2.52	0.43
167:c:510:UQ8:O5	167:c:510:UQ8:H4MB	2.19	0.43
97:DA:108:PHE:CE2	97:DA:152:LEU:HD12	2.54	0.43
97:DA:368:THR:O	97:DA:369:THR:OG1	2.36	0.43
98:DB:186:THR:HG21	98:DB:349:TRP:HB2	2.00	0.43
109:DN:218:ILE:H	109:DN:218:ILE:HD12	1.83	0.43
115:DT:259:THR:HG21	127:EF:149:ASN:HD22	1.83	0.43
119:DX:231:ASP:OD1	119:DX:233:THR:OG1	2.35	0.43
120:DY:206:LEU:HD23	120:DY:206:LEU:C	2.44	0.43
134:EM:51:GLN:NE2	134:EM:55:ASP:OD1	2.51	0.43
97:Da:654:ARG:CZ	115:Dt:199:LEU:HD11	2.49	0.43
110:Do:299:LEU:HD12	110:Do:299:LEU:N	2.33	0.43
121:Dz:25:ILE:HG22	121:Dz:26:TYR:CD2	2.54	0.43
122:Ea:168:LEU:HD23	122:Ea:168:LEU:C	2.44	0.43
12:AB:70:LEU:O	28:AR:166:LYS:NZ	2.40	0.43
28:AR:87:ILE:HD12	28:AR:158:PRO:HG3	2.01	0.43
29:AS:94:ARG:NH2	32:AV:97:ASP:OD1	2.52	0.43
30:AT:129:THR:HG22	30:AT:130:ALA:N	2.34	0.43
36:AZ:7:LEU:N	36:AZ:7:LEU:HD22	2.34	0.43
76:CF:209:TYR:HA	76:CF:212:ARG:HG2	2.01	0.43
85:a:292:MET:SD	85:a:294:ILE:HD11	2.59	0.43
91:g:194:ARG:HB2	91:g:197:ALA:CB	2.49	0.43
97:DA:401:THR:HG21	97:DA:535:ALA:HA	2.01	0.43
100:DD:283:TYR:O	100:DD:287:THR:HG23	2.19	0.43
114:DS:21:VAL:HG11	114:DS:330:VAL:HG23	2.00	0.43
114:DS:215:THR:OG1	167:EN:1205:UQ8:H30B	2.19	0.43
116:DU:100:ILE:C	116:DU:100:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:DZ:193:HIS:NE2	138:EQ:70:ASN:O	2.52	0.43
104:Dh:121:TYR:OH	123:Eb:72:ASP:OD1	2.27	0.43
105:Di:42:ASP:OD1	117:Dv:44:ARG:NH1	2.52	0.43
115:Dt:270:TRP:O	127:Ef:127:ASN:ND2	2.52	0.43
116:Du:227:GLN:OE1	116:Du:234:GLN:NE2	2.51	0.43
117:Dv:59:ILE:HD13	117:Dv:280:VAL:HG13	2.01	0.43
8:A7:138:THR:HG22	8:A7:139:ASP:N	2.34	0.42
11:AA:64:VAL:HG11	11:AA:76:PHE:HE1	1.83	0.42
13:AC:492:PHE:O	13:AC:496:ILE:HG22	2.19	0.42
14:AD:76:ILE:HG23	14:AD:256:MET:CE	2.48	0.42
35:AY:5:ILE:HD12	35:AY:5:ILE:N	2.34	0.42
51:BH:51:ASN:ND2	52:BI:81:CYS:O	2.52	0.42
66:BW:19:GLU:OE1	66:BW:19:GLU:N	2.47	0.42
73:CA:226:SER:O	73:CA:230:GLY:N	2.43	0.42
92:H:96:ASN:O	92:H:100:PHE:CD2	2.72	0.42
95:K:35:THR:HG22	95:K:36:LEU:HG	2.01	0.42
85:a:484:SER:O	85:a:488:ILE:HG23	2.18	0.42
103:DG:40:TYR:CZ	103:DG:44:ILE:HD11	2.54	0.42
109:DN:189:ILE:HD12	132:EK:50:GLN:OE1	2.19	0.42
112:DQ:333:THR:HG23	115:DT:74:VAL:HG21	2.00	0.42
114:DS:152:VAL:N	114:DS:153:PRO:HD2	2.33	0.42
118:DW:214:ASN:ND2	118:DW:228:GLN:OE1	2.52	0.42
119:DX:8:ARG:NE	150:DX:306:CDL:OA7	2.52	0.42
130:EI:79:ILE:O	130:EI:82:VAL:HG12	2.19	0.42
141:ET:37:LEU:C	141:ET:37:LEU:HD12	2.44	0.42
97:Da:581:LEU:HD21	97:Da:600:TRP:HB2	2.00	0.42
99:Dc:106:VAL:HG22	116:Du:247:PRO:HB2	2.00	0.42
150:Dh:201:CDL:H673	150:Dh:202:CDL:OB7	2.19	0.42
108:Dm:340:THR:O	108:Dm:344:VAL:HG23	2.19	0.42
111:Dp:164:ALA:HB3	111:Dp:275:THR:HG22	2.00	0.42
114:Ds:152:VAL:N	114:Ds:153:PRO:HD2	2.34	0.42
115:Dt:45:PRO:CG	115:Dt:50:ILE:HD11	2.47	0.42
115:Dt:158:THR:HG22	115:Dt:163:VAL:O	2.19	0.42
118:Dw:310:PHE:CE2	118:Dw:314:LEU:HD11	2.53	0.42
153:A6:303:PC1:O13	153:A6:303:PC1:H133	2.19	0.42
9:A8:227:ARG:NH2	14:AD:448:GLU:OE1	2.44	0.42
14:AD:209:GLU:OE1	160:AD:502:FMN:HM82	2.19	0.42
58:BO:98:SER:OG	58:BO:123:VAL:HG22	2.19	0.42
70:CH:114:ASN:OD1	70:CH:115:SER:N	2.52	0.42
86:B:207:VAL:HG22	86:B:462:VAL:HG21	2.01	0.42
99:DC:363:LEU:HD23	99:DC:363:LEU:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
100:DD:179:LEU:CD1	115:DT:193:VAL:HG13	2.49	0.42
104:DH:8:SER:OG	108:DM:451:GLN:OE1	2.37	0.42
108:DM:198:HIS:O	108:DM:202:GLY:N	2.51	0.42
109:DN:218:ILE:HD12	109:DN:218:ILE:N	2.34	0.42
112:DQ:117:THR:HG22	112:DQ:118:ILE:N	2.33	0.42
114:DS:25:VAL:HG23	114:DS:25:VAL:O	2.18	0.42
116:DU:258:ALA:HB2	116:DU:270:VAL:HG21	2.01	0.42
130:EI:120:VAL:HG13	142:EU:52:ASP:OD1	2.20	0.42
139:ER:90:GLN:OE1	139:ER:90:GLN:N	2.41	0.42
105:Di:33:TRP:HB2	105:Di:39:VAL:HG11	2.01	0.42
108:Dm:212:ASP:OD1	108:Dm:212:ASP:N	2.52	0.42
109:Dn:365:ARG:NH1	121:Dz:44:ASN:O	2.52	0.42
112:Dq:159:GLU:OE2	112:Dq:163:GLN:NE2	2.52	0.42
141:Et:6:ILE:N	141:Et:6:ILE:HD12	2.34	0.42
149:Dl:241:ASN:OD1	149:Dl:242:ILE:N	2.51	0.42
149:DL:306:PHE:HE2	149:DL:362:VAL:HG13	1.84	0.42
7:A6:124:LEU:HB3	7:A6:125:PRO:HD3	2.01	0.42
11:AA:247:ASP:OD1	11:AA:247:ASP:N	2.47	0.42
13:AC:409:PHE:CD1	150:AC:801:CDL:H273	2.54	0.42
19:AI:51:GLU:OE1	19:AI:74:LEU:HD22	2.19	0.42
45:BB:198:LEU:HB3	47:BD:184:ILE:HG21	2.01	0.42
49:BF:98:ILE:HG23	49:BF:99:ALA:N	2.34	0.42
86:B:384:LYS:NZ	86:B:480:LEU:O	2.45	0.42
91:G:181:ILE:HD12	150:c:509:CDL:HA21	2.01	0.42
88:d:204:HIS:HA	90:f:58:MET:HE1	2.01	0.42
89:e:218:CYS:CB	158:e:1102:FES:S2	3.08	0.42
103:DG:92:GLU:OE2	131:EV:66:ARG:NH2	2.52	0.42
110:DO:325:TYR:N	150:DO:501:CDL:OA3	2.51	0.42
97:Da:391:HIS:HB3	97:Da:392:PRO:HD3	2.01	0.42
98:Db:402:HIS:ND1	98:Db:403:LYS:O	2.50	0.42
99:Dc:259:TYR:O	99:Dc:263:VAL:HG13	2.19	0.42
99:Dc:457:PHE:O	99:Dc:460:ILE:HG13	2.19	0.42
109:Dn:24:ILE:HD12	125:Ed:5:ILE:HD12	2.02	0.42
150:Dn:502:CDL:H832	150:Dn:502:CDL:H872	2.01	0.42
111:Dp:225:GLN:N	111:Dp:225:GLN:OE1	2.52	0.42
111:Dp:323:VAL:HG23	111:Dp:323:VAL:O	2.17	0.42
114:Ds:302:THR:HG22	114:Ds:302:THR:O	2.18	0.42
137:Ep:52:CYS:SG	137:Ep:95:LEU:HD23	2.60	0.42
5:A4:98:LEU:HD23	5:A4:98:LEU:C	2.44	0.42
18:AH:176:PHE:CZ	43:B6:52:LEU:HD23	2.55	0.42
21:AK:160:ALA:HB3	23:AM:172:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AQ:108:ASP:OD1	27:AQ:109:GLU:N	2.52	0.42
42:B5:66:ASN:N	42:B5:69:GLU:OE2	2.52	0.42
45:BB:205:LEU:CD1	47:BD:188:ILE:HG23	2.50	0.42
48:BE:101:THR:HG22	48:BE:102:HIS:N	2.33	0.42
78:CK:41:VAL:HG12	78:CK:42:PHE:N	2.33	0.42
81:CN:34:VAL:HB	81:CN:35:PRO:HD3	2.02	0.42
87:C:37:PHE:CE2	87:C:237:ILE:HD12	2.54	0.42
150:C:505:CDL:OB3	93:i:67:GLN:NE2	2.52	0.42
167:C:512:UQ8:H3MA	167:C:512:UQ8:O2	2.18	0.42
86:b:98:VAL:HG22	86:b:243:ASN:HB3	2.02	0.42
89:e:203:ILE:HD12	89:e:203:ILE:N	2.35	0.42
97:DA:477:LEU:HD11	97:DA:492:MET:HE1	2.01	0.42
99:DC:126:ILE:O	99:DC:126:ILE:HG22	2.17	0.42
105:DI:146:ILE:N	105:DI:146:ILE:HD12	2.34	0.42
108:DM:80:ARG:NH2	108:DM:200:ASP:O	2.53	0.42
108:DM:448:PHE:O	108:DM:452:THR:HG22	2.19	0.42
109:DN:131:ASN:ND2	124:EC:77:LEU:HD13	2.34	0.42
110:DO:169:LEU:C	110:DO:169:LEU:HD12	2.45	0.42
150:DO:501:CDL:H181	150:DO:501:CDL:H871	2.01	0.42
112:DQ:136:TRP:NE1	112:DQ:198:TYR:OH	2.48	0.42
112:DQ:257:ASP:OD1	112:DQ:258:LEU:N	2.52	0.42
121:DZ:136:VAL:HG23	121:DZ:137:HIS:N	2.34	0.42
124:EC:131:ASP:OD2	124:EC:141:ARG:NH2	2.49	0.42
98:Db:195:ILE:HD12	98:Db:195:ILE:N	2.34	0.42
98:Db:203:LEU:HD13	98:Db:203:LEU:C	2.44	0.42
98:Db:588:VAL:HG13	98:Db:589:SER:N	2.34	0.42
112:Dq:240:TYR:CE2	112:Dq:244:LEU:HD11	2.55	0.42
1:A0:72:ILE:HD12	1:A0:72:ILE:N	2.34	0.42
1:A0:401:ILE:HG23	1:A0:443:VAL:HG21	2.01	0.42
4:A3:37:TYR:O	4:A3:41:ASN:N	2.53	0.42
150:AC:802:CDL:H471	51:BH:159:ILE:CD1	2.50	0.42
14:AD:41:ILE:O	14:AD:138:LYS:NZ	2.53	0.42
14:AD:407:TYR:OH	14:AD:452:ASP:OD2	2.37	0.42
18:AH:165:ILE:HD11	43:B6:36:ASN:ND2	2.35	0.42
18:AH:176:PHE:CE2	43:B6:55:VAL:HG21	2.55	0.42
26:AP:187:ILE:CG2	26:AP:192:ILE:HD12	2.50	0.42
30:AT:2:ARG:NH1	30:AT:161:THR:O	2.48	0.42
49:BF:116:GLN:OE1	63:BT:133:ASN:ND2	2.35	0.42
73:CA:604:ASP:OD2	73:CA:607:THR:OG1	2.37	0.42
87:C:23:MET:SD	167:C:512:UQ8:H3MB	2.59	0.42
87:C:288:TRP:CZ2	155:C:513:3PE:H3I3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:d:47:VAL:HG13	88:d:48:GLY:N	2.34	0.42
98:DB:16:ASN:ND2	98:DB:18:GLY:O	2.48	0.42
99:DC:518:TRP:CZ2	153:EO:204:PC1:H142	2.54	0.42
100:DD:502:TYR:CZ	100:DD:506:LEU:HD21	2.53	0.42
112:DQ:115:ASP:OD1	112:DQ:115:ASP:N	2.52	0.42
118:DW:154:THR:HG22	118:DW:165:GLY:HA2	2.02	0.42
153:DX:305:PC1:H143	153:DX:305:PC1:O13	2.19	0.42
100:Dd:286:TYR:CE2	100:Dd:290:LEU:HD11	2.54	0.42
100:Dd:328:ASP:OD1	101:De:43:ARG:NH2	2.42	0.42
150:Dg:201:CDL:H272	150:Dg:201:CDL:C47	2.50	0.42
110:Do:471:PRO:O	110:Do:472:SER:OG	2.24	0.42
112:Dq:247:TYR:CD1	115:Dt:316:ILE:HD11	2.54	0.42
114:Ds:254:TYR:O	114:Ds:258:VAL:HG23	2.19	0.42
120:Dy:97:VAL:O	120:Dy:97:VAL:HG12	2.18	0.42
4:A3:258:ASN:OD1	4:A3:259:TYR:N	2.45	0.42
5:A4:74:LEU:HD21	5:A4:229:GLU:CD	2.44	0.42
11:AA:93:PRO:HA	11:AA:96:ILE:HG22	2.01	0.42
12:AB:515:HIS:HB2	12:AB:521:ILE:HD11	2.01	0.42
43:B6:56:THR:CG2	56:BM:92:ILE:HD11	2.50	0.42
48:BE:115:LEU:HD21	48:BE:144:TYR:CD2	2.55	0.42
71:CM:16:LYS:NZ	77:CG:46:ASP:OD2	2.52	0.42
72:CL:54:TYR:OH	74:CI:92:PHE:O	2.37	0.42
85:A:513:VAL:HG22	92:h:44:SER:OG	2.18	0.42
85:a:97:ARG:NH2	85:a:283:GLU:O	2.52	0.42
96:l:3:ALA:N	96:l:4:PRO:CD	2.83	0.42
99:DC:458:VAL:HG11	153:DC:602:PC1:H3H1	2.01	0.42
100:DD:120:THR:HG21	100:DD:256:MET:HE3	2.02	0.42
115:DT:280:GLU:HG2	112:Dq:0:ACE:H2	2.01	0.42
120:DY:81:LEU:N	120:DY:82:PRO:CD	2.83	0.42
124:EC:7:GLU:O	124:EC:11:LEU:HD13	2.19	0.42
138:EQ:73:ILE:O	138:EQ:73:ILE:HD13	2.19	0.42
97:Da:342:THR:HB	97:Da:396:VAL:HG13	2.00	0.42
97:Da:500:VAL:HA	97:Da:503:PHE:HD2	1.84	0.42
97:Da:501:ALA:HB2	97:Da:529:ILE:CG2	2.44	0.42
98:Db:44:ILE:HD12	98:Db:44:ILE:N	2.35	0.42
100:Dd:350:ARG:NH1	100:Dd:387:TPO:O2P	2.48	0.42
104:Dh:8:SER:OG	108:Dm:451:GLN:NE2	2.53	0.42
112:Dq:242:GLU:HB2	112:Dq:249:LYS:HD3	2.02	0.42
113:Dr:124:TYR:CE2	113:Dr:128:VAL:HG21	2.54	0.42
114:Ds:13:SER:OG	123:Eb:178:PHE:N	2.51	0.42
126:Ee:124:HIS:CE1	126:Ee:128:THR:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
143:Ej:31:LEU:O	143:Ej:175:HIS:NE2	2.51	0.42
143:Ej:120:LEU:HD21	143:Ej:165:LEU:HD11	2.00	0.42
145:Ex:21:LEU:C	145:Ex:21:LEU:HD23	2.45	0.42
1:A0:465:LEU:HD12	1:A0:468:VAL:HG11	2.02	0.42
3:A2:160:VAL:HG11	3:A2:163:LYS:HD2	2.02	0.42
3:A2:281:VAL:HG21	39:B2:85:SER:HB2	2.00	0.42
6:A5:228:LEU:HD11	6:A5:240:VAL:HG21	2.01	0.42
7:A6:40:GLN:O	7:A6:44:HIS:N	2.52	0.42
7:A6:114:ARG:NE	7:A6:182:GLY:O	2.53	0.42
11:AA:587:LEU:N	11:AA:587:LEU:HD12	2.35	0.42
12:AB:207:ILE:HD12	12:AB:207:ILE:N	2.35	0.42
16:AF:117:ILE:HD11	16:AF:128:PHE:HZ	1.84	0.42
16:AF:220:SER:OG	16:AF:225:ILE:HG21	2.19	0.42
22:AL:108:ASN:O	22:AL:112:GLU:N	2.52	0.42
25:AO:95:LEU:HD13	25:AO:114:ILE:HD13	2.00	0.42
28:AR:107:LEU:HD23	28:AR:107:LEU:C	2.45	0.42
73:CA:129:MET:SD	73:CA:435:VAL:HG21	2.60	0.42
75:CB:179:TYR:O	75:CB:182:ILE:HG12	2.19	0.42
89:e:193:VAL:HG22	89:e:194:SER:N	2.35	0.42
97:DA:125:TYR:CE1	115:DT:208:ILE:HD12	2.55	0.42
97:DA:603:MET:HE1	167:DS:403:UQ8:H46B	2.01	0.42
98:DB:245:THR:HG1	98:DB:247:LYS:NZ	2.17	0.42
150:DD:704:CDL:HA61	106:DJ:65:LEU:HD22	2.01	0.42
102:DF:155:PHE:O	102:DF:158:VAL:HG13	2.20	0.42
108:DM:30:THR:HG22	108:DM:31:ALA:N	2.34	0.42
115:DT:135:LEU:O	115:DT:140:GLN:NE2	2.51	0.42
117:DV:118:HIS:N	153:DV:406:PC1:O14	2.53	0.42
127:EF:142:SER:OG	127:EF:149:ASN:OD1	2.24	0.42
97:Da:329:ARG:O	97:Da:337:ILE:HD11	2.20	0.42
101:De:43:ARG:NH2	101:De:62:GLU:OE1	2.52	0.42
102:Df:230:TYR:OH	133:El:8:PRO:O	2.34	0.42
108:Dm:404:VAL:HG23	108:Dm:404:VAL:O	2.19	0.42
117:Dv:248:GLN:NE2	117:Dv:259:TYR:O	2.48	0.42
120:Dy:70:ALA:CB	120:Dy:164:LEU:HD21	2.49	0.42
122:Ea:75:GLN:NE2	122:Ea:169:ASN:OD1	2.52	0.42
124:Ec:9:LEU:C	124:Ec:9:LEU:HD12	2.44	0.42
140:Es:45:ILE:HD11	140:Es:52:GLU:OE2	2.20	0.42
1:A0:72:ILE:HD11	1:A0:101:PHE:HB2	2.00	0.42
4:A3:275:ILE:O	4:A3:276:ARG:C	2.63	0.42
10:A9:52:TRP:CE2	88:D:26:ILE:HD13	2.53	0.42
18:AH:239:PHE:HA	18:AH:242:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AS:168:LYS:NZ	29:AS:169:PRO:O	2.37	0.42
35:AY:14:LEU:O	35:AY:18:ILE:HG12	2.20	0.42
44:BA:198:ASP:OD2	44:BA:201:HIS:N	2.44	0.42
49:BF:153:GLU:OE1	49:BF:153:GLU:N	2.44	0.42
70:CH:102:LEU:HD23	72:CL:11:ILE:HG23	2.01	0.42
77:CG:176:ASN:ND2	82:CC:2:ARG:O	2.42	0.42
79:CE:107:ALA:O	79:CE:109:VAL:HG23	2.19	0.42
86:B:303:VAL:HG22	86:B:305:LEU:CD1	2.50	0.42
87:C:143:ASP:HB2	87:C:265:ILE:HD11	2.02	0.42
88:D:64:THR:HG22	88:D:65:TYR:N	2.35	0.42
89:E:208:LEU:HD22	89:E:215:VAL:HG21	2.01	0.42
90:F:45:LEU:HD13	90:F:57:CYS:SG	2.59	0.42
87:c:121:PHE:CE2	87:c:195:LEU:HD21	2.55	0.42
98:DB:106:TRP:NE1	106:DJ:155:GLU:OE1	2.51	0.42
113:DR:222:ILE:HA	113:DR:238:THR:HG22	2.01	0.42
99:Dc:190:LEU:HD12	121:Dz:149:VAL:HG11	2.02	0.42
155:Dr:401:3PE:H3I3	155:Dr:401:3PE:H3C2	2.02	0.42
116:Du:135:LEU:HD21	116:Du:180:ILE:HD12	2.01	0.42
138:Eq:36:MET:O	138:Eq:102:LYS:NZ	2.50	0.42
1:A0:84:ARG:HA	1:A0:87:VAL:HG22	2.02	0.42
1:A0:110:ASP:OD1	1:A0:142:ARG:NH1	2.53	0.42
7:A6:225:ASP:O	7:A6:229:GLY:N	2.51	0.42
12:AB:602:LEU:HD23	12:AB:602:LEU:C	2.45	0.42
15:AE:52:ALA:O	15:AE:419:LYS:O	2.38	0.42
19:AI:47:GLU:OE1	19:AI:47:GLU:N	2.49	0.42
30:AT:95:SER:N	159:AT:201:SF4:S1	2.93	0.42
68:BY:43:PHE:O	68:BY:47:LYS:HB2	2.20	0.42
85:A:121:ARG:NH1	85:A:129:GLU:OE2	2.53	0.42
85:A:390:GLN:NE2	85:A:513:VAL:OXT	2.52	0.42
87:C:21:SER:OG	85:a:512:ILE:HD11	2.20	0.42
87:C:318:THR:HG22	87:C:323:ASN:OD1	2.19	0.42
167:C:512:UQ8:H42	167:C:512:UQ8:H46	1.82	0.42
88:D:42:GLU:N	88:D:42:GLU:OE1	2.53	0.42
93:I:24:TYR:O	93:I:27:VAL:HG22	2.19	0.42
87:c:273:PHE:CB	89:e:200:LEU:HD21	2.50	0.42
88:d:278:TYR:CE2	88:d:282:LEU:HD11	2.55	0.42
98:DB:337:LEU:HD22	98:DB:337:LEU:N	2.35	0.42
105:DI:142:SER:HG	150:DI:302:CDL:PB2	2.43	0.42
140:ES:50:ASN:OD1	140:ES:51:LEU:N	2.47	0.42
99:Dc:77:VAL:O	99:Dc:77:VAL:HG22	2.19	0.42
99:Dc:176:ILE:HD12	99:Dc:176:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
116:Du:51:GLN:HB3	116:Du:316:MET:HE1	2.01	0.42
119:Dx:84:PHE:CE2	119:Dx:88:LEU:HD11	2.55	0.42
141:Et:30:LEU:HD23	141:Et:30:LEU:C	2.44	0.42
149:Dl:306:PHE:HE2	149:Dl:362:VAL:HG13	1.85	0.42
9:A8:149:THR:HG22	9:A8:150:ASP:N	2.34	0.42
11:AA:68:HIS:CE1	118:Dw:82:LYS:HD3	2.55	0.42
11:AA:373:ILE:HD11	11:AA:391:ILE:CD1	2.50	0.42
153:AA:906:PC1:H3I2	153:AA:906:PC1:H3E1	2.02	0.42
14:AD:308:VAL:HG12	14:AD:309:ARG:N	2.35	0.42
16:AF:262:ILE:HG22	16:AF:263:ALA:N	2.34	0.42
19:AI:75:VAL:HG11	19:AI:83:VAL:HG13	2.00	0.42
62:BS:91:ASN:OD1	62:BS:92:GLY:N	2.52	0.42
71:CM:20:SER:O	79:CE:89:ASN:ND2	2.53	0.42
97:DA:34:ASN:HB2	121:DZ:25:ILE:HD12	2.02	0.42
97:DA:247:ALA:O	97:DA:251:VAL:HG11	2.20	0.42
97:DA:270:THR:OG1	97:DA:271:THR:N	2.53	0.42
97:DA:646:ILE:HD13	115:DT:146:ILE:HG21	2.01	0.42
99:DC:470:ARG:NH1	99:DC:473:GLU:OE2	2.53	0.42
106:DJ:155:GLU:O	106:DJ:189:ARG:NH2	2.48	0.42
114:DS:301:PHE:N	150:DS:401:CDL:OA3	2.53	0.42
97:Da:191:TYR:O	97:Da:191:TYR:CG	2.73	0.42
97:Da:335:VAL:CG2	97:Da:407:MET:HE2	2.50	0.42
100:Dd:572:TRP:N	150:Dd:705:CDL:OB4	2.49	0.42
150:Di:1103:CDL:H652	153:Dv:404:PC1:H3I2	2.02	0.42
106:Dj:28:VAL:O	106:Dj:28:VAL:HG12	2.19	0.42
108:Dm:300:VAL:HB	108:Dm:301:PRO:HD3	2.02	0.42
112:Dq:333:THR:HG23	115:Dt:74:VAL:HG21	2.01	0.42
113:Dr:225:MET:CE	113:Dr:320:ILE:HG21	2.50	0.42
114:Ds:163:GLY:O	114:Ds:166:THR:HG22	2.19	0.42
142:Eu:35:ASN:O	142:Eu:41:GLN:NE2	2.49	0.42
149:Dl:99:THR:O	149:Dl:105:ARG:NH2	2.52	0.42
4:A3:72:LEU:HD21	4:A3:115:THR:HG21	2.02	0.41
4:A3:133:TYR:O	4:A3:137:VAL:HG23	2.19	0.41
12:AB:338:GLN:O	12:AB:538:LYS:N	2.52	0.41
25:AO:95:LEU:HD11	25:AO:112:PHE:HB3	2.02	0.41
51:BH:120:ARG:NH1	52:BI:85:GLU:OE1	2.53	0.41
85:A:105:GLY:O	85:A:109:PHE:HD1	2.03	0.41
85:A:406:ILE:HD13	85:A:463:ILE:HG21	2.01	0.41
85:a:201:LEU:HA	85:a:204:ILE:HG12	2.01	0.41
85:a:474:LYS:O	85:a:501:THR:HG21	2.20	0.41
103:DG:24:GLU:OE1	103:DG:24:GLU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
104:DH:14:TYR:OH	108:DM:393:GLU:OE1	2.32	0.41
109:DN:126:ILE:HD12	109:DN:126:ILE:H	1.85	0.41
109:DN:392:LYS:N	109:DN:393:PRO:HD2	2.34	0.41
114:DS:248:LEU:HD21	150:DS:401:CDL:H271	2.01	0.41
115:DT:81:PRO:HG2	115:DT:89:MET:HE3	2.02	0.41
109:Dn:16:TYR:O	109:Dn:20:ASN:ND2	2.42	0.41
109:Dn:392:LYS:N	109:Dn:393:PRO:HD2	2.35	0.41
110:Do:447:VAL:HG22	110:Do:448:VAL:N	2.35	0.41
120:Dy:71:TYR:CE1	120:Dy:81:LEU:HD11	2.54	0.41
6:A5:248:VAL:HG22	6:A5:248:VAL:O	2.20	0.41
11:AA:565:LEU:HD21	11:AA:603:VAL:HG22	2.02	0.41
11:AA:567:LEU:HD22	11:AA:567:LEU:N	2.35	0.41
11:AA:577:LEU:HD23	11:AA:577:LEU:C	2.45	0.41
12:AB:182:ARG:NH2	12:AB:226:VAL:O	2.53	0.41
12:AB:276:PRO:HB3	12:AB:287:ILE:HG23	2.02	0.41
12:AB:422:THR:HA	12:AB:426:LEU:HB3	2.02	0.41
13:AC:269:THR:O	13:AC:273:ALA:HB2	2.20	0.41
14:AD:389:GLY:HA3	14:AD:420:ILE:HD11	2.02	0.41
30:AT:91:LEU:HD23	30:AT:91:LEU:C	2.45	0.41
50:BG:113:ASN:OD1	50:BG:128:GLN:NE2	2.45	0.41
64:BU:81:GLY:O	64:BU:84:SER:OG	2.26	0.41
64:BU:99:ARG:NH1	142:EU:4:ASP:OD1	2.51	0.41
85:A:101:LEU:HD11	93:I:32:LEU:CD1	2.49	0.41
87:C:120:VAL:O	87:C:124:LEU:HD13	2.20	0.41
91:G:181:ILE:O	91:G:181:ILE:HG22	2.19	0.41
91:G:313:ILE:HG22	91:G:314:LEU:N	2.36	0.41
97:DA:653:ILE:HG23	115:DT:133:LEU:HD22	2.02	0.41
98:DB:155:GLU:HB3	98:DB:158:THR:HG22	2.02	0.41
109:DN:213:ASN:OD1	124:EC:182:LYS:NZ	2.47	0.41
120:DY:81:LEU:N	120:DY:82:PRO:HD2	2.35	0.41
141:ET:30:LEU:HD23	141:ET:30:LEU:C	2.44	0.41
100:Dd:503:LEU:HB2	132:Ek:40:ILE:HD11	2.01	0.41
150:Dm:501:CDL:OA9	138:Eq:71:LEU:HD21	2.20	0.41
114:Ds:211:THR:HG21	114:Ds:249:ALA:HA	2.02	0.41
129:Eh:1:MET:HE3	129:Eh:1:MET:HB2	1.91	0.41
133:El:40:ALA:O	133:El:148:VAL:HG13	2.19	0.41
167:El:906:UQ8:C8	167:El:906:UQ8:H1M	2.50	0.41
138:Eq:20:THR:OG1	138:Eq:24:LYS:NZ	2.53	0.41
149:DL:298:GLN:N	149:DL:310:LEU:O	2.53	0.41
13:AC:108:TYR:OH	13:AC:164:THR:OG1	2.33	0.41
14:AD:116:ILE:HD12	14:AD:116:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AD:308:VAL:HG21	14:AD:315:LEU:HB2	2.01	0.41
18:AH:86:ASN:ND2	53:BJ:164:TRP:O	2.51	0.41
22:AL:190:ILE:O	22:AL:190:ILE:HG23	2.20	0.41
25:AO:37:ILE:HG23	25:AO:45:ILE:CD1	2.50	0.41
85:A:100:THR:HG22	85:A:101:LEU:N	2.36	0.41
99:DC:80:LEU:HD11	110:DO:272:GLU:HB3	2.02	0.41
99:DC:142:TYR:O	99:DC:144:ASP:N	2.54	0.41
150:DD:704:CDL:CA6	106:DJ:65:LEU:HD22	2.50	0.41
103:DG:9:ARG:NH1	127:EF:79:MET:HE1	2.34	0.41
115:DT:318:ILE:HD12	115:DT:318:ILE:C	2.45	0.41
144:EW:29:LEU:HD23	144:EW:29:LEU:O	2.20	0.41
97:Da:216:ILE:HG23	123:Eb:192:ASP:OD2	2.20	0.41
100:Dd:199:ARG:NH1	108:Dm:83:TYR:OH	2.54	0.41
105:Di:186:THR:HG22	105:Di:188:ASP:CG	2.44	0.41
112:Dq:293:THR:O	112:Dq:293:THR:HG22	2.19	0.41
114:Ds:209:THR:HG23	114:Ds:210:PHE:N	2.35	0.41
116:Du:246:TYR:N	116:Du:247:PRO:HD2	2.36	0.41
123:Eb:19:THR:HG23	123:Eb:20:PHE:CD2	2.55	0.41
140:Es:81:PHE:CE2	140:Es:85:LEU:HD11	2.55	0.41
149:DL:398:ILE:HD13	149:DL:412:THR:HG22	2.02	0.41
1:A0:349:MET:HE3	1:A0:369:LEU:CD1	2.50	0.41
9:A8:296:GLN:OE1	9:A8:296:GLN:N	2.53	0.41
14:AD:127:LYS:HB2	14:AD:276:LEU:HD23	2.03	0.41
18:AH:280:ASP:OD1	55:BL:3:ASN:ND2	2.52	0.41
30:AT:81:TYR:CB	30:AT:117:ILE:HD12	2.50	0.41
46:BC:148:SER:OG	46:BC:150:ILE:O	2.34	0.41
55:BL:108:ARG:HD2	60:BQ:99:THR:HG23	2.02	0.41
64:BU:108:SER:O	64:BU:109:THR:OG1	2.32	0.41
86:B:417:LEU:O	86:B:421:VAL:HG23	2.20	0.41
90:F:68:ILE:O	90:F:72:VAL:HG23	2.20	0.41
87:c:203:MET:HE1	167:c:510:UQ8:C3	2.51	0.41
88:d:64:THR:HG22	88:d:65:TYR:N	2.36	0.41
97:DA:132:VAL:HG21	97:DA:138:ASN:HB2	2.02	0.41
97:DA:335:VAL:HG21	97:DA:407:MET:HE2	2.01	0.41
99:DC:386:LYS:NZ	100:DD:91:GLU:O	2.54	0.41
99:DC:458:VAL:HG11	153:DC:602:PC1:C3H	2.51	0.41
109:DN:340:MET:O	150:DN:506:CDL:O1	2.36	0.41
111:DP:365:THR:HG22	111:DP:366:LYS:N	2.35	0.41
120:DY:176:ASN:OD1	120:DY:177:ASP:N	2.53	0.41
100:Dd:403:ASP:OD1	100:Dd:403:ASP:C	2.62	0.41
105:Di:118:TYR:N	105:Di:122:ASP:OD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:Dp:169:TRP:CD1	111:Dp:170:VAL:HG23	2.55	0.41
133:El:75:ILE:H	133:El:75:ILE:HD12	1.85	0.41
143:Ej:44:ASN:ND2	143:Ej:130:THR:OG1	2.46	0.41
149:DL:263:THR:HG22	149:DL:265:LEU:H	1.85	0.41
2:A1:53:PHE:CZ	2:A1:238:ILE:HD12	2.56	0.41
10:A9:13:TYR:CE2	10:A9:17:LEU:HD11	2.56	0.41
14:AD:129:ARG:NH2	14:AD:166:GLU:OE2	2.53	0.41
16:AF:138:ILE:HG22	16:AF:139:PRO:HD3	2.03	0.41
27:AQ:8:VAL:HG12	27:AQ:9:LYS:N	2.35	0.41
55:BL:43:PHE:O	55:BL:47:ILE:HG13	2.20	0.41
73:CA:511:HIS:ND1	73:CA:520:LEU:O	2.45	0.41
77:CG:65:ILE:HD12	77:CG:78:TYR:CE2	2.56	0.41
85:A:123:ARG:O	85:A:126:ILE:HG13	2.21	0.41
89:E:191:ILE:HD12	89:E:191:ILE:N	2.35	0.41
85:a:465:ARG:NE	86:b:34:LYS:O	2.49	0.41
87:c:115:ALA:HB2	87:c:203:MET:HA	2.02	0.41
97:DA:191:TYR:O	97:DA:191:TYR:CG	2.73	0.41
98:DB:532:SER:O	98:DB:534:HIS:ND1	2.52	0.41
100:DD:382:ARG:HA	100:DD:389:LEU:HD11	2.01	0.41
108:DM:212:ASP:OD1	108:DM:212:ASP:N	2.53	0.41
109:DN:190:LYS:NZ	132:EK:80:VAL:O	2.53	0.41
110:DO:245:GLN:O	110:DO:248:VAL:HG22	2.19	0.41
110:DO:299:LEU:N	110:DO:299:LEU:HD12	2.36	0.41
111:DP:184:LYS:HG2	111:DP:296:THR:HG22	2.03	0.41
112:DQ:34:THR:HG23	112:DQ:62:ARG:HH12	1.85	0.41
112:DQ:293:THR:O	112:DQ:293:THR:HG22	2.21	0.41
115:DT:158:THR:HG22	115:DT:163:VAL:O	2.21	0.41
127:EF:50:ILE:HG22	127:EF:51:THR:N	2.35	0.41
98:Db:1:MET:HE3	102:Df:78:MET:HG3	2.03	0.41
99:Dc:264:ARG:NH2	108:Dm:328:HIS:O	2.53	0.41
100:Dd:151:THR:CG2	100:Dd:197:LEU:HD11	2.50	0.41
110:Do:309:LEU:HD23	110:Do:309:LEU:C	2.46	0.41
133:El:129:ALA:O	133:El:133:THR:HG22	2.21	0.41
1:A0:464:THR:O	1:A0:464:THR:HG22	2.20	0.41
4:A3:268:LEU:HD23	4:A3:293:THR:HG21	2.03	0.41
6:A5:60:ILE:C	6:A5:60:ILE:HD12	2.45	0.41
9:A8:302:LEU:HD12	9:A8:305:LEU:HD11	2.01	0.41
11:AA:121:LEU:O	11:AA:123:THR:N	2.53	0.41
15:AE:128:LEU:HG	15:AE:157:LEU:HD13	2.01	0.41
20:AJ:47:TYR:CE1	20:AJ:51:VAL:HG11	2.56	0.41
22:AL:124:HIS:CD2	22:AL:181:CYS:SG	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AN:181:ARG:NE	24:AN:183:ASP:OD1	2.54	0.41
49:BF:67:LEU:HB3	49:BF:110:VAL:HG12	2.03	0.41
73:CA:299:CYS:SG	73:CA:300:ARG:N	2.93	0.41
87:C:38:THR:HG23	87:C:91:LEU:CD1	2.50	0.41
87:C:257:TYR:OH	153:C:509:PC1:H132	2.21	0.41
88:D:275:THR:HG21	87:c:229:ASN:HA	2.03	0.41
86:b:312:VAL:HG13	86:b:313:PRO:O	2.20	0.41
91:g:15:VAL:HG22	91:g:16:LYS:N	2.36	0.41
97:DA:335:VAL:CG2	97:DA:407:MET:HE2	2.50	0.41
99:DC:479:TYR:O	99:DC:483:VAL:HG23	2.20	0.41
105:DI:133:GLN:NE2	115:DT:207:GLU:O	2.50	0.41
108:DM:44:TYR:CE1	108:DM:113:LEU:HD13	2.56	0.41
150:DQ:1504:CDL:H271	150:Dg:202:CDL:H322	2.02	0.41
113:DR:140:PRO:HG2	113:DR:144:ILE:HD11	2.02	0.41
99:Dc:106:VAL:HG21	116:Du:248:LEU:HD23	2.02	0.41
111:Dp:219:VAL:O	111:Dp:219:VAL:HG22	2.21	0.41
113:Dr:137:ILE:HD12	113:Dr:137:ILE:N	2.35	0.41
118:Dw:257:GLU:OE1	118:Dw:257:GLU:N	2.43	0.41
129:Eh:130:LYS:NZ	129:Eh:165:LEU:HD12	2.35	0.41
130:Ei:74:SER:O	130:Ei:78:LEU:HD13	2.20	0.41
149:DL:450:LEU:HD23	149:DL:459:ALA:HB2	2.02	0.41
6:A5:127:ASP:O	6:A5:131:ASN:N	2.45	0.41
9:A8:313:ILE:N	9:A8:313:ILE:HD12	2.36	0.41
12:AB:69:ARG:NH2	12:AB:280:GLU:OE1	2.54	0.41
12:AB:162:GLU:CD	61:BR:106:THR:HG23	2.46	0.41
13:AC:243:THR:HA	13:AC:246:ILE:HG22	2.01	0.41
14:AD:359:ASP:O	14:AD:362:THR:HG22	2.21	0.41
15:AE:7:GLN:O	34:AX:120:ALA:N	2.52	0.41
15:AE:45:LEU:HD11	15:AE:426:LEU:CD2	2.51	0.41
16:AF:256:PHE:CZ	16:AF:299:LEU:HD11	2.56	0.41
26:AP:82:ASP:O	26:AP:89:SER:OG	2.38	0.41
29:AS:67:ILE:N	29:AS:68:PRO:HD2	2.36	0.41
43:B6:51:ASN:OD1	50:BG:61:GLN:NE2	2.46	0.41
87:C:13:ILE:HD12	91:g:181:ILE:HD13	2.03	0.41
88:D:130:ASP:OD1	88:D:131:GLU:N	2.48	0.41
87:c:121:PHE:CD2	87:c:195:LEU:HD21	2.56	0.41
89:e:223:TYR:HA	89:e:228:ARG:O	2.21	0.41
98:DB:407:ASP:OD1	102:DF:173:TYR:OH	2.24	0.41
98:DB:486:ARG:O	98:DB:490:ARG:HG3	2.21	0.41
109:DN:113:PHE:CE2	109:DN:117:ILE:HD11	2.55	0.41
116:DU:154:SER:O	116:DU:159:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
132:EK:61:ARG:O	132:EK:64:ILE:HG22	2.21	0.41
99:Dc:368:ILE:HD12	99:Dc:401:ILE:CD1	2.47	0.41
105:Di:105:TYR:OH	150:Di:1103:CDL:OA4	2.36	0.41
108:Dm:431:LEU:N	108:Dm:431:LEU:HD12	2.36	0.41
111:Dp:119:LEU:HD21	111:Dp:396:SER:HB2	2.02	0.41
117:Dv:137:SER:N	117:Dv:138:PRO:HD2	2.35	0.41
130:Ei:80:GLY:HA3	130:Ei:109:LEU:HD12	2.01	0.41
136:Eo:31:TYR:CZ	136:Eo:35:LEU:HD11	2.55	0.41
143:Ej:41:VAL:HG11	143:Ej:52:ILE:HD13	2.02	0.41
11:AA:149:TYR:O	11:AA:152:THR:OG1	2.35	0.41
11:AA:334:LYS:NZ	46:BC:67:SER:OG	2.39	0.41
16:AF:232:SER:HB3	39:B2:40:THR:HG21	2.03	0.41
18:AH:70:ASP:OD1	18:AH:70:ASP:C	2.62	0.41
19:AI:61:LEU:O	19:AI:61:LEU:HD23	2.20	0.41
31:AU:42:SER:OG	31:AU:45:ASP:OD2	2.27	0.41
46:BC:81:LYS:NZ	150:BC:302:CDL:OA4	2.43	0.41
73:CA:112:ASP:CG	73:CA:164:SER:HG	2.27	0.41
85:A:382:TYR:OH	92:H:1:MET:O	2.26	0.41
150:C:505:CDL:OB4	85:a:499:ARG:NH2	2.54	0.41
85:a:123:ARG:O	85:a:126:ILE:HG13	2.21	0.41
99:DC:101:GLU:CG	116:DU:271:LEU:HD21	2.48	0.41
99:DC:521:LEU:CD2	106:DJ:144:MET:HE1	2.50	0.41
102:DF:208:HIS:O	102:DF:212:THR:HG23	2.21	0.41
116:DU:246:TYR:N	116:DU:247:PRO:HD2	2.36	0.41
140:ES:81:PHE:CE2	140:ES:85:LEU:HD11	2.56	0.41
143:EJ:44:ASN:ND2	143:EJ:130:THR:OG1	2.46	0.41
145:EX:33:ASP:OD1	147:EZ:48:ARG:NH1	2.54	0.41
106:Dj:99:ASN:OD1	106:Dj:99:ASN:N	2.54	0.41
150:Dj:404:CDL:OB7	150:Dj:404:CDL:HB62	2.21	0.41
110:Do:64:ASN:O	110:Do:68:LEU:HD13	2.21	0.41
114:Ds:211:THR:CG2	114:Ds:249:ALA:HA	2.50	0.41
125:Ed:156:ILE:HG22	125:Ed:157:TRP:N	2.36	0.41
125:Ed:175:LEU:HD23	125:Ed:175:LEU:O	2.21	0.41
143:Ej:99:PHE:O	143:Ej:100:PRO:C	2.64	0.41
149:Dl:120:GLY:O	149:Dl:456:ILE:HD11	2.21	0.41
1:A0:204:VAL:O	1:A0:208:ILE:HG12	2.21	0.41
4:A3:53:THR:HG21	4:A3:88:VAL:HG11	2.01	0.41
8:A7:176:ASP:OD1	8:A7:176:ASP:C	2.64	0.41
13:AC:131:PHE:O	13:AC:134:ILE:HG22	2.21	0.41
13:AC:214:LEU:HD23	13:AC:214:LEU:C	2.46	0.41
15:AE:217:LYS:HB3	15:AE:221:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AE:232:LEU:HD12	25:AO:59:THR:CG2	2.51	0.41
16:AF:138:ILE:N	16:AF:139:PRO:CD	2.84	0.41
19:AI:69:MET:HB2	19:AI:70:PRO:HD3	2.01	0.41
19:AI:188:THR:O	19:AI:192:VAL:HG12	2.20	0.41
22:AL:173:THR:HG21	22:AL:203:HIS:CD2	2.55	0.41
25:AO:52:GLU:O	25:AO:56:SER:N	2.54	0.41
28:AR:172:MET:SD	28:AR:172:MET:N	2.94	0.41
40:B3:67:LEU:HD23	44:BA:112:ILE:HD13	2.03	0.41
43:B6:56:THR:HG21	56:BM:92:ILE:HD11	2.01	0.41
51:BH:3:ILE:HD11	51:BH:8:TRP:CH2	2.56	0.41
57:BN:70:VAL:N	69:BZ:1:MET:O	2.52	0.41
73:CA:56:ALA:HB2	73:CA:78:THR:HB	2.02	0.41
73:CA:327:SER:O	73:CA:331:VAL:HG23	2.20	0.41
73:CA:569:LEU:HD22	73:CA:610:THR:HB	2.03	0.41
75:CB:123:ARG:N	158:CB:1000:FES:S1	2.86	0.41
85:A:53:GLU:O	85:A:415:ARG:NH2	2.54	0.41
86:B:100:ARG:NH2	86:B:357:ASP:OD2	2.53	0.41
87:C:92:PHE:CE2	87:C:130:VAL:HG21	2.56	0.41
89:E:203:ILE:HD12	89:E:203:ILE:N	2.36	0.41
88:d:130:ASP:OD1	88:d:131:GLU:N	2.50	0.41
91:g:292:LEU:HD23	91:g:292:LEU:O	2.21	0.41
99:DC:311:ARG:NE	153:DC:605:PC1:O14	2.51	0.41
100:DD:120:THR:HG22	140:ES:25:TRP:CE3	2.56	0.41
100:DD:403:ASP:OD1	100:DD:403:ASP:C	2.64	0.41
100:DD:451:THR:HG22	100:DD:452:SER:H	1.85	0.41
104:DH:87:ILE:HD11	150:DN:502:CDL:H431	2.03	0.41
111:DP:236:PHE:HD2	111:DP:340:ILE:HG23	1.85	0.41
116:DU:213:GLN:N	116:DU:213:GLN:OE1	2.54	0.41
117:DV:59:ILE:HD12	117:DV:59:ILE:N	2.36	0.41
119:DX:228:ASN:O	119:DX:228:ASN:ND2	2.54	0.41
122:EA:79:ASP:OD1	122:EA:106:ARG:NH2	2.53	0.41
125:ED:128:LEU:HD23	125:ED:128:LEU:C	2.46	0.41
125:ED:149:TYR:CE2	125:ED:153:LEU:HD11	2.56	0.41
127:EF:128:VAL:HG12	127:EF:130:GLN:H	1.86	0.41
129:EH:32:ASP:OD1	129:EH:33:GLU:N	2.53	0.41
133:EL:131:TRP:CH2	167:EL:905:UQ8:H3MB	2.56	0.41
150:EN:1201:CDL:C45	167:EN:1205:UQ8:H15B	2.51	0.41
150:Da:709:CDL:H362	106:Dj:97:THR:HA	2.03	0.41
150:Dj:403:CDL:HB61	140:Es:63:THR:HG21	2.03	0.41
113:Dr:209:ILE:N	113:Dr:210:PRO:HD2	2.36	0.41
119:Dx:2:VAL:N	153:Dx:1209:PC1:O12	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
123:Eb:188:GLU:OE1	123:Eb:188:GLU:N	2.50	0.41
124:Ec:160:SER:OG	124:Ec:162:ASN:ND2	2.52	0.41
143:Ej:127:ASP:OD2	143:Ej:130:THR:OG1	2.39	0.41
149:DL:306:PHE:CE2	149:DL:362:VAL:HG13	2.55	0.41
11:AA:676:ASP:OD2	49:BF:87:THR:HG22	2.20	0.41
12:AB:382:ARG:NH2	12:AB:525:GLU:OE2	2.54	0.41
13:AC:101:ASN:ND2	13:AC:107:ASN:OD1	2.54	0.41
13:AC:179:LEU:C	13:AC:179:LEU:HD23	2.45	0.41
18:AH:103:THR:O	18:AH:103:THR:HG22	2.21	0.41
18:AH:107:ASN:ND2	18:AH:122:ASN:O	2.49	0.41
21:AK:32:GLU:N	21:AK:32:GLU:OE1	2.54	0.41
25:AO:145:ILE:N	25:AO:145:ILE:HD12	2.37	0.41
46:BC:144:THR:OG1	46:BC:145:GLY:N	2.53	0.41
89:E:167:GLU:HG3	89:E:167:GLU:O	2.21	0.41
92:H:102:PHE:HB3	92:H:103:PRO:HD3	2.02	0.41
85:a:114:VAL:HG21	85:a:168:LEU:HD23	2.03	0.41
85:a:169:GLN:OE1	85:a:269:THR:OG1	2.17	0.41
87:c:9:MET:SD	92:h:48:TYR:OH	2.70	0.41
91:g:22:ARG:NH1	91:g:205:GLU:OE2	2.51	0.41
97:DA:140:ILE:HA	109:DN:320:CYS:SG	2.61	0.41
97:DA:380:ILE:HD12	97:DA:445:VAL:HG11	2.03	0.41
99:DC:106:VAL:HG21	116:DU:248:LEU:HD23	2.02	0.41
107:DK:19:THR:O	107:DK:19:THR:HG22	2.21	0.41
112:DQ:305:ILE:HD11	137:EP:46:ALA:HB3	2.03	0.41
113:DR:209:ILE:N	113:DR:210:PRO:HD2	2.35	0.41
115:DT:282:MET:O	137:EP:47:LYS:NZ	2.44	0.41
97:Da:57:TYR:OH	97:Da:145:GLN:NE2	2.52	0.41
98:Db:175:VAL:HG22	98:Db:179:TRP:CE2	2.56	0.41
110:Do:57:LEU:HD22	110:Do:106:VAL:HG13	2.03	0.41
112:Dq:34:THR:OG1	112:Dq:34:THR:O	2.38	0.41
117:Dv:45:THR:O	117:Dv:45:THR:HG22	2.21	0.41
117:Dv:269:LEU:HD23	117:Dv:269:LEU:C	2.45	0.41
153:Eo:204:PC1:H2I3	153:Eo:204:PC1:C2E	2.51	0.41
6:A5:55:ASP:OD1	9:A8:151:TYR:OH	2.31	0.40
8:A7:133:GLU:OE2	50:BG:87:ARG:NH2	2.51	0.40
9:A8:101:ARG:NH1	9:A8:102:ASP:O	2.55	0.40
12:AB:128:ASP:O	12:AB:132:CYS:N	2.53	0.40
25:AO:141:GLU:HB2	25:AO:158:LEU:HD12	2.03	0.40
30:AT:62:LEU:HD21	30:AT:64:LEU:HD21	2.02	0.40
37:B0:42:LYS:NZ	50:BG:164:SER:O	2.54	0.40
73:CA:150:THR:OG1	73:CA:151:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B:177:THR:HG23	86:B:178:VAL:N	2.36	0.40
88:D:228:THR:CG2	88:D:229:PRO:HD3	2.51	0.40
96:L:3:ALA:N	96:L:4:PRO:CD	2.84	0.40
99:DC:378:THR:O	99:DC:378:THR:HG22	2.19	0.40
108:DM:44:TYR:O	108:DM:114:GLN:NE2	2.54	0.40
109:DN:86:LEU:HD23	109:DN:86:LEU:C	2.45	0.40
110:DO:305:LEU:HD23	110:DO:305:LEU:O	2.21	0.40
116:DU:211:ILE:HG23	116:DU:212:PHE:N	2.36	0.40
119:DX:228:ASN:O	119:DX:236:LEU:HD21	2.22	0.40
122:EA:168:LEU:C	122:EA:168:LEU:HD23	2.46	0.40
99:Dc:378:THR:O	99:Dc:378:THR:HG22	2.21	0.40
109:Dn:385:ILE:HD11	120:Dy:126:ILE:HD12	2.02	0.40
111:Dp:365:THR:HG22	111:Dp:366:LYS:N	2.36	0.40
115:Dt:123:THR:HG22	115:Dt:124:ARG:N	2.36	0.40
142:Eu:3:SER:OG	142:Eu:4:ASP:N	2.52	0.40
11:AA:232:LEU:N	11:AA:232:LEU:HD12	2.36	0.40
12:AB:74:GLY:O	14:AD:425:ILE:HD11	2.21	0.40
14:AD:410:ILE:HG23	14:AD:440:ILE:CD1	2.52	0.40
19:AI:42:PHE:CZ	19:AI:75:VAL:HG22	2.56	0.40
23:AM:64:PHE:HD2	23:AM:82:VAL:HG13	1.86	0.40
29:AS:62:LYS:NZ	29:AS:66:LEU:HD11	2.36	0.40
30:AT:8:THR:HB	30:AT:9:PRO:HD3	2.03	0.40
35:AY:18:ILE:HD11	150:B1:402:CDL:H762	2.03	0.40
35:AY:54:ILE:HD13	39:B2:6:TYR:HB2	2.02	0.40
36:AZ:25:ARG:NH2	36:AZ:58:ASP:OD1	2.54	0.40
49:BF:15:ILE:HG21	90:F:22:PHE:HE2	1.86	0.40
61:BR:37:LEU:N	61:BR:37:LEU:HD12	2.36	0.40
72:CL:38:GLU:OE1	72:CL:76:GLN:NE2	2.55	0.40
79:CE:19:GLY:O	79:CE:197:GLN:NE2	2.55	0.40
80:CJ:2:ASN:OD1	80:CJ:3:HIS:N	2.54	0.40
150:c:509:CDL:H442	167:c:510:UQ8:H30A	2.04	0.40
97:DA:215:VAL:O	97:DA:215:VAL:HG13	2.22	0.40
97:DA:328:ARG:HE	97:DA:328:ARG:HA	1.87	0.40
99:DC:190:LEU:HD11	121:DZ:170:LEU:HD11	2.03	0.40
99:DC:240:TRP:NE1	150:DC:601:CDL:OA4	2.46	0.40
153:DC:608:PC1:H2I1	150:EH:1601:CDL:H351	2.02	0.40
136:EO:40:TYR:OH	153:EO:205:PC1:O32	2.38	0.40
97:Da:562:MET:HE2	167:Ds:404:UQ8:O2	2.21	0.40
99:Dc:155:TYR:OH	110:Do:249:PRO:O	2.36	0.40
99:Dc:239:ILE:HD13	150:Dh:202:CDL:H221	2.04	0.40
102:Df:89:ASP:OD1	102:Df:89:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
102:Df:156:ASP:N	102:Df:156:ASP:OD1	2.54	0.40
108:Dm:159:ARG:NE	108:Dm:161:GLU:OE2	2.48	0.40
108:Dm:413:ALA:O	108:Dm:435:LYS:NZ	2.35	0.40
114:Ds:155:GLU:OE1	114:Ds:204:ARG:NH2	2.53	0.40
141:Et:37:LEU:HD12	141:Et:37:LEU:C	2.46	0.40
144:Ew:26:TYR:O	144:Ew:30:VAL:HG12	2.21	0.40
3:A2:44:TYR:HE2	3:A2:45:ARG:HH22	1.68	0.40
5:A4:40:TYR:OH	5:A4:97:ASP:OD2	2.33	0.40
8:A7:198:TYR:O	8:A7:201:CYS:SG	2.79	0.40
12:AB:189:GLN:O	12:AB:423:ARG:NH1	2.50	0.40
13:AC:32:PHE:CD1	13:AC:52:LEU:HD11	2.56	0.40
13:AC:269:THR:O	13:AC:273:ALA:CB	2.69	0.40
16:AF:332:ASP:OD1	52:BI:132:ARG:NH1	2.52	0.40
24:AN:43:HIS:HA	24:AN:110:MET:HE1	2.03	0.40
28:AR:47:VAL:HG11	28:AR:143:ILE:HD11	2.02	0.40
49:BF:74:ILE:HD11	49:BF:98:ILE:HG13	2.04	0.40
61:BR:100:VAL:HG22	61:BR:101:TYR:N	2.36	0.40
63:BT:29:CYS:HB3	63:BT:34:MET:HE2	2.04	0.40
73:CA:96:ALA:CB	73:CA:137:VAL:HG21	2.52	0.40
76:CF:207:LEU:O	76:CF:212:ARG:NH2	2.53	0.40
85:A:129:GLU:O	85:A:133:LEU:HG	2.21	0.40
87:C:38:THR:HG22	168:C:502:HEM:HMB1	2.02	0.40
88:d:168:ARG:NH1	166:d:802:HEC:O1A	2.49	0.40
89:e:158:THR:O	89:e:162:VAL:HG23	2.22	0.40
91:g:195:ASN:OD1	96:l:7:LEU:HD13	2.22	0.40
97:DA:386:PHE:O	97:DA:390:GLY:N	2.52	0.40
98:DB:376:ILE:N	98:DB:376:ILE:HD12	2.37	0.40
99:DC:419:ILE:CG2	99:DC:432:LEU:HD11	2.52	0.40
100:DD:287:THR:HG22	109:DN:279:VAL:HG13	1.99	0.40
101:DE:47:ILE:HG23	125:ED:170:TYR:HD1	1.87	0.40
111:DP:345:ILE:HD12	111:DP:345:ILE:N	2.37	0.40
115:DT:123:THR:HG22	115:DT:124:ARG:N	2.37	0.40
116:DU:125:PHE:O	116:DU:127:ARG:N	2.54	0.40
125:ED:33:MET:HE2	130:EI:67:THR:HG22	2.03	0.40
128:EG:93:LEU:HD13	130:EI:147:ALA:HB2	2.03	0.40
150:EL:901:CDL:H761	140:ES:68:ILE:HD13	2.04	0.40
99:Dc:311:ARG:HG2	99:Dc:315:ILE:HD11	2.03	0.40
105:Di:146:ILE:HD12	105:Di:146:ILE:N	2.36	0.40
153:Di:1104:PC1:H242	117:Dv:209:ILE:HG22	2.03	0.40
119:Dx:148:GLU:OE1	119:Dx:148:GLU:N	2.48	0.40
11:AA:582:VAL:HG12	11:AA:583:GLU:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:180:CYS:O	12:AB:181:THR:OG1	2.34	0.40
150:AC:802:CDL:H432	150:AC:802:CDL:H472	2.03	0.40
20:AJ:52:ASN:O	35:AY:22:LYS:NZ	2.50	0.40
27:AQ:96:LEU:HD23	27:AQ:96:LEU:C	2.46	0.40
45:BB:170:PRO:HB2	49:BF:62:ILE:HD12	2.03	0.40
52:BI:47:ILE:HG21	52:BI:160:ILE:HD12	2.04	0.40
57:BN:69:GLY:O	57:BN:73:ASN:N	2.54	0.40
57:BN:92:ARG:NH2	57:BN:103:ASP:OD2	2.55	0.40
64:BU:8:GLN:N	64:BU:9:PRO:HD2	2.37	0.40
68:BY:42:ILE:O	68:BY:46:GLU:HB3	2.22	0.40
89:E:182:LEU:HD22	89:E:191:ILE:HD11	2.03	0.40
92:H:61:HIS:NE2	88:d:288:GLU:OE2	2.54	0.40
95:K:50:PRO:HA	95:K:51:PRO:HD3	2.00	0.40
87:c:203:MET:HE2	168:c:505:HEM:HAA2	2.03	0.40
98:DB:203:LEU:C	98:DB:203:LEU:HD13	2.46	0.40
99:DC:92:ILE:HD12	99:DC:92:ILE:N	2.37	0.40
136:EO:2:VAL:HG12	136:EO:3:PHE:N	2.36	0.40
139:ER:37:CYS:O	139:ER:41:VAL:HG23	2.20	0.40
97:Da:68:GLY:C	97:Da:105:MET:HE2	2.46	0.40
99:Dc:328:PHE:CE2	99:Dc:332:LEU:HD11	2.57	0.40
118:Dw:195:THR:O	118:Dw:195:THR:HG23	2.20	0.40
118:Dw:257:GLU:O	118:Dw:284:GLN:NE2	2.55	0.40
120:Dy:120:LEU:HD23	120:Dy:120:LEU:C	2.46	0.40
122:Ea:158:VAL:HG23	122:Ea:159:LEU:N	2.36	0.40
129:Eh:12:ASP:OD1	129:Eh:13:ARG:N	2.45	0.40
130:Ei:101:LEU:O	130:Ei:105:ILE:HG22	2.21	0.40
142:Eu:53:LEU:O	142:Eu:53:LEU:HD23	2.20	0.40
146:Ey:5:LEU:HD21	148:Fa:14:VAL:CG1	2.46	0.40
1:A0:190:GLN:OE1	1:A0:190:GLN:N	2.49	0.40
3:A2:290:LEU:HD22	3:A2:290:LEU:N	2.36	0.40
7:A6:94:PRO:O	7:A6:163:ARG:NH2	2.49	0.40
11:AA:231:SER:O	59:BP:105:SER:OG	2.39	0.40
12:AB:78:MET:HA	12:AB:117:VAL:HG11	2.02	0.40
15:AE:248:ARG:NH2	15:AE:256:GLU:OE1	2.53	0.40
35:AY:19:LEU:C	35:AY:19:LEU:HD23	2.46	0.40
41:B4:71:LEU:O	41:B4:71:LEU:HD23	2.22	0.40
49:BF:39:ASN:O	90:F:8:GLN:HG3	2.20	0.40
57:BN:120:LYS:NZ	65:BV:7:GLY:O	2.36	0.40
81:CN:24:ASN:HA	81:CN:27:VAL:HG23	2.04	0.40
86:B:163:VAL:O	86:B:167:VAL:HG23	2.21	0.40
87:C:167:ILE:CG2	167:C:511:UQ8:H30A	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:C:283:ARG:NH1	87:C:371:SER:O	2.55	0.40
88:D:161:ASP:OD2	88:D:163:SER:OG	2.27	0.40
92:h:100:PHE:CD1	92:h:100:PHE:C	3.00	0.40
105:DI:85:VAL:HG13	113:DR:131:ILE:HG23	2.03	0.40
107:DK:40:GLN:NE2	107:DK:81:ARG:O	2.49	0.40
112:DQ:188:LEU:HD23	112:DQ:188:LEU:C	2.46	0.40
114:DS:338:ASN:ND2	114:DS:340:SER:O	2.55	0.40
122:EA:154:LEU:O	122:EA:158:VAL:HG22	2.22	0.40
125:ED:106:ILE:O	125:ED:110:SER:OG	2.35	0.40
131:EV:35:VAL:HG12	131:EV:36:ALA:N	2.36	0.40
137:EP:101:ILE:C	137:EP:101:ILE:HD12	2.47	0.40
134:Em:52:VAL:HG13	134:Em:53:GLU:N	2.37	0.40
138:Eq:12:THR:HG22	138:Eq:13:HIS:N	2.36	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AA	711/750 (95%)	694 (98%)	16 (2%)	1 (0%)	48	77
12	AB	686/718 (96%)	674 (98%)	12 (2%)	0	100	100
13	AC	503/505 (100%)	489 (97%)	14 (3%)	0	100	100
14	AD	439/474 (93%)	427 (97%)	12 (3%)	0	100	100
15	AE	439/442 (99%)	431 (98%)	8 (2%)	0	100	100
16	AF	357/360 (99%)	349 (98%)	8 (2%)	0	100	100
17	AG	344/346 (99%)	340 (99%)	4 (1%)	0	100	100
18	AH	281/284 (99%)	273 (97%)	8 (3%)	0	100	100
19	AI	229/274 (84%)	227 (99%)	2 (1%)	0	100	100
20	AJ	252/255 (99%)	245 (97%)	7 (3%)	0	100	100
21	AK	228/257 (89%)	219 (96%)	9 (4%)	0	100	100
22	AL	216/236 (92%)	209 (97%)	7 (3%)	0	100	100
23	AM	229/233 (98%)	223 (97%)	6 (3%)	0	100	100
24	AN	155/206 (75%)	154 (99%)	1 (1%)	0	100	100
25	AO	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	B5	52/71 (73%)	52 (100%)	0	0	100	100
43	B6	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
44	BA	197/212 (93%)	192 (98%)	5 (2%)	0	100	100
45	BB	165/214 (77%)	164 (99%)	1 (1%)	0	100	100
46	BC	171/207 (83%)	168 (98%)	3 (2%)	0	100	100
47	BD	146/205 (71%)	145 (99%)	1 (1%)	0	100	100
48	BE	166/189 (88%)	159 (96%)	7 (4%)	0	100	100
49	BF	175/188 (93%)	166 (95%)	9 (5%)	0	100	100
50	BG	158/175 (90%)	153 (97%)	5 (3%)	0	100	100
51	BH	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
52	BI	147/172 (86%)	146 (99%)	1 (1%)	0	100	100
53	BJ	142/166 (86%)	142 (100%)	0	0	100	100
54	BK	107/144 (74%)	105 (98%)	2 (2%)	0	100	100
55	BL	140/143 (98%)	139 (99%)	1 (1%)	0	100	100
56	BM	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
95	k	56/62 (90%)	56 (100%)	0	0	100	100
96	L	30/41 (73%)	30 (100%)	0	0	100	100
96	l	30/41 (73%)	30 (100%)	0	0	100	100
97	DA	669/688 (97%)	655 (98%)	14 (2%)	0	100	100
97	Da	669/688 (97%)	655 (98%)	14 (2%)	0	100	100
98	DB	602/604 (100%)	589 (98%)	13 (2%)	0	100	100
98	Db	602/604 (100%)	591 (98%)	11 (2%)	0	100	100
99	DC	580/594 (98%)	569 (98%)	10 (2%)	1 (0%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
111	DP	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
111	Dp	288/402 (72%)	279 (97%)	9 (3%)	0	100	100
112	DQ	382/386 (99%)	376 (98%)	6 (2%)	0	100	100
112	Dq	382/386 (99%)	369 (97%)	13 (3%)	0	100	100
113	DR	241/348 (69%)	234 (97%)	7 (3%)	0	100	100
113	Dr	241/348 (69%)	238 (99%)	3 (1%)	0	100	100
114	DS	345/347 (99%)	344 (100%)	1 (0%)	0	100	100
114	Ds	345/347 (99%)	343 (99%)	2 (1%)	0	100	100
115	DT	291/318 (92%)	287 (99%)	4 (1%)	0	100	100
115	Dt	291/318 (92%)	288 (99%)	3 (1%)	0	100	100
116	DU	327/330 (99%)	322 (98%)	5 (2%)	0	100	100
116	Du	327/330 (99%)	321 (98%)	6 (2%)	0	100	100
117	DV	317/319 (99%)	315 (99%)	2 (1%)	0	100	100
117	Dv	317/319 (99%)	312 (98%)	5 (2%)	0	100	100
118	DW	299/318 (94%)	297 (99%)	2 (1%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
126	Ee	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
127	EF	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
127	Ef	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
128	EG	96/100 (96%)	96 (100%)	0	0	100	100
128	Eg	96/100 (96%)	96 (100%)	0	0	100	100
129	EH	172/174 (99%)	171 (99%)	1 (1%)	0	100	100
129	Eh	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
130	EI	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
130	Ei	170/173 (98%)	165 (97%)	5 (3%)	0	100	100
131	EV	77/89 (86%)	76 (99%)	1 (1%)	0	100	100
131	Ev	77/89 (86%)	76 (99%)	1 (1%)	0	100	100
132	EK	167/170 (98%)	167 (100%)	0	0	100	100
132	Ek	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
133	EL	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
133	El	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
142	EU	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
142	Eu	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
143	EJ	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
143	Ej	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
144	EW	61/81 (75%)	61 (100%)	0	0	100	100
144	Ew	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
145	EX	67/72 (93%)	67 (100%)	0	0	100	100
145	Ex	67/72 (93%)	67 (100%)	0	0	100	100
146	EY	68/72 (94%)	68 (100%)	0	0	100	100
146	Ey	68/72 (94%)	68 (100%)	0	0	100	100
147	EZ	56/68 (82%)	55 (98%)	1 (2%)	0	100	100
147	Ez	56/68 (82%)	56 (100%)	0	0	100	100
148	FA	69/72 (96%)	69 (100%)	0	0	100	100
148	Fa	69/72 (96%)	69 (100%)	0	0	100	100
149	DL	378/462 (82%)	362 (96%)	16 (4%)	0	100	100
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

All (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
105	DI	119	GLU
11	AA	119	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	441/454 (97%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	BU	121/121 (100%)	121 (100%)	0	100	100
65	BV	102/102 (100%)	102 (100%)	0	100	100
66	BW	98/99 (99%)	98 (100%)	0	100	100
67	BX	81/97 (84%)	81 (100%)	0	100	100
68	BY	98/98 (100%)	98 (100%)	0	100	100
69	BZ	89/89 (100%)	89 (100%)	0	100	100
70	CH	100/184 (54%)	100 (100%)	0	100	100
71	CM	65/67 (97%)	65 (100%)	0	100	100
72	CL	82/83 (99%)	82 (100%)	0	100	100
73	CA	481/515 (93%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	455	ASP
1	A0	456	ASN
1	A0	462	VAL

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Mol	Chain	Res	Type
1	A0	465	LEU
2	A1	295	LEU
3	A2	194	ASP
4	A3	286	ASP
4	A3	289	ILE
7	A6	102	PHE
9	A8	301	GLU
10	A9	32	LYS
10	A9	134	ARG
11	AA	163	ASN
11	AA	165	ASP
11	AA	276	PHE
11	AA	363	ASN
11	AA	385	TYR
11	AA	435	VAL
11	AA	441	LEU
12	AB	386	LEU
13	AC	145	ASN
13	AC	205	TRP
13	AC	229	PHE
13	AC	327	GLN
14	AD	380	CYS
15	AE	9	TRP
15	AE	83	ASP
15	AE	432	THR
18	AH	166	PHE
18	AH	167	LEU
18	AH	172	ILE
18	AH	195	LEU
18	AH	245	TYR
19	AI	215	VAL
21	AK	130	TYR
22	AL	94	PHE
22	AL	121	ARG
22	AL	174	LYS
22	AL	175	CYS
23	AM	172	LEU
25	AO	196	VAL
27	AQ	5	TYR
28	AR	94	HIS
29	AS	19	ASN
30	AT	31	CYS

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Mol	Chain	Res	Type
30	AT	46	PHE
30	AT	144	LEU
31	AU	50	PHE
31	AU	73	LEU
34	AX	1	MET
34	AX	3	ASP
34	AX	57	ILE
35	AY	84	LEU
38	B1	33	TYR
47	BD	149	LEU
48	BE	133	ASN
48	BE	138	LEU
49	BF	96	HIS
55	BL	26	LEU
56	BM	10	PHE
60	BQ	65	LEU
60	BQ	99	THR
61	BR	94	ASN
63	BT	40	GLN
63	BT	48	ASN
63	BT	52	VAL
63	BT	122	LYS
63	BT	134	ASN
63	BT	141	GLN
73	CA	160	PHE
73	CA	345	VAL
75	CB	161	HIS
75	CB	231	HIS
77	CG	99	HIS
77	CG	169	HIS
78	CK	41	VAL
79	CE	3	LEU
79	CE	47	PHE
86	B	133	VAL
86	B	410	LEU
87	C	195	LEU
88	D	26	ILE
88	D	123	GLN
88	D	178	ILE
89	E	38	LEU
91	G	127	ARG
91	G	192	LEU

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Mol	Chain	Res	Type
92	H	41	VAL
93	I	65	LEU
93	I	67	GLN
93	I	79	HIS
96	L	11	ARG
85	a	118	THR
85	a	234	LYS
85	a	492	HIS
85	a	505	TYR
86	b	110	LEU
86	b	175	ARG
86	b	312	VAL
86	b	427	PHE
87	c	167	ILE
87	c	320	GLU
87	c	389	LEU
88	d	303	TYR
89	e	117	ARG
89	e	254	MET
90	f	26	GLU
91	g	72	LEU
91	g	93	LEU
91	g	192	LEU
93	i	3	TYR
97	DA	57	TYR
97	DA	232	MET
97	DA	429	VAL
97	DA	447	LEU
97	DA	630	ARG
98	DB	45	TRP
98	DB	104	ILE
98	DB	143	ILE
98	DB	175	VAL
98	DB	183	LEU
98	DB	224	PHE
98	DB	524	LYS
100	DD	214	ASN
100	DD	236	LYS
100	DD	247	GLU
102	DF	35	LYS
102	DF	90	ASP
103	DG	1	MET

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Mol	Chain	Res	Type
105	DI	115	GLU
105	DI	141	ILE
106	DJ	26	LYS
106	DJ	99	ASN
106	DJ	204	GLU
107	DK	96	GLU
108	DM	386	THR
108	DM	414	GLN
109	DN	249	ILE
109	DN	262	LEU
110	DO	272	GLU
111	DP	228	LEU
112	DQ	34	THR
112	DQ	49	LEU
113	DR	211	ARG
114	DS	58	GLU
114	DS	145	LEU
114	DS	232	GLN
116	DU	10	LYS
117	DV	108	LYS
118	DW	268	ASP
119	DX	157	GLU
121	DZ	125	GLN
123	EB	56	TYR
124	EC	56	LEU
125	ED	174	ARG
125	ED	175	LEU
127	EF	51	THR
127	EF	105	GLN
129	EH	70	HIS
130	EI	8	TYR
130	EI	132	VAL
132	EK	12	ASN
134	EM	137	GLU
135	EN	144	LEU
136	EO	124	LYS
138	EQ	2	GLU
138	EQ	65	PHE
138	EQ	73	ILE
141	ET	38	LEU
141	ET	83	GLU
143	EJ	21	VAL

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Mol	Chain	Res	Type
143	EJ	158	LEU
144	EW	62	LYS
145	EX	4	LYS
146	EY	67	LEU
147	EZ	23	CYS
148	FA	50	GLU
97	Da	57	TYR
97	Da	76	ARG
97	Da	429	VAL
97	Da	447	LEU
97	Da	503	PHE
97	Da	519	ASP
97	Da	526	HIS
97	Da	630	ARG
98	Db	45	TRP
98	Db	224	PHE
98	Db	230	TYR
98	Db	412	THR
98	Db	511	ASP
98	Db	524	LYS
98	Db	585	LEU
99	Dc	50	GLU
100	Dd	214	ASN
100	Dd	236	LYS
100	Dd	247	GLU
100	Dd	446	ARG
102	Df	35	LYS
104	Dh	122	GLU
105	Di	141	ILE
105	Di	208	ILE
106	Dj	26	LYS
106	Dj	204	GLU
108	Dm	103	LEU
108	Dm	372	ASP
108	Dm	386	THR
109	Dn	30	LEU
109	Dn	114	TYR
109	Dn	210	LEU
109	Dn	262	LEU
109	Dn	420	ASN
110	Do	272	GLU
111	Dp	228	LEU

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Mol	Chain	Res	Type
114	Ds	58	GLU
114	Ds	65	THR
114	Ds	145	LEU
114	Ds	232	GLN
116	Du	10	LYS
116	Du	91	VAL
116	Du	213	GLN
116	Du	250	VAL
116	Du	276	LYS
117	Dv	3	TYR
117	Dv	108	LYS
117	Dv	275	ILE
118	Dw	268	ASP
119	Dx	134	LEU
119	Dx	157	GLU
119	Dx	173	ILE
119	Dx	228	ASN
121	Dz	125	GLN
123	Eb	63	ARG
124	Ec	9	LEU
125	Ed	82	TYR
125	Ed	174	ARG
127	Ef	105	GLN
130	Ei	8	TYR
130	Ei	111	TYR
130	Ei	132	VAL
132	Ek	12	ASN
132	Ek	17	LEU
132	Ek	21	ARG
134	Em	137	GLU
135	En	144	LEU
136	Eo	124	LYS
138	Eq	2	GLU
138	Eq	65	PHE
138	Eq	73	ILE
141	Et	38	LEU
141	Et	58	CYS
141	Et	83	GLU
143	Ej	99	PHE
143	Ej	158	LEU
144	Ew	62	LYS
145	Ex	4	LYS

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Mol	Chain	Res	Type
147	Ez	23	CYS
148	Fa	50	GLU
148	Fa	72	LEU
149	Dl	326	GLN
149	DL	326	GLN
149	DL	366	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (314) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	45	ASN
1	A0	102	ASN
1	A0	132	ASN
1	A0	213	GLN
1	A0	435	HIS
1	A0	497	ASN
2	A1	73	HIS
2	A1	177	HIS
2	A1	181	HIS
2	A1	252	GLN
2	A1	334	GLN
3	A2	85	GLN
4	A3	266	GLN
4	A3	280	ASN
5	A4	145	ASN
5	A4	216	ASN
5	A4	249	HIS
5	A4	258	ASN
5	A4	283	HIS
6	A5	71	GLN
6	A5	260	HIS
8	A7	219	GLN
9	A8	107	ASN
9	A8	262	HIS
10	A9	12	HIS
10	A9	29	HIS
10	A9	101	HIS
10	A9	133	ASN
10	A9	145	ASN
10	A9	181	ASN
10	A9	227	GLN
11	AA	68	HIS

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Mol	Chain	Res	Type
11	AA	168	ASN
11	AA	290	ASN
12	AB	141	GLN
12	AB	263	GLN
12	AB	515	HIS
13	AC	41	GLN
14	AD	134	ASN
14	AD	314	ASN
15	AE	22	GLN
15	AE	58	HIS
15	AE	222	ASN
15	AE	265	ASN
15	AE	296	GLN
16	AF	39	ASN
16	AF	133	ASN
16	AF	188	ASN
17	AG	306	GLN
17	AG	321	ASN
20	AJ	114	HIS
20	AJ	118	ASN
21	AK	98	ASN
22	AL	40	HIS
24	AN	180	GLN
25	AO	99	ASN
25	AO	177	GLN
27	AQ	32	HIS
27	AQ	63	ASN
27	AQ	158	GLN
27	AQ	164	ASN
28	AR	9	GLN
29	AS	98	HIS
35	AY	94	ASN
35	AY	100	ASN
40	B3	38	ASN
41	B4	64	GLN
41	B4	73	GLN
43	B6	31	GLN
44	BA	56	HIS
44	BA	135	ASN
45	BB	92	HIS
45	BB	178	ASN
46	BC	158	ASN

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Mol	Chain	Res	Type
47	BD	68	GLN
47	BD	76	GLN
47	BD	177	ASN
47	BD	181	GLN
48	BE	150	ASN
51	BH	135	ASN
52	BI	53	GLN
52	BI	113	ASN
54	BK	84	GLN
54	BK	108	GLN
55	BL	111	HIS
55	BL	131	ASN
56	BM	101	HIS
56	BM	119	HIS
57	BN	104	GLN
58	BO	59	GLN
58	BO	109	GLN
61	BR	109	HIS
62	BS	103	HIS
64	BU	96	HIS
64	BU	112	GLN
65	BV	2	ASN
65	BV	52	GLN
66	BW	90	ASN
71	CM	64	ASN
71	CM	66	ASN
72	CL	76	GLN
73	CA	238	HIS
73	CA	365	HIS
73	CA	397	ASN
75	CB	56	HIS
75	CB	70	GLN
75	CB	231	HIS
76	CF	90	ASN
77	CG	99	HIS
79	CE	114	ASN
79	CE	238	ASN
79	CE	261	HIS
79	CE	265	ASN
79	CE	271	ASN
79	CE	290	ASN
80	CJ	34	HIS

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Mol	Chain	Res	Type
81	CN	43	GLN
81	CN	44	ASN
84	CD	23	ASN
84	CD	25	ASN
85	A	169	GLN
85	A	364	HIS
86	B	404	ASN
87	C	316	HIS
87	C	321	GLN
87	C	356	GLN
88	D	118	HIS
88	D	120	HIS
88	D	299	ASN
89	E	59	ASN
89	E	80	HIS
89	E	261	HIS
90	F	30	GLN
90	F	50	ASN
92	H	60	GLN
93	I	35	GLN
85	a	170	ASN
85	a	226	HIS
85	a	340	HIS
85	a	427	ASN
86	b	84	GLN
86	b	283	GLN
86	b	340	GLN
86	b	354	HIS
86	b	404	ASN
87	c	18	GLN
88	d	154	ASN
88	d	243	GLN
88	d	307	ASN
89	e	80	HIS
90	f	30	GLN
92	h	60	GLN
92	h	90	GLN
93	i	43	ASN
97	DA	50	HIS
97	DA	253	GLN
97	DA	472	ASN
97	DA	528	HIS

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Mol	Chain	Res	Type
98	DB	171	GLN
98	DB	198	GLN
98	DB	266	ASN
98	DB	373	HIS
99	DC	129	ASN
99	DC	135	ASN
99	DC	205	ASN
99	DC	224	ASN
100	DD	70	ASN
100	DD	130	ASN
100	DD	134	ASN
100	DD	427	ASN
100	DD	471	GLN
100	DD	477	HIS
100	DD	481	GLN
101	DE	73	GLN
105	DI	88	HIS
107	DK	41	GLN
107	DK	117	HIS
108	DM	67	HIS
108	DM	333	ASN
109	DN	57	ASN
109	DN	88	HIS
109	DN	122	ASN
109	DN	146	ASN
109	DN	298	ASN
109	DN	311	GLN
110	DO	90	GLN
110	DO	198	GLN
110	DO	251	GLN
110	DO	380	ASN
111	DP	133	HIS
111	DP	174	ASN
112	DQ	61	ASN
113	DR	125	ASN
113	DR	262	GLN
115	DT	160	GLN
115	DT	181	ASN
115	DT	258	ASN
116	DU	268	ASN
116	DU	318	GLN
117	DV	24	ASN

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Mol	Chain	Res	Type
117	DV	42	GLN
117	DV	69	HIS
117	DV	97	ASN
117	DV	143	ASN
118	DW	188	ASN
118	DW	203	HIS
118	DW	214	ASN
118	DW	232	HIS
118	DW	262	HIS
119	DX	228	ASN
120	DY	65	HIS
120	DY	200	ASN
121	DZ	110	ASN
121	DZ	168	ASN
123	EB	208	HIS
127	EF	150	ASN
128	EG	9	ASN
128	EG	13	ASN
129	EH	4	ASN
129	EH	80	HIS
130	EI	64	ASN
132	EK	28	GLN
133	EL	84	ASN
133	EL	117	GLN
136	EO	4	HIS
136	EO	112	GLN
137	EP	123	HIS
144	EW	40	GLN
146	EY	20	HIS
147	EZ	10	ASN
148	FA	52	HIS
97	Da	182	ASN
97	Da	514	ASN
97	Da	526	HIS
98	Db	198	GLN
98	Db	208	GLN
98	Db	266	ASN
98	Db	316	GLN
98	Db	548	GLN
98	Db	558	HIS
99	Dc	52	ASN
99	Dc	58	ASN

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Mol	Chain	Res	Type
99	Dc	72	ASN
99	Dc	75	ASN
99	Dc	129	ASN
99	Dc	297	GLN
99	Dc	382	ASN
100	Dd	262	HIS
100	Dd	427	ASN
100	Dd	471	GLN
100	Dd	485	ASN
101	De	56	ASN
101	De	73	GLN
102	Df	49	GLN
107	Dk	47	GLN
108	Dm	333	ASN
108	Dm	399	HIS
108	Dm	451	GLN
108	Dm	454	ASN
109	Dn	57	ASN
109	Dn	88	HIS
110	Do	107	ASN
110	Do	245	GLN
110	Do	438	GLN
111	Dp	133	HIS
111	Dp	174	ASN
112	Dq	54	ASN
112	Dq	296	HIS
113	Dr	262	GLN
114	Ds	20	ASN
114	Ds	327	GLN
114	Ds	339	ASN
115	Dt	72	ASN
115	Dt	166	GLN
115	Dt	220	ASN
116	Du	17	ASN
116	Du	56	HIS
116	Du	234	GLN
116	Du	268	ASN
116	Du	300	HIS
117	Dv	24	ASN
117	Dv	42	GLN
117	Dv	143	ASN
118	Dw	25	ASN

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Mol	Chain	Res	Type
118	Dw	81	ASN
118	Dw	232	HIS
119	Dx	47	GLN
123	Eb	34	ASN
123	Eb	208	HIS
124	Ec	44	HIS
124	Ec	202	GLN
125	Ed	133	ASN
127	Ef	56	GLN
128	Eg	9	ASN
128	Eg	13	ASN
130	Ei	166	ASN
132	Ek	28	GLN
132	Ek	84	HIS
132	Ek	101	GLN
132	Ek	105	ASN
132	Ek	163	HIS
133	El	38	ASN
133	El	62	ASN
137	Ep	41	ASN
138	Eq	64	ASN
139	Er	45	ASN
141	Et	60	ASN
144	Ew	40	GLN
147	Ez	37	HIS
149	Dl	260	ASN
149	DL	90	GLN
149	DL	141	ASN
149	DL	260	ASN
149	DL	386	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
100	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	-
100	SEP	Dd	520	100	-	0/5/8/10	-
100	TPO	DD	387	100	-	2/9/11/13	-

All (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
100	Dd	387	TPO	P-O1P	3.32	1.61	1.50

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
105	Di	120	SEP	OG-CB-CA	2.90	110.97	108.14
100	Dd	520	SEP	OG-CB-CA	2.88	110.95	108.14
105	DI	120	SEP	P-OG-CB	-2.84	110.47	118.30
105	Di	120	SEP	P-OG-CB	-2.81	110.56	118.30
105	DI	120	SEP	OG-CB-CA	2.52	110.59	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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
153	PC1	DV	404	-	53,53,53	0.29	0	59,61,61	0.27	0
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
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
169	DA	703	HEA	C3A-C2A	5.70	1.48	1.36
169	DA	702	HEA	C3B-C2B	5.55	1.47	1.34
169	Da	702	HEA	C3B-C2B	5.50	1.47	1.34
169	DA	703	HEA	FE-NB	5.49	2.11	1.94
169	Da	703	HEA	FE-NB	5.48	2.11	1.94
169	DA	703	HEA	C3B-C2B	5.46	1.47	1.34
169	Da	702	HEA	FE-NB	5.43	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	DA	702	HEA	FE-NB	5.43	2.11	1.94
169	DA	703	HEA	FE-ND	5.42	2.11	1.94
169	Da	703	HEA	FE-ND	5.42	2.11	1.94
169	Da	703	HEA	C3B-C2B	5.40	1.46	1.34
166	CE	401	HEC	CHB-C4A	5.36	1.48	1.38
169	Da	702	HEA	FE-ND	5.34	2.11	1.94
169	DA	702	HEA	FE-ND	5.29	2.11	1.94
166	D	401	HEC	C3D-C2D	5.23	1.47	1.36
166	d	802	HEC	C3B-C2B	5.23	1.47	1.36
166	CE	401	HEC	FE-NC	5.20	2.12	1.95
166	d	802	HEC	C3D-C2D	5.20	1.47	1.36
166	D	401	HEC	C3B-C2B	5.20	1.47	1.36
166	CE	401	HEC	FE-NB	5.14	2.10	1.94
166	CE	401	HEC	FE-NA	5.13	2.12	1.95
166	d	802	HEC	FE-NB	5.11	2.10	1.94
166	d	802	HEC	C2A-C3A	5.10	1.47	1.36
166	d	802	HEC	FE-ND	5.09	2.10	1.94
166	D	401	HEC	CHD-C1D	5.08	1.48	1.38
166	d	802	HEC	CHA-C1A	5.07	1.48	1.38
166	D	401	HEC	FE-ND	5.06	2.10	1.94
166	D	401	HEC	C2A-C3A	5.03	1.47	1.36
166	D	401	HEC	CHA-C1A	5.02	1.48	1.38
166	D	401	HEC	FE-NB	5.02	2.10	1.94
169	Da	702	HEA	C3D-C2D	4.90	1.47	1.36
169	Da	703	HEA	C3D-C2D	4.89	1.47	1.36
169	DA	703	HEA	C3D-C2D	4.89	1.47	1.36
166	d	802	HEC	CHD-C1D	4.85	1.48	1.38
169	DA	702	HEA	C3D-C2D	4.85	1.47	1.36
166	d	802	HEC	CHB-C4A	4.81	1.47	1.38
166	CE	401	HEC	CHC-C4B	4.81	1.48	1.38
169	DA	702	HEA	FE-NC	4.73	2.11	1.95
169	Da	702	HEA	FE-NC	4.72	2.11	1.95
166	D	401	HEC	CHC-C4B	4.70	1.48	1.38
166	d	802	HEC	CHC-C4B	4.69	1.48	1.38
166	D	401	HEC	CHB-C4A	4.68	1.47	1.38
169	Da	703	HEA	FE-NC	4.66	2.10	1.95
166	CE	401	HEC	CHA-C1A	4.66	1.47	1.38
169	DA	703	HEA	FE-NC	4.64	2.10	1.95
169	DA	703	HEA	CHC-C4B	4.59	1.47	1.38
166	CE	401	HEC	C3D-C2D	4.57	1.46	1.36
169	DA	702	HEA	CHB-C4A	4.55	1.47	1.38
169	Da	702	HEA	CHC-C4B	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	DA	702	HEA	CHC-C4B	4.51	1.47	1.38
166	D	401	HEC	FE-NC	4.51	2.10	1.95
169	Da	702	HEA	CHA-C1A	4.51	1.47	1.38
166	D	401	HEC	FE-NA	4.48	2.10	1.95
169	DA	702	HEA	CHA-C1A	4.48	1.47	1.38
169	Da	703	HEA	CHC-C4B	4.48	1.47	1.38
166	d	802	HEC	FE-NC	4.47	2.10	1.95
169	Da	703	HEA	CHB-C4A	4.44	1.47	1.38
169	Da	703	HEA	CHA-C1A	4.43	1.47	1.38
169	DA	703	HEA	CHB-C4A	4.40	1.46	1.38
166	d	802	HEC	FE-NA	4.40	2.10	1.95
169	DA	703	HEA	CHD-C1D	4.40	1.47	1.38
169	DA	703	HEA	CHA-C1A	4.40	1.46	1.38
169	Da	702	HEA	CHB-C4A	4.37	1.46	1.38
169	Da	702	HEA	CHD-C1D	4.35	1.47	1.38
169	DA	702	HEA	CHD-C1D	4.34	1.47	1.38
169	Da	703	HEA	CHD-C1D	4.34	1.47	1.38
166	CE	401	HEC	CHB-C1B	4.19	1.48	1.39
166	D	401	HEC	CHD-C4C	4.11	1.48	1.39
166	CE	401	HEC	CHD-C1D	4.01	1.46	1.38
166	CE	401	HEC	FE-ND	3.96	2.07	1.94
166	d	802	HEC	CHD-C4C	3.95	1.48	1.39
166	D	401	HEC	CHA-C4D	3.89	1.48	1.39
166	d	802	HEC	CHC-C1C	3.88	1.48	1.39
166	D	401	HEC	CHC-C1C	3.88	1.48	1.39
166	d	802	HEC	CHA-C4D	3.84	1.48	1.39
169	DA	703	HEA	CHC-C1C	3.79	1.47	1.39
169	Da	703	HEA	CHC-C1C	3.79	1.47	1.39
169	Da	702	HEA	CHD-C4C	3.77	1.47	1.39
169	Da	702	HEA	CHC-C1C	3.76	1.47	1.39
169	DA	702	HEA	CHC-C1C	3.70	1.47	1.39
169	DA	703	HEA	CHD-C4C	3.70	1.47	1.39
169	DA	702	HEA	CHD-C4C	3.68	1.47	1.39
169	Da	703	HEA	CHD-C4C	3.67	1.47	1.39
169	DA	702	HEA	CHB-C1B	3.61	1.47	1.39
169	DA	703	HEA	CHA-C4D	3.59	1.47	1.39
169	Da	703	HEA	CHB-C1B	3.56	1.47	1.39
169	Da	703	HEA	CHA-C4D	3.56	1.47	1.39
169	Da	702	HEA	CHB-C1B	3.54	1.47	1.39
169	Da	702	HEA	CHA-C4D	3.51	1.47	1.39
166	D	401	HEC	C3C-C2C	3.50	1.48	1.38
166	d	802	HEC	CHB-C1B	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	DA	703	HEA	CHB-C1B	3.47	1.47	1.39
168	ED	602	HEM	FE-NB	3.46	2.05	1.94
166	D	401	HEC	CHB-C1B	3.44	1.47	1.39
168	Ed	201	HEM	FE-NB	3.44	2.05	1.94
169	DA	702	HEA	CHA-C4D	3.43	1.47	1.39
166	CE	401	HEC	C4B-C3B	3.39	1.50	1.45
169	DA	702	HEA	C1A-NA	3.36	1.46	1.39
166	d	802	HEC	C3C-C2C	3.34	1.47	1.38
169	Da	702	HEA	C1A-NA	3.32	1.46	1.39
168	c	504	HEM	FE-NB	3.22	2.04	1.94
169	Da	703	HEA	C1A-NA	3.20	1.46	1.39
168	ED	602	HEM	FE-ND	3.19	2.04	1.94
168	c	505	HEM	FE-ND	3.18	2.04	1.94
168	C	502	HEM	FE-ND	3.17	2.04	1.94
166	CE	401	HEC	C3C-C2C	3.16	1.47	1.38
169	DA	703	HEA	C1A-NA	3.15	1.45	1.39
168	c	504	HEM	FE-ND	3.13	2.04	1.94
168	C	501	HEM	FE-ND	3.12	2.04	1.94
166	D	401	HEC	C4B-NB	-3.12	1.34	1.40
168	Ed	201	HEM	FE-NC	3.09	2.05	1.95
168	Ed	201	HEM	FE-ND	3.09	2.04	1.94
166	CE	401	HEC	CHA-C4D	3.05	1.46	1.39
166	CE	401	HEC	CHD-C4C	3.05	1.46	1.39
168	C	501	HEM	FE-NB	3.05	2.04	1.94
166	CE	401	HEC	C1A-C2A	3.04	1.50	1.45
168	ED	602	HEM	FE-NC	3.03	2.05	1.95
166	CE	401	HEC	CMB-C2B	3.02	1.57	1.50
166	CE	401	HEC	C4A-C3A	3.01	1.51	1.45
166	CE	401	HEC	CHC-C1C	3.00	1.46	1.39
166	d	802	HEC	C4B-NB	-3.00	1.35	1.40
166	CE	401	HEC	C1C-NC	-2.99	1.34	1.39
168	c	505	HEM	FE-NB	2.97	2.04	1.94
166	CE	401	HEC	C4B-NB	-2.97	1.35	1.40
166	CE	401	HEC	CAC-C3C	-2.97	1.43	1.51
168	ED	602	HEM	FE-NA	2.96	2.05	1.95
168	C	502	HEM	FE-NB	2.95	2.04	1.94
168	Ed	201	HEM	FE-NA	2.95	2.05	1.95
169	DA	703	HEA	C4B-C3B	2.92	1.49	1.44
168	Ed	201	HEM	CAC-C3C	2.91	1.55	1.47
166	CE	401	HEC	C1D-ND	-2.91	1.35	1.40
168	c	505	HEM	FE-NC	2.90	2.04	1.95
168	c	505	HEM	CAB-C3B	2.90	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
168	c	504	HEM	CAC-C3C	2.89	1.55	1.47
169	Da	703	HEA	C4B-C3B	2.89	1.49	1.44
168	ED	602	HEM	CAB-C3B	2.89	1.55	1.47
168	c	505	HEM	FE-NA	2.89	2.04	1.95
168	c	504	HEM	CAB-C3B	2.88	1.55	1.47
168	Ed	201	HEM	CAB-C3B	2.88	1.55	1.47
168	ED	602	HEM	CAC-C3C	2.88	1.55	1.47
168	C	501	HEM	CAB-C3B	2.88	1.55	1.47
168	C	502	HEM	CAB-C3B	2.86	1.55	1.47
168	c	505	HEM	CAC-C3C	2.86	1.55	1.47
168	C	501	HEM	CAC-C3C	2.86	1.55	1.47
168	C	502	HEM	CAC-C3C	2.86	1.55	1.47
169	Da	702	HEA	C1A-C2A	2.81	1.50	1.45
169	DA	702	HEA	C4B-C3B	2.80	1.49	1.44
169	DA	702	HEA	C1D-ND	-2.79	1.35	1.40
169	Da	703	HEA	C1D-ND	-2.78	1.35	1.40
166	d	802	HEC	C1D-ND	-2.77	1.35	1.40
169	DA	703	HEA	C1D-ND	-2.76	1.35	1.40
169	Da	702	HEA	C1D-ND	-2.76	1.35	1.40
166	D	401	HEC	C1D-ND	-2.72	1.35	1.40
169	Da	702	HEA	C4B-C3B	2.72	1.49	1.44
169	DA	702	HEA	C4A-NA	2.71	1.45	1.39
169	Da	702	HEA	C1C-C2C	2.71	1.49	1.43
169	DA	702	HEA	C1C-C2C	2.69	1.49	1.43
168	C	501	HEM	FE-NA	2.68	2.04	1.95
169	Da	702	HEA	C4B-NB	-2.68	1.35	1.40
169	DA	702	HEA	C1A-C2A	2.68	1.50	1.45
168	c	504	HEM	FE-NC	2.68	2.04	1.95
169	DA	703	HEA	C4A-NA	2.66	1.44	1.39
168	C	502	HEM	FE-NC	2.65	2.04	1.95
169	Da	703	HEA	C4A-NA	2.65	1.44	1.39
166	CE	401	HEC	C4D-C3D	2.64	1.49	1.45
168	C	501	HEM	FE-NC	2.64	2.04	1.95
169	DA	702	HEA	C4B-NB	-2.63	1.35	1.40
169	DA	703	HEA	C1C-C2C	2.62	1.49	1.43
169	Da	702	HEA	C4A-NA	2.59	1.44	1.39
169	Da	703	HEA	C1C-C2C	2.59	1.49	1.43
166	D	401	HEC	C1C-C2C	2.58	1.49	1.43
166	d	802	HEC	C1C-C2C	2.57	1.49	1.43
169	Da	703	HEA	C1A-C2A	2.57	1.49	1.45
169	DA	703	HEA	C1A-C2A	2.54	1.49	1.45
166	CE	401	HEC	C1B-C2B	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	Da	702	HEA	C3C-C4C	2.53	1.48	1.42
166	d	802	HEC	C4D-C3D	2.53	1.49	1.45
168	c	504	HEM	FE-NA	2.52	2.03	1.95
169	DA	702	HEA	C3C-C4C	2.52	1.48	1.42
169	DA	703	HEA	C4B-NB	-2.50	1.36	1.40
169	DA	703	HEA	C3C-C4C	2.50	1.48	1.42
169	Da	703	HEA	C3C-C4C	2.49	1.48	1.42
168	C	502	HEM	FE-NA	2.49	2.03	1.95
169	Da	703	HEA	C4B-NB	-2.48	1.36	1.40
166	D	401	HEC	C1D-C2D	2.47	1.49	1.44
166	d	802	HEC	C1B-C2B	2.45	1.49	1.44
169	DA	703	HEA	C4D-C3D	2.42	1.49	1.45
169	Da	703	HEA	C4D-C3D	2.37	1.49	1.45
166	D	401	HEC	C4D-C3D	2.35	1.49	1.45
166	d	802	HEC	C1D-C2D	2.35	1.49	1.44
166	D	401	HEC	C1B-C2B	2.30	1.49	1.44
166	d	802	HEC	C4A-NA	-2.27	1.35	1.39
166	D	401	HEC	C1A-C2A	2.27	1.49	1.45
166	D	401	HEC	C1A-NA	-2.23	1.35	1.39
166	d	802	HEC	C1A-NA	-2.23	1.35	1.39
169	Da	702	HEA	C1D-C2D	2.22	1.48	1.44
169	DA	702	HEA	C1D-C2D	2.22	1.48	1.44
169	Da	703	HEA	C4C-NC	-2.22	1.35	1.39
169	Da	702	HEA	C4D-C3D	2.21	1.48	1.45
166	D	401	HEC	C4A-NA	-2.18	1.35	1.39
169	DA	703	HEA	C1D-C2D	2.18	1.48	1.44
166	d	802	HEC	C4C-NC	-2.18	1.35	1.39
166	D	401	HEC	C4C-C3C	2.18	1.48	1.44
169	Da	703	HEA	C1D-C2D	2.16	1.48	1.44
166	CE	401	HEC	C4A-NA	-2.16	1.35	1.39
169	DA	702	HEA	C4C-NC	-2.16	1.35	1.39
169	Da	703	HEA	C1B-C2B	2.15	1.48	1.44
169	DA	703	HEA	C4C-NC	-2.15	1.35	1.39
166	d	802	HEC	C4B-C3B	2.14	1.48	1.45
169	DA	702	HEA	C1B-C2B	2.13	1.48	1.44
166	d	802	HEC	C4C-C3C	2.11	1.48	1.44
169	Da	702	HEA	C4C-NC	-2.11	1.35	1.39
166	CE	401	HEC	C4D-ND	-2.11	1.34	1.38
166	D	401	HEC	C4C-NC	-2.10	1.35	1.39
166	d	802	HEC	C1A-C2A	2.10	1.48	1.45
169	Da	702	HEA	C1B-C2B	2.09	1.48	1.44
169	DA	702	HEA	C4D-C3D	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	DA	703	HEA	C1B-C2B	2.07	1.48	1.44
166	D	401	HEC	C4B-C3B	2.03	1.48	1.45
168	C	502	HEM	CMB-C2B	2.00	1.55	1.50

All (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
169	Da	702	HEA	C3C-C4C-NC	6.82	114.45	110.25
169	Da	703	HEA	C3C-C4C-NC	6.82	114.44	110.25
166	d	802	HEC	C1B-C2B-C3B	-6.67	99.94	106.96
166	D	401	HEC	C2B-C1B-NB	6.15	117.25	109.88
169	DA	702	HEA	C3D-C4D-ND	6.04	116.21	110.36
166	d	802	HEC	C2B-C1B-NB	6.01	117.08	109.88
169	DA	703	HEA	C3D-C4D-ND	6.00	116.17	110.36
169	Da	702	HEA	C3D-C4D-ND	5.91	116.08	110.36
166	CE	401	HEC	CAB-C3B-C4B	5.89	132.46	124.81
169	Da	703	HEA	C3D-C4D-ND	5.89	116.06	110.36
169	DA	703	HEA	C2D-C1D-ND	5.38	116.21	109.84
166	d	802	HEC	C3D-C4D-ND	5.36	115.55	110.36
169	Da	703	HEA	C2D-C1D-ND	5.33	116.16	109.84
169	DA	703	HEA	C2B-C1B-NB	5.32	116.26	109.88
169	Da	702	HEA	C2B-C1B-NB	5.28	116.20	109.88
169	DA	702	HEA	C2D-C1D-ND	5.28	116.09	109.84
166	D	401	HEC	C3D-C4D-ND	5.24	115.43	110.36
169	Da	703	HEA	C2B-C1B-NB	5.24	116.16	109.88
166	D	401	HEC	C1C-C2C-C3C	-5.22	100.72	106.83
169	Da	702	HEA	C2D-C1D-ND	5.21	116.02	109.84
169	Da	702	HEA	C3C-C2C-C1C	-5.21	100.87	107.16
169	Da	702	HEA	C3B-C4B-NB	5.21	116.01	109.84
169	DA	702	HEA	C3C-C2C-C1C	-5.20	100.89	107.16
169	DA	702	HEA	C3B-C4B-NB	5.19	115.99	109.84
169	Da	703	HEA	C3B-C4B-NB	5.19	115.99	109.84
169	DA	702	HEA	C2B-C1B-NB	5.17	116.08	109.88
166	CE	401	HEC	C1A-C2A-C3A	-5.14	100.43	107.13
169	Da	703	HEA	C3C-C2C-C1C	-5.11	101.00	107.16
169	DA	703	HEA	C3C-C2C-C1C	-5.07	101.04	107.16
169	DA	703	HEA	C3B-C4B-NB	5.03	115.80	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	d	802	HEC	C1C-C2C-C3C	-4.97	101.02	106.83
166	CE	401	HEC	C1B-C2B-C3B	-4.83	101.88	106.96
166	CE	401	HEC	C3D-C4D-ND	4.80	115.01	110.36
166	D	401	HEC	C2A-C1A-NA	4.77	114.97	110.32
166	d	802	HEC	C2A-C1A-NA	4.76	114.95	110.32
166	CE	401	HEC	CBB-CAB-C3B	4.70	125.38	112.43
166	CE	401	HEC	C4A-NA-C1A	-4.58	100.86	105.35
166	CE	401	HEC	C2C-C1C-NC	4.58	117.05	110.08
166	CE	401	HEC	CHD-C1D-ND	4.41	129.81	124.37
166	d	802	HEC	C2D-C1D-ND	4.38	115.03	109.84
166	CE	401	HEC	CBC-CAC-C3C	4.38	124.50	112.43
169	DA	702	HEA	C1D-C2D-C3D	-4.18	102.56	106.96
169	Da	702	HEA	C2C-C1C-NC	4.18	116.45	110.08
169	DA	702	HEA	C2C-C1C-NC	4.17	116.42	110.08
169	Da	702	HEA	C1D-C2D-C3D	-4.10	102.64	106.96
169	Da	703	HEA	C2C-C1C-NC	4.10	116.32	110.08
166	d	802	HEC	CBC-CAC-C3C	4.09	123.70	112.43
169	DA	703	HEA	C2C-C1C-NC	4.09	116.30	110.08
166	CE	401	HEC	C3A-C4A-NA	4.05	117.16	109.69
166	D	401	HEC	C2C-C1C-NC	4.01	116.19	110.08
169	DA	703	HEA	C1D-C2D-C3D	-4.01	102.74	106.96
169	Da	703	HEA	C1D-C2D-C3D	-4.00	102.75	106.96
166	CE	401	HEC	CHD-C1D-C2D	-3.99	115.66	126.73
166	CE	401	HEC	C2D-C1D-ND	3.95	114.53	109.84
166	d	802	HEC	CBB-CAB-C3B	3.94	123.30	112.43
166	D	401	HEC	C2D-C1D-ND	3.93	114.50	109.84
167	El	906	UQ8	C7-C8-C9	3.89	133.27	126.79
166	D	401	HEC	CBC-CAC-C3C	3.89	123.15	112.43
166	d	802	HEC	C2C-C1C-NC	3.81	115.88	110.08
166	D	401	HEC	CBB-CAB-C3B	3.79	122.87	112.43
169	DA	703	HEA	C13-C12-C11	-3.78	108.67	114.35
167	EL	905	UQ8	C7-C8-C9	3.62	132.81	126.79
166	D	401	HEC	CHB-C1B-C2B	-3.56	119.42	124.98
169	Da	702	HEA	C1B-C2B-C3B	-3.53	102.58	106.80
167	El	906	UQ8	C8-C7-C6	3.50	121.47	112.05
166	d	802	HEC	C1D-C2D-C3D	-3.47	103.31	106.96
169	DA	703	HEA	C1B-C2B-C3B	-3.45	102.67	106.80
166	CE	401	HEC	C4D-C3D-C2D	-3.45	101.87	106.90
166	d	802	HEC	CHB-C1B-C2B	-3.43	119.62	124.98
169	DA	702	HEA	C1B-C2B-C3B	-3.40	102.73	106.80
168	Ed	201	HEM	C4D-ND-C1D	3.36	108.55	105.07
169	Da	703	HEA	C27-C19-C20	3.33	120.88	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
169	Da	703	HEA	C1B-C2B-C3B	-3.33	102.82	106.80
166	d	802	HEC	C3B-C4B-NB	3.32	113.87	110.17
166	D	401	HEC	C1D-C2D-C3D	-3.29	103.50	106.96
166	D	401	HEC	C3A-C4A-NA	3.29	115.75	109.69
166	D	401	HEC	C3B-C4B-NB	3.28	113.82	110.17
166	CE	401	HEC	CHA-C1A-C2A	-3.24	119.69	124.94
166	d	802	HEC	C4D-C3D-C2D	-3.23	102.19	106.90
169	DA	703	HEA	C26-C15-C16	3.23	120.70	115.27
166	CE	401	HEC	C2B-C1B-NB	3.21	113.73	109.88
166	CE	401	HEC	CAC-C3C-C4C	3.21	129.37	124.92
168	ED	602	HEM	C4D-ND-C1D	3.19	108.37	105.07
166	D	401	HEC	C4D-C3D-C2D	-3.19	102.24	106.90
166	d	802	HEC	C1A-C2A-C3A	-3.18	102.99	107.13
168	C	502	HEM	C4A-NA-C1A	3.17	108.45	105.35
166	D	401	HEC	C4A-C3A-C2A	-3.16	102.33	106.94
169	DA	703	HEA	CHB-C1B-C2B	-3.15	120.06	124.98
169	DA	702	HEA	CHA-C4D-C3D	-3.15	120.21	124.84
169	DA	703	HEA	C4D-C3D-C2D	-3.15	102.31	106.90
169	Da	703	HEA	C4D-C3D-C2D	-3.10	102.38	106.90
166	d	802	HEC	C3A-C4A-NA	3.10	115.40	109.69
166	CE	401	HEC	CHA-C4D-C3D	-3.09	120.30	124.84
168	c	505	HEM	C4D-ND-C1D	3.08	108.26	105.07
169	Da	702	HEA	CHB-C4A-NA	3.07	127.76	124.44
166	d	802	HEC	C3C-C4C-NC	3.06	113.57	110.15
166	CE	401	HEC	CHC-C1C-C2C	-3.05	118.63	127.24
166	D	401	HEC	C1A-C2A-C3A	-3.04	103.16	107.13
169	Da	702	HEA	C4D-C3D-C2D	-3.03	102.48	106.90
167	C	511	UQ8	C7-C8-C9	3.03	131.83	126.79
167	EL	905	UQ8	C8-C7-C6	3.03	120.20	112.05
169	DA	702	HEA	C4D-C3D-C2D	-3.02	102.50	106.90
168	c	505	HEM	C4A-NA-C1A	3.02	108.30	105.35
168	C	501	HEM	C4D-ND-C1D	3.00	108.18	105.07
166	D	401	HEC	C3C-C4C-NC	3.00	113.50	110.15
167	Ed	202	UQ8	C7-C8-C9	2.99	131.78	126.79
168	C	502	HEM	C4D-ND-C1D	2.98	108.16	105.07
169	Da	702	HEA	OMA-CMA-C3A	-2.98	118.94	125.69
166	d	802	HEC	C4A-C3A-C2A	-2.98	102.58	106.94
166	CE	401	HEC	CMC-C2C-C3C	2.98	132.06	125.61
168	c	504	HEM	C4D-ND-C1D	2.97	108.14	105.07
169	Da	702	HEA	CHA-C4D-C3D	-2.97	120.47	124.84
168	c	505	HEM	C1B-NB-C4B	2.97	108.14	105.07
169	Da	703	HEA	CHB-C1B-C2B	-2.95	120.38	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
168	c	504	HEM	C4A-NA-C1A	2.94	108.23	105.35
168	Ed	201	HEM	C4A-NA-C1A	2.93	108.21	105.35
150	Di	1101	CDL	CB2-C1-CA2	-2.91	104.22	112.79
167	ED	603	UQ8	C7-C8-C9	2.91	131.63	126.79
168	C	501	HEM	C4A-NA-C1A	2.91	108.19	105.35
169	DA	702	HEA	C4B-C3B-C2B	-2.89	102.47	107.41
169	Da	703	HEA	C4B-C3B-C2B	-2.89	102.48	107.41
150	EA	301	CDL	CB2-C1-CA2	-2.89	104.29	112.79
166	CE	401	HEC	C4A-C3A-C2A	-2.89	102.73	106.94
168	ED	602	HEM	C4A-NA-C1A	2.88	108.17	105.35
169	DA	703	HEA	C27-C19-C20	2.88	120.12	115.27
169	Da	703	HEA	C13-C12-C11	-2.87	110.03	114.35
169	Da	702	HEA	C3A-C2A-C1A	-2.87	104.34	107.08
150	BT	204	CDL	CB2-C1-CA2	-2.87	104.35	112.79
169	Da	702	HEA	CHB-C1B-C2B	-2.86	120.51	124.98
166	CE	401	HEC	CAD-C3D-C4D	2.85	129.64	124.66
168	C	502	HEM	C1B-NB-C4B	2.85	108.02	105.07
169	DA	702	HEA	CHB-C1B-C2B	-2.85	120.53	124.98
166	CE	401	HEC	CAC-C3C-C2C	-2.84	122.31	126.86
169	Da	702	HEA	CHB-C4A-C3A	-2.84	120.40	125.26
150	C	507	CDL	CB2-C1-CA2	-2.83	104.46	112.79
166	D	401	HEC	CMC-C2C-C3C	2.83	131.73	125.61
166	CE	401	HEC	C4B-NB-C1B	2.82	107.98	105.07
150	DV	401	CDL	CB2-C1-CA2	-2.81	104.51	112.79
151	A0	603	UDP	PA-O3A-PB	-2.81	123.18	132.83
169	Da	702	HEA	C4B-C3B-C2B	-2.81	102.62	107.41
168	ED	602	HEM	C4C-NC-C1C	2.80	108.09	105.35
169	DA	703	HEA	C4B-C3B-C2B	-2.80	102.62	107.41
166	D	401	HEC	CHA-C4D-C3D	-2.79	120.73	124.84
167	Ds	404	UQ8	C7-C8-C9	2.78	131.43	126.79
166	CE	401	HEC	CHB-C4A-C3A	-2.78	119.64	125.48
150	BL	301	CDL	CB2-C1-CA2	-2.78	104.60	112.79
150	Dv	403	CDL	CB2-C1-CA2	-2.78	104.61	112.79
150	El	901	CDL	CB2-C1-CA2	-2.77	104.63	112.79
169	Da	703	HEA	CAD-C3D-C4D	2.77	129.50	124.66
166	d	802	HEC	CMC-C2C-C3C	2.76	131.58	125.61
169	DA	703	HEA	CAD-C3D-C4D	2.76	129.48	124.66
150	AA	901	CDL	CB2-C1-CA2	-2.76	104.67	112.79
168	c	504	HEM	C4C-NC-C1C	2.75	108.04	105.35
168	C	501	HEM	C1B-NB-C4B	2.75	107.91	105.07
169	Da	703	HEA	C26-C15-C16	2.74	119.88	115.27
166	CE	401	HEC	CHA-C1A-NA	-2.74	121.48	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
167	c	510	UQ8	C8-C7-C6	2.73	119.40	112.05
150	BC	302	CDL	CB2-C1-CA2	-2.72	104.79	112.79
168	ED	602	HEM	C1B-NB-C4B	2.71	107.88	105.07
150	DN	503	CDL	CB2-C1-CA2	-2.71	104.82	112.79
150	Ek	201	CDL	CB2-C1-CA2	-2.70	104.85	112.79
166	d	802	HEC	CAD-C3D-C4D	2.69	129.37	124.66
168	C	501	HEM	C4C-NC-C1C	2.69	107.98	105.35
166	CE	401	HEC	C1D-C2D-C3D	-2.68	104.14	106.96
150	DU	402	CDL	CB2-C1-CA2	-2.68	104.91	112.79
150	ES	1101	CDL	CB2-C1-CA2	-2.67	104.92	112.79
168	c	504	HEM	C1B-NB-C4B	2.67	107.83	105.07
150	ED	604	CDL	CB2-C1-CA2	-2.66	104.95	112.79
169	DA	702	HEA	C3A-C2A-C1A	-2.66	104.53	107.08
168	Ed	201	HEM	C4C-NC-C1C	2.66	107.96	105.35
164	CA	702	FAD	P-O3P-PA	-2.66	123.69	132.83
150	DD	706	CDL	CB2-C1-CA2	-2.66	104.97	112.79
167	DS	403	UQ8	C7-C8-C9	2.66	131.21	126.79
150	DX	301	CDL	CB2-C1-CA2	-2.65	104.98	112.79
150	AC	801	CDL	CB2-C1-CA2	-2.65	104.98	112.79
166	CE	401	HEC	CAB-C3B-C2B	-2.65	122.99	127.53
150	Dg	202	CDL	CB2-C1-CA2	-2.65	104.99	112.79
150	EK	201	CDL	CB2-C1-CA2	-2.65	105.00	112.79
150	Dj	403	CDL	CB2-C1-CA2	-2.64	105.01	112.79
167	C	512	UQ8	C7-C8-C9	2.64	131.19	126.79
169	DA	703	HEA	CAA-CBA-CGA	-2.63	107.94	113.60
150	DU	404	CDL	CB2-C1-CA2	-2.63	105.06	112.79
150	Dd	706	CDL	CB2-C1-CA2	-2.62	105.07	112.79
150	DR	402	CDL	CB2-C1-CA2	-2.62	105.08	112.79
168	c	505	HEM	C4C-NC-C1C	2.62	107.91	105.35
150	Eg	101	CDL	CB2-C1-CA2	-2.62	105.09	112.79
150	Do	501	CDL	CB2-C1-CA2	-2.61	105.11	112.79
150	h	501	CDL	CB2-C1-CA2	-2.60	105.12	112.79
150	Eb	302	CDL	CB2-C1-CA2	-2.60	105.13	112.79
167	C	511	UQ8	C8-C7-C6	2.60	119.06	112.05
150	Da	709	CDL	CB2-C1-CA2	-2.60	105.14	112.79
150	Ds	402	CDL	CB2-C1-CA2	-2.60	105.15	112.79
150	DA	706	CDL	CB2-C1-CA2	-2.59	105.15	112.79
169	Da	703	HEA	CHA-C4D-C3D	-2.59	121.03	124.84
166	CE	401	HEC	C1C-CHC-C4B	2.59	132.48	126.34
169	DA	703	HEA	CHB-C4A-NA	2.59	127.24	124.44
168	C	502	HEM	C4C-NC-C1C	2.59	107.88	105.35
150	DS	401	CDL	CB2-C1-CA2	-2.58	105.18	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
169	DA	703	HEA	CHA-C4D-C3D	-2.58	121.04	124.84
150	CC	305	CDL	CB2-C1-CA2	-2.58	105.19	112.79
150	DO	501	CDL	CB2-C1-CA2	-2.58	105.20	112.79
169	Da	703	HEA	CHB-C4A-NA	2.58	127.23	124.44
166	d	802	HEC	CHA-C4D-C3D	-2.58	121.06	124.84
150	BT	202	CDL	CB2-C1-CA2	-2.57	105.21	112.79
150	Dc	601	CDL	CB2-C1-CA2	-2.57	105.23	112.79
169	Da	702	HEA	C13-C14-C15	-2.57	121.47	127.66
150	BE	201	CDL	CB2-C1-CA2	-2.57	105.23	112.79
169	Da	703	HEA	CHC-C1C-C2C	-2.56	120.00	127.24
169	Da	702	HEA	CAA-CBA-CGA	-2.56	108.09	113.60
167	EL	905	UQ8	C17-C18-C19	-2.56	121.49	127.66
150	CG	302	CDL	CB2-C1-CA2	-2.56	105.25	112.79
150	DV	403	CDL	CB2-C1-CA2	-2.56	105.26	112.79
150	Dn	502	CDL	CB2-C1-CA2	-2.56	105.26	112.79
168	Ed	201	HEM	C1B-NB-C4B	2.56	107.71	105.07
150	c	502	CDL	CB2-C1-CA2	-2.56	105.27	112.79
150	Dq	1403	CDL	CB2-C1-CA2	-2.56	105.27	112.79
150	DI	302	CDL	CB2-C1-CA2	-2.55	105.27	112.79
150	DD	704	CDL	CB2-C1-CA2	-2.55	105.27	112.79
150	DC	601	CDL	CB2-C1-CA2	-2.55	105.28	112.79
150	BG	201	CDL	CB2-C1-CA2	-2.55	105.28	112.79
150	E	301	CDL	CB2-C1-CA2	-2.54	105.31	112.79
169	Da	703	HEA	CMB-C2B-C1B	2.54	128.91	125.04
166	D	401	HEC	CAD-C3D-C4D	2.54	129.10	124.66
150	Dx	1204	CDL	CB2-C1-CA2	-2.54	105.32	112.79
166	D	401	HEC	CMB-C2B-C3B	2.54	133.00	126.12
150	DV	402	CDL	CB2-C1-CA2	-2.54	105.32	112.79
150	Dm	502	CDL	CB2-C1-CA2	-2.53	105.33	112.79
150	AC	802	CDL	CB2-C1-CA2	-2.53	105.35	112.79
150	DH	202	CDL	CB2-C1-CA2	-2.53	105.35	112.79
167	C	511	UQ8	C17-C18-C19	-2.52	121.59	127.66
169	DA	702	HEA	CHB-C4A-NA	2.52	127.16	124.44
169	Da	703	HEA	CHD-C1D-C2D	-2.52	119.73	126.73
150	Dr	403	CDL	CB2-C1-CA2	-2.52	105.38	112.79
167	Ed	202	UQ8	C8-C7-C6	2.51	118.82	112.05
150	Du	403	CDL	CB2-C1-CA2	-2.51	105.40	112.79
150	EL	901	CDL	CB2-C1-CA2	-2.51	105.40	112.79
169	Da	703	HEA	CAD-CBD-CGD	-2.51	108.20	113.60
150	CC	304	CDL	CB2-C1-CA2	-2.51	105.41	112.79
150	En	1201	CDL	CB2-C1-CA2	-2.50	105.42	112.79
169	DA	702	HEA	C13-C14-C15	-2.50	121.63	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
150	Dn	506	CDL	CB2-C1-CA2	-2.50	105.43	112.79
150	DQ	1502	CDL	CB2-C1-CA2	-2.50	105.44	112.79
150	Dq	1401	CDL	CB2-C1-CA2	-2.50	105.44	112.79
167	c	510	UQ8	C17-C18-C19	-2.50	121.65	127.66
150	Dh	201	CDL	CB2-C1-CA2	-2.49	105.45	112.79
150	DZ	501	CDL	CB2-C1-CA2	-2.49	105.46	112.79
169	Da	702	HEA	CHC-C1C-C2C	-2.49	120.21	127.24
150	Ea	502	CDL	CB2-C1-CA2	-2.48	105.47	112.79
150	CJ	201	CDL	CB2-C1-CA2	-2.48	105.49	112.79
150	Dj	404	CDL	CB2-C1-CA2	-2.48	105.49	112.79
150	A0	601	CDL	CB2-C1-CA2	-2.48	105.49	112.79
169	DA	703	HEA	CHC-C1C-C2C	-2.48	120.24	127.24
150	c	509	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	H	1302	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	Dn	503	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	Dx	1201	CDL	CB2-C1-CA2	-2.48	105.50	112.79
150	DM	501	CDL	CB2-C1-CA2	-2.47	105.51	112.79
150	DN	507	CDL	CB2-C1-CA2	-2.47	105.51	112.79
169	DA	703	HEA	CMD-C2D-C1D	2.47	128.80	125.04
150	DS	404	CDL	CB2-C1-CA2	-2.47	105.52	112.79
169	DA	702	HEA	CHC-C1C-C2C	-2.47	120.27	127.24
166	d	802	HEC	CHC-C1C-C2C	-2.47	120.27	127.24
150	Dj	401	CDL	CB2-C1-CA2	-2.46	105.55	112.79
150	B1	402	CDL	CB2-C1-CA2	-2.46	105.56	112.79
150	DN	506	CDL	CB2-C1-CA2	-2.46	105.56	112.79
150	B0	101	CDL	CB2-C1-CA2	-2.46	105.56	112.79
168	Ed	201	HEM	C3D-C4D-ND	-2.46	107.43	110.17
166	CE	401	HEC	CMC-C2C-C1C	2.45	129.11	125.37
150	DH	201	CDL	CB2-C1-CA2	-2.45	105.57	112.79
166	D	401	HEC	CHC-C1C-C2C	-2.45	120.31	127.24
166	D	401	HEC	CMD-C2D-C1D	2.45	128.78	125.04
169	Da	703	HEA	C25-C23-C24	2.45	120.02	114.60
169	DA	703	HEA	CHD-C1D-C2D	-2.45	119.92	126.73
167	CC	303	UQ8	C7-C8-C9	2.45	130.87	126.79
150	DQ	1504	CDL	CB2-C1-CA2	-2.44	105.60	112.79
150	c	501	CDL	CB2-C1-CA2	-2.44	105.60	112.79
169	DA	702	HEA	C25-C23-C24	2.44	120.00	114.60
150	DU	401	CDL	CB2-C1-CA2	-2.44	105.60	112.79
168	C	502	HEM	C2A-C1A-NA	-2.44	107.42	110.15
169	Da	703	HEA	C4B-NB-C1B	-2.44	102.56	105.07
150	BY	201	CDL	CB2-C1-CA2	-2.44	105.61	112.79
169	DA	703	HEA	C25-C23-C24	2.44	119.99	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
169	Da	702	HEA	CHD-C1D-C2D	-2.44	119.96	126.73
169	DA	702	HEA	CHD-C1D-C2D	-2.44	119.96	126.73
150	DJ	305	CDL	CB2-C1-CA2	-2.43	105.63	112.79
150	DN	502	CDL	CB2-C1-CA2	-2.43	105.64	112.79
166	D	401	HEC	CHB-C4A-C3A	-2.43	120.39	125.48
150	AP	301	CDL	CB2-C1-CA2	-2.43	105.64	112.79
150	Du	401	CDL	CB2-C1-CA2	-2.43	105.64	112.79
150	Ds	405	CDL	CB2-C1-CA2	-2.43	105.65	112.79
167	EN	1205	UQ8	C17-C18-C19	-2.43	121.82	127.66
169	DA	703	HEA	C1D-ND-C4D	-2.43	102.57	105.07
169	Da	702	HEA	C25-C23-C24	2.42	119.95	114.60
150	Ds	406	CDL	CB2-C1-CA2	-2.42	105.67	112.79
169	Da	702	HEA	C27-C19-C20	2.42	119.34	115.27
150	EB	302	CDL	CB2-C1-CA2	-2.41	105.68	112.79
150	EN	1202	CDL	CB2-C1-CA2	-2.41	105.69	112.79
150	Di	1103	CDL	CB2-C1-CA2	-2.41	105.71	112.79
150	CD	302	CDL	CB2-C1-CA2	-2.41	105.71	112.79
150	DA	709	CDL	CB2-C1-CA2	-2.41	105.71	112.79
169	DA	703	HEA	CHB-C4A-C3A	-2.40	121.15	125.26
169	Da	703	HEA	CAA-CBA-CGA	-2.40	108.43	113.60
150	Dv	401	CDL	CB2-C1-CA2	-2.40	105.72	112.79
167	ED	603	UQ8	C8-C7-C6	2.40	118.52	112.05
169	Da	702	HEA	C4B-NB-C1B	-2.40	102.59	105.07
150	Ea	501	CDL	CB2-C1-CA2	-2.40	105.73	112.79
150	DG	202	CDL	CB2-C1-CA2	-2.39	105.75	112.79
169	Da	703	HEA	C3A-C2A-C1A	-2.39	104.79	107.08
169	DA	702	HEA	C27-C19-C20	2.39	119.29	115.27
150	Dn	501	CDL	CB2-C1-CA2	-2.39	105.76	112.79
150	CD	301	CDL	CB2-C1-CA2	-2.39	105.77	112.79
169	Da	703	HEA	OMA-CMA-C3A	-2.38	120.31	125.69
169	DA	702	HEA	CAA-CBA-CGA	-2.37	108.50	113.60
169	DA	702	HEA	CMD-C2D-C1D	2.37	128.65	125.04
150	Du	402	CDL	CB2-C1-CA2	-2.37	105.82	112.79
150	EI	401	CDL	CB2-C1-CA2	-2.37	105.82	112.79
150	Dm	501	CDL	CB2-C1-CA2	-2.36	105.83	112.79
150	Dd	702	CDL	CB2-C1-CA2	-2.36	105.84	112.79
166	d	802	HEC	CHB-C4A-C3A	-2.36	120.53	125.48
150	DS	405	CDL	CB2-C1-CA2	-2.36	105.85	112.79
169	DA	702	HEA	C1D-ND-C4D	-2.36	102.64	105.07
169	DA	703	HEA	C4B-NB-C1B	-2.36	102.64	105.07
150	DU	403	CDL	CB2-C1-CA2	-2.36	105.85	112.79
150	Dr	402	CDL	CB2-C1-CA2	-2.36	105.85	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	Ed	204	CDL	CB2-C1-CA2	-2.36	105.85	112.79
150	Eh	1601	CDL	CB2-C1-CA2	-2.35	105.86	112.79
150	EO	202	CDL	CB2-C1-CA2	-2.35	105.87	112.79
150	ED	601	CDL	CB2-C1-CA2	-2.35	105.88	112.79
168	Ed	201	HEM	CAD-CBD-CGD	-2.35	108.55	113.60
150	C	506	CDL	CB2-C1-CA2	-2.35	105.88	112.79
150	EH	1601	CDL	CB2-C1-CA2	-2.35	105.89	112.79
166	d	802	HEC	CMB-C2B-C3B	2.34	132.48	126.12
150	EN	1201	CDL	CB2-C1-CA2	-2.34	105.89	112.79
150	BC	301	CDL	CB2-C1-CA2	-2.34	105.90	112.79
150	Ep	701	CDL	CB2-C1-CA2	-2.34	105.90	112.79
150	El	903	CDL	CB2-C1-CA2	-2.34	105.91	112.79
150	DG	201	CDL	CB2-C1-CA2	-2.34	105.91	112.79
169	Da	703	HEA	C1D-ND-C4D	-2.34	102.66	105.07
169	DA	703	HEA	CAD-CBD-CGD	-2.33	108.59	113.60
150	B0	102	CDL	CB2-C1-CA2	-2.33	105.93	112.79
150	DX	307	CDL	CB2-C1-CA2	-2.33	105.94	112.79
166	D	401	HEC	CMA-C3A-C4A	2.33	128.82	124.71
169	DA	703	HEA	C13-C14-C15	-2.33	122.06	127.66
167	CC	303	UQ8	C11-C9-C8	-2.33	116.41	121.12
150	Dj	407	CDL	CB2-C1-CA2	-2.32	105.95	112.79
166	CE	401	HEC	CAA-C2A-C1A	2.32	129.27	124.89
169	DA	702	HEA	CHB-C4A-C3A	-2.32	121.29	125.26
167	En	1202	UQ8	C7-C8-C9	2.32	130.65	126.79
150	DM	502	CDL	CB2-C1-CA2	-2.32	105.97	112.79
168	c	504	HEM	C2A-C1A-NA	-2.32	107.56	110.15
150	Dh	202	CDL	CB2-C1-CA2	-2.31	105.98	112.79
169	DA	702	HEA	OMA-CMA-C3A	-2.31	120.46	125.69
150	Ei	401	CDL	CB2-C1-CA2	-2.31	105.98	112.79
169	Da	702	HEA	CMD-C2D-C1D	2.31	128.56	125.04
169	Da	703	HEA	CHB-C4A-C3A	-2.30	121.32	125.26
150	Dg	201	CDL	CB2-C1-CA2	-2.30	106.02	112.79
169	DA	703	HEA	CMB-C2B-C1B	2.30	128.54	125.04
167	El	906	UQ8	C17-C18-C19	-2.29	122.14	127.66
168	C	502	HEM	C3D-C4D-ND	-2.29	107.62	110.17
167	EN	1205	UQ8	C7-C8-C9	2.29	130.60	126.79
150	Eu	101	CDL	CB2-C1-CA2	-2.29	106.06	112.79
168	ED	602	HEM	C3B-C2B-C1B	2.28	108.18	106.49
167	CC	303	UQ8	C8-C7-C6	2.28	118.18	112.05
168	C	501	HEM	C3B-C2B-C1B	2.28	108.17	106.49
166	D	401	HEC	CAA-C2A-C1A	2.28	129.18	124.89
150	DJ	303	CDL	CB2-C1-CA2	-2.27	106.09	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
150	DJ	302	CDL	CB2-C1-CA2	-2.27	106.10	112.79
169	Da	703	HEA	CMD-C2D-C1D	2.27	128.50	125.04
150	Ed	205	CDL	CB2-C1-CA2	-2.27	106.11	112.79
156	A6	301	LPP	P1-O5-C6	-2.27	112.04	118.30
168	c	505	HEM	C3D-C4D-ND	-2.27	107.64	110.17
150	C	505	CDL	CB2-C1-CA2	-2.27	106.12	112.79
169	DA	702	HEA	C4B-NB-C1B	-2.27	102.73	105.07
150	CG	301	CDL	CB2-C1-CA2	-2.27	106.12	112.79
150	EL	903	CDL	CB2-C1-CA2	-2.26	106.12	112.79
168	Ed	201	HEM	C2A-C1A-NA	-2.26	107.62	110.15
150	DQ	1501	CDL	CB2-C1-CA2	-2.26	106.15	112.79
150	Dq	1402	CDL	CB2-C1-CA2	-2.25	106.17	112.79
168	c	505	HEM	C2A-C1A-NA	-2.24	107.64	110.15
150	Ds	401	CDL	CB2-C1-CA2	-2.24	106.19	112.79
169	DA	703	HEA	OMA-CMA-C3A	-2.24	120.62	125.69
169	DA	703	HEA	C3A-C2A-C1A	-2.24	104.94	107.08
166	d	802	HEC	CHA-C1A-C2A	-2.24	121.31	124.94
150	DX	306	CDL	CB2-C1-CA2	-2.24	106.20	112.79
150	Dd	705	CDL	CB2-C1-CA2	-2.24	106.20	112.79
168	ED	602	HEM	C3D-C4D-ND	-2.24	107.68	110.17
169	Da	702	HEA	CAD-C3D-C4D	2.23	128.56	124.66
167	Ed	202	UQ8	C21-C19-C18	2.23	125.64	121.12
169	Da	702	HEA	C1D-ND-C4D	-2.22	102.78	105.07
150	Dc	608	CDL	CB2-C1-CA2	-2.22	106.25	112.79
150	Dv	402	CDL	CB2-C1-CA2	-2.22	106.25	112.79
151	A0	603	UDP	O3B-PB-O3A	2.22	112.08	104.64
150	BV	201	CDL	CB2-C1-CA2	-2.22	106.27	112.79
168	Ed	201	HEM	C3B-C2B-C1B	2.21	108.13	106.49
169	DA	702	HEA	CMB-C2B-C1B	2.21	128.41	125.04
150	Dj	405	CDL	CB2-C1-CA2	-2.20	106.30	112.79
169	Da	702	HEA	C17-C18-C19	-2.20	122.36	127.66
150	AF	401	CDL	CB2-C1-CA2	-2.20	106.31	112.79
150	H	1301	CDL	CB2-C1-CA2	-2.19	106.34	112.79
150	ED	605	CDL	CB2-C1-CA2	-2.19	106.35	112.79
150	AF	402	CDL	CB2-C1-CA2	-2.18	106.37	112.79
150	Dy	301	CDL	CB2-C1-CA2	-2.17	106.40	112.79
166	CE	401	HEC	CHB-C1B-C2B	-2.17	121.59	124.98
169	DA	702	HEA	CHC-C4B-C3B	-2.17	120.22	125.80
169	Da	702	HEA	CHC-C4B-C3B	-2.16	120.23	125.80
169	Da	702	HEA	CMB-C2B-C1B	2.16	128.32	125.04
166	CE	401	HEC	CAA-CBA-CGA	-2.15	108.97	113.60
150	C	504	CDL	CB2-C1-CA2	-2.15	106.47	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
169	DA	702	HEA	C26-C15-C16	2.14	118.86	115.27
150	Dj	402	CDL	CB2-C1-CA2	-2.13	106.51	112.79
168	ED	602	HEM	C2A-C1A-NA	-2.13	107.77	110.15
169	DA	702	HEA	C2A-C1A-NA	2.13	112.39	110.32
150	DJ	307	CDL	CB2-C1-CA2	-2.12	106.56	112.79
150	DY	301	CDL	CB2-C1-CA2	-2.11	106.58	112.79
150	DD	703	CDL	CB2-C1-CA2	-2.11	106.59	112.79
168	c	504	HEM	C3B-C2B-C1B	2.10	108.05	106.49
169	Da	703	HEA	C16-C17-C18	-2.10	104.97	111.88
166	CE	401	HEC	CHC-C4B-NB	-2.10	121.78	124.37
168	Ed	201	HEM	C2D-C1D-ND	-2.10	107.36	109.88
150	AA	908	CDL	CB2-C1-CA2	-2.10	106.61	112.79
169	Da	702	HEA	C26-C15-C16	2.10	118.80	115.27
169	DA	702	HEA	CAD-C3D-C4D	2.10	128.33	124.66
150	A0	602	CDL	CB2-C1-CA2	-2.10	106.62	112.79
169	DA	702	HEA	C17-C18-C19	-2.09	122.62	127.66
168	ED	602	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
173	Er	201	ATP	PB-O3B-PG	2.08	139.98	132.83
150	DR	403	CDL	CB2-C1-CA2	-2.08	106.66	112.79
150	c	506	CDL	CB2-C1-CA2	-2.08	106.66	112.79
166	D	401	HEC	CHA-C1A-C2A	-2.08	121.57	124.94
167	CC	303	UQ8	C17-C18-C19	-2.08	122.65	127.66
166	d	802	HEC	CMA-C3A-C4A	2.07	128.36	124.71
169	Da	703	HEA	CHC-C4B-C3B	-2.07	120.47	125.80
167	C	512	UQ8	C8-C7-C6	2.06	117.61	112.05
169	Da	702	HEA	C2A-C1A-NA	2.06	112.33	110.32
168	c	505	HEM	C3B-C2B-C1B	2.06	108.02	106.49
173	ER	201	ATP	PB-O3B-PG	2.06	139.88	132.83
169	DA	703	HEA	C16-C17-C18	-2.05	105.13	111.88
150	h	501	CDL	OB6-CB4-CB6	-2.05	100.96	108.40
167	ED	603	UQ8	C21-C19-C18	2.05	125.27	121.12
150	DJ	304	CDL	CB2-C1-CA2	-2.04	106.78	112.79
166	d	802	HEC	CMD-C2D-C1D	2.04	128.14	125.04
150	EL	902	CDL	CB2-C1-CA2	-2.03	106.81	112.79
150	Dv	401	CDL	OA6-CA4-CA6	-2.02	101.08	108.40
169	Da	703	HEA	CMC-C2C-C3C	2.02	131.47	126.59
150	g	801	CDL	CB2-C1-CA2	-2.02	106.85	112.79
150	BC	302	CDL	OA6-CA4-CA6	-2.02	101.10	108.40
167	En	1202	UQ8	C17-C18-C19	-2.01	122.81	127.66
168	C	501	HEM	C2A-C1A-NA	-2.01	107.90	110.15
150	El	902	CDL	CB2-C1-CA2	-2.01	106.86	112.79
168	C	501	HEM	C3D-C4D-ND	-2.01	107.93	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
167	C	512	UQ8	C17-C18-C19	-2.00	122.84	127.66

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

All (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
150	A0	602	CDL	CA3-OA5-PA1-OA3
150	A0	602	CDL	C1-CB2-OB2-PB2
150	A0	602	CDL	CB3-OB5-PB2-OB2
150	A0	602	CDL	CB3-OB5-PB2-OB3
150	A0	602	CDL	OB5-CB3-CB4-OB6
150	A0	602	CDL	C51-CB5-OB6-CB4
150	A1	402	CDL	CB2-C1-CA2-OA2
150	A1	402	CDL	O1-C1-CB2-OB2
150	A1	402	CDL	CA3-OA5-PA1-OA2
150	A1	402	CDL	CA3-OA5-PA1-OA3
150	A1	402	CDL	CA3-OA5-PA1-OA4
150	A1	402	CDL	CB3-OB5-PB2-OB3
150	AA	901	CDL	C51-CB5-OB6-CB4
150	AA	908	CDL	C11-CA5-OA6-CA4
150	AA	908	CDL	C51-CB5-OB6-CB4
150	AC	801	CDL	CA3-OA5-PA1-OA2
150	AC	801	CDL	CA3-OA5-PA1-OA3
150	AC	801	CDL	CA3-OA5-PA1-OA4
150	AC	801	CDL	CB2-OB2-PB2-OB3
150	AC	801	CDL	CB2-OB2-PB2-OB5
150	AC	801	CDL	CB3-OB5-PB2-OB3
150	AC	801	CDL	CB3-OB5-PB2-OB4
150	AC	802	CDL	CB2-OB2-PB2-OB3
150	AC	802	CDL	CB2-OB2-PB2-OB4
150	AC	802	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
150	AF	401	CDL	CA3-OA5-PA1-OA2
150	AF	401	CDL	CA3-OA5-PA1-OA3
150	AF	401	CDL	CA3-OA5-PA1-OA4
150	AF	401	CDL	OB7-CB5-OB6-CB4
150	AF	402	CDL	CA2-OA2-PA1-OA3
150	AM	301	CDL	CA2-OA2-PA1-OA4
150	AM	301	CDL	C11-CA5-OA6-CA4
150	AM	301	CDL	CB2-OB2-PB2-OB3
150	AM	301	CDL	CB2-OB2-PB2-OB5
150	AP	301	CDL	CA3-OA5-PA1-OA2
150	AP	301	CDL	CA3-OA5-PA1-OA3
150	AP	301	CDL	CA3-OA5-PA1-OA4
150	AP	301	CDL	C11-CA5-OA6-CA4
150	AP	301	CDL	CB2-OB2-PB2-OB4
150	AP	301	CDL	C51-CB5-OB6-CB4
150	B0	101	CDL	CA2-OA2-PA1-OA4
150	B0	101	CDL	C11-CA5-OA6-CA4
150	B0	101	CDL	CB2-OB2-PB2-OB3
150	B0	101	CDL	CB2-OB2-PB2-OB4
150	B0	101	CDL	CB3-OB5-PB2-OB4
150	B0	101	CDL	OB7-CB5-OB6-CB4
150	B0	101	CDL	C51-CB5-OB6-CB4
150	B0	102	CDL	O1-C1-CB2-OB2
150	B0	102	CDL	CA2-C1-CB2-OB2
150	B0	102	CDL	OA6-CA4-CA6-OA8
150	B1	402	CDL	CA3-OA5-PA1-OA3
150	B1	402	CDL	CB2-OB2-PB2-OB3
150	B1	402	CDL	CB2-OB2-PB2-OB4
150	BC	302	CDL	CA3-OA5-PA1-OA2
150	BC	302	CDL	CA3-OA5-PA1-OA3
150	BC	302	CDL	CB2-OB2-PB2-OB3
150	BC	302	CDL	CB3-OB5-PB2-OB4
150	BE	201	CDL	O1-C1-CB2-OB2
150	BE	201	CDL	CA2-C1-CB2-OB2
150	BE	201	CDL	CA2-OA2-PA1-OA4
150	BE	201	CDL	CA3-OA5-PA1-OA3
150	BE	201	CDL	C11-CA5-OA6-CA4
150	BE	201	CDL	CB2-OB2-PB2-OB3
150	BE	201	CDL	CB2-OB2-PB2-OB5
150	BE	201	CDL	OB7-CB5-OB6-CB4
150	BG	201	CDL	CA2-OA2-PA1-OA3
150	BG	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
150	BG	201	CDL	CB2-OB2-PB2-OB3
150	BG	201	CDL	CB3-OB5-PB2-OB3
150	BL	301	CDL	O1-C1-CA2-OA2
150	BL	301	CDL	CB3-OB5-PB2-OB3
150	BT	202	CDL	CA2-C1-CB2-OB2
150	BT	202	CDL	C11-CA5-OA6-CA4
150	BT	202	CDL	CB2-OB2-PB2-OB3
150	BT	202	CDL	CB2-OB2-PB2-OB4
150	BT	202	CDL	CB3-OB5-PB2-OB3
150	BT	202	CDL	CB3-OB5-PB2-OB4
150	BT	202	CDL	C51-CB5-OB6-CB4
150	BT	204	CDL	CA2-OA2-PA1-OA3
150	BT	204	CDL	CA3-OA5-PA1-OA3
150	BT	204	CDL	OA7-CA5-OA6-CA4
150	BT	204	CDL	CB2-OB2-PB2-OB3
150	BT	204	CDL	CB2-OB2-PB2-OB4
150	BT	204	CDL	CB2-OB2-PB2-OB5
150	BV	201	CDL	C51-CB5-OB6-CB4
150	BY	201	CDL	CB2-OB2-PB2-OB5
150	BY	201	CDL	CB4-CB3-OB5-PB2
150	BY	201	CDL	C51-CB5-OB6-CB4
150	CG	301	CDL	CA2-OA2-PA1-OA3
150	CG	301	CDL	CA2-OA2-PA1-OA4
150	CG	301	CDL	CA2-OA2-PA1-OA5
150	CG	301	CDL	CB2-OB2-PB2-OB3
150	CG	302	CDL	CA2-OA2-PA1-OA3
150	CG	302	CDL	CA2-OA2-PA1-OA4
150	CG	302	CDL	CA3-OA5-PA1-OA3
150	CG	302	CDL	C11-CA5-OA6-CA4
150	CG	302	CDL	C1-CB2-OB2-PB2
150	CJ	201	CDL	O1-C1-CA2-OA2
150	CC	304	CDL	CA2-OA2-PA1-OA3
150	CC	304	CDL	CB2-OB2-PB2-OB3
150	CC	304	CDL	OB6-CB4-CB6-OB8
150	CC	305	CDL	CB2-OB2-PB2-OB3
150	CC	305	CDL	CB2-OB2-PB2-OB4
150	CC	305	CDL	CB2-OB2-PB2-OB5
150	CC	305	CDL	CB3-OB5-PB2-OB2
150	CC	305	CDL	OB7-CB5-OB6-CB4
150	CD	301	CDL	CA2-OA2-PA1-OA4
150	CD	301	CDL	CA2-OA2-PA1-OA5
150	CD	301	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
150	CD	301	CDL	CB2-OB2-PB2-OB3
150	CD	301	CDL	CB2-OB2-PB2-OB4
150	CD	301	CDL	CB3-OB5-PB2-OB3
150	CD	302	CDL	CA3-OA5-PA1-OA2
150	CD	302	CDL	CA3-OA5-PA1-OA3
150	CD	302	CDL	CA4-CA3-OA5-PA1
150	CD	302	CDL	C11-CA5-OA6-CA4
150	CD	302	CDL	CB2-OB2-PB2-OB3
150	C	503	CDL	O1-C1-CA2-OA2
150	C	504	CDL	CA2-OA2-PA1-OA3
150	C	504	CDL	CA2-OA2-PA1-OA4
150	C	504	CDL	CA3-OA5-PA1-OA3
150	C	504	CDL	OA5-CA3-CA4-OA6
150	C	504	CDL	C1-CB2-OB2-PB2
150	C	504	CDL	CB2-OB2-PB2-OB3
150	C	505	CDL	CA3-OA5-PA1-OA2
150	C	505	CDL	CA3-OA5-PA1-OA3
150	C	505	CDL	CA3-OA5-PA1-OA4
150	C	505	CDL	C11-CA5-OA6-CA4
150	C	506	CDL	CA3-OA5-PA1-OA3
150	C	506	CDL	C11-CA5-OA6-CA4
150	C	506	CDL	CB3-OB5-PB2-OB3
150	C	506	CDL	CB3-OB5-PB2-OB4
150	C	506	CDL	C51-CB5-OB6-CB4
150	C	507	CDL	O1-C1-CB2-OB2
150	C	507	CDL	CA3-OA5-PA1-OA4
150	C	507	CDL	OA7-CA5-OA6-CA4
150	C	507	CDL	CB3-OB5-PB2-OB3
150	E	301	CDL	CA3-OA5-PA1-OA2
150	E	301	CDL	CA3-OA5-PA1-OA3
150	E	301	CDL	CA3-OA5-PA1-OA4
150	H	1301	CDL	C11-CA5-OA6-CA4
150	H	1301	CDL	CB2-OB2-PB2-OB3
150	H	1301	CDL	CB2-OB2-PB2-OB4
150	H	1301	CDL	CB3-OB5-PB2-OB3
150	H	1301	CDL	CB3-OB5-PB2-OB4
150	H	1302	CDL	CA2-C1-CB2-OB2
150	H	1302	CDL	CA2-OA2-PA1-OA3
150	H	1302	CDL	CA2-OA2-PA1-OA4
150	H	1302	CDL	OA7-CA5-OA6-CA4
150	H	1302	CDL	C11-CA5-OA6-CA4
150	H	1302	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
150	c	501	CDL	CA3-OA5-PA1-OA2
150	c	501	CDL	CA3-OA5-PA1-OA3
150	c	501	CDL	CA3-OA5-PA1-OA4
150	c	501	CDL	C11-CA5-OA6-CA4
150	c	501	CDL	CB2-OB2-PB2-OB3
150	c	501	CDL	CB2-OB2-PB2-OB4
150	c	502	CDL	CA2-OA2-PA1-OA4
150	c	502	CDL	CB2-OB2-PB2-OB3
150	c	502	CDL	CB2-OB2-PB2-OB4
150	c	502	CDL	CB2-OB2-PB2-OB5
150	c	506	CDL	CA2-C1-CB2-OB2
150	c	506	CDL	CA2-OA2-PA1-OA3
150	c	506	CDL	CA3-OA5-PA1-OA3
150	c	506	CDL	C11-CA5-OA6-CA4
150	c	506	CDL	CB2-OB2-PB2-OB3
150	c	509	CDL	CA2-OA2-PA1-OA3
150	c	509	CDL	CA2-OA2-PA1-OA4
150	c	509	CDL	CA2-OA2-PA1-OA5
150	c	509	CDL	C1-CB2-OB2-PB2
150	c	509	CDL	CB3-OB5-PB2-OB3
150	g	801	CDL	CA2-C1-CB2-OB2
150	g	801	CDL	CA2-OA2-PA1-OA3
150	g	801	CDL	CB2-OB2-PB2-OB3
150	g	801	CDL	OB6-CB4-CB6-OB8
150	g	801	CDL	C51-CB5-OB6-CB4
150	h	501	CDL	CB2-OB2-PB2-OB3
150	h	501	CDL	CB2-OB2-PB2-OB4
150	h	501	CDL	C51-CB5-OB6-CB4
150	DA	706	CDL	CA2-OA2-PA1-OA3
150	DA	706	CDL	CB3-OB5-PB2-OB4
150	DA	709	CDL	CA3-OA5-PA1-OA3
150	DA	709	CDL	CA3-OA5-PA1-OA4
150	DA	709	CDL	C11-CA5-OA6-CA4
150	DC	601	CDL	CA2-OA2-PA1-OA4
150	DC	601	CDL	CA3-OA5-PA1-OA4
150	DC	601	CDL	CB2-OB2-PB2-OB4
150	DC	601	CDL	CB3-OB5-PB2-OB4
150	DD	703	CDL	CA3-OA5-PA1-OA4
150	DD	703	CDL	C11-CA5-OA6-CA4
150	DD	704	CDL	CB2-OB2-PB2-OB3
150	DD	705	CDL	CA2-OA2-PA1-OA3
150	DD	705	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
150	DD	705	CDL	CA3-OA5-PA1-OA3
150	DD	705	CDL	C51-CB5-OB6-CB4
150	DD	706	CDL	CA2-OA2-PA1-OA3
150	DD	706	CDL	CA2-OA2-PA1-OA4
150	DD	706	CDL	CA3-OA5-PA1-OA3
150	DD	706	CDL	CB3-OB5-PB2-OB3
150	DG	201	CDL	CB2-OB2-PB2-OB3
150	DG	201	CDL	CB3-OB5-PB2-OB2
150	DG	201	CDL	CB4-CB3-OB5-PB2
150	DG	201	CDL	C51-CB5-OB6-CB4
150	DG	202	CDL	CA2-OA2-PA1-OA4
150	DG	202	CDL	CB3-OB5-PB2-OB4
150	DH	201	CDL	CB2-C1-CA2-OA2
150	DH	201	CDL	CA3-OA5-PA1-OA3
150	DH	201	CDL	OA6-CA4-CA6-OA8
150	DH	202	CDL	CA3-OA5-PA1-OA2
150	DH	202	CDL	CA3-OA5-PA1-OA3
150	DH	202	CDL	CA3-OA5-PA1-OA4
150	DH	202	CDL	CB3-OB5-PB2-OB2
150	DH	202	CDL	CB3-OB5-PB2-OB3
150	DI	302	CDL	C11-CA5-OA6-CA4
150	DI	302	CDL	CB2-OB2-PB2-OB3
150	DI	302	CDL	CB2-OB2-PB2-OB4
150	DI	302	CDL	CB3-OB5-PB2-OB3
150	DI	302	CDL	C51-CB5-OB6-CB4
150	DJ	302	CDL	CA4-CA6-OA8-CA7
150	DJ	302	CDL	C1-CB2-OB2-PB2
150	DJ	302	CDL	CB2-OB2-PB2-OB3
150	DJ	302	CDL	CB3-OB5-PB2-OB4
150	DJ	302	CDL	C51-CB5-OB6-CB4
150	DJ	303	CDL	C1-CA2-OA2-PA1
150	DJ	303	CDL	CB2-OB2-PB2-OB5
150	DJ	303	CDL	CB3-OB5-PB2-OB4
150	DJ	304	CDL	CA2-OA2-PA1-OA3
150	DJ	304	CDL	CA2-OA2-PA1-OA4
150	DJ	304	CDL	CA2-OA2-PA1-OA5
150	DJ	304	CDL	C11-CA5-OA6-CA4
150	DJ	305	CDL	O1-C1-CA2-OA2
150	DJ	305	CDL	CB2-C1-CA2-OA2
150	DJ	305	CDL	CA3-OA5-PA1-OA4
150	DJ	305	CDL	OA7-CA5-OA6-CA4
150	DJ	307	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
150	DJ	307	CDL	CB3-OB5-PB2-OB4
150	DJ	307	CDL	OB5-CB3-CB4-OB6
150	DJ	307	CDL	OB7-CB5-OB6-CB4
150	DJ	307	CDL	C51-CB5-OB6-CB4
150	DM	501	CDL	C1-CA2-OA2-PA1
150	DM	501	CDL	CA2-OA2-PA1-OA3
150	DM	501	CDL	CB2-OB2-PB2-OB3
150	DM	501	CDL	CB2-OB2-PB2-OB4
150	DM	501	CDL	OB7-CB5-OB6-CB4
150	DM	501	CDL	C51-CB5-OB6-CB4
150	DN	502	CDL	CA2-OA2-PA1-OA3
150	DN	502	CDL	CA2-OA2-PA1-OA4
150	DN	502	CDL	CA2-OA2-PA1-OA5
150	DN	502	CDL	CA3-OA5-PA1-OA3
150	DN	502	CDL	CA3-OA5-PA1-OA4
150	DN	502	CDL	CB2-OB2-PB2-OB3
150	DN	503	CDL	CA2-OA2-PA1-OA3
150	DN	503	CDL	CA2-OA2-PA1-OA4
150	DN	503	CDL	CA2-OA2-PA1-OA5
150	DN	503	CDL	CB2-OB2-PB2-OB4
150	DN	506	CDL	CB3-OB5-PB2-OB3
150	DN	506	CDL	C51-CB5-OB6-CB4
150	DN	507	CDL	C1-CA2-OA2-PA1
150	DN	507	CDL	CA2-OA2-PA1-OA4
150	DN	507	CDL	CA3-OA5-PA1-OA3
150	DN	507	CDL	CA3-OA5-PA1-OA4
150	DN	507	CDL	C11-CA5-OA6-CA4
150	DN	507	CDL	CB3-OB5-PB2-OB2
150	DN	507	CDL	CB3-OB5-PB2-OB3
150	DO	501	CDL	CA3-OA5-PA1-OA2
150	DO	501	CDL	CA3-OA5-PA1-OA3
150	DO	501	CDL	C11-CA5-OA6-CA4
150	DO	501	CDL	CB2-OB2-PB2-OB3
150	DO	501	CDL	CB3-OB5-PB2-OB2
150	DO	501	CDL	CB3-OB5-PB2-OB3
150	DO	501	CDL	C51-CB5-OB6-CB4
150	DQ	1501	CDL	CA3-OA5-PA1-OA3
150	DQ	1501	CDL	CA3-OA5-PA1-OA4
150	DQ	1502	CDL	CA2-OA2-PA1-OA3
150	DQ	1502	CDL	CA3-OA5-PA1-OA2
150	DQ	1502	CDL	CA3-OA5-PA1-OA3
150	DQ	1502	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
150	DQ	1502	CDL	CB3-OB5-PB2-OB2
150	DQ	1502	CDL	CB3-OB5-PB2-OB3
150	DQ	1504	CDL	OA5-CA3-CA4-OA6
150	DQ	1504	CDL	OA7-CA5-OA6-CA4
150	DR	402	CDL	CA3-OA5-PA1-OA3
150	DR	402	CDL	CA3-OA5-PA1-OA4
150	DR	402	CDL	CB2-OB2-PB2-OB3
150	DR	402	CDL	CB2-OB2-PB2-OB4
150	DR	402	CDL	CB2-OB2-PB2-OB5
150	DR	402	CDL	OB6-CB4-CB6-OB8
150	DR	403	CDL	OB6-CB4-CB6-OB8
150	DS	401	CDL	CA2-OA2-PA1-OA3
150	DS	401	CDL	CB4-CB3-OB5-PB2
150	DS	404	CDL	CB3-OB5-PB2-OB2
150	DS	404	CDL	CB3-OB5-PB2-OB3
150	DS	404	CDL	CB3-OB5-PB2-OB4
150	DS	404	CDL	C51-CB5-OB6-CB4
150	DS	405	CDL	CA2-OA2-PA1-OA3
150	DS	405	CDL	CA2-OA2-PA1-OA4
150	DS	405	CDL	CB2-OB2-PB2-OB3
150	DS	405	CDL	CB3-OB5-PB2-OB3
150	DS	405	CDL	CB3-OB5-PB2-OB4
150	DU	401	CDL	CA2-OA2-PA1-OA3
150	DU	401	CDL	CA2-OA2-PA1-OA4
150	DU	401	CDL	CB2-OB2-PB2-OB3
150	DU	402	CDL	C11-CA5-OA6-CA4
150	DU	402	CDL	CB2-OB2-PB2-OB3
150	DU	402	CDL	CB2-OB2-PB2-OB4
150	DU	402	CDL	CB2-OB2-PB2-OB5
150	DU	402	CDL	CB3-OB5-PB2-OB3
150	DU	402	CDL	CB3-OB5-PB2-OB4
150	DU	403	CDL	CB3-OB5-PB2-OB3
150	DU	404	CDL	CA3-OA5-PA1-OA3
150	DU	404	CDL	CA3-CA4-OA6-CA5
150	DU	404	CDL	CB2-OB2-PB2-OB3
150	DU	404	CDL	CB2-OB2-PB2-OB4
150	DV	401	CDL	CA3-OA5-PA1-OA3
150	DV	401	CDL	CA3-OA5-PA1-OA4
150	DV	401	CDL	OA7-CA5-OA6-CA4
150	DV	401	CDL	C51-CB5-OB6-CB4
150	DV	402	CDL	CA3-OA5-PA1-OA4
150	DV	403	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
150	DV	403	CDL	CA2-OA2-PA1-OA4
150	DV	403	CDL	CA3-OA5-PA1-OA3
150	DV	403	CDL	CB3-OB5-PB2-OB3
150	DV	403	CDL	C51-CB5-OB6-CB4
150	DX	301	CDL	CA2-OA2-PA1-OA5
150	DX	301	CDL	CB2-OB2-PB2-OB3
150	DX	301	CDL	CB2-OB2-PB2-OB4
150	DX	301	CDL	CB2-OB2-PB2-OB5
150	DX	306	CDL	CA3-OA5-PA1-OA3
150	DX	306	CDL	CA4-CA3-OA5-PA1
150	DX	306	CDL	OA7-CA5-OA6-CA4
150	DX	306	CDL	C11-CA5-OA6-CA4
150	DX	306	CDL	CB2-OB2-PB2-OB3
150	DX	306	CDL	CB3-OB5-PB2-OB4
150	DX	307	CDL	CA2-OA2-PA1-OA4
150	DY	301	CDL	CA3-OA5-PA1-OA3
150	DY	301	CDL	CA3-OA5-PA1-OA4
150	DY	301	CDL	C11-CA5-OA6-CA4
150	DY	301	CDL	CB2-OB2-PB2-OB3
150	DY	301	CDL	OB6-CB4-CB6-OB8
150	DY	301	CDL	C51-CB5-OB6-CB4
150	EA	301	CDL	CA2-OA2-PA1-OA3
150	EA	301	CDL	CA2-OA2-PA1-OA4
150	EA	301	CDL	CA2-OA2-PA1-OA5
150	EA	301	CDL	OA9-CA7-OA8-CA6
150	EA	301	CDL	CB2-OB2-PB2-OB3
150	EA	301	CDL	CB2-OB2-PB2-OB4
150	EB	302	CDL	CA3-OA5-PA1-OA3
150	EB	302	CDL	CA3-OA5-PA1-OA4
150	EB	302	CDL	C11-CA5-OA6-CA4
150	EB	302	CDL	CB2-OB2-PB2-OB3
150	EB	302	CDL	CB2-OB2-PB2-OB4
150	EB	302	CDL	CB3-OB5-PB2-OB3
150	EB	302	CDL	OB7-CB5-OB6-CB4
150	ED	601	CDL	O1-C1-CA2-OA2
150	ED	601	CDL	CA2-OA2-PA1-OA3
150	ED	601	CDL	CA2-OA2-PA1-OA5
150	ED	601	CDL	CA3-OA5-PA1-OA3
150	ED	601	CDL	OA7-CA5-OA6-CA4
150	ED	601	CDL	C11-CA5-OA6-CA4
150	ED	601	CDL	CB3-OB5-PB2-OB3
150	ED	604	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
150	ED	605	CDL	CA3-OA5-PA1-OA2
150	ED	605	CDL	CA3-OA5-PA1-OA3
150	ED	605	CDL	CA3-OA5-PA1-OA4
150	ED	605	CDL	CB2-OB2-PB2-OB3
150	ED	605	CDL	CB3-OB5-PB2-OB4
150	EH	1601	CDL	C11-CA5-OA6-CA4
150	EH	1601	CDL	CB3-OB5-PB2-OB3
150	EH	1601	CDL	C51-CB5-OB6-CB4
150	EI	401	CDL	CB3-OB5-PB2-OB3
150	EK	201	CDL	CA2-OA2-PA1-OA3
150	EK	201	CDL	CA2-OA2-PA1-OA4
150	EK	201	CDL	CA2-OA2-PA1-OA5
150	EK	201	CDL	CA3-OA5-PA1-OA3
150	EL	902	CDL	C11-CA5-OA6-CA4
150	EL	902	CDL	CB2-OB2-PB2-OB3
150	EL	902	CDL	CB2-OB2-PB2-OB4
150	EL	902	CDL	CB3-OB5-PB2-OB2
150	EL	902	CDL	CB3-OB5-PB2-OB3
150	EL	902	CDL	CB3-OB5-PB2-OB4
150	EL	903	CDL	CA2-OA2-PA1-OA4
150	EL	903	CDL	CB2-OB2-PB2-OB3
150	EL	903	CDL	CB2-OB2-PB2-OB4
150	EL	903	CDL	CB3-OB5-PB2-OB3
150	EL	903	CDL	CB3-OB5-PB2-OB4
150	EN	1201	CDL	O1-C1-CA2-OA2
150	EN	1201	CDL	CA2-OA2-PA1-OA4
150	EN	1202	CDL	CA3-OA5-PA1-OA4
150	EN	1202	CDL	CB3-OB5-PB2-OB3
150	EN	1202	CDL	C51-CB5-OB6-CB4
150	EO	202	CDL	C11-CA5-OA6-CA4
150	EO	202	CDL	CB2-OB2-PB2-OB3
150	EO	202	CDL	C51-CB5-OB6-CB4
150	ES	1101	CDL	CA2-OA2-PA1-OA5
150	ES	1101	CDL	CB3-OB5-PB2-OB2
150	ES	1101	CDL	CB3-OB5-PB2-OB3
150	ES	1101	CDL	OB5-CB3-CB4-OB6
150	Da	709	CDL	CA2-OA2-PA1-OA3
150	Da	709	CDL	CA3-OA5-PA1-OA4
150	Da	709	CDL	OA7-CA5-OA6-CA4
150	Da	709	CDL	C11-CA5-OA6-CA4
150	Da	709	CDL	CB3-OB5-PB2-OB3
150	Da	709	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
150	Dc	601	CDL	CA2-OA2-PA1-OA4
150	Dc	601	CDL	CB2-OB2-PB2-OB4
150	Dc	601	CDL	CB3-OB5-PB2-OB4
150	Dc	608	CDL	O1-C1-CB2-OB2
150	Dc	608	CDL	OA7-CA5-OA6-CA4
150	Dc	608	CDL	C11-CA5-OA6-CA4
150	Dc	608	CDL	CB2-OB2-PB2-OB5
150	Dc	608	CDL	CB3-OB5-PB2-OB2
150	Dc	608	CDL	CB3-OB5-PB2-OB3
150	Dc	608	CDL	CB3-OB5-PB2-OB4
150	Dd	702	CDL	C1-CA2-OA2-PA1
150	Dd	702	CDL	CA3-OA5-PA1-OA3
150	Dd	702	CDL	CA3-OA5-PA1-OA4
150	Dd	702	CDL	C11-CA5-OA6-CA4
150	Dd	704	CDL	O1-C1-CA2-OA2
150	Dd	704	CDL	CB2-C1-CA2-OA2
150	Dd	704	CDL	C1-CB2-OB2-PB2
150	Dd	705	CDL	CA3-OA5-PA1-OA4
150	Dd	706	CDL	CA2-C1-CB2-OB2
150	Dd	706	CDL	CA2-OA2-PA1-OA4
150	Dg	201	CDL	CB2-C1-CA2-OA2
150	Dg	201	CDL	CA2-OA2-PA1-OA4
150	Dg	201	CDL	OA7-CA5-OA6-CA4
150	Dg	201	CDL	C11-CA5-OA6-CA4
150	Dg	201	CDL	CB3-OB5-PB2-OB2
150	Dg	201	CDL	CB4-CB3-OB5-PB2
150	Dg	202	CDL	CA2-OA2-PA1-OA3
150	Dg	202	CDL	CA2-OA2-PA1-OA4
150	Dg	202	CDL	CA3-OA5-PA1-OA3
150	Dh	201	CDL	CB2-C1-CA2-OA2
150	Dh	201	CDL	CA3-OA5-PA1-OA3
150	Dh	201	CDL	OA6-CA4-CA6-OA8
150	Dh	201	CDL	CB2-OB2-PB2-OB3
150	Dh	201	CDL	CB2-OB2-PB2-OB5
150	Dh	202	CDL	CA3-OA5-PA1-OA3
150	Dh	202	CDL	CA3-OA5-PA1-OA4
150	Dh	202	CDL	CB2-OB2-PB2-OB3
150	Dh	202	CDL	CB2-OB2-PB2-OB4
150	Dh	202	CDL	CB3-OB5-PB2-OB2
150	Dh	202	CDL	CB3-OB5-PB2-OB3
150	Di	1101	CDL	CB3-OB5-PB2-OB4
150	Di	1103	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
150	Di	1103	CDL	CB3-OB5-PB2-OB2
150	Di	1103	CDL	OB7-CB5-OB6-CB4
150	Di	1103	CDL	C51-CB5-OB6-CB4
150	Dj	401	CDL	CA2-OA2-PA1-OA3
150	Dj	401	CDL	CA2-OA2-PA1-OA4
150	Dj	401	CDL	CB2-OB2-PB2-OB3
150	Dj	401	CDL	CB3-OB5-PB2-OB3
150	Dj	401	CDL	CB3-OB5-PB2-OB4
150	Dj	401	CDL	OB7-CB5-OB6-CB4
150	Dj	401	CDL	C51-CB5-OB6-CB4
150	Dj	402	CDL	CB2-C1-CA2-OA2
150	Dj	402	CDL	C11-CA5-OA6-CA4
150	Dj	402	CDL	CB3-OB5-PB2-OB4
150	Dj	403	CDL	CA2-OA2-PA1-OA4
150	Dj	403	CDL	CA3-OA5-PA1-OA2
150	Dj	403	CDL	CA3-OA5-PA1-OA3
150	Dj	403	CDL	CA3-OA5-PA1-OA4
150	Dj	403	CDL	OB5-CB3-CB4-OB6
150	Dj	404	CDL	CA3-OA5-PA1-OA2
150	Dj	404	CDL	CA3-OA5-PA1-OA3
150	Dj	404	CDL	CA3-OA5-PA1-OA4
150	Dj	404	CDL	OA7-CA5-OA6-CA4
150	Dj	404	CDL	CB3-OB5-PB2-OB2
150	Dj	404	CDL	C51-CB5-OB6-CB4
150	Dj	405	CDL	OA7-CA5-OA6-CA4
150	Dj	405	CDL	CB2-OB2-PB2-OB3
150	Dj	405	CDL	CB2-OB2-PB2-OB5
150	Dj	407	CDL	OA6-CA4-CA6-OA8
150	Dj	407	CDL	C51-CB5-OB6-CB4
150	Dm	501	CDL	CA3-OA5-PA1-OA4
150	Dm	501	CDL	C1-CB2-OB2-PB2
150	Dm	501	CDL	CB2-OB2-PB2-OB4
150	Dm	501	CDL	C51-CB5-OB6-CB4
150	Dm	502	CDL	CA2-OA2-PA1-OA3
150	Dm	502	CDL	CA3-OA5-PA1-OA3
150	Dm	502	CDL	CA3-OA5-PA1-OA4
150	Dm	502	CDL	C11-CA5-OA6-CA4
150	Dn	501	CDL	CA2-OA2-PA1-OA3
150	Dn	501	CDL	CA2-OA2-PA1-OA4
150	Dn	501	CDL	CA2-OA2-PA1-OA5
150	Dn	502	CDL	CA3-OA5-PA1-OA2
150	Dn	502	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
150	Dn	502	CDL	CA3-OA5-PA1-OA4
150	Dn	502	CDL	CA4-CA3-OA5-PA1
150	Dn	503	CDL	CA2-OA2-PA1-OA3
150	Dn	503	CDL	CA2-OA2-PA1-OA5
150	Dn	503	CDL	CA3-OA5-PA1-OA2
150	Dn	503	CDL	CA3-OA5-PA1-OA3
150	Dn	506	CDL	CB3-OB5-PB2-OB3
150	Dn	506	CDL	OB7-CB5-OB6-CB4
150	Dn	506	CDL	C51-CB5-OB6-CB4
150	Do	501	CDL	CA2-OA2-PA1-OA4
150	Do	501	CDL	CA3-OA5-PA1-OA3
150	Do	501	CDL	CA3-OA5-PA1-OA4
150	Do	501	CDL	CB3-OB5-PB2-OB2
150	Do	501	CDL	C51-CB5-OB6-CB4
150	Dq	1401	CDL	OA7-CA5-OA6-CA4
150	Dq	1401	CDL	CB3-OB5-PB2-OB2
150	Dq	1401	CDL	C51-CB5-OB6-CB4
150	Dq	1402	CDL	CA2-OA2-PA1-OA5
150	Dq	1402	CDL	CA3-OA5-PA1-OA3
150	Dq	1402	CDL	CA3-OA5-PA1-OA4
150	Dq	1403	CDL	CB3-OB5-PB2-OB3
150	Dr	402	CDL	CA3-OA5-PA1-OA4
150	Dr	402	CDL	CB2-OB2-PB2-OB4
150	Dr	403	CDL	OB6-CB4-CB6-OB8
150	Ds	401	CDL	CA3-OA5-PA1-OA4
150	Ds	401	CDL	CB3-OB5-PB2-OB3
150	Ds	401	CDL	C51-CB5-OB6-CB4
150	Ds	402	CDL	CA2-OA2-PA1-OA3
150	Ds	402	CDL	CB4-CB3-OB5-PB2
150	Ds	405	CDL	CB3-OB5-PB2-OB2
150	Ds	405	CDL	CB3-OB5-PB2-OB3
150	Ds	405	CDL	CB3-OB5-PB2-OB4
150	Ds	405	CDL	C51-CB5-OB6-CB4
150	Ds	406	CDL	CA2-OA2-PA1-OA3
150	Ds	406	CDL	CA3-OA5-PA1-OA3
150	Ds	406	CDL	CB2-OB2-PB2-OB3
150	Ds	406	CDL	CB3-OB5-PB2-OB3
150	Du	401	CDL	C1-CA2-OA2-PA1
150	Du	401	CDL	CA2-OA2-PA1-OA3
150	Du	401	CDL	CA3-OA5-PA1-OA3
150	Du	401	CDL	CB2-OB2-PB2-OB3
150	Du	401	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
150	Du	401	CDL	CB2-OB2-PB2-OB5
150	Du	402	CDL	CA2-OA2-PA1-OA5
150	Du	402	CDL	CA3-OA5-PA1-OA3
150	Du	402	CDL	CB3-OB5-PB2-OB2
150	Du	402	CDL	CB3-OB5-PB2-OB3
150	Du	402	CDL	CB3-OB5-PB2-OB4
150	Du	403	CDL	CB3-OB5-PB2-OB3
150	Dv	401	CDL	CA3-OA5-PA1-OA2
150	Dv	401	CDL	CA3-OA5-PA1-OA3
150	Dv	401	CDL	CA3-OA5-PA1-OA4
150	Dv	401	CDL	OA7-CA5-OA6-CA4
150	Dv	401	CDL	CB2-OB2-PB2-OB4
150	Dv	402	CDL	CA3-OA5-PA1-OA2
150	Dv	402	CDL	CA3-OA5-PA1-OA3
150	Dv	402	CDL	CA3-OA5-PA1-OA4
150	Dv	402	CDL	CB2-OB2-PB2-OB3
150	Dv	403	CDL	CB3-OB5-PB2-OB2
150	Dv	403	CDL	CB3-OB5-PB2-OB3
150	Dv	403	CDL	OB5-CB3-CB4-OB6
150	Dv	403	CDL	C51-CB5-OB6-CB4
150	Dx	1201	CDL	CA2-OA2-PA1-OA3
150	Dx	1201	CDL	CA2-OA2-PA1-OA4
150	Dx	1201	CDL	CA2-OA2-PA1-OA5
150	Dx	1201	CDL	CB2-OB2-PB2-OB4
150	Dx	1204	CDL	OB5-CB3-CB4-OB6
150	Dx	1204	CDL	C51-CB5-OB6-CB4
150	Dy	301	CDL	CA3-OA5-PA1-OA2
150	Dy	301	CDL	CA3-OA5-PA1-OA3
150	Dy	301	CDL	CA3-OA5-PA1-OA4
150	Dy	301	CDL	C11-CA5-OA6-CA4
150	Dy	301	CDL	C51-CB5-OB6-CB4
150	Ea	501	CDL	CA2-OA2-PA1-OA3
150	Ea	501	CDL	CA2-OA2-PA1-OA5
150	Ea	501	CDL	CB2-OB2-PB2-OB3
150	Ea	502	CDL	C11-CA5-OA6-CA4
150	Ea	502	CDL	CB2-OB2-PB2-OB3
150	Eb	302	CDL	O1-C1-CA2-OA2
150	Eb	302	CDL	CA2-OA2-PA1-OA5
150	Eb	302	CDL	CB2-OB2-PB2-OB4
150	Eb	302	CDL	CB3-OB5-PB2-OB4
150	Eb	302	CDL	OB7-CB5-OB6-CB4
150	Ed	204	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
150	Ed	204	CDL	CA2-OA2-PA1-OA5
150	Ed	204	CDL	CA3-OA5-PA1-OA3
150	Ed	204	CDL	CA3-OA5-PA1-OA4
150	Ed	204	CDL	C11-CA5-OA6-CA4
150	Ed	204	CDL	OA9-CA7-OA8-CA6
150	Ed	204	CDL	CB2-OB2-PB2-OB3
150	Ed	204	CDL	CB2-OB2-PB2-OB4
150	Ed	204	CDL	CB2-OB2-PB2-OB5
150	Ed	205	CDL	CA3-OA5-PA1-OA3
150	Ed	205	CDL	CA3-OA5-PA1-OA4
150	Ed	205	CDL	CB3-OB5-PB2-OB3
150	Eg	101	CDL	O1-C1-CA2-OA2
150	Eg	101	CDL	CA2-OA2-PA1-OA3
150	Eg	101	CDL	CA2-OA2-PA1-OA5
150	Eg	101	CDL	C11-CA5-OA6-CA4
150	Eh	1601	CDL	CA2-OA2-PA1-OA3
150	Eh	1601	CDL	CA2-OA2-PA1-OA5
150	Eh	1601	CDL	C11-CA5-OA6-CA4
150	Eh	1601	CDL	CB3-OB5-PB2-OB3
150	Ei	401	CDL	CA2-OA2-PA1-OA4
150	Ei	401	CDL	C11-CA5-OA6-CA4
150	Ei	401	CDL	CB3-OB5-PB2-OB4
150	Ei	401	CDL	CB4-CB3-OB5-PB2
150	Ek	201	CDL	CA2-OA2-PA1-OA3
150	Ek	201	CDL	CA2-OA2-PA1-OA4
150	Ek	201	CDL	CA2-OA2-PA1-OA5
150	Ek	201	CDL	CA3-OA5-PA1-OA2
150	Ek	201	CDL	CA3-OA5-PA1-OA3
150	Ek	201	CDL	CA3-OA5-PA1-OA4
150	Ek	201	CDL	OA7-CA5-OA6-CA4
150	Ek	201	CDL	C11-CA5-OA6-CA4
150	El	901	CDL	CA3-OA5-PA1-OA4
150	El	901	CDL	OB6-CB4-CB6-OB8
150	El	901	CDL	C51-CB5-OB6-CB4
150	El	902	CDL	CA2-C1-CB2-OB2
150	El	902	CDL	C1-CB2-OB2-PB2
150	El	902	CDL	CB3-OB5-PB2-OB2
150	El	902	CDL	CB3-OB5-PB2-OB3
150	El	902	CDL	CB3-OB5-PB2-OB4
150	El	903	CDL	CA2-OA2-PA1-OA4
150	El	903	CDL	CA3-OA5-PA1-OA4
150	El	903	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
150	El	903	CDL	CB2-OB2-PB2-OB3
150	El	903	CDL	CB3-OB5-PB2-OB2
150	El	903	CDL	CB3-OB5-PB2-OB3
150	El	903	CDL	CB3-OB5-PB2-OB4
150	El	903	CDL	C51-CB5-OB6-CB4
150	En	1201	CDL	O1-C1-CA2-OA2
150	En	1201	CDL	CA2-OA2-PA1-OA5
150	En	1201	CDL	CB2-OB2-PB2-OB5
150	Ep	701	CDL	CB2-C1-CA2-OA2
150	Ep	701	CDL	C1-CA2-OA2-PA1
150	Eu	101	CDL	CB2-OB2-PB2-OB3
150	Eu	101	CDL	CB2-OB2-PB2-OB5
151	A0	603	UDP	C5'-O5'-PA-O2A
153	A0	605	PC1	C1-O11-P-O12
153	A0	605	PC1	C1-O11-P-O14
153	A0	605	PC1	C1-O11-P-O13
153	A1	403	PC1	O11-C1-C2-O21
153	A1	403	PC1	O22-C21-O21-C2
153	A2	402	PC1	C22-C21-O21-C2
153	A6	303	PC1	C11-O13-P-O14
153	A9	601	PC1	O13-C11-C12-N
153	A9	603	PC1	C11-O13-P-O14
153	A9	603	PC1	C1-O11-P-O12
153	A9	603	PC1	O22-C21-O21-C2
153	A9	603	PC1	C22-C21-O21-C2
153	AA	904	PC1	C22-C21-O21-C2
153	AA	905	PC1	C11-O13-P-O12
153	AA	905	PC1	C11-O13-P-O14
153	AA	905	PC1	C1-O11-P-O14
153	AA	905	PC1	C1-O11-P-O13
153	AA	905	PC1	O13-C11-C12-N
153	AA	906	PC1	C11-O13-P-O14
153	AA	907	PC1	C1-O11-P-O12
153	AA	907	PC1	C1-O11-P-O14
153	AA	907	PC1	C1-O11-P-O13
153	AA	907	PC1	O13-C11-C12-N
153	AA	907	PC1	C2-C1-O11-P
153	AC	804	PC1	C11-O13-P-O14
153	AC	804	PC1	C11-O13-P-O11
153	AH	301	PC1	C11-O13-P-O14
153	AJ	501	PC1	C1-O11-P-O12
153	AJ	501	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
153	AJ	501	PC1	C1-O11-P-O13
153	AJ	501	PC1	O13-C11-C12-N
153	AL	303	PC1	O13-C11-C12-N
153	AL	303	PC1	O22-C21-O21-C2
153	AM	302	PC1	C11-O13-P-O12
153	AM	302	PC1	C1-O11-P-O12
153	AM	302	PC1	C1-O11-P-O14
153	AM	302	PC1	C1-O11-P-O13
153	AQ	202	PC1	C11-O13-P-O14
153	AQ	202	PC1	C1-O11-P-O14
153	AU	202	PC1	O21-C2-C3-O31
153	B1	401	PC1	C11-O13-P-O14
153	B1	401	PC1	C1-O11-P-O12
153	B1	401	PC1	C1-O11-P-O14
153	B1	401	PC1	C2-C1-O11-P
153	B1	401	PC1	O21-C2-C3-O31
153	B1	403	PC1	C11-O13-P-O14
153	B1	403	PC1	C11-O13-P-O11
153	BG	202	PC1	C11-O13-P-O12
153	BG	202	PC1	C12-C11-O13-P
153	BG	202	PC1	O13-C11-C12-N
153	BS	1301	PC1	C11-O13-P-O12
153	BS	1301	PC1	C11-O13-P-O11
153	BS	1301	PC1	C1-O11-P-O14
153	BS	1301	PC1	O22-C21-O21-C2
153	BS	1301	PC1	C22-C21-O21-C2
153	BS	1302	PC1	C11-O13-P-O12
153	BS	1302	PC1	C1-O11-P-O12
153	BS	1302	PC1	C1-O11-P-O13
153	BT	203	PC1	C11-O13-P-O14
153	BT	203	PC1	C1-O11-P-O12
153	BT	203	PC1	C1-O11-P-O14
153	BT	203	PC1	C1-O11-P-O13
153	BT	203	PC1	O22-C21-O21-C2
153	BT	203	PC1	C22-C21-O21-C2
153	CC	302	PC1	C1-O11-P-O12
153	CC	302	PC1	C1-O11-P-O14
153	CC	302	PC1	O21-C2-C3-O31
153	A	1201	PC1	C11-O13-P-O14
153	A	1201	PC1	C11-O13-P-O11
153	C	509	PC1	C11-O13-P-O12
153	C	509	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
153	C	509	PC1	C12-C11-O13-P
153	C	509	PC1	O13-C11-C12-N
153	C	509	PC1	O22-C21-O21-C2
153	C	509	PC1	C22-C21-O21-C2
153	C	510	PC1	C11-O13-P-O14
153	D	402	PC1	C11-O13-P-O14
153	E	303	PC1	C11-O13-P-O14
153	E	303	PC1	C22-C21-O21-C2
153	K	501	PC1	C11-O13-P-O14
153	K	501	PC1	C1-O11-P-O14
153	K	501	PC1	C1-O11-P-O13
153	K	501	PC1	O13-C11-C12-N
153	K	502	PC1	C11-O13-P-O12
153	K	502	PC1	C22-C21-O21-C2
153	c	503	PC1	O13-C11-C12-N
153	c	503	PC1	O22-C21-O21-C2
153	c	503	PC1	C22-C21-O21-C2
153	c	507	PC1	O13-C11-C12-N
153	c	508	PC1	C22-C21-O21-C2
153	d	801	PC1	C1-O11-P-O14
153	e	1101	PC1	C11-O13-P-O14
153	e	1101	PC1	C11-O13-P-O11
153	g	802	PC1	C11-O13-P-O12
153	g	802	PC1	C1-O11-P-O14
153	g	802	PC1	C22-C21-O21-C2
153	k	301	PC1	C11-O13-P-O11
153	k	301	PC1	O13-C11-C12-N
153	DA	707	PC1	C11-O13-P-O14
153	DA	708	PC1	C1-O11-P-O12
153	DB	702	PC1	O22-C21-O21-C2
153	DC	602	PC1	C11-O13-P-O14
153	DC	602	PC1	C1-O11-P-O12
153	DC	602	PC1	C1-O11-P-O14
153	DC	603	PC1	O13-C11-C12-N
153	DC	604	PC1	C11-O13-P-O12
153	DC	604	PC1	C11-O13-P-O14
153	DC	604	PC1	C11-O13-P-O11
153	DC	605	PC1	C22-C21-O21-C2
153	DC	608	PC1	C11-O13-P-O12
153	DC	608	PC1	O22-C21-O21-C2
153	DC	608	PC1	C22-C21-O21-C2
153	DI	303	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
153	DI	303	PC1	C1-O11-P-O14
153	DI	303	PC1	C1-O11-P-O13
153	DJ	306	PC1	C11-O13-P-O12
153	DJ	306	PC1	C11-O13-P-O14
153	DS	406	PC1	C11-O13-P-O14
153	DS	406	PC1	C11-O13-P-O11
153	DS	406	PC1	C1-O11-P-O12
153	DS	406	PC1	C1-O11-P-O14
153	DS	406	PC1	C12-C11-O13-P
153	DV	404	PC1	C11-O13-P-O12
153	DV	406	PC1	C11-O13-P-O12
153	DV	406	PC1	C11-O13-P-O14
153	DV	406	PC1	C1-O11-P-O12
153	DV	406	PC1	C1-O11-P-O14
153	DX	305	PC1	C22-C21-O21-C2
153	DX	308	PC1	O13-C11-C12-N
153	DY	302	PC1	O13-C11-C12-N
153	DY	302	PC1	O22-C21-O21-C2
153	EB	301	PC1	C11-O13-P-O11
153	EB	301	PC1	C1-O11-P-O14
153	EB	303	PC1	O13-C11-C12-N
153	EN	1203	PC1	C11-O13-P-O14
153	EN	1203	PC1	O21-C2-C3-O31
153	EO	201	PC1	C12-C11-O13-P
153	EO	201	PC1	O13-C11-C12-N
153	EO	204	PC1	C11-O13-P-O12
153	EO	204	PC1	C1-O11-P-O12
153	EO	205	PC1	C11-O13-P-O12
153	EO	205	PC1	C11-O13-P-O14
153	EO	205	PC1	C11-O13-P-O11
153	EO	205	PC1	C22-C21-O21-C2
153	EO	206	PC1	C11-O13-P-O12
153	EO	206	PC1	C11-O13-P-O14
153	EO	206	PC1	C11-O13-P-O11
153	EO	206	PC1	C22-C21-O21-C2
153	Da	706	PC1	C11-O13-P-O14
153	Da	706	PC1	O21-C2-C3-O31
153	Da	707	PC1	C1-O11-P-O12
153	Da	707	PC1	C1-O11-P-O14
153	Da	707	PC1	C1-O11-P-O13
153	Da	707	PC1	O13-C11-C12-N
153	Db	702	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
153	Db	702	PC1	C22-C21-O21-C2
153	Dc	602	PC1	C1-O11-P-O12
153	Dc	602	PC1	C1-O11-P-O14
153	Dc	602	PC1	C1-O11-P-O13
153	Dc	604	PC1	C1-O11-P-O12
153	Dc	604	PC1	C1-O11-P-O14
153	Dc	605	PC1	C11-O13-P-O14
153	Dc	605	PC1	C1-O11-P-O14
153	Dc	605	PC1	O22-C21-O21-C2
153	Dc	605	PC1	C22-C21-O21-C2
153	Dc	609	PC1	C11-O13-P-O12
153	Dc	609	PC1	O22-C21-O21-C2
153	Dc	609	PC1	C22-C21-O21-C2
153	Dg	203	PC1	C22-C21-O21-C2
153	Di	1104	PC1	C1-O11-P-O14
153	Dj	406	PC1	C11-O13-P-O12
153	Dj	406	PC1	C1-O11-P-O14
153	Dj	406	PC1	C1-O11-P-O13
153	Ds	407	PC1	O21-C2-C3-O31
153	Dv	405	PC1	C11-O13-P-O14
153	Dv	405	PC1	C11-O13-P-O11
153	Dv	405	PC1	C1-O11-P-O12
153	Dv	405	PC1	C1-O11-P-O14
153	Dv	405	PC1	C1-O11-P-O13
153	Dv	407	PC1	C11-O13-P-O12
153	Dv	407	PC1	C11-O13-P-O14
153	Dv	407	PC1	C1-O11-P-O12
153	Dx	1203	PC1	C1-O11-P-O12
153	Dx	1203	PC1	C1-O11-P-O14
153	Dx	1203	PC1	O13-C11-C12-N
153	Dx	1203	PC1	O11-C1-C2-O21
153	Dx	1205	PC1	C11-O13-P-O14
153	Dy	302	PC1	O13-C11-C12-N
153	Dy	302	PC1	O22-C21-O21-C2
153	Eb	301	PC1	C1-O11-P-O14
153	Eb	303	PC1	O13-C11-C12-N
153	Ef	501	PC1	C11-O13-P-O14
153	Ef	501	PC1	C1-O11-P-O12
153	El	904	PC1	C11-O13-P-O12
153	El	904	PC1	C1-O11-P-O12
153	Eo	201	PC1	C12-C11-O13-P
153	Eo	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
153	Eo	204	PC1	C11-O13-P-O12
153	Eo	204	PC1	C11-O13-P-O14
153	Eo	204	PC1	C22-C21-O21-C2
153	Eo	205	PC1	C11-O13-P-O12
153	Eo	205	PC1	C11-O13-P-O14
153	Eo	205	PC1	C22-C21-O21-C2
154	A1	401	NDP	C5B-O5B-PA-O1A
155	A2	401	3PE	O11-C1-C2-O21
155	A9	602	3PE	C1-O11-P-O12
155	AJ	502	3PE	C11-O13-P-O14
155	BA	301	3PE	C11-O13-P-O14
155	BP	201	3PE	C1-O11-P-O14
155	BT	201	3PE	C1-O11-P-O12
155	BT	201	3PE	C1-O11-P-O14
155	BT	201	3PE	C11-O13-P-O14
155	BT	201	3PE	C22-C21-O21-C2
155	CD	303	3PE	C1-O11-P-O12
155	CD	303	3PE	C1-O11-P-O14
155	C	513	3PE	C11-O13-P-O11
155	C	513	3PE	C11-O13-P-O12
155	C	513	3PE	C11-O13-P-O14
155	G	401	3PE	C1-O11-P-O14
155	G	401	3PE	C11-O13-P-O12
155	G	401	3PE	C11-O13-P-O14
155	DC	606	3PE	C1-O11-P-O12
155	DC	606	3PE	C1-O11-P-O14
155	DC	607	3PE	C11-O13-P-O14
155	DG	204	3PE	C11-O13-P-O12
155	DG	204	3PE	C11-O13-P-O14
155	DI	301	3PE	C1-O11-P-O14
155	DI	301	3PE	O21-C2-C3-O31
155	DJ	301	3PE	C1-O11-P-O12
155	DR	401	3PE	O21-C2-C3-O31
155	DS	402	3PE	C1-O11-P-O14
155	DS	402	3PE	C11-O13-P-O11
155	DX	302	3PE	C11-O13-P-O12
155	DX	302	3PE	C11-O13-P-O14
155	DX	302	3PE	O13-C11-C12-N
155	DX	303	3PE	C1-O11-P-O12
155	DX	303	3PE	C1-O11-P-O13
155	DX	303	3PE	C1-O11-P-O14
155	DX	303	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
155	DX	304	3PE	C1-O11-P-O12
155	DX	304	3PE	C1-O11-P-O13
155	DX	304	3PE	C1-O11-P-O14
155	DX	304	3PE	C11-O13-P-O12
155	DX	304	3PE	C11-O13-P-O14
155	EL	904	3PE	C1-O11-P-O12
155	EL	904	3PE	C1-O11-P-O14
155	EL	904	3PE	C11-O13-P-O14
155	EM	901	3PE	C1-O11-P-O12
155	EM	901	3PE	C1-O11-P-O13
155	EM	901	3PE	C1-O11-P-O14
155	EN	1204	3PE	C11-O13-P-O12
155	EO	203	3PE	C1-O11-P-O12
155	EO	203	3PE	C1-O11-P-O14
155	Da	708	3PE	C1-O11-P-O12
155	Da	708	3PE	C1-O11-P-O14
155	Da	708	3PE	C11-O13-P-O14
155	Dc	607	3PE	C1-O11-P-O14
155	Dc	607	3PE	C11-O13-P-O11
155	Dc	607	3PE	C11-O13-P-O12
155	Dc	607	3PE	C11-O13-P-O14
155	Dd	703	3PE	C1-O11-P-O12
155	Dd	703	3PE	C11-O13-P-O14
155	Dg	204	3PE	C1-O11-P-O13
155	Di	1102	3PE	C1-O11-P-O13
155	Di	1102	3PE	C1-O11-P-O14
155	Di	1102	3PE	O21-C2-C3-O31
155	Dr	401	3PE	C1-O11-P-O13
155	Dr	404	3PE	C1-O11-P-O13
155	Ds	403	3PE	C1-O11-P-O14
155	Ds	403	3PE	C11-O13-P-O11
155	Dx	1202	3PE	C1-O11-P-O12
155	Dx	1202	3PE	C1-O11-P-O14
155	Dx	1202	3PE	C11-O13-P-O14
155	Dx	1202	3PE	O21-C2-C3-O31
155	Dx	1202	3PE	C22-C21-O21-C2
155	Dx	1206	3PE	C1-O11-P-O12
155	Dx	1206	3PE	C1-O11-P-O13
155	Dx	1206	3PE	C1-O11-P-O14
155	Dx	1206	3PE	C11-O13-P-O11
155	Dx	1206	3PE	C11-O13-P-O12
155	Dx	1206	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
155	Dx	1206	3PE	O13-C11-C12-N
155	Dx	1207	3PE	C1-O11-P-O14
155	Dx	1207	3PE	C11-O13-P-O12
155	Dx	1207	3PE	C11-O13-P-O14
155	Dx	1208	3PE	C1-O11-P-O12
155	Dx	1208	3PE	C1-O11-P-O13
155	Dx	1208	3PE	C1-O11-P-O14
155	Dx	1208	3PE	C11-O13-P-O12
155	El	905	3PE	C1-O11-P-O12
155	El	905	3PE	C11-O13-P-O14
155	Em	901	3PE	C1-O11-P-O12
155	Em	901	3PE	C1-O11-P-O13
155	Em	901	3PE	C1-O11-P-O14
155	Eo	202	3PE	O22-C21-O21-C2
155	Eo	202	3PE	C22-C21-O21-C2
155	Eo	203	3PE	C1-O11-P-O12
155	Eo	203	3PE	C1-O11-P-O13
155	Eo	203	3PE	C1-O11-P-O14
156	AA	902	LPP	C6-O5-P1-O2
156	AA	902	LPP	C6-O5-P1-O3
156	AA	902	LPP	C6-O5-P1-O4
156	DA	710	LPP	C6-O5-P1-O2
156	DA	710	LPP	C6-O5-P1-O3
156	DA	710	LPP	C6-O5-P1-O4
156	DN	504	LPP	C6-O5-P1-O2
156	DN	504	LPP	C6-O5-P1-O3
156	DN	504	LPP	C6-O5-P1-O4
156	Dn	504	LPP	C6-O5-P1-O2
156	Dn	504	LPP	C6-O5-P1-O4
156	Dl	1101	LPP	C6-O5-P1-O2
156	Dl	1101	LPP	C6-O5-P1-O4
157	A8	401	ADP	PA-O3A-PB-O2B
161	AS	200	8Q1	C28-C29-C32-C34
161	AS	200	8Q1	C28-C29-C32-O33
161	AS	200	8Q1	C30-C29-C32-C34
161	AS	200	8Q1	C30-C29-C32-O33
161	AS	200	8Q1	C31-C29-C32-C34
161	AS	200	8Q1	C31-C29-C32-O33
161	AS	200	8Q1	C42-C43-S44-C1
164	CA	702	FAD	C5B-O5B-PA-O1A
164	CA	702	FAD	C5B-O5B-PA-O2A
164	CA	702	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
164	CA	702	FAD	N10-C1'-C2'-C3'
164	CA	702	FAD	C5'-O5'-P-O1P
164	CA	702	FAD	C5'-O5'-P-O2P
164	CA	702	FAD	C5'-O5'-P-O3P
166	CE	401	HEC	C2B-C3B-CAB-CBB
166	CE	401	HEC	C4B-C3B-CAB-CBB
167	CC	303	UQ8	C12-C11-C9-C10
167	CC	303	UQ8	C12-C11-C9-C8
167	C	511	UQ8	C30-C29-C31-C32
167	C	511	UQ8	C28-C29-C31-C32
167	C	511	UQ8	C5-C6-C7-C8
167	C	512	UQ8	C9-C11-C12-C13
167	c	510	UQ8	C1-C6-C7-C8
167	c	510	UQ8	C5-C6-C7-C8
167	EL	905	UQ8	C30-C29-C31-C32
167	EL	905	UQ8	C28-C29-C31-C32
167	EL	905	UQ8	C1-C6-C7-C8
167	EL	905	UQ8	C5-C6-C7-C8
167	Ds	404	UQ8	C35-C34-C36-C37
167	Ds	404	UQ8	C33-C34-C36-C37
167	El	906	UQ8	C30-C29-C31-C32
167	El	906	UQ8	C28-C29-C31-C32
167	El	906	UQ8	C1-C6-C7-C8
167	El	906	UQ8	C5-C6-C7-C8
167	En	1202	UQ8	C25-C24-C26-C27
167	En	1202	UQ8	C23-C24-C26-C27
173	ER	201	ATP	C5'-O5'-PA-O2A
150	A0	602	CDL	OA9-CA7-OA8-CA6
150	AF	402	CDL	OB9-CB7-OB8-CB6
150	BG	201	CDL	OB9-CB7-OB8-CB6
150	CD	302	CDL	OA9-CA7-OA8-CA6
150	H	1301	CDL	OB9-CB7-OB8-CB6
150	DD	704	CDL	OA9-CA7-OA8-CA6
150	DV	402	CDL	OA9-CA7-OA8-CA6
150	EI	401	CDL	OA9-CA7-OA8-CA6
150	EK	201	CDL	OB9-CB7-OB8-CB6
150	EL	901	CDL	OB9-CB7-OB8-CB6
150	Dd	704	CDL	OA9-CA7-OA8-CA6
150	Dj	402	CDL	OA9-CA7-OA8-CA6
150	Dj	403	CDL	OA9-CA7-OA8-CA6
150	Dj	405	CDL	OB9-CB7-OB8-CB6
150	Dn	506	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	Du	402	CDL	OB9-CB7-OB8-CB6
150	Dv	403	CDL	OA9-CA7-OA8-CA6
150	Ei	401	CDL	OA9-CA7-OA8-CA6
153	AA	906	PC1	O32-C31-O31-C3
153	D	402	PC1	O32-C31-O31-C3
153	c	508	PC1	O32-C31-O31-C3
153	e	1101	PC1	O32-C31-O31-C3
153	DJ	306	PC1	O32-C31-O31-C3
153	EB	301	PC1	O32-C31-O31-C3
153	Dj	406	PC1	O32-C31-O31-C3
155	BT	201	3PE	O32-C31-O31-C3
166	CE	401	HEC	C2C-C3C-CAC-CBC
166	CE	401	HEC	C4C-C3C-CAC-CBC
150	DG	202	CDL	CA4-CA6-OA8-CA7
150	A0	602	CDL	C31-CA7-OA8-CA6
150	EA	301	CDL	C31-CA7-OA8-CA6
150	Dj	402	CDL	C31-CA7-OA8-CA6
150	Ei	401	CDL	C31-CA7-OA8-CA6
153	c	508	PC1	C32-C31-O31-C3
153	e	1101	PC1	C32-C31-O31-C3
153	EB	301	PC1	C32-C31-O31-C3
155	BT	201	3PE	C32-C31-O31-C3
166	D	401	HEC	C2B-C3B-CAB-CBB
166	D	401	HEC	C4B-C3B-CAB-CBB
166	d	802	HEC	C2B-C3B-CAB-CBB
166	d	802	HEC	C4B-C3B-CAB-CBB
150	A1	402	CDL	OB9-CB7-OB8-CB6
150	B0	102	CDL	OA9-CA7-OA8-CA6
150	B1	402	CDL	OB9-CB7-OB8-CB6
150	CG	301	CDL	OB9-CB7-OB8-CB6
150	C	506	CDL	OA9-CA7-OA8-CA6
150	H	1302	CDL	OA9-CA7-OA8-CA6
150	c	509	CDL	OB9-CB7-OB8-CB6
150	g	801	CDL	OA9-CA7-OA8-CA6
150	g	801	CDL	OB9-CB7-OB8-CB6
150	DD	704	CDL	OB9-CB7-OB8-CB6
150	DG	201	CDL	OB9-CB7-OB8-CB6
150	DH	202	CDL	OB9-CB7-OB8-CB6
150	DJ	302	CDL	OB9-CB7-OB8-CB6
150	DJ	305	CDL	OB9-CB7-OB8-CB6
150	DJ	307	CDL	OA9-CA7-OA8-CA6
150	DN	502	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
150	DN	506	CDL	OA9-CA7-OA8-CA6
150	DS	401	CDL	OB9-CB7-OB8-CB6
150	DS	404	CDL	OA9-CA7-OA8-CA6
150	DS	405	CDL	OB9-CB7-OB8-CB6
150	DU	402	CDL	OB9-CB7-OB8-CB6
150	DV	403	CDL	OA9-CA7-OA8-CA6
150	DX	301	CDL	OA9-CA7-OA8-CA6
150	DX	306	CDL	OA9-CA7-OA8-CA6
150	ED	604	CDL	OA9-CA7-OA8-CA6
150	ED	604	CDL	OB9-CB7-OB8-CB6
150	EH	1601	CDL	OB9-CB7-OB8-CB6
150	EO	202	CDL	OB9-CB7-OB8-CB6
150	ES	1101	CDL	OA9-CA7-OA8-CA6
150	Dd	704	CDL	OB9-CB7-OB8-CB6
150	Dg	201	CDL	OB9-CB7-OB8-CB6
150	Dh	202	CDL	OB9-CB7-OB8-CB6
150	Dj	401	CDL	OB9-CB7-OB8-CB6
150	Dj	404	CDL	OB9-CB7-OB8-CB6
150	Dj	407	CDL	OA9-CA7-OA8-CA6
150	Dn	501	CDL	OB9-CB7-OB8-CB6
150	Dn	503	CDL	OB9-CB7-OB8-CB6
150	Dq	1401	CDL	OA9-CA7-OA8-CA6
150	Ds	406	CDL	OB9-CB7-OB8-CB6
150	Ea	502	CDL	OA9-CA7-OA8-CA6
150	El	902	CDL	OB9-CB7-OB8-CB6
150	Ep	701	CDL	OB9-CB7-OB8-CB6
150	Eu	101	CDL	OA9-CA7-OA8-CA6
153	AA	904	PC1	O32-C31-O31-C3
153	AA	907	PC1	O32-C31-O31-C3
153	B1	403	PC1	O32-C31-O31-C3
153	c	503	PC1	O32-C31-O31-C3
153	Eb	301	PC1	O32-C31-O31-C3
153	Ef	501	PC1	O32-C31-O31-C3
155	BA	301	3PE	O32-C31-O31-C3
155	CK	101	3PE	O32-C31-O31-C3
155	CD	303	3PE	O32-C31-O31-C3
155	C	513	3PE	O32-C31-O31-C3
155	Da	708	3PE	O32-C31-O31-C3
155	Dr	401	3PE	O32-C31-O31-C3
166	D	401	HEC	C4C-C3C-CAC-CBC
166	d	802	HEC	C4C-C3C-CAC-CBC
166	D	401	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
166	d	802	HEC	C2C-C3C-CAC-CBC
150	A0	601	CDL	OA7-CA5-OA6-CA4
150	A0	601	CDL	OB7-CB5-OB6-CB4
150	A0	602	CDL	OB7-CB5-OB6-CB4
150	AA	908	CDL	OA7-CA5-OA6-CA4
150	AA	908	CDL	OB7-CB5-OB6-CB4
150	AM	301	CDL	OA7-CA5-OA6-CA4
150	AP	301	CDL	OA7-CA5-OA6-CA4
150	AP	301	CDL	OB7-CB5-OB6-CB4
150	B0	101	CDL	OA7-CA5-OA6-CA4
150	BC	301	CDL	OA7-CA5-OA6-CA4
150	BE	201	CDL	OA7-CA5-OA6-CA4
150	BG	201	CDL	OA7-CA5-OA6-CA4
150	BL	301	CDL	OA7-CA5-OA6-CA4
150	BT	202	CDL	OA7-CA5-OA6-CA4
150	BT	202	CDL	OB7-CB5-OB6-CB4
150	BV	201	CDL	OB7-CB5-OB6-CB4
150	BY	201	CDL	OB7-CB5-OB6-CB4
150	CG	302	CDL	OA7-CA5-OA6-CA4
150	CD	302	CDL	OA7-CA5-OA6-CA4
150	C	505	CDL	OA7-CA5-OA6-CA4
150	C	506	CDL	OA7-CA5-OA6-CA4
150	C	506	CDL	OB7-CB5-OB6-CB4
150	H	1301	CDL	OA7-CA5-OA6-CA4
150	c	506	CDL	OA7-CA5-OA6-CA4
150	g	801	CDL	OB7-CB5-OB6-CB4
150	h	501	CDL	OB7-CB5-OB6-CB4
150	DA	709	CDL	OA7-CA5-OA6-CA4
150	DD	703	CDL	OA7-CA5-OA6-CA4
150	DD	705	CDL	OB7-CB5-OB6-CB4
150	DG	201	CDL	OB7-CB5-OB6-CB4
150	DI	302	CDL	OA7-CA5-OA6-CA4
150	DI	302	CDL	OB7-CB5-OB6-CB4
150	DJ	302	CDL	OB7-CB5-OB6-CB4
150	DJ	304	CDL	OA7-CA5-OA6-CA4
150	DJ	305	CDL	OB7-CB5-OB6-CB4
150	DM	502	CDL	OA7-CA5-OA6-CA4
150	DM	502	CDL	OB7-CB5-OB6-CB4
150	DN	506	CDL	OB7-CB5-OB6-CB4
150	DN	507	CDL	OA7-CA5-OA6-CA4
150	DO	501	CDL	OA7-CA5-OA6-CA4
150	DO	501	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
150	DS	404	CDL	OA7-CA5-OA6-CA4
150	DU	402	CDL	OA7-CA5-OA6-CA4
150	DV	401	CDL	OB7-CB5-OB6-CB4
150	DV	403	CDL	OB7-CB5-OB6-CB4
150	DY	301	CDL	OA7-CA5-OA6-CA4
150	DY	301	CDL	OB7-CB5-OB6-CB4
150	EB	302	CDL	OA7-CA5-OA6-CA4
150	ED	604	CDL	OA7-CA5-OA6-CA4
150	EH	1601	CDL	OB7-CB5-OB6-CB4
150	EL	902	CDL	OA7-CA5-OA6-CA4
150	EL	903	CDL	OB7-CB5-OB6-CB4
150	EN	1202	CDL	OA7-CA5-OA6-CA4
150	EN	1202	CDL	OB7-CB5-OB6-CB4
150	EO	202	CDL	OB7-CB5-OB6-CB4
150	Dd	702	CDL	OA7-CA5-OA6-CA4
150	Dg	201	CDL	OB7-CB5-OB6-CB4
150	Di	1103	CDL	OA7-CA5-OA6-CA4
150	Dj	402	CDL	OA7-CA5-OA6-CA4
150	Dj	404	CDL	OB7-CB5-OB6-CB4
150	Dj	407	CDL	OB7-CB5-OB6-CB4
150	Dm	501	CDL	OB7-CB5-OB6-CB4
150	Dm	502	CDL	OA7-CA5-OA6-CA4
150	Dm	502	CDL	OB7-CB5-OB6-CB4
150	Do	501	CDL	OB7-CB5-OB6-CB4
150	Dq	1401	CDL	OB7-CB5-OB6-CB4
150	Du	401	CDL	OB7-CB5-OB6-CB4
150	Dv	403	CDL	OB7-CB5-OB6-CB4
150	Dx	1204	CDL	OB7-CB5-OB6-CB4
150	Dy	301	CDL	OB7-CB5-OB6-CB4
150	Ea	502	CDL	OA7-CA5-OA6-CA4
150	Eb	302	CDL	OA7-CA5-OA6-CA4
150	Ed	204	CDL	OA7-CA5-OA6-CA4
150	Eg	101	CDL	OA7-CA5-OA6-CA4
150	Ei	401	CDL	OA7-CA5-OA6-CA4
150	El	901	CDL	OB7-CB5-OB6-CB4
150	El	902	CDL	OB7-CB5-OB6-CB4
150	El	903	CDL	OB7-CB5-OB6-CB4
153	A2	402	PC1	O22-C21-O21-C2
153	AA	904	PC1	O22-C21-O21-C2
153	AM	302	PC1	O22-C21-O21-C2
153	A	1201	PC1	O22-C21-O21-C2
153	E	303	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
153	K	502	PC1	O22-C21-O21-C2
153	c	508	PC1	O22-C21-O21-C2
153	DC	605	PC1	O22-C21-O21-C2
153	DG	203	PC1	O22-C21-O21-C2
153	DX	305	PC1	O22-C21-O21-C2
153	EO	205	PC1	O22-C21-O21-C2
153	EO	206	PC1	O22-C21-O21-C2
153	Db	702	PC1	O22-C21-O21-C2
153	Dg	203	PC1	O22-C21-O21-C2
153	Eo	204	PC1	O22-C21-O21-C2
153	Eo	205	PC1	O22-C21-O21-C2
155	BT	201	3PE	O22-C21-O21-C2
155	Dx	1202	3PE	O22-C21-O21-C2
150	Ds	405	CDL	OA9-CA7-OA8-CA6
150	Dg	202	CDL	CA4-CA6-OA8-CA7
150	AF	402	CDL	C71-CB7-OB8-CB6
150	B0	102	CDL	C31-CA7-OA8-CA6
150	BG	201	CDL	C71-CB7-OB8-CB6
150	CD	302	CDL	C31-CA7-OA8-CA6
150	H	1301	CDL	C71-CB7-OB8-CB6
150	H	1302	CDL	C31-CA7-OA8-CA6
150	DD	704	CDL	C31-CA7-OA8-CA6
150	DG	201	CDL	C71-CB7-OB8-CB6
150	DJ	302	CDL	C71-CB7-OB8-CB6
150	DJ	305	CDL	C71-CB7-OB8-CB6
150	DN	506	CDL	C31-CA7-OA8-CA6
150	DQ	1504	CDL	C71-CB7-OB8-CB6
150	DS	405	CDL	C71-CB7-OB8-CB6
150	DV	402	CDL	C31-CA7-OA8-CA6
150	DX	301	CDL	C31-CA7-OA8-CA6
150	ED	604	CDL	C71-CB7-OB8-CB6
150	EI	401	CDL	C31-CA7-OA8-CA6
150	EK	201	CDL	C71-CB7-OB8-CB6
150	EL	901	CDL	C71-CB7-OB8-CB6
150	EL	903	CDL	C71-CB7-OB8-CB6
150	ES	1101	CDL	C31-CA7-OA8-CA6
150	Da	709	CDL	C71-CB7-OB8-CB6
150	Dd	704	CDL	C31-CA7-OA8-CA6
150	Dd	704	CDL	C71-CB7-OB8-CB6
150	Dg	201	CDL	C71-CB7-OB8-CB6
150	Dj	403	CDL	C31-CA7-OA8-CA6
150	Dj	405	CDL	C71-CB7-OB8-CB6

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

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Mol	Chain	Res	Type	Atoms
150	Dm	502	CDL	C51-CB5-OB6-CB4
150	Dq	1401	CDL	C11-CA5-OA6-CA4
150	Du	401	CDL	C51-CB5-OB6-CB4
150	Dv	401	CDL	C11-CA5-OA6-CA4
150	Eb	302	CDL	C11-CA5-OA6-CA4
150	Eb	302	CDL	C51-CB5-OB6-CB4
150	El	902	CDL	C51-CB5-OB6-CB4
153	A1	403	PC1	C22-C21-O21-C2
153	AL	303	PC1	C22-C21-O21-C2
153	AM	302	PC1	C22-C21-O21-C2
153	A	1201	PC1	C22-C21-O21-C2
153	DB	702	PC1	C22-C21-O21-C2
153	DG	203	PC1	C22-C21-O21-C2
153	DY	302	PC1	C22-C21-O21-C2
153	Dy	302	PC1	C22-C21-O21-C2
150	Dx	1201	CDL	OB9-CB7-OB8-CB6
150	DV	401	CDL	OA9-CA7-OA8-CA6
150	Dg	201	CDL	OA9-CA7-OA8-CA6
150	Di	1101	CDL	OB9-CB7-OB8-CB6
150	A1	402	CDL	C31-CA7-OA8-CA6
150	A1	402	CDL	C71-CB7-OB8-CB6
150	B1	402	CDL	C71-CB7-OB8-CB6
150	BT	204	CDL	C31-CA7-OA8-CA6
150	CG	301	CDL	C71-CB7-OB8-CB6
150	CJ	201	CDL	C31-CA7-OA8-CA6
150	C	503	CDL	C31-CA7-OA8-CA6
150	C	506	CDL	C31-CA7-OA8-CA6
150	c	509	CDL	C71-CB7-OB8-CB6
150	g	801	CDL	C31-CA7-OA8-CA6
150	g	801	CDL	C71-CB7-OB8-CB6
150	DD	704	CDL	C71-CB7-OB8-CB6
150	DH	202	CDL	C31-CA7-OA8-CA6
150	DH	202	CDL	C71-CB7-OB8-CB6
150	DJ	307	CDL	C31-CA7-OA8-CA6
150	DN	502	CDL	C71-CB7-OB8-CB6
150	DS	401	CDL	C71-CB7-OB8-CB6
150	DS	404	CDL	C31-CA7-OA8-CA6
150	DU	402	CDL	C71-CB7-OB8-CB6
150	DV	403	CDL	C31-CA7-OA8-CA6
150	DX	306	CDL	C31-CA7-OA8-CA6
150	EA	301	CDL	C71-CB7-OB8-CB6
150	ED	604	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	EH	1601	CDL	C71-CB7-OB8-CB6
150	EN	1201	CDL	C71-CB7-OB8-CB6
150	EO	202	CDL	C71-CB7-OB8-CB6
150	Dh	202	CDL	C31-CA7-OA8-CA6
150	Dh	202	CDL	C71-CB7-OB8-CB6
150	Dj	401	CDL	C71-CB7-OB8-CB6
150	Dj	404	CDL	C71-CB7-OB8-CB6
150	Dj	407	CDL	C31-CA7-OA8-CA6
150	Dn	503	CDL	C71-CB7-OB8-CB6
150	Dr	402	CDL	C31-CA7-OA8-CA6
150	Ds	405	CDL	C31-CA7-OA8-CA6
150	Dv	401	CDL	C31-CA7-OA8-CA6
150	Dx	1204	CDL	C31-CA7-OA8-CA6
150	Eg	101	CDL	C31-CA7-OA8-CA6
150	Ek	201	CDL	C71-CB7-OB8-CB6
150	El	902	CDL	C71-CB7-OB8-CB6
150	Ep	701	CDL	C71-CB7-OB8-CB6
150	Eu	101	CDL	C31-CA7-OA8-CA6
153	A9	601	PC1	C32-C31-O31-C3
153	AA	907	PC1	C32-C31-O31-C3
153	c	503	PC1	C32-C31-O31-C3
153	c	507	PC1	C32-C31-O31-C3
153	DC	602	PC1	C32-C31-O31-C3
153	DC	604	PC1	C32-C31-O31-C3
153	Dc	604	PC1	C32-C31-O31-C3
153	Ds	407	PC1	C32-C31-O31-C3
153	Eb	301	PC1	C32-C31-O31-C3
153	Ef	501	PC1	C32-C31-O31-C3
155	CK	101	3PE	C32-C31-O31-C3
155	CD	303	3PE	C32-C31-O31-C3
155	Dr	401	3PE	C32-C31-O31-C3
150	AA	901	CDL	OB7-CB5-OB6-CB4
150	c	501	CDL	OA7-CA5-OA6-CA4
150	DS	404	CDL	OB7-CB5-OB6-CB4
150	EH	1601	CDL	OA7-CA5-OA6-CA4
150	EO	202	CDL	OA7-CA5-OA6-CA4
150	Ds	401	CDL	OB7-CB5-OB6-CB4
150	Ds	405	CDL	OB7-CB5-OB6-CB4
150	Dy	301	CDL	OA7-CA5-OA6-CA4
150	Eh	1601	CDL	OA7-CA5-OA6-CA4
153	D	402	PC1	O22-C21-O21-C2
153	g	802	PC1	O22-C21-O21-C2

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

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Mol	Chain	Res	Type	Atoms
150	DJ	307	CDL	O1-C1-CB2-OB2
150	DM	502	CDL	O1-C1-CB2-OB2
150	DN	507	CDL	O1-C1-CA2-OA2
150	DR	403	CDL	O1-C1-CA2-OA2
150	DU	403	CDL	O1-C1-CB2-OB2
150	DX	306	CDL	O1-C1-CA2-OA2
150	EB	302	CDL	O1-C1-CA2-OA2
150	ED	605	CDL	O1-C1-CB2-OB2
150	EH	1601	CDL	O1-C1-CB2-OB2
150	EK	201	CDL	O1-C1-CA2-OA2
150	Da	709	CDL	O1-C1-CA2-OA2
150	Dd	702	CDL	O1-C1-CA2-OA2
150	Dd	706	CDL	O1-C1-CB2-OB2
150	Dh	202	CDL	O1-C1-CA2-OA2
150	Dj	402	CDL	O1-C1-CA2-OA2
150	Dj	403	CDL	O1-C1-CB2-OB2
150	Dm	501	CDL	O1-C1-CB2-OB2
150	Dn	503	CDL	O1-C1-CA2-OA2
150	Dr	403	CDL	O1-C1-CA2-OA2
150	Du	403	CDL	O1-C1-CA2-OA2
150	Dv	401	CDL	O1-C1-CB2-OB2
150	Dv	402	CDL	O1-C1-CB2-OB2
150	Dv	403	CDL	O1-C1-CA2-OA2
150	Dx	1204	CDL	O1-C1-CA2-OA2
150	Ed	204	CDL	O1-C1-CB2-OB2
150	Ed	205	CDL	O1-C1-CB2-OB2
150	Ei	401	CDL	O1-C1-CA2-OA2
150	El	902	CDL	O1-C1-CA2-OA2
150	Eu	101	CDL	O1-C1-CA2-OA2
150	A0	601	CDL	C71-CB7-OB8-CB6
150	B0	102	CDL	C71-CB7-OB8-CB6
150	B1	402	CDL	C31-CA7-OA8-CA6
150	CD	301	CDL	C31-CA7-OA8-CA6
150	C	505	CDL	C31-CA7-OA8-CA6
150	DA	709	CDL	C31-CA7-OA8-CA6
150	DC	601	CDL	C71-CB7-OB8-CB6
150	ED	601	CDL	C31-CA7-OA8-CA6
150	EL	902	CDL	C71-CB7-OB8-CB6
150	Dc	601	CDL	C71-CB7-OB8-CB6
150	Dg	201	CDL	C31-CA7-OA8-CA6
150	Dh	201	CDL	C71-CB7-OB8-CB6
150	Dq	1401	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
150	Dx	1201	CDL	C71-CB7-OB8-CB6
150	El	901	CDL	C71-CB7-OB8-CB6
150	Ep	701	CDL	C31-CA7-OA8-CA6
153	DV	405	PC1	C32-C31-O31-C3
153	DX	308	PC1	C32-C31-O31-C3
153	EN	1203	PC1	C32-C31-O31-C3
153	Dc	602	PC1	C32-C31-O31-C3
150	A0	601	CDL	OB9-CB7-OB8-CB6
150	BT	204	CDL	OA9-CA7-OA8-CA6
150	EL	902	CDL	OB9-CB7-OB8-CB6
150	Da	709	CDL	OB9-CB7-OB8-CB6
150	Dc	601	CDL	OB9-CB7-OB8-CB6
150	Eh	1601	CDL	OB9-CB7-OB8-CB6
153	DC	602	PC1	O32-C31-O31-C3
150	AC	802	CDL	C11-CA5-OA6-CA4
150	C	503	CDL	C11-CA5-OA6-CA4
150	c	502	CDL	C11-CA5-OA6-CA4
150	DM	501	CDL	C11-CA5-OA6-CA4
150	DQ	1501	CDL	C11-CA5-OA6-CA4
150	DQ	1502	CDL	C11-CA5-OA6-CA4
150	DR	403	CDL	C11-CA5-OA6-CA4
150	DU	401	CDL	C11-CA5-OA6-CA4
150	DU	401	CDL	C51-CB5-OB6-CB4
150	DU	404	CDL	C11-CA5-OA6-CA4
150	EK	201	CDL	C11-CA5-OA6-CA4
150	EK	201	CDL	C51-CB5-OB6-CB4
150	ES	1101	CDL	C11-CA5-OA6-CA4
150	Dj	403	CDL	C11-CA5-OA6-CA4
150	Dj	407	CDL	C11-CA5-OA6-CA4
150	Dm	501	CDL	C11-CA5-OA6-CA4
150	Dn	503	CDL	C11-CA5-OA6-CA4
150	Do	501	CDL	C11-CA5-OA6-CA4
150	Dq	1402	CDL	C51-CB5-OB6-CB4
150	Dr	403	CDL	C11-CA5-OA6-CA4
150	Dv	401	CDL	C51-CB5-OB6-CB4
150	Eu	101	CDL	C11-CA5-OA6-CA4
153	AX	401	PC1	C22-C21-O21-C2
153	D	402	PC1	C22-C21-O21-C2
153	k	301	PC1	C22-C21-O21-C2
153	Dv	405	PC1	C22-C21-O21-C2
153	Dx	1209	PC1	C22-C21-O21-C2
155	DG	204	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
150	Dd	705	CDL	CA5-C11-C12-C13
153	A9	601	PC1	O32-C31-O31-C3
151	A0	603	UDP	C3'-C4'-C5'-O5'
164	CA	702	FAD	O4B-C4B-C5B-O5B
164	CA	702	FAD	C3B-C4B-C5B-O5B
150	CC	304	CDL	C71-CB7-OB8-CB6
150	DA	706	CDL	C71-CB7-OB8-CB6
150	DQ	1504	CDL	C31-CA7-OA8-CA6
150	DV	401	CDL	C31-CA7-OA8-CA6
150	Di	1101	CDL	C71-CB7-OB8-CB6
150	Dv	402	CDL	C31-CA7-OA8-CA6
155	EO	203	3PE	C32-C31-O31-C3
150	DM	501	CDL	OA7-CA5-OA6-CA4
150	DQ	1501	CDL	OA7-CA5-OA6-CA4
150	DU	401	CDL	OB7-CB5-OB6-CB4
150	EK	201	CDL	OA7-CA5-OA6-CA4
150	ES	1101	CDL	OA7-CA5-OA6-CA4
150	Dj	407	CDL	OA7-CA5-OA6-CA4
150	Do	501	CDL	OA7-CA5-OA6-CA4
150	Dr	403	CDL	OA7-CA5-OA6-CA4
150	Dv	401	CDL	OB7-CB5-OB6-CB4
150	DU	401	CDL	C1-CA2-OA2-PA1
150	Dg	201	CDL	C1-CA2-OA2-PA1
150	Di	1101	CDL	CB4-CB3-OB5-PB2
150	Dj	405	CDL	C1-CB2-OB2-PB2
150	Ea	501	CDL	C1-CB2-OB2-PB2
153	A0	605	PC1	C2-C1-O11-P
153	AU	201	PC1	C2-C1-O11-P
155	CD	303	3PE	C2-C1-O11-P
150	Dh	201	CDL	OB9-CB7-OB8-CB6
150	Dh	202	CDL	OA9-CA7-OA8-CA6
150	Dr	402	CDL	OA9-CA7-OA8-CA6
150	Dx	1204	CDL	OA9-CA7-OA8-CA6
153	DV	405	PC1	O32-C31-O31-C3
153	DX	308	PC1	O32-C31-O31-C3
153	Dc	604	PC1	O32-C31-O31-C3
167	C	511	UQ8	C40-C39-C41-C42
167	C	512	UQ8	C20-C19-C21-C22
167	DS	403	UQ8	C35-C34-C36-C37
167	EN	1205	UQ8	C25-C24-C26-C27
167	C	511	UQ8	C38-C39-C41-C42
167	C	512	UQ8	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
167	EN	1205	UQ8	C23-C24-C26-C27
150	B0	102	CDL	OB9-CB7-OB8-CB6
150	C	505	CDL	OA9-CA7-OA8-CA6
150	DA	709	CDL	OA9-CA7-OA8-CA6
150	DC	601	CDL	OB9-CB7-OB8-CB6
150	EN	1201	CDL	OB9-CB7-OB8-CB6
150	Dq	1401	CDL	OB9-CB7-OB8-CB6
150	Eg	101	CDL	OA9-CA7-OA8-CA6
167	C	511	UQ8	C34-C36-C37-C38
167	C	512	UQ8	C24-C26-C27-C28
167	ED	603	UQ8	C39-C41-C42-C43
167	En	1202	UQ8	C34-C36-C37-C38
167	En	1202	UQ8	C19-C21-C22-C23
169	DA	703	HEA	C15-C16-C17-C18
169	Da	703	HEA	C19-C20-C21-C22
150	B0	101	CDL	C71-CB7-OB8-CB6
150	C	505	CDL	C71-CB7-OB8-CB6
150	c	501	CDL	C31-CA7-OA8-CA6
150	DN	502	CDL	C31-CA7-OA8-CA6
150	DZ	501	CDL	C71-CB7-OB8-CB6
150	Dn	501	CDL	C31-CA7-OA8-CA6
153	CC	302	PC1	C32-C31-O31-C3
153	K	502	PC1	C32-C31-O31-C3
155	G	401	3PE	C32-C31-O31-C3
155	DJ	301	3PE	C32-C31-O31-C3
150	B1	402	CDL	OA9-CA7-OA8-CA6
150	ED	601	CDL	OA9-CA7-OA8-CA6
150	Ep	701	CDL	OA9-CA7-OA8-CA6
150	Dj	405	CDL	C51-CB5-OB6-CB4
150	Dr	402	CDL	C51-CB5-OB6-CB4
150	Ds	401	CDL	C11-CA5-OA6-CA4
150	El	902	CDL	C11-CA5-OA6-CA4
153	Da	707	PC1	C22-C21-O21-C2
155	A2	401	3PE	C22-C21-O21-C2
150	B0	101	CDL	CA2-C1-CB2-OB2
150	BC	301	CDL	CA2-C1-CB2-OB2
150	C	504	CDL	CA2-C1-CB2-OB2
150	C	507	CDL	CA2-C1-CB2-OB2
150	DA	709	CDL	CA2-C1-CB2-OB2
150	DD	706	CDL	CA2-C1-CB2-OB2
150	DG	201	CDL	CB2-C1-CA2-OA2
150	DJ	302	CDL	CB2-C1-CA2-OA2

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

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Mol	Chain	Res	Type	Atoms
150	EN	1202	CDL	C31-CA7-OA8-CA6
150	Da	709	CDL	C31-CA7-OA8-CA6
150	Dc	608	CDL	C71-CB7-OB8-CB6
150	Dg	202	CDL	C31-CA7-OA8-CA6
150	Dn	503	CDL	C31-CA7-OA8-CA6
150	Do	501	CDL	C31-CA7-OA8-CA6
150	Ea	501	CDL	C71-CB7-OB8-CB6
150	El	903	CDL	C71-CB7-OB8-CB6
153	AH	301	PC1	C32-C31-O31-C3
153	AQ	202	PC1	C32-C31-O31-C3
153	DA	707	PC1	C32-C31-O31-C3
153	DC	608	PC1	C32-C31-O31-C3
153	DQ	1503	PC1	C32-C31-O31-C3
153	Da	706	PC1	C32-C31-O31-C3
153	Dq	1404	PC1	C32-C31-O31-C3
153	Dv	406	PC1	C32-C31-O31-C3
153	Dx	1205	PC1	C32-C31-O31-C3
155	DC	607	3PE	C32-C31-O31-C3
155	DS	402	3PE	C32-C31-O31-C3
155	Dc	607	3PE	C32-C31-O31-C3
155	Dr	404	3PE	C32-C31-O31-C3
155	Ds	403	3PE	C32-C31-O31-C3
154	A1	401	NDP	O4D-C1D-N1N-C6N
153	DA	708	PC1	C3C-C3D-C3E-C3F
150	Dh	201	CDL	C38-C39-C40-C41
150	Dj	404	CDL	C77-C78-C79-C80
150	BL	301	CDL	OB5-CB3-CB4-OB6
150	DV	403	CDL	OB5-CB3-CB4-OB6
150	EB	302	CDL	OB5-CB3-CB4-OB6
153	DQ	1503	PC1	O11-C1-C2-O21
150	Dq	1402	CDL	C19-C20-C21-C22
153	d	801	PC1	C3E-C3F-C3G-C3H
153	Da	707	PC1	C3C-C3D-C3E-C3F
150	A1	402	CDL	O1-C1-CA2-OA2
150	BT	202	CDL	O1-C1-CB2-OB2
150	BT	204	CDL	O1-C1-CA2-OA2
150	c	506	CDL	O1-C1-CB2-OB2
150	g	801	CDL	O1-C1-CB2-OB2
150	DH	201	CDL	O1-C1-CA2-OA2
150	DQ	1501	CDL	O1-C1-CA2-OA2
150	DQ	1502	CDL	O1-C1-CA2-OA2
150	DX	301	CDL	O1-C1-CA2-OA2

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

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Mol	Chain	Res	Type	Atoms
155	Dg	204	3PE	C22-C21-O21-C2
150	Dg	201	CDL	C23-C24-C25-C26
150	h	501	CDL	CA5-C11-C12-C13
150	DS	404	CDL	CA5-C11-C12-C13
150	Ei	401	CDL	CA5-C11-C12-C13
150	c	506	CDL	OA9-CA7-OA8-CA6
150	DO	501	CDL	OA9-CA7-OA8-CA6
150	El	903	CDL	OB9-CB7-OB8-CB6
153	Da	706	PC1	O32-C31-O31-C3
155	DC	607	3PE	O32-C31-O31-C3
155	Dr	404	3PE	O32-C31-O31-C3
150	AA	908	CDL	C61-C62-C63-C64
150	DQ	1501	CDL	C19-C20-C21-C22
153	AA	905	PC1	C32-C31-O31-C3
155	DG	205	3PE	C32-C31-O31-C3
155	Em	901	3PE	C32-C31-O31-C3
150	B0	101	CDL	CA5-C11-C12-C13
150	BC	302	CDL	CB5-C51-C52-C53
150	DN	503	CDL	CA5-C11-C12-C13
150	DU	404	CDL	CA5-C11-C12-C13
150	Dc	608	CDL	CA5-C11-C12-C13
150	Dg	202	CDL	CB7-C71-C72-C73
150	Dh	202	CDL	CA5-C11-C12-C13
150	Dm	501	CDL	CA5-C11-C12-C13
150	Du	403	CDL	CA5-C11-C12-C13
150	El	901	CDL	CA5-C11-C12-C13
150	DR	402	CDL	OA9-CA7-OA8-CA6
150	CG	302	CDL	OA9-CA7-OA8-CA6
155	Ds	403	3PE	O32-C31-O31-C3
150	A0	602	CDL	CA5-C11-C12-C13
150	AF	401	CDL	CA5-C11-C12-C13
150	B0	102	CDL	CA5-C11-C12-C13
150	C	507	CDL	CB5-C51-C52-C53
150	E	301	CDL	CA5-C11-C12-C13
150	H	1302	CDL	CA5-C11-C12-C13
150	DG	202	CDL	CA5-C11-C12-C13
150	DH	202	CDL	CA5-C11-C12-C13
150	DQ	1504	CDL	CB5-C51-C52-C53
150	DZ	501	CDL	CA5-C11-C12-C13
150	ED	601	CDL	CA5-C11-C12-C13
150	EH	1601	CDL	CA5-C11-C12-C13
150	Dc	601	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
150	Dn	503	CDL	CA5-C11-C12-C13
150	Ds	405	CDL	CA5-C11-C12-C13
150	El	902	CDL	CA5-C11-C12-C13
155	EM	901	3PE	C21-C22-C23-C24
156	AA	902	LPP	C11-C12-C13-C14
151	A0	603	UDP	O4'-C4'-C5'-O5'
150	c	502	CDL	C31-CA7-OA8-CA6
150	DH	201	CDL	C71-CB7-OB8-CB6
150	DY	301	CDL	C31-CA7-OA8-CA6
150	Dd	706	CDL	C71-CB7-OB8-CB6
150	Dn	502	CDL	C31-CA7-OA8-CA6
153	A1	403	PC1	C32-C31-O31-C3
155	Dc	607	3PE	C2-C3-O31-C31
150	EO	202	CDL	C77-C78-C79-C80
150	C	503	CDL	OA7-CA5-OA6-CA4
150	c	502	CDL	OA7-CA5-OA6-CA4
150	DU	404	CDL	OA7-CA5-OA6-CA4
150	Dj	405	CDL	OB7-CB5-OB6-CB4
150	Dq	1402	CDL	OB7-CB5-OB6-CB4
150	AC	802	CDL	CA4-CA3-OA5-PA1
155	DG	205	3PE	C2-C1-O11-P
150	DZ	501	CDL	CB7-C71-C72-C73
150	EL	901	CDL	CA5-C11-C12-C13
150	Dq	1402	CDL	CA5-C11-C12-C13
150	Dy	301	CDL	CA5-C11-C12-C13
153	EO	201	PC1	C31-C32-C33-C34
156	A6	301	LPP	C11-C12-C13-C14
150	DJ	307	CDL	C11-CA5-OA6-CA4
150	Dc	601	CDL	C51-CB5-OB6-CB4
153	B1	401	PC1	C22-C21-O21-C2
150	AM	301	CDL	OA9-CA7-OA8-CA6
150	DR	402	CDL	OB9-CB7-OB8-CB6
150	Dc	608	CDL	OB9-CB7-OB8-CB6
150	Dn	503	CDL	OA9-CA7-OA8-CA6
150	Ea	501	CDL	OB9-CB7-OB8-CB6
153	AH	301	PC1	O32-C31-O31-C3
153	DA	707	PC1	O32-C31-O31-C3
153	DC	608	PC1	O32-C31-O31-C3
153	Dq	1404	PC1	O32-C31-O31-C3
153	Dx	1205	PC1	O32-C31-O31-C3
150	ED	601	CDL	OB9-CB7-OB8-CB6
150	Da	709	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	Do	501	CDL	OA9-CA7-OA8-CA6
153	AQ	202	PC1	O32-C31-O31-C3
153	DQ	1503	PC1	O32-C31-O31-C3
153	Dv	406	PC1	O32-C31-O31-C3
167	EN	1205	UQ8	C34-C36-C37-C38
167	EN	1205	UQ8	C19-C21-C22-C23
167	Ed	202	UQ8	C39-C41-C42-C43
167	El	906	UQ8	C14-C16-C17-C18
150	AA	908	CDL	CA5-C11-C12-C13
150	AC	801	CDL	CA5-C11-C12-C13
151	A0	603	UDP	O4'-C1'-N1-C2
150	C	504	CDL	O1-C1-CB2-OB2
150	C	505	CDL	O1-C1-CB2-OB2
150	H	1302	CDL	O1-C1-CB2-OB2
150	DD	705	CDL	O1-C1-CA2-OA2
150	DJ	302	CDL	O1-C1-CA2-OA2
150	DV	402	CDL	O1-C1-CB2-OB2
150	DY	301	CDL	O1-C1-CA2-OA2
150	EL	902	CDL	O1-C1-CB2-OB2
150	Dd	704	CDL	O1-C1-CB2-OB2
150	Dg	201	CDL	O1-C1-CA2-OA2
150	Ds	402	CDL	O1-C1-CB2-OB2
150	El	902	CDL	O1-C1-CB2-OB2
150	CG	302	CDL	OB7-CB5-OB6-CB4
150	Dr	402	CDL	OB7-CB5-OB6-CB4
150	Ds	401	CDL	OA7-CA5-OA6-CA4
150	Ds	405	CDL	OA7-CA5-OA6-CA4
150	El	902	CDL	OA7-CA5-OA6-CA4
153	Da	707	PC1	O22-C21-O21-C2
155	Ds	403	3PE	C2-C3-O31-C31
153	DI	303	PC1	C32-C31-O31-C3
155	Di	1102	3PE	C32-C31-O31-C3
150	ES	1101	CDL	C35-C36-C37-C38
150	B0	101	CDL	OB9-CB7-OB8-CB6
150	C	505	CDL	OB9-CB7-OB8-CB6
150	c	501	CDL	OA9-CA7-OA8-CA6
150	c	501	CDL	OB9-CB7-OB8-CB6
150	DD	706	CDL	OB9-CB7-OB8-CB6
150	Dg	202	CDL	OA9-CA7-OA8-CA6
150	Dn	501	CDL	OA9-CA7-OA8-CA6
153	A1	403	PC1	O32-C31-O31-C3
153	AA	905	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
153	CC	302	PC1	O32-C31-O31-C3
155	Dc	607	3PE	O32-C31-O31-C3
155	Em	901	3PE	O32-C31-O31-C3
150	DU	401	CDL	CA5-C11-C12-C13
150	DS	405	CDL	C38-C39-C40-C41
150	Dj	402	CDL	C54-C55-C56-C57
155	DG	205	3PE	O32-C31-O31-C3
150	c	501	CDL	C51-CB5-OB6-CB4
150	DD	705	CDL	C11-CA5-OA6-CA4
150	DH	202	CDL	C11-CA5-OA6-CA4
150	DJ	303	CDL	C11-CA5-OA6-CA4
150	DN	502	CDL	C11-CA5-OA6-CA4
150	Dq	1403	CDL	C11-CA5-OA6-CA4
155	Ds	408	3PE	C22-C21-O21-C2
155	Eo	203	3PE	C22-C21-O21-C2
150	AC	801	CDL	C34-C35-C36-C37
150	A0	601	CDL	CB3-OB5-PB2-OB2
150	A0	602	CDL	CA3-OA5-PA1-OA2
150	A1	402	CDL	CB2-OB2-PB2-OB5
150	AA	901	CDL	CA3-OA5-PA1-OA2
150	AA	901	CDL	CB2-OB2-PB2-OB5
150	AC	801	CDL	CB3-OB5-PB2-OB2
150	AC	802	CDL	CB2-OB2-PB2-OB5
150	AC	802	CDL	CB3-OB5-PB2-OB2
150	AM	301	CDL	CA2-OA2-PA1-OA5
150	AM	301	CDL	CB3-OB5-PB2-OB2
150	AP	301	CDL	CB2-OB2-PB2-OB5
150	B0	101	CDL	CA2-OA2-PA1-OA5
150	B0	101	CDL	CB2-OB2-PB2-OB5
150	B1	402	CDL	CA3-OA5-PA1-OA2
150	B1	402	CDL	CB2-OB2-PB2-OB5
150	BC	301	CDL	CA2-OA2-PA1-OA5
150	BC	302	CDL	CB2-OB2-PB2-OB5
150	BC	302	CDL	CB3-OB5-PB2-OB2
150	BE	201	CDL	CA2-OA2-PA1-OA5
150	BG	201	CDL	CA2-OA2-PA1-OA5
150	BT	202	CDL	CB2-OB2-PB2-OB5
150	BT	202	CDL	CB3-OB5-PB2-OB2
150	CG	301	CDL	CB2-OB2-PB2-OB5
150	CG	302	CDL	CA2-OA2-PA1-OA5
150	CG	302	CDL	CB3-OB5-PB2-OB2
150	CC	304	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
150	CC	305	CDL	CA3-OA5-PA1-OA2
150	CD	301	CDL	CA3-OA5-PA1-OA2
150	CD	301	CDL	CB2-OB2-PB2-OB5
150	CD	302	CDL	CB2-OB2-PB2-OB5
150	C	503	CDL	CA2-OA2-PA1-OA5
150	C	503	CDL	CA3-OA5-PA1-OA2
150	C	503	CDL	CB2-OB2-PB2-OB5
150	C	504	CDL	CA2-OA2-PA1-OA5
150	C	504	CDL	CA3-OA5-PA1-OA2
150	C	504	CDL	CB2-OB2-PB2-OB5
150	C	505	CDL	CA2-OA2-PA1-OA5
150	C	506	CDL	CB3-OB5-PB2-OB2
150	C	507	CDL	CA3-OA5-PA1-OA2
150	E	301	CDL	CA2-OA2-PA1-OA5
150	E	301	CDL	CB2-OB2-PB2-OB5
150	H	1301	CDL	CB2-OB2-PB2-OB5
150	H	1301	CDL	CB3-OB5-PB2-OB2
150	H	1302	CDL	CA2-OA2-PA1-OA5
150	H	1302	CDL	CA3-OA5-PA1-OA2
150	H	1302	CDL	CB3-OB5-PB2-OB2
150	c	501	CDL	CB2-OB2-PB2-OB5
150	h	501	CDL	CA2-OA2-PA1-OA5
150	h	501	CDL	CB2-OB2-PB2-OB5
150	DA	709	CDL	CA3-OA5-PA1-OA2
150	DC	601	CDL	CA3-OA5-PA1-OA2
150	DC	601	CDL	CB2-OB2-PB2-OB5
150	DC	601	CDL	CB3-OB5-PB2-OB2
150	DD	705	CDL	CA2-OA2-PA1-OA5
150	DD	706	CDL	CA2-OA2-PA1-OA5
150	DD	706	CDL	CA3-OA5-PA1-OA2
150	DD	706	CDL	CB3-OB5-PB2-OB2
150	DH	202	CDL	CB2-OB2-PB2-OB5
150	DI	302	CDL	CB2-OB2-PB2-OB5
150	DJ	302	CDL	CB3-OB5-PB2-OB2
150	DJ	305	CDL	CB2-OB2-PB2-OB5
150	DJ	307	CDL	CB2-OB2-PB2-OB5
150	DJ	307	CDL	CB3-OB5-PB2-OB2
150	DM	501	CDL	CB2-OB2-PB2-OB5
150	DM	502	CDL	CA2-OA2-PA1-OA5
150	DM	502	CDL	CB2-OB2-PB2-OB5
150	DN	502	CDL	CA3-OA5-PA1-OA2
150	DN	502	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
150	DN	503	CDL	CB2-OB2-PB2-OB5
150	DN	506	CDL	CB3-OB5-PB2-OB2
150	DN	507	CDL	CA2-OA2-PA1-OA5
150	DN	507	CDL	CA3-OA5-PA1-OA2
150	DQ	1501	CDL	CA3-OA5-PA1-OA2
150	DQ	1504	CDL	CA2-OA2-PA1-OA5
150	DR	402	CDL	CA3-OA5-PA1-OA2
150	DR	403	CDL	CA2-OA2-PA1-OA5
150	DS	405	CDL	CA2-OA2-PA1-OA5
150	DS	405	CDL	CB3-OB5-PB2-OB2
150	DU	401	CDL	CA2-OA2-PA1-OA5
150	DU	401	CDL	CB2-OB2-PB2-OB5
150	DU	402	CDL	CB3-OB5-PB2-OB2
150	DU	403	CDL	CA2-OA2-PA1-OA5
150	DU	403	CDL	CB3-OB5-PB2-OB2
150	DU	404	CDL	CB2-OB2-PB2-OB5
150	DV	401	CDL	CA3-OA5-PA1-OA2
150	DV	402	CDL	CA3-OA5-PA1-OA2
150	DV	403	CDL	CA2-OA2-PA1-OA5
150	DV	403	CDL	CB2-OB2-PB2-OB5
150	DX	306	CDL	CA2-OA2-PA1-OA5
150	DX	306	CDL	CB3-OB5-PB2-OB2
150	DX	307	CDL	CA2-OA2-PA1-OA5
150	DY	301	CDL	CA3-OA5-PA1-OA2
150	DZ	501	CDL	CA2-OA2-PA1-OA5
150	EA	301	CDL	CB2-OB2-PB2-OB5
150	EB	302	CDL	CA3-OA5-PA1-OA2
150	EB	302	CDL	CB2-OB2-PB2-OB5
150	ED	604	CDL	CA3-OA5-PA1-OA2
150	ED	604	CDL	CB3-OB5-PB2-OB2
150	ED	605	CDL	CB3-OB5-PB2-OB2
150	EH	1601	CDL	CA2-OA2-PA1-OA5
150	EH	1601	CDL	CB3-OB5-PB2-OB2
150	EI	401	CDL	CB3-OB5-PB2-OB2
150	EL	902	CDL	CB2-OB2-PB2-OB5
150	EL	903	CDL	CB2-OB2-PB2-OB5
150	EL	903	CDL	CB3-OB5-PB2-OB2
150	EN	1201	CDL	CA2-OA2-PA1-OA5
150	ES	1101	CDL	CA3-OA5-PA1-OA2
150	Da	709	CDL	CB3-OB5-PB2-OB2
150	Dc	601	CDL	CA3-OA5-PA1-OA2
150	Dc	601	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
150	Dc	601	CDL	CB3-OB5-PB2-OB2
150	Dd	702	CDL	CA3-OA5-PA1-OA2
150	Dd	704	CDL	CB2-OB2-PB2-OB5
150	Dg	201	CDL	CA2-OA2-PA1-OA5
150	Dg	202	CDL	CA2-OA2-PA1-OA5
150	Dh	202	CDL	CA3-OA5-PA1-OA2
150	Dh	202	CDL	CB2-OB2-PB2-OB5
150	Di	1101	CDL	CB3-OB5-PB2-OB2
150	Dj	401	CDL	CA2-OA2-PA1-OA5
150	Dj	401	CDL	CB3-OB5-PB2-OB2
150	Dj	402	CDL	CA3-OA5-PA1-OA2
150	Dj	403	CDL	CA2-OA2-PA1-OA5
150	Dj	404	CDL	CA2-OA2-PA1-OA5
150	Dj	407	CDL	CA2-OA2-PA1-OA5
150	Dj	407	CDL	CB2-OB2-PB2-OB5
150	Dm	501	CDL	CA3-OA5-PA1-OA2
150	Dm	501	CDL	CB2-OB2-PB2-OB5
150	Dm	502	CDL	CA3-OA5-PA1-OA2
150	Dn	502	CDL	CB3-OB5-PB2-OB2
150	Dn	506	CDL	CB3-OB5-PB2-OB2
150	Do	501	CDL	CA3-OA5-PA1-OA2
150	Dq	1401	CDL	CA2-OA2-PA1-OA5
150	Dq	1402	CDL	CA3-OA5-PA1-OA2
150	Dq	1403	CDL	CA2-OA2-PA1-OA5
150	Dq	1403	CDL	CA3-OA5-PA1-OA2
150	Dr	402	CDL	CA3-OA5-PA1-OA2
150	Dr	402	CDL	CB2-OB2-PB2-OB5
150	Dr	403	CDL	CA2-OA2-PA1-OA5
150	Ds	401	CDL	CA3-OA5-PA1-OA2
150	Ds	406	CDL	CA2-OA2-PA1-OA5
150	Ds	406	CDL	CB3-OB5-PB2-OB2
150	Du	401	CDL	CA2-OA2-PA1-OA5
150	Du	401	CDL	CB3-OB5-PB2-OB2
150	Dv	401	CDL	CB2-OB2-PB2-OB5
150	Dv	403	CDL	CA2-OA2-PA1-OA5
150	Dv	403	CDL	CA3-OA5-PA1-OA2
150	Dv	403	CDL	CB2-OB2-PB2-OB5
150	Dx	1201	CDL	CB2-OB2-PB2-OB5
150	Dx	1201	CDL	CB3-OB5-PB2-OB2
150	Dx	1204	CDL	CA2-OA2-PA1-OA5
150	Dx	1204	CDL	CA3-OA5-PA1-OA2
150	Dx	1204	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
150	Ea	502	CDL	CA2-OA2-PA1-OA5
150	Ea	502	CDL	CB2-OB2-PB2-OB5
150	Eb	302	CDL	CB2-OB2-PB2-OB5
150	Eb	302	CDL	CB3-OB5-PB2-OB2
150	Ed	204	CDL	CA3-OA5-PA1-OA2
150	Ed	204	CDL	CB3-OB5-PB2-OB2
150	Ed	205	CDL	CA3-OA5-PA1-OA2
150	Eg	101	CDL	CB3-OB5-PB2-OB2
150	Eh	1601	CDL	CB3-OB5-PB2-OB2
150	Ei	401	CDL	CA2-OA2-PA1-OA5
150	Ei	401	CDL	CB3-OB5-PB2-OB2
150	El	903	CDL	CA2-OA2-PA1-OA5
150	El	903	CDL	CB2-OB2-PB2-OB5
150	Ep	701	CDL	CA3-OA5-PA1-OA2
150	Eu	101	CDL	CB3-OB5-PB2-OB2
153	A9	603	PC1	C11-O13-P-O11
153	AA	903	PC1	C1-O11-P-O13
153	AA	905	PC1	C11-O13-P-O11
153	AA	906	PC1	C11-O13-P-O11
153	AA	907	PC1	C11-O13-P-O11
153	AQ	202	PC1	C1-O11-P-O13
153	AU	201	PC1	C11-O13-P-O11
153	AU	201	PC1	C1-O11-P-O13
153	AX	401	PC1	C1-O11-P-O13
153	B1	401	PC1	C11-O13-P-O11
153	B1	401	PC1	C1-O11-P-O13
153	B1	403	PC1	C1-O11-P-O13
153	BG	202	PC1	C11-O13-P-O11
153	BS	1301	PC1	C1-O11-P-O13
153	BS	1302	PC1	C11-O13-P-O11
153	CC	302	PC1	C1-O11-P-O13
153	C	508	PC1	C11-O13-P-O11
153	C	508	PC1	C1-O11-P-O13
153	C	509	PC1	C11-O13-P-O11
153	C	510	PC1	C11-O13-P-O11
153	K	501	PC1	C11-O13-P-O11
153	K	502	PC1	C11-O13-P-O11
153	c	508	PC1	C11-O13-P-O11
153	d	801	PC1	C1-O11-P-O13
153	g	802	PC1	C11-O13-P-O11
153	DA	708	PC1	C1-O11-P-O13
153	DB	702	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
153	DC	602	PC1	C11-O13-P-O11
153	DC	602	PC1	C1-O11-P-O13
153	DC	603	PC1	C11-O13-P-O11
153	DC	604	PC1	C1-O11-P-O13
153	DC	605	PC1	C1-O11-P-O13
153	DC	608	PC1	C11-O13-P-O11
153	DI	303	PC1	C11-O13-P-O11
153	DJ	306	PC1	C11-O13-P-O11
153	DJ	306	PC1	C1-O11-P-O13
153	DQ	1503	PC1	C11-O13-P-O11
153	DS	406	PC1	C1-O11-P-O13
153	DV	404	PC1	C11-O13-P-O11
153	DV	405	PC1	C11-O13-P-O11
153	DV	406	PC1	C11-O13-P-O11
153	DV	406	PC1	C1-O11-P-O13
153	DX	305	PC1	C11-O13-P-O11
153	DX	308	PC1	C1-O11-P-O13
153	EB	301	PC1	C1-O11-P-O13
153	EO	201	PC1	C11-O13-P-O11
153	EO	204	PC1	C11-O13-P-O11
153	EO	204	PC1	C1-O11-P-O13
153	Da	706	PC1	C11-O13-P-O11
153	Db	702	PC1	C11-O13-P-O11
153	Dc	602	PC1	C11-O13-P-O11
153	Dc	603	PC1	C11-O13-P-O11
153	Dc	604	PC1	C11-O13-P-O11
153	Dc	604	PC1	C1-O11-P-O13
153	Dc	605	PC1	C1-O11-P-O13
153	Dc	609	PC1	C11-O13-P-O11
153	Di	1104	PC1	C11-O13-P-O11
153	Di	1104	PC1	C1-O11-P-O13
153	Dj	406	PC1	C11-O13-P-O11
153	Dq	1404	PC1	C11-O13-P-O11
153	Dv	406	PC1	C11-O13-P-O11
153	Dv	407	PC1	C11-O13-P-O11
153	Dv	407	PC1	C1-O11-P-O13
153	Dx	1203	PC1	C1-O11-P-O13
153	Ef	501	PC1	C1-O11-P-O13
153	El	904	PC1	C11-O13-P-O11
153	El	904	PC1	C1-O11-P-O13
153	Eo	201	PC1	C11-O13-P-O11
153	Eo	204	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
153	Eo	205	PC1	C11-O13-P-O11
155	A9	602	3PE	C1-O11-P-O13
155	AJ	502	3PE	C11-O13-P-O11
155	BA	301	3PE	C11-O13-P-O11
155	BT	201	3PE	C1-O11-P-O13
155	CD	303	3PE	C1-O11-P-O13
155	G	401	3PE	C11-O13-P-O11
155	DC	606	3PE	C1-O11-P-O13
155	DC	607	3PE	C11-O13-P-O11
155	DG	204	3PE	C1-O11-P-O13
155	DG	204	3PE	C11-O13-P-O11
155	DI	301	3PE	C1-O11-P-O13
155	DJ	301	3PE	C1-O11-P-O13
155	DS	402	3PE	C1-O11-P-O13
155	DX	302	3PE	C11-O13-P-O11
155	DX	303	3PE	C11-O13-P-O11
155	DX	304	3PE	C11-O13-P-O11
155	EL	904	3PE	C1-O11-P-O13
155	EL	904	3PE	C11-O13-P-O11
155	EN	1204	3PE	C11-O13-P-O11
155	EO	203	3PE	C1-O11-P-O13
155	Da	708	3PE	C1-O11-P-O13
155	Dd	703	3PE	C1-O11-P-O13
155	Ds	403	3PE	C1-O11-P-O13
155	Dx	1202	3PE	C1-O11-P-O13
155	Dx	1202	3PE	C11-O13-P-O11
155	Dx	1207	3PE	C1-O11-P-O13
155	Dx	1207	3PE	C11-O13-P-O11
155	El	905	3PE	C1-O11-P-O13
155	El	905	3PE	C11-O13-P-O11
150	Dm	502	CDL	CB7-C71-C72-C73
155	EN	1204	3PE	C21-C22-C23-C24
150	C	507	CDL	C71-CB7-OB8-CB6
150	DV	403	CDL	C71-CB7-OB8-CB6
150	Dx	1204	CDL	C71-CB7-OB8-CB6
150	En	1201	CDL	C71-CB7-OB8-CB6
153	Di	1104	PC1	C32-C31-O31-C3
155	A2	401	3PE	C32-C31-O31-C3
150	BV	201	CDL	CA5-C11-C12-C13
150	DM	502	CDL	CB7-C71-C72-C73
150	Dx	1201	CDL	CA5-C11-C12-C13
150	A0	601	CDL	CA2-C1-CB2-OB2

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

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Mol	Chain	Res	Type	Atoms
153	A9	603	PC1	C32-C31-O31-C3
153	d	801	PC1	C32-C31-O31-C3
153	Dc	609	PC1	C32-C31-O31-C3
150	C	506	CDL	C20-C21-C22-C23
150	Dd	704	CDL	C38-C39-C40-C41
150	Ds	406	CDL	C38-C39-C40-C41
155	BA	301	3PE	C24-C25-C26-C27
150	BG	201	CDL	CA5-C11-C12-C13
150	c	502	CDL	C57-C58-C59-C60
150	c	509	CDL	C12-C13-C14-C15
150	DX	301	CDL	C14-C15-C16-C17
150	Ds	405	CDL	C77-C78-C79-C80
150	BG	201	CDL	C51-CB5-OB6-CB4
150	C	505	CDL	C51-CB5-OB6-CB4
150	DN	503	CDL	C11-CA5-OA6-CA4
150	DQ	1501	CDL	C51-CB5-OB6-CB4
150	DQ	1504	CDL	C51-CB5-OB6-CB4
150	DZ	501	CDL	C51-CB5-OB6-CB4
150	EL	902	CDL	C51-CB5-OB6-CB4
150	EL	903	CDL	C11-CA5-OA6-CA4
150	Dg	202	CDL	C11-CA5-OA6-CA4
150	Ds	402	CDL	C11-CA5-OA6-CA4
150	Du	403	CDL	C11-CA5-OA6-CA4
150	Dv	402	CDL	C11-CA5-OA6-CA4
150	El	903	CDL	C11-CA5-OA6-CA4
153	A0	605	PC1	C22-C21-O21-C2
153	A9	601	PC1	C22-C21-O21-C2
153	DA	708	PC1	C22-C21-O21-C2
150	AA	908	CDL	C73-C74-C75-C76
150	B1	402	CDL	C80-C81-C82-C83
150	BE	201	CDL	C11-C12-C13-C14
150	C	505	CDL	C23-C24-C25-C26
150	DA	709	CDL	C17-C18-C19-C20
150	DG	201	CDL	C14-C15-C16-C17
150	DG	202	CDL	C80-C81-C82-C83
150	DJ	307	CDL	C54-C55-C56-C57
150	DN	507	CDL	C16-C17-C18-C19
150	DO	501	CDL	C76-C77-C78-C79
150	DQ	1502	CDL	C51-C52-C53-C54
150	DU	402	CDL	C61-C62-C63-C64
150	Dd	704	CDL	C22-C23-C24-C25
150	Dj	403	CDL	C17-C18-C19-C20

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

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Mol	Chain	Res	Type	Atoms
153	A0	605	PC1	O22-C21-O21-C2
150	C	504	CDL	CA7-C31-C32-C33
150	A0	601	CDL	C13-C14-C15-C16
150	A1	402	CDL	C40-C41-C42-C43
150	H	1301	CDL	C33-C34-C35-C36
150	DU	404	CDL	C11-C12-C13-C14
150	ED	605	CDL	C16-C17-C18-C19
150	EL	901	CDL	C37-C38-C39-C40
150	Da	709	CDL	C76-C77-C78-C79
150	Dd	705	CDL	C13-C14-C15-C16
150	Dn	501	CDL	C73-C74-C75-C76
150	Dn	506	CDL	C37-C38-C39-C40
150	Dq	1403	CDL	C51-C52-C53-C54
150	Dv	402	CDL	C54-C55-C56-C57
150	Ea	501	CDL	C42-C43-C44-C45
150	Ea	501	CDL	C77-C78-C79-C80
150	Eg	101	CDL	C16-C17-C18-C19
150	El	903	CDL	C74-C75-C76-C77
153	B1	403	PC1	C36-C37-C38-C39
153	EO	206	PC1	C3E-C3F-C3G-C3H
153	Eb	301	PC1	C27-C28-C29-C2A
150	CD	301	CDL	C1-CB2-OB2-PB2
150	CD	302	CDL	C1-CB2-OB2-PB2
150	DD	705	CDL	CA4-CA3-OA5-PA1
150	EK	201	CDL	C1-CA2-OA2-PA1
155	BP	201	3PE	C2-C1-O11-P
150	B1	402	CDL	C56-C57-C58-C59
150	BC	302	CDL	C34-C35-C36-C37
150	DJ	302	CDL	C35-C36-C37-C38
150	Dj	403	CDL	C55-C56-C57-C58
150	Dj	407	CDL	C55-C56-C57-C58
150	Ds	406	CDL	C11-C12-C13-C14
150	Ed	205	CDL	C51-C52-C53-C54
150	El	901	CDL	C80-C81-C82-C83
153	AJ	501	PC1	C3C-C3D-C3E-C3F
155	Dd	703	3PE	C25-C26-C27-C28
150	A0	601	CDL	O1-C1-CB2-OB2
150	DJ	307	CDL	O1-C1-CA2-OA2
150	Dg	202	CDL	O1-C1-CA2-OA2
150	Dg	202	CDL	O1-C1-CB2-OB2
150	Dj	407	CDL	O1-C1-CA2-OA2
150	Dq	1403	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
150	Ds	401	CDL	O1-C1-CA2-OA2
150	Du	401	CDL	O1-C1-CB2-OB2
150	DG	201	CDL	C12-C13-C14-C15
150	Dg	201	CDL	C11-C12-C13-C14
150	Dq	1401	CDL	C13-C14-C15-C16
150	Dv	401	CDL	C54-C55-C56-C57
153	c	507	PC1	C24-C25-C26-C27
153	Dc	605	PC1	C29-C2A-C2B-C2C
150	C	503	CDL	CA5-C11-C12-C13
150	DH	201	CDL	CA5-C11-C12-C13
150	DV	401	CDL	CA5-C11-C12-C13
150	EN	1201	CDL	CA5-C11-C12-C13
153	Eo	201	PC1	C31-C32-C33-C34
150	EL	901	CDL	OB6-CB4-CB6-OB8
150	BC	302	CDL	C31-CA7-OA8-CA6
150	DJ	303	CDL	C71-CB7-OB8-CB6
150	DQ	1502	CDL	C71-CB7-OB8-CB6
153	AC	804	PC1	C32-C31-O31-C3
150	AA	908	CDL	C41-C42-C43-C44
150	C	503	CDL	C81-C82-C83-C84
150	DA	709	CDL	C16-C17-C18-C19
150	DI	302	CDL	C13-C14-C15-C16
150	DQ	1504	CDL	C11-C12-C13-C14
150	DS	404	CDL	C14-C15-C16-C17
150	DU	404	CDL	C33-C34-C35-C36
150	DV	401	CDL	C54-C55-C56-C57
150	DX	301	CDL	C11-C12-C13-C14
150	EL	903	CDL	C63-C64-C65-C66
150	Dg	201	CDL	C58-C59-C60-C61
150	Dj	407	CDL	C13-C14-C15-C16
150	Ds	406	CDL	C14-C15-C16-C17
150	Dx	1204	CDL	C19-C20-C21-C22
150	Eh	1601	CDL	C61-C62-C63-C64
150	El	902	CDL	C39-C40-C41-C42
153	k	301	PC1	C3D-C3E-C3F-C3G
153	DJ	306	PC1	C3D-C3E-C3F-C3G
153	Eo	204	PC1	C2C-C2D-C2E-C2F
155	BA	301	3PE	C2D-C2E-C2F-C2G
150	Dc	601	CDL	OA9-CA7-OA8-CA6
150	Dd	706	CDL	OB9-CB7-OB8-CB6
153	Dc	609	PC1	O32-C31-O31-C3
167	El	906	UQ8	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
150	B0	101	CDL	C52-C53-C54-C55
150	C	505	CDL	C21-C22-C23-C24
150	c	506	CDL	C36-C37-C38-C39
150	DJ	304	CDL	C62-C63-C64-C65
150	DN	502	CDL	C73-C74-C75-C76
150	DU	404	CDL	C80-C81-C82-C83
150	EL	901	CDL	C39-C40-C41-C42
150	Dj	403	CDL	C39-C40-C41-C42
150	Dq	1402	CDL	C12-C13-C14-C15
150	Dr	402	CDL	C51-C52-C53-C54
150	Dr	402	CDL	C57-C58-C59-C60
150	Ds	402	CDL	C61-C62-C63-C64
150	Ds	405	CDL	C14-C15-C16-C17
150	Dx	1201	CDL	C14-C15-C16-C17
150	Ed	205	CDL	C16-C17-C18-C19
153	Eo	205	PC1	C3E-C3F-C3G-C3H
156	AA	902	LPP	C17-C18-C19-C20
150	Dj	402	CDL	CA4-CA6-OA8-CA7
150	Dj	407	CDL	CA5-C11-C12-C13
150	Dv	401	CDL	CA5-C11-C12-C13
150	Ea	501	CDL	CB7-C71-C72-C73
150	CD	301	CDL	C61-C62-C63-C64
150	C	503	CDL	C41-C42-C43-C44
150	C	504	CDL	C53-C54-C55-C56
150	C	504	CDL	C55-C56-C57-C58
150	DA	706	CDL	C41-C42-C43-C44
150	DH	202	CDL	C21-C22-C23-C24
150	DI	302	CDL	C42-C43-C44-C45
150	DJ	303	CDL	C40-C41-C42-C43
150	DM	501	CDL	C55-C56-C57-C58
150	EA	301	CDL	C11-C12-C13-C14
150	EK	201	CDL	C40-C41-C42-C43
150	ES	1101	CDL	C13-C14-C15-C16
150	Di	1101	CDL	C41-C42-C43-C44
150	Di	1103	CDL	C71-C72-C73-C74
150	Dj	402	CDL	C62-C63-C64-C65
150	Du	402	CDL	C37-C38-C39-C40
150	Ek	201	CDL	C40-C41-C42-C43
155	CD	303	3PE	C27-C28-C29-C2A
150	c	502	CDL	OA9-CA7-OA8-CA6
150	DY	301	CDL	OA9-CA7-OA8-CA6
150	Dn	502	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	Dx	1204	CDL	OB9-CB7-OB8-CB6
155	A2	401	3PE	O32-C31-O31-C3
150	B0	102	CDL	C13-C14-C15-C16
150	BG	201	CDL	C34-C35-C36-C37
150	DM	502	CDL	C14-C15-C16-C17
150	DO	501	CDL	C32-C33-C34-C35
150	DU	402	CDL	C21-C22-C23-C24
150	DX	301	CDL	C19-C20-C21-C22
150	EN	1202	CDL	C57-C58-C59-C60
150	El	903	CDL	C20-C21-C22-C23
153	Dy	302	PC1	C2E-C2F-C2G-C2H
150	BG	201	CDL	OB7-CB5-OB6-CB4
150	DC	601	CDL	OB7-CB5-OB6-CB4
150	EL	902	CDL	OB7-CB5-OB6-CB4
150	Dh	201	CDL	OA7-CA5-OA6-CA4
150	Ea	501	CDL	OB7-CB5-OB6-CB4
153	A9	601	PC1	O22-C21-O21-C2
153	DA	708	PC1	O22-C21-O21-C2
150	AC	801	CDL	C51-CB5-OB6-CB4
150	DA	706	CDL	C51-CB5-OB6-CB4
150	DC	601	CDL	C51-CB5-OB6-CB4
150	Dc	601	CDL	C11-CA5-OA6-CA4
150	Dh	201	CDL	C11-CA5-OA6-CA4
150	Dn	501	CDL	C11-CA5-OA6-CA4
150	Dn	503	CDL	C51-CB5-OB6-CB4
150	Ea	501	CDL	C51-CB5-OB6-CB4
153	BG	202	PC1	C22-C21-O21-C2
150	CG	302	CDL	C20-C21-C22-C23
150	c	506	CDL	C56-C57-C58-C59
150	DC	601	CDL	C40-C41-C42-C43
150	DD	706	CDL	C75-C76-C77-C78
150	DN	503	CDL	C13-C14-C15-C16
150	ED	601	CDL	C17-C18-C19-C20
150	EK	201	CDL	C74-C75-C76-C77
150	EL	903	CDL	C81-C82-C83-C84
150	EO	202	CDL	C11-C12-C13-C14
150	ES	1101	CDL	C17-C18-C19-C20
150	Dd	705	CDL	C36-C37-C38-C39
150	Di	1103	CDL	C74-C75-C76-C77
150	Eb	302	CDL	C20-C21-C22-C23
153	AA	904	PC1	C3D-C3E-C3F-C3G
153	DI	303	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
153	EO	206	PC1	C3B-C3C-C3D-C3E
153	Dc	602	PC1	C3C-C3D-C3E-C3F
153	Dj	406	PC1	C3D-C3E-C3F-C3G
150	EA	301	CDL	CB7-C71-C72-C73
150	Dy	301	CDL	CB5-C51-C52-C53
150	AA	908	CDL	C59-C60-C61-C62
150	BY	201	CDL	C56-C57-C58-C59
150	CD	301	CDL	C72-C73-C74-C75
150	CD	302	CDL	C39-C40-C41-C42
150	CD	302	CDL	C61-C62-C63-C64
150	g	801	CDL	C11-C12-C13-C14
150	DD	704	CDL	C75-C76-C77-C78
150	DJ	302	CDL	C11-C12-C13-C14
150	DR	403	CDL	C11-C12-C13-C14
150	DR	403	CDL	C13-C14-C15-C16
150	DS	404	CDL	C75-C76-C77-C78
150	DV	403	CDL	C79-C80-C81-C82
150	DX	301	CDL	C38-C39-C40-C41
150	DX	306	CDL	C72-C73-C74-C75
150	EN	1201	CDL	C77-C78-C79-C80
150	Da	709	CDL	C14-C15-C16-C17
150	Di	1103	CDL	C37-C38-C39-C40
150	Di	1103	CDL	C42-C43-C44-C45
150	Di	1103	CDL	C77-C78-C79-C80
150	Dj	404	CDL	C11-C12-C13-C14
150	Dj	404	CDL	C16-C17-C18-C19
150	Ds	402	CDL	C74-C75-C76-C77
150	Ds	405	CDL	C20-C21-C22-C23
150	Du	402	CDL	C34-C35-C36-C37
150	Du	403	CDL	C80-C81-C82-C83
150	Dv	401	CDL	C80-C81-C82-C83
150	Dx	1201	CDL	C77-C78-C79-C80
150	Dx	1204	CDL	C40-C41-C42-C43
150	Eu	101	CDL	C11-C12-C13-C14
153	A9	603	PC1	C3C-C3D-C3E-C3F
153	AU	202	PC1	C3C-C3D-C3E-C3F
153	C	509	PC1	C35-C36-C37-C38
153	DB	702	PC1	C27-C28-C29-C2A
153	DC	602	PC1	C3C-C3D-C3E-C3F
153	Dx	1205	PC1	C24-C25-C26-C27
155	DJ	301	3PE	C32-C33-C34-C35
156	EI	402	LPP	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
155	DS	402	3PE	C2-C3-O31-C31
150	DR	402	CDL	C61-C62-C63-C64
150	DS	401	CDL	C61-C62-C63-C64
150	DS	404	CDL	C20-C21-C22-C23
150	DX	307	CDL	C32-C33-C34-C35
150	DY	301	CDL	C12-C13-C14-C15
150	DY	301	CDL	C35-C36-C37-C38
150	EO	202	CDL	C16-C17-C18-C19
150	Dd	704	CDL	C63-C64-C65-C66
150	Dh	202	CDL	C37-C38-C39-C40
150	Dj	403	CDL	C13-C14-C15-C16
150	Du	401	CDL	C11-C12-C13-C14
150	Du	402	CDL	C14-C15-C16-C17
150	Dx	1204	CDL	C35-C36-C37-C38
153	C	508	PC1	C2B-C2C-C2D-C2E
153	k	301	PC1	C2E-C2F-C2G-C2H
153	DY	302	PC1	C2E-C2F-C2G-C2H
153	Dc	603	PC1	C2A-C2B-C2C-C2D
155	DC	607	3PE	O13-C11-C12-N
150	AA	908	CDL	C12-C13-C14-C15
150	AM	301	CDL	C82-C83-C84-C85
150	B0	101	CDL	C38-C39-C40-C41
150	B1	402	CDL	C34-C35-C36-C37
150	BC	302	CDL	C32-C33-C34-C35
150	c	509	CDL	C75-C76-C77-C78
150	DJ	303	CDL	C60-C61-C62-C63
150	DV	401	CDL	C57-C58-C59-C60
150	DX	307	CDL	C11-C12-C13-C14
150	ED	605	CDL	C11-C12-C13-C14
150	ED	605	CDL	C23-C24-C25-C26
150	Dj	405	CDL	C20-C21-C22-C23
150	Dn	506	CDL	C35-C36-C37-C38
150	Ds	405	CDL	C75-C76-C77-C78
150	Dx	1204	CDL	C60-C61-C62-C63
150	Ek	201	CDL	C74-C75-C76-C77
150	El	901	CDL	C23-C24-C25-C26
153	k	301	PC1	C35-C36-C37-C38
153	DS	406	PC1	C3B-C3C-C3D-C3E
150	Dd	702	CDL	CB7-C71-C72-C73
150	Dr	402	CDL	CA7-C31-C32-C33
150	DJ	304	CDL	OB9-CB7-OB8-CB6
150	Ds	401	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	Dv	403	CDL	OB9-CB7-OB8-CB6
153	A9	603	PC1	O32-C31-O31-C3
153	d	801	PC1	O32-C31-O31-C3
150	AA	901	CDL	C23-C24-C25-C26
150	AA	901	CDL	C36-C37-C38-C39
150	AF	401	CDL	C63-C64-C65-C66
150	c	502	CDL	C73-C74-C75-C76
150	DD	704	CDL	C63-C64-C65-C66
150	DI	302	CDL	C71-C72-C73-C74
150	DV	403	CDL	C72-C73-C74-C75
150	Dh	202	CDL	C21-C22-C23-C24
150	Dh	202	CDL	C63-C64-C65-C66
150	Do	501	CDL	C77-C78-C79-C80
150	Du	403	CDL	C57-C58-C59-C60
150	Eh	1601	CDL	C20-C21-C22-C23
150	h	501	CDL	C71-CB7-OB8-CB6
150	AC	801	CDL	C55-C56-C57-C58
150	CC	305	CDL	C11-C12-C13-C14
150	DI	302	CDL	C37-C38-C39-C40
150	DI	302	CDL	C62-C63-C64-C65
150	DQ	1504	CDL	C17-C18-C19-C20
150	DS	401	CDL	C16-C17-C18-C19
150	DX	306	CDL	C36-C37-C38-C39
150	EB	302	CDL	C20-C21-C22-C23
150	EO	202	CDL	C63-C64-C65-C66
150	Ds	401	CDL	C37-C38-C39-C40
150	Ed	205	CDL	C11-C12-C13-C14
150	Eh	1601	CDL	C55-C56-C57-C58
150	Ek	201	CDL	C77-C78-C79-C80
150	El	901	CDL	C12-C13-C14-C15
150	El	903	CDL	C81-C82-C83-C84
155	Eo	202	3PE	C36-C37-C38-C39
150	AC	802	CDL	C13-C14-C15-C16
150	AF	402	CDL	C71-C72-C73-C74
150	C	507	CDL	C22-C23-C24-C25
150	DN	502	CDL	C57-C58-C59-C60
150	DN	507	CDL	C60-C61-C62-C63
150	EI	401	CDL	C61-C62-C63-C64
150	EL	903	CDL	C20-C21-C22-C23
150	EN	1202	CDL	C36-C37-C38-C39
150	Dc	601	CDL	C40-C41-C42-C43
150	Di	1103	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
150	Ea	501	CDL	C34-C35-C36-C37
153	DB	702	PC1	C3C-C3D-C3E-C3F
153	Di	1104	PC1	C27-C28-C29-C2A
155	BA	301	3PE	C34-C35-C36-C37
164	CA	702	FAD	O3'-C3'-C4'-C5'
153	DI	303	PC1	O32-C31-O31-C3
153	Di	1104	PC1	O32-C31-O31-C3
155	Di	1102	3PE	O32-C31-O31-C3
150	AC	802	CDL	C62-C63-C64-C65
150	AF	401	CDL	C61-C62-C63-C64
150	CG	301	CDL	C63-C64-C65-C66
150	CJ	201	CDL	C76-C77-C78-C79
150	H	1301	CDL	C80-C81-C82-C83
150	g	801	CDL	C79-C80-C81-C82
150	DD	705	CDL	C62-C63-C64-C65
150	DH	202	CDL	C37-C38-C39-C40
150	DJ	307	CDL	C82-C83-C84-C85
150	DV	401	CDL	C80-C81-C82-C83
150	EH	1601	CDL	C20-C21-C22-C23
150	EL	902	CDL	C38-C39-C40-C41
150	EN	1201	CDL	C17-C18-C19-C20
150	EN	1202	CDL	C23-C24-C25-C26
150	ES	1101	CDL	C55-C56-C57-C58
150	Da	709	CDL	C74-C75-C76-C77
150	Dd	706	CDL	C75-C76-C77-C78
150	Dn	501	CDL	C57-C58-C59-C60
150	Do	501	CDL	C32-C33-C34-C35
150	Do	501	CDL	C40-C41-C42-C43
150	Ds	401	CDL	C11-C12-C13-C14
150	Ds	401	CDL	C23-C24-C25-C26
150	Ds	402	CDL	C16-C17-C18-C19
150	Ds	405	CDL	C37-C38-C39-C40
150	Dv	403	CDL	C13-C14-C15-C16
150	Dv	403	CDL	C72-C73-C74-C75
150	Dx	1201	CDL	C20-C21-C22-C23
150	Dx	1204	CDL	C17-C18-C19-C20
150	Dy	301	CDL	C35-C36-C37-C38
150	Ed	205	CDL	C23-C24-C25-C26
150	Eg	101	CDL	C60-C61-C62-C63
150	Eg	101	CDL	C63-C64-C65-C66
150	Eh	1601	CDL	C23-C24-C25-C26
150	Ei	401	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
150	El	901	CDL	C37-C38-C39-C40
150	El	903	CDL	C56-C57-C58-C59
155	Ds	408	3PE	C27-C28-C29-C2A
150	A0	601	CDL	CA3-CA4-CA6-OA8
150	BV	201	CDL	CB3-CB4-CB6-OB8
150	DU	401	CDL	CA3-CA4-CA6-OA8
150	EL	902	CDL	CA3-CA4-CA6-OA8
150	Ds	402	CDL	CA3-CA4-CA6-OA8
153	DC	605	PC1	C1-C2-C3-O31
153	EO	205	PC1	C1-C2-C3-O31
155	EN	1204	3PE	C1-C2-C3-O31
150	Dn	501	CDL	OA7-CA5-OA6-CA4
150	C	507	CDL	C17-C18-C19-C20
150	c	506	CDL	C60-C61-C62-C63
150	DG	202	CDL	C14-C15-C16-C17
150	DQ	1504	CDL	C51-C52-C53-C54
150	DS	404	CDL	C37-C38-C39-C40
150	EK	201	CDL	C77-C78-C79-C80
150	Dd	704	CDL	C17-C18-C19-C20
150	Dv	401	CDL	C57-C58-C59-C60
150	Dv	403	CDL	C79-C80-C81-C82
150	Dv	403	CDL	C82-C83-C84-C85
150	Dx	1201	CDL	C74-C75-C76-C77
150	El	901	CDL	C61-C62-C63-C64
153	DC	603	PC1	C2A-C2B-C2C-C2D
150	Dh	201	CDL	CA5-C11-C12-C13
153	AC	804	PC1	C21-C22-C23-C24
150	AC	801	CDL	C54-C55-C56-C57
150	AC	802	CDL	C80-C81-C82-C83
150	DN	506	CDL	C35-C36-C37-C38
150	DX	306	CDL	C11-C12-C13-C14
150	Dc	601	CDL	C12-C13-C14-C15
150	Dn	506	CDL	C14-C15-C16-C17
150	Dq	1401	CDL	C17-C18-C19-C20
150	Eu	101	CDL	C36-C37-C38-C39
155	DX	302	3PE	C39-C3A-C3B-C3C
150	En	1201	CDL	OB9-CB7-OB8-CB6
150	Dj	401	CDL	C31-CA7-OA8-CA6
150	Dr	403	CDL	C71-CB7-OB8-CB6
155	DR	401	3PE	C32-C31-O31-C3
167	c	510	UQ8	C28-C29-C31-C32
167	El	906	UQ8	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
150	A0	602	CDL	C11-CA5-OA6-CA4
150	h	501	CDL	C11-CA5-OA6-CA4
150	DC	601	CDL	C11-CA5-OA6-CA4
150	DV	402	CDL	C11-CA5-OA6-CA4
150	ED	605	CDL	C11-CA5-OA6-CA4
150	Dq	1402	CDL	C11-CA5-OA6-CA4
150	Ea	501	CDL	C11-CA5-OA6-CA4
153	Ef	501	PC1	C22-C21-O21-C2
155	AJ	502	3PE	C22-C21-O21-C2
155	DG	205	3PE	C22-C21-O21-C2
155	Dd	703	3PE	C22-C21-O21-C2
150	Dj	401	CDL	CA4-CA6-OA8-CA7
150	DA	709	CDL	C12-C13-C14-C15
150	DQ	1504	CDL	C34-C35-C36-C37
150	ED	605	CDL	C61-C62-C63-C64
150	EL	901	CDL	C61-C62-C63-C64
150	Dv	403	CDL	C17-C18-C19-C20
150	Dy	301	CDL	C82-C83-C84-C85
150	Ea	502	CDL	C74-C75-C76-C77
153	BS	1302	PC1	C36-C37-C38-C39
150	AC	802	CDL	C73-C74-C75-C76
150	BC	302	CDL	C12-C13-C14-C15
150	DC	601	CDL	C14-C15-C16-C17
150	DD	705	CDL	C36-C37-C38-C39
150	DM	501	CDL	C79-C80-C81-C82
150	DO	501	CDL	C40-C41-C42-C43
150	DV	403	CDL	C82-C83-C84-C85
150	DY	301	CDL	C82-C83-C84-C85
150	EL	901	CDL	C82-C83-C84-C85
150	EN	1201	CDL	C34-C35-C36-C37
150	EO	202	CDL	C31-C32-C33-C34
150	El	901	CDL	C39-C40-C41-C42
150	El	902	CDL	C34-C35-C36-C37
153	A9	601	PC1	C3B-C3C-C3D-C3E
155	EL	904	3PE	C26-C27-C28-C29
155	EN	1204	3PE	C38-C39-C3A-C3B
150	C	507	CDL	OB9-CB7-OB8-CB6
150	DV	403	CDL	OB9-CB7-OB8-CB6
156	EI	402	LPP	C11-C12-C13-C14
150	C	504	CDL	C43-C44-C45-C46
150	EL	901	CDL	C19-C20-C21-C22
150	Dj	401	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
150	El	902	CDL	C75-C76-C77-C78
153	C	508	PC1	C3D-C3E-C3F-C3G
150	CG	301	CDL	O1-C1-CB2-OB2
150	Dd	706	CDL	O1-C1-CA2-OA2
150	CC	304	CDL	C13-C14-C15-C16
150	DU	402	CDL	C14-C15-C16-C17
150	Dh	202	CDL	C74-C75-C76-C77
150	Di	1103	CDL	C80-C81-C82-C83
150	Dj	405	CDL	C37-C38-C39-C40
150	Dj	407	CDL	C82-C83-C84-C85
150	Dr	403	CDL	C34-C35-C36-C37
150	Ei	401	CDL	C12-C13-C14-C15
153	AQ	202	PC1	C26-C27-C28-C29
153	e	1101	PC1	C25-C26-C27-C28
155	Dx	1207	3PE	C3D-C3E-C3F-C3G
150	AA	901	CDL	C11-C12-C13-C14
150	DC	601	CDL	C80-C81-C82-C83
150	DH	202	CDL	C63-C64-C65-C66
150	DM	501	CDL	C81-C82-C83-C84
150	DR	403	CDL	C17-C18-C19-C20
150	DS	405	CDL	C58-C59-C60-C61
150	DS	405	CDL	C62-C63-C64-C65
150	EO	202	CDL	C37-C38-C39-C40
150	Dd	704	CDL	C82-C83-C84-C85
150	Ed	205	CDL	C61-C62-C63-C64
150	Eh	1601	CDL	C53-C54-C55-C56
150	El	903	CDL	C76-C77-C78-C79
153	c	507	PC1	C3C-C3D-C3E-C3F
150	DJ	307	CDL	OB9-CB7-OB8-CB6
150	Dm	502	CDL	OB9-CB7-OB8-CB6
150	Ed	204	CDL	OB9-CB7-OB8-CB6
150	BT	202	CDL	CA5-C11-C12-C13
150	CJ	201	CDL	CB2-C1-CA2-OA2
150	DS	404	CDL	CA2-C1-CB2-OB2
150	DX	301	CDL	CA2-C1-CB2-OB2
150	DX	307	CDL	CB2-C1-CA2-OA2
150	ED	601	CDL	CB2-C1-CA2-OA2
150	Dd	705	CDL	CA2-C1-CB2-OB2
150	Dg	202	CDL	CB2-C1-CA2-OA2
150	Ea	502	CDL	CA2-C1-CB2-OB2
150	AA	908	CDL	C53-C54-C55-C56
150	AA	908	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
150	AC	802	CDL	C42-C43-C44-C45
150	CD	302	CDL	C51-C52-C53-C54
150	DD	703	CDL	C74-C75-C76-C77
150	DJ	307	CDL	C59-C60-C61-C62
150	EL	903	CDL	C56-C57-C58-C59
150	Dc	608	CDL	C57-C58-C59-C60
150	Dg	201	CDL	C63-C64-C65-C66
150	Dq	1402	CDL	C36-C37-C38-C39
150	Dx	1201	CDL	C11-C12-C13-C14
153	AL	303	PC1	C3C-C3D-C3E-C3F
150	AC	801	CDL	OB7-CB5-OB6-CB4
150	h	501	CDL	OA7-CA5-OA6-CA4
150	DA	706	CDL	OB7-CB5-OB6-CB4
150	DC	601	CDL	OA7-CA5-OA6-CA4
150	DJ	304	CDL	OB7-CB5-OB6-CB4
150	DV	402	CDL	OA7-CA5-OA6-CA4
150	ED	605	CDL	OA7-CA5-OA6-CA4
150	Dc	601	CDL	OA7-CA5-OA6-CA4
150	Dn	503	CDL	OB7-CB5-OB6-CB4
150	Dq	1402	CDL	OA7-CA5-OA6-CA4
150	Dq	1403	CDL	OB7-CB5-OB6-CB4
150	Ea	501	CDL	OA7-CA5-OA6-CA4
153	BG	202	PC1	O22-C21-O21-C2
153	Ef	501	PC1	O22-C21-O21-C2
155	DG	205	3PE	O22-C21-O21-C2
155	Dd	703	3PE	O22-C21-O21-C2
150	AP	301	CDL	C74-C75-C76-C77
150	BL	301	CDL	C21-C22-C23-C24
150	BY	201	CDL	C36-C37-C38-C39
150	H	1302	CDL	C59-C60-C61-C62
150	DG	201	CDL	C63-C64-C65-C66
150	Dn	506	CDL	C40-C41-C42-C43
150	Dr	403	CDL	C11-C12-C13-C14
150	Du	402	CDL	C12-C13-C14-C15
150	Dv	402	CDL	C13-C14-C15-C16
150	Ek	201	CDL	C53-C54-C55-C56
153	AA	903	PC1	C34-C35-C36-C37
153	BS	1302	PC1	C32-C33-C34-C35
155	DX	303	3PE	C3D-C3E-C3F-C3G
155	Ds	408	3PE	C38-C39-C3A-C3B
150	AC	801	CDL	C1-CB2-OB2-PB2
150	DJ	305	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
150	Dj	401	CDL	C1-CB2-OB2-PB2
150	Eh	1601	CDL	OA9-CA7-OA8-CA6
150	AC	802	CDL	C55-C56-C57-C58
150	AF	402	CDL	C37-C38-C39-C40
150	BT	204	CDL	C43-C44-C45-C46
150	BV	201	CDL	C37-C38-C39-C40
150	C	503	CDL	C32-C33-C34-C35
150	c	501	CDL	C13-C14-C15-C16
150	DD	705	CDL	C41-C42-C43-C44
150	DJ	305	CDL	C20-C21-C22-C23
150	DN	503	CDL	C41-C42-C43-C44
150	DS	404	CDL	C60-C61-C62-C63
150	DU	402	CDL	C56-C57-C58-C59
150	DZ	501	CDL	C38-C39-C40-C41
150	EL	901	CDL	C80-C81-C82-C83
150	EN	1201	CDL	C53-C54-C55-C56
150	Dj	405	CDL	C77-C78-C79-C80
150	Ds	405	CDL	C60-C61-C62-C63
150	Ea	501	CDL	C16-C17-C18-C19
150	Eb	302	CDL	C54-C55-C56-C57
150	Ek	201	CDL	C33-C34-C35-C36
150	El	902	CDL	C12-C13-C14-C15
150	El	902	CDL	C63-C64-C65-C66
150	Eu	101	CDL	C17-C18-C19-C20
153	DB	702	PC1	C32-C33-C34-C35
155	EN	1204	3PE	C27-C28-C29-C2A
150	DA	709	CDL	CA5-C11-C12-C13
150	DC	601	CDL	CA5-C11-C12-C13
150	DD	703	CDL	CA5-C11-C12-C13
150	B0	101	CDL	C40-C41-C42-C43
150	BE	201	CDL	C19-C20-C21-C22
150	C	506	CDL	C71-C72-C73-C74
150	DJ	307	CDL	C51-C52-C53-C54
150	DV	401	CDL	C39-C40-C41-C42
150	DV	403	CDL	C17-C18-C19-C20
150	DX	306	CDL	C17-C18-C19-C20
150	ED	605	CDL	C51-C52-C53-C54
150	Dd	705	CDL	C62-C63-C64-C65
150	Dj	405	CDL	C41-C42-C43-C44
150	Dj	407	CDL	C59-C60-C61-C62
150	Ds	406	CDL	C62-C63-C64-C65
150	Dx	1201	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
150	Ed	204	CDL	C80-C81-C82-C83
150	En	1201	CDL	C82-C83-C84-C85
153	D	402	PC1	C3C-C3D-C3E-C3F
153	DC	605	PC1	C29-C2A-C2B-C2C
155	DC	606	3PE	C3E-C3F-C3G-C3H
155	Dx	1202	3PE	C36-C37-C38-C39
150	DD	705	CDL	C71-CB7-OB8-CB6
150	DV	401	CDL	C71-CB7-OB8-CB6
150	Dq	1403	CDL	C71-CB7-OB8-CB6
150	Ds	402	CDL	C71-CB7-OB8-CB6
150	Du	403	CDL	C71-CB7-OB8-CB6
153	AU	201	PC1	C32-C31-O31-C3
153	BG	202	PC1	C32-C31-O31-C3
153	EO	206	PC1	C32-C31-O31-C3
166	CE	401	HEC	C2A-CAA-CBA-CGA
150	CC	304	CDL	C51-CB5-OB6-CB4
150	CD	302	CDL	C51-CB5-OB6-CB4
150	E	301	CDL	C51-CB5-OB6-CB4
150	DJ	304	CDL	C51-CB5-OB6-CB4
150	ED	605	CDL	C51-CB5-OB6-CB4
150	EN	1201	CDL	C11-CA5-OA6-CA4
150	Dd	702	CDL	C51-CB5-OB6-CB4
150	Dq	1403	CDL	C51-CB5-OB6-CB4
150	Ed	205	CDL	C11-CA5-OA6-CA4
150	Eh	1601	CDL	C51-CB5-OB6-CB4
150	Ek	201	CDL	C51-CB5-OB6-CB4
150	Ep	701	CDL	C11-CA5-OA6-CA4
155	El	905	3PE	C22-C21-O21-C2
150	AC	802	CDL	C60-C61-C62-C63
150	B0	102	CDL	C58-C59-C60-C61
150	BG	201	CDL	C60-C61-C62-C63
150	BT	202	CDL	C82-C83-C84-C85
150	h	501	CDL	C14-C15-C16-C17
150	DD	704	CDL	C82-C83-C84-C85
150	DI	302	CDL	C74-C75-C76-C77
150	DJ	305	CDL	C37-C38-C39-C40
150	DJ	305	CDL	C41-C42-C43-C44
150	DJ	307	CDL	C77-C78-C79-C80
150	DN	506	CDL	C37-C38-C39-C40
150	DN	506	CDL	C40-C41-C42-C43
150	DV	403	CDL	C12-C13-C14-C15
150	DX	307	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
150	DZ	501	CDL	C34-C35-C36-C37
150	Dc	601	CDL	C80-C81-C82-C83
150	Dc	608	CDL	C42-C43-C44-C45
150	Dd	706	CDL	C80-C81-C82-C83
150	Dh	201	CDL	C56-C57-C58-C59
150	Dm	501	CDL	C11-C12-C13-C14
150	Du	401	CDL	C36-C37-C38-C39
150	Dv	401	CDL	C39-C40-C41-C42
150	Dv	402	CDL	C36-C37-C38-C39
150	Dv	402	CDL	C62-C63-C64-C65
150	Dx	1204	CDL	C56-C57-C58-C59
150	Ea	502	CDL	C81-C82-C83-C84
150	Eb	302	CDL	C34-C35-C36-C37
150	Eu	101	CDL	C63-C64-C65-C66
153	DX	305	PC1	C3D-C3E-C3F-C3G
155	BA	301	3PE	C25-C26-C27-C28
155	DS	402	3PE	C37-C38-C39-C3A
155	EL	904	3PE	C37-C38-C39-C3A
155	Dx	1202	3PE	C3C-C3D-C3E-C3F
156	Ed	203	LPP	C19-C20-C21-C22
150	BC	302	CDL	OA9-CA7-OA8-CA6
150	DJ	303	CDL	OB9-CB7-OB8-CB6
150	DQ	1502	CDL	OB9-CB7-OB8-CB6
150	Di	1103	CDL	CA7-C31-C32-C33
150	Ea	501	CDL	CA5-C11-C12-C13
150	DG	201	CDL	C56-C57-C58-C59
150	DN	503	CDL	C36-C37-C38-C39
150	Dn	501	CDL	C35-C36-C37-C38
150	Dr	402	CDL	C20-C21-C22-C23
150	Ds	406	CDL	C53-C54-C55-C56
155	DN	501	3PE	C28-C29-C2A-C2B
150	CG	302	CDL	C42-C43-C44-C45
150	DU	401	CDL	C36-C37-C38-C39
150	DX	307	CDL	C63-C64-C65-C66
150	Dr	403	CDL	C17-C18-C19-C20
153	c	507	PC1	C28-C29-C2A-C2B
153	k	301	PC1	C22-C23-C24-C25
153	Dv	406	PC1	C3C-C3D-C3E-C3F
155	Ds	403	3PE	C37-C38-C39-C3A
167	DS	403	UQ8	C33-C34-C36-C37
167	Ed	202	UQ8	C33-C34-C36-C37
150	h	501	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
150	Dj	401	CDL	OA9-CA7-OA8-CA6
150	Dr	403	CDL	OB9-CB7-OB8-CB6
153	AC	804	PC1	O32-C31-O31-C3
155	DR	401	3PE	O32-C31-O31-C3
150	CG	302	CDL	C78-C79-C80-C81
150	c	509	CDL	C43-C44-C45-C46
150	DJ	304	CDL	C40-C41-C42-C43
150	DQ	1502	CDL	C75-C76-C77-C78
150	DS	405	CDL	C53-C54-C55-C56
150	DV	402	CDL	C81-C82-C83-C84
150	EN	1201	CDL	C39-C40-C41-C42
150	EO	202	CDL	C62-C63-C64-C65
150	Dg	201	CDL	C44-C45-C46-C47
150	Dn	503	CDL	C56-C57-C58-C59
150	Dn	506	CDL	C56-C57-C58-C59
150	Ds	406	CDL	C55-C56-C57-C58
150	Dx	1204	CDL	C36-C37-C38-C39
150	Eg	101	CDL	C81-C82-C83-C84
150	Eh	1601	CDL	C57-C58-C59-C60
150	El	901	CDL	C33-C34-C35-C36
150	El	901	CDL	C51-C52-C53-C54
153	AC	804	PC1	C29-C2A-C2B-C2C
150	A0	602	CDL	OA7-CA5-OA6-CA4
150	A1	402	CDL	OA7-CA5-OA6-CA4
150	c	506	CDL	OB7-CB5-OB6-CB4
150	DH	201	CDL	OA7-CA5-OA6-CA4
150	DU	403	CDL	OA7-CA5-OA6-CA4
150	DX	307	CDL	OB7-CB5-OB6-CB4
150	Du	401	CDL	OA7-CA5-OA6-CA4
150	El	901	CDL	OA7-CA5-OA6-CA4
153	DX	308	PC1	O22-C21-O21-C2
153	Dq	1404	PC1	O22-C21-O21-C2
155	AJ	502	3PE	O22-C21-O21-C2
155	C	513	3PE	O22-C21-O21-C2
155	DN	501	3PE	O22-C21-O21-C2
150	BY	201	CDL	CA5-C11-C12-C13
150	DR	403	CDL	CA7-C31-C32-C33
150	Ea	501	CDL	CA7-C31-C32-C33
155	Em	901	3PE	C21-C22-C23-C24
150	BT	204	CDL	C71-CB7-OB8-CB6
150	C	504	CDL	C71-CB7-OB8-CB6
150	DN	507	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
150	DX	306	CDL	C71-CB7-OB8-CB6
150	ED	605	CDL	C71-CB7-OB8-CB6
150	Du	401	CDL	C71-CB7-OB8-CB6
150	Du	402	CDL	C31-CA7-OA8-CA6
153	A6	303	PC1	C32-C31-O31-C3
153	BS	1301	PC1	C32-C31-O31-C3
153	Da	707	PC1	C32-C31-O31-C3
155	AJ	502	3PE	C32-C31-O31-C3
150	A1	402	CDL	C82-C83-C84-C85
150	BT	204	CDL	C83-C84-C85-C86
150	CC	305	CDL	C58-C59-C60-C61
150	DA	709	CDL	C40-C41-C42-C43
150	DN	507	CDL	C55-C56-C57-C58
150	DQ	1504	CDL	C40-C41-C42-C43
150	DR	403	CDL	C12-C13-C14-C15
150	DS	405	CDL	C55-C56-C57-C58
150	Dj	404	CDL	C31-C32-C33-C34
150	Dn	506	CDL	C82-C83-C84-C85
150	Dq	1401	CDL	C40-C41-C42-C43
150	Dr	403	CDL	C12-C13-C14-C15
150	En	1201	CDL	C21-C22-C23-C24
153	D	402	PC1	C25-C26-C27-C28
150	A0	602	CDL	C40-C41-C42-C43
150	B0	101	CDL	C13-C14-C15-C16
150	C	505	CDL	C75-C76-C77-C78
150	DA	706	CDL	C17-C18-C19-C20
150	DN	506	CDL	C56-C57-C58-C59
150	DV	403	CDL	C53-C54-C55-C56
150	ED	604	CDL	C80-C81-C82-C83
150	EK	201	CDL	C53-C54-C55-C56
150	Eh	1601	CDL	C83-C84-C85-C86
150	En	1201	CDL	C17-C18-C19-C20
153	A0	605	PC1	C2C-C2D-C2E-C2F
153	AQ	202	PC1	C2B-C2C-C2D-C2E
153	Dx	1209	PC1	C3D-C3E-C3F-C3G
150	C	503	CDL	C79-C80-C81-C82
150	h	501	CDL	C71-C72-C73-C74
150	DG	201	CDL	C53-C54-C55-C56
150	DH	201	CDL	C56-C57-C58-C59
150	DN	507	CDL	C80-C81-C82-C83
150	DX	301	CDL	C74-C75-C76-C77
150	DY	301	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
150	EB	302	CDL	C34-C35-C36-C37
150	EK	201	CDL	C33-C34-C35-C36
150	ES	1101	CDL	C23-C24-C25-C26
150	ES	1101	CDL	C60-C61-C62-C63
150	Di	1101	CDL	C17-C18-C19-C20
150	Dj	401	CDL	C37-C38-C39-C40
150	Dj	403	CDL	C60-C61-C62-C63
150	Dy	301	CDL	C43-C44-C45-C46
150	Eh	1601	CDL	C81-C82-C83-C84
153	AQ	202	PC1	C3C-C3D-C3E-C3F
153	E	303	PC1	C3C-C3D-C3E-C3F
153	EO	206	PC1	C3C-C3D-C3E-C3F
153	Eo	204	PC1	C3A-C3B-C3C-C3D
150	Eh	1601	CDL	CA5-C11-C12-C13
150	Ek	201	CDL	CA5-C11-C12-C13
153	B1	403	PC1	C31-C32-C33-C34
150	AC	801	CDL	C78-C79-C80-C81
150	B0	102	CDL	C43-C44-C45-C46
150	CC	305	CDL	C36-C37-C38-C39
150	DD	704	CDL	C17-C18-C19-C20
150	DD	706	CDL	C23-C24-C25-C26
150	DJ	302	CDL	C17-C18-C19-C20
150	DJ	302	CDL	C39-C40-C41-C42
150	DJ	305	CDL	C77-C78-C79-C80
150	DQ	1504	CDL	C57-C58-C59-C60
150	DU	404	CDL	C23-C24-C25-C26
150	DX	301	CDL	C12-C13-C14-C15
150	DX	307	CDL	C43-C44-C45-C46
150	EL	901	CDL	C33-C34-C35-C36
150	EN	1201	CDL	C21-C22-C23-C24
150	Da	709	CDL	C16-C17-C18-C19
150	Dd	705	CDL	C40-C41-C42-C43
150	Dj	407	CDL	C51-C52-C53-C54
150	Ds	406	CDL	C58-C59-C60-C61
150	En	1201	CDL	C39-C40-C41-C42
153	A6	302	PC1	C3C-C3D-C3E-C3F
153	BG	202	PC1	C35-C36-C37-C38
153	DC	608	PC1	C2C-C2D-C2E-C2F
153	EO	205	PC1	C3A-C3B-C3C-C3D
153	Ds	407	PC1	C2B-C2C-C2D-C2E
155	AJ	502	3PE	C3E-C3F-C3G-C3H
155	DN	501	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
155	DS	402	3PE	C39-C3A-C3B-C3C
155	Dr	404	3PE	C3E-C3F-C3G-C3H
155	Ds	408	3PE	C35-C36-C37-C38
155	Dx	1208	3PE	C27-C28-C29-C2A
150	CG	301	CDL	C53-C54-C55-C56
150	DJ	304	CDL	C19-C20-C21-C22
150	DQ	1504	CDL	C61-C62-C63-C64
150	DR	402	CDL	C82-C83-C84-C85
150	DX	301	CDL	C61-C62-C63-C64
150	DX	306	CDL	C63-C64-C65-C66
150	DZ	501	CDL	C16-C17-C18-C19
150	EH	1601	CDL	C83-C84-C85-C86
150	Dh	202	CDL	C71-C72-C73-C74
150	Dj	402	CDL	C16-C17-C18-C19
150	Dj	402	CDL	C52-C53-C54-C55
150	Dx	1204	CDL	C76-C77-C78-C79
153	AC	804	PC1	C2E-C2F-C2G-C2H
153	K	502	PC1	C3D-C3E-C3F-C3G
153	DV	405	PC1	C3C-C3D-C3E-C3F
153	Dj	406	PC1	C22-C23-C24-C25
155	DG	205	3PE	C3E-C3F-C3G-C3H
153	Eo	204	PC1	C32-C31-O31-C3
150	BG	201	CDL	C53-C54-C55-C56
150	c	506	CDL	C17-C18-C19-C20
150	c	506	CDL	C20-C21-C22-C23
150	DH	202	CDL	C42-C43-C44-C45
150	DJ	302	CDL	C82-C83-C84-C85
150	DJ	304	CDL	C33-C34-C35-C36
150	DN	502	CDL	C35-C36-C37-C38
150	DQ	1504	CDL	C36-C37-C38-C39
150	EL	902	CDL	C83-C84-C85-C86
150	Dd	704	CDL	C11-C12-C13-C14
150	Dj	402	CDL	C58-C59-C60-C61
150	Dj	404	CDL	C19-C20-C21-C22
150	Dj	405	CDL	C11-C12-C13-C14
150	Dv	402	CDL	C81-C82-C83-C84
150	Dy	301	CDL	C79-C80-C81-C82
150	En	1201	CDL	C54-C55-C56-C57
153	AA	903	PC1	C38-C39-C3A-C3B
153	EN	1203	PC1	C2B-C2C-C2D-C2E
153	Di	1104	PC1	C3A-C3B-C3C-C3D
155	Eo	202	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
150	DR	402	CDL	CA7-C31-C32-C33
153	A1	403	PC1	C31-C32-C33-C34
150	A1	402	CDL	C11-CA5-OA6-CA4
150	A1	402	CDL	C51-CB5-OB6-CB4
150	AC	801	CDL	C11-CA5-OA6-CA4
150	AM	301	CDL	C51-CB5-OB6-CB4
150	B0	102	CDL	C51-CB5-OB6-CB4
150	BC	302	CDL	C11-CA5-OA6-CA4
150	CJ	201	CDL	C51-CB5-OB6-CB4
150	CD	301	CDL	C51-CB5-OB6-CB4
150	c	506	CDL	C51-CB5-OB6-CB4
150	DD	703	CDL	C51-CB5-OB6-CB4
150	DD	704	CDL	C11-CA5-OA6-CA4
150	DH	201	CDL	C11-CA5-OA6-CA4
150	DN	506	CDL	C11-CA5-OA6-CA4
150	DQ	1502	CDL	C51-CB5-OB6-CB4
150	DS	401	CDL	C11-CA5-OA6-CA4
150	DS	405	CDL	C51-CB5-OB6-CB4
150	DU	403	CDL	C11-CA5-OA6-CA4
150	DX	307	CDL	C51-CB5-OB6-CB4
150	Dd	705	CDL	C11-CA5-OA6-CA4
150	Dd	705	CDL	C51-CB5-OB6-CB4
150	Ds	402	CDL	C51-CB5-OB6-CB4
150	Ds	406	CDL	C51-CB5-OB6-CB4
150	Du	401	CDL	C11-CA5-OA6-CA4
150	Du	402	CDL	C11-CA5-OA6-CA4
150	El	901	CDL	C11-CA5-OA6-CA4
153	A6	303	PC1	C22-C21-O21-C2
153	AA	905	PC1	C22-C21-O21-C2
153	AU	202	PC1	C22-C21-O21-C2
153	c	507	PC1	C22-C21-O21-C2
153	e	1101	PC1	C22-C21-O21-C2
153	DS	406	PC1	C22-C21-O21-C2
153	DX	308	PC1	C22-C21-O21-C2
153	Dq	1404	PC1	C22-C21-O21-C2
153	Dx	1203	PC1	C22-C21-O21-C2
155	CD	303	3PE	C22-C21-O21-C2
155	C	513	3PE	C22-C21-O21-C2
155	DC	606	3PE	C22-C21-O21-C2
155	DN	501	3PE	C22-C21-O21-C2
155	DX	303	3PE	C22-C21-O21-C2
155	EO	203	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
155	Dc	606	3PE	C22-C21-O21-C2
155	Dx	1207	3PE	C22-C21-O21-C2
150	AA	908	CDL	OA5-CA3-CA4-OA6
150	BT	202	CDL	OB5-CB3-CB4-OB6
150	CD	302	CDL	OB5-CB3-CB4-OB6
150	DX	301	CDL	OB5-CB3-CB4-OB6
150	ED	605	CDL	OB5-CB3-CB4-OB6
150	EH	1601	CDL	OA5-CA3-CA4-OA6
150	Du	401	CDL	OA5-CA3-CA4-OA6
150	Ed	205	CDL	OB5-CB3-CB4-OB6
153	Dq	1404	PC1	O11-C1-C2-O21
150	AA	908	CDL	C38-C39-C40-C41
150	AA	908	CDL	C82-C83-C84-C85
150	DC	601	CDL	C33-C34-C35-C36
150	DG	201	CDL	C13-C14-C15-C16
150	DM	501	CDL	C58-C59-C60-C61
150	DN	506	CDL	C82-C83-C84-C85
150	DR	403	CDL	C41-C42-C43-C44
150	DV	402	CDL	C23-C24-C25-C26
150	EL	902	CDL	C63-C64-C65-C66
150	EL	902	CDL	C74-C75-C76-C77
150	Dv	403	CDL	C53-C54-C55-C56
150	Dx	1204	CDL	C32-C33-C34-C35
150	Eg	101	CDL	C42-C43-C44-C45
153	DC	602	PC1	C3D-C3E-C3F-C3G
155	DX	303	3PE	C26-C27-C28-C29
155	Eo	202	3PE	C2C-C2D-C2E-C2F
156	AL	304	LPP	C20-C21-C22-C23
156	Dn	504	LPP	C31-C32-C33-C34
150	BT	204	CDL	C36-C37-C38-C39
150	DO	501	CDL	C15-C16-C17-C18
150	Dj	401	CDL	C53-C54-C55-C56
150	Ep	701	CDL	C11-C12-C13-C14
153	Db	702	PC1	C27-C28-C29-C2A
150	AM	301	CDL	OB7-CB5-OB6-CB4
150	B0	102	CDL	OB7-CB5-OB6-CB4
150	CD	302	CDL	OB7-CB5-OB6-CB4
150	E	301	CDL	OB7-CB5-OB6-CB4
150	DQ	1502	CDL	OB7-CB5-OB6-CB4
150	DS	401	CDL	OA7-CA5-OA6-CA4
150	DS	405	CDL	OB7-CB5-OB6-CB4
150	ED	605	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
150	EN	1201	CDL	OA7-CA5-OA6-CA4
150	Dd	702	CDL	OB7-CB5-OB6-CB4
150	Dd	705	CDL	OA7-CA5-OA6-CA4
150	Dd	705	CDL	OB7-CB5-OB6-CB4
150	Ds	406	CDL	OB7-CB5-OB6-CB4
150	Ed	205	CDL	OA7-CA5-OA6-CA4
150	Ek	201	CDL	OB7-CB5-OB6-CB4
153	e	1101	PC1	O22-C21-O21-C2
155	CD	303	3PE	O22-C21-O21-C2
155	DC	606	3PE	O22-C21-O21-C2
155	EO	203	3PE	O22-C21-O21-C2
155	El	905	3PE	O22-C21-O21-C2
150	DY	301	CDL	C57-C58-C59-C60
150	DZ	501	CDL	C77-C78-C79-C80
150	EA	301	CDL	C81-C82-C83-C84
150	EI	401	CDL	C11-C12-C13-C14
150	Dn	502	CDL	C12-C13-C14-C15
156	AC	803	LPP	C39-C40-C41-C42
150	AF	402	CDL	OB6-CB4-CB6-OB8
150	c	502	CDL	OB6-CB4-CB6-OB8
150	DA	709	CDL	OA6-CA4-CA6-OA8
150	DD	703	CDL	OB6-CB4-CB6-OB8
150	DJ	304	CDL	OB6-CB4-CB6-OB8
150	Da	709	CDL	OA6-CA4-CA6-OA8
150	Dg	201	CDL	OA6-CA4-CA6-OA8
150	Dn	503	CDL	OB6-CB4-CB6-OB8
150	En	1201	CDL	OA6-CA4-CA6-OA8
153	AA	907	PC1	O21-C2-C3-O31
153	DV	406	PC1	O21-C2-C3-O31
153	EO	205	PC1	O21-C2-C3-O31
155	DN	501	3PE	O21-C2-C3-O31
156	AC	803	LPP	O9-C7-C8-O27
150	DV	402	CDL	C36-C37-C38-C39
150	DX	306	CDL	C40-C41-C42-C43
150	EA	301	CDL	C13-C14-C15-C16
150	EH	1601	CDL	C81-C82-C83-C84
150	Dj	401	CDL	C82-C83-C84-C85
153	BS	1301	PC1	C2C-C2D-C2E-C2F
153	d	801	PC1	C25-C26-C27-C28
153	EO	205	PC1	C33-C34-C35-C36
155	EN	1204	3PE	C35-C36-C37-C38
155	Dx	1202	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
153	BG	202	PC1	O32-C31-O31-C3
150	AF	402	CDL	C39-C40-C41-C42
150	DD	705	CDL	C82-C83-C84-C85
150	DG	201	CDL	C31-C32-C33-C34
150	DJ	303	CDL	C13-C14-C15-C16
150	DJ	304	CDL	C51-C52-C53-C54
150	DS	404	CDL	C17-C18-C19-C20
150	DV	403	CDL	C13-C14-C15-C16
150	ES	1101	CDL	C79-C80-C81-C82
150	Dr	402	CDL	C60-C61-C62-C63
150	Dv	402	CDL	C23-C24-C25-C26
150	Dx	1204	CDL	C20-C21-C22-C23
150	El	902	CDL	C78-C79-C80-C81
153	A9	601	PC1	C23-C24-C25-C26
153	B1	401	PC1	C2E-C2F-C2G-C2H
155	El	905	3PE	C26-C27-C28-C29
155	Eo	202	3PE	C27-C28-C29-C2A
167	c	510	UQ8	C30-C29-C31-C32
150	A1	402	CDL	CB7-C71-C72-C73
167	CC	303	UQ8	C13-C14-C16-C17
150	AM	301	CDL	C11-C12-C13-C14
150	DN	507	CDL	C42-C43-C44-C45
150	DU	403	CDL	C36-C37-C38-C39
150	Dv	403	CDL	C12-C13-C14-C15
150	Ed	204	CDL	C76-C77-C78-C79
155	Ds	403	3PE	C39-C3A-C3B-C3C
155	Dx	1202	3PE	C27-C28-C29-C2A
156	EI	402	LPP	C20-C21-C22-C23
168	C	501	HEM	C3A-C2A-CAA-CBA
150	EK	201	CDL	CA4-CA6-OA8-CA7
150	DG	202	CDL	C51-C52-C53-C54
150	DX	307	CDL	C14-C15-C16-C17
150	Dd	705	CDL	C82-C83-C84-C85
150	Dx	1204	CDL	C54-C55-C56-C57
153	BS	1301	PC1	C34-C35-C36-C37
153	E	303	PC1	C33-C34-C35-C36
153	DI	303	PC1	C2C-C2D-C2E-C2F
155	Dr	404	3PE	C22-C23-C24-C25
156	EI	402	LPP	C15-C16-C17-C18
150	AC	801	CDL	C76-C77-C78-C79
150	DJ	302	CDL	C53-C54-C55-C56
150	DJ	303	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
150	Dc	608	CDL	C60-C61-C62-C63
150	Dg	202	CDL	C17-C18-C19-C20
150	Dq	1403	CDL	C38-C39-C40-C41
150	Dr	402	CDL	C82-C83-C84-C85
150	Dv	403	CDL	C43-C44-C45-C46
153	DJ	306	PC1	C22-C23-C24-C25
153	Da	707	PC1	C3E-C3F-C3G-C3H
153	Db	702	PC1	C32-C33-C34-C35
153	Di	1104	PC1	C2C-C2D-C2E-C2F
153	Eo	201	PC1	C3B-C3C-C3D-C3E
155	BT	201	3PE	C3D-C3E-C3F-C3G
155	EM	901	3PE	C26-C27-C28-C29
155	Dc	607	3PE	C34-C35-C36-C37
155	Dx	1207	3PE	C26-C27-C28-C29
150	DM	501	CDL	C71-CB7-OB8-CB6
150	Ed	205	CDL	C71-CB7-OB8-CB6
150	AC	801	CDL	C19-C20-C21-C22
150	Ds	405	CDL	C17-C18-C19-C20
150	Dv	402	CDL	C75-C76-C77-C78
153	DA	707	PC1	C24-C25-C26-C27
153	EO	204	PC1	C3C-C3D-C3E-C3F
150	BT	204	CDL	OB9-CB7-OB8-CB6
150	DD	705	CDL	OB9-CB7-OB8-CB6
150	DV	401	CDL	OB9-CB7-OB8-CB6
150	Dq	1403	CDL	OB9-CB7-OB8-CB6
150	Ds	402	CDL	OB9-CB7-OB8-CB6
150	Du	403	CDL	OB9-CB7-OB8-CB6
153	AU	201	PC1	O32-C31-O31-C3
153	EO	206	PC1	O32-C31-O31-C3
150	A1	402	CDL	OB7-CB5-OB6-CB4
150	AC	801	CDL	OA7-CA5-OA6-CA4
150	CC	304	CDL	OB7-CB5-OB6-CB4
150	CD	301	CDL	OB7-CB5-OB6-CB4
150	DD	703	CDL	OB7-CB5-OB6-CB4
150	DD	704	CDL	OA7-CA5-OA6-CA4
150	DG	201	CDL	OA7-CA5-OA6-CA4
150	DN	506	CDL	OA7-CA5-OA6-CA4
150	Du	402	CDL	OA7-CA5-OA6-CA4
150	Eh	1601	CDL	OB7-CB5-OB6-CB4
150	Ep	701	CDL	OA7-CA5-OA6-CA4
153	AA	905	PC1	O22-C21-O21-C2
153	Dx	1203	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
155	DX	303	3PE	O22-C21-O21-C2
155	Dc	606	3PE	O22-C21-O21-C2
155	Dx	1207	3PE	O22-C21-O21-C2
150	DG	201	CDL	C11-CA5-OA6-CA4
150	Dx	1201	CDL	C11-CA5-OA6-CA4
155	DJ	301	3PE	C22-C21-O21-C2
150	BT	204	CDL	C37-C38-C39-C40
150	CD	302	CDL	C12-C13-C14-C15
150	DQ	1501	CDL	C43-C44-C45-C46
150	Dg	202	CDL	C35-C36-C37-C38
150	Ds	405	CDL	C16-C17-C18-C19
150	Dv	401	CDL	C21-C22-C23-C24
153	B1	401	PC1	C3B-C3C-C3D-C3E
155	El	905	3PE	C3E-C3F-C3G-C3H
155	Em	901	3PE	C2A-C2B-C2C-C2D
156	DN	504	LPP	C35-C36-C37-C38
150	A0	602	CDL	CA2-OA2-PA1-OA5
150	BG	201	CDL	CB3-OB5-PB2-OB2
150	g	801	CDL	CA2-OA2-PA1-OA5
150	g	801	CDL	CB2-OB2-PB2-OB5
150	DA	706	CDL	CB3-OB5-PB2-OB2
150	DC	601	CDL	CA2-OA2-PA1-OA5
150	DD	703	CDL	CA3-OA5-PA1-OA2
150	DD	703	CDL	CB2-OB2-PB2-OB5
150	DD	704	CDL	CB2-OB2-PB2-OB5
150	DG	202	CDL	CA2-OA2-PA1-OA5
150	DG	202	CDL	CB3-OB5-PB2-OB2
150	DI	302	CDL	CB3-OB5-PB2-OB2
150	DJ	305	CDL	CA3-OA5-PA1-OA2
150	DM	501	CDL	CA2-OA2-PA1-OA5
150	DN	502	CDL	CB2-OB2-PB2-OB5
150	DU	401	CDL	CB3-OB5-PB2-OB2
150	DV	403	CDL	CA3-OA5-PA1-OA2
150	DY	301	CDL	CB2-OB2-PB2-OB5
150	ED	601	CDL	CB2-OB2-PB2-OB5
150	EK	201	CDL	CA3-OA5-PA1-OA2
150	EL	901	CDL	CB2-OB2-PB2-OB5
150	EL	903	CDL	CA2-OA2-PA1-OA5
150	EN	1202	CDL	CA3-OA5-PA1-OA2
150	Dd	706	CDL	CA2-OA2-PA1-OA5
150	Di	1101	CDL	CB2-OB2-PB2-OB5
150	Dj	401	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
150	Dj	402	CDL	CB3-OB5-PB2-OB2
150	Dj	403	CDL	CB2-OB2-PB2-OB5
150	Dn	501	CDL	CA3-OA5-PA1-OA2
150	Dq	1403	CDL	CB3-OB5-PB2-OB2
150	Du	402	CDL	CA3-OA5-PA1-OA2
150	Du	403	CDL	CB3-OB5-PB2-OB2
150	Dv	402	CDL	CB3-OB5-PB2-OB2
150	El	901	CDL	CA3-OA5-PA1-OA2
150	El	902	CDL	CB2-OB2-PB2-OB5
150	El	903	CDL	CA3-OA5-PA1-OA2
153	AM	302	PC1	C11-O13-P-O11
153	BG	202	PC1	C1-O11-P-O13
153	D	402	PC1	C11-O13-P-O11
153	DA	707	PC1	C11-O13-P-O11
153	DX	308	PC1	C11-O13-P-O11
153	EN	1203	PC1	C11-O13-P-O11
153	Dx	1203	PC1	C11-O13-P-O11
153	Eb	301	PC1	C1-O11-P-O13
155	BT	201	3PE	C11-O13-P-O11
155	DJ	301	3PE	C11-O13-P-O11
155	Dd	703	3PE	C11-O13-P-O11
155	Dx	1208	3PE	C11-O13-P-O11
150	BG	201	CDL	C13-C14-C15-C16
150	DQ	1501	CDL	C36-C37-C38-C39
150	DS	401	CDL	C80-C81-C82-C83
150	DZ	501	CDL	C12-C13-C14-C15
150	Dc	608	CDL	C21-C22-C23-C24
150	Dg	201	CDL	C83-C84-C85-C86
150	Dj	403	CDL	C23-C24-C25-C26
150	Do	501	CDL	C15-C16-C17-C18
150	Dr	403	CDL	C54-C55-C56-C57
155	EM	901	3PE	C2A-C2B-C2C-C2D
150	C	504	CDL	CA5-C11-C12-C13
150	DD	703	CDL	CB7-C71-C72-C73
150	DG	201	CDL	CA4-CA3-OA5-PA1
150	DH	202	CDL	C1-CB2-OB2-PB2
150	EL	902	CDL	C1-CB2-OB2-PB2
150	ES	1101	CDL	CA4-CA3-OA5-PA1
150	Ds	401	CDL	C1-CA2-OA2-PA1
153	Da	706	PC1	C2-C1-O11-P
150	DG	201	CDL	C58-C59-C60-C61
150	Dh	202	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
150	Dq	1403	CDL	C75-C76-C77-C78
150	Eu	101	CDL	C72-C73-C74-C75
153	c	507	PC1	C2E-C2F-C2G-C2H
155	AJ	502	3PE	O32-C31-O31-C3
153	AA	903	PC1	C32-C31-O31-C3
153	C	508	PC1	C32-C31-O31-C3
150	A0	602	CDL	OB5-CB3-CB4-CB6
150	AM	301	CDL	OA5-CA3-CA4-CA6
150	BC	301	CDL	OA5-CA3-CA4-CA6
150	CD	301	CDL	OA5-CA3-CA4-CA6
150	C	505	CDL	OB5-CB3-CB4-CB6
150	c	502	CDL	OA5-CA3-CA4-CA6
150	DA	706	CDL	OB5-CB3-CB4-CB6
150	DC	601	CDL	OB5-CB3-CB4-CB6
150	DG	201	CDL	OA5-CA3-CA4-CA6
150	DJ	307	CDL	OB5-CB3-CB4-CB6
150	DU	404	CDL	OB5-CB3-CB4-CB6
150	ED	601	CDL	OB5-CB3-CB4-CB6
150	ED	604	CDL	OB5-CB3-CB4-CB6
150	EI	401	CDL	OB5-CB3-CB4-CB6
150	ES	1101	CDL	OB5-CB3-CB4-CB6
150	Dc	601	CDL	OB5-CB3-CB4-CB6
150	Dd	705	CDL	OA5-CA3-CA4-CA6
150	Dn	502	CDL	OB5-CB3-CB4-CB6
150	Do	501	CDL	OA5-CA3-CA4-CA6
150	Dq	1401	CDL	OB5-CB3-CB4-CB6
150	Dq	1403	CDL	OB5-CB3-CB4-CB6
150	Ds	406	CDL	OB5-CB3-CB4-CB6
153	A1	403	PC1	O11-C1-C2-C3
153	AA	905	PC1	O11-C1-C2-C3
153	AJ	501	PC1	O11-C1-C2-C3
153	AU	201	PC1	O11-C1-C2-C3
153	B1	403	PC1	O11-C1-C2-C3
153	C	509	PC1	O11-C1-C2-C3
153	D	402	PC1	O11-C1-C2-C3
153	EN	1203	PC1	O11-C1-C2-C3
153	Dc	603	PC1	O11-C1-C2-C3
153	Di	1104	PC1	O11-C1-C2-C3
155	A2	401	3PE	O11-C1-C2-C3
155	Dc	606	3PE	O11-C1-C2-C3
150	CC	305	CDL	C52-C53-C54-C55
150	Dc	601	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
150	Dg	202	CDL	C63-C64-C65-C66
150	Ds	401	CDL	C32-C33-C34-C35
150	Ds	402	CDL	C22-C23-C24-C25
153	AA	904	PC1	C3F-C3G-C3H-C3I
151	A0	603	UDP	O4'-C1'-N1-C6
150	Dg	202	CDL	CA5-C11-C12-C13
150	BY	201	CDL	C20-C21-C22-C23
150	DS	404	CDL	C12-C13-C14-C15
150	Dn	502	CDL	C41-C42-C43-C44
150	Ea	501	CDL	C12-C13-C14-C15
150	En	1201	CDL	C53-C54-C55-C56
153	Dc	609	PC1	C2C-C2D-C2E-C2F
153	Dx	1203	PC1	C2B-C2C-C2D-C2E
155	BT	201	3PE	C35-C36-C37-C38
155	DX	304	3PE	C27-C28-C29-C2A
150	DM	502	CDL	CA4-CA6-OA8-CA7
150	EH	1601	CDL	CA4-CA6-OA8-CA7
150	CG	302	CDL	C52-C53-C54-C55
150	DS	404	CDL	C57-C58-C59-C60
150	Dy	301	CDL	C56-C57-C58-C59
150	En	1201	CDL	C34-C35-C36-C37
153	A	1201	PC1	C3B-C3C-C3D-C3E
153	DC	603	PC1	C35-C36-C37-C38
153	Eo	201	PC1	C25-C26-C27-C28
156	DN	504	LPP	C31-C32-C33-C34
150	CG	302	CDL	C72-C73-C74-C75
150	c	506	CDL	C58-C59-C60-C61
150	DN	507	CDL	C12-C13-C14-C15
150	EB	302	CDL	C57-C58-C59-C60
150	EH	1601	CDL	C73-C74-C75-C76
150	EI	401	CDL	C76-C77-C78-C79
150	EL	901	CDL	C55-C56-C57-C58
150	Dj	404	CDL	C18-C19-C20-C21
150	Dm	501	CDL	C82-C83-C84-C85
150	Dn	506	CDL	C43-C44-C45-C46
153	DQ	1503	PC1	C34-C35-C36-C37
153	EO	205	PC1	C2D-C2E-C2F-C2G
156	DN	504	LPP	C37-C38-C39-C40
150	BT	204	CDL	CA5-C11-C12-C13
150	DR	402	CDL	C23-C24-C25-C26
150	EL	901	CDL	C23-C24-C25-C26
150	Di	1101	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
150	Ds	406	CDL	C12-C13-C14-C15
150	El	903	CDL	C61-C62-C63-C64
153	Dx	1209	PC1	C24-C25-C26-C27
150	DQ	1501	CDL	C71-CB7-OB8-CB6
150	A1	402	CDL	CA2-C1-CB2-OB2
150	C	503	CDL	CB2-C1-CA2-OA2
150	DJ	303	CDL	CB2-C1-CA2-OA2
150	EN	1201	CDL	CB2-C1-CA2-OA2
150	Eb	302	CDL	CB2-C1-CA2-OA2
150	Ds	402	CDL	OB7-CB5-OB6-CB4
150	AA	901	CDL	C82-C83-C84-C85
150	CJ	201	CDL	C79-C80-C81-C82
150	CJ	201	CDL	C81-C82-C83-C84
150	C	505	CDL	C11-C12-C13-C14
150	DR	402	CDL	C33-C34-C35-C36
150	DV	403	CDL	C43-C44-C45-C46
150	ED	601	CDL	C56-C57-C58-C59
150	EL	902	CDL	C36-C37-C38-C39
150	Dj	403	CDL	C58-C59-C60-C61
150	Dn	506	CDL	C36-C37-C38-C39
153	AU	201	PC1	C23-C24-C25-C26
153	B1	403	PC1	C2C-C2D-C2E-C2F
153	EO	201	PC1	C3B-C3C-C3D-C3E
153	Dv	406	PC1	C2D-C2E-C2F-C2G
150	BT	202	CDL	C73-C74-C75-C76
150	CD	302	CDL	C20-C21-C22-C23
150	DA	709	CDL	C42-C43-C44-C45
150	DR	403	CDL	C54-C55-C56-C57
150	DU	402	CDL	C42-C43-C44-C45
150	DV	401	CDL	C21-C22-C23-C24
150	Dg	201	CDL	C17-C18-C19-C20
150	Dg	201	CDL	C52-C53-C54-C55
150	Dq	1402	CDL	C17-C18-C19-C20
150	Dr	403	CDL	C41-C42-C43-C44
150	Ds	405	CDL	C76-C77-C78-C79
150	Eu	101	CDL	C40-C41-C42-C43
153	Da	706	PC1	C24-C25-C26-C27
153	Dq	1404	PC1	C34-C35-C36-C37
153	El	904	PC1	C3C-C3D-C3E-C3F
150	AF	401	CDL	C11-CA5-OA6-CA4
150	C	504	CDL	C51-CB5-OB6-CB4
150	DU	402	CDL	C51-CB5-OB6-CB4

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

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Mol	Chain	Res	Type	Atoms
150	Dc	601	CDL	C14-C15-C16-C17
150	Dc	608	CDL	CA3-CA4-CA6-OA8
150	Dd	702	CDL	CA3-CA4-CA6-OA8
150	Dd	704	CDL	CB3-CB4-CB6-OB8
150	Dg	201	CDL	CB3-CB4-CB6-OB8
150	Dh	201	CDL	CA3-CA4-CA6-OA8
150	Di	1103	CDL	CA3-CA4-CA6-OA8
150	Dj	401	CDL	CA3-CA4-CA6-OA8
150	Dm	502	CDL	CA3-CA4-CA6-OA8
150	Dn	501	CDL	CA3-CA4-CA6-OA8
150	Dr	403	CDL	CB3-CB4-CB6-OB8
150	Dv	403	CDL	CA3-CA4-CA6-OA8
150	Dv	403	CDL	C40-C41-C42-C43
150	Dx	1201	CDL	CA3-CA4-CA6-OA8
150	Eb	302	CDL	CB3-CB4-CB6-OB8
150	Eh	1601	CDL	C14-C15-C16-C17
150	Eh	1601	CDL	CB3-CB4-CB6-OB8
150	Ei	401	CDL	CA3-CA4-CA6-OA8
150	El	901	CDL	CB3-CB4-CB6-OB8
150	El	902	CDL	CA3-CA4-CA6-OA8
153	A2	402	PC1	C1-C2-C3-O31
153	A6	303	PC1	C1-C2-C3-O31
153	BT	203	PC1	C1-C2-C3-O31
153	C	508	PC1	C1-C2-C3-O31
153	C	509	PC1	C1-C2-C3-O31
153	K	501	PC1	C1-C2-C3-O31
153	d	801	PC1	C1-C2-C3-O31
153	g	802	PC1	C1-C2-C3-O31
153	DA	708	PC1	C1-C2-C3-O31
153	DC	608	PC1	C1-C2-C3-O31
153	DX	308	PC1	C1-C2-C3-O31
153	DY	302	PC1	C1-C2-C3-O31
153	EN	1203	PC1	C1-C2-C3-O31
153	EO	206	PC1	C1-C2-C3-O31
153	Dc	605	PC1	C1-C2-C3-O31
153	Ds	407	PC1	C1-C2-C3-O31
153	Dv	404	PC1	C1-C2-C3-O31
153	Dy	302	PC1	C1-C2-C3-O31
153	Ef	501	PC1	C33-C34-C35-C36
153	Eo	201	PC1	C1-C2-C3-O31
155	C	513	3PE	C1-C2-C3-O31
155	DR	401	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
155	DX	304	3PE	C1-C2-C3-O31
155	DX	304	3PE	C39-C3A-C3B-C3C
155	EL	904	3PE	C3E-C3F-C3G-C3H
155	EM	901	3PE	C1-C2-C3-O31
155	Da	708	3PE	C28-C29-C2A-C2B
155	Dx	1202	3PE	C1-C2-C3-O31
155	Em	901	3PE	C26-C27-C28-C29
156	DA	710	LPP	C40-C41-C42-C43
156	Dn	504	LPP	C37-C38-C39-C40
150	c	506	CDL	C13-C14-C15-C16
150	DQ	1502	CDL	C38-C39-C40-C41
150	Dd	704	CDL	C12-C13-C14-C15
150	Eg	101	CDL	C79-C80-C81-C82
153	A6	302	PC1	C28-C29-C2A-C2B
153	DJ	306	PC1	C37-C38-C39-C3A
153	DV	404	PC1	C3B-C3C-C3D-C3E
167	CC	303	UQ8	C1-C6-C7-C8
167	C	511	UQ8	C1-C6-C7-C8
150	DQ	1504	CDL	CB4-CB6-OB8-CB7
150	DX	307	CDL	CA4-CA6-OA8-CA7
150	BC	301	CDL	C35-C36-C37-C38
150	DM	501	CDL	C14-C15-C16-C17
150	DV	401	CDL	C18-C19-C20-C21
150	EL	902	CDL	C79-C80-C81-C82
150	Da	709	CDL	C18-C19-C20-C21
150	Da	709	CDL	C21-C22-C23-C24
150	Dj	401	CDL	C13-C14-C15-C16
150	Eg	101	CDL	C11-C12-C13-C14
153	C	508	PC1	C38-C39-C3A-C3B
153	DI	303	PC1	C3A-C3B-C3C-C3D
155	Dx	1208	3PE	C39-C3A-C3B-C3C
150	c	501	CDL	C19-C20-C21-C22
150	EL	903	CDL	C77-C78-C79-C80
150	Dj	404	CDL	C61-C62-C63-C64
155	DI	301	3PE	C35-C36-C37-C38
150	Dv	401	CDL	C72-C71-CB7-OB8
150	CC	305	CDL	CB5-C51-C52-C53
150	DJ	304	CDL	CA5-C11-C12-C13
150	Ds	402	CDL	CB5-C51-C52-C53
150	C	504	CDL	OB9-CB7-OB8-CB6
150	AA	901	CDL	C22-C23-C24-C25
150	DH	202	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
150	Dj	404	CDL	C63-C64-C65-C66
150	Dr	402	CDL	C13-C14-C15-C16
150	Dr	403	CDL	C35-C36-C37-C38
150	Dx	1201	CDL	C38-C39-C40-C41
153	DC	608	PC1	C3D-C3E-C3F-C3G
153	Dv	404	PC1	C3F-C3G-C3H-C3I
167	CC	303	UQ8	C39-C41-C42-C43
150	AP	301	CDL	C60-C61-C62-C63
150	c	502	CDL	C14-C15-C16-C17
150	DH	202	CDL	C73-C74-C75-C76
150	DU	401	CDL	C60-C61-C62-C63
150	DV	402	CDL	C62-C63-C64-C65
150	EN	1202	CDL	C37-C38-C39-C40
150	Dd	702	CDL	C32-C33-C34-C35
150	Dn	503	CDL	C83-C84-C85-C86
153	A9	601	PC1	C2D-C2E-C2F-C2G
153	C	509	PC1	C2E-C2F-C2G-C2H
153	D	402	PC1	C2B-C2C-C2D-C2E
156	AL	304	LPP	C40-C41-C42-C43
150	CD	301	CDL	CB4-CB6-OB8-CB7
150	h	501	CDL	CA4-CA6-OA8-CA7
150	DD	703	CDL	C23-C24-C25-C26
150	DX	301	CDL	C35-C36-C37-C38
150	Dv	401	CDL	C18-C19-C20-C21
153	EB	301	PC1	C36-C37-C38-C39
153	Dg	203	PC1	C3D-C3E-C3F-C3G
153	Eo	204	PC1	C3F-C3G-C3H-C3I
155	AJ	502	3PE	C2B-C2C-C2D-C2E
164	CA	702	FAD	O3'-C3'-C4'-O4'
150	ED	605	CDL	OB9-CB7-OB8-CB6
153	Da	707	PC1	O32-C31-O31-C3
153	AA	906	PC1	C21-C22-C23-C24
150	C	507	CDL	C14-C15-C16-C17
150	DH	202	CDL	C51-C52-C53-C54
150	EH	1601	CDL	C78-C79-C80-C81
150	Dd	704	CDL	C20-C21-C22-C23
150	Du	401	CDL	C60-C61-C62-C63
150	El	902	CDL	C52-C53-C54-C55
153	Dc	604	PC1	C3F-C3G-C3H-C3I
150	B1	402	CDL	C51-CB5-OB6-CB4
150	Dx	1204	CDL	C11-CA5-OA6-CA4
153	AA	906	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
150	DS	405	CDL	C43-C44-C45-C46
150	Du	402	CDL	C19-C20-C21-C22
167	DS	403	UQ8	C30-C29-C31-C32
167	Ds	404	UQ8	C30-C29-C31-C32
150	AC	801	CDL	C62-C63-C64-C65
150	Dd	702	CDL	C37-C38-C39-C40
150	Dx	1201	CDL	C32-C33-C34-C35
153	Db	702	PC1	C2C-C2D-C2E-C2F
155	DC	607	3PE	C25-C26-C27-C28
167	DS	403	UQ8	C28-C29-C31-C32
157	A8	401	ADP	PA-O3A-PB-O1B
157	AQ	201	ADP	PA-O3A-PB-O1B
150	ES	1101	CDL	CA5-C11-C12-C13
150	CD	301	CDL	C71-CB7-OB8-CB6
150	Dm	501	CDL	C71-CB7-OB8-CB6
150	Ds	402	CDL	C31-CA7-OA8-CA6
153	Dc	603	PC1	C32-C31-O31-C3
150	DJ	302	CDL	C37-C38-C39-C40
150	DV	402	CDL	C75-C76-C77-C78
150	Dg	201	CDL	C19-C20-C21-C22
153	DV	404	PC1	C3F-C3G-C3H-C3I
153	Dv	404	PC1	C2A-C2B-C2C-C2D
150	A0	601	CDL	C11-C12-C13-C14
150	DN	506	CDL	C36-C37-C38-C39
150	DO	501	CDL	C11-C12-C13-C14
150	DS	404	CDL	C16-C17-C18-C19
150	DU	401	CDL	C13-C14-C15-C16
150	DY	301	CDL	C56-C57-C58-C59
150	EO	202	CDL	C53-C54-C55-C56
150	Dj	403	CDL	C34-C35-C36-C37
150	Ds	402	CDL	C11-C12-C13-C14
153	DA	707	PC1	C29-C2A-C2B-C2C
153	DX	305	PC1	C24-C25-C26-C27
150	AC	802	CDL	CA6-CA4-OA6-CA5
150	CD	302	CDL	CA3-CA4-OA6-CA5
150	c	501	CDL	CB6-CB4-OB6-CB5
150	DJ	305	CDL	CB6-CB4-OB6-CB5
150	DN	503	CDL	CA6-CA4-OA6-CA5
150	DQ	1502	CDL	CB6-CB4-OB6-CB5
150	Dj	405	CDL	CB6-CB4-OB6-CB5
150	Dq	1403	CDL	CB6-CB4-OB6-CB5
150	Dx	1204	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
150	El	903	CDL	CA3-CA4-OA6-CA5
153	A	1201	PC1	C3-C2-O21-C21
153	k	301	PC1	C3-C2-O21-C21
153	Eo	204	PC1	C1-C2-O21-C21
155	BT	201	3PE	C1-C2-O21-C21
153	AU	202	PC1	O22-C21-O21-C2
150	DH	202	CDL	C44-C45-C46-C47
150	DR	402	CDL	C20-C21-C22-C23
150	EN	1202	CDL	C32-C33-C34-C35
150	Dj	401	CDL	C39-C40-C41-C42
153	C	510	PC1	C28-C29-C2A-C2B
153	DB	702	PC1	C2D-C2E-C2F-C2G
153	DB	702	PC1	C2E-C2F-C2G-C2H
153	Dg	203	PC1	C28-C29-C2A-C2B
153	Dv	405	PC1	C3B-C3C-C3D-C3E
153	El	904	PC1	C3B-C3C-C3D-C3E
150	BV	201	CDL	C17-C18-C19-C20
150	c	509	CDL	C41-C42-C43-C44
150	DD	705	CDL	C84-C85-C86-C87
150	DN	506	CDL	C43-C44-C45-C46
150	EI	401	CDL	C20-C21-C22-C23
150	EL	901	CDL	C42-C43-C44-C45
150	Dd	706	CDL	C20-C21-C22-C23
150	Dg	202	CDL	C14-C15-C16-C17
150	Dj	404	CDL	C53-C54-C55-C56
150	Dq	1402	CDL	C53-C54-C55-C56
153	Eo	204	PC1	C33-C34-C35-C36
150	EI	401	CDL	C1-CA2-OA2-PA1
156	Dn	504	LPP	C6-O5-P1-O3
156	Dl	1101	LPP	C6-O5-P1-O3
150	AA	908	CDL	C39-C40-C41-C42
150	B0	101	CDL	C15-C16-C17-C18
150	C	505	CDL	C38-C39-C40-C41
150	DN	506	CDL	C14-C15-C16-C17
150	Dn	502	CDL	C19-C20-C21-C22
150	Dv	403	CDL	C41-C42-C43-C44
150	Eb	302	CDL	C57-C58-C59-C60
153	B1	403	PC1	C2D-C2E-C2F-C2G
153	c	503	PC1	C3C-C3D-C3E-C3F
153	c	503	PC1	C3D-C3E-C3F-C3G
153	Dc	603	PC1	C35-C36-C37-C38
155	Ds	408	3PE	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
150	CG	302	CDL	C71-CB7-OB8-CB6
150	DD	703	CDL	C31-CA7-OA8-CA6
150	DJ	302	CDL	C31-CA7-OA8-CA6
150	DJ	303	CDL	C31-CA7-OA8-CA6
150	DV	402	CDL	C71-CB7-OB8-CB6
153	A	1201	PC1	C32-C31-O31-C3
155	DI	301	3PE	C32-C31-O31-C3
150	AA	901	CDL	OA5-CA3-CA4-OA6
150	AF	402	CDL	OA5-CA3-CA4-OA6
150	AM	301	CDL	OA5-CA3-CA4-OA6
150	B1	402	CDL	OB5-CB3-CB4-OB6
150	DC	601	CDL	OB5-CB3-CB4-OB6
150	DJ	307	CDL	OA5-CA3-CA4-OA6
150	DU	404	CDL	OB5-CB3-CB4-OB6
150	Dj	402	CDL	OB5-CB3-CB4-OB6
150	Dq	1401	CDL	OA5-CA3-CA4-OA6
150	Eb	302	CDL	OA5-CA3-CA4-OA6
150	Eb	302	CDL	OB5-CB3-CB4-OB6
153	A9	601	PC1	O11-C1-C2-O21
153	AA	903	PC1	O11-C1-C2-O21
153	AA	905	PC1	O11-C1-C2-O21
153	c	503	PC1	O11-C1-C2-O21
153	DB	702	PC1	O11-C1-C2-O21
153	DX	308	PC1	O11-C1-C2-O21
153	EN	1203	PC1	O11-C1-C2-O21
155	Ds	403	3PE	O11-C1-C2-O21
150	B1	402	CDL	C76-C77-C78-C79
150	BT	204	CDL	C44-C45-C46-C47
150	DS	401	CDL	C72-C73-C74-C75
150	ES	1101	CDL	C72-C73-C74-C75
150	Dd	705	CDL	C84-C85-C86-C87
150	Ds	405	CDL	C57-C58-C59-C60
150	Dv	401	CDL	C14-C15-C16-C17
153	DV	404	PC1	C2A-C2B-C2C-C2D
155	EN	1204	3PE	C3E-C3F-C3G-C3H
150	DM	502	CDL	C19-C20-C21-C22
150	Ds	406	CDL	C43-C44-C45-C46
153	DV	405	PC1	C2D-C2E-C2F-C2G
155	DC	607	3PE	C34-C35-C36-C37
150	El	901	CDL	O1-C1-CA2-OA2
150	DM	501	CDL	OB9-CB7-OB8-CB6
150	DN	507	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
150	Ed	205	CDL	OB9-CB7-OB8-CB6
153	AA	903	PC1	O32-C31-O31-C3
153	Eo	204	PC1	O32-C31-O31-C3
150	Dj	401	CDL	C17-C18-C19-C20
150	BV	201	CDL	CB5-C51-C52-C53
150	DU	402	CDL	CA5-C11-C12-C13
155	Di	1102	3PE	C35-C36-C37-C38
150	Ek	201	CDL	CA4-CA6-OA8-CA7
150	A0	601	CDL	OA6-CA4-CA6-OA8
150	A1	402	CDL	OA6-CA4-CA6-OA8
150	AM	301	CDL	OB6-CB4-CB6-OB8
150	BC	302	CDL	OB6-CB4-CB6-OB8
150	BG	201	CDL	OA6-CA4-CA6-OA8
150	c	509	CDL	OB6-CB4-CB6-OB8
150	DD	704	CDL	OA6-CA4-CA6-OA8
150	EN	1201	CDL	OA6-CA4-CA6-OA8
150	Dm	502	CDL	OA6-CA4-CA6-OA8
153	C	509	PC1	O21-C2-C3-O31
153	DA	708	PC1	O21-C2-C3-O31
153	DS	406	PC1	O21-C2-C3-O31
153	DX	308	PC1	O21-C2-C3-O31
155	EN	1204	3PE	O21-C2-C3-O31
150	DU	403	CDL	C12-C13-C14-C15
150	DY	301	CDL	C14-C15-C16-C17
150	DZ	501	CDL	C73-C74-C75-C76
150	Do	501	CDL	C11-C12-C13-C14
153	c	507	PC1	C39-C3A-C3B-C3C
153	DG	203	PC1	C28-C29-C2A-C2B
153	Dj	406	PC1	C37-C38-C39-C3A
150	BC	302	CDL	OA7-CA5-OA6-CA4
150	CJ	201	CDL	OB7-CB5-OB6-CB4
153	c	507	PC1	O22-C21-O21-C2
153	C	508	PC1	O32-C31-O31-C3
150	B1	402	CDL	C77-C78-C79-C80
150	C	503	CDL	C55-C56-C57-C58
150	C	506	CDL	C44-C45-C46-C47
150	H	1301	CDL	C38-C39-C40-C41
150	DV	403	CDL	C40-C41-C42-C43
150	Dh	201	CDL	C12-C13-C14-C15
150	Dn	501	CDL	C76-C77-C78-C79
153	D	402	PC1	C3F-C3G-C3H-C3I
153	DG	203	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
153	Db	702	PC1	C2A-C2B-C2C-C2D
156	Dn	504	LPP	C35-C36-C37-C38
150	A0	602	CDL	C13-C14-C15-C16
150	A1	402	CDL	C84-C85-C86-C87
150	AP	301	CDL	C14-C15-C16-C17
150	B1	402	CDL	C11-C12-C13-C14
150	CG	302	CDL	C73-C74-C75-C76
150	C	504	CDL	C75-C76-C77-C78
150	DQ	1504	CDL	C53-C54-C55-C56
150	Dd	702	CDL	C23-C24-C25-C26
150	Ei	401	CDL	C20-C21-C22-C23
155	Dc	607	3PE	C25-C26-C27-C28
167	Ds	404	UQ8	C28-C29-C31-C32
150	CJ	201	CDL	C73-C74-C75-C76
150	DI	302	CDL	C79-C80-C81-C82
150	Dj	401	CDL	C35-C36-C37-C38
150	Dm	501	CDL	C81-C82-C83-C84
153	Db	702	PC1	C2E-C2F-C2G-C2H
155	DS	402	3PE	C2B-C2C-C2D-C2E
155	Di	1102	3PE	C39-C3A-C3B-C3C
150	AA	901	CDL	C81-C82-C83-C84
150	B0	101	CDL	C18-C19-C20-C21
150	BY	201	CDL	C76-C77-C78-C79
150	E	301	CDL	C14-C15-C16-C17
150	DI	302	CDL	C19-C20-C21-C22
150	DM	501	CDL	C82-C83-C84-C85
150	DV	402	CDL	C11-C12-C13-C14
150	EB	302	CDL	C55-C56-C57-C58
150	Dn	502	CDL	C36-C37-C38-C39
153	EO	205	PC1	C2E-C2F-C2G-C2H
153	Da	706	PC1	C29-C2A-C2B-C2C
153	Eb	301	PC1	C36-C37-C38-C39
150	c	509	CDL	C31-CA7-OA8-CA6
150	Dm	502	CDL	C31-CA7-OA8-CA6
150	El	901	CDL	C31-CA7-OA8-CA6
153	DS	406	PC1	C32-C31-O31-C3
153	Dv	405	PC1	C32-C31-O31-C3
155	Dx	1202	3PE	C32-C31-O31-C3
150	Dg	201	CDL	C56-C57-C58-C59
150	Dh	202	CDL	C44-C45-C46-C47
153	BT	203	PC1	C33-C34-C35-C36
153	DB	702	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
153	DC	604	PC1	C3F-C3G-C3H-C3I
150	B1	402	CDL	C55-C56-C57-C58
150	DM	501	CDL	C77-C78-C79-C80
150	Dc	608	CDL	C20-C21-C22-C23
150	Do	501	CDL	C12-C13-C14-C15
153	AH	301	PC1	C3C-C3D-C3E-C3F
153	DS	406	PC1	C3F-C3G-C3H-C3I
153	EO	204	PC1	C3B-C3C-C3D-C3E
153	Dc	605	PC1	C3F-C3G-C3H-C3I
150	BG	201	CDL	C11-C12-C13-C14
150	CJ	201	CDL	C17-C18-C19-C20
150	C	505	CDL	C72-C73-C74-C75
150	DJ	305	CDL	C22-C23-C24-C25
150	DU	403	CDL	C14-C15-C16-C17
150	Dc	601	CDL	C36-C37-C38-C39
153	EO	201	PC1	C2B-C2C-C2D-C2E
153	Dv	405	PC1	C3F-C3G-C3H-C3I
150	DD	706	CDL	CA4-CA6-OA8-CA7
150	DD	705	CDL	CA2-C1-CB2-OB2
150	Dy	301	CDL	CA2-C1-CB2-OB2
153	A6	303	PC1	O22-C21-O21-C2
150	CG	301	CDL	C11-CA5-OA6-CA4
150	DN	502	CDL	C51-CB5-OB6-CB4
150	DX	307	CDL	C11-CA5-OA6-CA4
155	Dx	1206	3PE	C22-C21-O21-C2
150	AF	402	CDL	C20-C21-C22-C23
150	c	501	CDL	C12-C13-C14-C15
150	DA	706	CDL	C15-C16-C17-C18
150	DJ	303	CDL	C84-C85-C86-C87
150	DR	402	CDL	C84-C85-C86-C87
150	DS	404	CDL	C76-C77-C78-C79
150	DV	402	CDL	C82-C83-C84-C85
150	Dr	402	CDL	C59-C60-C61-C62
150	Ep	701	CDL	C84-C85-C86-C87
155	Dd	703	3PE	C35-C36-C37-C38
150	AF	402	CDL	C31-CA7-OA8-CA6
150	DS	401	CDL	C31-CA7-OA8-CA6
150	DU	401	CDL	C31-CA7-OA8-CA6
150	ED	605	CDL	C31-CA7-OA8-CA6
150	Dj	402	CDL	C71-CB7-OB8-CB6
150	Dy	301	CDL	C31-CA7-OA8-CA6
150	En	1201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	Eu	101	CDL	C71-CB7-OB8-CB6
150	DS	401	CDL	C11-C12-C13-C14
150	Dg	201	CDL	C12-C13-C14-C15
150	Dj	403	CDL	CA5-C11-C12-C13
150	Do	501	CDL	C20-C21-C22-C23
156	Dl	1101	LPP	C41-C42-C43-C44
169	DA	703	HEA	C4D-C3D-CAD-CBD
169	Da	703	HEA	C4D-C3D-CAD-CBD
150	Ds	402	CDL	OA9-CA7-OA8-CA6
150	DN	506	CDL	C20-C21-C22-C23
150	DR	402	CDL	C13-C14-C15-C16
150	DV	403	CDL	C41-C42-C43-C44
150	Ds	405	CDL	C42-C43-C44-C45
150	Dv	402	CDL	C82-C83-C84-C85
153	DX	308	PC1	C2B-C2C-C2D-C2E
150	Dd	706	CDL	CA4-CA6-OA8-CA7
150	A1	402	CDL	OA5-CA3-CA4-CA6
150	AA	901	CDL	OA5-CA3-CA4-CA6
150	BC	302	CDL	OB5-CB3-CB4-CB6
150	CG	301	CDL	OA5-CA3-CA4-CA6
150	CC	304	CDL	OA5-CA3-CA4-CA6
150	C	503	CDL	OB5-CB3-CB4-CB6
150	DQ	1502	CDL	OB5-CB3-CB4-CB6
150	DQ	1504	CDL	OA5-CA3-CA4-CA6
150	DQ	1504	CDL	OB5-CB3-CB4-CB6
150	DS	405	CDL	OB5-CB3-CB4-CB6
150	DU	401	CDL	OB5-CB3-CB4-CB6
150	DX	307	CDL	OB5-CB3-CB4-CB6
150	DZ	501	CDL	OB5-CB3-CB4-CB6
150	EA	301	CDL	OA5-CA3-CA4-CA6
150	EB	302	CDL	OA5-CA3-CA4-CA6
150	ED	604	CDL	OA5-CA3-CA4-CA6
150	EL	901	CDL	OB5-CB3-CB4-CB6
150	Di	1101	CDL	OB5-CB3-CB4-CB6
150	Di	1103	CDL	OB5-CB3-CB4-CB6
150	Dn	502	CDL	OA5-CA3-CA4-CA6
150	Dn	503	CDL	OB5-CB3-CB4-CB6
150	Ds	402	CDL	OB5-CB3-CB4-CB6
150	Du	401	CDL	OB5-CB3-CB4-CB6
150	Du	403	CDL	OB5-CB3-CB4-CB6
150	Dx	1204	CDL	OB5-CB3-CB4-CB6
150	Ea	501	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
150	Eb	302	CDL	OA5-CA3-CA4-CA6
150	El	901	CDL	OA5-CA3-CA4-CA6
153	A9	601	PC1	O11-C1-C2-C3
153	AA	903	PC1	O11-C1-C2-C3
153	DQ	1503	PC1	O11-C1-C2-C3
153	Dq	1404	PC1	O11-C1-C2-C3
153	Dx	1203	PC1	O11-C1-C2-C3
155	BP	201	3PE	O11-C1-C2-C3
155	Da	708	3PE	O11-C1-C2-C3
155	Dr	404	3PE	O11-C1-C2-C3
155	Dx	1207	3PE	O11-C1-C2-C3
150	DJ	304	CDL	C16-C17-C18-C19
150	Dn	502	CDL	C11-C12-C13-C14
150	Dr	402	CDL	C84-C85-C86-C87
150	Ds	402	CDL	C77-C78-C79-C80
153	Eo	204	PC1	C2A-C2B-C2C-C2D
150	c	509	CDL	CA5-C11-C12-C13
155	DN	501	3PE	O13-C11-C12-N
155	Dg	204	3PE	O13-C11-C12-N
150	Dh	201	CDL	C19-C20-C21-C22
150	C	504	CDL	C31-CA7-OA8-CA6
150	Dg	202	CDL	C71-CB7-OB8-CB6
150	Dv	401	CDL	C71-CB7-OB8-CB6
150	Dv	402	CDL	C71-CB7-OB8-CB6
153	Dc	603	PC1	O32-C31-O31-C3
150	DQ	1501	CDL	C12-C13-C14-C15
150	DU	403	CDL	C15-C16-C17-C18
167	C	511	UQ8	C25-C24-C26-C27
169	DA	702	HEA	C26-C15-C16-C17
169	Da	702	HEA	C26-C15-C16-C17
150	Dn	501	CDL	CB7-C71-C72-C73
150	C	506	CDL	C12-C13-C14-C15
150	c	506	CDL	C15-C16-C17-C18
150	EL	901	CDL	C44-C45-C46-C47
150	Du	401	CDL	C71-C72-C73-C74
150	BC	301	CDL	O1-C1-CB2-OB2
150	Dx	1201	CDL	OA7-CA5-OA6-CA4
153	DS	406	PC1	O22-C21-O21-C2
150	DQ	1501	CDL	OB9-CB7-OB8-CB6
150	Dh	202	CDL	C51-C52-C53-C54
155	DI	301	3PE	C39-C3A-C3B-C3C
164	CA	702	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
150	DH	202	CDL	C53-C54-C55-C56
150	EB	302	CDL	C12-C13-C14-C15
150	Dd	702	CDL	C20-C21-C22-C23
150	Dj	407	CDL	C77-C78-C79-C80
150	Ds	405	CDL	C12-C13-C14-C15
153	CC	302	PC1	C35-C36-C37-C38
150	CD	301	CDL	C11-CA5-OA6-CA4
150	AF	401	CDL	C31-CA7-OA8-CA6
150	DU	403	CDL	C31-CA7-OA8-CA6
150	Ed	205	CDL	C31-CA7-OA8-CA6
153	AM	302	PC1	C32-C31-O31-C3
153	DY	302	PC1	C32-C31-O31-C3
153	Db	702	PC1	C32-C31-O31-C3
153	DC	604	PC1	O21-C21-C22-C23
150	Dd	704	CDL	CA5-C11-C12-C13
150	C	504	CDL	C24-C25-C26-C27
150	Dm	501	CDL	C58-C59-C60-C61
153	EO	205	PC1	C2B-C2C-C2D-C2E
155	Ds	403	3PE	C2B-C2C-C2D-C2E
150	A0	602	CDL	C1-CA2-OA2-PA1
150	A1	402	CDL	CB4-CB3-OB5-PB2
150	AF	401	CDL	C1-CB2-OB2-PB2
150	B0	102	CDL	CA4-CA3-OA5-PA1
150	CG	301	CDL	C1-CB2-OB2-PB2
150	C	507	CDL	C1-CA2-OA2-PA1
150	DD	704	CDL	CB4-CB3-OB5-PB2
150	DS	405	CDL	C1-CA2-OA2-PA1
150	DU	404	CDL	C1-CB2-OB2-PB2
150	ED	604	CDL	CA4-CA3-OA5-PA1
150	EI	401	CDL	CB4-CB3-OB5-PB2
150	EO	202	CDL	CA4-CA3-OA5-PA1
150	Dh	202	CDL	C1-CB2-OB2-PB2
150	Di	1101	CDL	CA4-CA3-OA5-PA1
150	Eg	101	CDL	C1-CA2-OA2-PA1
150	Eu	101	CDL	CA4-CA3-OA5-PA1
153	A	1201	PC1	C2-C1-O11-P
153	DA	707	PC1	C2-C1-O11-P
155	BA	301	3PE	C2-C1-O11-P
150	CC	304	CDL	C40-C41-C42-C43
150	DM	502	CDL	C11-C12-C13-C14
150	DM	502	CDL	C52-C53-C54-C55
150	DN	503	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
150	DS	401	CDL	C22-C23-C24-C25
153	BS	1301	PC1	C3E-C3F-C3G-C3H
150	B0	101	CDL	C31-C32-C33-C34
150	DD	704	CDL	C60-C61-C62-C63
150	DS	404	CDL	C42-C43-C44-C45
150	DV	403	CDL	C31-C32-C33-C34
150	EL	903	CDL	C61-C62-C63-C64
150	Di	1103	CDL	C19-C20-C21-C22
150	Dn	506	CDL	C11-C12-C13-C14
150	Dx	1204	CDL	C64-C65-C66-C67
153	BG	202	PC1	C23-C24-C25-C26
156	EI	402	LPP	C18-C19-C20-C21
150	El	901	CDL	CB5-C51-C52-C53
150	Dm	501	CDL	OB9-CB7-OB8-CB6
150	CG	301	CDL	C71-C72-C73-C74
150	DH	201	CDL	C63-C64-C65-C66
150	AA	908	CDL	C31-CA7-OA8-CA6
150	DD	705	CDL	C31-CA7-OA8-CA6
150	DU	401	CDL	C71-CB7-OB8-CB6
150	EL	901	CDL	C31-CA7-OA8-CA6
150	Dm	501	CDL	C31-CA7-OA8-CA6
153	B1	401	PC1	C32-C31-O31-C3
153	DC	603	PC1	C32-C31-O31-C3
150	DH	201	CDL	C21-C22-C23-C24
150	Dr	402	CDL	C75-C76-C77-C78
150	Ep	701	CDL	C60-C61-C62-C63
150	AA	908	CDL	CA3-CA4-CA6-OA8
150	BE	201	CDL	CB3-CB4-CB6-OB8
150	BV	201	CDL	CA3-CA4-CA6-OA8
150	CD	301	CDL	CB3-CB4-CB6-OB8
150	C	504	CDL	CB3-CB4-CB6-OB8
150	C	505	CDL	CA3-CA4-CA6-OA8
150	c	506	CDL	CA3-CA4-CA6-OA8
150	g	801	CDL	CB3-CB4-CB6-OB8
150	h	501	CDL	CA3-CA4-CA6-OA8
150	DA	706	CDL	CA3-CA4-CA6-OA8
150	DA	706	CDL	CB3-CB4-CB6-OB8
150	DA	709	CDL	CA3-CA4-CA6-OA8
150	DD	705	CDL	CA3-CA4-CA6-OA8
150	DH	201	CDL	CA3-CA4-CA6-OA8
150	DJ	304	CDL	CB3-CB4-CB6-OB8
150	DJ	307	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
150	DR	403	CDL	CB3-CB4-CB6-OB8
150	ED	605	CDL	CA3-CA4-CA6-OA8
150	Da	709	CDL	CA3-CA4-CA6-OA8
150	Dc	601	CDL	CA3-CA4-CA6-OA8
150	Dg	201	CDL	CA3-CA4-CA6-OA8
150	Dg	202	CDL	CB3-CB4-CB6-OB8
150	Di	1101	CDL	CB3-CB4-CB6-OB8
150	Dj	407	CDL	CA3-CA4-CA6-OA8
150	Dr	402	CDL	CA3-CA4-CA6-OA8
150	Ed	205	CDL	CA3-CA4-CA6-OA8
153	A6	302	PC1	C1-C2-C3-O31
153	AA	906	PC1	C1-C2-C3-O31
153	AA	907	PC1	C1-C2-C3-O31
153	B1	401	PC1	C1-C2-C3-O31
153	BS	1301	PC1	C1-C2-C3-O31
153	CC	302	PC1	C1-C2-C3-O31
153	C	510	PC1	C1-C2-C3-O31
153	DA	707	PC1	C1-C2-C3-O31
153	DS	406	PC1	C1-C2-C3-O31
153	DV	404	PC1	C1-C2-C3-O31
153	DV	406	PC1	C1-C2-C3-O31
153	Da	706	PC1	C1-C2-C3-O31
153	Dc	609	PC1	C1-C2-C3-O31
155	BA	301	3PE	C1-C2-C3-O31
155	CC	301	3PE	C1-C2-C3-O31
155	DN	501	3PE	C1-C2-C3-O31
155	EL	904	3PE	C1-C2-C3-O31
155	Da	708	3PE	C1-C2-C3-O31
155	El	905	3PE	C1-C2-C3-O31
155	Em	901	3PE	C1-C2-C3-O31
156	AC	803	LPP	C6-C7-C8-O27
150	B1	402	CDL	OB7-CB5-OB6-CB4
155	DJ	301	3PE	O22-C21-O21-C2
150	DD	705	CDL	C40-C41-C42-C43
150	Ea	502	CDL	C11-C12-C13-C14
153	DC	608	PC1	C3C-C3D-C3E-C3F
153	Dg	203	PC1	C26-C27-C28-C29
150	DY	301	CDL	CA5-C11-C12-C13
150	CG	302	CDL	OB9-CB7-OB8-CB6
150	DV	402	CDL	OB9-CB7-OB8-CB6
150	B0	102	CDL	C15-C16-C17-C18
150	C	505	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
150	Da	709	CDL	C39-C40-C41-C42
150	Dg	201	CDL	C72-C73-C74-C75
153	Dc	603	PC1	C3D-C3E-C3F-C3G
155	DI	301	3PE	C38-C39-C3A-C3B
155	Dc	607	3PE	C2F-C2G-C2H-C2I
150	Dj	403	CDL	C11-C12-C13-C14
153	DB	702	PC1	C38-C39-C3A-C3B
153	DC	603	PC1	C2C-C2D-C2E-C2F
150	CD	301	CDL	OB9-CB7-OB8-CB6
167	ED	603	UQ8	C40-C39-C41-C42
169	DA	702	HEA	C14-C15-C16-C17
150	DJ	304	CDL	C59-C60-C61-C62
150	ES	1101	CDL	C58-C59-C60-C61
153	AQ	202	PC1	C28-C29-C2A-C2B
150	Dd	702	CDL	C14-C15-C16-C17
150	Dd	706	CDL	C77-C78-C79-C80
150	Dj	402	CDL	C51-C52-C53-C54
153	Eo	205	PC1	C3B-C3C-C3D-C3E
150	AF	402	CDL	CA2-OA2-PA1-OA5
150	B0	101	CDL	CA3-OA5-PA1-OA2
150	B0	101	CDL	CB3-OB5-PB2-OB2
150	BE	201	CDL	CA3-OA5-PA1-OA2
150	BT	204	CDL	CA2-OA2-PA1-OA5
150	BY	201	CDL	CA3-OA5-PA1-OA2
150	c	506	CDL	CA3-OA5-PA1-OA2
150	DX	306	CDL	CA3-OA5-PA1-OA2
150	Dd	705	CDL	CA3-OA5-PA1-OA2
150	Di	1103	CDL	CB2-OB2-PB2-OB5
150	Dj	402	CDL	CA2-OA2-PA1-OA5
150	Du	402	CDL	CB2-OB2-PB2-OB5
150	Ed	205	CDL	CB3-OB5-PB2-OB2
153	A6	303	PC1	C11-O13-P-O11
153	A9	603	PC1	C1-O11-P-O13
153	d	801	PC1	C11-O13-P-O11
153	g	802	PC1	C1-O11-P-O13
153	EB	303	PC1	C1-O11-P-O13
155	BP	201	3PE	C1-O11-P-O13
155	G	401	3PE	C1-O11-P-O13
155	DG	205	3PE	C1-O11-P-O13
150	DG	201	CDL	CA5-C11-C12-C13
150	DD	703	CDL	OA9-CA7-OA8-CA6
153	A	1201	PC1	O32-C31-O31-C3

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

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Mol	Chain	Res	Type	Atoms
155	DI	301	3PE	O32-C31-O31-C3
150	DV	401	CDL	CB5-C51-C52-C53
150	EL	903	CDL	CA7-C31-C32-C33
150	C	506	CDL	C24-C25-C26-C27
150	Dq	1401	CDL	C35-C36-C37-C38
153	Dx	1205	PC1	C3D-C3E-C3F-C3G
150	BV	201	CDL	C72-C71-CB7-OB8
150	CD	301	CDL	C32-C31-CA7-OA8
153	Dv	406	PC1	O31-C31-C32-C33
150	DD	706	CDL	C44-C45-C46-C47
150	Dn	506	CDL	C84-C85-C86-C87
153	DA	707	PC1	C37-C38-C39-C3A
153	DC	603	PC1	C3D-C3E-C3F-C3G
155	Dx	1206	3PE	C2F-C2G-C2H-C2I
150	c	509	CDL	OA9-CA7-OA8-CA6
150	El	901	CDL	OA9-CA7-OA8-CA6
150	AM	301	CDL	C37-C38-C39-C40
150	CG	302	CDL	C14-C15-C16-C17
150	C	505	CDL	C19-C20-C21-C22
150	DD	704	CDL	C11-C12-C13-C14
153	C	509	PC1	C3E-C3F-C3G-C3H
167	Ed	202	UQ8	C2-C3-O3-C3M
150	Dr	402	CDL	CB7-C71-C72-C73
150	DU	404	CDL	C13-C14-C15-C16
150	AF	401	CDL	OA6-CA4-CA6-OA8
150	BE	201	CDL	OB6-CB4-CB6-OB8
150	BT	204	CDL	OB6-CB4-CB6-OB8
150	BV	201	CDL	OB6-CB4-CB6-OB8
150	BY	201	CDL	OA6-CA4-CA6-OA8
150	CD	301	CDL	OB6-CB4-CB6-OB8
150	DJ	303	CDL	OA6-CA4-CA6-OA8
150	DM	501	CDL	OA6-CA4-CA6-OA8
150	DS	401	CDL	OA6-CA4-CA6-OA8
150	DU	401	CDL	OA6-CA4-CA6-OA8
150	DX	307	CDL	OA6-CA4-CA6-OA8
150	ED	604	CDL	OA6-CA4-CA6-OA8
150	EI	401	CDL	OA6-CA4-CA6-OA8
150	EL	902	CDL	OA6-CA4-CA6-OA8
150	EL	902	CDL	OB6-CB4-CB6-OB8
150	Dc	608	CDL	OA6-CA4-CA6-OA8
150	Dd	702	CDL	OB6-CB4-CB6-OB8
150	Dd	704	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
150	Dg	202	CDL	OB6-CB4-CB6-OB8
150	Di	1103	CDL	OA6-CA4-CA6-OA8
150	Dj	401	CDL	OA6-CA4-CA6-OA8
150	Dn	501	CDL	OA6-CA4-CA6-OA8
150	Ds	402	CDL	OA6-CA4-CA6-OA8
150	Dy	301	CDL	OA6-CA4-CA6-OA8
150	Eh	1601	CDL	OB6-CB4-CB6-OB8
150	Ei	401	CDL	OA6-CA4-CA6-OA8
150	El	902	CDL	OA6-CA4-CA6-OA8
153	A2	402	PC1	O21-C2-C3-O31
153	A6	302	PC1	O21-C2-C3-O31
153	AA	903	PC1	O21-C2-C3-O31
153	BS	1301	PC1	O21-C2-C3-O31
153	C	508	PC1	O21-C2-C3-O31
153	K	501	PC1	O21-C2-C3-O31
153	d	801	PC1	O21-C2-C3-O31
153	EO	206	PC1	O21-C2-C3-O31
153	Dy	302	PC1	O21-C2-C3-O31
155	BA	301	3PE	O21-C2-C3-O31
155	CC	301	3PE	O21-C2-C3-O31
155	DC	607	3PE	O21-C2-C3-O31
155	DX	304	3PE	O21-C2-C3-O31
155	Dc	607	3PE	O21-C2-C3-O31
155	Dr	401	3PE	O21-C2-C3-O31
155	Em	901	3PE	O21-C2-C3-O31
150	AC	801	CDL	C71-CB7-OB8-CB6
153	A0	605	PC1	C32-C31-O31-C3
153	Dy	302	PC1	C32-C31-O31-C3
153	c	507	PC1	O21-C21-C22-C23
150	DN	503	CDL	C11-C12-C13-C14
150	DU	402	CDL	C60-C61-C62-C63
150	Di	1101	CDL	C77-C78-C79-C80
150	Eb	302	CDL	C37-C38-C39-C40
150	Dc	608	CDL	C51-CB5-OB6-CB4
150	Eu	101	CDL	C51-CB5-OB6-CB4
153	d	801	PC1	C22-C21-O21-C2
150	Dm	501	CDL	C76-C77-C78-C79
153	DC	602	PC1	C3F-C3G-C3H-C3I
150	DD	703	CDL	CB2-C1-CA2-OA2
150	Ds	405	CDL	CA2-C1-CB2-OB2
150	Dv	401	CDL	CA2-C1-CB2-OB2
150	Ed	204	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
150	El	901	CDL	CA2-C1-CB2-OB2
167	ED	603	UQ8	C24-C26-C27-C28
150	AC	801	CDL	C39-C40-C41-C42
150	DR	403	CDL	C37-C38-C39-C40
150	DS	405	CDL	C14-C15-C16-C17
150	El	901	CDL	C36-C37-C38-C39
150	AF	401	CDL	OA7-CA5-OA6-CA4
150	CG	301	CDL	OA7-CA5-OA6-CA4
150	CC	305	CDL	OA7-CA5-OA6-CA4
150	C	504	CDL	OB7-CB5-OB6-CB4
150	DN	502	CDL	OB7-CB5-OB6-CB4
150	DU	402	CDL	OB7-CB5-OB6-CB4
150	DX	306	CDL	OB7-CB5-OB6-CB4
150	DX	307	CDL	OA7-CA5-OA6-CA4
150	Dx	1204	CDL	OA7-CA5-OA6-CA4
153	AA	906	PC1	O22-C21-O21-C2
155	Dx	1206	3PE	O22-C21-O21-C2
167	EN	1205	UQ8	C40-C39-C41-C42
167	ED	603	UQ8	C38-C39-C41-C42
169	Da	702	HEA	C14-C15-C16-C17
150	DA	706	CDL	C75-C76-C77-C78
150	DA	706	CDL	C77-C78-C79-C80
150	EL	902	CDL	C52-C53-C54-C55
150	EL	903	CDL	C43-C44-C45-C46
150	Dg	202	CDL	C80-C81-C82-C83
150	Ds	402	CDL	C80-C81-C82-C83
150	El	903	CDL	C23-C24-C25-C26
153	Dc	603	PC1	C2C-C2D-C2E-C2F
153	Dg	203	PC1	O31-C31-C32-C33
150	DQ	1501	CDL	CB5-C51-C52-C53
150	DA	706	CDL	C55-C56-C57-C58
150	DG	201	CDL	C17-C18-C19-C20
150	EN	1201	CDL	C40-C41-C42-C43
150	Ea	501	CDL	C44-C45-C46-C47
153	Eo	205	PC1	C29-C2A-C2B-C2C
150	DG	202	CDL	C72-C73-C74-C75
150	Eh	1601	CDL	C73-C74-C75-C76
153	AA	905	PC1	C3B-C3C-C3D-C3E
153	Db	702	PC1	C38-C39-C3A-C3B
150	AA	901	CDL	CA4-CA3-OA5-PA1
150	AC	802	CDL	CB4-CB3-OB5-PB2
150	AP	301	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
150	AP	301	CDL	CB4-CB3-OB5-PB2
150	BG	201	CDL	C1-CB2-OB2-PB2
150	BL	301	CDL	CA4-CA3-OA5-PA1
150	C	506	CDL	C1-CB2-OB2-PB2
150	c	501	CDL	CB4-CB3-OB5-PB2
150	c	502	CDL	C1-CA2-OA2-PA1
150	DA	706	CDL	CB4-CB3-OB5-PB2
150	DN	503	CDL	CA4-CA3-OA5-PA1
150	DN	507	CDL	CA4-CA3-OA5-PA1
150	DR	402	CDL	CA4-CA3-OA5-PA1
150	DV	402	CDL	C1-CA2-OA2-PA1
150	DX	307	CDL	C1-CB2-OB2-PB2
150	DZ	501	CDL	C1-CB2-OB2-PB2
150	EA	301	CDL	CA4-CA3-OA5-PA1
150	EN	1202	CDL	C1-CA2-OA2-PA1
150	Dj	403	CDL	CA4-CA3-OA5-PA1
150	Dj	404	CDL	C1-CB2-OB2-PB2
150	Dj	404	CDL	CB4-CB3-OB5-PB2
150	Dn	502	CDL	C1-CB2-OB2-PB2
150	Dn	506	CDL	C1-CB2-OB2-PB2
150	Du	402	CDL	C1-CA2-OA2-PA1
150	Du	403	CDL	C1-CA2-OA2-PA1
150	Dv	401	CDL	C1-CA2-OA2-PA1
150	Dv	402	CDL	C1-CB2-OB2-PB2
150	Dx	1204	CDL	CA4-CA3-OA5-PA1
150	Ea	502	CDL	CA4-CA3-OA5-PA1
150	Ed	204	CDL	C1-CA2-OA2-PA1
150	Eh	1601	CDL	C1-CA2-OA2-PA1
150	Ek	201	CDL	C1-CA2-OA2-PA1
150	El	902	CDL	CA4-CA3-OA5-PA1
153	AC	804	PC1	C2-C1-O11-P
153	C	508	PC1	C2-C1-O11-P
153	C	509	PC1	C2-C1-O11-P
153	Db	702	PC1	C2-C1-O11-P
155	DG	204	3PE	C2-C1-O11-P
155	Dc	607	3PE	C2-C1-O11-P
150	Dm	502	CDL	OA9-CA7-OA8-CA6
153	DS	406	PC1	O32-C31-O31-C3
153	Dv	405	PC1	O32-C31-O31-C3
155	Dx	1202	3PE	O32-C31-O31-C3
150	AC	802	CDL	C38-C39-C40-C41
150	B1	402	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
150	CD	301	CDL	C37-C38-C39-C40
150	DG	202	CDL	C34-C35-C36-C37
150	DS	404	CDL	C11-C12-C13-C14
150	DU	404	CDL	C17-C18-C19-C20
150	Ds	405	CDL	C11-C12-C13-C14
153	AA	904	PC1	C11-C12-N-C13
153	EO	205	PC1	C11-C12-N-C13
153	Di	1104	PC1	C11-C12-N-C14
150	Dx	1204	CDL	CA7-C31-C32-C33
150	g	801	CDL	C13-C14-C15-C16
150	DG	202	CDL	C35-C36-C37-C38
150	Dd	705	CDL	C44-C45-C46-C47
150	Di	1103	CDL	C33-C34-C35-C36
150	Dr	402	CDL	C34-C35-C36-C37
153	BT	203	PC1	C3B-C3C-C3D-C3E
155	DR	401	3PE	C35-C36-C37-C38
156	EI	402	LPP	C38-C39-C40-C41
150	BE	201	CDL	C42-C43-C44-C45
150	DN	507	CDL	C38-C39-C40-C41
150	EL	903	CDL	C84-C85-C86-C87
150	Dh	201	CDL	C31-CA7-OA8-CA6
150	EL	901	CDL	C11-C12-C13-C14
153	Da	706	PC1	C37-C38-C39-C3A
168	C	502	HEM	C3D-CAD-CBD-CGD
150	CD	301	CDL	OA7-CA5-OA6-CA4
150	Dn	502	CDL	OA7-CA5-OA6-CA4
150	Eu	101	CDL	OB7-CB5-OB6-CB4
150	CC	305	CDL	C11-CA5-OA6-CA4
150	DS	405	CDL	C11-CA5-OA6-CA4
150	DZ	501	CDL	C11-CA5-OA6-CA4
150	Dn	502	CDL	C11-CA5-OA6-CA4
153	C	510	PC1	C22-C21-O21-C2
155	EL	904	3PE	C22-C21-O21-C2
150	BY	201	CDL	C11-C12-C13-C14
150	EL	901	CDL	C12-C13-C14-C15
150	Da	709	CDL	C40-C41-C42-C43
150	Dj	403	CDL	C79-C80-C81-C82
153	DA	708	PC1	C3E-C3F-C3G-C3H
150	A0	602	CDL	C14-C15-C16-C17
150	DN	502	CDL	C76-C77-C78-C79
150	Dd	704	CDL	C23-C24-C25-C26
150	Dd	706	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
150	Dj	403	CDL	C63-C64-C65-C66
150	DG	201	CDL	C24-C25-C26-C27
150	DU	402	CDL	C20-C21-C22-C23
150	Dh	201	CDL	C21-C22-C23-C24
164	CA	702	FAD	P-O3P-PA-O5B
150	AF	401	CDL	C64-C65-C66-C67
150	DG	202	CDL	C63-C64-C65-C66
150	DI	302	CDL	C33-C34-C35-C36
150	Eb	302	CDL	C12-C13-C14-C15
153	Dc	602	PC1	C3D-C3E-C3F-C3G
156	Dl	1101	LPP	C39-C40-C41-C42
150	DS	401	CDL	OA9-CA7-OA8-CA6
150	ED	605	CDL	OA9-CA7-OA8-CA6
153	Dc	602	PC1	C3F-C3G-C3H-C3I
156	Dl	1101	LPP	C18-C19-C20-C21
150	AC	801	CDL	OA5-CA3-CA4-CA6
150	B0	101	CDL	OA5-CA3-CA4-CA6
150	BC	302	CDL	OA5-CA3-CA4-CA6
150	BL	301	CDL	OB5-CB3-CB4-CB6
150	BY	201	CDL	OA5-CA3-CA4-CA6
150	CG	302	CDL	OB5-CB3-CB4-CB6
150	CD	302	CDL	OB5-CB3-CB4-CB6
150	E	301	CDL	OB5-CB3-CB4-CB6
150	DS	401	CDL	OB5-CB3-CB4-CB6
150	DZ	501	CDL	OA5-CA3-CA4-CA6
150	EB	302	CDL	OB5-CB3-CB4-CB6
150	Dj	403	CDL	OB5-CB3-CB4-CB6
150	Dm	501	CDL	OA5-CA3-CA4-CA6
150	Dv	403	CDL	OB5-CB3-CB4-CB6
150	Ep	701	CDL	OA5-CA3-CA4-CA6
150	Eu	101	CDL	OA5-CA3-CA4-CA6
153	A6	302	PC1	O11-C1-C2-C3
153	AA	904	PC1	O11-C1-C2-C3
153	AA	907	PC1	O11-C1-C2-C3
153	AL	303	PC1	O11-C1-C2-C3
153	BG	202	PC1	O11-C1-C2-C3
153	K	501	PC1	O11-C1-C2-C3
153	DB	702	PC1	O11-C1-C2-C3
153	DI	303	PC1	O11-C1-C2-C3
153	Dg	203	PC1	O11-C1-C2-C3
155	DS	402	3PE	O11-C1-C2-C3
156	AC	803	LPP	O5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
150	Ed	205	CDL	O1-C1-CA2-OA2
150	BC	302	CDL	C11-C12-C13-C14
150	c	502	CDL	C34-C35-C36-C37
150	DN	506	CDL	C11-C12-C13-C14
150	DU	403	CDL	C44-C45-C46-C47
150	Ds	402	CDL	C78-C79-C80-C81
150	Ep	701	CDL	C80-C81-C82-C83
153	k	301	PC1	C2C-C2D-C2E-C2F
150	DU	401	CDL	OA9-CA7-OA8-CA6
150	Dj	402	CDL	OB9-CB7-OB8-CB6
150	A0	602	CDL	C37-C38-C39-C40
150	BT	202	CDL	C37-C38-C39-C40
150	DG	201	CDL	C42-C43-C44-C45
150	DJ	304	CDL	C13-C14-C15-C16
150	DQ	1502	CDL	C12-C13-C14-C15
155	Di	1102	3PE	C38-C39-C3A-C3B
156	Dn	505	LPP	C35-C36-C37-C38
150	DU	403	CDL	C84-C85-C86-C87
150	Di	1103	CDL	C16-C17-C18-C19
150	Dj	402	CDL	C57-C58-C59-C60
155	DS	402	3PE	C27-C28-C29-C2A
150	Dc	608	CDL	OB7-CB5-OB6-CB4
150	C	506	CDL	CB7-C71-C72-C73
150	EL	902	CDL	CA5-C11-C12-C13
150	BG	201	CDL	C31-CA7-OA8-CA6
150	AA	908	CDL	C40-C41-C42-C43
150	c	501	CDL	C60-C61-C62-C63
150	DR	402	CDL	C42-C43-C44-C45
150	AA	901	CDL	C32-C31-CA7-OA8
150	BC	302	CDL	C32-C31-CA7-OA8
150	Dg	202	CDL	OB9-CB7-OB8-CB6
150	Dy	301	CDL	OA9-CA7-OA8-CA6
155	CD	303	3PE	C2C-C2D-C2E-C2F
155	Di	1102	3PE	C34-C35-C36-C37
150	Ds	406	CDL	C11-CA5-OA6-CA4
150	DI	302	CDL	C16-C17-C18-C19
156	AC	803	LPP	C6-O5-P1-O2
156	AC	803	LPP	C6-O5-P1-O4
150	Dd	704	CDL	C74-C75-C76-C77
150	Dn	503	CDL	C12-C13-C14-C15
153	DS	406	PC1	C29-C2A-C2B-C2C
153	Db	702	PC1	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
153	DI	303	PC1	C11-C12-N-C13
150	CC	305	CDL	C71-CB7-OB8-CB6
150	DU	403	CDL	C71-CB7-OB8-CB6
153	AX	401	PC1	C32-C31-O31-C3
153	EO	205	PC1	C32-C31-O31-C3
150	DN	506	CDL	C16-C17-C18-C19
150	DO	501	CDL	C77-C78-C79-C80
150	EL	902	CDL	C13-C14-C15-C16
150	AC	801	CDL	C37-C38-C39-C40
150	CG	301	CDL	C32-C33-C34-C35
150	DN	507	CDL	C73-C74-C75-C76
150	ED	601	CDL	C20-C21-C22-C23
150	Dh	202	CDL	C53-C54-C55-C56
153	e	1101	PC1	C3C-C3D-C3E-C3F
150	A1	402	CDL	C20-C21-C22-C23
150	c	501	CDL	C84-C85-C86-C87
150	Eh	1601	CDL	C40-C41-C42-C43
153	EO	205	PC1	C2A-C2B-C2C-C2D
150	AP	301	CDL	CA3-CA4-OA6-CA5
150	DC	601	CDL	CB6-CB4-OB6-CB5
150	DG	201	CDL	CB3-CB4-OB6-CB5
150	DJ	304	CDL	CB3-CB4-OB6-CB5
150	DN	502	CDL	CB6-CB4-OB6-CB5
150	DO	501	CDL	CB6-CB4-OB6-CB5
150	DZ	501	CDL	CB6-CB4-OB6-CB5
150	EA	301	CDL	CA6-CA4-OA6-CA5
150	EB	302	CDL	CA6-CA4-OA6-CA5
150	Dg	201	CDL	CB3-CB4-OB6-CB5
150	Dj	404	CDL	CB3-CB4-OB6-CB5
150	Dn	501	CDL	CB6-CB4-OB6-CB5
150	Dn	502	CDL	CA6-CA4-OA6-CA5
150	Du	403	CDL	CA3-CA4-OA6-CA5
153	AA	906	PC1	C3-C2-O21-C21
153	CC	302	PC1	C1-C2-O21-C21
153	DS	406	PC1	C1-C2-O21-C21
155	Dx	1202	3PE	C1-C2-O21-C21
155	Eo	203	3PE	C3-C2-O21-C21
150	DZ	501	CDL	OA7-CA5-OA6-CA4
150	AF	402	CDL	C78-C79-C80-C81
150	DS	405	CDL	C33-C34-C35-C36
150	DU	401	CDL	C32-C33-C34-C35
150	El	901	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
150	BL	301	CDL	C20-C21-C22-C23
150	DG	201	CDL	C44-C45-C46-C47
150	EN	1201	CDL	C14-C15-C16-C17
150	Dh	202	CDL	C34-C35-C36-C37
153	k	301	PC1	C37-C38-C39-C3A
155	A9	602	3PE	C2F-C2G-C2H-C2I
150	En	1201	CDL	OA9-CA7-OA8-CA6
150	CD	302	CDL	C71-CB7-OB8-CB6
150	DD	703	CDL	C71-CB7-OB8-CB6
153	DC	605	PC1	C32-C31-O31-C3
167	ED	603	UQ8	C35-C34-C36-C37
150	Dg	201	CDL	C75-C76-C77-C78
167	EN	1205	UQ8	C38-C39-C41-C42
150	AC	802	CDL	C44-C45-C46-C47
150	DM	501	CDL	C40-C41-C42-C43
150	DX	307	CDL	C42-C43-C44-C45
155	Da	708	3PE	C3A-C3B-C3C-C3D
155	Dc	607	3PE	C3B-C3C-C3D-C3E
150	CJ	201	CDL	CB5-C51-C52-C53
150	DI	302	CDL	CA7-C31-C32-C33
150	AC	802	CDL	CA3-CA4-CA6-OA8
150	AF	401	CDL	CB4-CB3-OB5-PB2
150	AF	402	CDL	CB3-CB4-CB6-OB8
150	CC	304	CDL	CB3-CB4-CB6-OB8
150	CD	302	CDL	CA3-CA4-CA6-OA8
150	h	501	CDL	CB3-CB4-CB6-OB8
150	DA	706	CDL	CA4-CA3-OA5-PA1
150	DC	601	CDL	CA3-CA4-CA6-OA8
150	DG	201	CDL	C1-CB2-OB2-PB2
150	DH	202	CDL	CB3-CB4-CB6-OB8
150	DJ	305	CDL	CB3-CB4-CB6-OB8
150	DN	502	CDL	CA3-CA4-CA6-OA8
150	EA	301	CDL	CB3-CB4-CB6-OB8
150	EK	201	CDL	CB4-CB3-OB5-PB2
150	EL	901	CDL	CA3-CA4-CA6-OA8
150	Dd	705	CDL	C1-CB2-OB2-PB2
150	Dh	202	CDL	CB3-CB4-CB6-OB8
150	Di	1101	CDL	CA3-CA4-CA6-OA8
150	Di	1101	CDL	C1-CB2-OB2-PB2
150	Dj	405	CDL	CB3-CB4-CB6-OB8
150	Dn	502	CDL	C1-CA2-OA2-PA1
150	Du	402	CDL	CB3-CB4-CB6-OB8

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

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Mol	Chain	Res	Type	Atoms
153	AA	904	PC1	O11-C1-C2-O21
153	BS	1302	PC1	O11-C1-C2-O21
153	E	303	PC1	O11-C1-C2-O21
153	K	501	PC1	O11-C1-C2-O21
153	DG	203	PC1	O11-C1-C2-O21
153	Di	1104	PC1	O11-C1-C2-O21
155	DS	402	3PE	O11-C1-C2-O21
155	Da	708	3PE	O11-C1-C2-O21
155	Dg	204	3PE	O11-C1-C2-O21
155	Dr	404	3PE	O11-C1-C2-O21
155	Dx	1207	3PE	O11-C1-C2-O21
150	DV	401	CDL	C72-C71-CB7-OB8
150	En	1201	CDL	C12-C11-CA5-OA6
153	DV	405	PC1	O31-C31-C32-C33
150	Eg	101	CDL	C73-C74-C75-C76
150	c	506	CDL	C21-C22-C23-C24
150	DU	401	CDL	C11-C12-C13-C14
150	EL	901	CDL	C51-C52-C53-C54
150	EL	902	CDL	C84-C85-C86-C87
153	A0	605	PC1	C3C-C3D-C3E-C3F
153	C	508	PC1	C26-C27-C28-C29
153	Dv	405	PC1	C29-C2A-C2B-C2C
150	AC	801	CDL	OB9-CB7-OB8-CB6
150	C	504	CDL	C17-C18-C19-C20
150	BC	302	CDL	CA2-C1-CB2-OB2
150	Dy	301	CDL	CB2-C1-CA2-OA2
150	Ed	204	CDL	CB2-C1-CA2-OA2
150	Eg	101	CDL	CB2-C1-CA2-OA2
150	En	1201	CDL	CB2-C1-CA2-OA2
150	BV	201	CDL	O1-C1-CA2-OA2
150	CD	301	CDL	O1-C1-CB2-OB2
150	DS	405	CDL	OA7-CA5-OA6-CA4
150	Ds	406	CDL	OA7-CA5-OA6-CA4
153	d	801	PC1	O22-C21-O21-C2
155	EL	904	3PE	O22-C21-O21-C2
150	Ea	501	CDL	CA4-CA6-OA8-CA7
157	AQ	201	ADP	PA-O3A-PB-O2B
150	EI	401	CDL	C52-C51-CB5-OB6
153	A0	605	PC1	O31-C31-C32-C33
150	BT	202	CDL	C34-C35-C36-C37
150	Dn	506	CDL	C60-C61-C62-C63
150	AF	401	CDL	OA9-CA7-OA8-CA6

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

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Mol	Chain	Res	Type	Atoms
150	Ds	401	CDL	OB6-CB4-CB6-OB8
150	Eb	302	CDL	OB6-CB4-CB6-OB8
150	Ed	205	CDL	OB6-CB4-CB6-OB8
150	Eg	101	CDL	OA6-CA4-CA6-OA8
150	Ek	201	CDL	OA6-CA4-CA6-OA8
150	Ep	701	CDL	OB6-CB4-CB6-OB8
153	A6	303	PC1	O21-C2-C3-O31
153	AA	906	PC1	O21-C2-C3-O31
153	BT	203	PC1	O21-C2-C3-O31
153	DV	404	PC1	O21-C2-C3-O31
153	DY	302	PC1	O21-C2-C3-O31
153	Dc	609	PC1	O21-C2-C3-O31
153	Dv	404	PC1	O21-C2-C3-O31
153	Eo	204	PC1	O21-C2-C3-O31
155	EL	904	3PE	O21-C2-C3-O31
155	Dx	1208	3PE	O21-C2-C3-O31
155	El	905	3PE	O21-C2-C3-O31
155	Eo	202	3PE	O21-C2-C3-O31
150	BG	201	CDL	C74-C75-C76-C77
150	BG	201	CDL	C75-C76-C77-C78
150	BT	204	CDL	C71-C72-C73-C74
150	c	509	CDL	C17-C18-C19-C20
150	EA	301	CDL	C60-C61-C62-C63
150	Dx	1204	CDL	C72-C73-C74-C75
150	El	902	CDL	C13-C14-C15-C16
153	AA	905	PC1	C3D-C3E-C3F-C3G
150	DN	502	CDL	CB7-C71-C72-C73
150	DD	705	CDL	OA9-CA7-OA8-CA6
150	DU	401	CDL	OB9-CB7-OB8-CB6
150	Dm	501	CDL	OA9-CA7-OA8-CA6
150	Dv	401	CDL	OB9-CB7-OB8-CB6
150	Eu	101	CDL	OB9-CB7-OB8-CB6
153	AX	401	PC1	O32-C31-O31-C3
153	DC	603	PC1	O32-C31-O31-C3
155	Dd	703	3PE	O32-C31-O31-C3
150	BT	202	CDL	C15-C16-C17-C18
150	DX	306	CDL	C32-C33-C34-C35
150	EA	301	CDL	C37-C38-C39-C40
150	ED	601	CDL	C12-C13-C14-C15
153	AA	904	PC1	C11-C12-N-C14
153	Di	1104	PC1	C11-C12-N-C13
154	A1	401	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
173	ER	201	ATP	C5'-O5'-PA-O3A
150	B1	402	CDL	C17-C18-C19-C20
150	DX	301	CDL	C33-C34-C35-C36
150	El	902	CDL	C44-C45-C46-C47
150	EL	901	CDL	C11-CA5-OA6-CA4
150	DQ	1501	CDL	C53-C54-C55-C56
150	En	1201	CDL	C40-C41-C42-C43
150	AA	908	CDL	OA9-CA7-OA8-CA6
150	C	504	CDL	OA9-CA7-OA8-CA6
150	DU	403	CDL	OA9-CA7-OA8-CA6
153	DY	302	PC1	O32-C31-O31-C3
150	AP	301	CDL	C13-C14-C15-C16
150	H	1301	CDL	C11-C12-C13-C14
150	Ds	402	CDL	C82-C83-C84-C85
150	Eh	1601	CDL	C18-C19-C20-C21
150	Eh	1601	CDL	C74-C75-C76-C77
150	DN	507	CDL	OB7-CB5-OB6-CB4
150	EL	901	CDL	OA7-CA5-OA6-CA4
153	C	510	PC1	O22-C21-O21-C2
150	H	1302	CDL	C15-C16-C17-C18
150	DM	501	CDL	C59-C60-C61-C62
150	DN	502	CDL	C12-C13-C14-C15
150	DQ	1502	CDL	C60-C61-C62-C63
150	DR	402	CDL	C41-C42-C43-C44
150	Ed	204	CDL	C13-C14-C15-C16
153	AA	906	PC1	C3E-C3F-C3G-C3H
153	DB	702	PC1	C3B-C3C-C3D-C3E
150	BG	201	CDL	OA9-CA7-OA8-CA6
150	DM	502	CDL	CA5-C11-C12-C13
150	BE	201	CDL	C15-C16-C17-C18
150	DJ	304	CDL	C75-C76-C77-C78
150	DN	506	CDL	C59-C60-C61-C62
150	DQ	1501	CDL	C17-C18-C19-C20
150	DR	402	CDL	C34-C35-C36-C37
150	c	502	CDL	C37-C38-C39-C40
153	A9	601	PC1	C3D-C3E-C3F-C3G
153	DC	603	PC1	C3B-C3C-C3D-C3E
150	AC	802	CDL	C72-C71-CB7-OB8
150	Dn	506	CDL	C20-C21-C22-C23
153	Ef	501	PC1	C23-C24-C25-C26
150	CC	305	CDL	OB9-CB7-OB8-CB6
150	Dh	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	DH	201	CDL	C19-C20-C21-C22
169	DA	703	HEA	C2D-C3D-CAD-CBD
169	Da	703	HEA	C2D-C3D-CAD-CBD
150	c	506	CDL	C62-C63-C64-C65
150	DH	202	CDL	C20-C21-C22-C23
150	DH	202	CDL	C52-C53-C54-C55
150	EN	1201	CDL	C13-C14-C15-C16
150	Eb	302	CDL	C55-C56-C57-C58
153	Eo	205	PC1	C3C-C3D-C3E-C3F
168	C	501	HEM	C1A-C2A-CAA-CBA
150	BT	204	CDL	C74-C75-C76-C77
150	CJ	201	CDL	C44-C45-C46-C47
150	ED	604	CDL	C74-C75-C76-C77
150	Dg	201	CDL	C21-C22-C23-C24
153	k	301	PC1	C36-C37-C38-C39
150	BC	301	CDL	CA5-C11-C12-C13
150	EL	903	CDL	C31-CA7-OA8-CA6
153	DX	305	PC1	C32-C31-O31-C3
150	Dj	404	CDL	C55-C56-C57-C58
150	BC	301	CDL	CB2-OB2-PB2-OB5
150	BG	201	CDL	CB2-OB2-PB2-OB5
150	BT	204	CDL	CA3-OA5-PA1-OA2
150	CJ	201	CDL	CA2-OA2-PA1-OA5
150	CC	304	CDL	CB2-OB2-PB2-OB5
150	C	506	CDL	CA2-OA2-PA1-OA5
150	c	502	CDL	CA2-OA2-PA1-OA5
150	c	506	CDL	CA2-OA2-PA1-OA5
150	DA	706	CDL	CA2-OA2-PA1-OA5
150	DA	709	CDL	CB2-OB2-PB2-OB5
150	DD	705	CDL	CB3-OB5-PB2-OB2
150	DH	201	CDL	CA3-OA5-PA1-OA2
150	DJ	302	CDL	CB2-OB2-PB2-OB5
150	DJ	303	CDL	CB3-OB5-PB2-OB2
150	DQ	1502	CDL	CA2-OA2-PA1-OA5
150	DS	401	CDL	CA2-OA2-PA1-OA5
150	DS	401	CDL	CB3-OB5-PB2-OB2
150	DV	403	CDL	CB3-OB5-PB2-OB2
150	DX	306	CDL	CB2-OB2-PB2-OB5
150	ED	605	CDL	CB2-OB2-PB2-OB5
150	EO	202	CDL	CB3-OB5-PB2-OB2
150	Da	709	CDL	CA2-OA2-PA1-OA5
150	Da	709	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
150	Dc	601	CDL	CA2-OA2-PA1-OA5
150	Do	501	CDL	CA2-OA2-PA1-OA5
150	Ds	402	CDL	CA2-OA2-PA1-OA5
150	Ds	402	CDL	CB3-OB5-PB2-OB2
153	AH	301	PC1	C11-O13-P-O11
153	AU	202	PC1	C11-O13-P-O11
153	BT	203	PC1	C11-O13-P-O11
153	Dc	605	PC1	C11-O13-P-O11
153	Dx	1205	PC1	C11-O13-P-O11
153	Eb	301	PC1	C11-O13-P-O11
155	Da	708	3PE	C11-O13-P-O11
155	Ds	408	3PE	C11-O13-P-O11
150	DD	705	CDL	C59-C60-C61-C62
150	DD	706	CDL	C13-C14-C15-C16
153	Dv	404	PC1	C3B-C3C-C3D-C3E
150	Dn	502	CDL	O1-C1-CB2-OB2
150	Dj	404	CDL	C62-C63-C64-C65
155	DC	607	3PE	C3B-C3C-C3D-C3E
150	BG	201	CDL	CB4-CB3-OB5-PB2
150	BY	201	CDL	C1-CB2-OB2-PB2
150	CG	302	CDL	CB4-CB3-OB5-PB2
150	CC	304	CDL	C1-CB2-OB2-PB2
150	c	506	CDL	CB4-CB3-OB5-PB2
150	DD	703	CDL	C1-CA2-OA2-PA1
150	DD	704	CDL	C1-CB2-OB2-PB2
150	DG	201	CDL	C1-CA2-OA2-PA1
150	DM	501	CDL	CB4-CB3-OB5-PB2
150	DN	506	CDL	C1-CB2-OB2-PB2
150	DQ	1504	CDL	C1-CA2-OA2-PA1
150	DR	403	CDL	CA4-CA3-OA5-PA1
150	DR	403	CDL	C1-CB2-OB2-PB2
150	DX	301	CDL	CA4-CA3-OA5-PA1
150	EL	903	CDL	C1-CB2-OB2-PB2
150	EO	202	CDL	C1-CB2-OB2-PB2
150	EO	202	CDL	CB4-CB3-OB5-PB2
150	Dg	201	CDL	CA4-CA3-OA5-PA1
150	Dm	501	CDL	CA4-CA3-OA5-PA1
150	Ds	406	CDL	C1-CA2-OA2-PA1
150	Dv	403	CDL	C1-CA2-OA2-PA1
150	Ei	401	CDL	C1-CB2-OB2-PB2
150	Ek	201	CDL	CB4-CB3-OB5-PB2
150	El	901	CDL	C1-CA2-OA2-PA1

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

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Mol	Chain	Res	Type	Atoms
150	C	503	CDL	CB2-OB2-PB2-OB3
150	C	504	CDL	CA3-OA5-PA1-OA4
150	C	504	CDL	CB2-OB2-PB2-OB4
150	C	505	CDL	CA2-OA2-PA1-OA3
150	C	506	CDL	CA3-OA5-PA1-OA4
150	C	507	CDL	CA2-OA2-PA1-OA4
150	C	507	CDL	CA3-OA5-PA1-OA3
150	C	507	CDL	CB3-OB5-PB2-OB4
150	E	301	CDL	CA2-OA2-PA1-OA3
150	E	301	CDL	CB2-OB2-PB2-OB3
150	H	1302	CDL	CA3-OA5-PA1-OA3
150	c	502	CDL	CA2-OA2-PA1-OA3
150	c	506	CDL	CB2-OB2-PB2-OB4
150	g	801	CDL	CA2-OA2-PA1-OA4
150	g	801	CDL	CB2-OB2-PB2-OB4
150	h	501	CDL	CA2-OA2-PA1-OA3
150	DA	706	CDL	CA2-OA2-PA1-OA4
150	DA	706	CDL	CB3-OB5-PB2-OB3
150	DC	601	CDL	CA2-OA2-PA1-OA3
150	DC	601	CDL	CA3-OA5-PA1-OA3
150	DC	601	CDL	CB2-OB2-PB2-OB3
150	DC	601	CDL	CB3-OB5-PB2-OB3
150	DD	703	CDL	CA3-OA5-PA1-OA3
150	DD	706	CDL	CB3-OB5-PB2-OB4
150	DG	202	CDL	CA2-OA2-PA1-OA3
150	DG	202	CDL	CB3-OB5-PB2-OB3
150	DH	202	CDL	CB2-OB2-PB2-OB3
150	DI	302	CDL	CB3-OB5-PB2-OB4
150	DJ	302	CDL	CB3-OB5-PB2-OB3
150	DJ	303	CDL	CB3-OB5-PB2-OB3
150	DJ	305	CDL	CA3-OA5-PA1-OA3
150	DJ	305	CDL	CB2-OB2-PB2-OB3
150	DJ	307	CDL	CB2-OB2-PB2-OB3
150	DJ	307	CDL	CB3-OB5-PB2-OB3
150	DM	501	CDL	CA2-OA2-PA1-OA4
150	DM	502	CDL	CA2-OA2-PA1-OA4
150	DM	502	CDL	CB2-OB2-PB2-OB3
150	DN	502	CDL	CB3-OB5-PB2-OB4
150	DN	506	CDL	CB3-OB5-PB2-OB4
150	DN	507	CDL	CA2-OA2-PA1-OA3
150	DO	501	CDL	CB2-OB2-PB2-OB4
150	DQ	1504	CDL	CA2-OA2-PA1-OA3

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

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

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

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

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

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Mol	Chain	Res	Type	Atoms
150	c	509	CDL	OA5-CA3-CA4-CA6
150	DD	704	CDL	OB5-CB3-CB4-CB6
150	DN	506	CDL	OB5-CB3-CB4-CB6
150	DO	501	CDL	OA5-CA3-CA4-CA6
150	ED	605	CDL	OB5-CB3-CB4-CB6
150	EH	1601	CDL	OB5-CB3-CB4-CB6
150	EL	903	CDL	OA5-CA3-CA4-CA6
150	Dd	704	CDL	OA5-CA3-CA4-CA6
150	Dd	706	CDL	OB5-CB3-CB4-CB6
150	Dj	401	CDL	OA5-CA3-CA4-CA6
153	AH	301	PC1	O11-C1-C2-C3
153	BS	1302	PC1	O11-C1-C2-C3
153	c	503	PC1	O11-C1-C2-C3
153	DG	203	PC1	O11-C1-C2-C3
155	DX	302	3PE	O11-C1-C2-C3
155	Dd	703	3PE	O11-C1-C2-C3
155	Dg	204	3PE	O11-C1-C2-C3
155	Ds	403	3PE	O11-C1-C2-C3
167	Ds	404	UQ8	C39-C41-C42-C43
150	A1	402	CDL	C15-C16-C17-C18
150	DN	506	CDL	C13-C14-C15-C16
150	EL	903	CDL	C23-C24-C25-C26
150	Dg	202	CDL	C31-C32-C33-C34
150	Ds	401	CDL	C36-C37-C38-C39
150	Du	401	CDL	C37-C38-C39-C40
150	Dv	401	CDL	C43-C44-C45-C46
155	EL	904	3PE	C2B-C2C-C2D-C2E
150	CD	302	CDL	OB9-CB7-OB8-CB6
150	BT	204	CDL	C60-C61-C62-C63
150	DC	601	CDL	C79-C80-C81-C82
150	Dn	506	CDL	C18-C19-C20-C21
150	H	1302	CDL	C34-C35-C36-C37
150	EO	202	CDL	C18-C19-C20-C21
150	Dn	501	CDL	C77-C78-C79-C80
150	Ds	405	CDL	C72-C73-C74-C75
150	Ds	406	CDL	C33-C34-C35-C36
153	AJ	501	PC1	C2F-C2G-C2H-C2I
153	c	507	PC1	C3E-C3F-C3G-C3H
153	Dx	1205	PC1	C25-C26-C27-C28
167	Ds	404	UQ8	C5-C4-O4-C4M
150	BT	204	CDL	C16-C17-C18-C19
150	DD	706	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
150	DS	401	CDL	C74-C75-C76-C77
150	DZ	501	CDL	C11-C12-C13-C14
153	A9	603	PC1	C12-C11-O13-P
153	DB	702	PC1	C12-C11-O13-P
153	Db	702	PC1	C12-C11-O13-P
153	Dv	405	PC1	C12-C11-O13-P
153	Dx	1203	PC1	C12-C11-O13-P
155	BP	201	3PE	C12-C11-O13-P
155	CC	301	3PE	C12-C11-O13-P
155	C	513	3PE	C12-C11-O13-P
155	DI	301	3PE	C12-C11-O13-P
155	DX	302	3PE	C12-C11-O13-P
155	Dg	204	3PE	C12-C11-O13-P
155	Di	1102	3PE	C12-C11-O13-P
155	Dx	1206	3PE	C12-C11-O13-P
150	Dg	201	CDL	CA5-C11-C12-C13
150	AF	402	CDL	C43-C44-C45-C46
150	BT	204	CDL	C42-C43-C44-C45
150	CD	302	CDL	C19-C20-C21-C22
150	EL	902	CDL	C17-C18-C19-C20
153	AA	907	PC1	C22-C23-C24-C25
153	EB	301	PC1	C3C-C3D-C3E-C3F
153	Ef	501	PC1	C26-C27-C28-C29
153	DC	605	PC1	O32-C31-O31-C3
150	AA	901	CDL	C63-C64-C65-C66
153	DG	203	PC1	C3B-C3C-C3D-C3E
150	E	301	CDL	C16-C17-C18-C19
150	DM	501	CDL	C62-C63-C64-C65
153	DG	203	PC1	C23-C24-C25-C26
150	AP	301	CDL	CB7-C71-C72-C73
150	BT	204	CDL	CB5-C51-C52-C53
150	Dd	702	CDL	CA5-C11-C12-C13
153	EN	1203	PC1	C3C-C3D-C3E-C3F
155	Ds	403	3PE	C27-C28-C29-C2A
150	Eb	302	CDL	C31-CA7-OA8-CA6
150	Du	402	CDL	CA2-C1-CB2-OB2
150	Dx	1201	CDL	OB7-CB5-OB6-CB4
150	A0	602	CDL	C39-C40-C41-C42
150	DJ	304	CDL	C74-C75-C76-C77
150	Dh	201	CDL	C63-C64-C65-C66
150	Dr	402	CDL	C40-C41-C42-C43
150	Ei	401	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
153	EO	201	PC1	C32-C33-C34-C35
150	AF	402	CDL	OB5-CB3-CB4-OB6
150	B1	402	CDL	OA5-CA3-CA4-OA6
150	BY	201	CDL	OA5-CA3-CA4-OA6
150	CJ	201	CDL	OB5-CB3-CB4-OB6
150	E	301	CDL	OB5-CB3-CB4-OB6
150	c	502	CDL	OA5-CA3-CA4-OA6
150	DD	705	CDL	OB5-CB3-CB4-OB6
150	DM	501	CDL	OB5-CB3-CB4-OB6
150	DO	501	CDL	OA5-CA3-CA4-OA6
150	DQ	1502	CDL	OB5-CB3-CB4-OB6
150	DQ	1504	CDL	OB5-CB3-CB4-OB6
150	DS	405	CDL	OB5-CB3-CB4-OB6
150	DV	403	CDL	OA5-CA3-CA4-OA6
150	DX	307	CDL	OB5-CB3-CB4-OB6
150	EB	302	CDL	OA5-CA3-CA4-OA6
150	ED	604	CDL	OA5-CA3-CA4-OA6
150	ED	604	CDL	OB5-CB3-CB4-OB6
150	Da	709	CDL	OB5-CB3-CB4-OB6
150	Dj	401	CDL	OA5-CA3-CA4-OA6
150	Dn	502	CDL	OB5-CB3-CB4-OB6
150	Dq	1403	CDL	OB5-CB3-CB4-OB6
150	Ds	402	CDL	OB5-CB3-CB4-OB6
150	Du	401	CDL	OB5-CB3-CB4-OB6
150	Eg	101	CDL	OB5-CB3-CB4-OB6
150	Eh	1601	CDL	OA5-CA3-CA4-OA6
153	AH	301	PC1	O11-C1-C2-O21
153	AJ	501	PC1	O11-C1-C2-O21
153	AL	303	PC1	O11-C1-C2-O21
153	AQ	202	PC1	O11-C1-C2-O21
153	B1	403	PC1	O11-C1-C2-O21
153	C	509	PC1	O11-C1-C2-O21
153	c	507	PC1	O11-C1-C2-O21
153	Db	702	PC1	O11-C1-C2-O21
153	Dc	603	PC1	O11-C1-C2-O21
153	Dg	203	PC1	O11-C1-C2-O21
155	AJ	502	3PE	O11-C1-C2-O21
155	BP	201	3PE	O11-C1-C2-O21
155	Dc	606	3PE	O11-C1-C2-O21
155	Dd	703	3PE	O11-C1-C2-O21
156	AC	803	LPP	O5-C6-C7-O9
150	C	504	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
150	C	506	CDL	C11-C12-C13-C14
150	DO	501	CDL	C36-C37-C38-C39
150	DQ	1504	CDL	C13-C14-C15-C16
150	Da	709	CDL	C22-C23-C24-C25
150	Di	1103	CDL	C57-C58-C59-C60
150	Dn	502	CDL	C84-C85-C86-C87
150	Dq	1402	CDL	C78-C79-C80-C81
150	Dq	1403	CDL	C12-C13-C14-C15
150	AC	802	CDL	C61-C62-C63-C64
150	ED	604	CDL	C12-C13-C14-C15
150	E	301	CDL	C18-C19-C20-C21
153	A2	402	PC1	C37-C38-C39-C3A
153	AA	907	PC1	C37-C38-C39-C3A
155	BP	201	3PE	C36-C37-C38-C39
150	Dx	1201	CDL	C51-CB5-OB6-CB4
153	Dx	1205	PC1	C22-C21-O21-C2
150	DX	307	CDL	C78-C79-C80-C81
150	EN	1202	CDL	C11-C12-C13-C14
150	Dj	401	CDL	C36-C37-C38-C39
150	Du	402	CDL	C57-C58-C59-C60
155	DS	402	3PE	C34-C35-C36-C37
150	DD	703	CDL	OB9-CB7-OB8-CB6
150	DR	403	CDL	O1-C1-CB2-OB2
150	Dm	502	CDL	O1-C1-CB2-OB2
150	C	506	CDL	C34-C35-C36-C37
150	DX	301	CDL	C24-C25-C26-C27
150	Dh	202	CDL	C80-C81-C82-C83
150	Ds	405	CDL	C58-C59-C60-C61
150	El	902	CDL	C83-C84-C85-C86
153	EB	303	PC1	C2E-C2F-C2G-C2H
153	EO	201	PC1	C29-C2A-C2B-C2C
153	Dc	605	PC1	C3E-C3F-C3G-C3H
153	EN	1203	PC1	C11-C12-N-C13
153	Eo	204	PC1	C11-C12-N-C15
150	c	509	CDL	C11-C12-C13-C14
150	g	801	CDL	C37-C38-C39-C40
150	Du	403	CDL	C61-C62-C63-C64
155	DJ	301	3PE	C35-C36-C37-C38
150	DU	404	CDL	CA4-CA6-OA8-CA7
156	Dl	1101	LPP	O27-C29-C30-C31
150	CG	301	CDL	CB3-CB4-CB6-OB8
150	DD	704	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
150	DH	201	CDL	CB3-CB4-CB6-OB8
150	DJ	303	CDL	C57-C58-C59-C60
150	DN	502	CDL	CB3-CB4-CB6-OB8
150	DY	301	CDL	CB3-CB4-CB6-OB8
150	Dc	601	CDL	C34-C35-C36-C37
150	Dh	201	CDL	CB3-CB4-CB6-OB8
150	Dn	501	CDL	CB3-CB4-CB6-OB8
150	Dy	301	CDL	CB3-CB4-CB6-OB8
153	A2	402	PC1	O13-C11-C12-N
153	A9	603	PC1	O13-C11-C12-N
153	AA	906	PC1	O13-C11-C12-N
153	AH	301	PC1	O13-C11-C12-N
153	AQ	202	PC1	O13-C11-C12-N
153	AU	201	PC1	O13-C11-C12-N
153	AU	202	PC1	O13-C11-C12-N
153	B1	403	PC1	O13-C11-C12-N
153	CC	302	PC1	O13-C11-C12-N
153	K	502	PC1	O13-C11-C12-N
153	d	801	PC1	O13-C11-C12-N
153	e	1101	PC1	O13-C11-C12-N
153	g	802	PC1	O13-C11-C12-N
153	DB	702	PC1	O13-C11-C12-N
153	DC	604	PC1	O13-C11-C12-N
153	DS	406	PC1	O13-C11-C12-N
153	DV	405	PC1	O13-C11-C12-N
153	EO	204	PC1	O13-C11-C12-N
153	Db	702	PC1	O13-C11-C12-N
153	Dc	604	PC1	O13-C11-C12-N
153	Dc	605	PC1	O13-C11-C12-N
153	Dg	203	PC1	C23-C24-C25-C26
153	Dv	405	PC1	O13-C11-C12-N
153	Dv	406	PC1	O13-C11-C12-N
153	Ef	501	PC1	C1-C2-C3-O31
153	El	904	PC1	O13-C11-C12-N
155	Dx	1208	3PE	C1-C2-C3-O31
150	BE	201	CDL	OA6-CA4-CA6-OA8
150	BL	301	CDL	OB6-CB4-CB6-OB8
150	BV	201	CDL	OA6-CA4-CA6-OA8
150	CD	302	CDL	OA6-CA4-CA6-OA8
150	H	1302	CDL	OB6-CB4-CB6-OB8
150	c	509	CDL	OA6-CA4-CA6-OA8
150	h	501	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
150	DD	706	CDL	OB6-CB4-CB6-OB8
150	DI	302	CDL	OA6-CA4-CA6-OA8
150	DN	502	CDL	OA6-CA4-CA6-OA8
150	DN	502	CDL	OB6-CB4-CB6-OB8
150	DX	301	CDL	OB6-CB4-CB6-OB8
150	DZ	501	CDL	OA6-CA4-CA6-OA8
150	ED	601	CDL	OA6-CA4-CA6-OA8
150	ED	605	CDL	OA6-CA4-CA6-OA8
150	EK	201	CDL	OA6-CA4-CA6-OA8
150	EN	1202	CDL	OB6-CB4-CB6-OB8
150	EO	202	CDL	OB6-CB4-CB6-OB8
150	Dd	704	CDL	OB6-CB4-CB6-OB8
150	Dg	201	CDL	OB6-CB4-CB6-OB8
150	Dh	201	CDL	OB6-CB4-CB6-OB8
150	Dh	202	CDL	OB6-CB4-CB6-OB8
150	Dj	401	CDL	OB6-CB4-CB6-OB8
150	Dj	402	CDL	OB6-CB4-CB6-OB8
150	Dj	404	CDL	OA6-CA4-CA6-OA8
150	Dn	501	CDL	OB6-CB4-CB6-OB8
150	Dq	1402	CDL	OA6-CA4-CA6-OA8
150	Dr	402	CDL	OA6-CA4-CA6-OA8
153	A1	403	PC1	O21-C2-C3-O31
153	C	510	PC1	O21-C2-C3-O31
153	g	802	PC1	O21-C2-C3-O31
153	DC	605	PC1	O21-C2-C3-O31
153	DC	608	PC1	O21-C2-C3-O31
153	Dc	604	PC1	O21-C2-C3-O31
153	Dc	605	PC1	O21-C2-C3-O31
153	Eo	201	PC1	O21-C2-C3-O31
155	EM	901	3PE	O21-C2-C3-O31
150	AA	908	CDL	C33-C34-C35-C36
150	EL	901	CDL	C78-C79-C80-C81
150	Dx	1201	CDL	C73-C74-C75-C76
150	El	902	CDL	C79-C80-C81-C82
150	C	504	CDL	C40-C41-C42-C43
150	DD	706	CDL	C84-C85-C86-C87
153	Db	702	PC1	C3B-C3C-C3D-C3E
150	EA	301	CDL	CA5-C11-C12-C13
168	C	502	HEM	C4D-C3D-CAD-CBD
150	E	301	CDL	C75-C76-C77-C78
150	c	501	CDL	C80-C81-C82-C83
150	Di	1101	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
150	B0	101	CDL	C75-C76-C77-C78
150	Dn	506	CDL	C74-C75-C76-C77
150	Eh	1601	CDL	C13-C14-C15-C16
153	c	503	PC1	C24-C25-C26-C27
150	AC	801	CDL	C1-CA2-OA2-PA1
150	DD	705	CDL	CB4-CB3-OB5-PB2
150	DM	501	CDL	C1-CB2-OB2-PB2
150	Dr	402	CDL	CA4-CA3-OA5-PA1
150	Eg	101	CDL	CB4-CB3-OB5-PB2
150	DU	401	CDL	C37-C38-C39-C40
150	EL	902	CDL	OA9-CA7-OA8-CA6
153	DA	708	PC1	O32-C31-O31-C3
150	DN	503	CDL	C31-CA7-OA8-CA6
150	Dd	705	CDL	C71-CB7-OB8-CB6
150	AF	402	CDL	C12-C13-C14-C15
150	C	504	CDL	C77-C78-C79-C80
150	c	502	CDL	C60-C61-C62-C63
150	DG	202	CDL	C31-C32-C33-C34
150	DH	202	CDL	C36-C37-C38-C39
150	Dm	501	CDL	C52-C51-CB5-OB6
150	DH	202	CDL	C80-C81-C82-C83
150	DN	503	CDL	C57-C58-C59-C60
150	DZ	501	CDL	C39-C40-C41-C42
150	ES	1101	CDL	C11-C12-C13-C14
150	Dr	402	CDL	C71-C72-C73-C74
150	Dx	1204	CDL	C44-C45-C46-C47
153	Eb	303	PC1	C2E-C2F-C2G-C2H
153	C	509	PC1	O32-C31-O31-C3
153	DX	305	PC1	O32-C31-O31-C3
150	C	506	CDL	C80-C81-C82-C83
150	H	1301	CDL	C20-C21-C22-C23
150	DU	402	CDL	C17-C18-C19-C20
150	Dm	501	CDL	C40-C41-C42-C43
150	Do	501	CDL	C36-C37-C38-C39
153	DI	303	PC1	C35-C36-C37-C38
155	BA	301	3PE	C26-C27-C28-C29
150	A1	402	CDL	C80-C81-C82-C83
150	C	504	CDL	C73-C74-C75-C76
150	DY	301	CDL	C17-C18-C19-C20
150	Dn	502	CDL	C57-C58-C59-C60
150	Du	403	CDL	C40-C41-C42-C43
153	k	301	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
155	El	905	3PE	C22-C23-C24-C25
167	CC	303	UQ8	C14-C16-C17-C18
167	C	511	UQ8	C24-C26-C27-C28
167	EN	1205	UQ8	C14-C16-C17-C18
150	AC	802	CDL	C51-C52-C53-C54
150	ED	601	CDL	C35-C36-C37-C38
153	A6	302	PC1	C36-C37-C38-C39
153	A9	603	PC1	C24-C25-C26-C27
153	AM	302	PC1	C3C-C3D-C3E-C3F
153	Eo	201	PC1	C2B-C2C-C2D-C2E
150	EL	903	CDL	OA9-CA7-OA8-CA6
150	AC	801	CDL	C63-C64-C65-C66
150	DS	404	CDL	C72-C73-C74-C75
150	DU	404	CDL	C20-C21-C22-C23
150	Dh	201	CDL	C77-C78-C79-C80
150	El	903	CDL	C43-C44-C45-C46
150	En	1201	CDL	C44-C45-C46-C47
155	Di	1102	3PE	C32-C33-C34-C35
150	C	507	CDL	C16-C17-C18-C19
150	DZ	501	CDL	C43-C44-C45-C46
150	AP	301	CDL	CA5-C11-C12-C13
153	AJ	501	PC1	C21-C22-C23-C24
153	AA	904	PC1	C11-C12-N-C15
153	DI	303	PC1	C11-C12-N-C15
153	Di	1104	PC1	C11-C12-N-C15
150	CD	301	CDL	C74-C75-C76-C77
150	DR	402	CDL	C73-C74-C75-C76
150	EL	901	CDL	C77-C78-C79-C80
150	Eb	302	CDL	C14-C15-C16-C17
153	DV	405	PC1	C3B-C3C-C3D-C3E
153	Ds	407	PC1	C3C-C3D-C3E-C3F
150	DQ	1504	CDL	C32-C33-C34-C35
150	EK	201	CDL	C34-C35-C36-C37
150	Dx	1201	CDL	C36-C37-C38-C39
153	AA	906	PC1	C3B-C3C-C3D-C3E
153	Dc	609	PC1	C2B-C2C-C2D-C2E
150	DU	403	CDL	O1-C1-CA2-OA2
150	Dq	1402	CDL	O1-C1-CA2-OA2
150	El	901	CDL	O1-C1-CB2-OB2
150	Dd	706	CDL	OB7-CB5-OB6-CB4
150	E	301	CDL	C55-C56-C57-C58
150	H	1302	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
150	c	506	CDL	C61-C62-C63-C64
150	DO	501	CDL	C80-C81-C82-C83
153	Dc	603	PC1	C34-C35-C36-C37
167	EL	905	UQ8	C2-C3-O3-C3M
167	EL	905	UQ8	C5-C4-O4-C4M
167	EN	1205	UQ8	C2-C3-O3-C3M
167	Ds	404	UQ8	C2-C3-O3-C3M
150	c	506	CDL	C71-C72-C73-C74
150	Di	1101	CDL	C15-C16-C17-C18
150	Dn	501	CDL	C12-C13-C14-C15
150	Dx	1201	CDL	C71-C72-C73-C74
150	DR	403	CDL	OB9-CB7-OB8-CB6
150	c	506	CDL	C34-C35-C36-C37
150	c	509	CDL	C44-C45-C46-C47
150	DD	706	CDL	C34-C35-C36-C37
150	EA	301	CDL	C64-C65-C66-C67
150	Dg	202	CDL	C13-C14-C15-C16
150	AC	801	CDL	C14-C15-C16-C17
150	DO	501	CDL	C71-C72-C73-C74
150	EO	202	CDL	C58-C59-C60-C61
150	Dn	502	CDL	C73-C74-C75-C76
150	El	901	CDL	C40-C41-C42-C43
153	D	402	PC1	C3E-C3F-C3G-C3H
150	DJ	307	CDL	C72-C71-CB7-OB8
150	c	506	CDL	C73-C74-C75-C76
150	DQ	1501	CDL	C81-C82-C83-C84
150	DU	403	CDL	C52-C53-C54-C55
150	A1	402	CDL	CB6-CB4-OB6-CB5
150	AA	908	CDL	CB3-CB4-OB6-CB5
150	AM	301	CDL	CB3-CB4-OB6-CB5
150	BY	201	CDL	CB6-CB4-OB6-CB5
150	CG	302	CDL	CB6-CB4-OB6-CB5
150	CC	305	CDL	CA6-CA4-OA6-CA5
150	CD	301	CDL	CB3-CB4-OB6-CB5
150	H	1302	CDL	CA6-CA4-OA6-CA5
150	c	509	CDL	CA3-CA4-OA6-CA5
150	c	509	CDL	CA6-CA4-OA6-CA5
150	DD	704	CDL	CB3-CB4-OB6-CB5
150	DS	401	CDL	CB3-CB4-OB6-CB5
150	DV	401	CDL	CB6-CB4-OB6-CB5
150	Dc	601	CDL	CB6-CB4-OB6-CB5
150	Dd	704	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
150	Ds	402	CDL	CB3-CB4-OB6-CB5
150	Dv	401	CDL	CB6-CB4-OB6-CB5
150	Ea	501	CDL	CB6-CB4-OB6-CB5
150	Ea	502	CDL	CA6-CA4-OA6-CA5
150	Eb	302	CDL	CA6-CA4-OA6-CA5
150	Eh	1601	CDL	CB3-CB4-OB6-CB5
153	A1	403	PC1	C1-C2-O21-C21
153	AM	302	PC1	C3-C2-O21-C21
153	DC	608	PC1	C1-C2-O21-C21
153	EO	206	PC1	C1-C2-O21-C21
153	Dc	605	PC1	C3-C2-O21-C21
153	Dv	405	PC1	C1-C2-O21-C21
155	BP	201	3PE	C3-C2-O21-C21
155	DC	606	3PE	C1-C2-O21-C21
155	EO	203	3PE	C1-C2-O21-C21
155	Dr	401	3PE	C1-C2-O21-C21
150	BT	204	CDL	OB5-CB3-CB4-CB6
150	DD	706	CDL	OA5-CA3-CA4-CA6
150	DN	507	CDL	OA5-CA3-CA4-CA6
150	DO	501	CDL	OB5-CB3-CB4-CB6
150	DV	403	CDL	OB5-CB3-CB4-CB6
150	Da	709	CDL	OB5-CB3-CB4-CB6
150	Dd	706	CDL	OA5-CA3-CA4-CA6
150	Ea	501	CDL	OA5-CA3-CA4-CA6
150	Eg	101	CDL	OA5-CA3-CA4-CA6
150	Eh	1601	CDL	OA5-CA3-CA4-CA6
153	AQ	202	PC1	O11-C1-C2-C3
153	c	507	PC1	O11-C1-C2-C3
150	DM	501	CDL	C54-C55-C56-C57
150	Dn	501	CDL	C40-C41-C42-C43
150	C	507	CDL	OB7-CB5-OB6-CB4
150	Di	1101	CDL	OB7-CB5-OB6-CB4
153	Dx	1205	PC1	O22-C21-O21-C2
150	DR	403	CDL	C71-CB7-OB8-CB6
150	Dq	1401	CDL	C32-C33-C34-C35
150	Dq	1401	CDL	C59-C60-C61-C62
150	ES	1101	CDL	CA7-C31-C32-C33
150	Dn	502	CDL	CA5-C11-C12-C13
150	BE	201	CDL	C51-C52-C53-C54
153	A	1201	PC1	C3C-C3D-C3E-C3F
153	Eb	303	PC1	C34-C35-C36-C37
150	BE	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
150	Dd	705	CDL	OB9-CB7-OB8-CB6
150	Eb	302	CDL	OA9-CA7-OA8-CA6
150	DR	402	CDL	C31-C32-C33-C34
150	Dh	202	CDL	C79-C80-C81-C82
153	AA	906	PC1	C2C-C2D-C2E-C2F
155	El	905	3PE	C33-C34-C35-C36
150	BG	201	CDL	C63-C64-C65-C66
150	DJ	304	CDL	C1-CB2-OB2-PB2
150	ES	1101	CDL	C1-CB2-OB2-PB2
150	Dg	201	CDL	C1-CB2-OB2-PB2
150	Do	501	CDL	C1-CA2-OA2-PA1
156	AC	803	LPP	C6-O5-P1-O3
150	AM	301	CDL	C75-C76-C77-C78
150	Dn	501	CDL	C78-C79-C80-C81
153	c	503	PC1	C29-C2A-C2B-C2C
155	Ds	403	3PE	C28-C29-C2A-C2B
150	BE	201	CDL	C31-CA7-OA8-CA6
150	BY	201	CDL	C71-CB7-OB8-CB6
150	DN	503	CDL	OA9-CA7-OA8-CA6
150	Ea	501	CDL	OB5-CB3-CB4-OB6
153	AM	302	PC1	O11-C1-C2-O21
153	AU	201	PC1	O11-C1-C2-O21
153	Dc	609	PC1	O11-C1-C2-O21
150	DG	202	CDL	C17-C18-C19-C20
150	DH	201	CDL	C17-C18-C19-C20
150	DN	506	CDL	C81-C82-C83-C84
150	Di	1103	CDL	C62-C63-C64-C65
153	EN	1203	PC1	C11-C12-N-C15
153	EO	205	PC1	C11-C12-N-C14
150	CG	302	CDL	C12-C13-C14-C15
150	DD	704	CDL	C14-C15-C16-C17
150	ED	601	CDL	C51-C52-C53-C54
150	Dj	401	CDL	C59-C60-C61-C62
150	Dq	1403	CDL	C78-C79-C80-C81
153	A9	603	PC1	C3D-C3E-C3F-C3G
153	C	510	PC1	C3B-C3C-C3D-C3E
155	BA	301	3PE	C2B-C2C-C2D-C2E
167	C	511	UQ8	C23-C24-C26-C27
150	BY	201	CDL	OB9-CB7-OB8-CB6
150	CD	301	CDL	C55-C56-C57-C58
153	Dc	603	PC1	C3B-C3C-C3D-C3E
168	C	502	HEM	C2D-C3D-CAD-CBD

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

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

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Mol	Chain	Res	Type	Atoms
150	Ds	401	CDL	CA2-OA2-PA1-OA5
150	Ds	401	CDL	CB2-OB2-PB2-OB5
150	Du	403	CDL	CA2-OA2-PA1-OA5
150	Du	403	CDL	CA3-OA5-PA1-OA2
150	Dy	301	CDL	CA2-OA2-PA1-OA5
150	Dy	301	CDL	CB3-OB5-PB2-OB2
150	Ei	401	CDL	CA3-OA5-PA1-OA2
150	Ep	701	CDL	CB2-OB2-PB2-OB5
150	Eu	101	CDL	CA2-OA2-PA1-OA5
153	A6	302	PC1	C11-O13-P-O11
153	A9	601	PC1	C1-O11-P-O13
153	AA	904	PC1	C1-O11-P-O13
153	AC	804	PC1	C1-O11-P-O13
153	D	402	PC1	C1-O11-P-O13
153	Dv	406	PC1	C1-O11-P-O13
153	Eb	303	PC1	C1-O11-P-O13
153	Ef	501	PC1	C11-O13-P-O11
155	BP	201	3PE	C11-O13-P-O11
155	DI	301	3PE	C11-O13-P-O11
155	DR	401	3PE	C1-O11-P-O13
155	DX	302	3PE	C1-O11-P-O13
155	Di	1102	3PE	C11-O13-P-O11
155	Ds	408	3PE	C1-O11-P-O13
155	Eo	202	3PE	C11-O13-P-O11
150	AF	401	CDL	C84-C85-C86-C87
150	BT	204	CDL	C12-C13-C14-C15
150	Dh	202	CDL	C52-C53-C54-C55
155	DG	205	3PE	C29-C2A-C2B-C2C
155	Ds	403	3PE	C34-C35-C36-C37
155	El	905	3PE	C2F-C2G-C2H-C2I
150	g	801	CDL	C39-C40-C41-C42
150	EN	1201	CDL	C12-C13-C14-C15
150	Di	1103	CDL	C76-C77-C78-C79
153	AA	906	PC1	C3D-C3E-C3F-C3G
150	H	1301	CDL	C14-C15-C16-C17
150	DR	403	CDL	C34-C35-C36-C37
150	Dh	202	CDL	C20-C21-C22-C23
153	Dy	302	PC1	C3B-C3C-C3D-C3E
156	DA	710	LPP	C18-C19-C20-C21
150	Du	403	CDL	CA4-CA6-OA8-CA7
150	DA	706	CDL	C63-C64-C65-C66
150	DM	502	CDL	C12-C13-C14-C15

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

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Mol	Chain	Res	Type	Atoms
153	C	508	PC1	C28-C29-C2A-C2B
150	EK	201	CDL	CA5-C11-C12-C13
155	CD	303	3PE	C21-C22-C23-C24
150	C	504	CDL	C11-C12-C13-C14
150	DD	706	CDL	C56-C57-C58-C59
150	DN	506	CDL	C18-C19-C20-C21
150	EN	1202	CDL	C12-C13-C14-C15
150	El	903	CDL	C84-C85-C86-C87
153	AL	303	PC1	C23-C24-C25-C26
153	Eo	201	PC1	C3F-C3G-C3H-C3I
150	Dn	506	CDL	C59-C60-C61-C62
153	AL	303	PC1	C29-C2A-C2B-C2C
153	c	503	PC1	C2A-C2B-C2C-C2D
150	DC	601	CDL	C31-CA7-OA8-CA6
153	AU	202	PC1	C32-C31-O31-C3
150	DI	302	CDL	O1-C1-CB2-OB2
150	A0	601	CDL	C1-CA2-OA2-PA1
150	AM	301	CDL	CB4-CB3-OB5-PB2
150	B1	402	CDL	C1-CA2-OA2-PA1
150	C	503	CDL	C1-CA2-OA2-PA1
150	c	502	CDL	CB4-CB3-OB5-PB2
150	DN	502	CDL	CB4-CB3-OB5-PB2
150	DV	401	CDL	C1-CA2-OA2-PA1
150	DV	401	CDL	CB4-CB3-OB5-PB2
150	DV	402	CDL	C1-CB2-OB2-PB2
150	DV	403	CDL	CB4-CB3-OB5-PB2
150	ED	601	CDL	C1-CB2-OB2-PB2
150	ED	605	CDL	C1-CB2-OB2-PB2
150	EL	902	CDL	CA4-CA3-OA5-PA1
150	Dd	702	CDL	CB4-CB3-OB5-PB2
150	Dd	704	CDL	CB4-CB3-OB5-PB2
150	Dm	501	CDL	C1-CA2-OA2-PA1
150	Dq	1401	CDL	C1-CA2-OA2-PA1
150	Dr	403	CDL	CA4-CA3-OA5-PA1
150	Dr	403	CDL	C1-CB2-OB2-PB2
150	Ea	501	CDL	CA4-CA3-OA5-PA1
153	AL	303	PC1	C2-C1-O11-P
155	DX	303	3PE	C2-C1-O11-P
155	Dd	703	3PE	C2-C1-O11-P
150	CC	304	CDL	C55-C56-C57-C58
153	Eb	301	PC1	C3C-C3D-C3E-C3F
155	DI	301	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
169	DA	703	HEA	CAA-CBA-CGA-O1A
150	c	509	CDL	C35-C36-C37-C38
150	DS	404	CDL	C78-C79-C80-C81
153	DA	707	PC1	C35-C36-C37-C38
150	AM	301	CDL	CB4-CB6-OB8-CB7
150	Dv	401	CDL	C72-C71-CB7-OB9
150	C	504	CDL	C13-C14-C15-C16
150	Dq	1403	CDL	C59-C60-C61-C62
150	BL	301	CDL	CB2-C1-CA2-OA2
150	E	301	CDL	CA2-C1-CB2-OB2
150	DG	201	CDL	CA2-C1-CB2-OB2
150	DH	202	CDL	CA2-C1-CB2-OB2
150	Dc	608	CDL	CA2-C1-CB2-OB2
150	Dd	706	CDL	OA7-CA5-OA6-CA4
150	Dn	506	CDL	OA7-CA5-OA6-CA4
150	Ed	205	CDL	OB7-CB5-OB6-CB4
150	DN	502	CDL	C61-C62-C63-C64
150	Dc	608	CDL	C12-C13-C14-C15
155	Dx	1208	3PE	C2B-C2C-C2D-C2E
150	Dh	202	CDL	CB7-C71-C72-C73
150	Dn	503	CDL	CB5-C51-C52-C53
150	Dr	403	CDL	CB7-C71-C72-C73
150	A1	402	CDL	C11-C12-C13-C14
150	DS	404	CDL	C32-C33-C34-C35
150	DU	403	CDL	C33-C34-C35-C36
150	DV	403	CDL	C14-C15-C16-C17
150	Dn	503	CDL	C23-C24-C25-C26
150	C	503	CDL	C71-CB7-OB8-CB6
150	c	506	CDL	C71-CB7-OB8-CB6
150	EB	302	CDL	C31-CA7-OA8-CA6
150	Eg	101	CDL	C71-CB7-OB8-CB6
150	AC	802	CDL	C17-C18-C19-C20
150	DR	402	CDL	C43-C44-C45-C46
156	AA	902	LPP	C34-C35-C36-C37
150	DC	601	CDL	OA9-CA7-OA8-CA6
150	AM	301	CDL	C39-C40-C41-C42
150	DQ	1504	CDL	C75-C76-C77-C78
150	AC	801	CDL	C59-C60-C61-C62
150	DN	507	CDL	C53-C54-C55-C56
150	DS	404	CDL	C40-C41-C42-C43
150	DU	401	CDL	C71-C72-C73-C74
150	Dc	608	CDL	C17-C18-C19-C20

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

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Mol	Chain	Res	Type	Atoms
150	Ds	405	CDL	C79-C80-C81-C82
150	DM	501	CDL	C12-C13-C14-C15
150	DX	301	CDL	C78-C79-C80-C81
153	A2	402	PC1	C3D-C3E-C3F-C3G
150	c	506	CDL	OB9-CB7-OB8-CB6
150	Eg	101	CDL	OB9-CB7-OB8-CB6
153	AU	202	PC1	O32-C31-O31-C3
150	CG	301	CDL	CA5-C11-C12-C13
150	BT	204	CDL	C24-C25-C26-C27
150	c	501	CDL	C24-C25-C26-C27
150	DJ	302	CDL	C33-C34-C35-C36
150	DX	301	CDL	C34-C35-C36-C37
153	DC	604	PC1	C27-C28-C29-C2A
150	AA	901	CDL	O1-C1-CA2-OA2
150	AC	802	CDL	O1-C1-CA2-OA2
150	DU	401	CDL	O1-C1-CB2-OB2
155	BP	201	3PE	O22-C21-O21-C2
150	A1	402	CDL	C17-C18-C19-C20
150	DA	709	CDL	C77-C78-C79-C80
150	Dn	503	CDL	C73-C74-C75-C76
150	Du	403	CDL	C13-C14-C15-C16
150	DH	201	CDL	C12-C13-C14-C15
150	DH	201	CDL	C60-C61-C62-C63
150	EH	1601	CDL	C64-C65-C66-C67
150	BE	201	CDL	CA5-C11-C12-C13
150	DH	201	CDL	CB5-C51-C52-C53
150	Dd	702	CDL	C80-C81-C82-C83
150	Ea	502	CDL	C37-C38-C39-C40
150	El	901	CDL	C19-C20-C21-C22
150	EL	902	CDL	C33-C34-C35-C36
150	Dh	202	CDL	C55-C56-C57-C58
155	A9	602	3PE	C2E-C2F-C2G-C2H
155	C	513	3PE	C33-C34-C35-C36
150	c	506	CDL	OA6-CA4-CA6-OA8
150	Ed	205	CDL	OA6-CA4-CA6-OA8
153	Dv	407	PC1	O21-C2-C3-O31
155	A2	401	3PE	O21-C2-C3-O31
150	BT	202	CDL	C59-C60-C61-C62
150	CG	301	CDL	C56-C57-C58-C59
150	DD	706	CDL	C76-C77-C78-C79
153	Dv	405	PC1	O31-C31-C32-C33
167	C	512	UQ8	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
150	C	505	CDL	C57-C58-C59-C60
150	DX	306	CDL	C13-C14-C15-C16
150	EB	302	CDL	C11-C12-C13-C14
150	BY	201	CDL	CA4-CA3-OA5-PA1
150	CJ	201	CDL	CA4-CA3-OA5-PA1
150	DD	703	CDL	CB4-CB3-OB5-PB2
150	EL	901	CDL	CB4-CB3-OB5-PB2
150	Eh	1601	CDL	CB4-CB3-OB5-PB2
153	El	904	PC1	C2-C1-O11-P
156	Dn	505	LPP	C7-C6-O5-P1
160	AD	502	FMN	C4'-C5'-O5'-P
150	AC	802	CDL	C34-C35-C36-C37
150	DI	302	CDL	C73-C74-C75-C76
150	EO	202	CDL	C13-C14-C15-C16
150	H	1302	CDL	OB7-CB5-OB6-CB4
150	DJ	303	CDL	OB7-CB5-OB6-CB4
153	K	501	PC1	O22-C21-O21-C2
167	El	906	UQ8	C2-C3-O3-C3M
150	Dj	407	CDL	C72-C71-CB7-OB8
153	DC	608	PC1	O31-C31-C32-C33
150	Dy	301	CDL	C57-C58-C59-C60
150	El	902	CDL	C55-C56-C57-C58
155	Dx	1207	3PE	C3F-C3G-C3H-C3I
150	c	506	CDL	CA4-CA6-OA8-CA7
150	c	501	CDL	C22-C23-C24-C25
150	DZ	501	CDL	C19-C20-C21-C22
150	EK	201	CDL	C15-C16-C17-C18
150	EN	1201	CDL	C62-C63-C64-C65
150	EO	202	CDL	C40-C41-C42-C43
155	Di	1102	3PE	C3A-C3B-C3C-C3D
169	Da	703	HEA	CAA-CBA-CGA-O1A
167	DS	403	UQ8	C40-C39-C41-C42
167	Ds	404	UQ8	C40-C39-C41-C42
150	A1	402	CDL	C71-C72-C73-C74
150	Dg	201	CDL	C18-C19-C20-C21
150	Dm	502	CDL	C38-C39-C40-C41
153	Dg	203	PC1	C3F-C3G-C3H-C3I
150	BT	204	CDL	C11-C12-C13-C14
150	Dq	1401	CDL	C71-C72-C73-C74
155	Dr	404	3PE	C29-C2A-C2B-C2C
155	AJ	502	3PE	O21-C21-C22-C23
150	H	1301	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
150	DX	301	CDL	C17-C18-C19-C20
153	D	402	PC1	C24-C25-C26-C27
155	DR	401	3PE	C3D-C3E-C3F-C3G
168	C	502	HEM	CAA-CBA-CGA-O1A
161	AS	200	8Q1	O40-C39-N41-C42
150	AC	801	CDL	C79-C80-C81-C82
150	CG	302	CDL	C77-C78-C79-C80
150	C	503	CDL	C73-C74-C75-C76
150	C	506	CDL	C63-C64-C65-C66
150	Dj	401	CDL	C12-C13-C14-C15
150	Du	403	CDL	C84-C85-C86-C87
150	Dv	402	CDL	C12-C13-C14-C15
156	DA	710	LPP	C17-C18-C19-C20
150	CC	304	CDL	C43-C44-C45-C46
150	DJ	304	CDL	C34-C35-C36-C37
150	DJ	305	CDL	C14-C15-C16-C17
150	Di	1101	CDL	C62-C63-C64-C65
150	Dn	502	CDL	C61-C62-C63-C64
150	CJ	201	CDL	CA3-CA4-CA6-OA8
150	C	503	CDL	CB3-CB4-CB6-OB8
150	c	502	CDL	CB2-C1-CA2-OA2
150	Dd	702	CDL	CA2-C1-CB2-OB2
150	Dd	706	CDL	CB3-CB4-CB6-OB8
150	Dj	404	CDL	CA3-CA4-CA6-OA8
150	Ds	402	CDL	CB3-CB4-CB6-OB8
150	Ds	405	CDL	CB3-CB4-CB6-OB8
153	AA	905	PC1	C1-C2-C3-O31
153	Dv	407	PC1	C1-C2-C3-O31
153	Eo	204	PC1	C1-C2-C3-O31
155	Ds	403	3PE	C1-C2-C3-O31
153	CC	302	PC1	O22-C21-O21-C2
150	BC	302	CDL	C36-C37-C38-C39
150	DQ	1501	CDL	C54-C55-C56-C57
150	Ds	405	CDL	C82-C83-C84-C85
150	Eg	101	CDL	C22-C23-C24-C25
150	ED	605	CDL	CB7-C71-C72-C73
150	BT	202	CDL	C16-C17-C18-C19
150	Ea	502	CDL	C60-C61-C62-C63
150	AA	901	CDL	C13-C14-C15-C16
150	DC	601	CDL	C77-C78-C79-C80
150	DJ	307	CDL	C15-C16-C17-C18
150	DJ	307	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
150	DQ	1501	CDL	O1-C1-CB2-OB2
150	DI	302	CDL	C57-C58-C59-C60
150	DQ	1502	CDL	C78-C79-C80-C81
150	H	1301	CDL	C37-C38-C39-C40
150	DN	507	CDL	C81-C82-C83-C84
150	Dq	1402	CDL	C21-C22-C23-C24
153	AU	202	PC1	C3B-C3C-C3D-C3E
153	Eo	201	PC1	C33-C34-C35-C36
150	BC	301	CDL	C11-C12-C13-C14
150	C	503	CDL	C52-C53-C54-C55
153	A2	402	PC1	C33-C34-C35-C36
155	DX	303	3PE	C3F-C3G-C3H-C3I
150	El	902	CDL	CB4-CB6-OB8-CB7
150	Dr	403	CDL	CA7-C31-C32-C33
150	Ed	204	CDL	CA5-C11-C12-C13
150	AF	402	CDL	C51-C52-C53-C54
150	BC	301	CDL	C71-C72-C73-C74
150	c	502	CDL	C32-C33-C34-C35
150	DY	301	CDL	C20-C21-C22-C23
150	Dj	403	CDL	C44-C45-C46-C47
150	Dq	1401	CDL	C60-C61-C62-C63
150	Dr	402	CDL	C74-C75-C76-C77
150	c	501	CDL	CA6-CA4-OA6-CA5
150	DJ	307	CDL	CB6-CB4-OB6-CB5
150	DN	506	CDL	CA3-CA4-OA6-CA5
150	DQ	1504	CDL	CA6-CA4-OA6-CA5
150	EK	201	CDL	CB3-CB4-OB6-CB5
150	EO	202	CDL	CB3-CB4-OB6-CB5
150	EO	202	CDL	CB6-CB4-OB6-CB5
150	Da	709	CDL	CA3-CA4-OA6-CA5
150	Dg	201	CDL	CA3-CA4-OA6-CA5
150	Dn	506	CDL	CA3-CA4-OA6-CA5
150	Do	501	CDL	CB3-CB4-OB6-CB5
150	Do	501	CDL	CB6-CB4-OB6-CB5
150	Dq	1401	CDL	CA6-CA4-OA6-CA5
150	Dq	1402	CDL	CA6-CA4-OA6-CA5
150	Du	403	CDL	CB3-CB4-OB6-CB5
150	Dv	401	CDL	CB3-CB4-OB6-CB5
153	A1	403	PC1	C3-C2-O21-C21
153	AQ	202	PC1	C1-C2-O21-C21
153	C	508	PC1	C3-C2-O21-C21
153	Db	702	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
153	Dc	609	PC1	C1-C2-O21-C21
153	Dc	609	PC1	C3-C2-O21-C21
153	Eo	205	PC1	C1-C2-O21-C21
153	Eo	205	PC1	C3-C2-O21-C21
167	C	512	UQ8	C35-C34-C36-C37
167	EN	1205	UQ8	C12-C11-C9-C10
167	En	1202	UQ8	C35-C34-C36-C37
150	Dh	201	CDL	C17-C18-C19-C20
150	Di	1101	CDL	C63-C64-C65-C66
150	Dn	501	CDL	C52-C53-C54-C55
150	Dy	301	CDL	C15-C16-C17-C18
153	AU	202	PC1	C3E-C3F-C3G-C3H
153	EN	1203	PC1	C11-C12-N-C14
153	Eo	204	PC1	C11-C12-N-C14
150	DD	706	CDL	OB7-CB5-OB6-CB4
153	DQ	1503	PC1	O22-C21-O21-C2
153	K	501	PC1	C22-C21-O21-C2
150	DH	202	CDL	C79-C80-C81-C82
150	EN	1202	CDL	C33-C34-C35-C36
150	Dv	402	CDL	C11-C12-C13-C14
155	DJ	301	3PE	C3C-C3D-C3E-C3F
150	DX	301	CDL	CA7-C31-C32-C33
150	CG	301	CDL	C20-C21-C22-C23
150	c	501	CDL	C57-C58-C59-C60
150	Dq	1403	CDL	C60-C61-C62-C63
150	A1	402	CDL	CB3-OB5-PB2-OB2
150	AC	802	CDL	CA2-OA2-PA1-OA5
150	H	1302	CDL	CB2-OB2-PB2-OB5
150	DJ	304	CDL	CB3-OB5-PB2-OB2
150	Dj	405	CDL	CA2-OA2-PA1-OA5
150	Ds	406	CDL	CA3-OA5-PA1-OA2
150	Du	401	CDL	CA3-OA5-PA1-OA2
150	Dv	402	CDL	CB2-OB2-PB2-OB5
155	Dr	401	3PE	C11-O13-P-O11
167	EL	905	UQ8	C4-C3-O3-C3M
150	AA	901	CDL	C19-C20-C21-C22
150	DS	404	CDL	C82-C83-C84-C85
153	DC	604	PC1	C26-C27-C28-C29
153	Dv	406	PC1	O21-C21-C22-C23
150	DX	307	CDL	C71-CB7-OB8-CB6
169	DA	703	HEA	CAA-CBA-CGA-O2A
169	Da	703	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
150	DR	403	CDL	C52-C53-C54-C55
150	ES	1101	CDL	C78-C79-C80-C81
150	A0	602	CDL	C12-C13-C14-C15
150	AM	301	CDL	C32-C33-C34-C35
150	ES	1101	CDL	C40-C41-C42-C43
150	Du	402	CDL	C80-C81-C82-C83
150	Ep	701	CDL	C20-C21-C22-C23
150	Eu	101	CDL	C13-C14-C15-C16
150	Dn	503	CDL	CB4-CB3-OB5-PB2
155	DI	301	3PE	C2-C1-O11-P
156	AA	902	LPP	C7-C6-O5-P1
150	Dj	401	CDL	C18-C19-C20-C21
150	Dj	402	CDL	C44-C45-C46-C47
150	H	1301	CDL	OA5-CA3-CA4-OA6
150	DJ	305	CDL	OA5-CA3-CA4-OA6
150	EL	901	CDL	OA5-CA3-CA4-OA6
150	Di	1103	CDL	OB5-CB3-CB4-OB6
150	Dy	301	CDL	OB5-CB3-CB4-OB6
153	DC	608	PC1	O11-C1-C2-O21
155	El	905	3PE	O11-C1-C2-O21
150	A0	602	CDL	C42-C43-C44-C45
150	AP	301	CDL	C11-C12-C13-C14
150	EH	1601	CDL	C13-C14-C15-C16
150	EL	901	CDL	C53-C54-C55-C56
150	Di	1103	CDL	C32-C33-C34-C35
150	Ek	201	CDL	C15-C16-C17-C18
150	DM	501	CDL	OB5-CB3-CB4-CB6
150	DX	306	CDL	OA5-CA3-CA4-CA6
150	ES	1101	CDL	OA5-CA3-CA4-CA6
150	Dj	405	CDL	OB5-CB3-CB4-CB6
150	Do	501	CDL	OB5-CB3-CB4-CB6
150	Eg	101	CDL	OB5-CB3-CB4-CB6
153	e	1101	PC1	O11-C1-C2-C3
153	Db	702	PC1	O11-C1-C2-C3
153	Ds	407	PC1	O11-C1-C2-C3
155	El	905	3PE	O11-C1-C2-C3
150	BC	301	CDL	C13-C14-C15-C16
150	c	502	CDL	C75-C76-C77-C78
150	Dj	402	CDL	C20-C21-C22-C23
150	Eb	302	CDL	C61-C62-C63-C64
153	AA	906	PC1	C2F-C2G-C2H-C2I
150	Dy	301	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
167	C	512	UQ8	C15-C14-C16-C17
150	c	501	CDL	C73-C74-C75-C76
153	k	301	PC1	C23-C24-C25-C26
150	DX	307	CDL	CA5-C11-C12-C13
150	DQ	1504	CDL	O1-C1-CB2-OB2
150	DU	404	CDL	O1-C1-CA2-OA2
150	Dj	404	CDL	O1-C1-CB2-OB2
150	BT	204	CDL	C82-C83-C84-C85
150	DM	501	CDL	C17-C18-C19-C20
150	DS	404	CDL	C18-C19-C20-C21
153	BT	203	PC1	C32-C31-O31-C3
166	CE	401	HEC	CAD-CBD-CGD-O1D
166	CE	401	HEC	CAD-CBD-CGD-O2D
169	DA	703	HEA	CAD-CBD-CGD-O1D
169	DA	703	HEA	CAD-CBD-CGD-O2D
169	Da	702	HEA	CAD-CBD-CGD-O1D
150	DR	402	CDL	C24-C25-C26-C27
155	BT	201	3PE	C23-C24-C25-C26
150	CG	302	CDL	C54-C55-C56-C57
153	AC	804	PC1	C2F-C2G-C2H-C2I
156	Dn	505	LPP	C37-C38-C39-C40
150	EL	901	CDL	OB7-CB5-OB6-CB4
153	Di	1104	PC1	O22-C21-O21-C2
155	Dr	401	3PE	O22-C21-O21-C2
150	DN	507	CDL	C20-C21-C22-C23
150	DS	405	CDL	C78-C79-C80-C81
150	Dd	704	CDL	C59-C60-C61-C62
150	Dr	403	CDL	C62-C63-C64-C65
150	B1	402	CDL	C12-C13-C14-C15
150	c	502	CDL	C40-C41-C42-C43
150	Dd	706	CDL	C34-C35-C36-C37
150	Dj	401	CDL	C60-C61-C62-C63
150	Dj	407	CDL	C32-C33-C34-C35
150	Dq	1401	CDL	C39-C40-C41-C42
150	Dq	1401	CDL	C74-C75-C76-C77
153	BT	203	PC1	O32-C31-O31-C3
150	B0	102	CDL	OB6-CB4-CB6-OB8
150	DQ	1504	CDL	OA6-CA4-CA6-OA8
150	EL	903	CDL	OB6-CB4-CB6-OB8
150	Dd	705	CDL	OB6-CB4-CB6-OB8
153	D	402	PC1	O21-C2-C3-O31
153	e	1101	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
153	Da	707	PC1	O21-C2-C3-O31
153	Ef	501	PC1	O21-C2-C3-O31
155	DC	606	3PE	O21-C2-C3-O31
150	BL	301	CDL	C42-C43-C44-C45
150	BY	201	CDL	C40-C41-C42-C43
150	c	509	CDL	C54-C55-C56-C57
150	Dd	705	CDL	C38-C39-C40-C41
150	Du	401	CDL	C32-C33-C34-C35
150	En	1201	CDL	C14-C15-C16-C17
150	EL	902	CDL	CB4-CB6-OB8-CB7
166	d	802	HEC	CAA-CBA-CGA-O2A
169	Da	702	HEA	CAD-CBD-CGD-O2D
150	DX	307	CDL	OB9-CB7-OB8-CB6
150	DQ	1504	CDL	C72-C73-C74-C75
150	EL	902	CDL	C44-C45-C46-C47
150	Eg	101	CDL	C12-C13-C14-C15
167	EN	1205	UQ8	C11-C12-C13-C14
153	B1	403	PC1	C37-C38-C39-C3A
156	Dl	1101	LPP	C17-C18-C19-C20
150	BL	301	CDL	C71-C72-C73-C74
155	EL	904	3PE	C2F-C2G-C2H-C2I
150	C	505	CDL	CA2-C1-CB2-OB2
150	C	506	CDL	CA2-C1-CB2-OB2
150	DJ	303	CDL	CA2-C1-CB2-OB2
169	Da	703	HEA	CAA-CBA-CGA-O2A
169	Da	703	HEA	CAD-CBD-CGD-O2D
150	DN	503	CDL	CA4-CA6-OA8-CA7
150	DN	502	CDL	C52-C53-C54-C55
150	BV	201	CDL	C13-C14-C15-C16
155	BT	201	3PE	C29-C2A-C2B-C2C
167	DS	403	UQ8	C38-C39-C41-C42
155	Ds	403	3PE	C3E-C3F-C3G-C3H
150	Ds	405	CDL	C18-C19-C20-C21
150	DU	403	CDL	C17-C18-C19-C20
150	DC	601	CDL	C36-C37-C38-C39
155	EM	901	3PE	C25-C26-C27-C28
168	C	502	HEM	CAA-CBA-CGA-O2A
150	c	509	CDL	C32-C33-C34-C35
150	A0	601	CDL	CA4-CA3-OA5-PA1
153	DB	702	PC1	C2-C1-O11-P
153	Eb	303	PC1	C2-C1-O11-P
155	BP	201	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
156	Dn	504	LPP	C7-C6-O5-P1
150	DH	201	CDL	C18-C19-C20-C21
153	Dc	605	PC1	O32-C31-O31-C3
150	Dm	502	CDL	O1-C1-CA2-OA2
150	AF	402	CDL	C76-C77-C78-C79
150	DM	502	CDL	C74-C75-C76-C77
150	Dn	502	CDL	C42-C43-C44-C45
150	Dq	1401	CDL	C57-C58-C59-C60
153	Dv	406	PC1	C3B-C3C-C3D-C3E
155	DX	302	3PE	C2B-C2C-C2D-C2E
150	En	1201	CDL	C77-C78-C79-C80
153	DB	702	PC1	O32-C31-O31-C3
150	AC	801	CDL	C41-C42-C43-C44
153	EO	201	PC1	C28-C29-C2A-C2B
150	DM	501	CDL	C52-C51-CB5-OB6
150	Dh	202	CDL	C72-C71-CB7-OB8
153	DS	406	PC1	O31-C31-C32-C33
153	Dc	609	PC1	O31-C31-C32-C33
150	H	1301	CDL	CA3-CA4-CA6-OA8
150	DC	601	CDL	CB3-CB4-CB6-OB8
150	DN	503	CDL	CA3-CA4-CA6-OA8
150	DX	307	CDL	CB3-CB4-CB6-OB8
150	DZ	501	CDL	CA3-CA4-CA6-OA8
150	Dd	705	CDL	CA3-CA4-CA6-OA8
150	Dj	402	CDL	CB3-CB4-CB6-OB8
150	Dq	1403	CDL	CB3-CB4-CB6-OB8
150	Ea	501	CDL	CB3-CB4-CB6-OB8
153	e	1101	PC1	C1-C2-C3-O31
153	g	802	PC1	C38-C39-C3A-C3B
153	Da	707	PC1	C1-C2-C3-O31
150	AF	402	CDL	C79-C80-C81-C82
150	C	504	CDL	C16-C17-C18-C19
150	DJ	303	CDL	C11-C12-C13-C14
150	DQ	1501	CDL	C51-C52-C53-C54
150	ED	601	CDL	C80-C81-C82-C83
150	Dd	705	CDL	C59-C60-C61-C62
150	Di	1101	CDL	C61-C62-C63-C64
150	Dy	301	CDL	C51-C52-C53-C54
155	DX	304	3PE	C35-C36-C37-C38
155	Dr	401	3PE	C3D-C3E-C3F-C3G
153	Dc	605	PC1	C32-C31-O31-C3
150	AC	801	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
150	B0	102	CDL	C32-C33-C34-C35
150	C	505	CDL	C71-C72-C73-C74
150	ES	1101	CDL	C44-C45-C46-C47
167	ED	603	UQ8	C25-C24-C26-C27
167	EN	1205	UQ8	C15-C14-C16-C17
167	En	1202	UQ8	C30-C29-C31-C32
169	Da	703	HEA	C27-C19-C20-C21
150	CJ	201	CDL	C51-C52-C53-C54
150	DQ	1501	CDL	C38-C39-C40-C41
150	Du	402	CDL	C39-C40-C41-C42
155	DR	401	3PE	C3F-C3G-C3H-C3I
155	DX	303	3PE	C32-C33-C34-C35
155	Ds	408	3PE	C36-C37-C38-C39
167	Ds	404	UQ8	C38-C39-C41-C42
167	Ed	202	UQ8	C38-C39-C41-C42
167	En	1202	UQ8	C33-C34-C36-C37
168	C	501	HEM	C2A-CAA-CBA-CGA
150	C	505	CDL	C13-C14-C15-C16
150	Dj	402	CDL	C21-C22-C23-C24
150	Ds	405	CDL	C40-C41-C42-C43
150	Dx	1204	CDL	C14-C15-C16-C17
155	Em	901	3PE	C25-C26-C27-C28
150	Dn	506	CDL	C11-CA5-OA6-CA4
150	Dm	502	CDL	C59-C60-C61-C62
153	Eo	205	PC1	C3D-C3E-C3F-C3G
155	DI	301	3PE	C3A-C3B-C3C-C3D
167	Ds	404	UQ8	C31-C32-C33-C34
150	BL	301	CDL	C11-C12-C13-C14
150	E	301	CDL	C11-C12-C13-C14
150	H	1302	CDL	C36-C37-C38-C39
150	DD	706	CDL	C11-C12-C13-C14
150	DV	402	CDL	C77-C78-C79-C80
150	Dg	202	CDL	C78-C79-C80-C81
150	Dj	404	CDL	C60-C61-C62-C63
150	Dq	1402	CDL	C32-C33-C34-C35
153	c	503	PC1	C26-C27-C28-C29
153	DJ	306	PC1	C23-C24-C25-C26
153	Dg	203	PC1	O32-C31-O31-C3
153	Dc	604	PC1	O21-C21-C22-C23
150	BY	201	CDL	C80-C81-C82-C83
150	Ed	204	CDL	C54-C55-C56-C57
155	Dx	1206	3PE	C3A-C3B-C3C-C3D

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

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

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Mol	Chain	Res	Type	Atoms
150	C	503	CDL	CB5-C51-C52-C53
153	Db	702	PC1	C21-C22-C23-C24
150	Dd	702	CDL	C71-CB7-OB8-CB6
153	Dg	203	PC1	C32-C31-O31-C3
150	CJ	201	CDL	C77-C78-C79-C80
150	DU	403	CDL	C57-C58-C59-C60
150	Dv	401	CDL	C52-C53-C54-C55
150	BT	202	CDL	C64-C65-C66-C67
150	CC	305	CDL	C77-C78-C79-C80
150	DM	501	CDL	C44-C45-C46-C47
150	DS	401	CDL	C55-C56-C57-C58
150	Da	709	CDL	C43-C44-C45-C46
150	Ea	501	CDL	C33-C34-C35-C36
150	Ei	401	CDL	C12-C11-CA5-OA6
155	CC	301	3PE	O31-C31-C32-C33
155	DX	302	3PE	O21-C21-C22-C23
150	Dn	502	CDL	CA4-CA6-OA8-CA7
150	A0	602	CDL	C80-C81-C82-C83
150	c	502	CDL	C62-C63-C64-C65
150	DC	601	CDL	C54-C55-C56-C57
150	DI	302	CDL	C55-C56-C57-C58
150	Dv	402	CDL	C56-C57-C58-C59
150	E	301	CDL	C51-C52-C53-C54
150	DV	401	CDL	C14-C15-C16-C17
150	Dc	608	CDL	C22-C23-C24-C25
150	Dx	1201	CDL	C37-C38-C39-C40
173	Er	201	ATP	PG-O3B-PB-O3A
150	C	507	CDL	C34-C35-C36-C37
150	DH	201	CDL	C61-C62-C63-C64
150	EL	901	CDL	C83-C84-C85-C86
153	DV	406	PC1	C3D-C3E-C3F-C3G
167	C	511	UQ8	C36-C37-C38-C39
167	El	906	UQ8	C11-C12-C13-C14
150	BV	201	CDL	C76-C77-C78-C79
150	DX	306	CDL	C38-C39-C40-C41
150	DZ	501	CDL	C33-C34-C35-C36
150	EH	1601	CDL	C77-C78-C79-C80
150	Dq	1403	CDL	C44-C45-C46-C47
150	Dv	402	CDL	C43-C44-C45-C46
153	c	507	PC1	C3F-C3G-C3H-C3I
161	AS	200	8Q1	O33-C32-C34-N36
150	DD	704	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
150	BC	301	CDL	C12-C11-CA5-OA6
150	BC	302	CDL	C72-C71-CB7-OB8
150	DN	506	CDL	C72-C71-CB7-OB8
150	Du	402	CDL	C32-C31-CA7-OA8
150	Eh	1601	CDL	C52-C51-CB5-OB6
155	BT	201	3PE	O21-C21-C22-C23
156	Dn	504	LPP	O27-C29-C30-C31
150	Di	1103	CDL	CB4-CB6-OB8-CB7
150	H	1302	CDL	C23-C24-C25-C26
150	h	501	CDL	C18-C19-C20-C21
167	EL	905	UQ8	C15-C14-C16-C17
167	EN	1205	UQ8	C35-C34-C36-C37
150	CC	305	CDL	C35-C36-C37-C38
150	C	504	CDL	C19-C20-C21-C22
150	DD	703	CDL	C38-C39-C40-C41
153	c	508	PC1	C38-C39-C3A-C3B
150	EK	201	CDL	CB3-OB5-PB2-OB2
150	Dh	202	CDL	CA2-OA2-PA1-OA5
150	Di	1103	CDL	CA2-OA2-PA1-OA5
150	Dr	403	CDL	CB2-OB2-PB2-OB5
153	A1	403	PC1	C1-O11-P-O13
153	AA	903	PC1	C11-O13-P-O11
153	c	507	PC1	C11-O13-P-O11
153	Dv	404	PC1	C1-O11-P-O13
155	DG	205	3PE	C11-O13-P-O11
167	C	512	UQ8	C13-C14-C16-C17
167	EN	1205	UQ8	C13-C14-C16-C17
167	EN	1205	UQ8	C12-C11-C9-C8
150	Do	501	CDL	C31-C32-C33-C34
150	Ep	701	CDL	C33-C34-C35-C36
150	DZ	501	CDL	C31-CA7-OA8-CA6
153	DB	702	PC1	C32-C31-O31-C3
150	B0	102	CDL	C12-C11-CA5-OA6
150	E	301	CDL	C32-C31-CA7-OA8
150	h	501	CDL	C52-C51-CB5-OB6
150	DQ	1502	CDL	C32-C31-CA7-OA8
150	Di	1103	CDL	C72-C71-CB7-OB8
153	EO	206	PC1	O21-C21-C22-C23
155	DJ	301	3PE	O21-C21-C22-C23
155	Di	1102	3PE	O21-C21-C22-C23
155	Dx	1207	3PE	O21-C21-C22-C23
150	DN	502	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
150	DU	404	CDL	C40-C41-C42-C43
155	DX	304	3PE	C26-C27-C28-C29
155	Di	1102	3PE	C36-C37-C38-C39
150	DU	402	CDL	OA9-CA7-OA8-CA6
150	CG	302	CDL	C41-C42-C43-C44
150	DR	403	CDL	C71-C72-C73-C74
150	Du	401	CDL	C13-C14-C15-C16
153	D	402	PC1	C3D-C3E-C3F-C3G
153	K	502	PC1	C27-C28-C29-C2A
155	DC	607	3PE	C2F-C2G-C2H-C2I
155	EL	904	3PE	C34-C35-C36-C37
167	CC	303	UQ8	C5-C6-C7-C8
150	A0	602	CDL	C73-C74-C75-C76
150	DV	401	CDL	C78-C79-C80-C81
150	Dd	706	CDL	C63-C64-C65-C66
150	Dg	201	CDL	C51-C52-C53-C54
150	Dj	405	CDL	C32-C33-C34-C35
150	Dj	405	CDL	C53-C54-C55-C56
150	Dj	405	CDL	C61-C62-C63-C64
150	Dn	502	CDL	C38-C39-C40-C41
150	CC	304	CDL	C73-C74-C75-C76
150	DN	506	CDL	C74-C75-C76-C77
150	DQ	1504	CDL	C19-C20-C21-C22
150	DV	401	CDL	C52-C53-C54-C55
150	EA	301	CDL	C78-C79-C80-C81
155	DX	304	3PE	C2E-C2F-C2G-C2H
150	EB	302	CDL	O1-C1-CB2-OB2
150	Do	501	CDL	O1-C1-CB2-OB2
150	Dd	702	CDL	OB9-CB7-OB8-CB6
150	Dn	502	CDL	OB9-CB7-OB8-CB6
150	A1	402	CDL	C52-C51-CB5-OB6
150	B1	402	CDL	C72-C71-CB7-OB8
150	H	1302	CDL	C32-C31-CA7-OA8
150	DS	405	CDL	C32-C31-CA7-OA8
150	DU	403	CDL	C32-C31-CA7-OA8
150	Da	709	CDL	C12-C11-CA5-OA6
150	Dq	1403	CDL	C72-C71-CB7-OB8
153	BG	202	PC1	O21-C21-C22-C23
153	K	502	PC1	O31-C31-C32-C33
153	EO	205	PC1	O31-C31-C32-C33
153	Dv	404	PC1	O31-C31-C32-C33
150	AC	802	CDL	C53-C54-C55-C56

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

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

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Mol	Chain	Res	Type	Atoms
150	El	902	CDL	C52-C51-CB5-OB6
153	AU	202	PC1	O31-C31-C32-C33
153	B1	401	PC1	O31-C31-C32-C33
153	DC	602	PC1	O21-C21-C22-C23
153	DC	603	PC1	O21-C21-C22-C23
155	DS	402	3PE	O21-C21-C22-C23
150	A0	602	CDL	C33-C34-C35-C36
150	DA	706	CDL	C71-C72-C73-C74
150	DI	302	CDL	C84-C85-C86-C87
156	AA	902	LPP	C31-C32-C33-C34
150	DD	703	CDL	C14-C15-C16-C17
150	DN	506	CDL	C60-C61-C62-C63
150	EL	903	CDL	C38-C39-C40-C41
150	Dh	202	CDL	C23-C24-C25-C26
150	Dv	403	CDL	C23-C24-C25-C26
153	EO	201	PC1	C23-C24-C25-C26
153	Dc	602	PC1	C2E-C2F-C2G-C2H
155	DI	301	3PE	C32-C33-C34-C35
155	DI	301	3PE	C36-C37-C38-C39
155	DS	402	3PE	C28-C29-C2A-C2B
150	AA	901	CDL	C1-CA2-OA2-PA1
150	CD	301	CDL	CA3-CA4-CA6-OA8
150	DD	703	CDL	CB3-CB4-CB6-OB8
150	DI	302	CDL	CB3-CB4-CB6-OB8
150	DU	403	CDL	C1-CB2-OB2-PB2
150	EB	302	CDL	CB3-CB4-CB6-OB8
150	ED	604	CDL	CA3-CA4-CA6-OA8
150	EL	901	CDL	CB3-CB4-CB6-OB8
150	Ds	401	CDL	CA3-CA4-CA6-OA8
150	Dx	1204	CDL	CB3-CB4-CB6-OB8
150	En	1201	CDL	CA3-CA4-CA6-OA8
155	A2	401	3PE	C1-C2-C3-O31
155	DC	607	3PE	C1-C2-C3-O31
155	Eo	202	3PE	C1-C2-C3-O31
166	CE	401	HEC	CAA-CBA-CGA-O2A
150	BC	301	CDL	C73-C74-C75-C76
150	BT	202	CDL	C55-C56-C57-C58
150	E	301	CDL	C19-C20-C21-C22
150	CD	301	CDL	C32-C31-CA7-OA9
150	BC	301	CDL	OB9-CB7-OB8-CB6
150	DD	706	CDL	C51-CB5-OB6-CB4
150	AC	802	CDL	C23-C24-C25-C26

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

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Mol	Chain	Res	Type	Atoms
153	DV	404	PC1	O31-C31-C32-C33
153	Eb	301	PC1	O31-C31-C32-C33
155	EM	901	3PE	O21-C21-C22-C23
155	Eo	202	3PE	O31-C31-C32-C33
150	Dd	702	CDL	OA9-CA7-OA8-CA6
150	AC	801	CDL	C44-C45-C46-C47
150	BV	201	CDL	C42-C43-C44-C45
153	DB	702	PC1	C26-C27-C28-C29
153	Di	1104	PC1	C34-C35-C36-C37
150	A1	402	CDL	C37-C38-C39-C40
150	g	801	CDL	C75-C76-C77-C78
150	EO	202	CDL	C41-C42-C43-C44
150	Dh	201	CDL	C57-C58-C59-C60
150	Eb	302	CDL	C23-C24-C25-C26
150	EK	201	CDL	CB2-C1-CA2-OA2
150	BE	201	CDL	O1-C1-CA2-OA2
150	g	801	CDL	O1-C1-CA2-OA2
150	Di	1101	CDL	O1-C1-CB2-OB2
150	Du	402	CDL	C79-C80-C81-C82
153	DC	602	PC1	C2E-C2F-C2G-C2H
150	DJ	304	CDL	CA4-CA6-OA8-CA7
153	c	507	PC1	O22-C21-C22-C23
173	ER	201	ATP	PB-O3B-PG-O3G
166	CE	401	HEC	CAA-CBA-CGA-O1A
150	ED	605	CDL	C12-C11-CA5-OA6
150	Dm	501	CDL	C12-C11-CA5-OA6
150	Dv	403	CDL	C52-C51-CB5-OB6
150	El	901	CDL	C32-C31-CA7-OA8
153	A0	605	PC1	O21-C21-C22-C23
155	DJ	301	3PE	O31-C31-C32-C33
169	Da	703	HEA	C18-C19-C20-C21
150	A0	602	CDL	C51-C52-C53-C54
150	EH	1601	CDL	C11-C12-C13-C14
155	Dx	1208	3PE	C35-C36-C37-C38
155	Eo	202	3PE	C26-C27-C28-C29
150	DJ	303	CDL	C51-CB5-OB6-CB4
173	ER	201	ATP	PG-O3B-PB-O3A
150	BY	201	CDL	C17-C18-C19-C20
150	Dj	405	CDL	C44-C45-C46-C47
150	Dq	1401	CDL	C58-C59-C60-C61
150	Du	401	CDL	C20-C21-C22-C23
150	Ed	204	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
150	AM	301	CDL	OB5-CB3-CB4-CB6
150	CD	301	CDL	OB5-CB3-CB4-CB6
150	C	507	CDL	OB5-CB3-CB4-CB6
150	DJ	304	CDL	OB5-CB3-CB4-CB6
150	DM	502	CDL	OA5-CA3-CA4-CA6
150	DN	502	CDL	OB5-CB3-CB4-CB6
150	DR	403	CDL	OA5-CA3-CA4-CA6
150	DX	301	CDL	OB5-CB3-CB4-CB6
150	EH	1601	CDL	OA5-CA3-CA4-CA6
150	Dd	704	CDL	OB5-CB3-CB4-CB6
150	Du	401	CDL	OA5-CA3-CA4-CA6
150	Eh	1601	CDL	OB5-CB3-CB4-CB6
153	C	510	PC1	O11-C1-C2-C3
153	E	303	PC1	O11-C1-C2-C3
153	DC	603	PC1	O11-C1-C2-C3
155	AJ	502	3PE	O11-C1-C2-C3
150	E	301	CDL	C12-C13-C14-C15
150	Du	402	CDL	C17-C18-C19-C20
150	Ei	401	CDL	C84-C85-C86-C87
150	En	1201	CDL	C43-C44-C45-C46
150	A0	602	CDL	C72-C71-CB7-OB8
150	H	1301	CDL	C32-C31-CA7-OA8
150	DI	302	CDL	C72-C71-CB7-OB8
150	EN	1201	CDL	C52-C51-CB5-OB6
150	Dd	702	CDL	C72-C71-CB7-OB8
153	A6	302	PC1	O31-C31-C32-C33
153	AA	904	PC1	O21-C21-C22-C23
153	Dc	602	PC1	O21-C21-C22-C23
153	Eo	205	PC1	O21-C21-C22-C23
155	BA	301	3PE	O21-C21-C22-C23
155	DG	205	3PE	O21-C21-C22-C23
155	DX	303	3PE	O31-C31-C32-C33
155	Dx	1207	3PE	O31-C31-C32-C33
150	DI	302	CDL	C34-C35-C36-C37
150	DQ	1502	CDL	C37-C38-C39-C40
150	Dh	201	CDL	C20-C21-C22-C23
150	Dq	1401	CDL	C16-C17-C18-C19
150	Dq	1401	CDL	C51-C52-C53-C54
150	AA	908	CDL	OA6-CA4-CA6-OA8
150	E	301	CDL	OA6-CA4-CA6-OA8
150	h	501	CDL	OB6-CB4-CB6-OB8
150	Da	709	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
150	Dn	502	CDL	OB6-CB4-CB6-OB8
150	Dq	1402	CDL	OB6-CB4-CB6-OB8
150	Dv	403	CDL	OA6-CA4-CA6-OA8
153	AC	804	PC1	O21-C2-C3-O31
153	AM	302	PC1	O21-C2-C3-O31
155	AJ	502	3PE	O21-C2-C3-O31
155	BT	201	3PE	O21-C2-C3-O31
150	DU	401	CDL	CB5-C51-C52-C53
150	DD	703	CDL	C20-C21-C22-C23
150	Dq	1402	CDL	C13-C14-C15-C16
150	Eu	101	CDL	C14-C15-C16-C17
155	A9	602	3PE	C29-C2A-C2B-C2C
150	Eg	101	CDL	C74-C75-C76-C77
150	Dn	501	CDL	OB7-CB5-OB6-CB4
150	AM	301	CDL	C32-C31-CA7-OA8
150	BT	204	CDL	C12-C11-CA5-OA6
150	DQ	1501	CDL	C72-C71-CB7-OB8
150	EL	903	CDL	C12-C11-CA5-OA6
150	Dd	705	CDL	C12-C11-CA5-OA6
150	Dj	402	CDL	C12-C11-CA5-OA6
150	Dn	503	CDL	C32-C31-CA7-OA8
150	Dq	1401	CDL	C32-C31-CA7-OA8
150	Dr	402	CDL	C52-C51-CB5-OB6
150	Ea	502	CDL	C52-C51-CB5-OB6
150	El	903	CDL	C32-C31-CA7-OA8
153	AJ	501	PC1	O31-C31-C32-C33
153	g	802	PC1	O21-C21-C22-C23
153	DC	608	PC1	O21-C21-C22-C23
153	EO	205	PC1	O21-C21-C22-C23
155	DG	205	3PE	O31-C31-C32-C33
155	Dx	1206	3PE	O21-C21-C22-C23
150	BV	201	CDL	C72-C71-CB7-OB9
150	H	1302	CDL	CB4-CB6-OB8-CB7
150	DZ	501	CDL	CA4-CA6-OA8-CA7
150	Dm	502	CDL	C19-C20-C21-C22
150	Du	402	CDL	C52-C53-C54-C55
150	Ek	201	CDL	C34-C35-C36-C37
155	CD	303	3PE	C32-C33-C34-C35
169	DA	702	HEA	CAD-CBD-CGD-O2D
151	A0	603	UDP	C5'-O5'-PA-O3A
154	A1	401	NDP	C2B-O2B-P2B-O3X
164	CA	702	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
150	DN	507	CDL	C77-C78-C79-C80
150	DZ	501	CDL	C44-C45-C46-C47
150	Dn	502	CDL	C18-C19-C20-C21
155	DN	501	3PE	C2C-C2D-C2E-C2F
150	DI	302	CDL	C71-CB7-OB8-CB6
150	Di	1101	CDL	C16-C17-C18-C19
153	C	509	PC1	C25-C26-C27-C28
153	Di	1104	PC1	C22-C21-O21-C2
150	AF	402	CDL	C72-C71-CB7-OB8
150	BT	204	CDL	C32-C31-CA7-OA8
150	DD	705	CDL	C72-C71-CB7-OB8
150	Dd	705	CDL	C72-C71-CB7-OB8
150	Dj	407	CDL	C32-C31-CA7-OA8
150	Ea	502	CDL	C12-C11-CA5-OA6
150	Ek	201	CDL	C32-C31-CA7-OA8
153	AM	302	PC1	O21-C21-C22-C23
153	AM	302	PC1	O31-C31-C32-C33
153	DX	308	PC1	O31-C31-C32-C33
155	Dd	703	3PE	O31-C31-C32-C33
150	Dm	501	CDL	C84-C85-C86-C87
153	Dc	609	PC1	C3C-C3D-C3E-C3F
155	Dr	401	3PE	C3F-C3G-C3H-C3I
150	BT	202	CDL	C17-C18-C19-C20
150	Eh	1601	CDL	C21-C22-C23-C24
153	EO	206	PC1	C3D-C3E-C3F-C3G
150	Ed	205	CDL	CB7-C71-C72-C73
150	DX	301	CDL	C32-C33-C34-C35
150	Dv	402	CDL	C77-C78-C79-C80
167	EN	1205	UQ8	C33-C34-C36-C37
167	El	906	UQ8	C12-C11-C9-C8
167	En	1202	UQ8	C12-C11-C9-C8
150	DN	506	CDL	CA4-CA3-OA5-PA1
150	EL	902	CDL	CB4-CB3-OB5-PB2
150	Dj	407	CDL	C1-CA2-OA2-PA1
150	AC	801	CDL	C20-C21-C22-C23
150	ES	1101	CDL	C31-C32-C33-C34
150	El	901	CDL	C62-C63-C64-C65
153	BG	202	PC1	C34-C35-C36-C37
150	BL	301	CDL	C32-C31-CA7-OA8
150	DA	709	CDL	C72-C71-CB7-OB8
150	DJ	302	CDL	C72-C71-CB7-OB8
150	DU	403	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
150	Dv	402	CDL	C72-C71-CB7-OB8
150	Dx	1204	CDL	C12-C11-CA5-OA6
150	Ea	502	CDL	C72-C71-CB7-OB8
155	EN	1204	3PE	O21-C21-C22-C23
150	Dn	503	CDL	C14-C15-C16-C17
161	AS	200	8Q1	C9-C10-C11-C12
155	BT	201	3PE	C31-C32-C33-C34
167	CC	303	UQ8	C9-C11-C12-C13
167	C	511	UQ8	C14-C16-C17-C18
167	C	511	UQ8	C9-C11-C12-C13
150	CC	304	CDL	C20-C21-C22-C23
150	ED	604	CDL	O1-C1-CA2-OA2
150	DD	705	CDL	C20-C21-C22-C23
150	DM	501	CDL	C13-C14-C15-C16
150	DQ	1501	CDL	C80-C81-C82-C83
150	EN	1201	CDL	C18-C19-C20-C21
167	Ds	404	UQ8	C3-C4-O4-C4M
167	Ed	202	UQ8	C4-C3-O3-C3M
154	A1	401	NDP	O4B-C4B-C5B-O5B
150	BY	201	CDL	CA7-C31-C32-C33
150	Dq	1402	CDL	CB5-C51-C52-C53
150	El	902	CDL	CB7-C71-C72-C73
150	CG	302	CDL	C56-C57-C58-C59
150	EH	1601	CDL	C14-C15-C16-C17
153	B1	403	PC1	C39-C3A-C3B-C3C
153	BG	202	PC1	C3E-C3F-C3G-C3H
153	C	508	PC1	C37-C38-C39-C3A
155	Dr	404	3PE	C28-C29-C2A-C2B
155	Eo	202	3PE	C38-C39-C3A-C3B
155	EM	901	3PE	C32-C31-O31-C3
150	c	509	CDL	C72-C71-CB7-OB8
150	DJ	304	CDL	C32-C31-CA7-OA8
150	DJ	304	CDL	C72-C71-CB7-OB8
150	Eu	101	CDL	C72-C71-CB7-OB8
153	Eo	201	PC1	O31-C31-C32-C33
153	DC	602	PC1	O22-C21-C22-C23
173	ER	201	ATP	PG-O3B-PB-O1B
150	c	506	CDL	C38-C39-C40-C41
150	DI	302	CDL	OB9-CB7-OB8-CB6
150	AA	908	CDL	C75-C76-C77-C78
150	DR	403	CDL	C62-C63-C64-C65
150	EH	1601	CDL	C35-C36-C37-C38

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

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Mol	Chain	Res	Type	Atoms
150	Dj	407	CDL	C52-C51-CB5-OB7
153	AU	202	PC1	O32-C31-C32-C33
153	BG	202	PC1	O22-C21-C22-C23
153	EO	205	PC1	O32-C31-C32-C33
155	Dx	1207	3PE	O22-C21-C22-C23
150	c	509	CDL	C51-C52-C53-C54
150	DQ	1502	CDL	C22-C23-C24-C25
167	c	510	UQ8	C40-C39-C41-C42
150	A0	602	CDL	C32-C33-C34-C35
150	Dg	202	CDL	C59-C60-C61-C62
150	Dn	506	CDL	C81-C82-C83-C84
150	Eg	101	CDL	C56-C57-C58-C59
150	En	1201	CDL	C32-C33-C34-C35
153	d	801	PC1	C22-C23-C24-C25
155	EM	901	3PE	O32-C31-O31-C3
167	c	510	UQ8	C12-C11-C9-C8
150	DU	401	CDL	C32-C31-CA7-OA8
150	DD	704	CDL	C40-C41-C42-C43
150	DN	507	CDL	C74-C75-C76-C77
150	Dq	1401	CDL	C11-C12-C13-C14
150	Dr	402	CDL	C54-C55-C56-C57
150	En	1201	CDL	C52-C53-C54-C55
150	DU	403	CDL	C52-C51-CB5-OB7
153	DA	707	PC1	O32-C31-C32-C33
153	Dg	203	PC1	O32-C31-C32-C33
155	BT	201	3PE	O22-C21-C22-C23
150	CC	305	CDL	C44-C45-C46-C47
150	g	801	CDL	C42-C43-C44-C45
150	Dh	201	CDL	C18-C19-C20-C21
155	Dx	1208	3PE	C2E-C2F-C2G-C2H
150	H	1301	CDL	C31-CA7-OA8-CA6
150	CD	301	CDL	C39-C40-C41-C42
150	ES	1101	CDL	C36-C37-C38-C39
150	Dg	201	CDL	C34-C35-C36-C37
150	Di	1101	CDL	C73-C74-C75-C76
150	Dq	1401	CDL	C19-C20-C21-C22
150	Dv	403	CDL	C34-C35-C36-C37
150	Dx	1201	CDL	C82-C83-C84-C85
153	EB	303	PC1	C34-C35-C36-C37
155	DN	501	3PE	C2D-C2E-C2F-C2G
155	Em	901	3PE	C3B-C3C-C3D-C3E
150	Dj	403	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
150	Du	401	CDL	CA2-C1-CB2-OB2
150	Du	401	CDL	C61-C62-C63-C64
150	E	301	CDL	C32-C31-CA7-OA9
150	DA	709	CDL	C72-C71-CB7-OB9
150	DD	704	CDL	C52-C51-CB5-OB7
150	Di	1103	CDL	C72-C71-CB7-OB9
150	Dn	502	CDL	C32-C31-CA7-OA9
150	Dr	403	CDL	C52-C51-CB5-OB7
153	C	509	PC1	O32-C31-C32-C33
155	DX	302	3PE	O22-C21-C22-C23
155	Di	1102	3PE	O22-C21-C22-C23
156	Dn	504	LPP	O28-C29-C30-C31
150	AF	402	CDL	C52-C51-CB5-OB6
150	Di	1101	CDL	C52-C51-CB5-OB6
150	c	501	CDL	C23-C24-C25-C26
150	DG	201	CDL	C34-C35-C36-C37
150	ES	1101	CDL	C83-C84-C85-C86
150	CD	302	CDL	C23-C24-C25-C26
150	g	801	CDL	C24-C25-C26-C27
150	DO	501	CDL	C23-C24-C25-C26
150	Dc	608	CDL	C59-C60-C61-C62
150	Di	1101	CDL	C53-C54-C55-C56
150	Ea	501	CDL	C43-C44-C45-C46
150	A1	402	CDL	C52-C51-CB5-OB7
150	B0	102	CDL	C12-C11-CA5-OA7
150	BC	301	CDL	C12-C11-CA5-OA7
150	BC	302	CDL	C72-C71-CB7-OB9
150	h	501	CDL	C52-C51-CB5-OB7
150	DM	502	CDL	C72-C71-CB7-OB9
150	ED	605	CDL	C12-C11-CA5-OA7
150	Dq	1403	CDL	C72-C71-CB7-OB9
150	Ds	406	CDL	C32-C31-CA7-OA9
150	Du	402	CDL	C32-C31-CA7-OA9
150	Eh	1601	CDL	C52-C51-CB5-OB7
150	Ei	401	CDL	C12-C11-CA5-OA7
150	Ep	701	CDL	C12-C11-CA5-OA7
153	DV	404	PC1	O32-C31-C32-C33
155	DG	204	3PE	O22-C21-C22-C23
155	DJ	301	3PE	O32-C31-C32-C33
155	Dd	703	3PE	O22-C21-C22-C23
155	Dg	204	3PE	O22-C21-C22-C23
150	c	502	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
150	DJ	302	CDL	CB3-CB4-CB6-OB8
150	DN	506	CDL	CA3-CA4-CA6-OA8
150	DQ	1502	CDL	CB3-CB4-CB6-OB8
150	DU	402	CDL	CB3-CB4-CB6-OB8
150	Ek	201	CDL	CB3-CB4-CB6-OB8
153	AA	903	PC1	C1-C2-C3-O31
153	c	503	PC1	C1-C2-C3-O31
153	DC	603	PC1	C1-C2-C3-O31
153	Dc	602	PC1	C1-C2-C3-O31
153	BG	202	PC1	O31-C31-C32-C33
150	BV	201	CDL	C11-C12-C13-C14
150	Ds	405	CDL	C34-C35-C36-C37
153	DA	707	PC1	C2C-C2D-C2E-C2F
153	DY	302	PC1	C3E-C3F-C3G-C3H
150	CG	302	CDL	CB2-OB2-PB2-OB5
150	CD	301	CDL	CB3-OB5-PB2-OB2
150	Ds	406	CDL	CB2-OB2-PB2-OB5
150	Ea	501	CDL	CB2-OB2-PB2-OB5
150	AC	801	CDL	C74-C75-C76-C77
150	DD	704	CDL	C51-C52-C53-C54
150	Ek	201	CDL	C11-C12-C13-C14
150	DU	402	CDL	O1-C1-CA2-OA2
150	ES	1101	CDL	O1-C1-CA2-OA2
150	C	507	CDL	CA5-C11-C12-C13
155	Da	708	3PE	C31-C32-C33-C34
150	C	507	CDL	C72-C71-CB7-OB9
150	H	1301	CDL	C52-C51-CB5-OB7
150	DN	506	CDL	C72-C71-CB7-OB9
150	Eb	302	CDL	C72-C71-CB7-OB9
150	El	902	CDL	C52-C51-CB5-OB7
153	EO	204	PC1	O22-C21-C22-C23
153	EO	206	PC1	O22-C21-C22-C23
155	A9	602	3PE	O22-C21-C22-C23
155	CC	301	3PE	O32-C31-C32-C33
155	DG	205	3PE	O32-C31-C32-C33
155	DI	301	3PE	O22-C21-C22-C23
155	EN	1204	3PE	O22-C21-C22-C23
156	AC	803	LPP	O28-C29-C30-C31
150	AF	401	CDL	C82-C83-C84-C85
150	CG	301	CDL	C72-C73-C74-C75
150	DJ	303	CDL	C55-C56-C57-C58
150	DN	507	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
150	DY	301	CDL	C77-C78-C79-C80
150	Da	709	CDL	C52-C53-C54-C55
150	Dc	601	CDL	C15-C16-C17-C18
150	Dq	1401	CDL	C12-C13-C14-C15
150	Eb	302	CDL	C33-C34-C35-C36
150	En	1201	CDL	C36-C37-C38-C39
150	DX	307	CDL	C39-C40-C41-C42
150	EB	302	CDL	C23-C24-C25-C26
150	Dd	705	CDL	C34-C35-C36-C37
150	Dj	401	CDL	C80-C81-C82-C83
150	Dj	404	CDL	C15-C16-C17-C18
153	K	502	PC1	C2E-C2F-C2G-C2H
156	EI	402	LPP	C21-C22-C23-C24
150	Dn	502	CDL	C52-C51-CB5-OB6
150	Ea	501	CDL	C32-C31-CA7-OA8
150	Ed	205	CDL	C12-C11-CA5-OA6
150	DJ	305	CDL	CB4-CB3-OB5-PB2
150	Dj	407	CDL	C1-CB2-OB2-PB2
150	Dq	1403	CDL	CA4-CA3-OA5-PA1
150	Ds	405	CDL	C1-CA2-OA2-PA1
153	EB	303	PC1	C2-C1-O11-P
153	EO	204	PC1	C2-C1-O11-P
155	A2	401	3PE	C2-C1-O11-P
150	A1	402	CDL	C31-C32-C33-C34
150	BG	201	CDL	C39-C40-C41-C42
150	Dj	407	CDL	C15-C16-C17-C18
150	Dm	501	CDL	C54-C55-C56-C57
150	Dj	401	CDL	C72-C71-CB7-OB9
150	Dm	501	CDL	C12-C11-CA5-OA7
150	Dv	403	CDL	C52-C51-CB5-OB7
150	Ea	502	CDL	C12-C11-CA5-OA7
150	Ea	502	CDL	C72-C71-CB7-OB9
150	El	901	CDL	C32-C31-CA7-OA9
155	DJ	301	3PE	O22-C21-C22-C23
155	Eo	202	3PE	O32-C31-C32-C33
150	ES	1101	CDL	C84-C85-C86-C87
150	Dn	506	CDL	C13-C14-C15-C16
150	BE	201	CDL	OB9-CB7-OB8-CB6
150	Dy	301	CDL	OB9-CB7-OB8-CB6
150	Dm	502	CDL	C60-C61-C62-C63
150	Do	501	CDL	C37-C38-C39-C40
155	DS	402	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
150	A0	602	CDL	CA2-OA2-PA1-OA3
150	AC	802	CDL	CA2-OA2-PA1-OA3
150	AF	402	CDL	CB3-OB5-PB2-OB3
150	B0	101	CDL	CA3-OA5-PA1-OA3
150	B0	102	CDL	CA2-OA2-PA1-OA3
150	BV	201	CDL	CA2-OA2-PA1-OA3
150	BV	201	CDL	CA2-OA2-PA1-OA4
150	BY	201	CDL	CA3-OA5-PA1-OA3
150	BY	201	CDL	CB2-OB2-PB2-OB4
150	BY	201	CDL	CB3-OB5-PB2-OB4
150	CG	302	CDL	CB2-OB2-PB2-OB3
150	CC	305	CDL	CB3-OB5-PB2-OB4
150	C	505	CDL	CB3-OB5-PB2-OB4
150	C	507	CDL	CA2-OA2-PA1-OA3
150	H	1302	CDL	CB2-OB2-PB2-OB3
150	DD	703	CDL	CB2-OB2-PB2-OB3
150	DD	703	CDL	CB2-OB2-PB2-OB4
150	DG	202	CDL	CA3-OA5-PA1-OA3
150	DH	202	CDL	CA2-OA2-PA1-OA3
150	DI	302	CDL	CA2-OA2-PA1-OA3
150	DJ	303	CDL	CB2-OB2-PB2-OB4
150	DJ	304	CDL	CB3-OB5-PB2-OB3
150	DJ	307	CDL	CA2-OA2-PA1-OA3
150	DN	506	CDL	CA2-OA2-PA1-OA3
150	DU	401	CDL	CB3-OB5-PB2-OB3
150	DX	301	CDL	CB3-OB5-PB2-OB3
150	DY	301	CDL	CA2-OA2-PA1-OA3
150	EA	301	CDL	CB3-OB5-PB2-OB3
150	ED	601	CDL	CB2-OB2-PB2-OB3
150	EI	401	CDL	CA2-OA2-PA1-OA3
150	EL	901	CDL	CA3-OA5-PA1-OA3
150	EL	901	CDL	CB2-OB2-PB2-OB3
150	EL	901	CDL	CB3-OB5-PB2-OB3
150	Dd	702	CDL	CA2-OA2-PA1-OA3
150	Dh	201	CDL	CB3-OB5-PB2-OB3
150	Dh	202	CDL	CA2-OA2-PA1-OA3
150	Di	1101	CDL	CB2-OB2-PB2-OB3
150	Di	1101	CDL	CB2-OB2-PB2-OB4
150	Di	1103	CDL	CB2-OB2-PB2-OB3
150	Dj	405	CDL	CA2-OA2-PA1-OA3
150	Dj	405	CDL	CA3-OA5-PA1-OA3
150	Dm	502	CDL	CB2-OB2-PB2-OB3

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

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

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Mol	Chain	Res	Type	Atoms
155	Da	708	3PE	O13-C11-C12-N
150	A0	602	CDL	C72-C71-CB7-OB9
150	BL	301	CDL	C32-C31-CA7-OA9
150	CJ	201	CDL	C32-C31-CA7-OA9
150	DI	302	CDL	C72-C71-CB7-OB9
150	ED	604	CDL	C72-C71-CB7-OB9
150	Da	709	CDL	C12-C11-CA5-OA7
150	Eu	101	CDL	C72-C71-CB7-OB9
153	K	501	PC1	O32-C31-C32-C33
153	Dc	602	PC1	O22-C21-C22-C23
153	Dx	1205	PC1	O32-C31-C32-C33
156	Dn	505	LPP	O28-C29-C30-C31
150	DS	405	CDL	C41-C42-C43-C44
150	Dh	201	CDL	C32-C33-C34-C35
150	Dn	501	CDL	C82-C83-C84-C85
150	Dr	402	CDL	C41-C42-C43-C44
150	Dx	1204	CDL	C51-C52-C53-C54
153	BS	1301	PC1	C3C-C3D-C3E-C3F
150	BL	301	CDL	C72-C71-CB7-OB8
150	C	505	CDL	C32-C31-CA7-OA8
150	C	506	CDL	C32-C31-CA7-OA8
150	Da	709	CDL	C32-C31-CA7-OA8
150	Dd	706	CDL	C32-C31-CA7-OA8
150	Ds	402	CDL	C12-C11-CA5-OA6
150	El	903	CDL	C52-C51-CB5-OB6
155	BP	201	3PE	O21-C21-C22-C23
150	AF	401	CDL	CB4-CB6-OB8-CB7
155	BA	301	3PE	O22-C21-O21-C2
150	Du	403	CDL	C17-C18-C19-C20
150	Dy	301	CDL	C34-C35-C36-C37
153	DA	707	PC1	C2D-C2E-C2F-C2G
150	Dy	301	CDL	C71-CB7-OB8-CB6
150	AA	901	CDL	C32-C31-CA7-OA9
150	H	1302	CDL	C32-C31-CA7-OA9
150	Di	1101	CDL	C72-C71-CB7-OB9
150	Dx	1204	CDL	C12-C11-CA5-OA7
153	g	802	PC1	O22-C21-C22-C23
153	Da	706	PC1	O32-C31-C32-C33
153	Dc	603	PC1	O22-C21-C22-C23
155	Dx	1207	3PE	O32-C31-C32-C33
150	DN	502	CDL	C75-C76-C77-C78
150	Ep	701	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
150	CC	304	CDL	C18-C19-C20-C21
150	Ds	401	CDL	C33-C34-C35-C36
153	DA	707	PC1	C3A-C3B-C3C-C3D
169	DA	702	HEA	CAD-CBD-CGD-O1D
150	BT	202	CDL	C72-C71-CB7-OB8
153	AH	301	PC1	O21-C21-C22-C23
153	DQ	1503	PC1	O31-C31-C32-C33
153	Dx	1203	PC1	O21-C21-C22-C23
150	B0	101	CDL	C24-C25-C26-C27
150	B1	402	CDL	C51-C52-C53-C54
150	ES	1101	CDL	C37-C38-C39-C40
150	Da	709	CDL	C71-C72-C73-C74
150	Dn	501	CDL	C44-C45-C46-C47
150	El	902	CDL	C36-C37-C38-C39
153	CC	302	PC1	C3D-C3E-C3F-C3G
153	Dv	407	PC1	C3C-C3D-C3E-C3F
155	DX	302	3PE	C26-C27-C28-C29
150	BC	302	CDL	C32-C31-CA7-OA9
150	DI	302	CDL	CB4-CB6-OB8-CB7
150	DV	401	CDL	C72-C71-CB7-OB9
150	Dr	402	CDL	C52-C51-CB5-OB7
153	A0	605	PC1	O22-C21-C22-C23
153	Dv	404	PC1	O32-C31-C32-C33
155	BA	301	3PE	O22-C21-C22-C23
167	c	510	UQ8	C25-C24-C26-C27
150	BV	201	CDL	C21-C22-C23-C24
150	C	503	CDL	C14-C15-C16-C17
150	DJ	304	CDL	C38-C39-C40-C41
150	En	1201	CDL	C19-C20-C21-C22
156	AA	902	LPP	C35-C36-C37-C38
167	En	1202	UQ8	C16-C17-C18-C19
150	CG	301	CDL	C74-C75-C76-C77
150	h	501	CDL	C41-C42-C43-C44
153	Da	706	PC1	C2D-C2E-C2F-C2G
150	A1	402	CDL	CA3-CA4-OA6-CA5
150	Dd	704	CDL	CB6-CB4-OB6-CB5
150	Dj	404	CDL	CB6-CB4-OB6-CB5
150	Dr	403	CDL	CA3-CA4-OA6-CA5
150	Dy	301	CDL	CB3-CB4-OB6-CB5
153	A2	402	PC1	C12-C11-O13-P
153	A6	303	PC1	C12-C11-O13-P
153	AJ	501	PC1	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
153	AU	202	PC1	C12-C11-O13-P
153	AX	401	PC1	C1-C2-O21-C21
153	C	508	PC1	C12-C11-O13-P
153	E	303	PC1	C12-C11-O13-P
153	c	507	PC1	C12-C11-O13-P
153	d	801	PC1	C12-C11-O13-P
153	g	802	PC1	C12-C11-O13-P
153	DX	308	PC1	C12-C11-O13-P
153	EB	301	PC1	C12-C11-O13-P
153	EN	1203	PC1	C12-C11-O13-P
153	Eb	301	PC1	C12-C11-O13-P
155	A9	602	3PE	C12-C11-O13-P
155	BT	201	3PE	C12-C11-O13-P
155	CK	101	3PE	C12-C11-O13-P
155	DG	204	3PE	C12-C11-O13-P
155	DN	501	3PE	C12-C11-O13-P
155	Dx	1202	3PE	C12-C11-O13-P
169	DA	703	HEA	C3B-C11-C12-C13
150	H	1301	CDL	OA9-CA7-OA8-CA6
150	AM	301	CDL	C32-C31-CA7-OA9
150	g	801	CDL	C52-C51-CB5-OB7
150	DJ	302	CDL	C72-C71-CB7-OB9
150	DQ	1501	CDL	C72-C71-CB7-OB9
150	Da	709	CDL	C52-C51-CB5-OB7
150	Dj	402	CDL	C12-C11-CA5-OA7
150	Dn	503	CDL	C32-C31-CA7-OA9
150	Ds	405	CDL	C12-C11-CA5-OA7
150	El	903	CDL	C32-C31-CA7-OA9
153	B1	401	PC1	O32-C31-C32-C33
153	BT	203	PC1	O32-C31-C32-C33
153	DX	308	PC1	O32-C31-C32-C33
153	El	904	PC1	O22-C21-C22-C23
155	DG	205	3PE	O22-C21-C22-C23
155	EM	901	3PE	O22-C21-C22-C23
155	Ds	403	3PE	O22-C21-C22-C23
150	DS	401	CDL	C13-C14-C15-C16
150	DX	301	CDL	C59-C60-C61-C62
150	EB	302	CDL	C14-C15-C16-C17
150	Dq	1403	CDL	C37-C38-C39-C40
153	DV	404	PC1	C29-C2A-C2B-C2C
150	Dq	1402	CDL	C72-C71-CB7-OB8
153	DC	605	PC1	O21-C21-C22-C23

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

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

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

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Mol	Chain	Res	Type	Atoms
155	Dr	401	3PE	O11-C1-C2-O21
156	A6	301	LPP	O5-C6-C7-O9
156	DN	504	LPP	O5-C6-C7-O9
167	En	1202	UQ8	C28-C29-C31-C32
150	AF	402	CDL	C72-C71-CB7-OB9
150	DD	706	CDL	C32-C31-CA7-OA9
150	DG	201	CDL	C32-C31-CA7-OA9
150	DV	402	CDL	C52-C51-CB5-OB7
150	EL	903	CDL	C12-C11-CA5-OA7
150	Di	1101	CDL	C52-C51-CB5-OB7
150	Dj	407	CDL	C32-C31-CA7-OA9
150	Dm	502	CDL	C12-C11-CA5-OA7
150	Ek	201	CDL	C32-C31-CA7-OA9
153	AA	906	PC1	O22-C21-C22-C23
153	AM	302	PC1	O32-C31-C32-C33
153	BG	202	PC1	O32-C31-C32-C33
153	DC	605	PC1	O22-C21-C22-C23
153	Eo	205	PC1	O22-C21-C22-C23
156	AA	902	LPP	O28-C29-C30-C31
150	c	502	CDL	C79-C80-C81-C82
150	DD	703	CDL	C37-C38-C39-C40
153	BT	203	PC1	C2B-C2C-C2D-C2E
150	BC	301	CDL	C52-C51-CB5-OB6
150	DN	503	CDL	C52-C51-CB5-OB6
150	DQ	1502	CDL	C72-C71-CB7-OB8
150	DR	403	CDL	C52-C51-CB5-OB6
150	DS	404	CDL	C52-C51-CB5-OB6
150	Dc	608	CDL	C32-C31-CA7-OA8
150	Dm	502	CDL	C12-C11-CA5-OA6
150	Dy	301	CDL	C72-C71-CB7-OB8
150	Eb	302	CDL	C12-C11-CA5-OA6
150	Eg	101	CDL	C12-C11-CA5-OA6
150	Ei	401	CDL	C72-C71-CB7-OB8
150	El	901	CDL	C72-C71-CB7-OB8
150	En	1201	CDL	C52-C51-CB5-OB6
153	A9	603	PC1	O21-C21-C22-C23
153	AA	906	PC1	O21-C21-C22-C23
153	AA	907	PC1	O31-C31-C32-C33
153	C	509	PC1	O21-C21-C22-C23
153	DG	203	PC1	O31-C31-C32-C33
153	Dc	609	PC1	O21-C21-C22-C23
155	DC	607	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
156	DN	504	LPP	O27-C29-C30-C31
150	BT	204	CDL	C57-C58-C59-C60
150	Du	403	CDL	C44-C45-C46-C47
150	Dv	402	CDL	C37-C38-C39-C40
153	Dx	1203	PC1	C2A-C2B-C2C-C2D
150	DH	202	CDL	C55-C56-C57-C58
150	DM	502	CDL	C59-C60-C61-C62
150	B0	101	CDL	C52-C51-CB5-OB7
150	H	1301	CDL	C32-C31-CA7-OA9
150	DJ	304	CDL	C32-C31-CA7-OA9
150	DU	401	CDL	C32-C31-CA7-OA9
150	DV	401	CDL	C52-C51-CB5-OB7
150	DV	402	CDL	C72-C71-CB7-OB9
150	ED	605	CDL	C72-C71-CB7-OB9
150	Dc	608	CDL	C32-C31-CA7-OA9
150	Dn	502	CDL	C52-C51-CB5-OB7
150	Dq	1402	CDL	C52-C51-CB5-OB7
150	Dv	402	CDL	C52-C51-CB5-OB7
150	Ed	205	CDL	C12-C11-CA5-OA7
150	Ep	701	CDL	C72-C71-CB7-OB9
168	c	504	HEM	C4D-C3D-CAD-CBD
150	A0	602	CDL	C55-C56-C57-C58
150	AA	901	CDL	C37-C38-C39-C40
150	AA	908	CDL	C64-C65-C66-C67
150	DX	306	CDL	C14-C15-C16-C17
150	DZ	501	CDL	C35-C36-C37-C38
150	EA	301	CDL	C56-C57-C58-C59
150	ED	601	CDL	C34-C35-C36-C37
150	Dy	301	CDL	C38-C39-C40-C41
150	AF	401	CDL	C72-C71-CB7-OB8
150	BC	302	CDL	C12-C11-CA5-OA6
150	DA	709	CDL	C12-C11-CA5-OA6
150	DO	501	CDL	C72-C71-CB7-OB8
150	Dm	501	CDL	C72-C71-CB7-OB8
153	DI	303	PC1	O21-C21-C22-C23
153	Eo	204	PC1	O21-C21-C22-C23
150	Da	709	CDL	C38-C39-C40-C41
153	AJ	501	PC1	C34-C35-C36-C37
153	C	509	PC1	C22-C23-C24-C25
167	EL	905	UQ8	C3-C4-O4-C4M
167	Ds	404	UQ8	C4-C3-O3-C3M
150	AA	901	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
150	BC	302	CDL	C73-C74-C75-C76
150	CG	302	CDL	C71-C72-C73-C74
150	C	503	CDL	C33-C34-C35-C36
150	c	509	CDL	C20-C21-C22-C23
150	DH	202	CDL	C78-C79-C80-C81
150	DC	601	CDL	C72-C71-CB7-OB9
150	DJ	304	CDL	C72-C71-CB7-OB9
150	DM	501	CDL	C12-C11-CA5-OA7
150	EI	401	CDL	C72-C71-CB7-OB9
150	EN	1201	CDL	C52-C51-CB5-OB7
150	ES	1101	CDL	C72-C71-CB7-OB9
150	Dc	601	CDL	C72-C71-CB7-OB9
150	Dg	201	CDL	C32-C31-CA7-OA9
150	Dv	401	CDL	C52-C51-CB5-OB7
150	Ea	501	CDL	C32-C31-CA7-OA9
153	AA	907	PC1	O22-C21-C22-C23
153	AA	907	PC1	O32-C31-C32-C33
153	C	509	PC1	O22-C21-C22-C23
153	Dc	605	PC1	O22-C21-C22-C23
153	Dx	1203	PC1	O22-C21-C22-C23
155	Dd	703	3PE	O32-C31-C32-C33
155	Em	901	3PE	O22-C21-C22-C23
167	c	510	UQ8	C24-C26-C27-C28
167	Ed	202	UQ8	C24-C26-C27-C28
166	D	401	HEC	CAA-CBA-CGA-O2A
150	E	301	CDL	C11-CA5-OA6-CA4
150	DH	201	CDL	C14-C15-C16-C17
150	EL	901	CDL	C36-C37-C38-C39
150	EN	1202	CDL	C59-C60-C61-C62
150	DA	706	CDL	C39-C40-C41-C42
150	DD	704	CDL	C39-C40-C41-C42
150	BG	201	CDL	O1-C1-CA2-OA2
150	B0	102	CDL	C32-C31-CA7-OA8
150	BC	301	CDL	C32-C31-CA7-OA8
150	BT	202	CDL	C52-C51-CB5-OB6
150	CC	305	CDL	C12-C11-CA5-OA6
150	DD	704	CDL	C12-C11-CA5-OA6
150	DN	503	CDL	C32-C31-CA7-OA8
150	DV	401	CDL	C52-C51-CB5-OB6
150	Du	401	CDL	C32-C31-CA7-OA8
153	Ds	407	PC1	O31-C31-C32-C33
153	Dx	1205	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
150	DJ	304	CDL	C52-C53-C54-C55
150	DV	402	CDL	C42-C43-C44-C45
150	Dh	201	CDL	C61-C62-C63-C64
150	Dv	402	CDL	C44-C45-C46-C47
150	DD	705	CDL	C72-C71-CB7-OB9
150	DN	502	CDL	C72-C71-CB7-OB9
150	DR	403	CDL	C52-C51-CB5-OB7
150	DY	301	CDL	C72-C71-CB7-OB9
150	Dd	705	CDL	C72-C71-CB7-OB9
150	El	903	CDL	C52-C51-CB5-OB7
153	A9	603	PC1	O32-C31-C32-C33
153	Dx	1203	PC1	O32-C31-C32-C33
168	C	501	HEM	C2D-C3D-CAD-CBD
169	Da	702	HEA	CAA-CBA-CGA-O1A
150	BT	202	CDL	C83-C84-C85-C86
150	C	504	CDL	C37-C38-C39-C40
153	Eo	204	PC1	C2F-C2G-C2H-C2I
155	DX	303	3PE	C38-C39-C3A-C3B
155	Em	901	3PE	C39-C3A-C3B-C3C
150	C	505	CDL	C12-C13-C14-C15
150	DR	402	CDL	C53-C54-C55-C56
150	EL	901	CDL	C73-C74-C75-C76
150	Dd	704	CDL	C57-C58-C59-C60
150	Do	501	CDL	C71-C72-C73-C74
150	C	507	CDL	C52-C51-CB5-OB7
150	DN	503	CDL	C52-C51-CB5-OB7
150	EK	201	CDL	C32-C31-CA7-OA9
150	Dn	503	CDL	C12-C11-CA5-OA7
150	Do	501	CDL	C72-C71-CB7-OB9
150	Dq	1402	CDL	C72-C71-CB7-OB9
150	Ds	405	CDL	C32-C31-CA7-OA9
150	En	1201	CDL	C52-C51-CB5-OB7
153	A9	603	PC1	O22-C21-C22-C23
155	Dx	1206	3PE	C2-C3-O31-C31
150	CJ	201	CDL	C31-C32-C33-C34
150	DJ	302	CDL	C80-C81-C82-C83
150	ED	605	CDL	C24-C25-C26-C27
150	EL	902	CDL	C15-C16-C17-C18
150	Ds	406	CDL	C34-C35-C36-C37
150	Dx	1204	CDL	C75-C76-C77-C78
153	A1	403	PC1	C2A-C2B-C2C-C2D
153	DJ	306	PC1	C28-C29-C2A-C2B

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

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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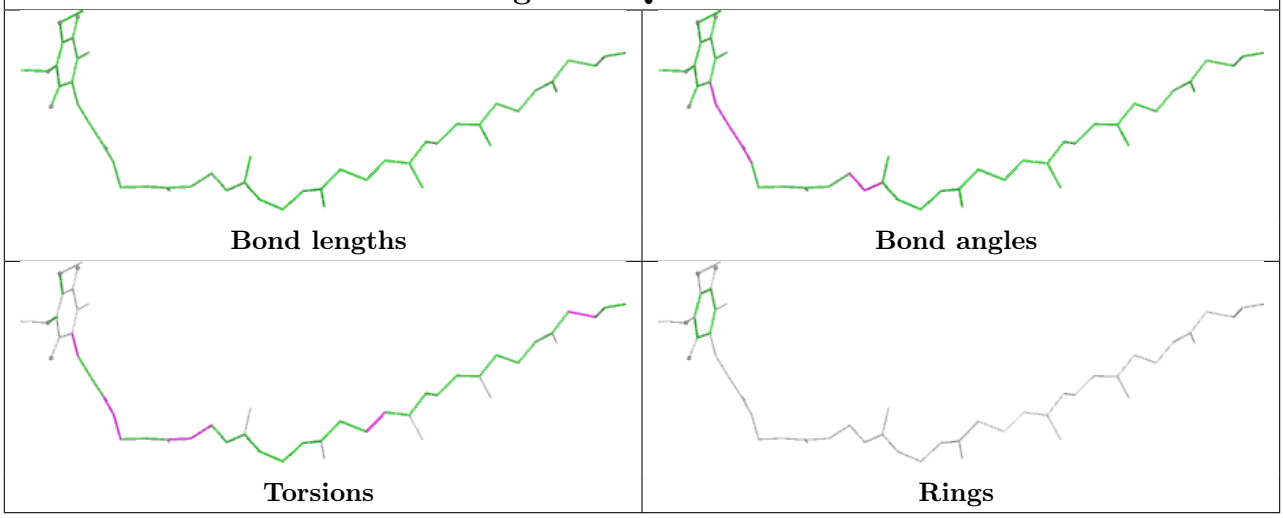
Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	EO	204	PC1	1	0
168	C	502	HEM	6	0
169	DA	703	HEA	1	0
155	Dr	401	3PE	2	0
167	En	1202	UQ8	4	0
155	EO	203	3PE	1	0
153	DV	406	PC1	1	0
153	K	502	PC1	1	0
150	Ds	401	CDL	3	0
150	Dd	704	CDL	1	0
155	Dg	204	3PE	1	0
150	BC	302	CDL	2	0
150	DH	202	CDL	1	0
153	AL	303	PC1	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
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

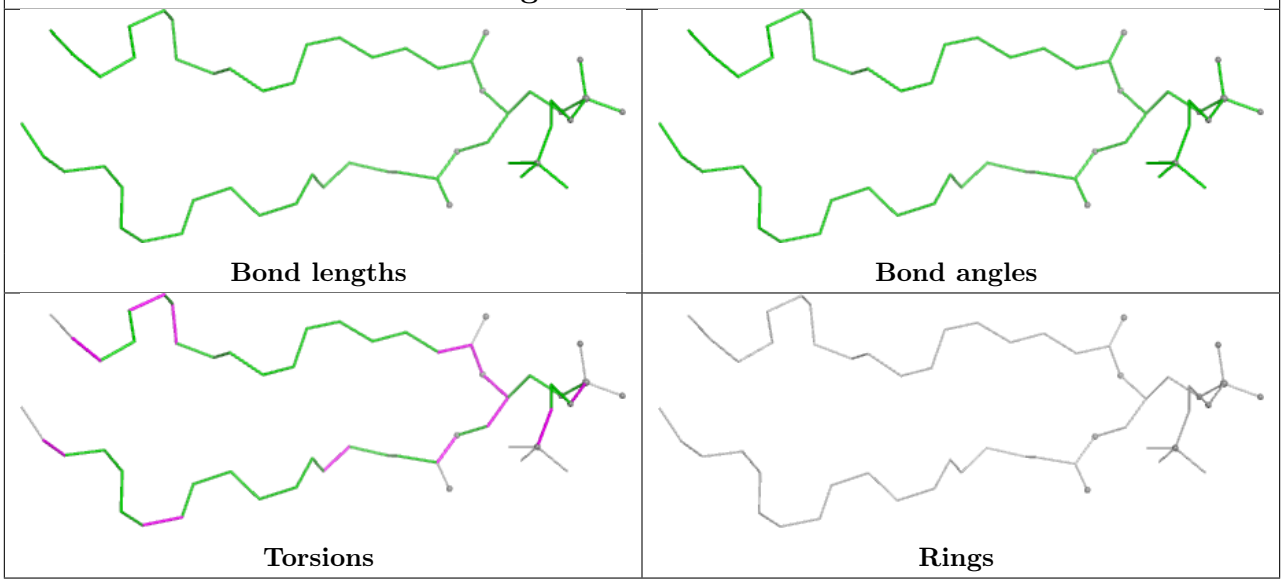
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

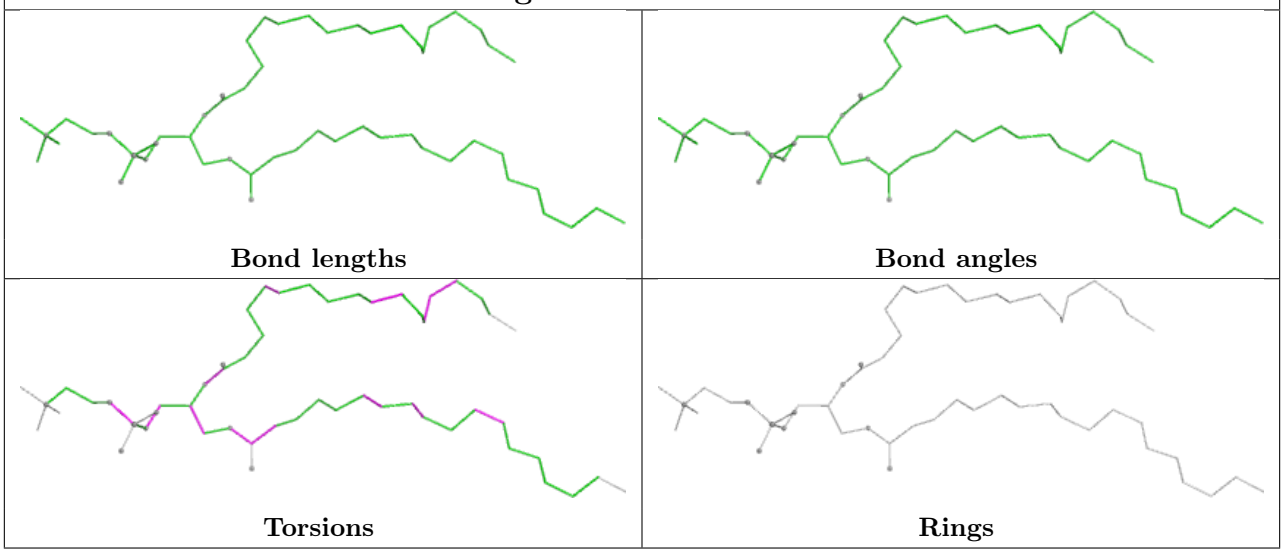
Ligand UQ8 CC 303



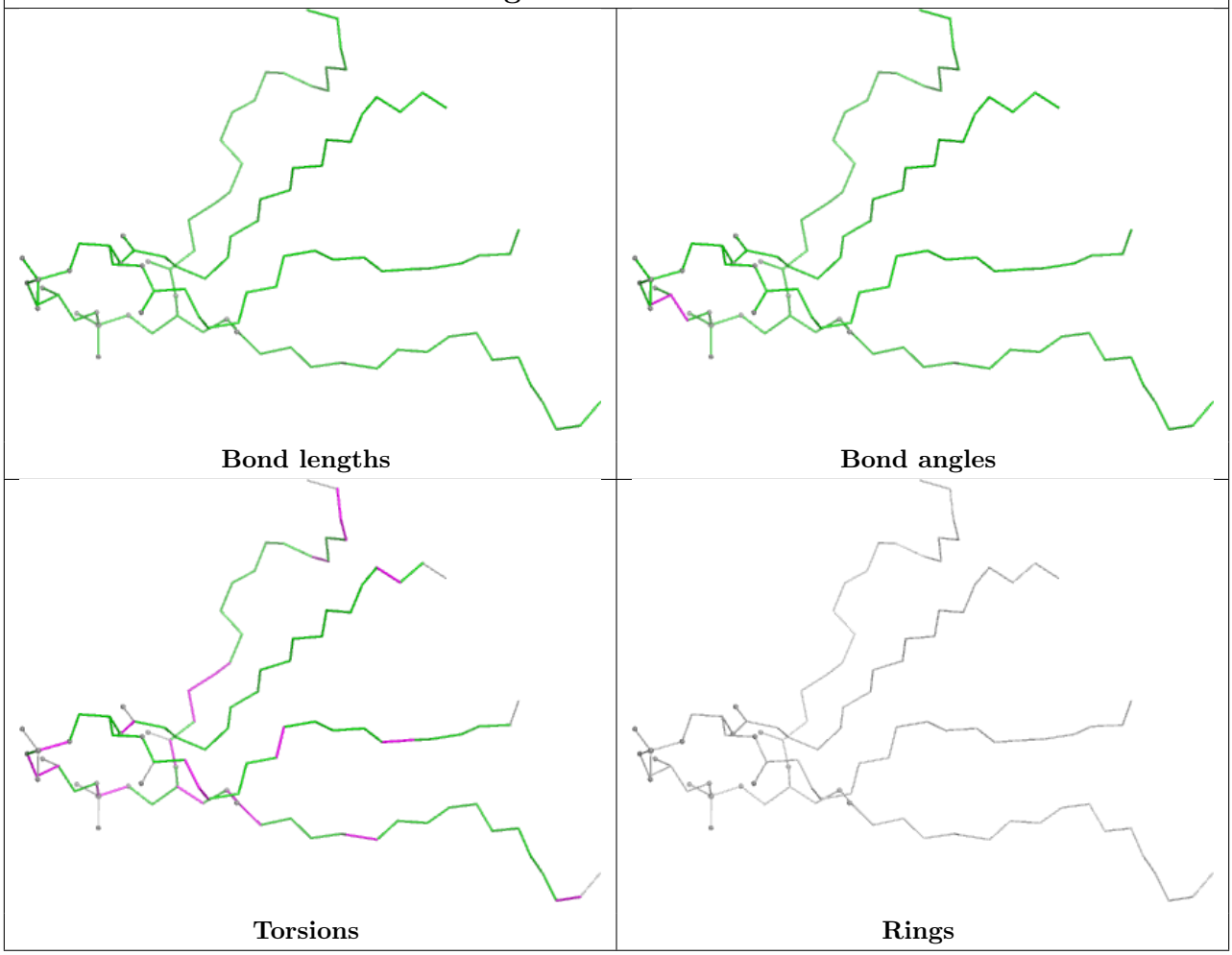
Ligand PC1 Eo 204



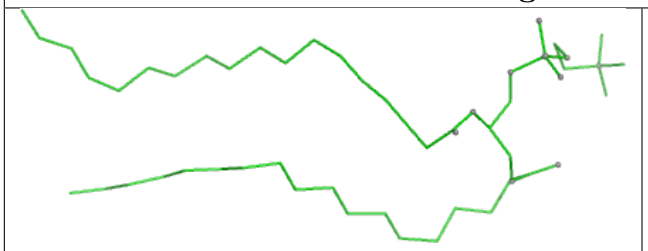
Ligand PC1 DA 707



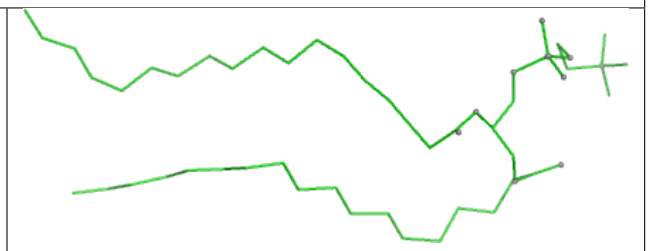
Ligand CDL C 506



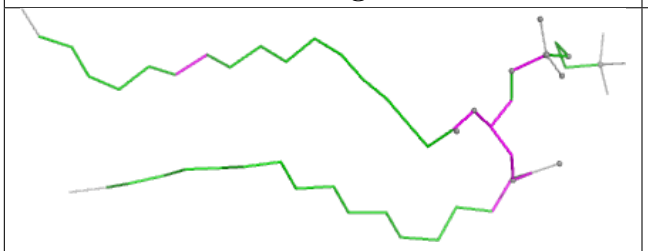
Ligand PC1 A1 403



Bond lengths



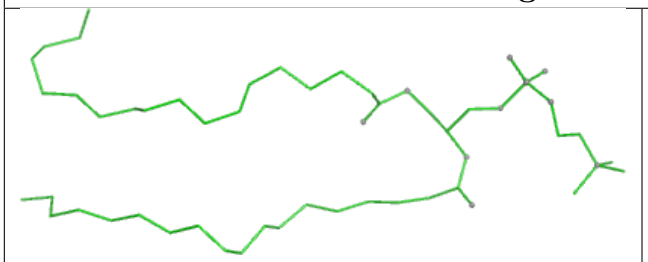
Bond angles



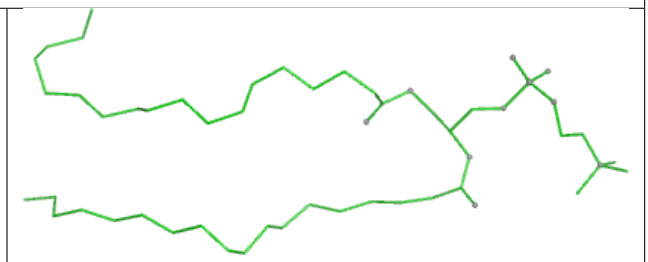
Torsions

Rings

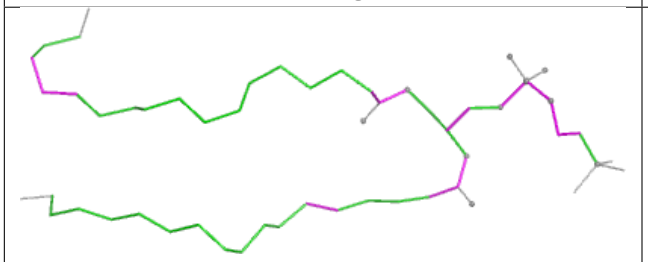
Ligand PC1 A9 603



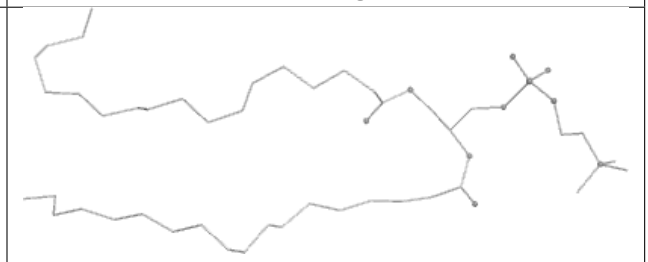
Bond lengths



Bond angles

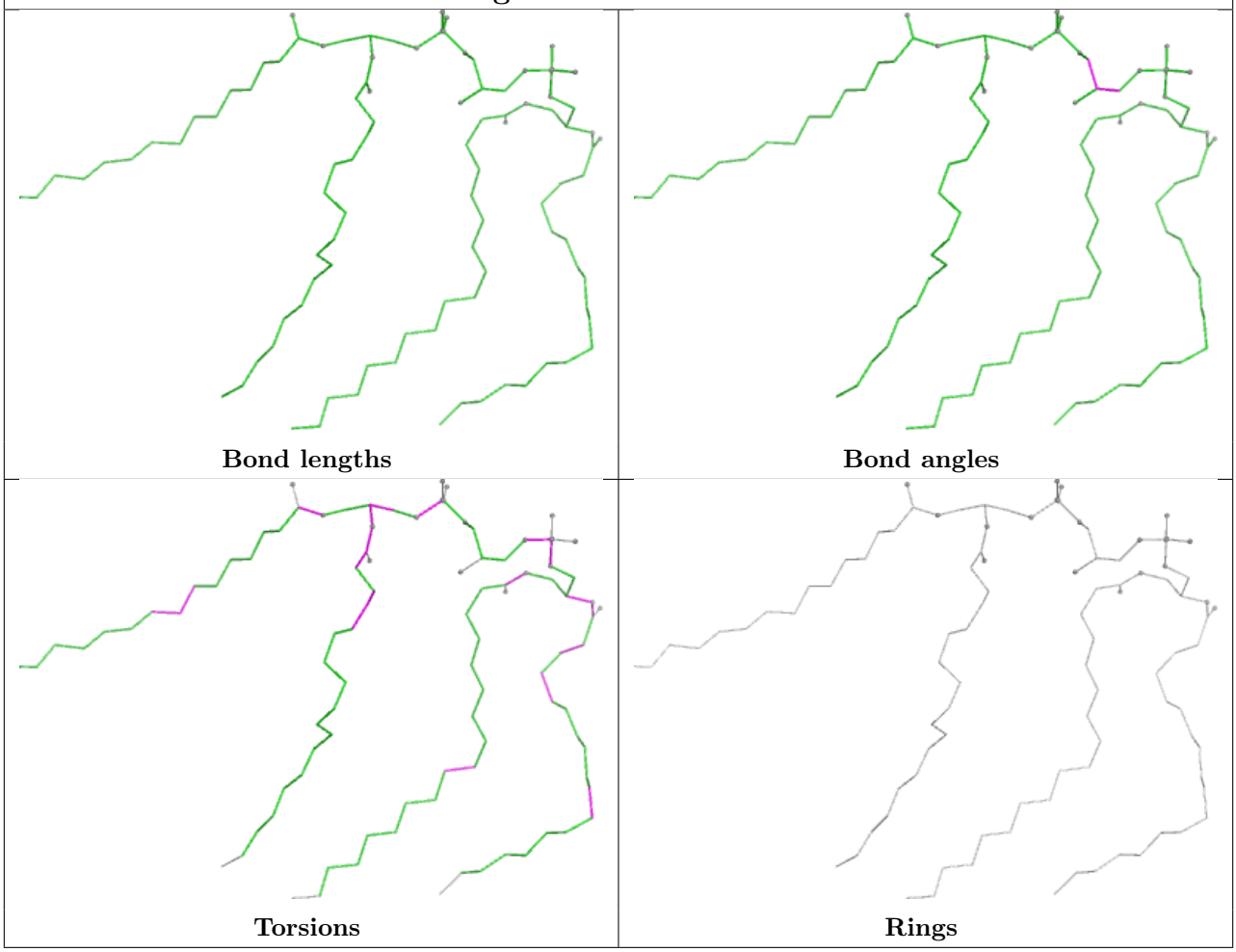


Torsions

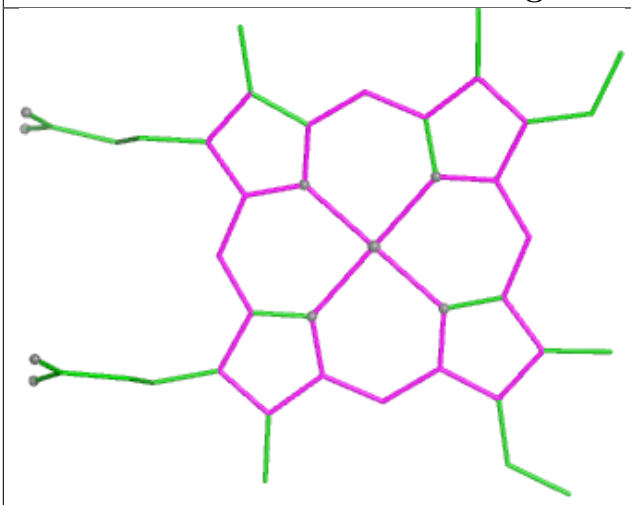


Rings

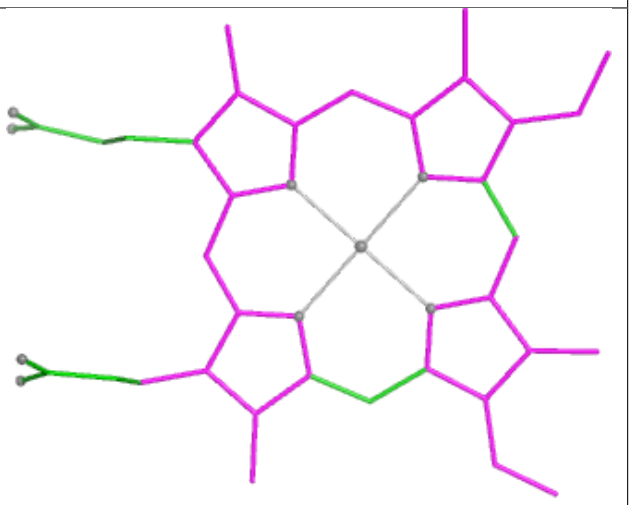
Ligand CDL CC 305



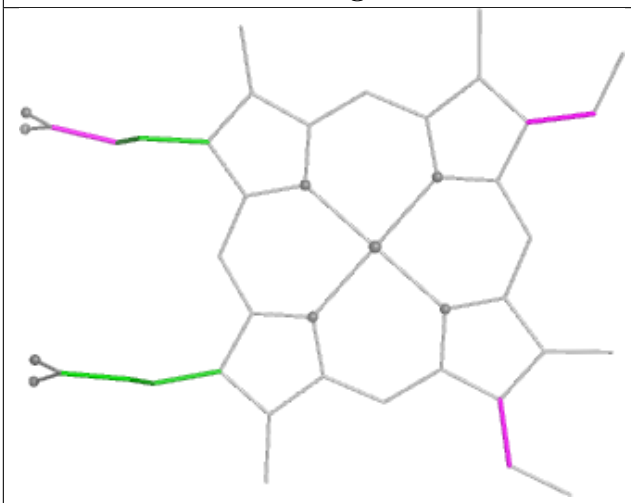
Ligand HEC d 802



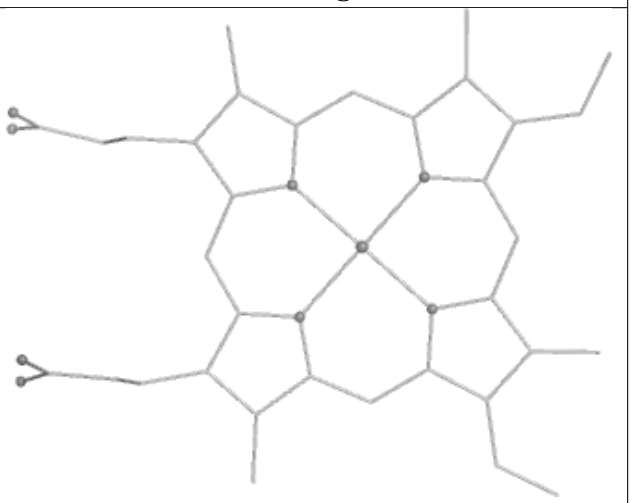
Bond lengths



Bond angles

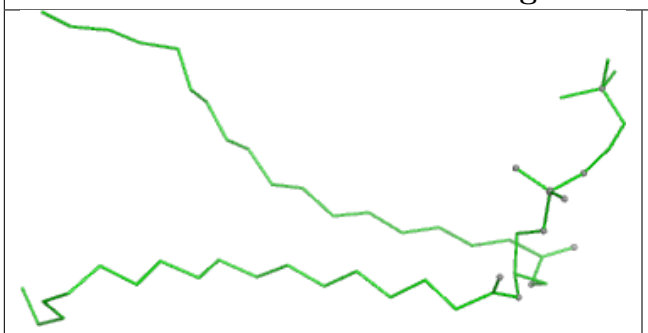


Torsions

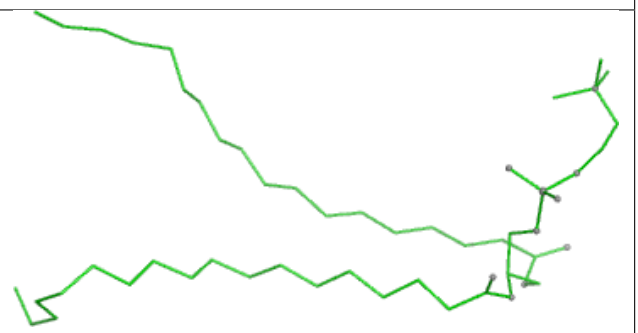


Rings

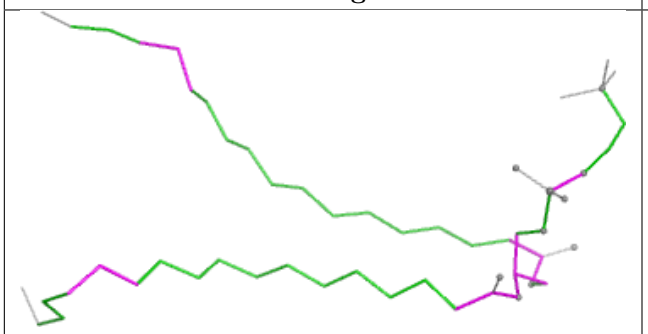
Ligand PC1 Dc 609



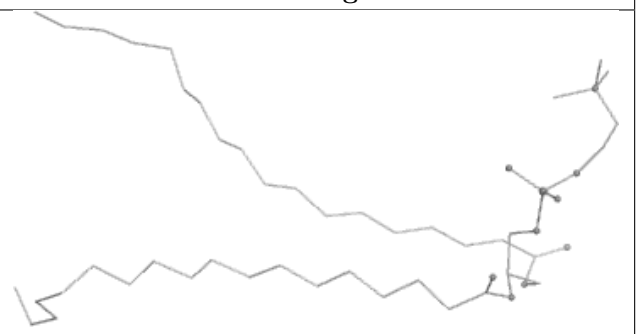
Bond lengths



Bond angles

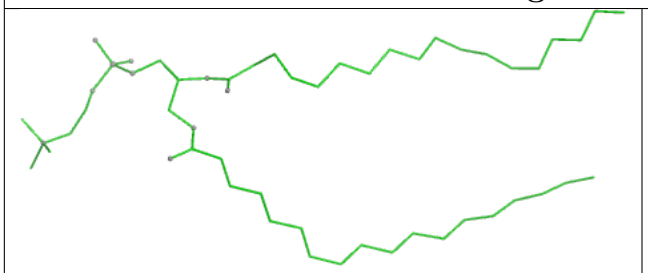


Torsions

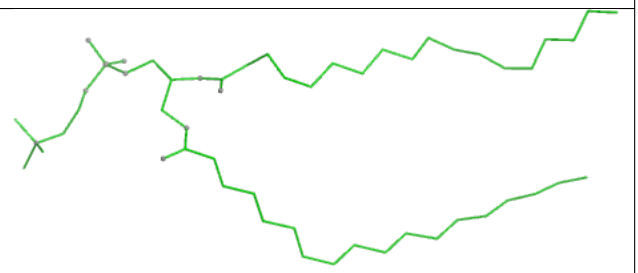


Rings

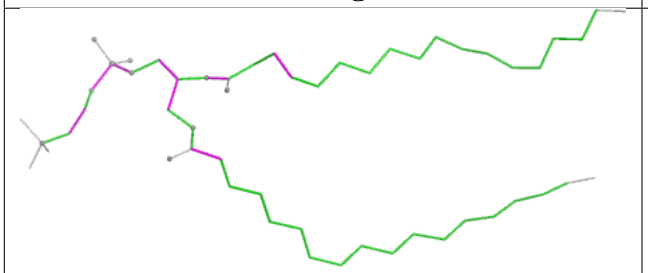
Ligand PC1 K 501



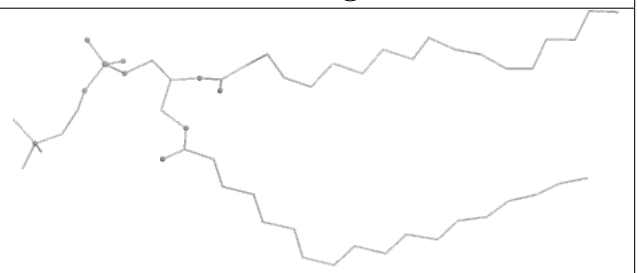
Bond lengths



Bond angles

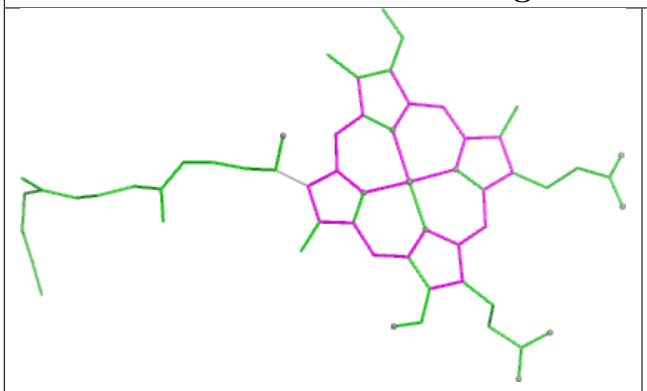


Torsions

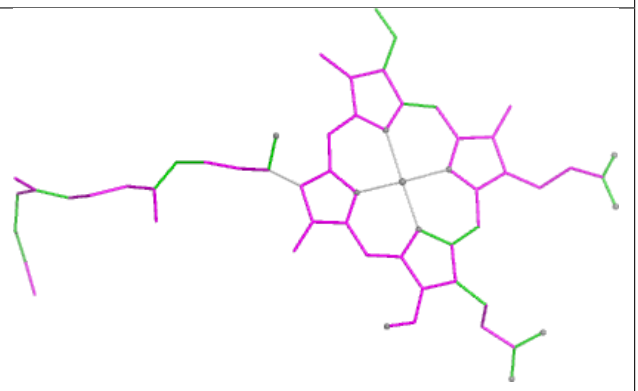


Rings

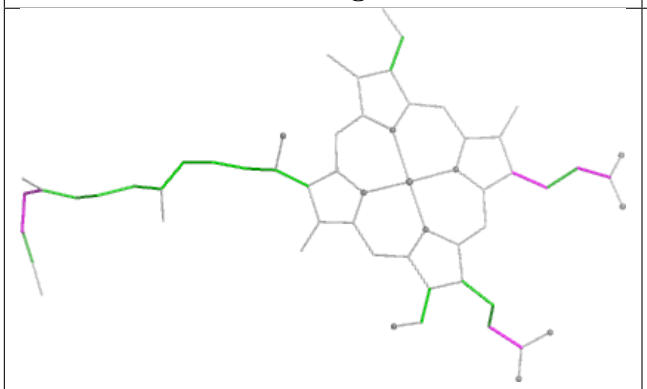
Ligand HEA Da 703



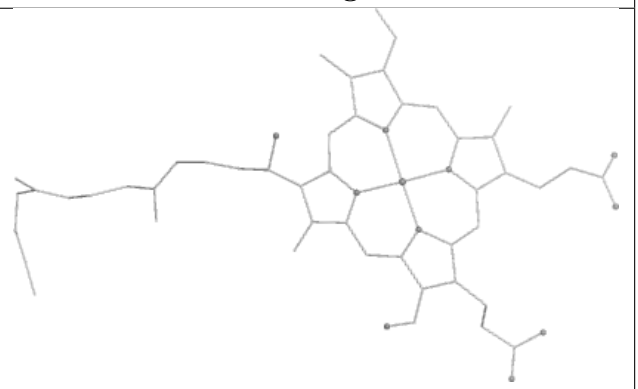
Bond lengths



Bond angles

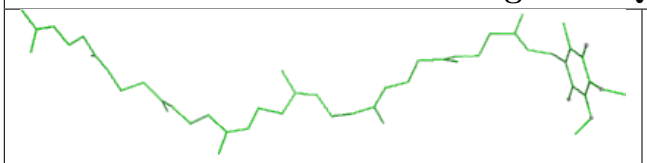


Torsions



Rings

Ligand UQ8 EN 1205



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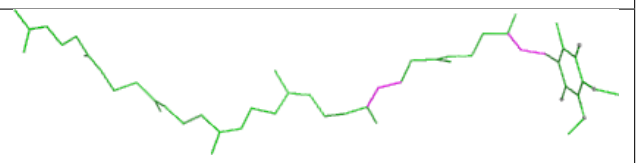
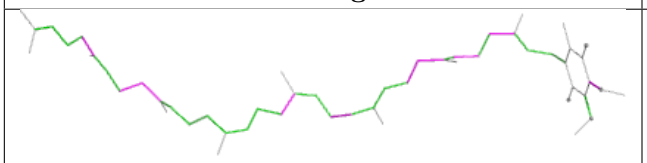


Bond angles



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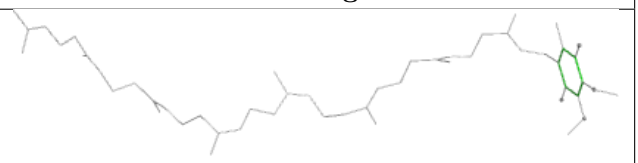
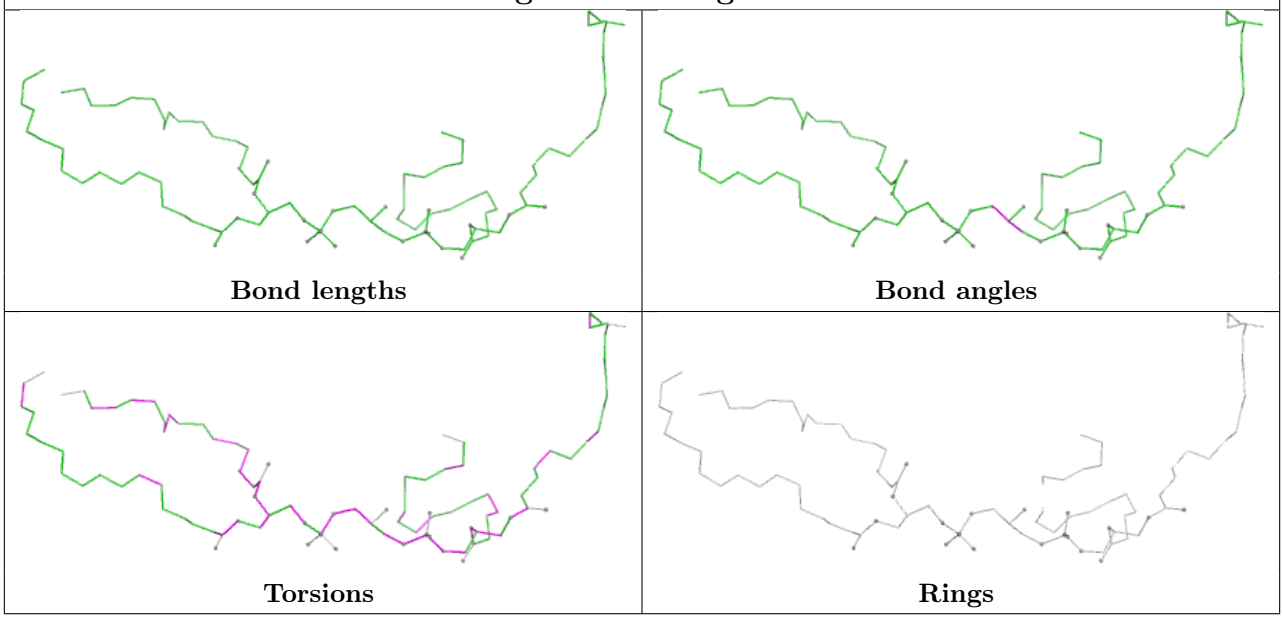
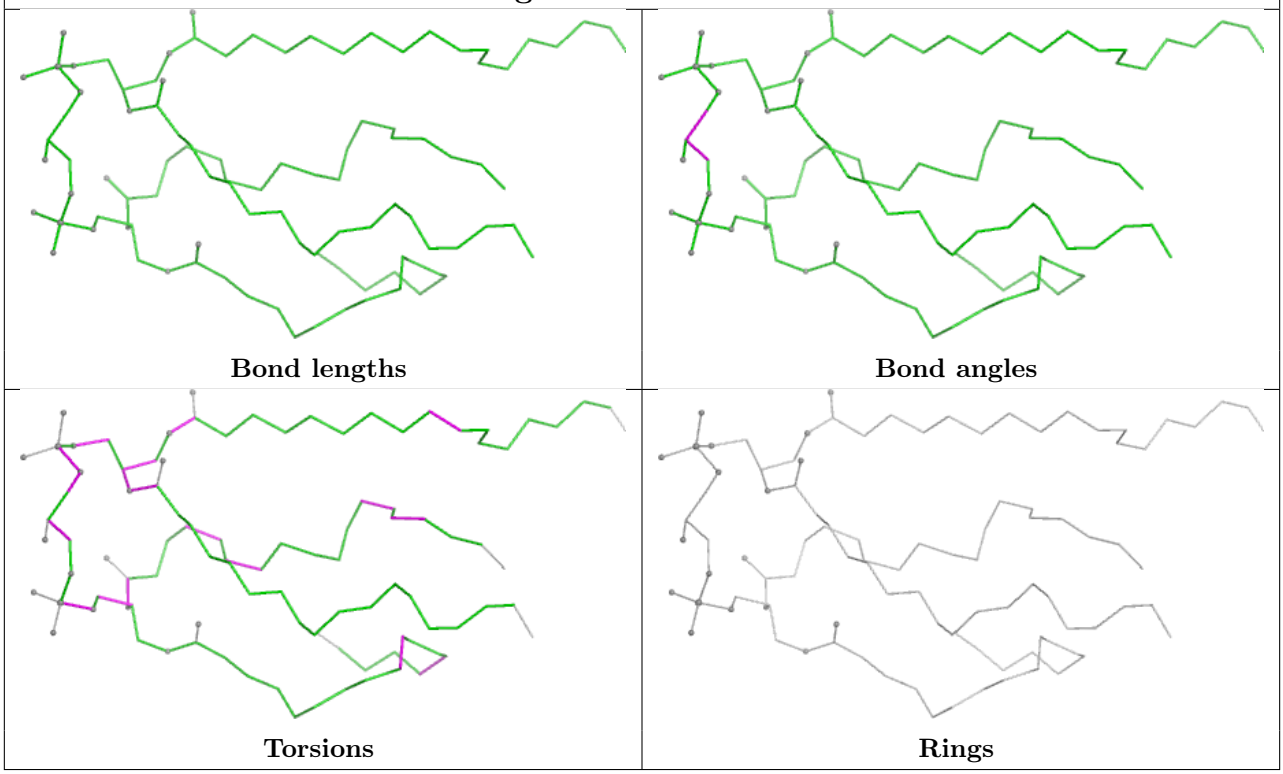


Rings

Ligand CDL Dg 201



Ligand CDL DJ 305



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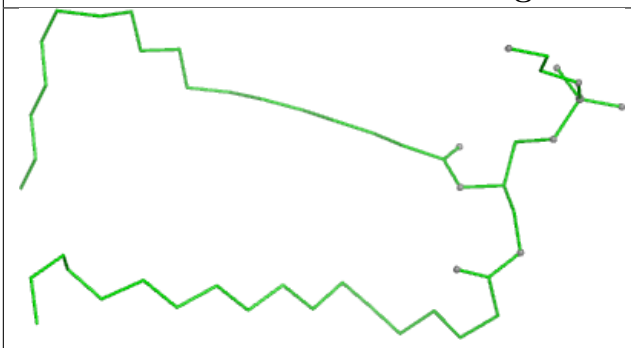
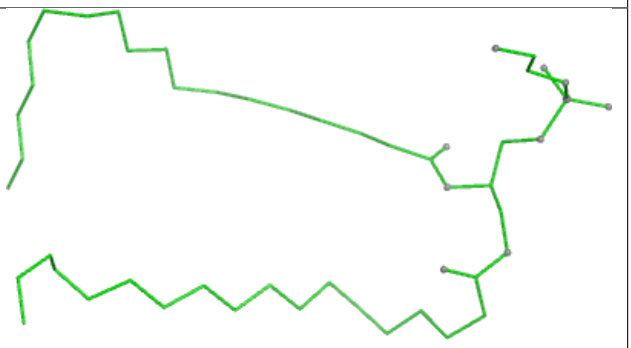
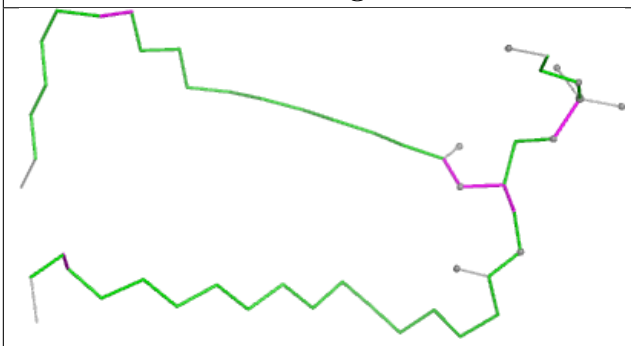
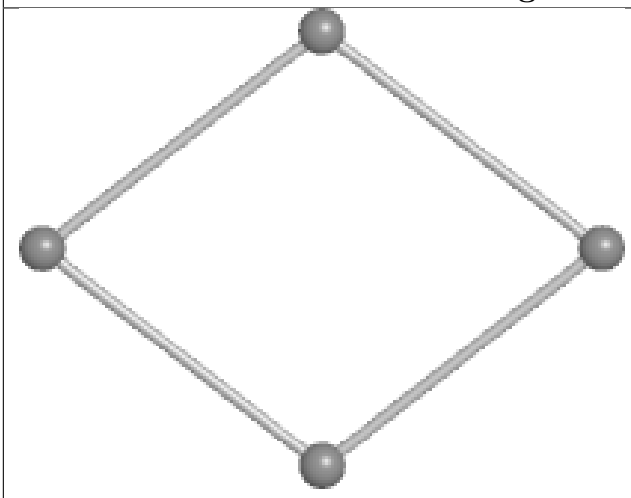
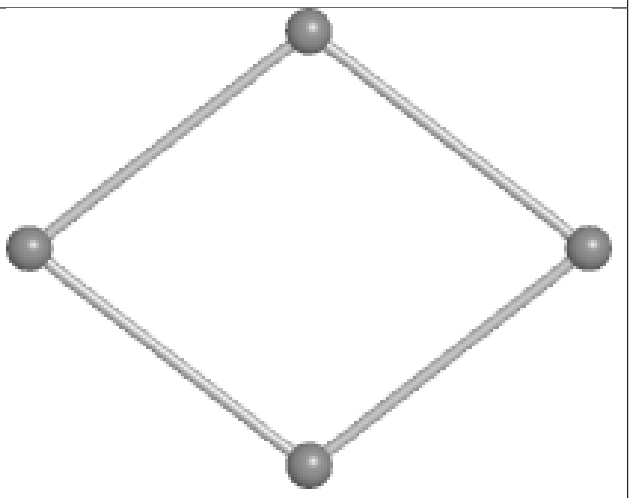
 Bond lengths	 Bond angles
 Torsions	Rings

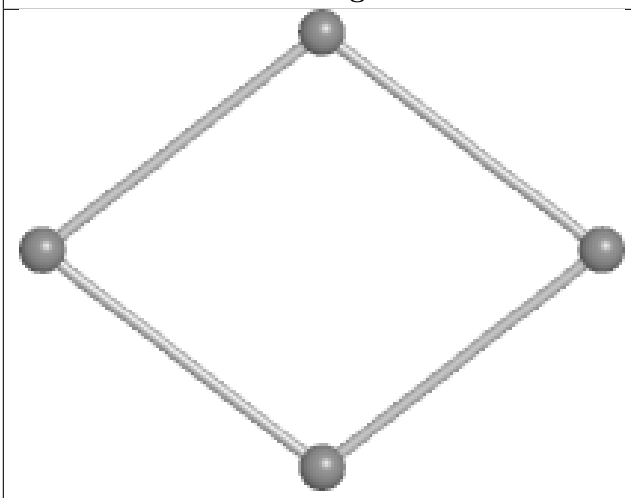
Ligand FES EF 201



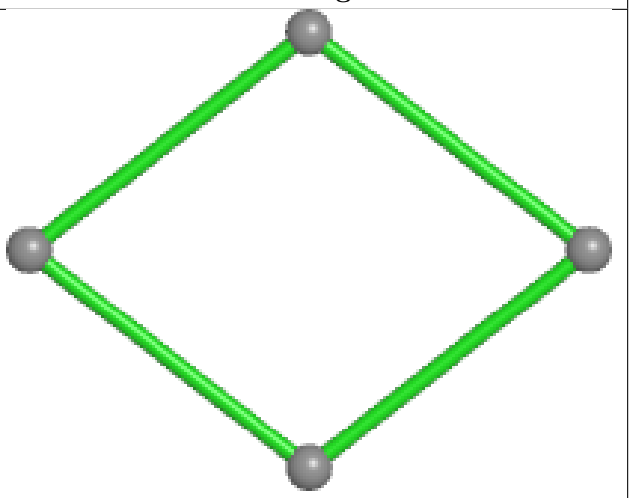
Bond lengths



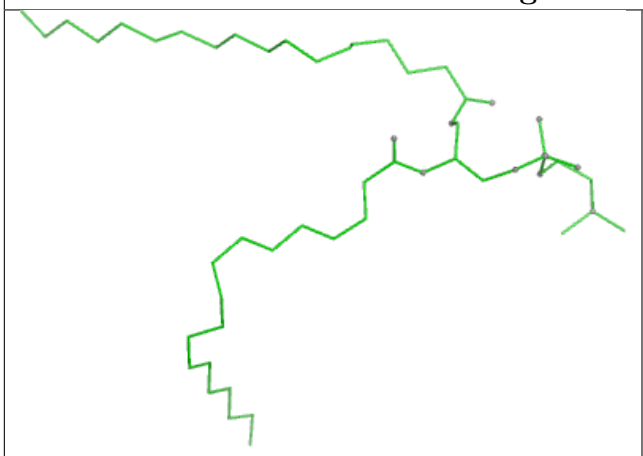
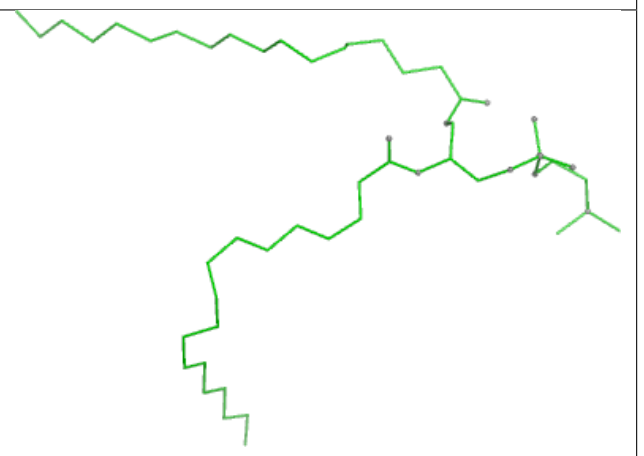
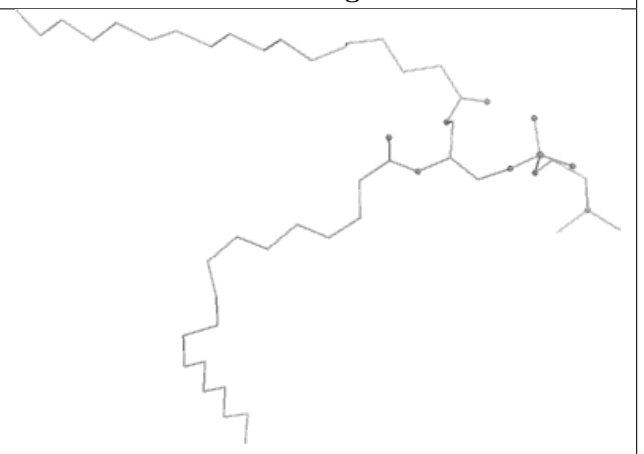
Bond angles

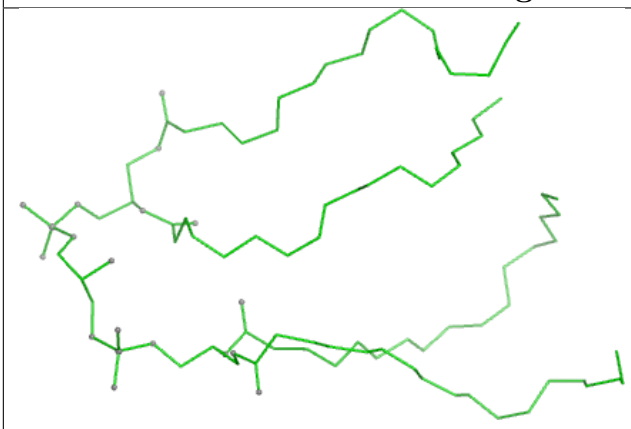
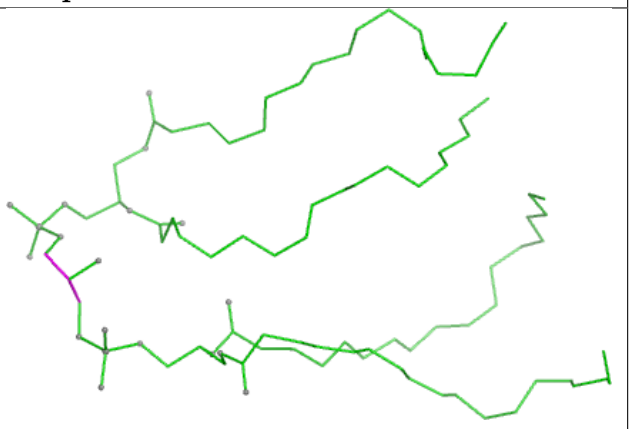
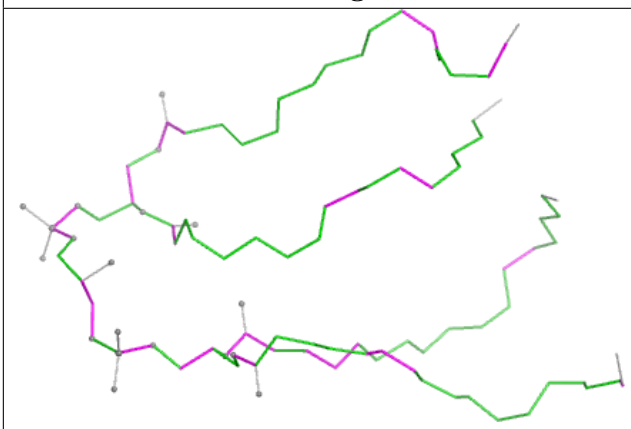
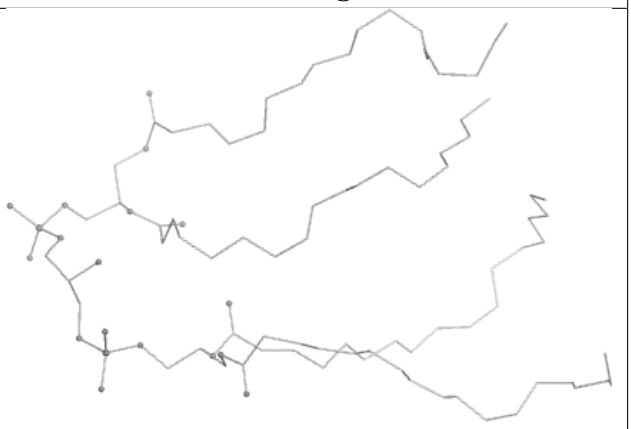


Torsions



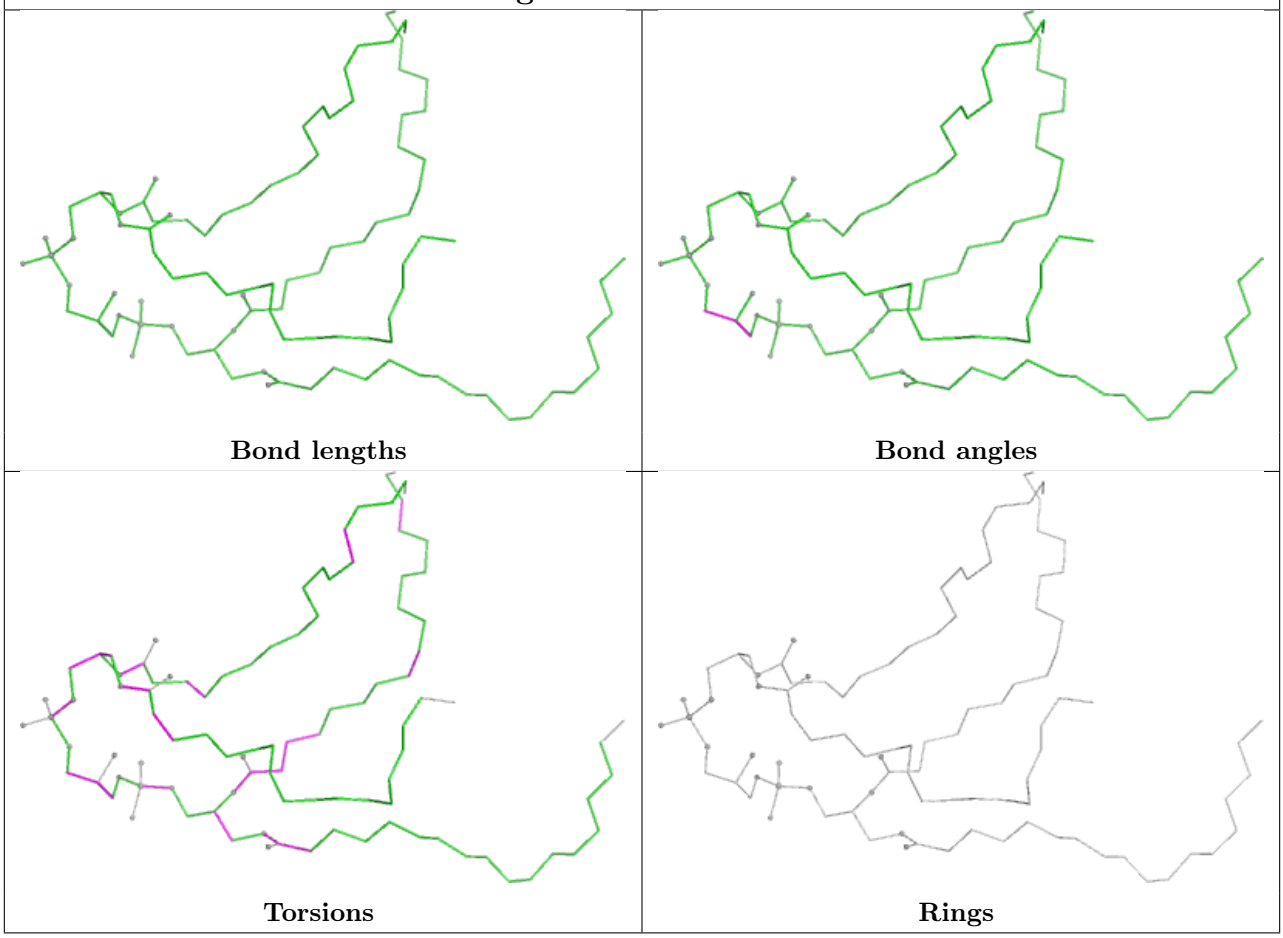
Rings

Ligand PC1 Eb 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

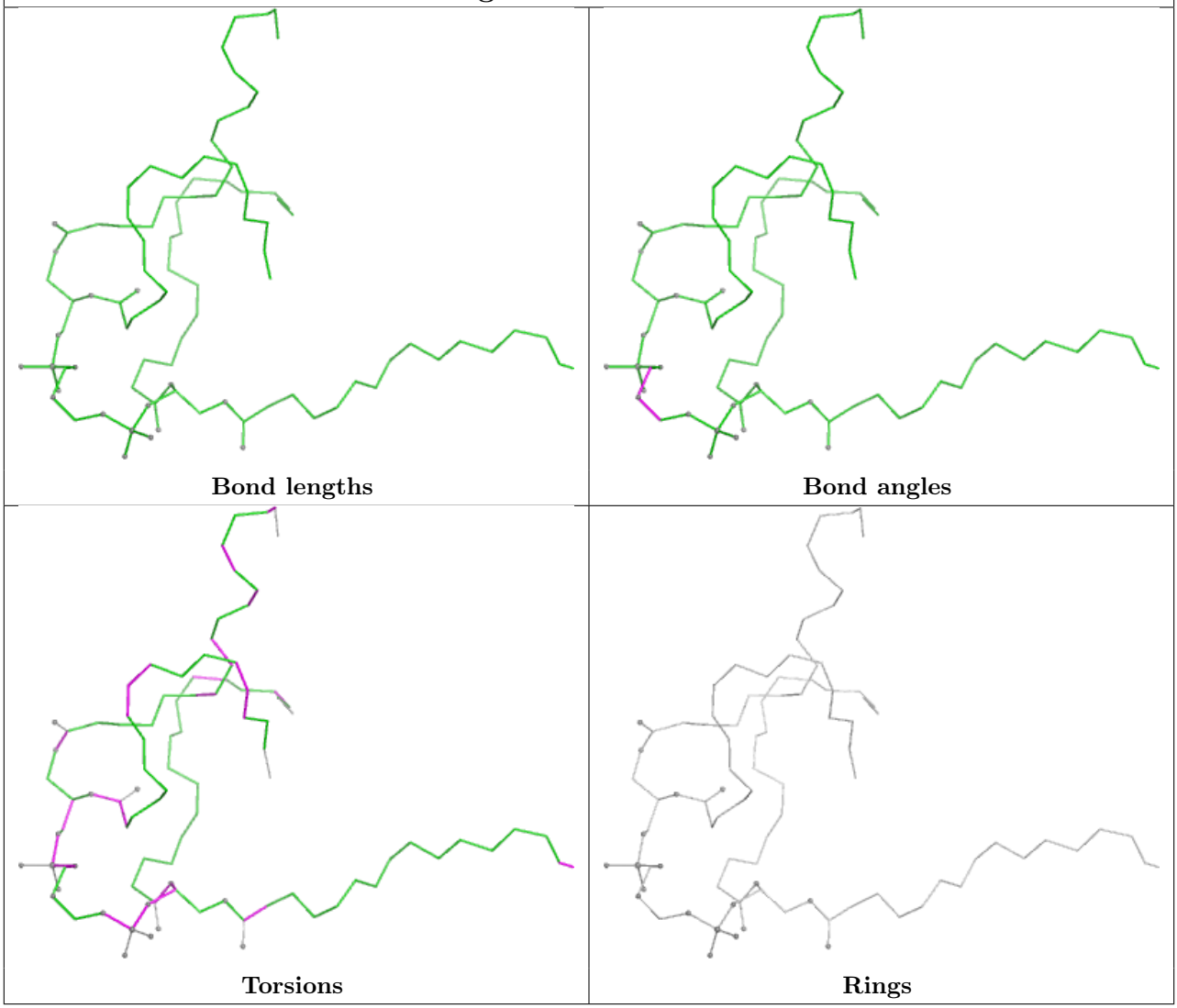
Ligand CDL Ep 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL BL 301

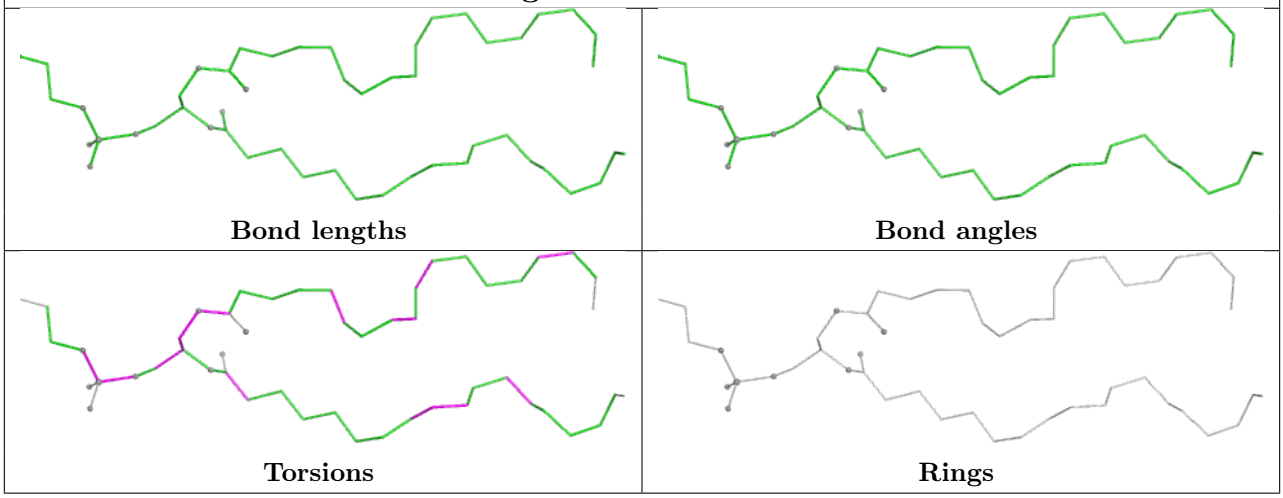
Ligand CDL Ed 205



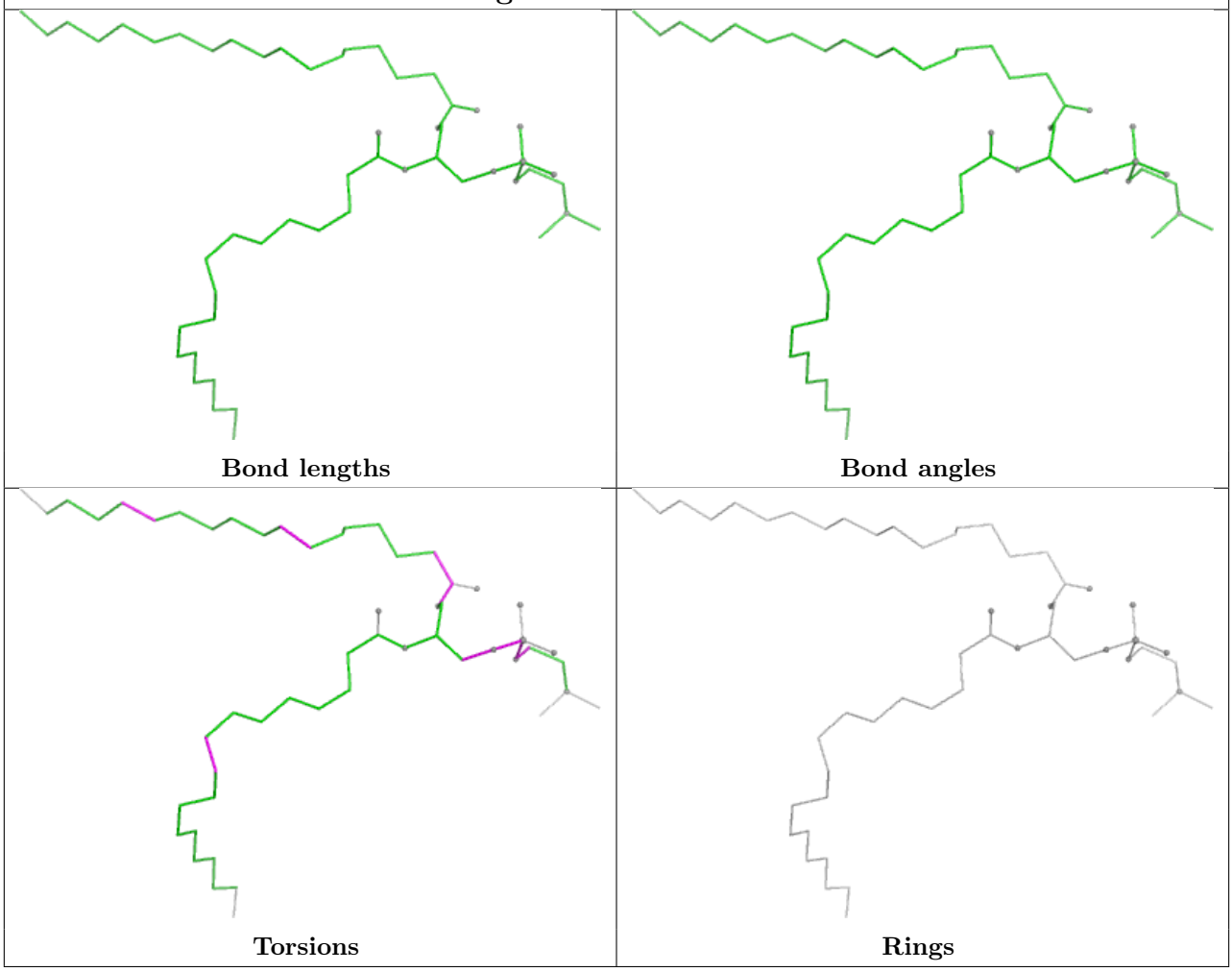
Ligand CDL El 903



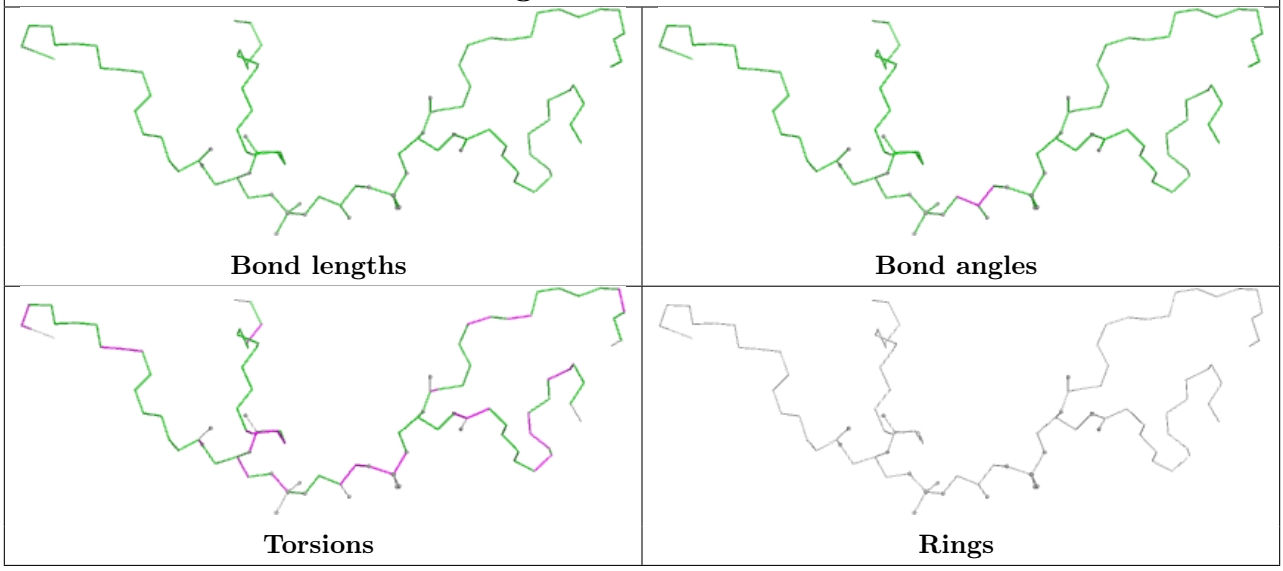
Ligand 3PE Ds 403



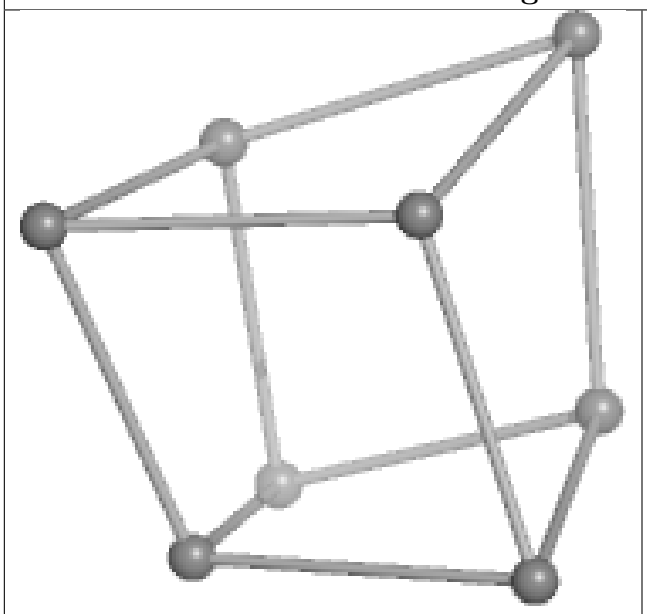
Ligand PC1 EB 301



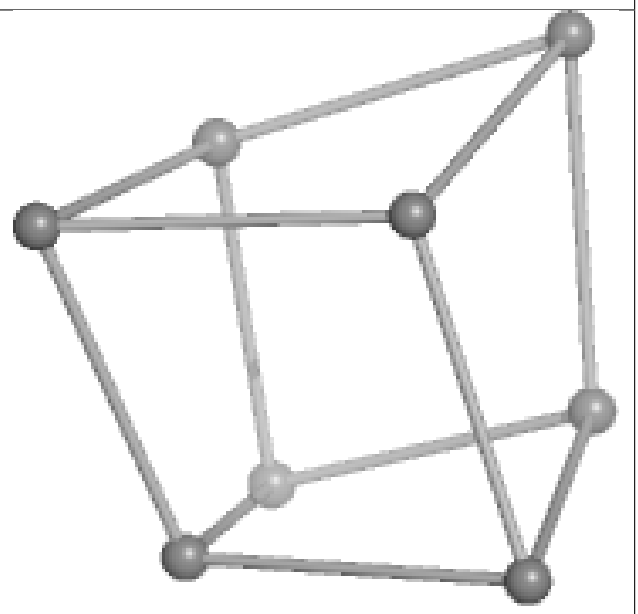
Ligand CDL Dv 402



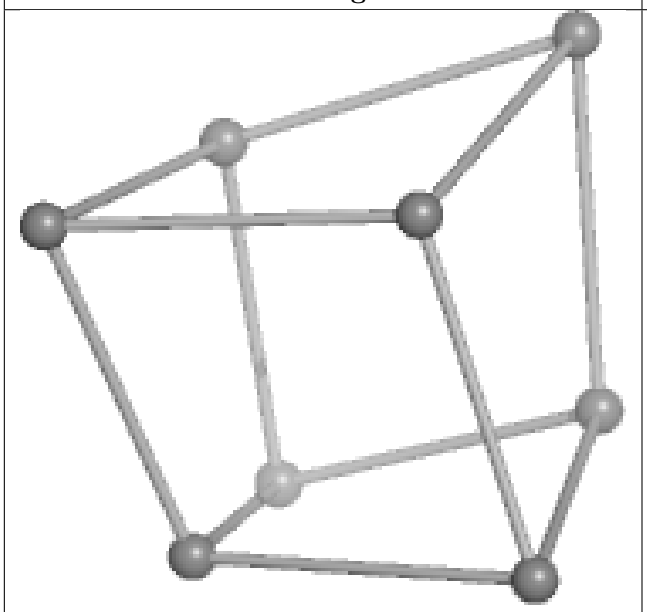
Ligand SF4 AL 302



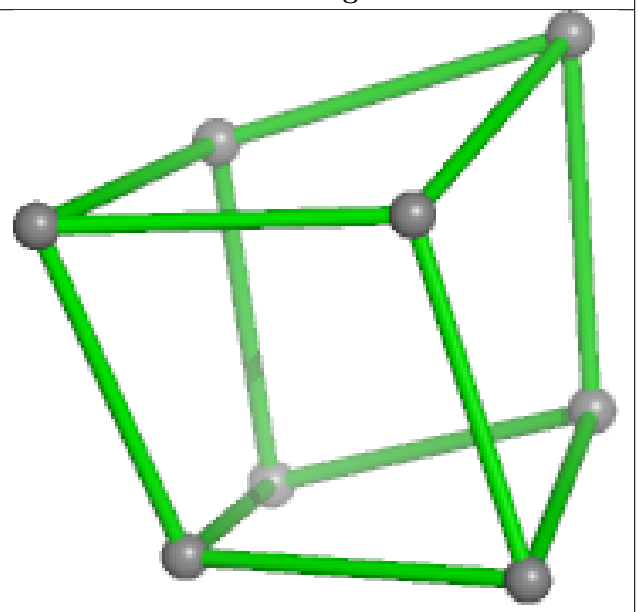
Bond lengths



Bond angles



Torsions



Rings

Ligand PC1 Eb 303

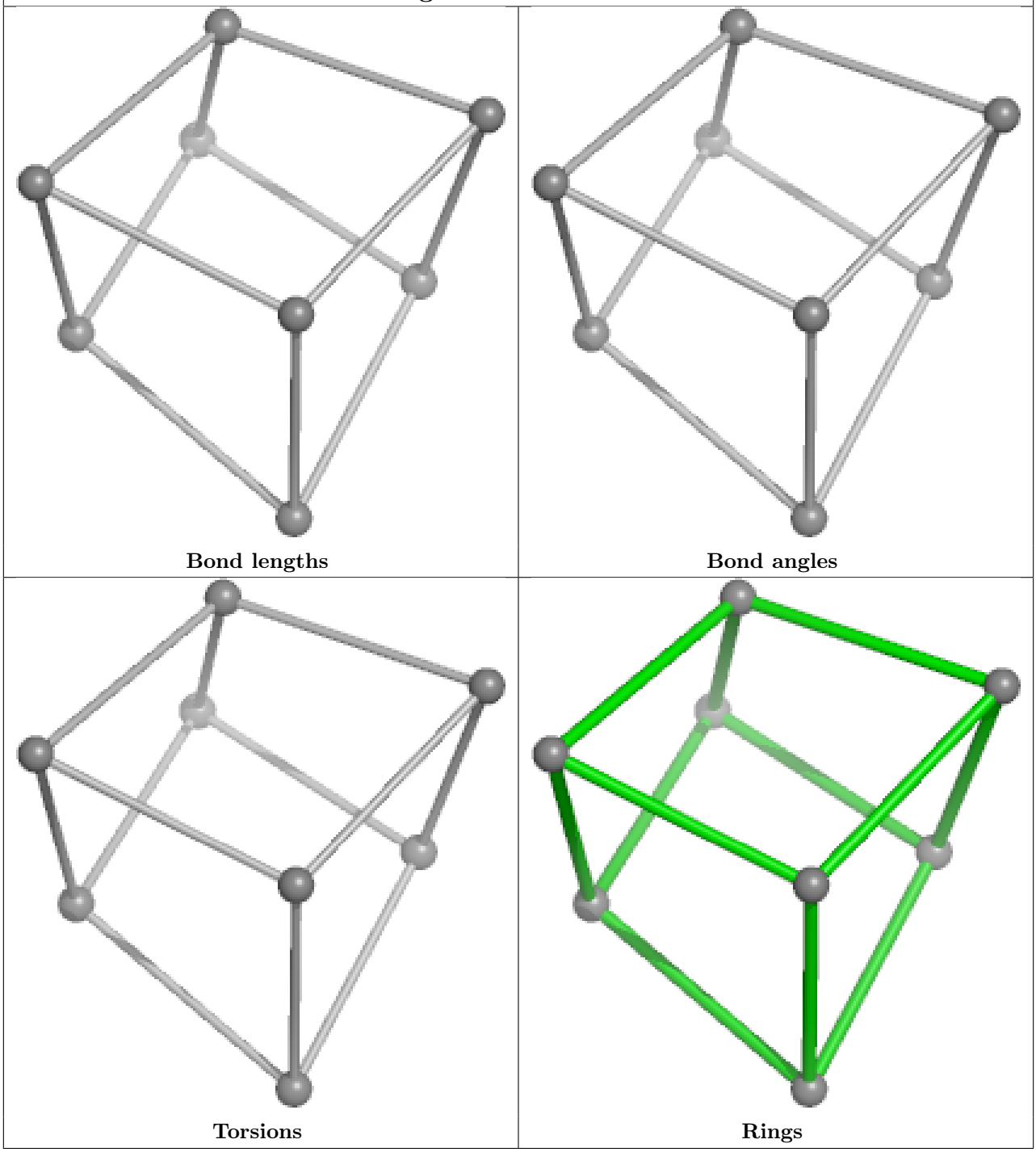
Bond lengths

Bond angles

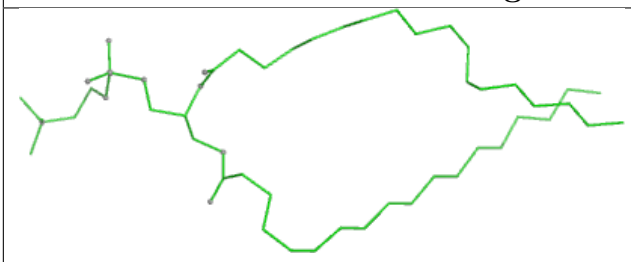
Torsions

Rings

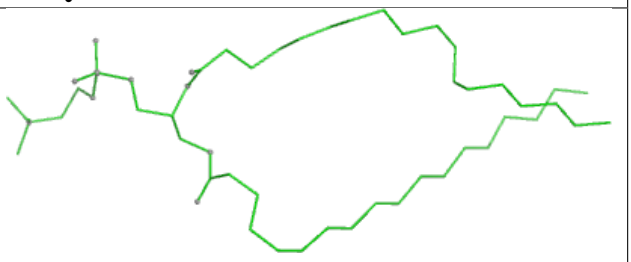
Ligand SF4 AB 803



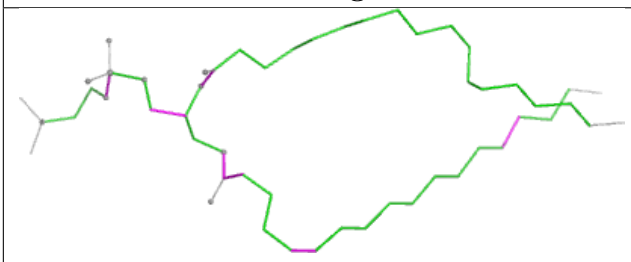
Ligand PC1 DQ 1503



Bond lengths



Bond angles



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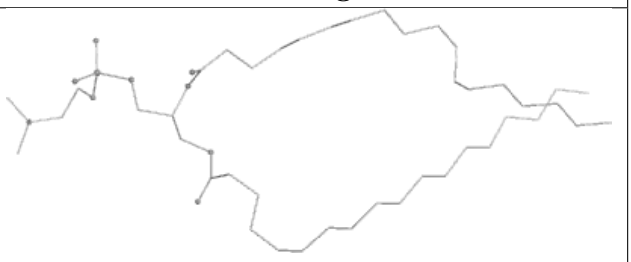
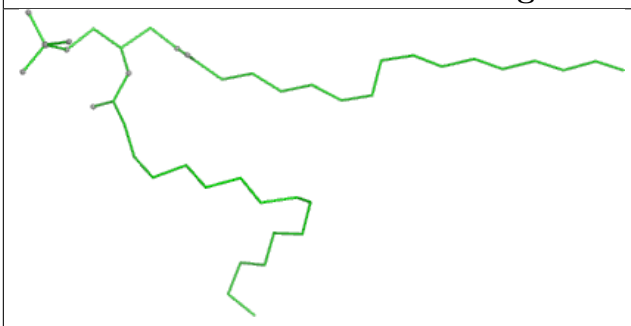
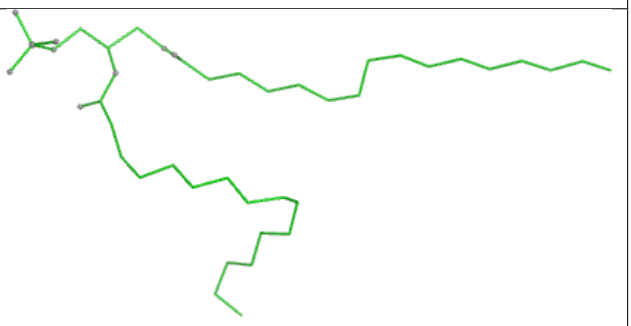


Rings

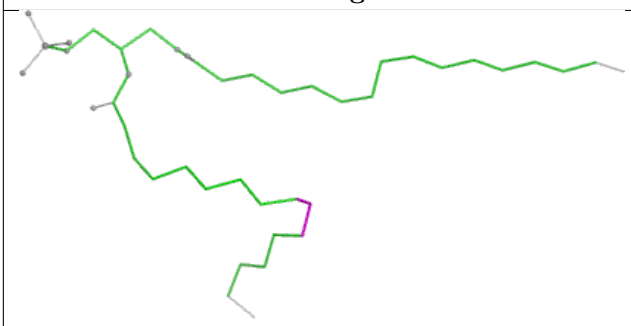
Ligand LPP Ed 203



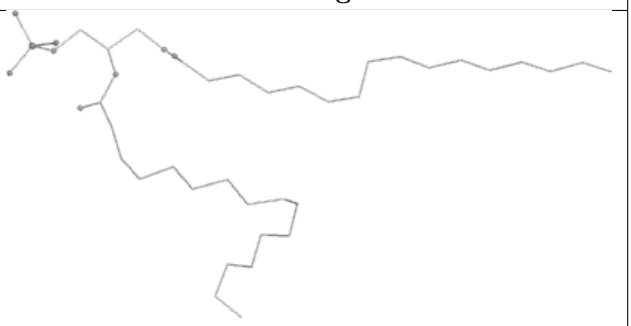
Bond lengths



Bond angles

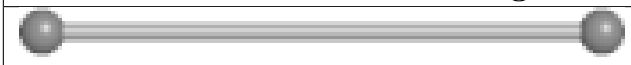


Torsions

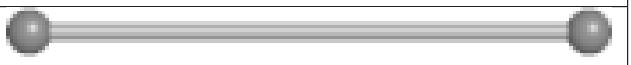


Rings

Ligand CUA Db 701

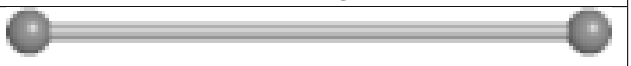


Bond lengths



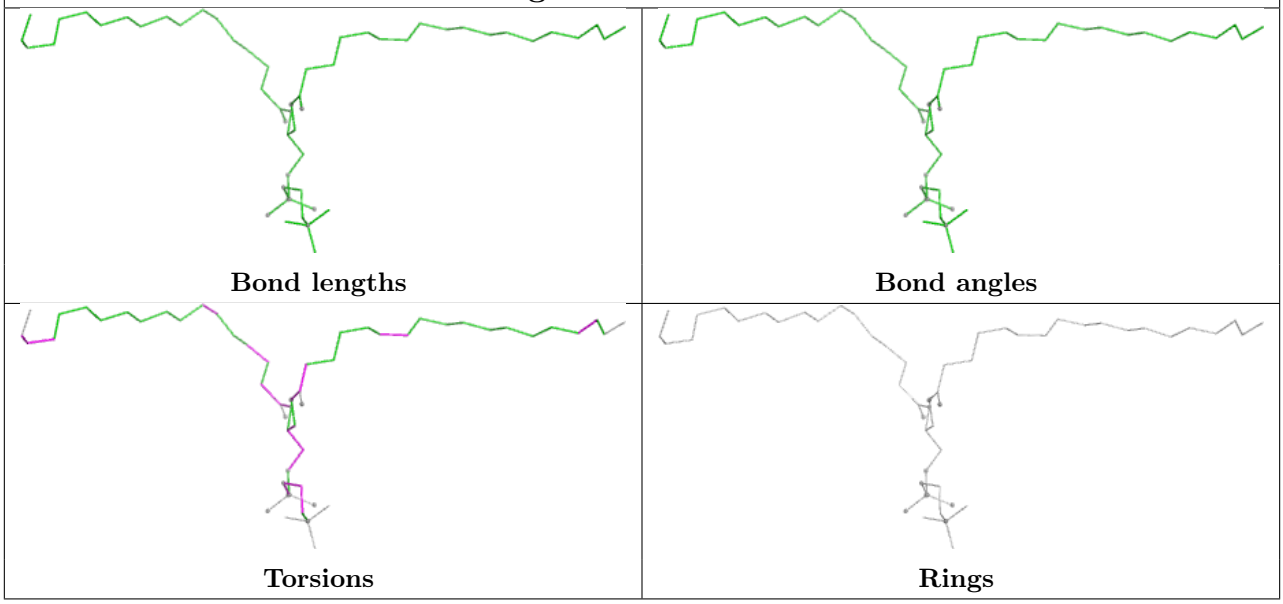
Bond angles

Torsions

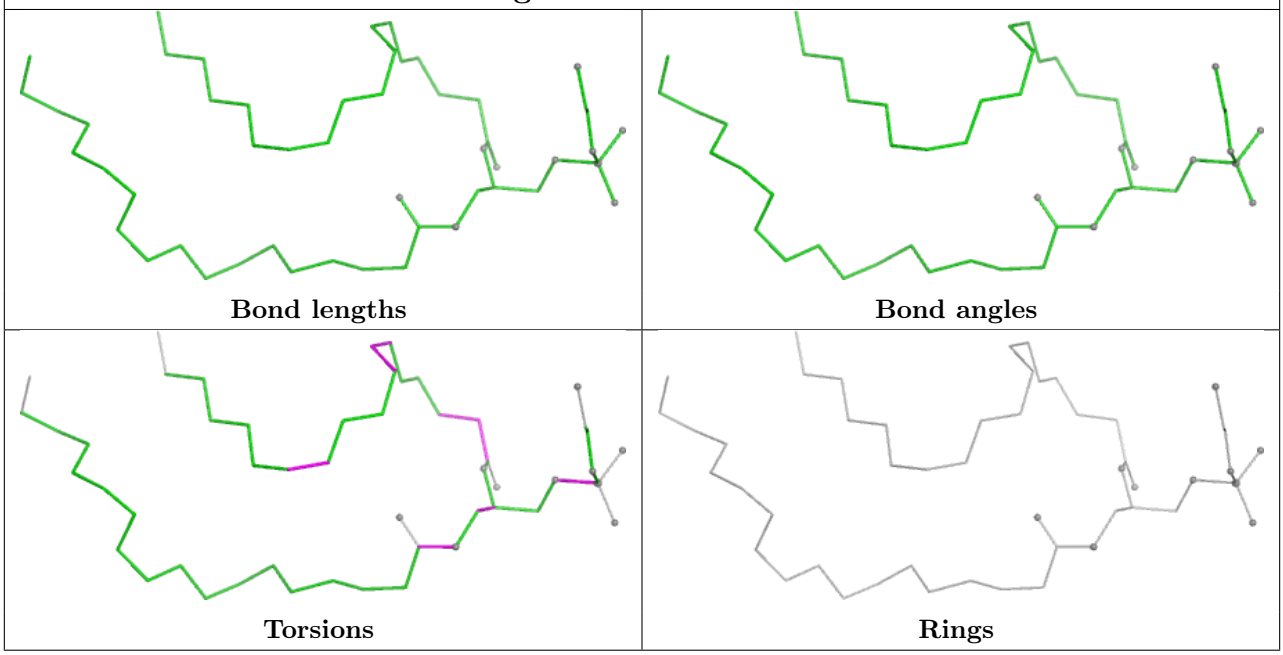


Rings

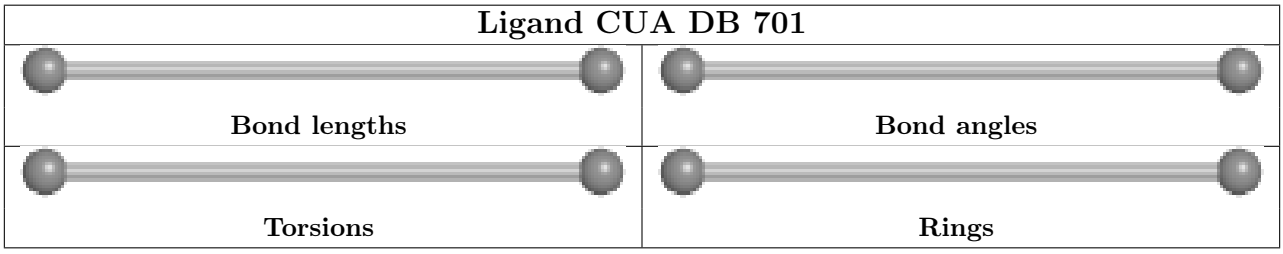
Ligand PC1 C 509



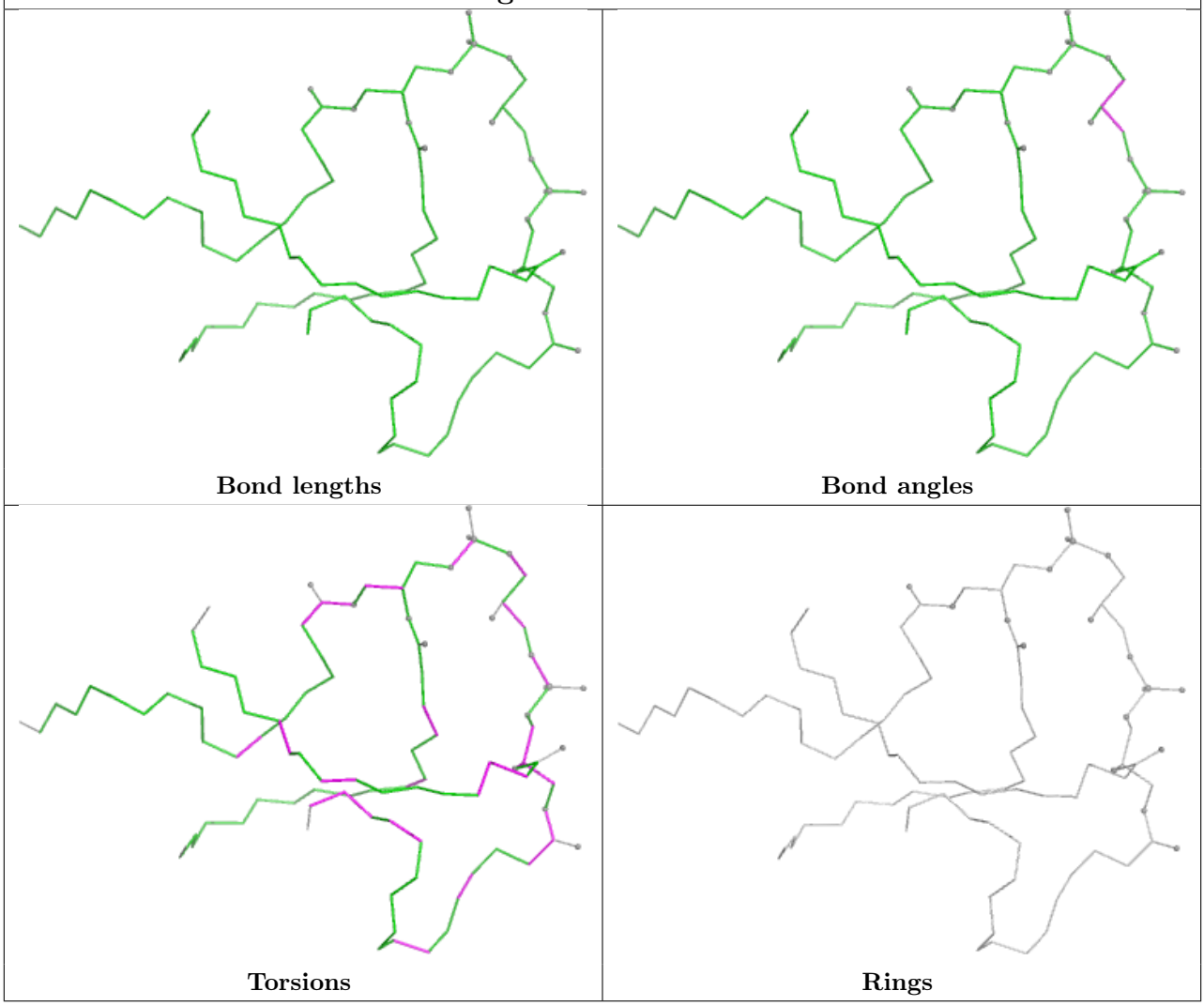
Ligand 3PE EM 901



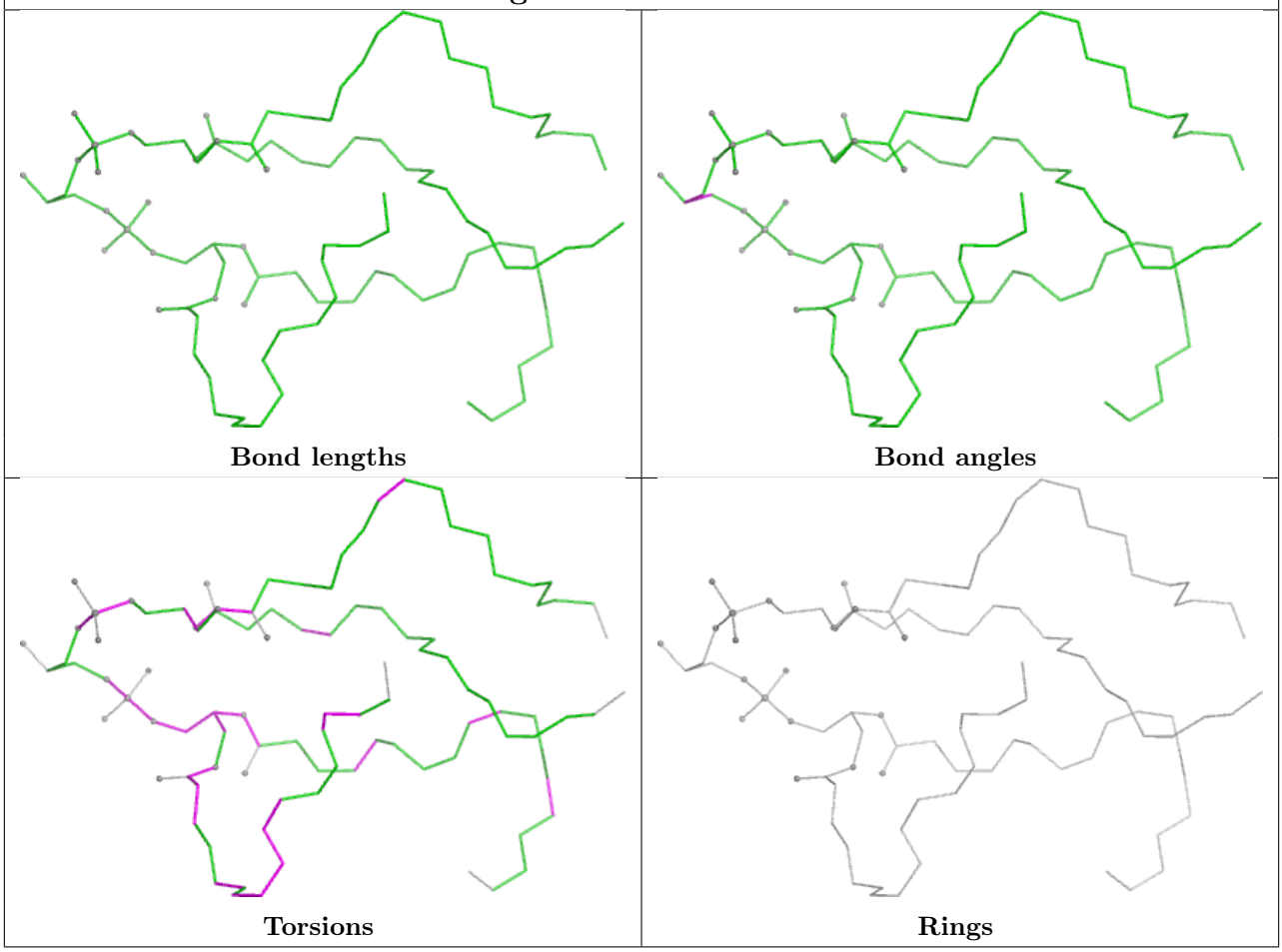
Ligand CUA DB 701



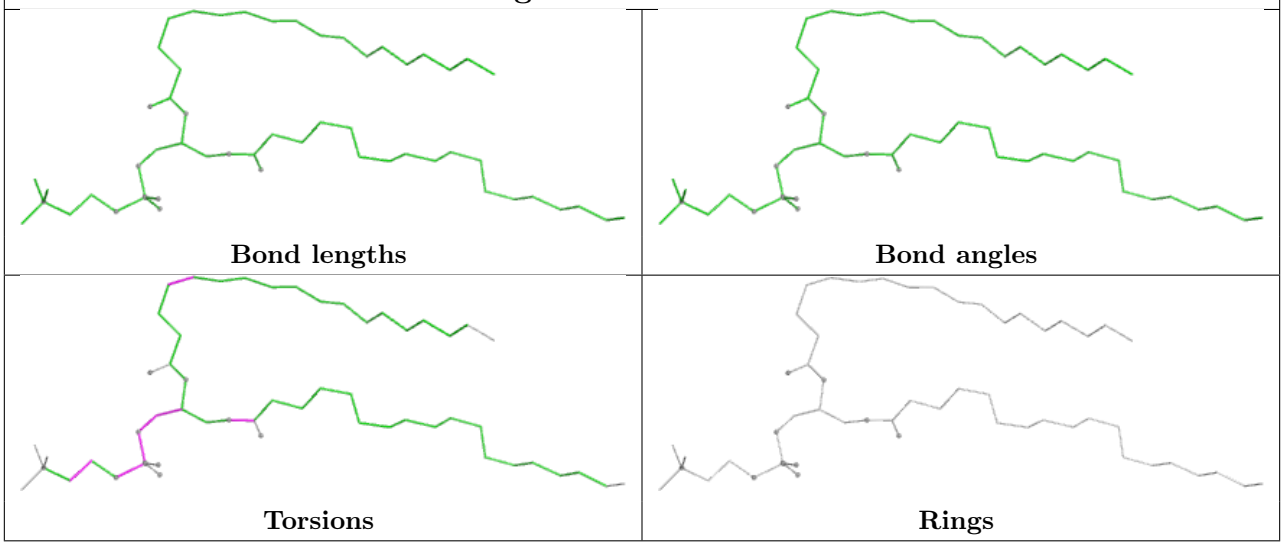
Ligand CDL c 509



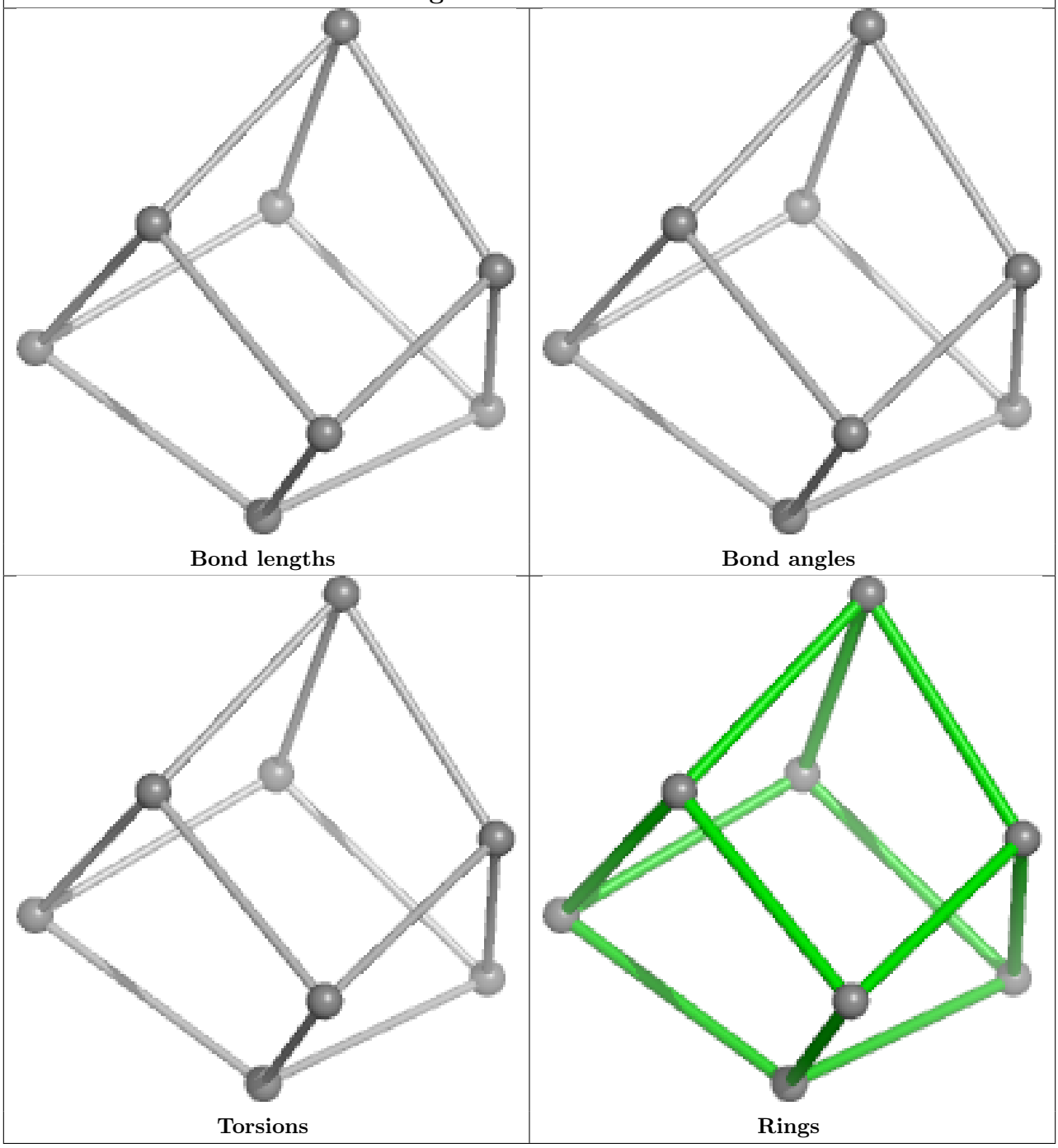
Ligand CDL DN 502



Ligand PC1 AU 201



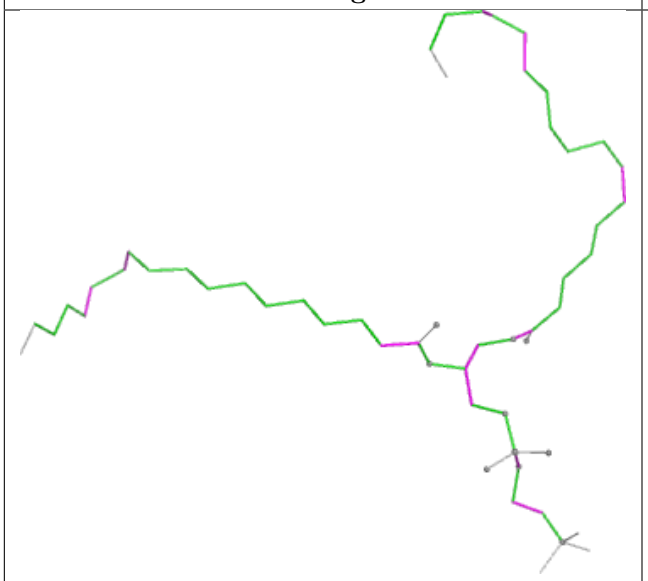
Ligand SF4 AT 201



Ligand PC1 DC 603

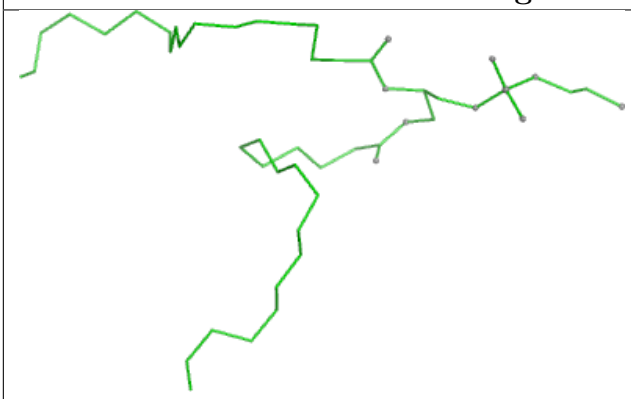
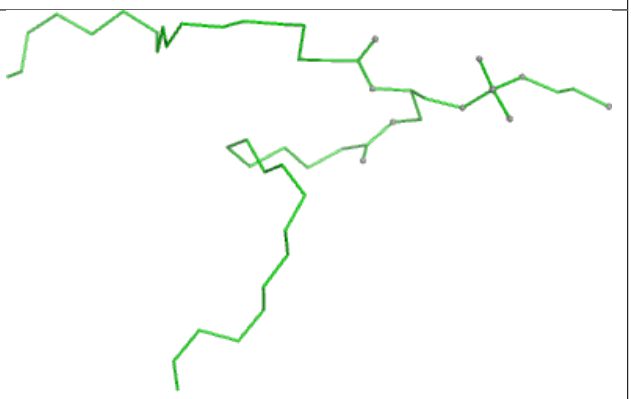
Bond lengths

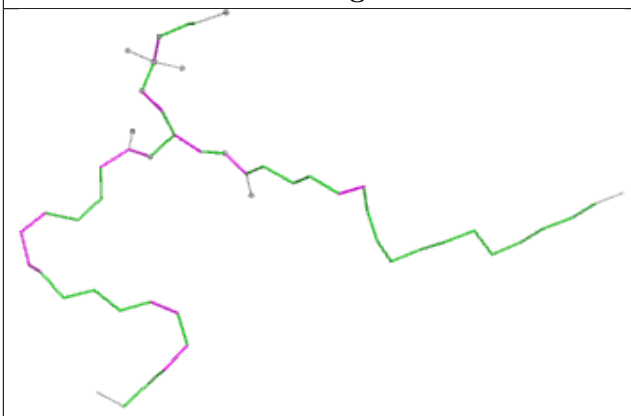
Bond angles



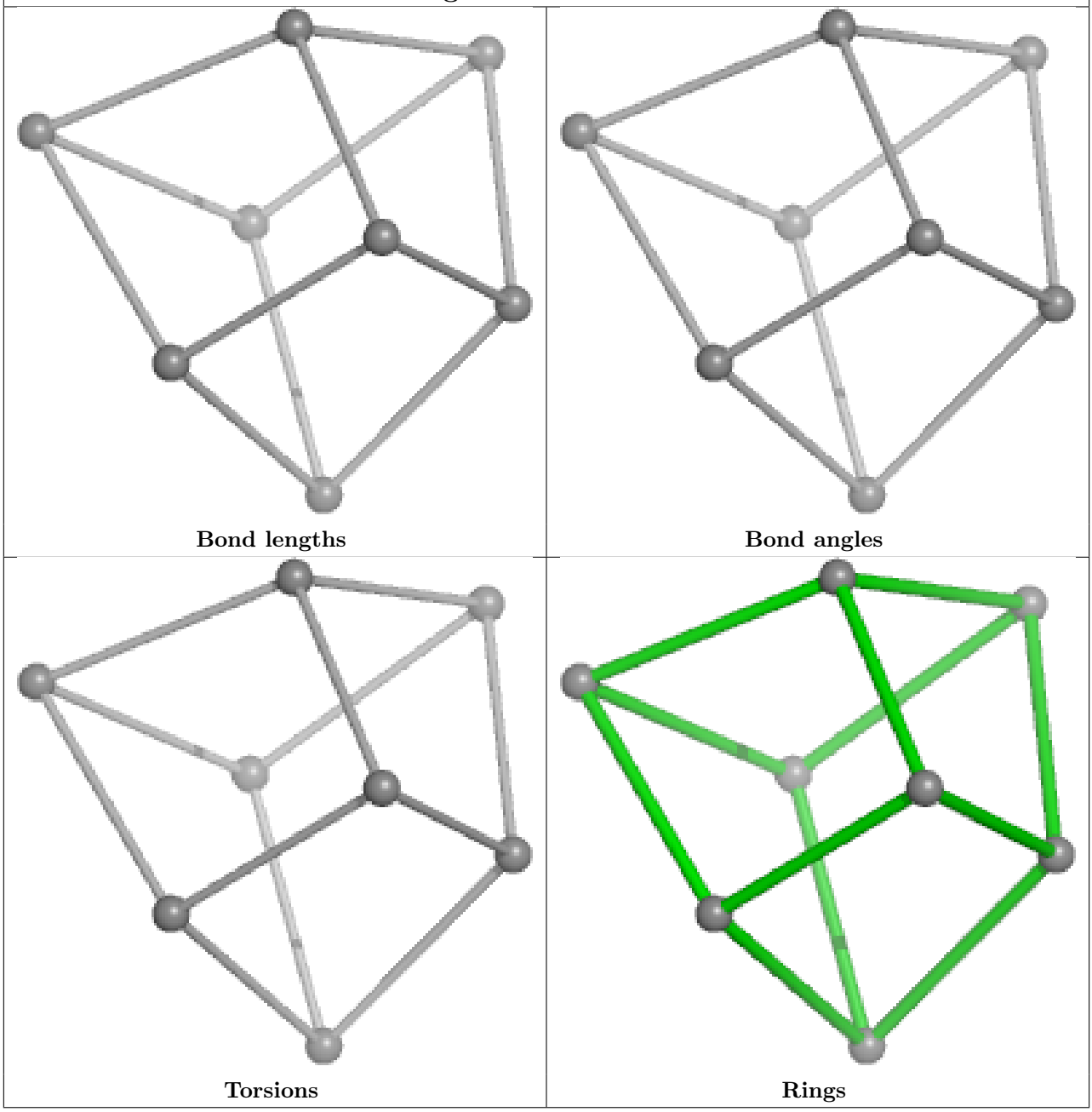
Torsions

Rings

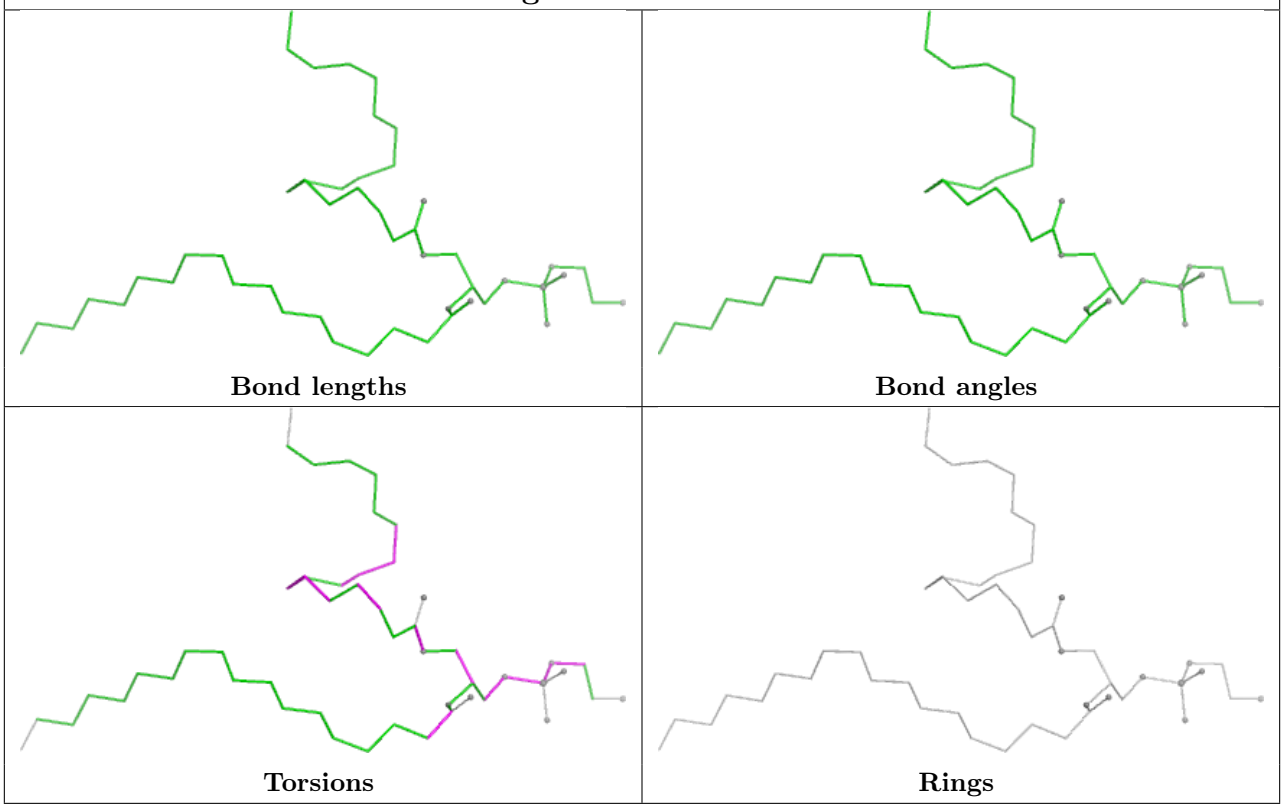
Ligand 3PE DX 304	
	
Bond lengths	**Bond angles**
Torsions	**Rings**

Ligand 3PE BA 301	
Bond lengths	Bond angles
 Torsions	Rings

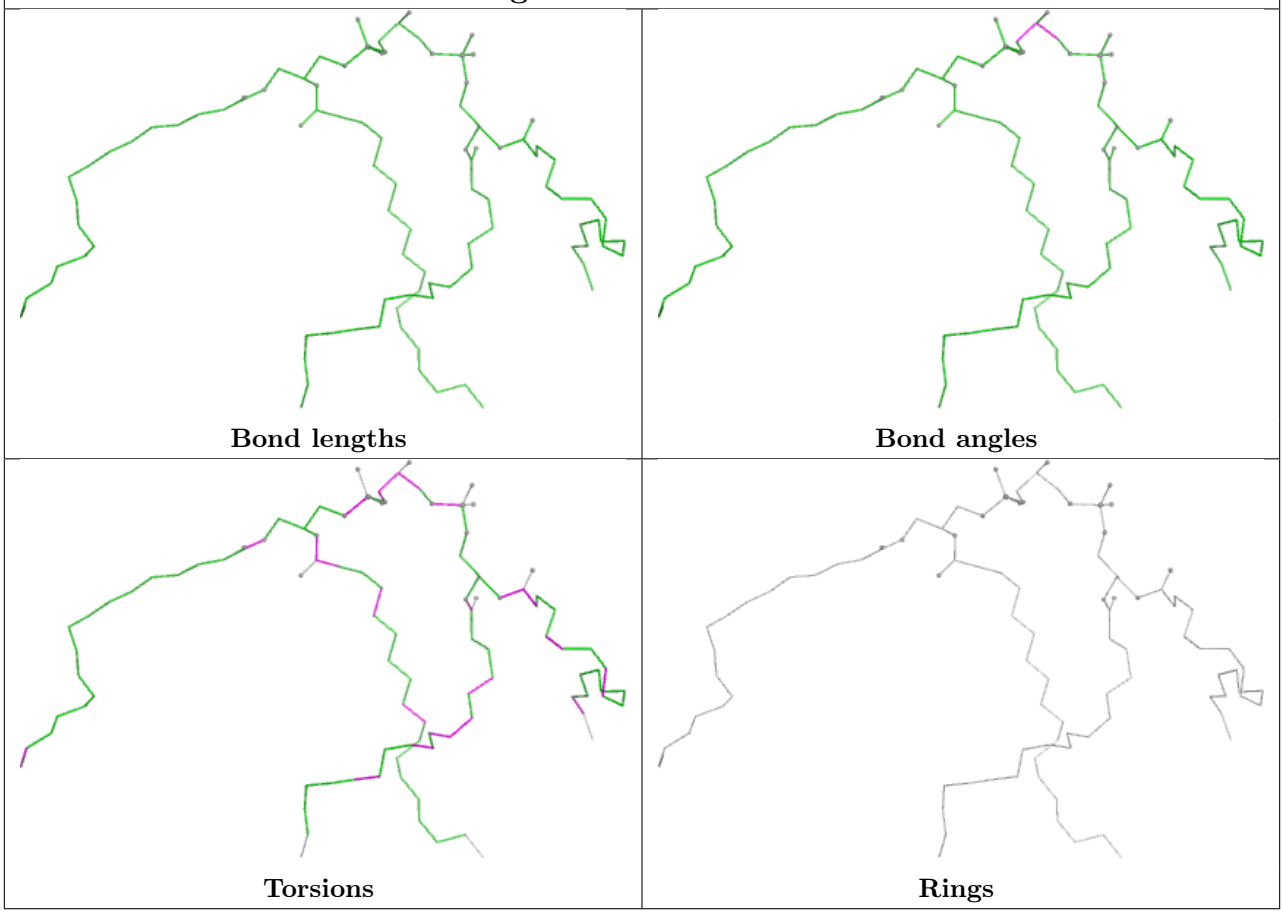
Ligand SF4 AL 301



Ligand 3PE DI 301



Ligand CDL DU 403



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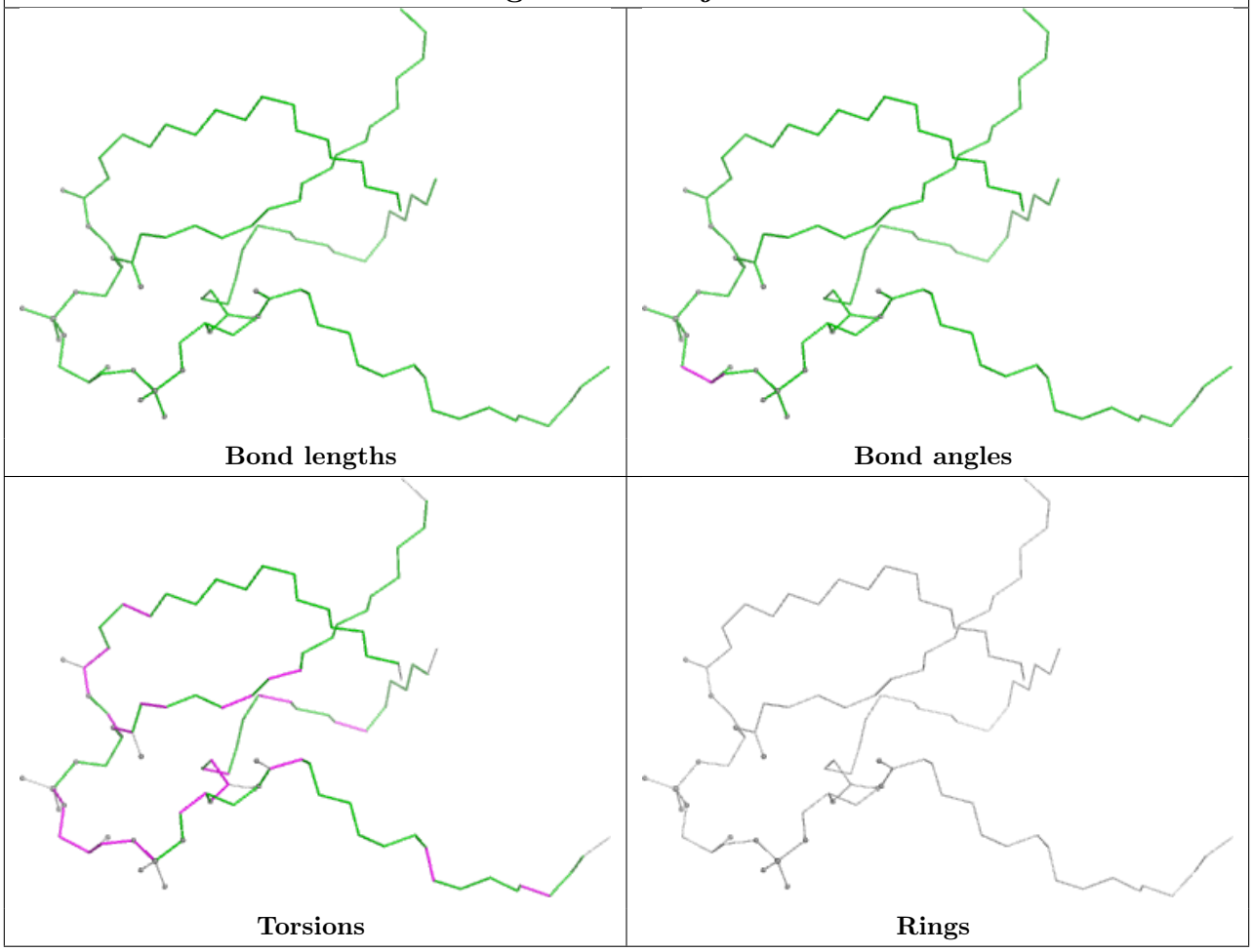

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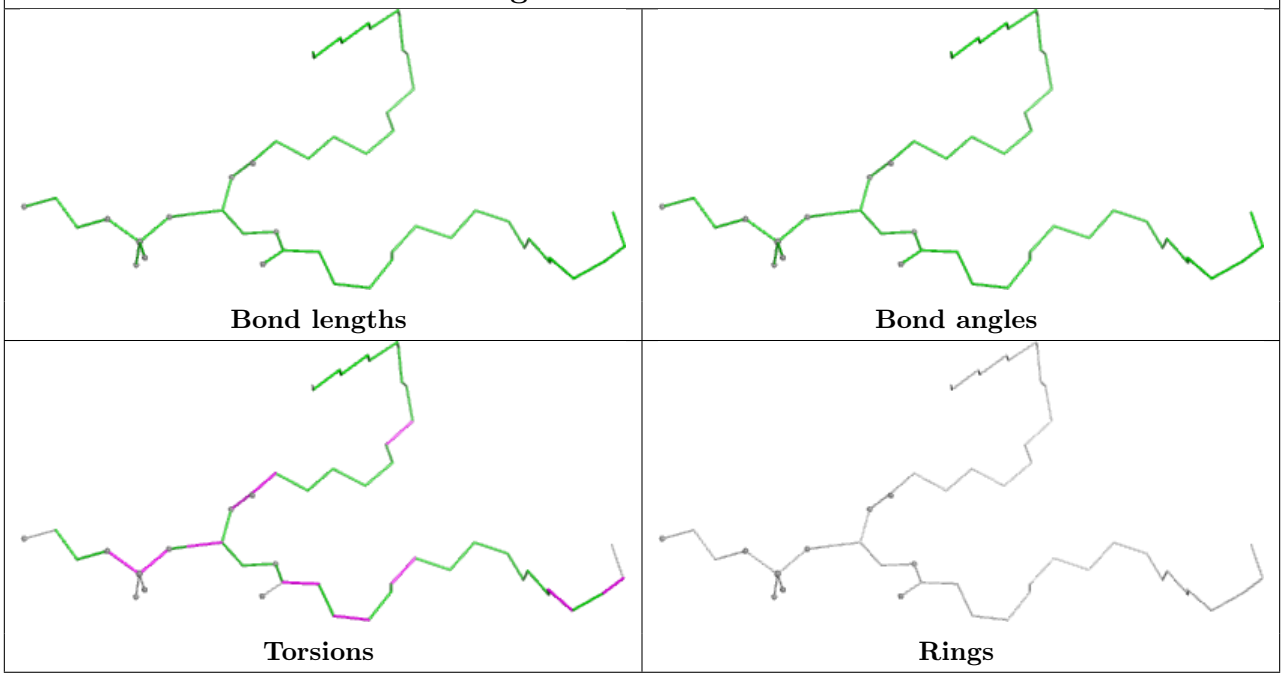

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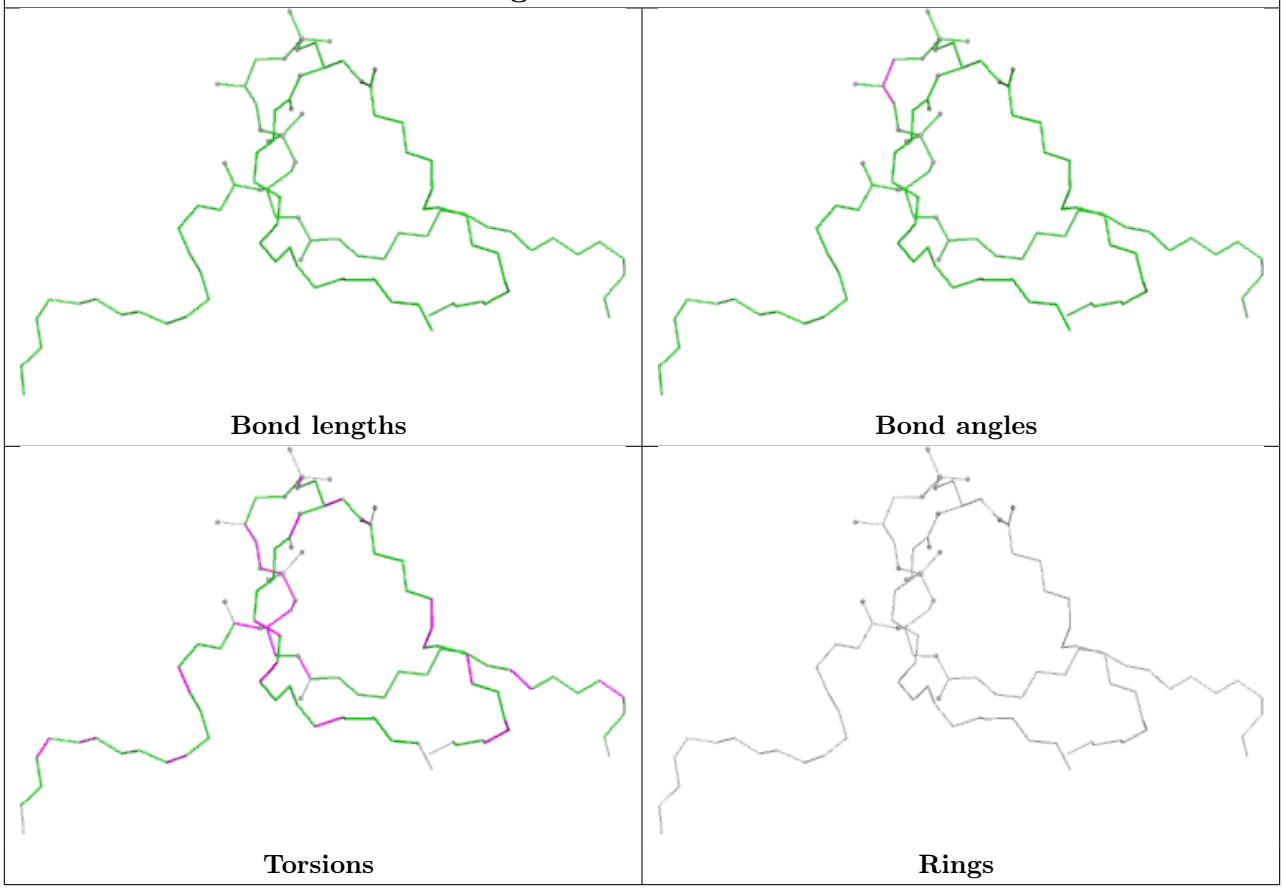

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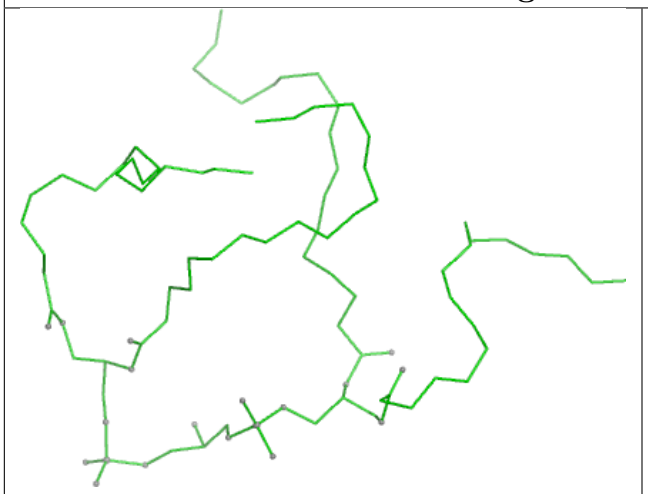
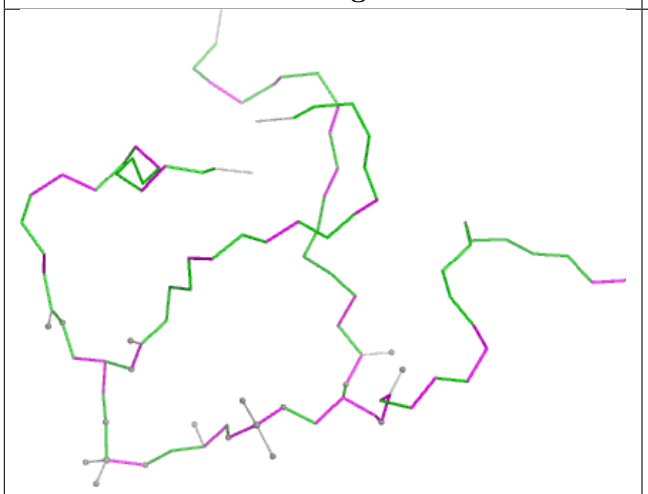


Bond lengths

Bond angles



Torsions

Rings

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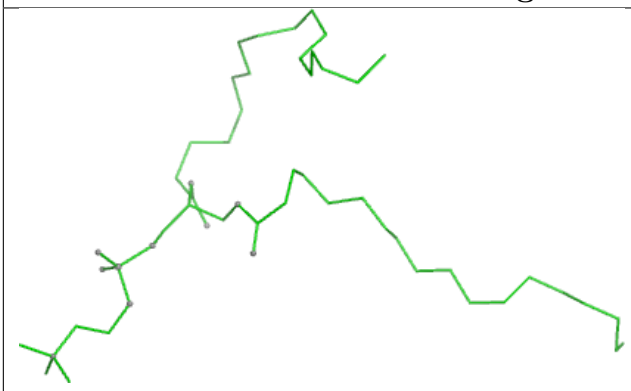
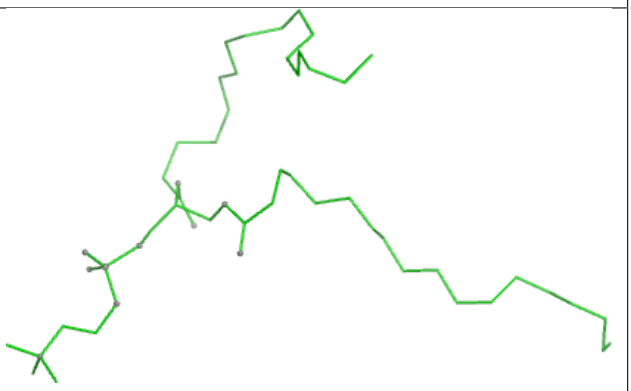
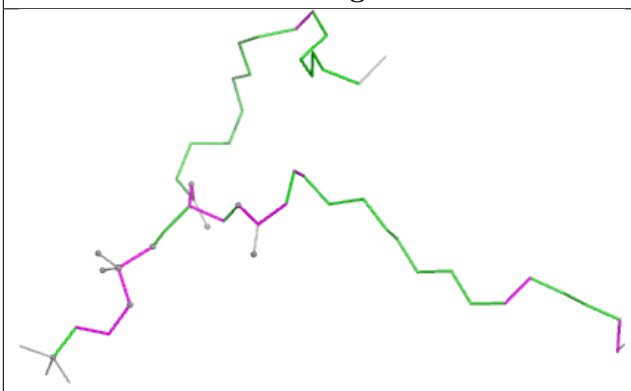
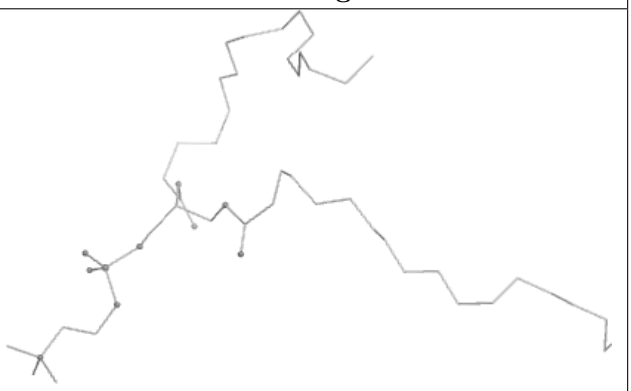
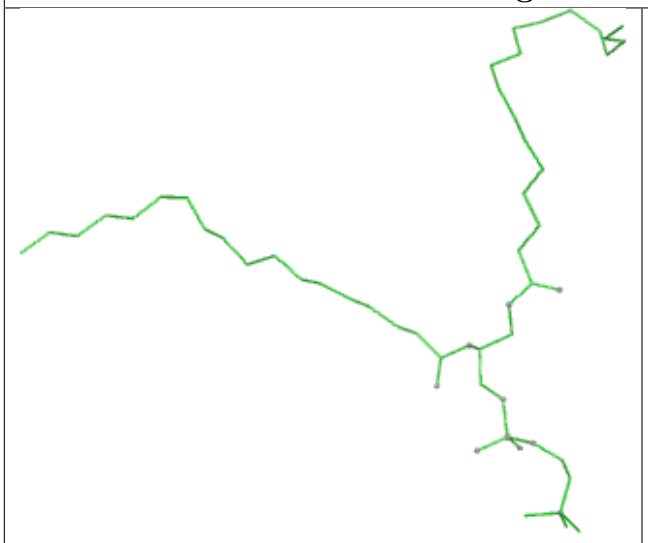
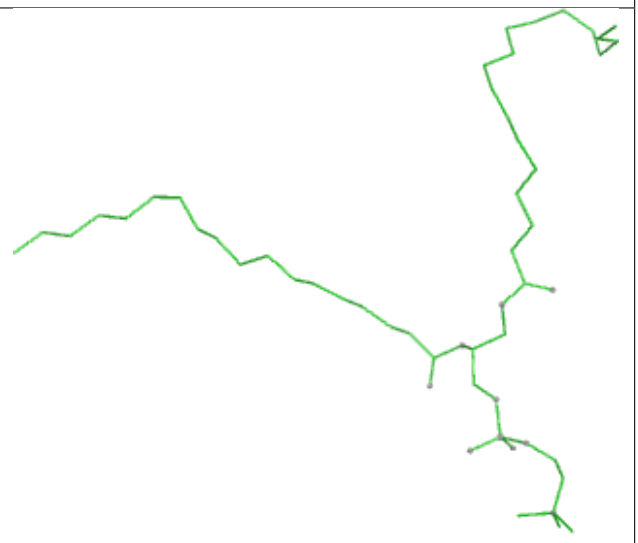
 Bond lengths	 Bond angles
 Torsions	 Rings

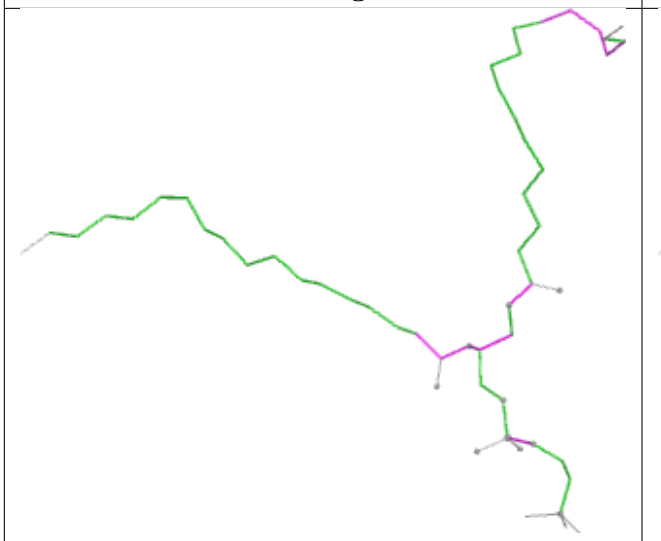
Ligand PC1 EO 206



Bond lengths



Bond angles



Torsions

Rings

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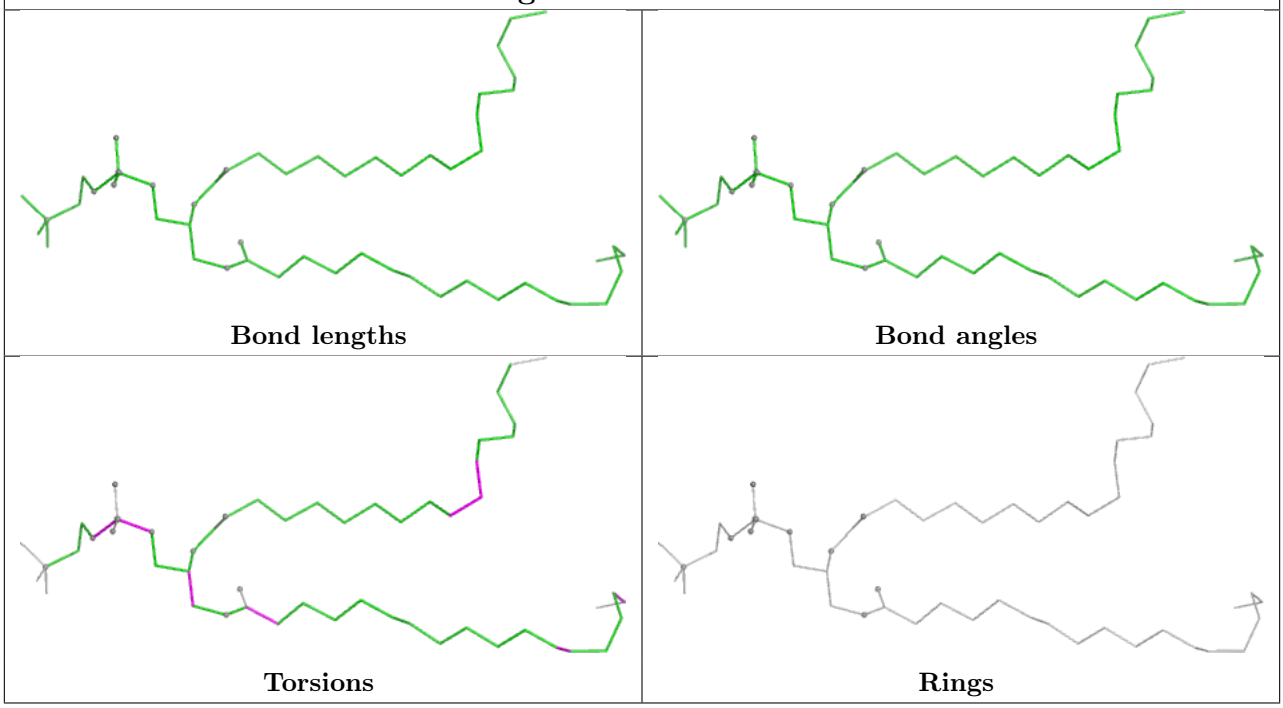

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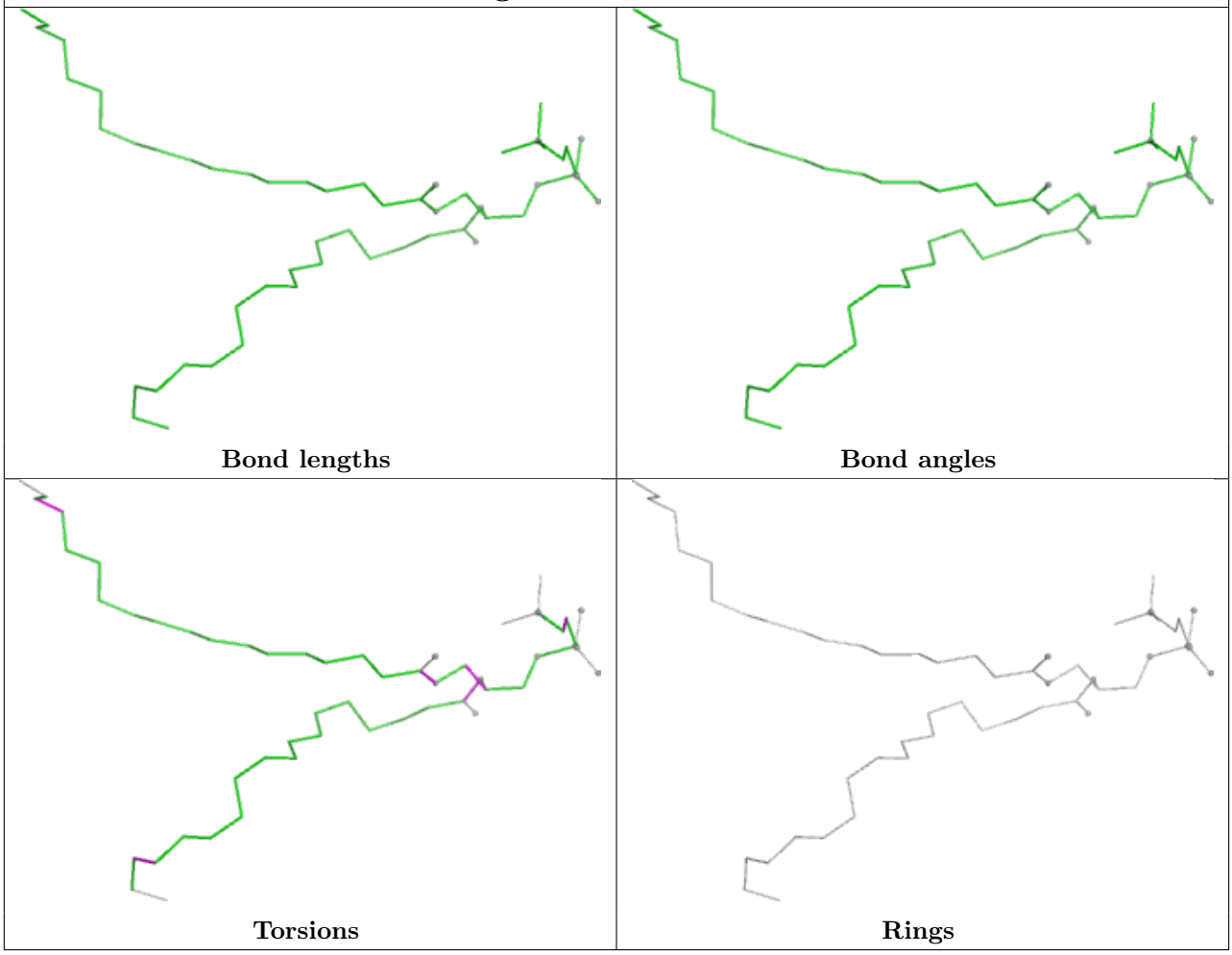
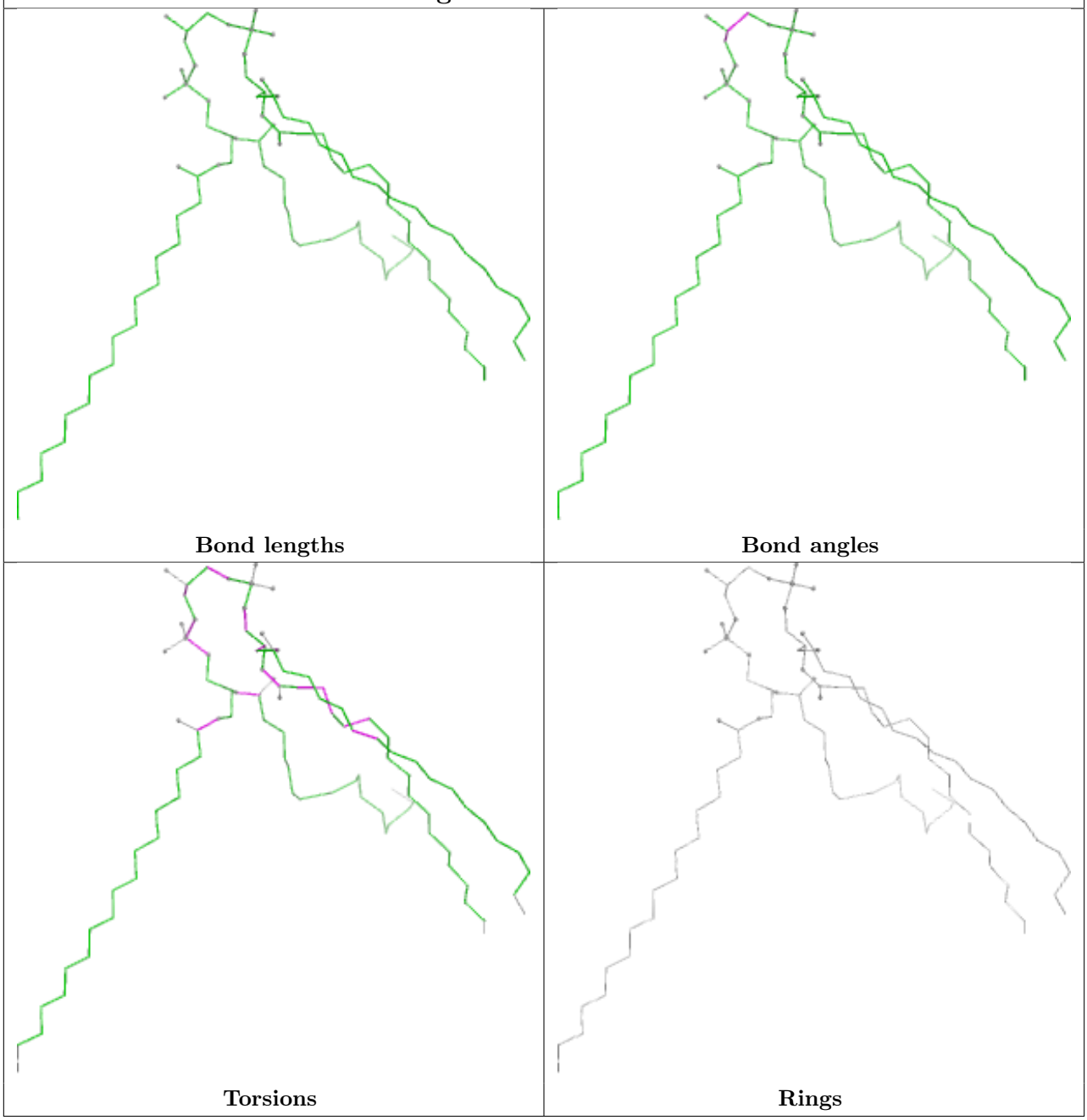
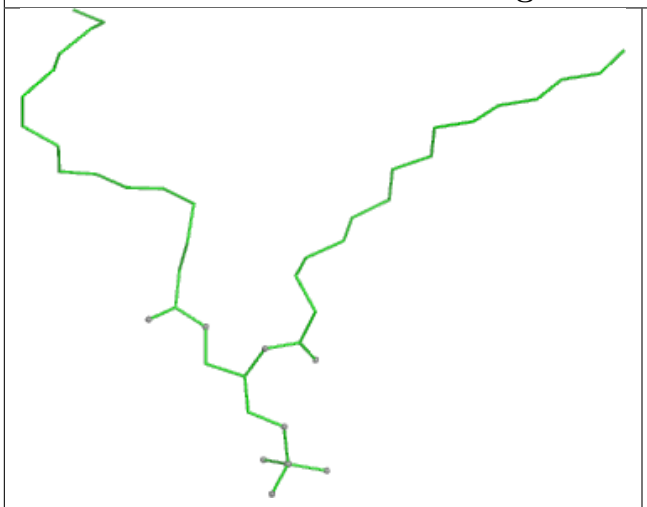


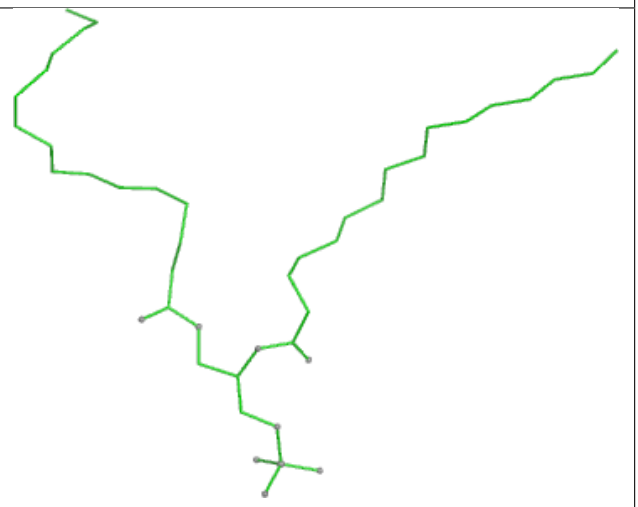
Ligand CDL A0 601



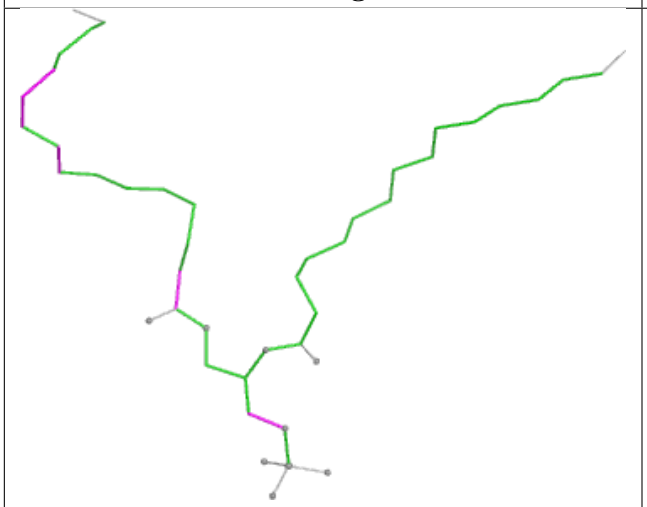
Ligand LPP Dn 505



Bond lengths



Bond angles



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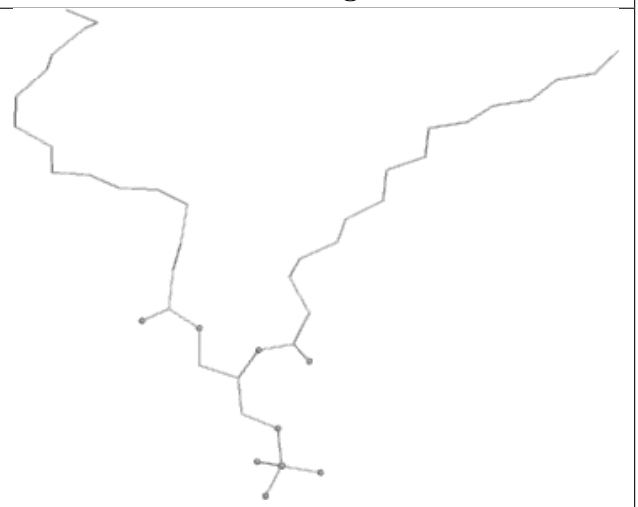

Rings

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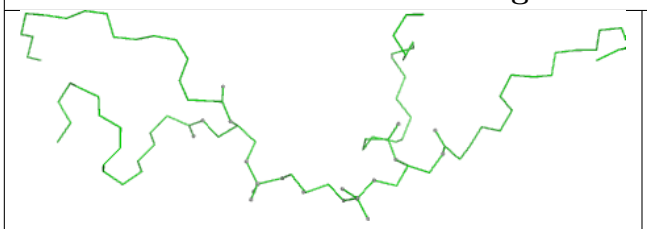

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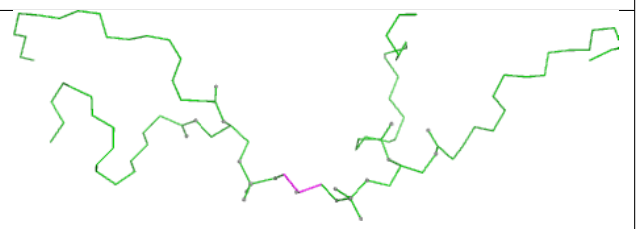
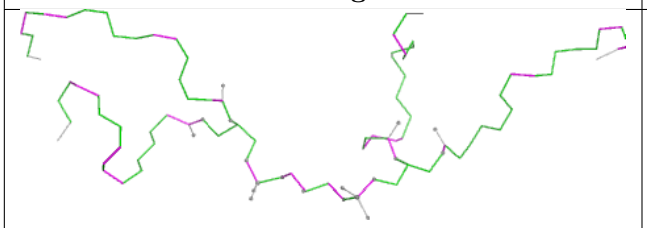


Bond angles



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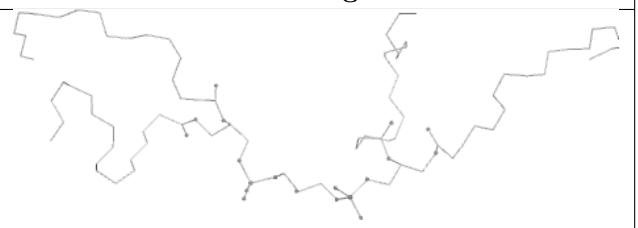
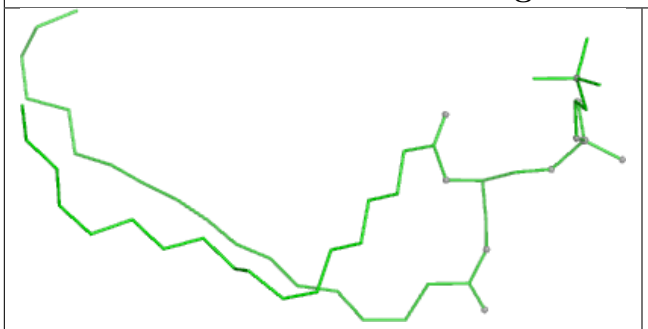


Rings

Ligand PC1 DC 604



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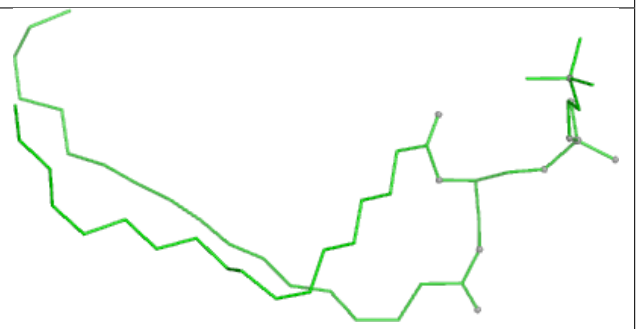
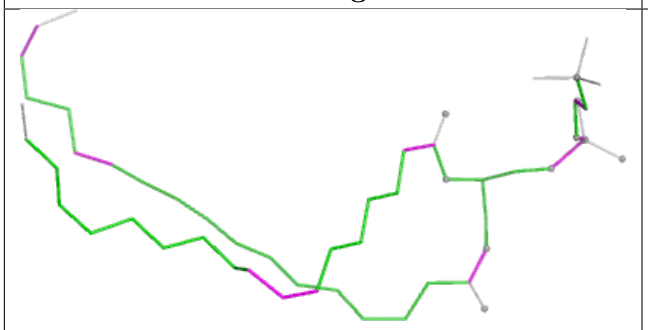


Bond angles



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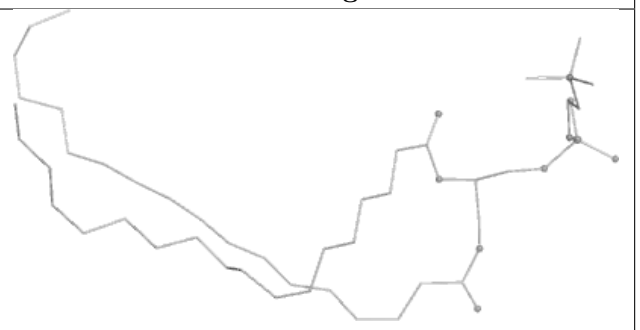
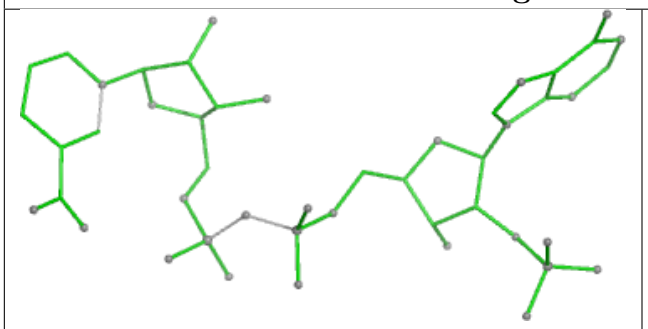
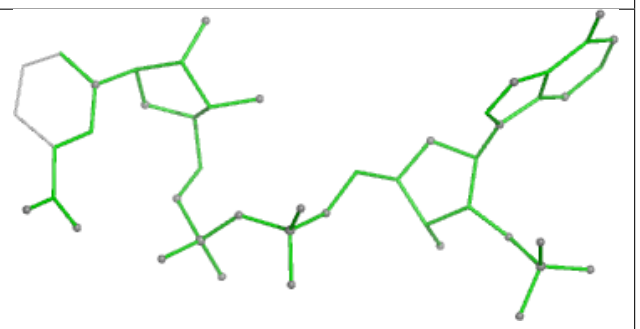


Rings

Ligand NDP A1 401



Bond lengths



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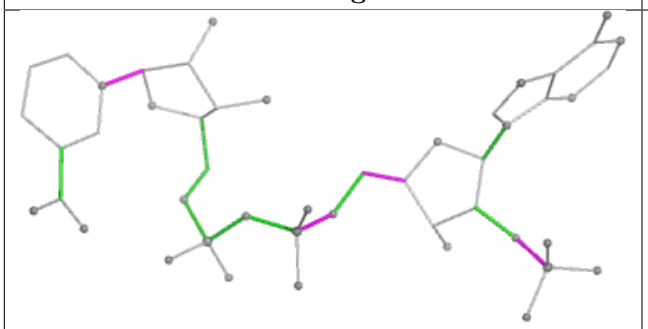

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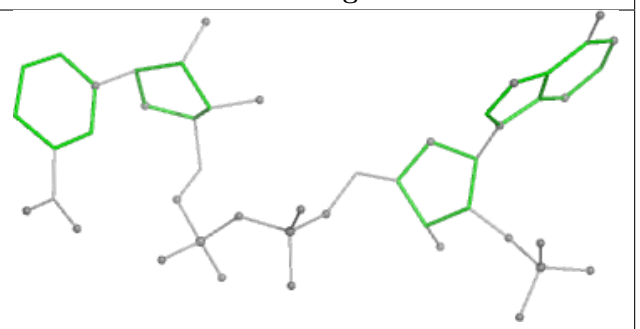
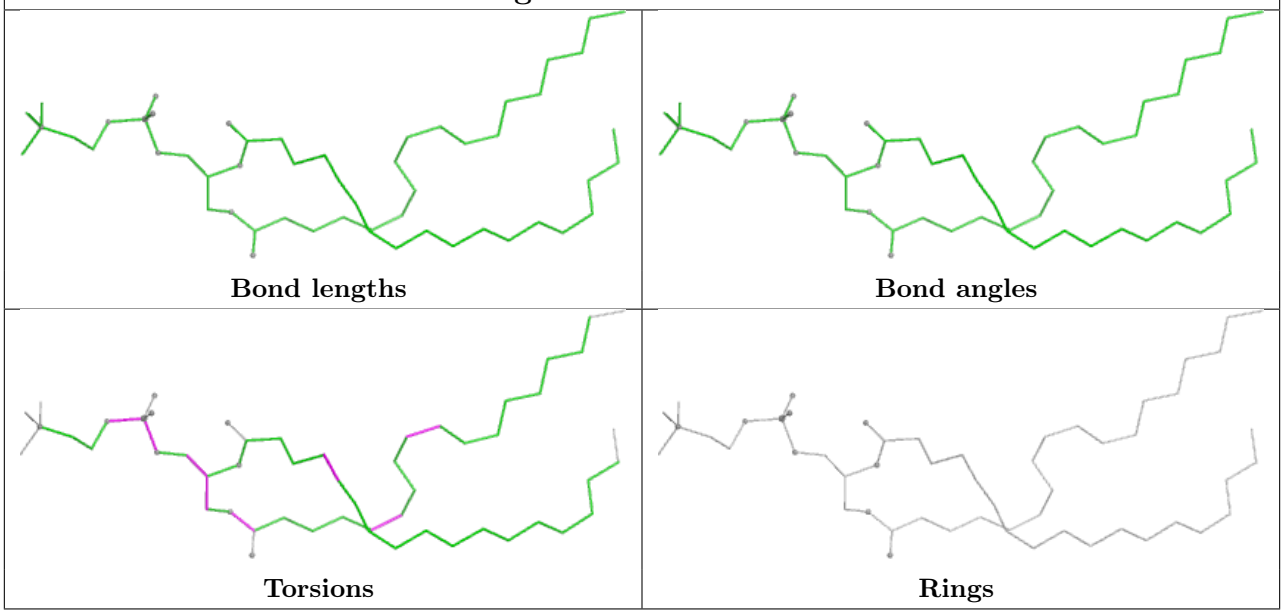
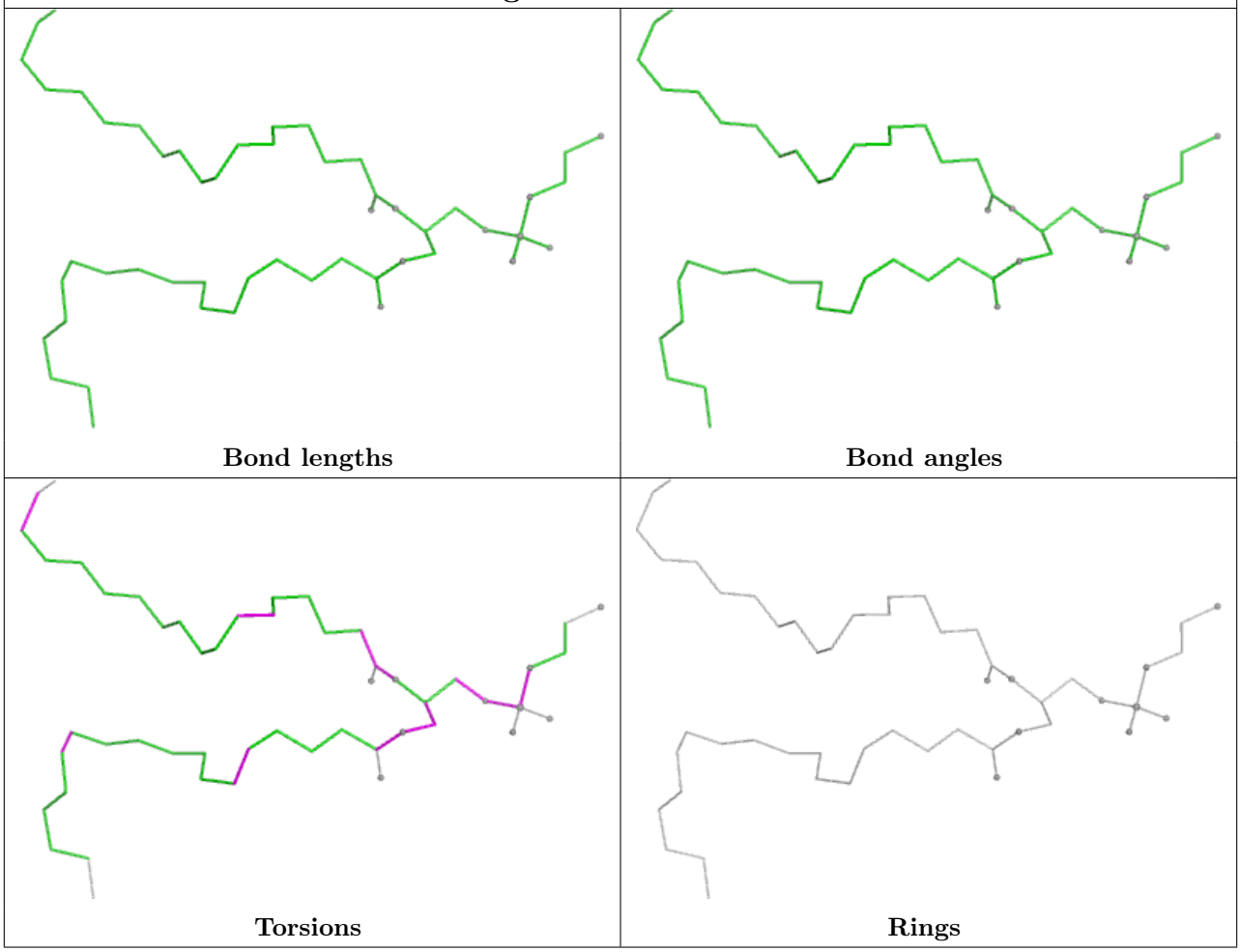


Rings

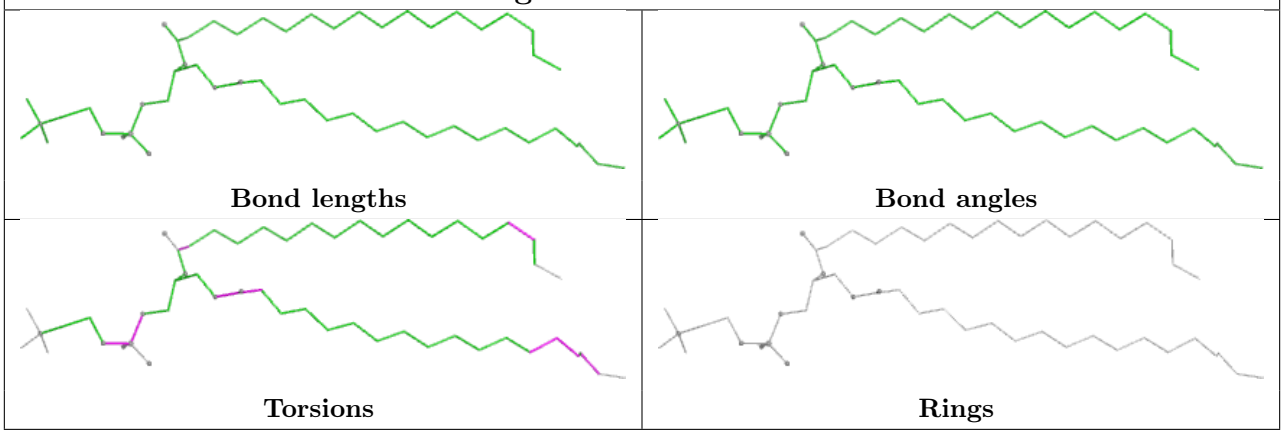
Ligand PC1 AA 903



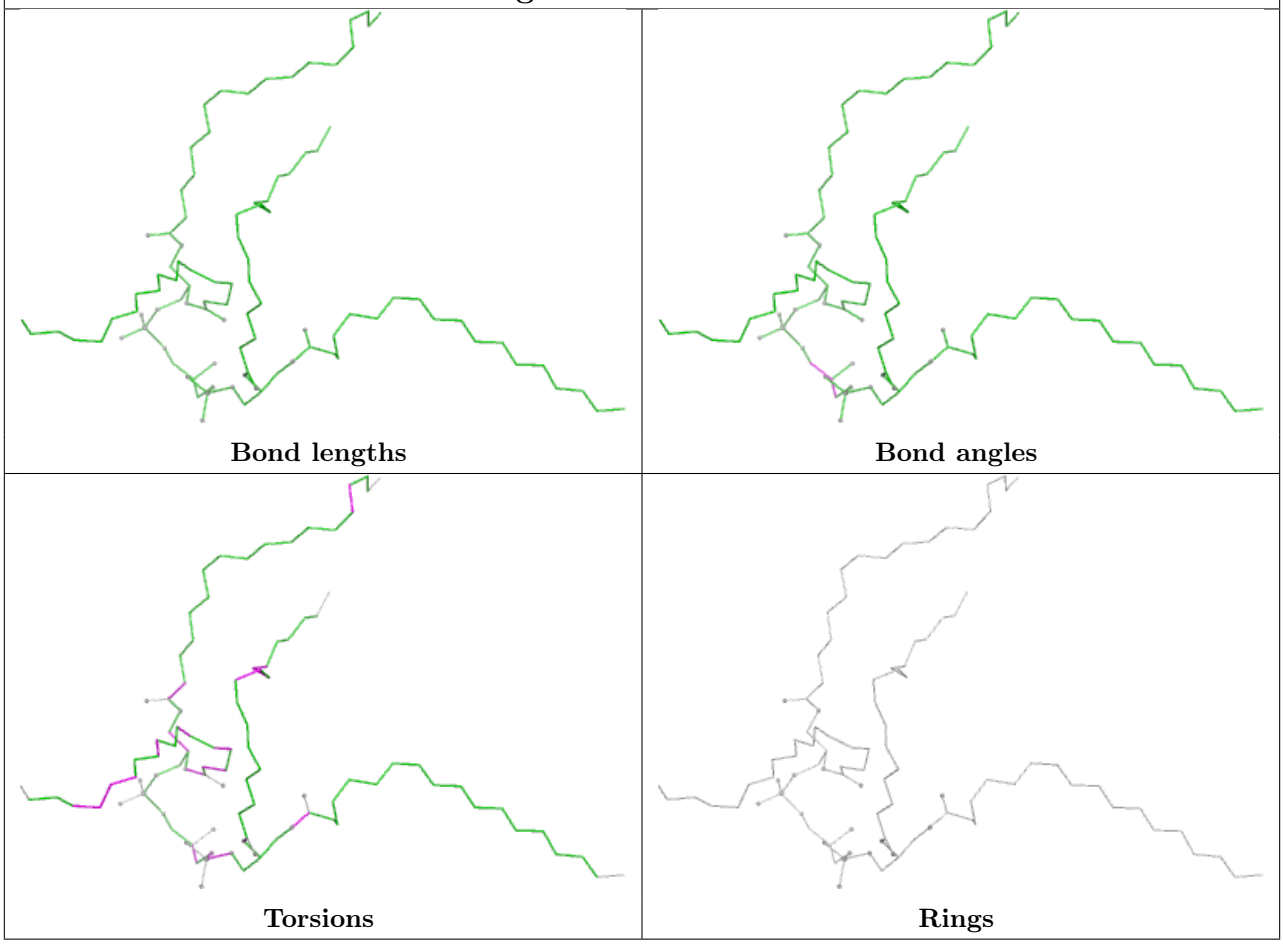
Ligand 3PE Dc 607

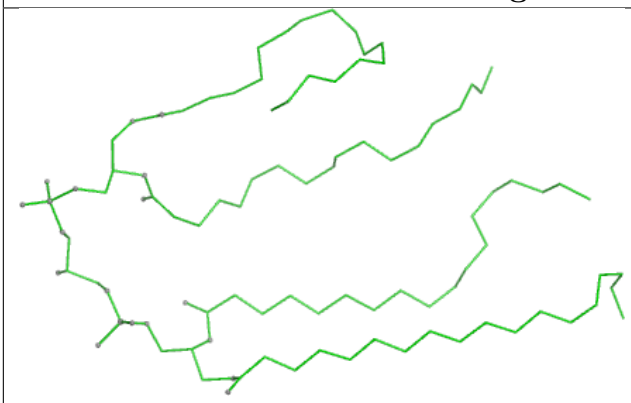
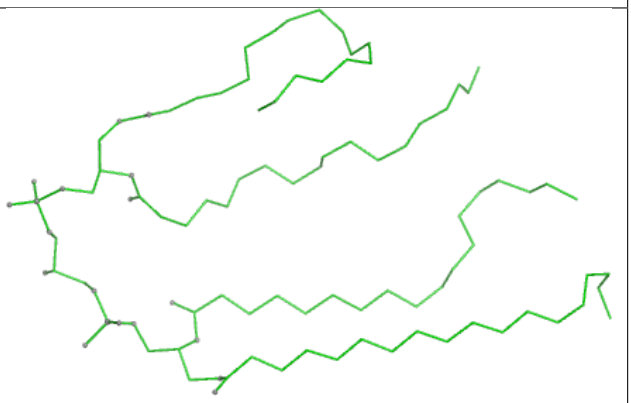
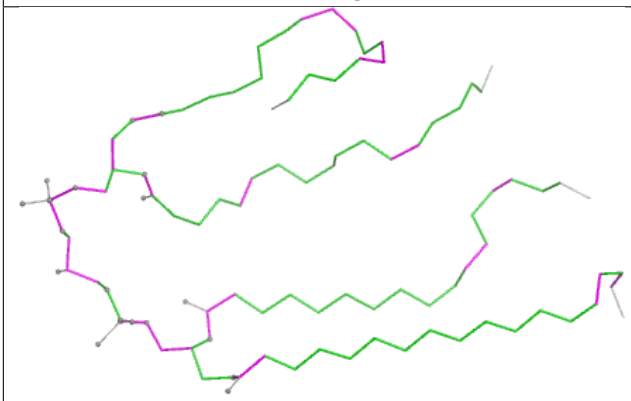


Ligand PC1 DC 602

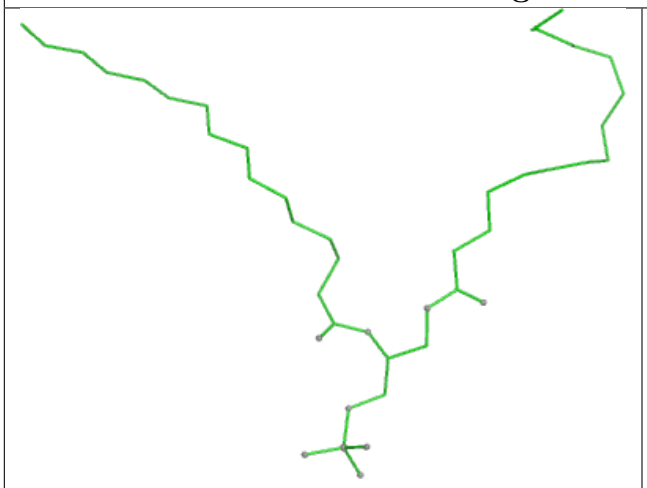


Ligand CDL Dc 608

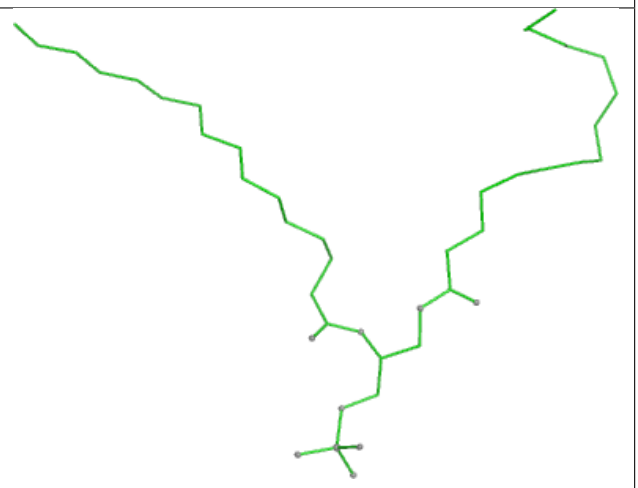


Ligand CDL DD 705	
 Bond lengths	 Bond angles
 Torsions	Rings

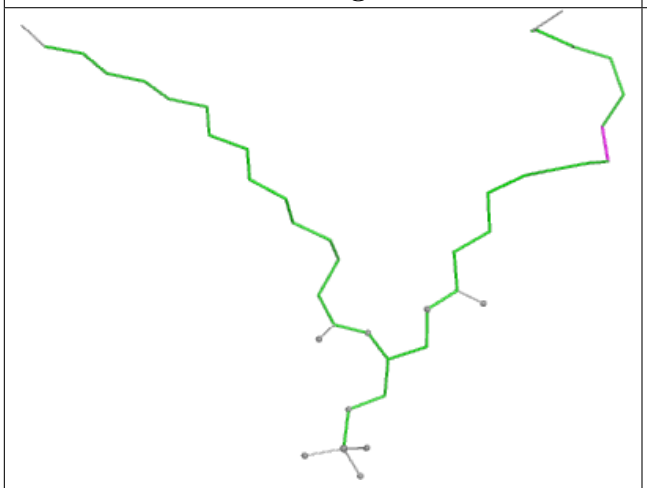
Ligand LPP DN 505



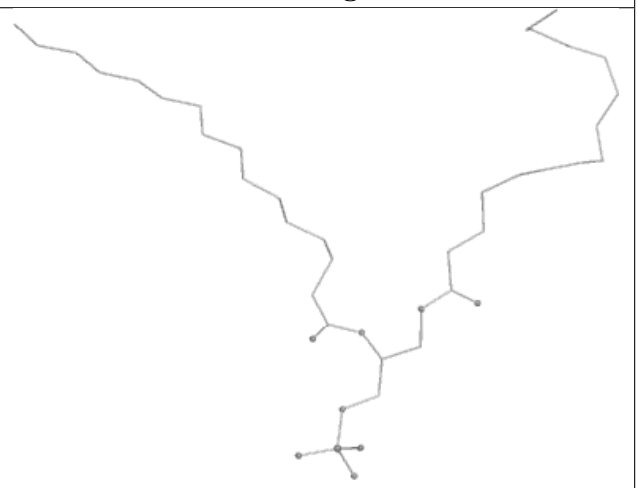
Bond lengths



Bond angles

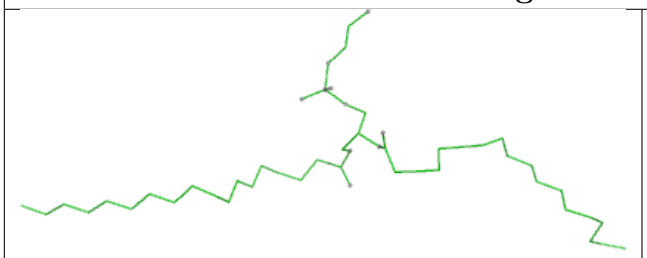


Torsions



Rings

Ligand 3PE CD 303



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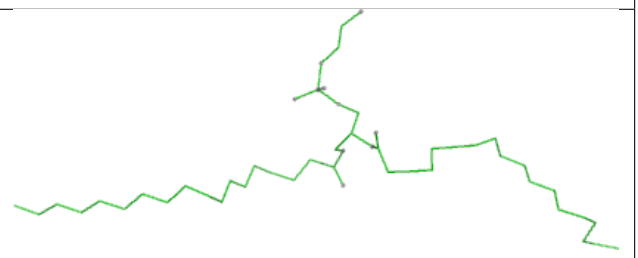
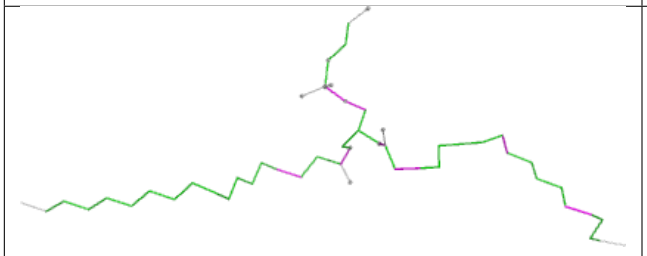


Bond angles



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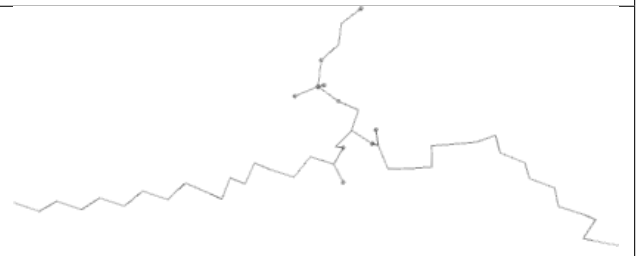
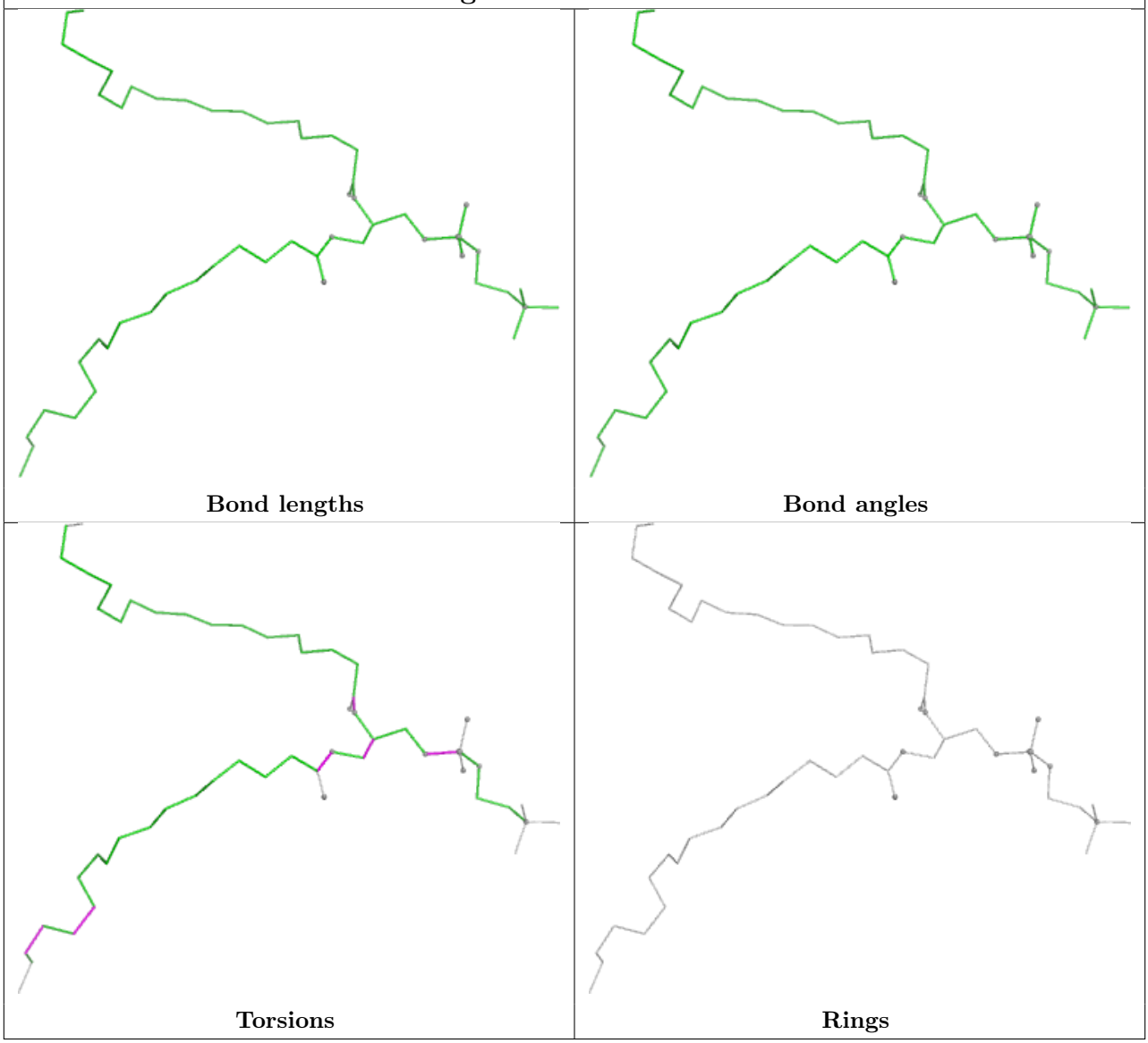
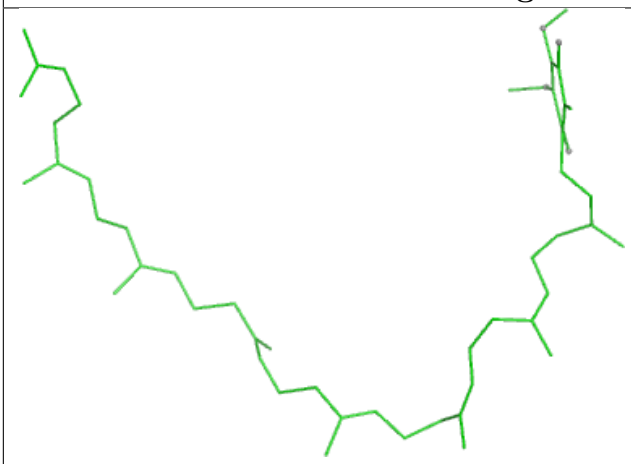


Rings

Ligand PC1 DA 708



Ligand UQ8 Ed 202



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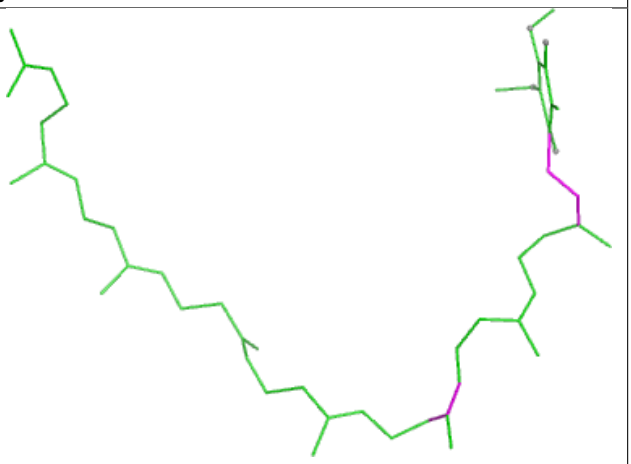
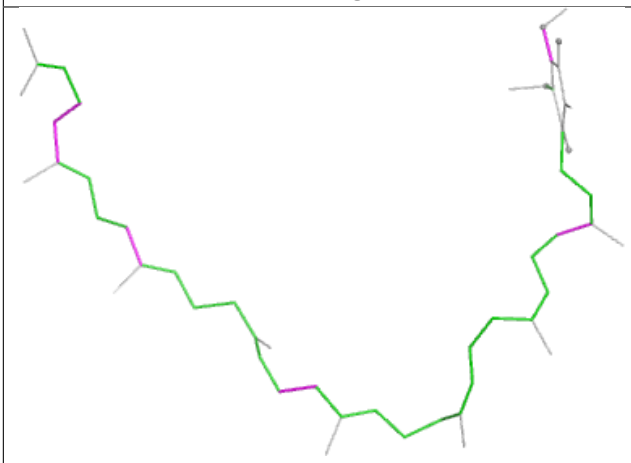


Bond angles



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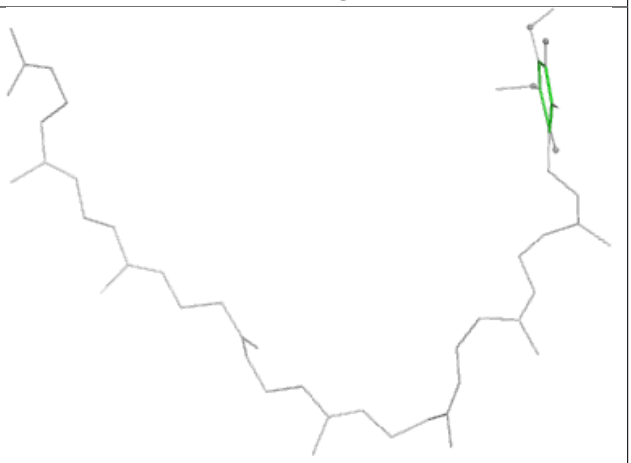
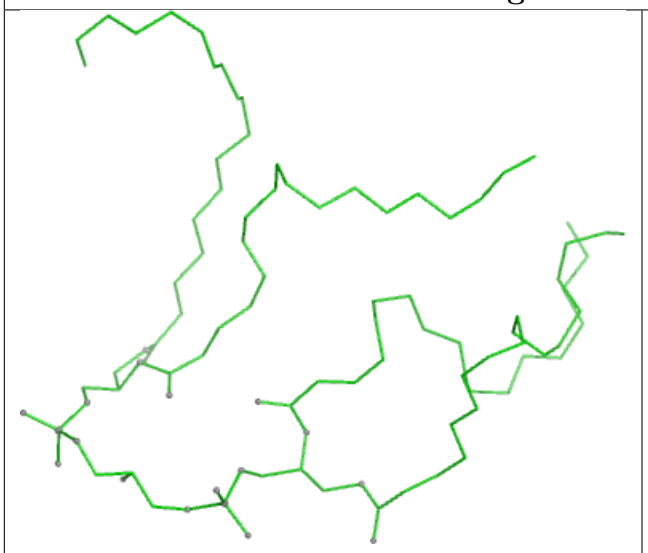


Rings

Ligand CDL DM 501



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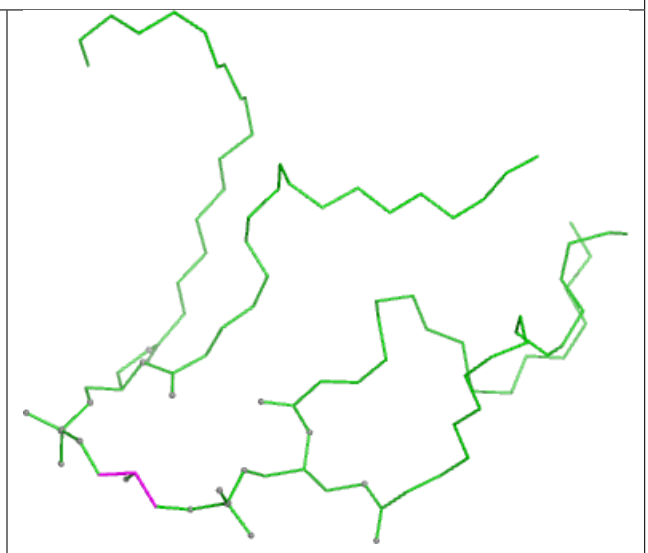
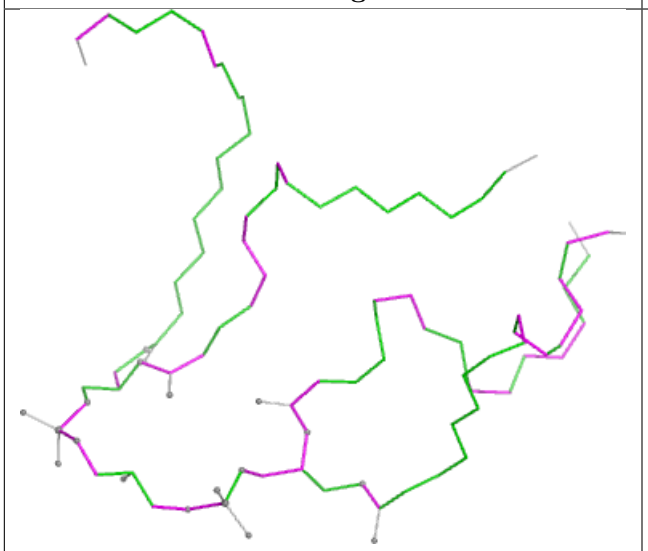


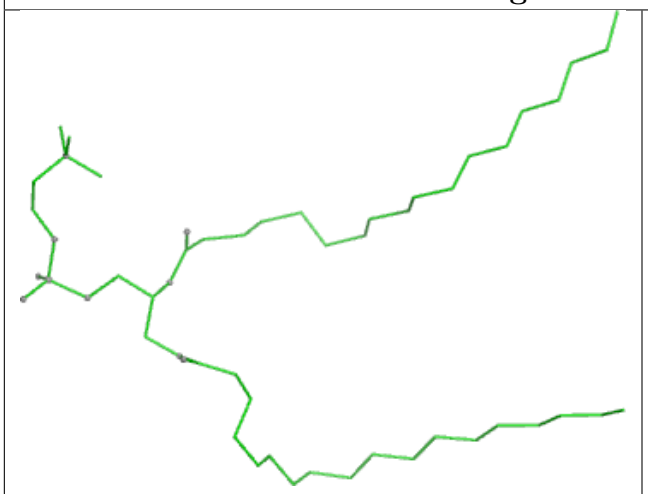
Bond angles



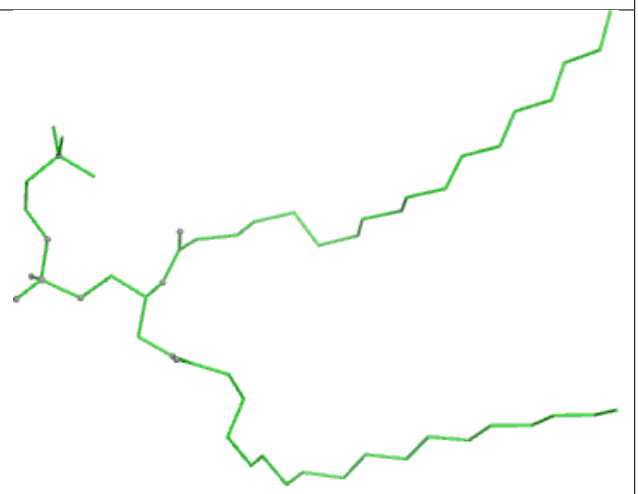
Torsions

Rings

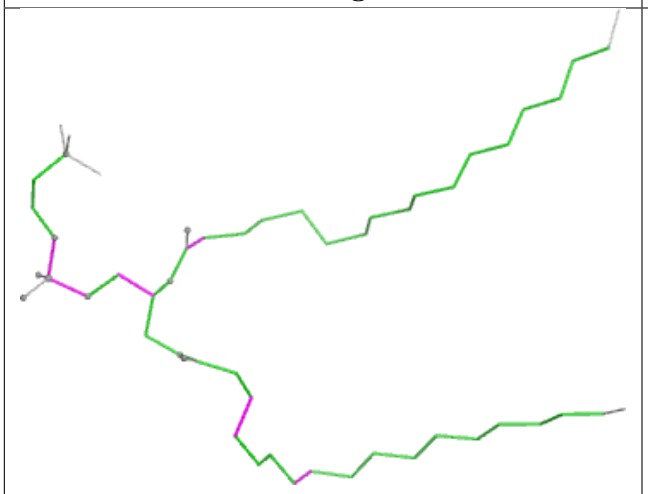
Ligand PC1 BS 1302



Bond lengths



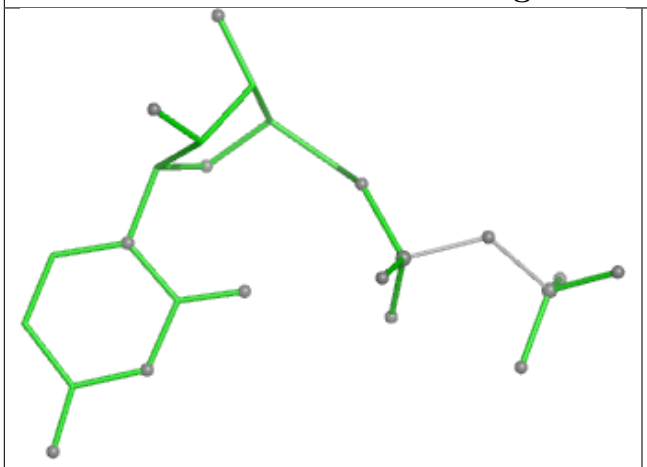
Bond angles



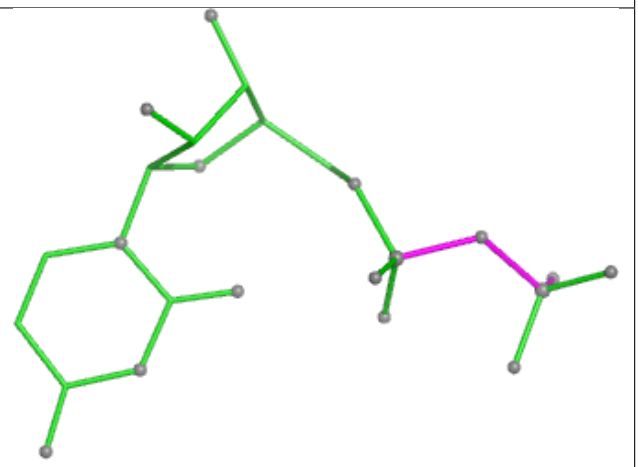
Torsions

Rings

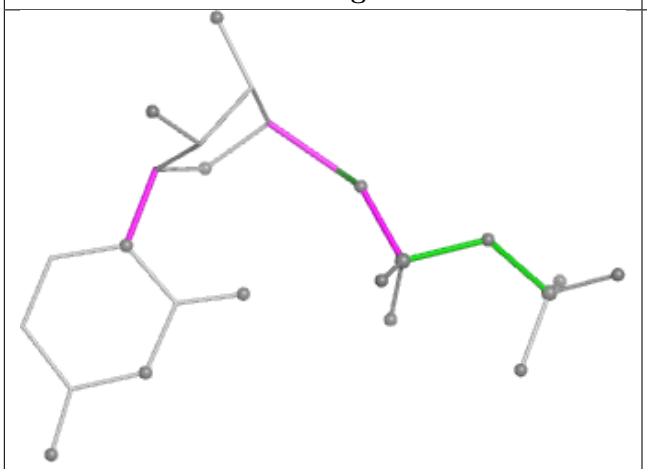
Ligand UDP A0 603



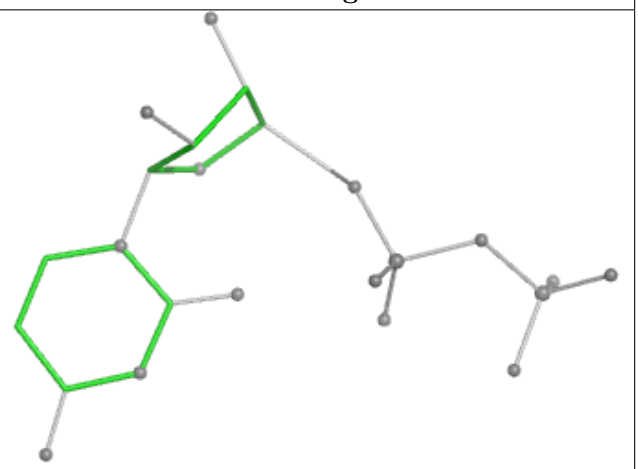
Bond lengths



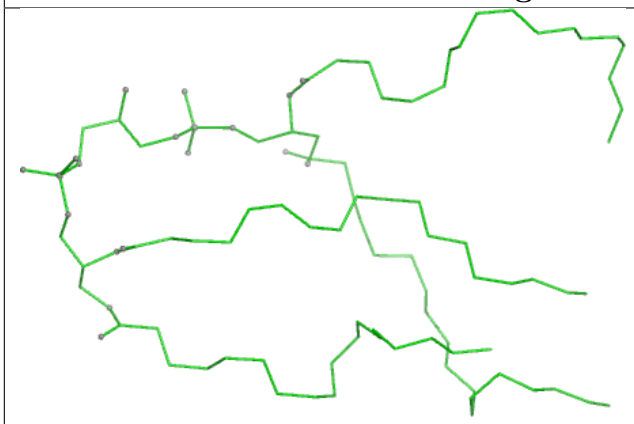
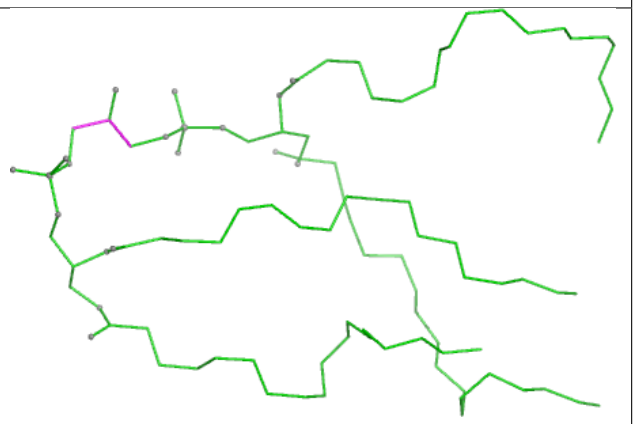
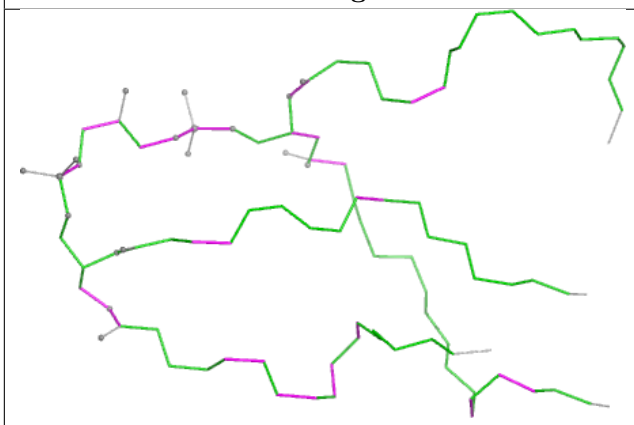
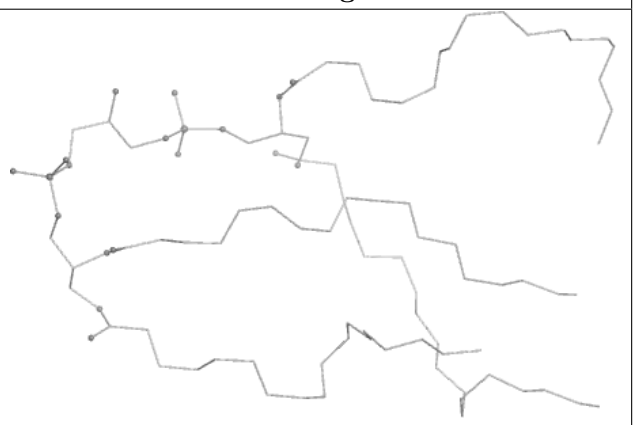
Bond angles



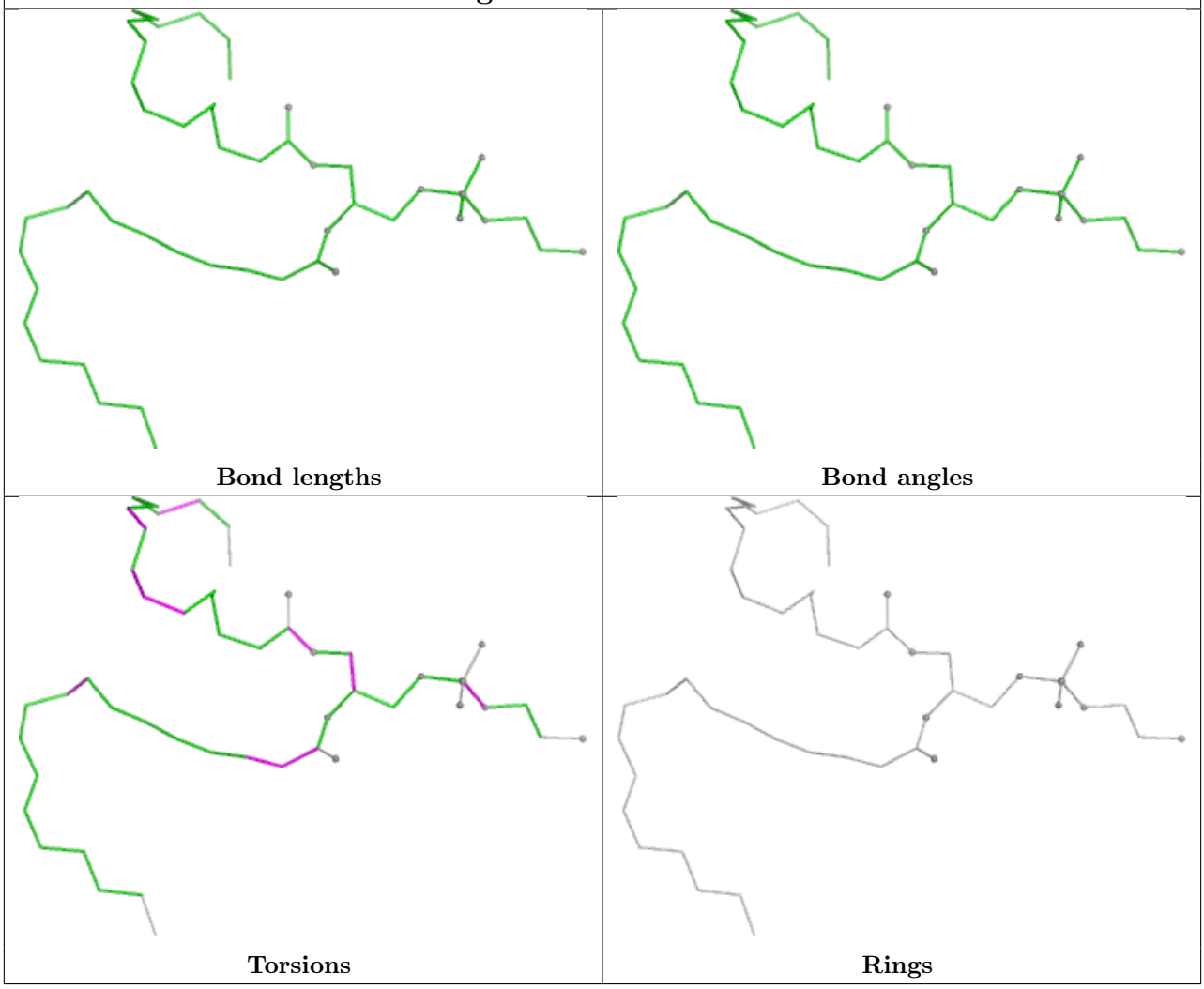
Torsions

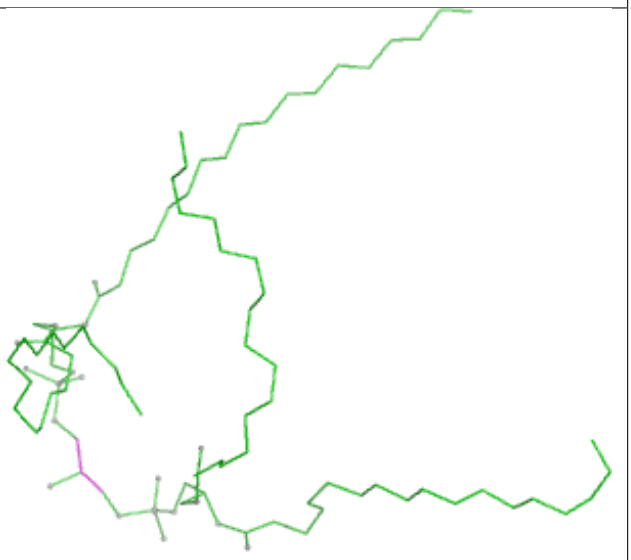
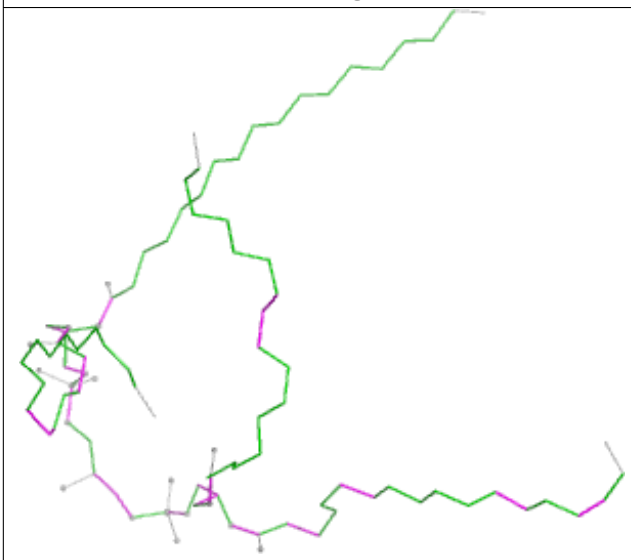


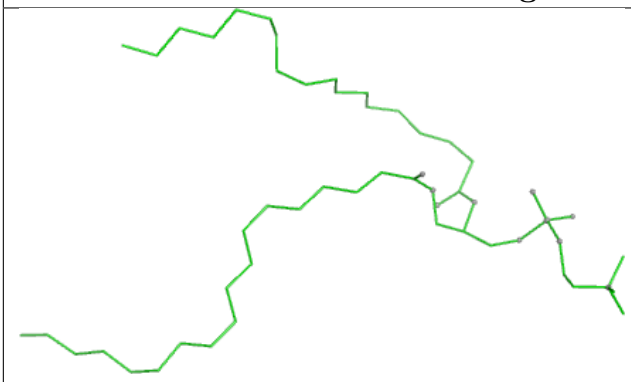
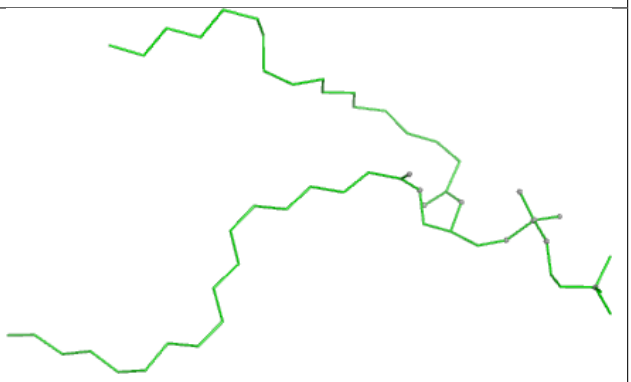
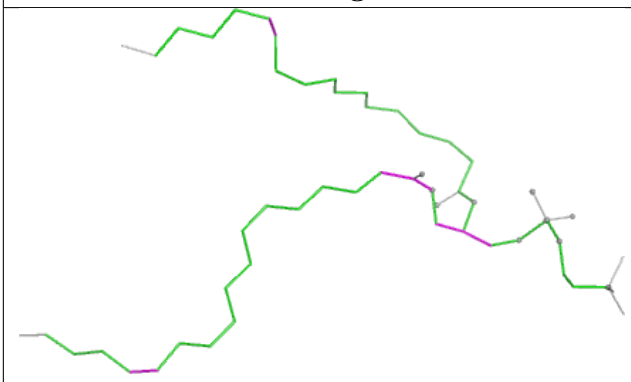
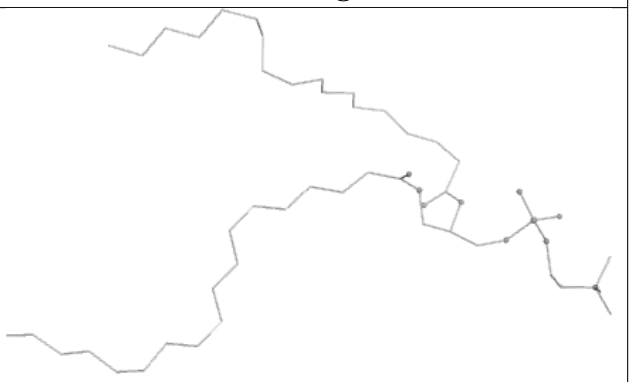
Rings

Ligand CDL DJ 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE EN 1204



Ligand CDL DD 703	
Bond lengths	 Bond angles
 Torsions	Rings

Ligand PC1 Ds 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

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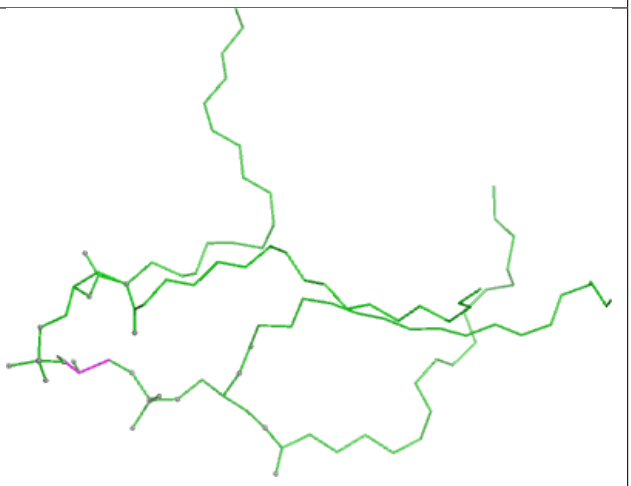
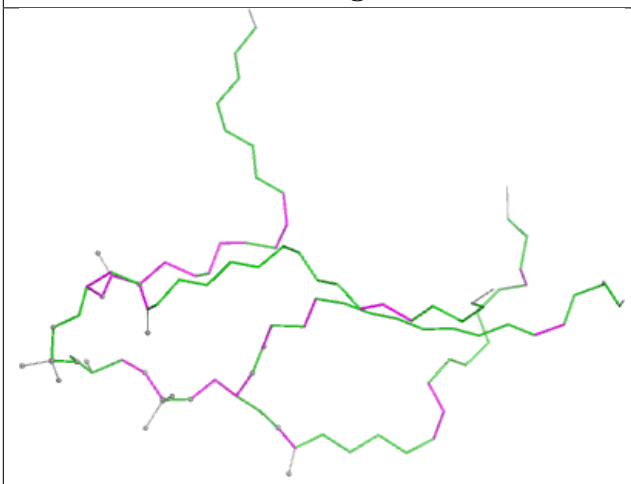
Bond lengths	 Bond angles
 Torsions	Rings

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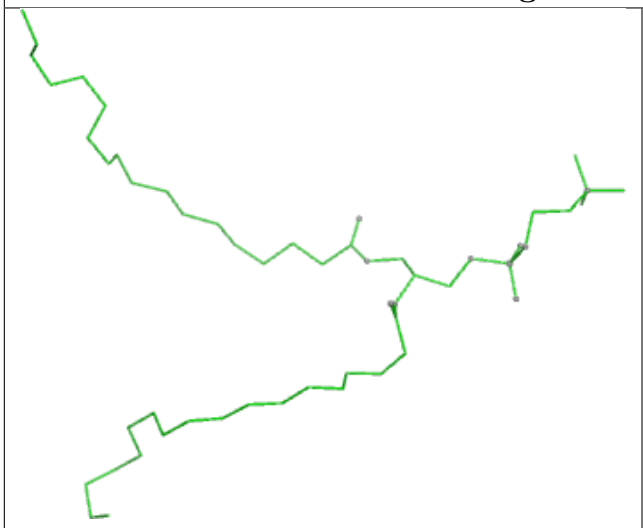
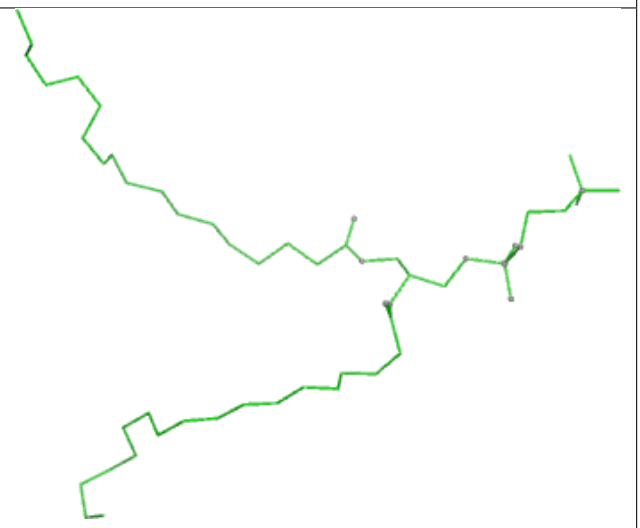
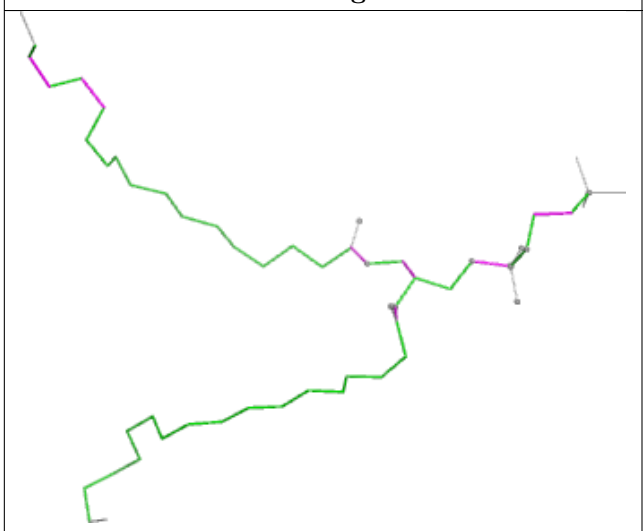
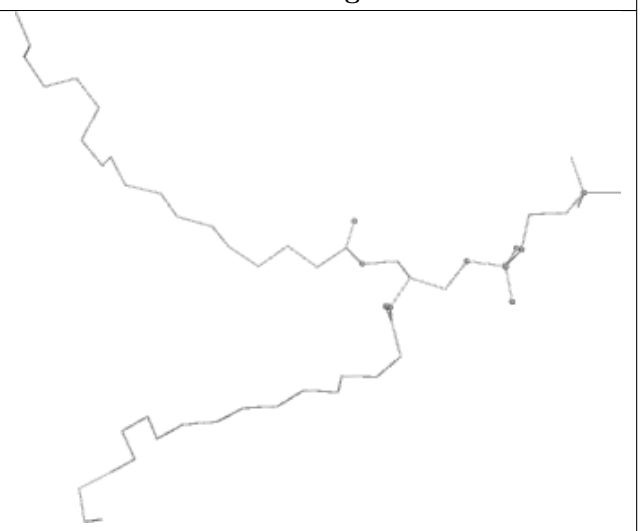
 Bond lengths	 Bond angles
 Torsions	 Rings

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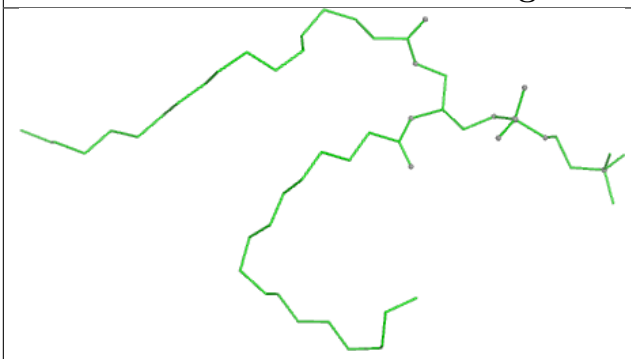
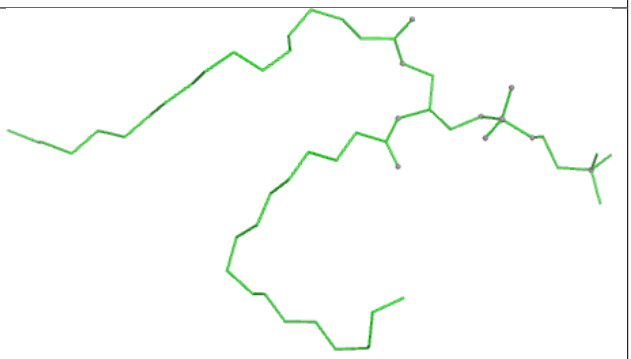
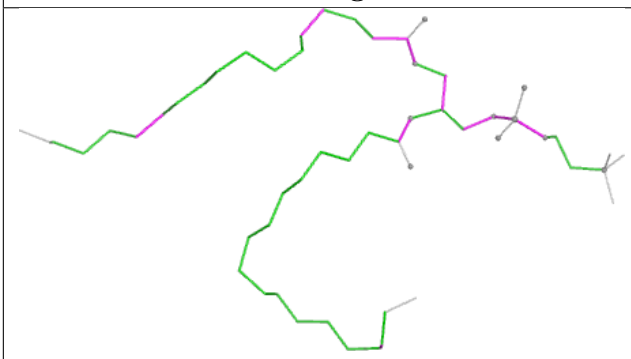
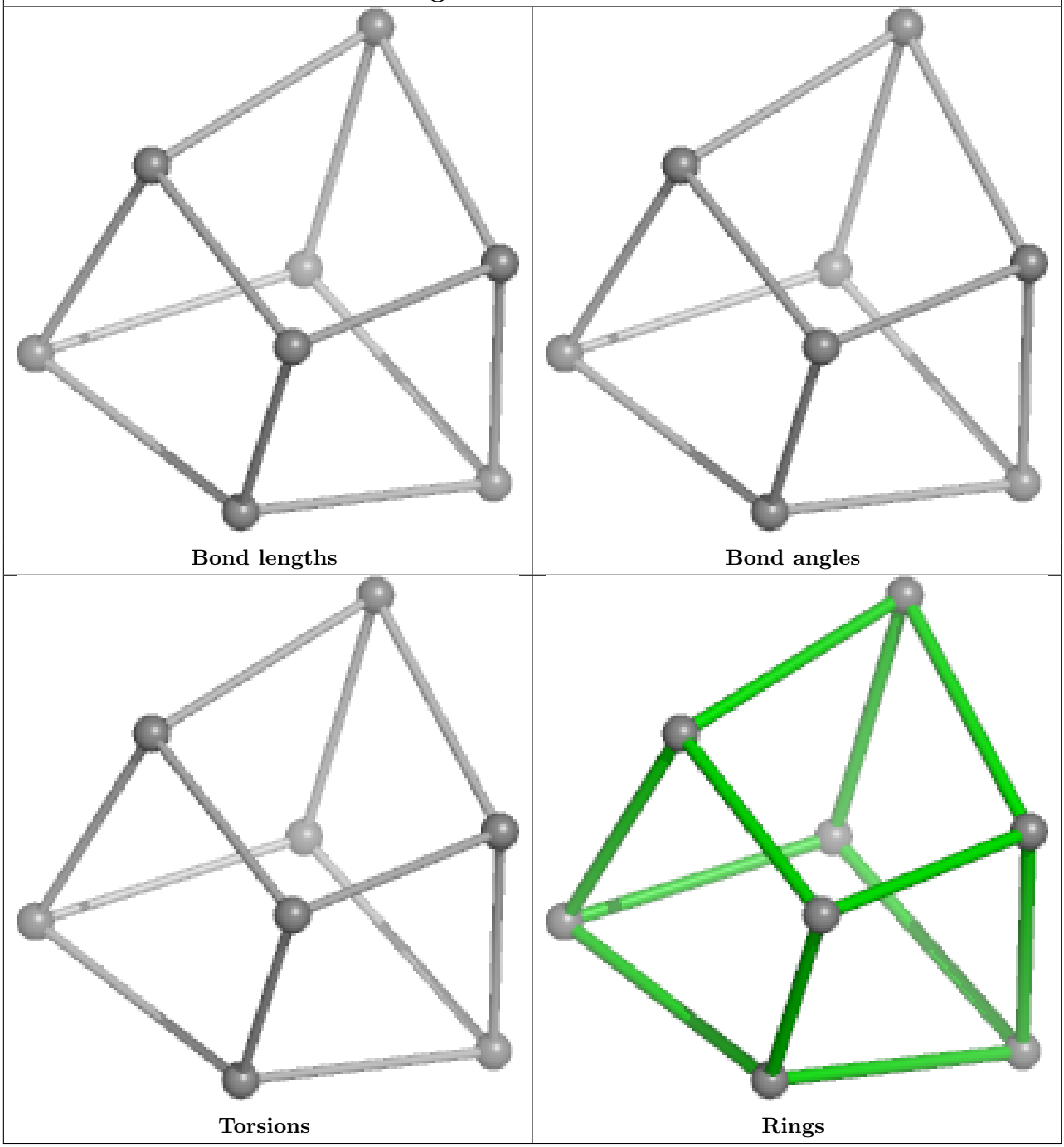
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand SF4 AB 802



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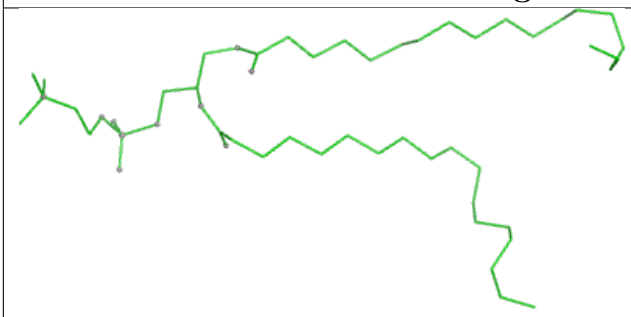
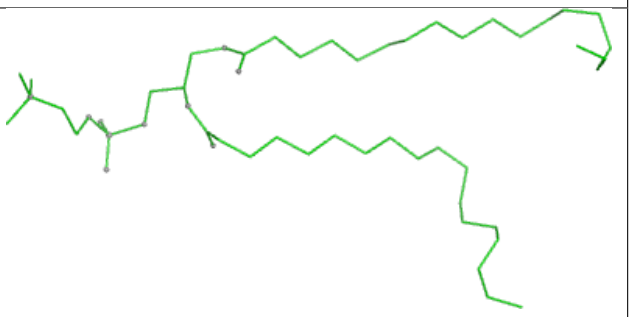
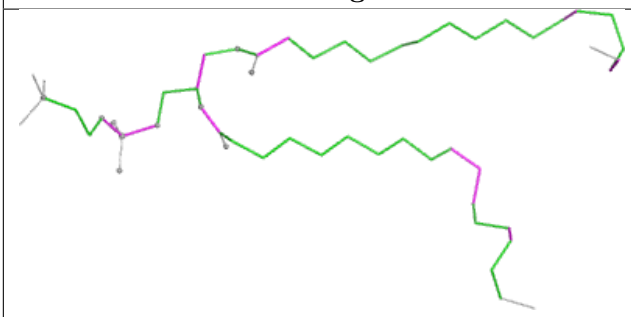
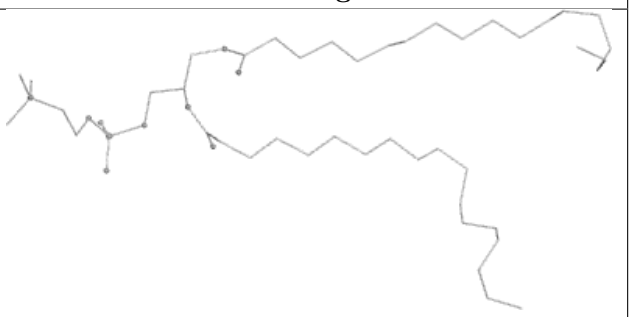
 Bond lengths	 Bond angles
 Torsions	 Rings

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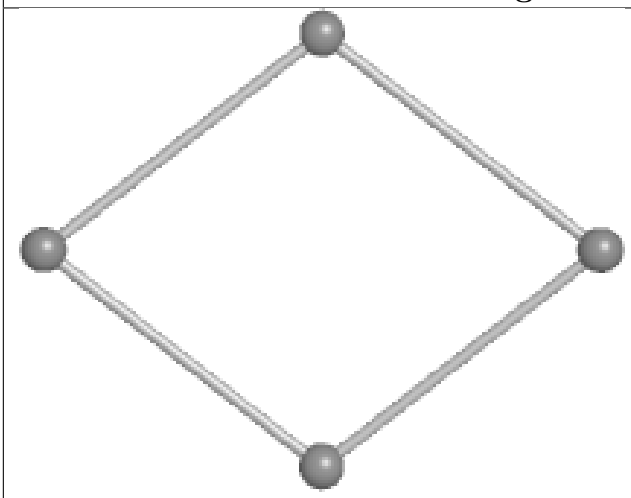
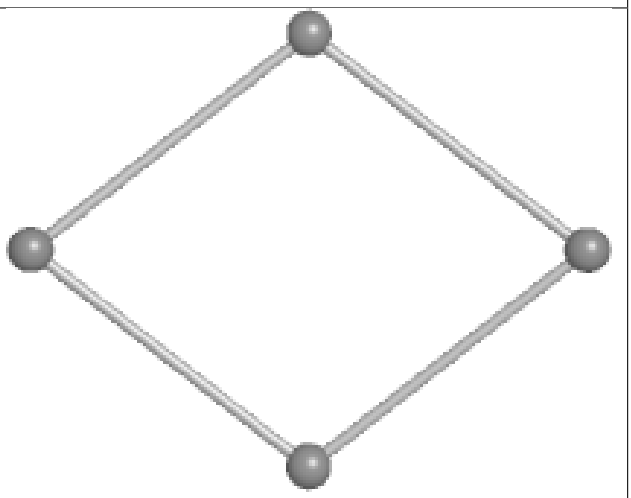
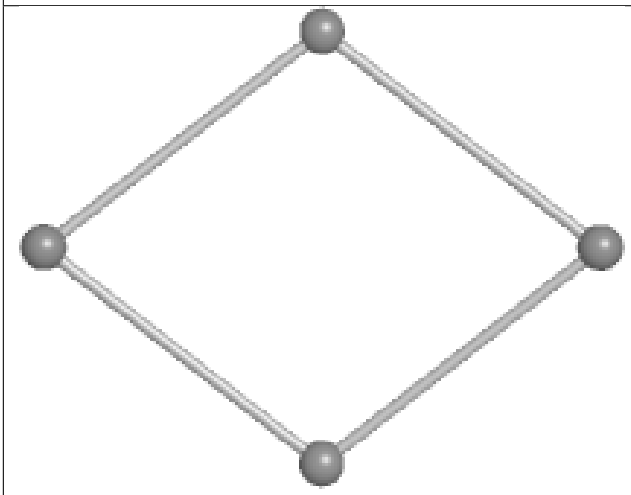


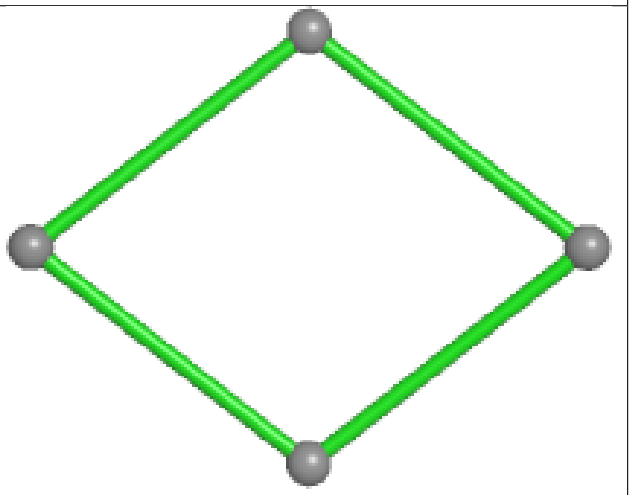
Bond lengths



Bond angles

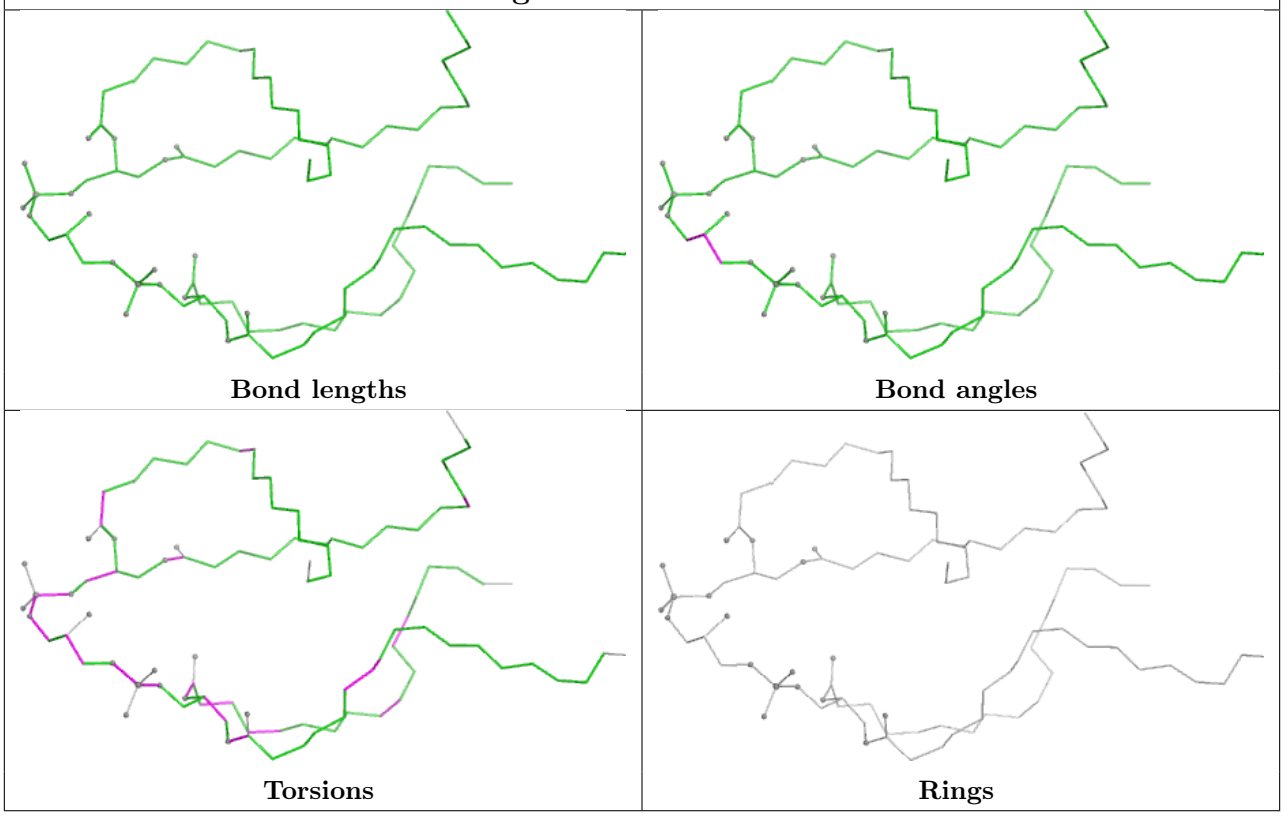


Torsions

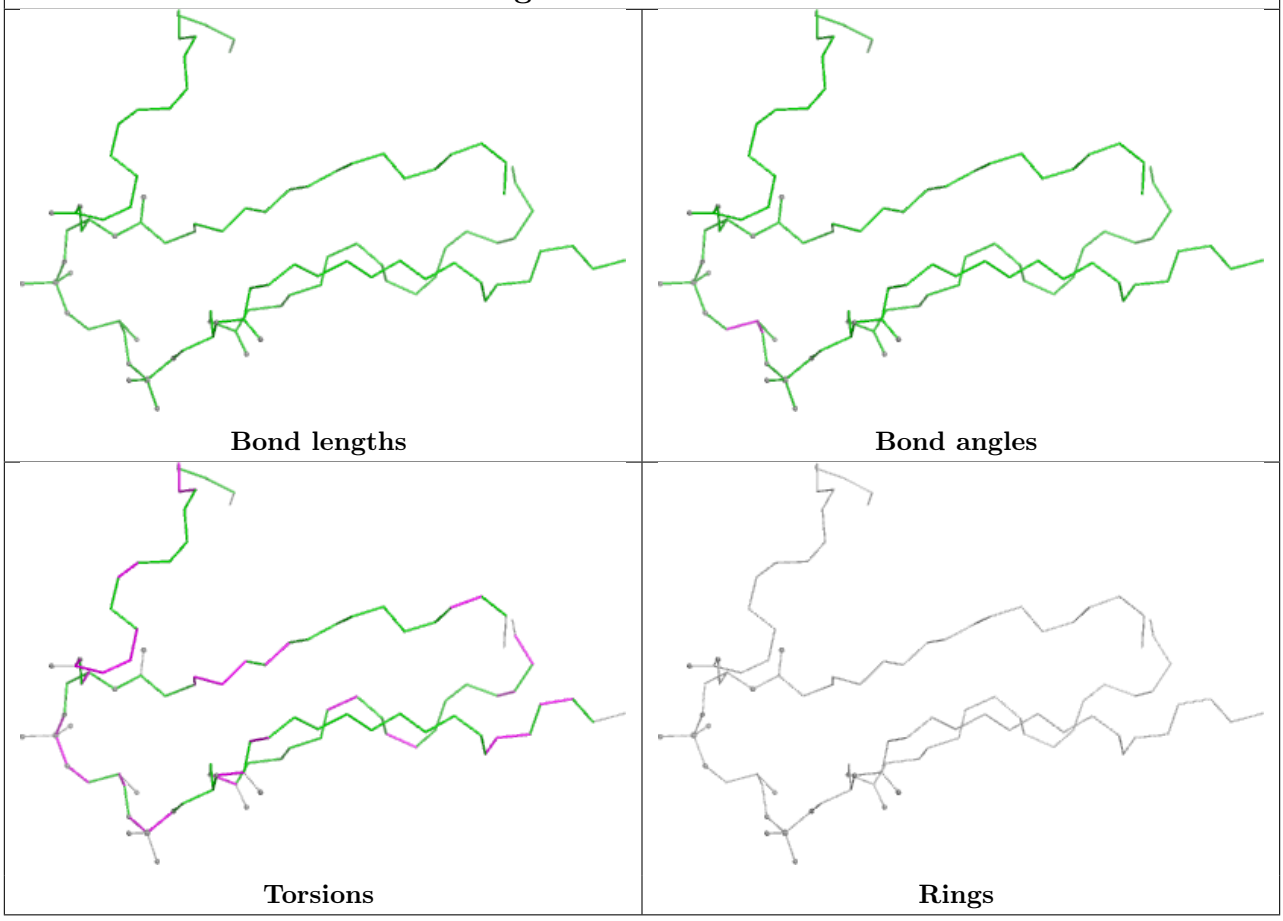


Rings

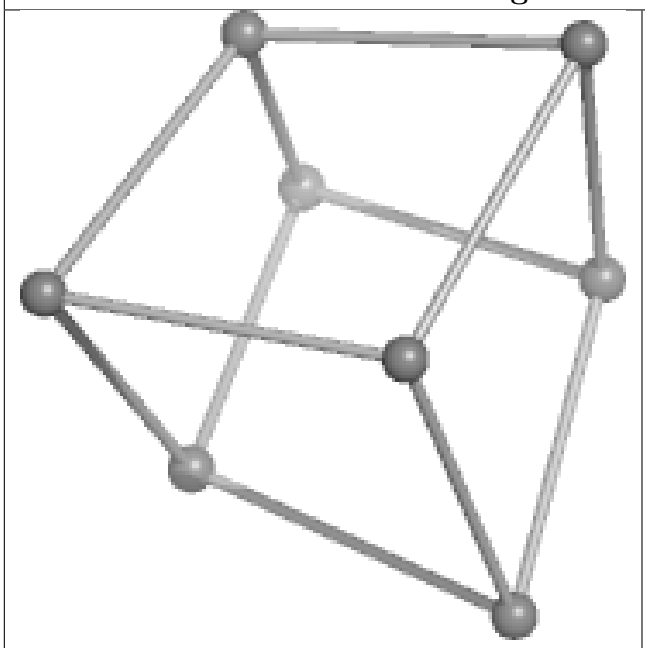
Ligand CDL ED 601



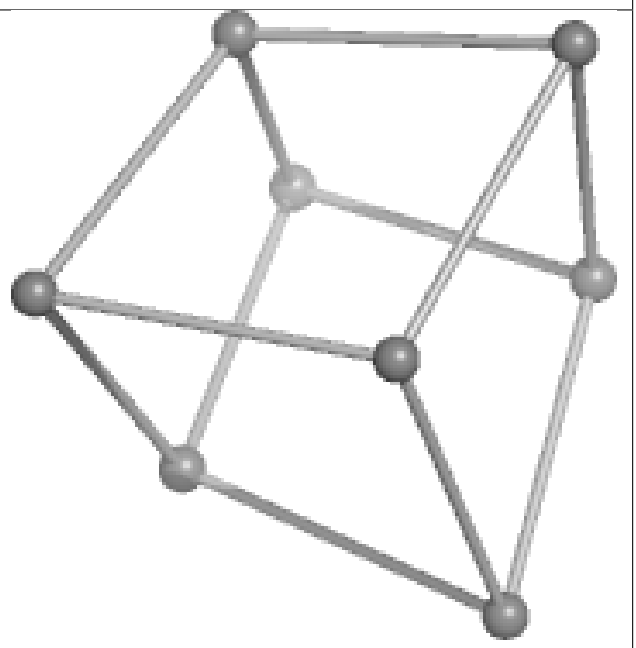
Ligand CDL Dh 202



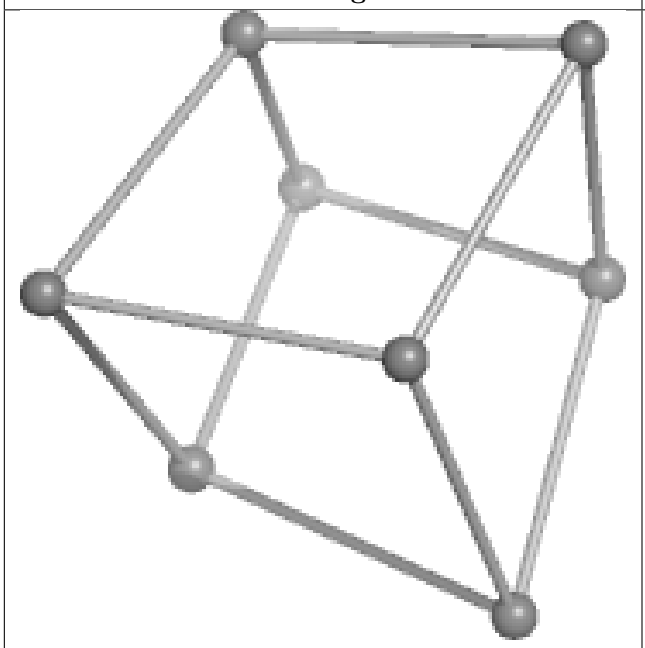
Ligand SF4 CB 1001



Bond lengths



Bond angles



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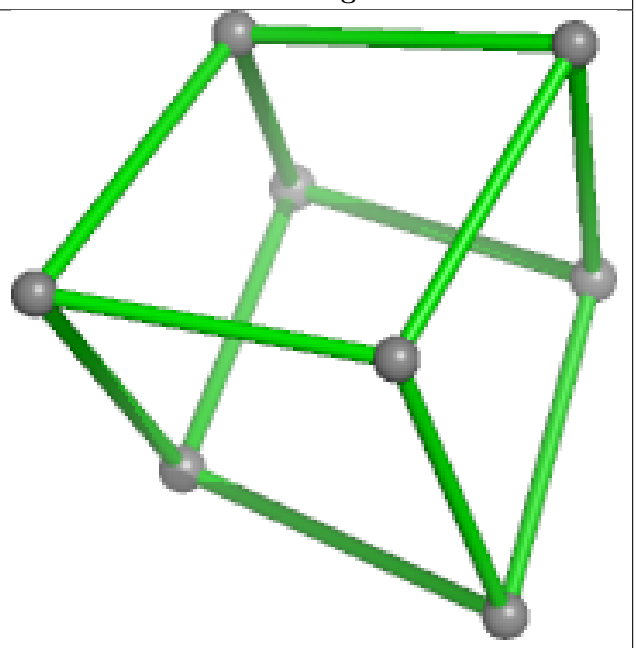
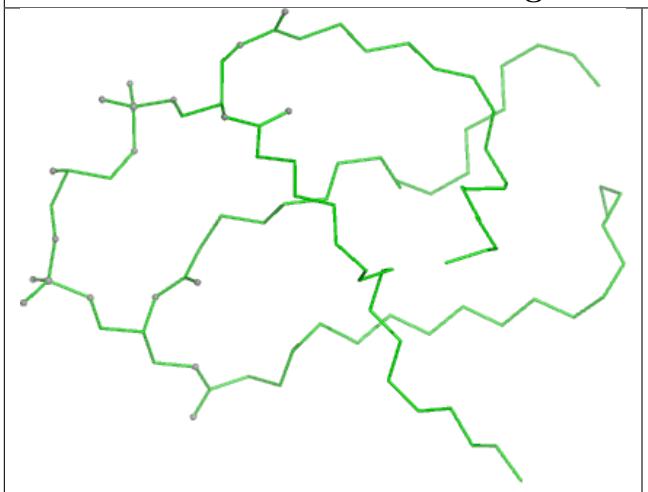


Rings

Ligand CDL C 504



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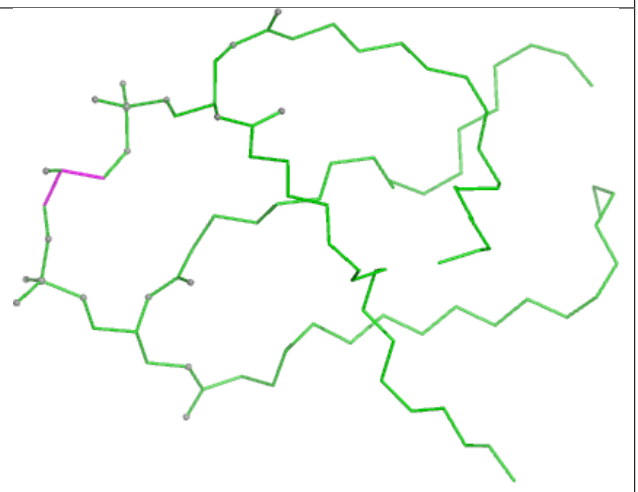
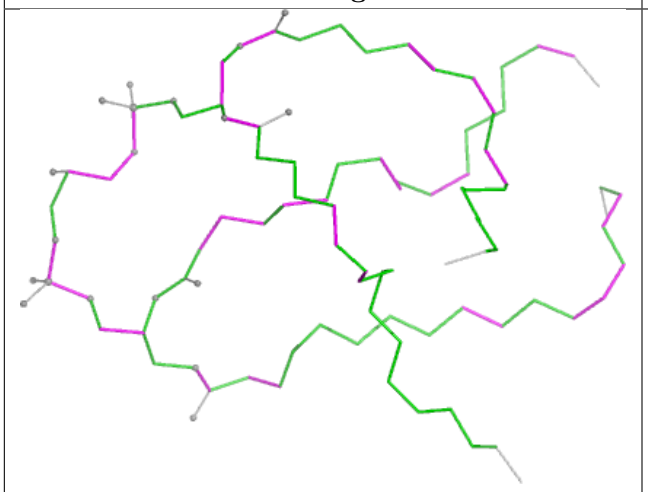


Bond angles



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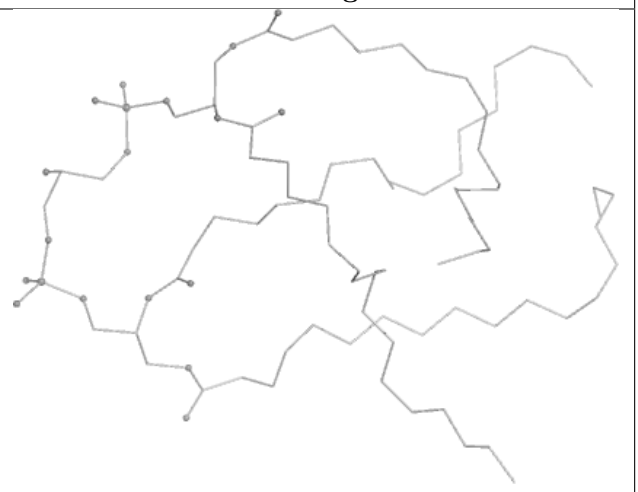
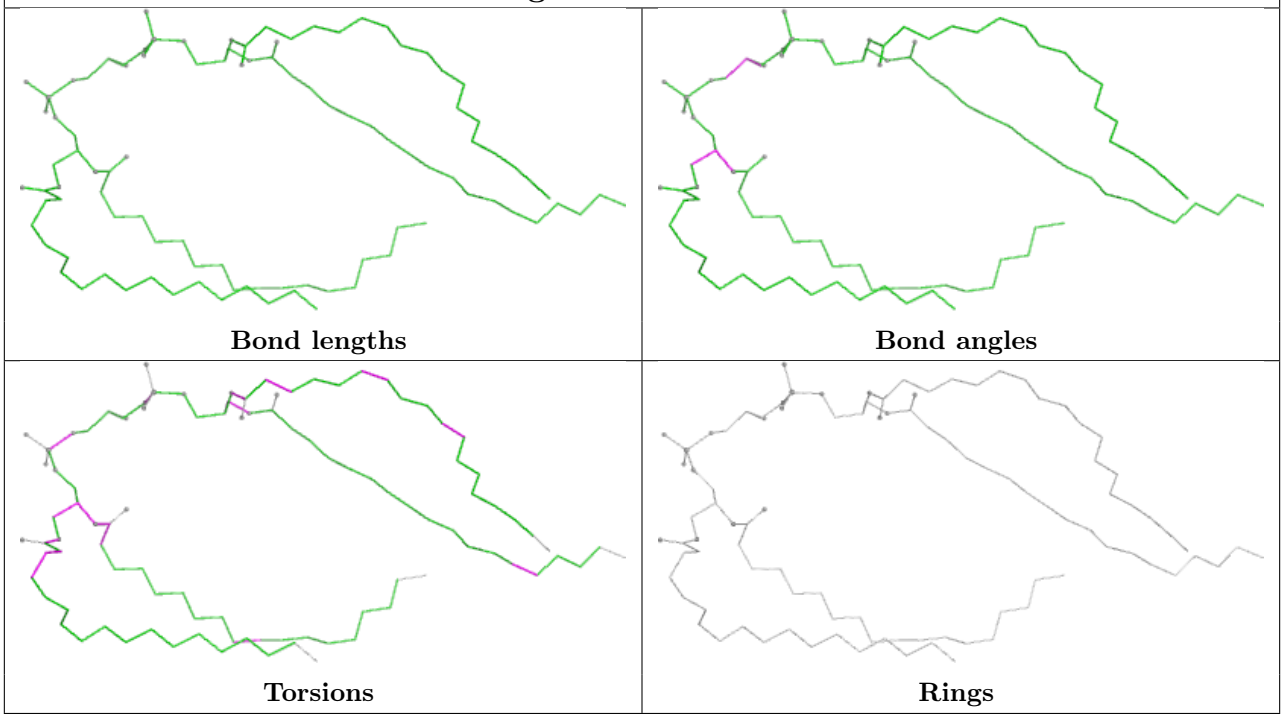
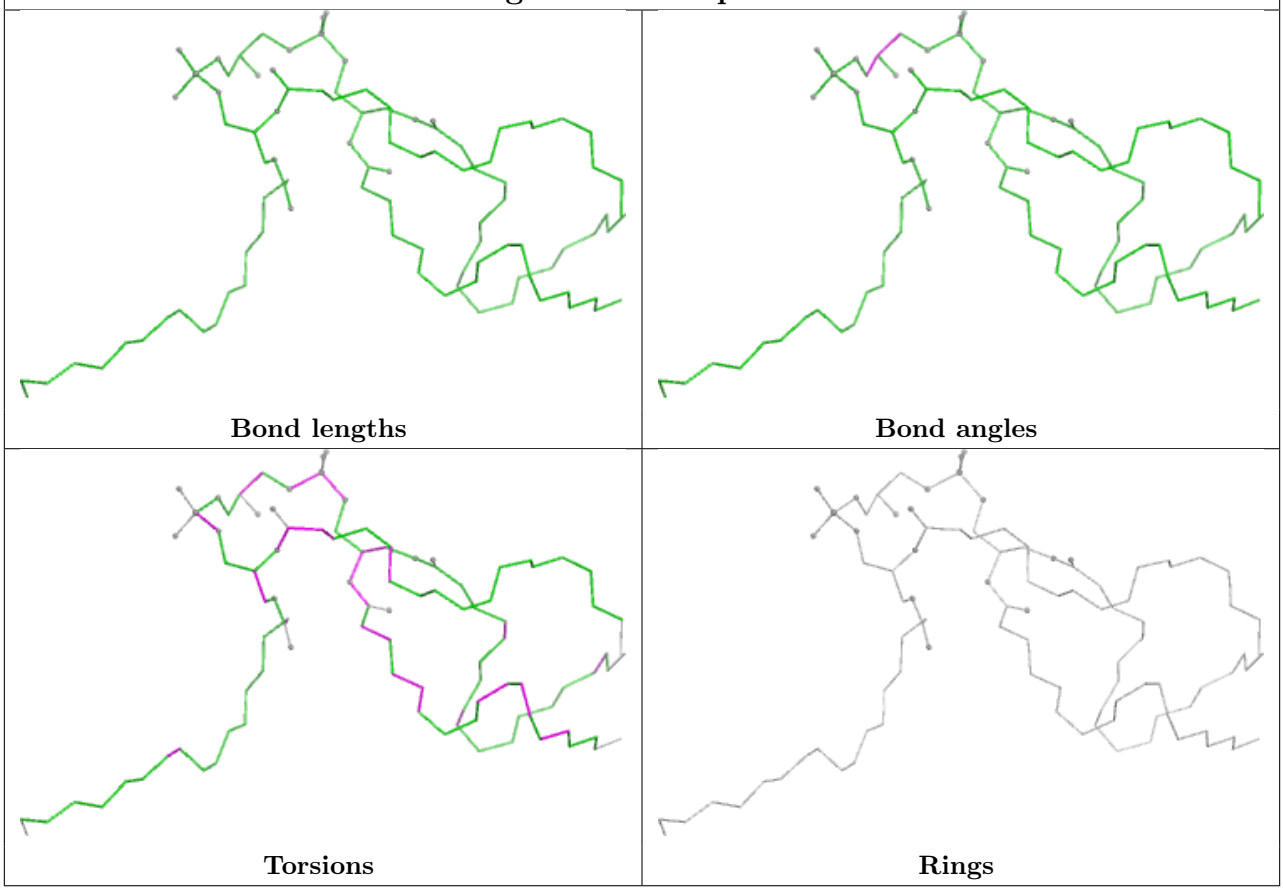


Rings

Ligand CDL h 501



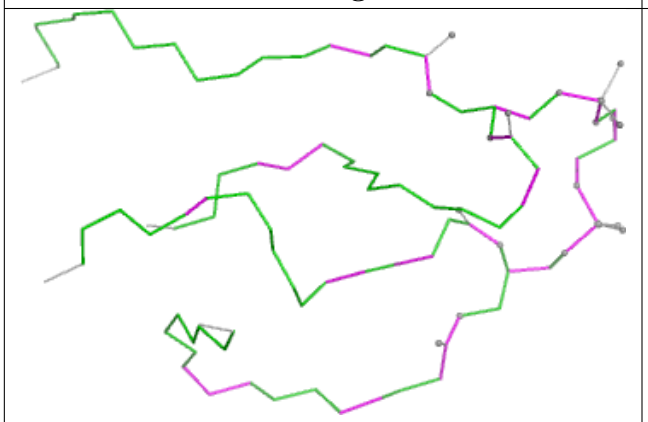
Ligand CDL Dq 1402



Ligand CDL Du 401

Bond lengths

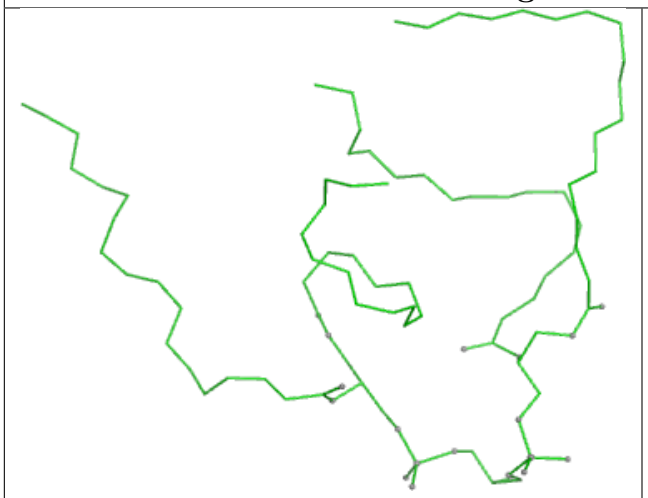
Bond angles



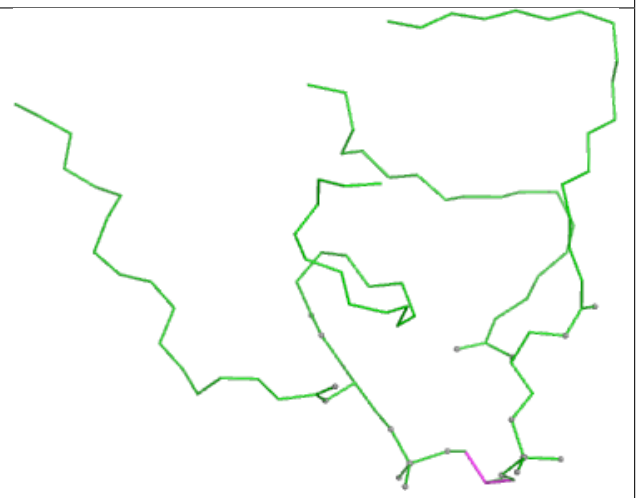
Torsions

Rings

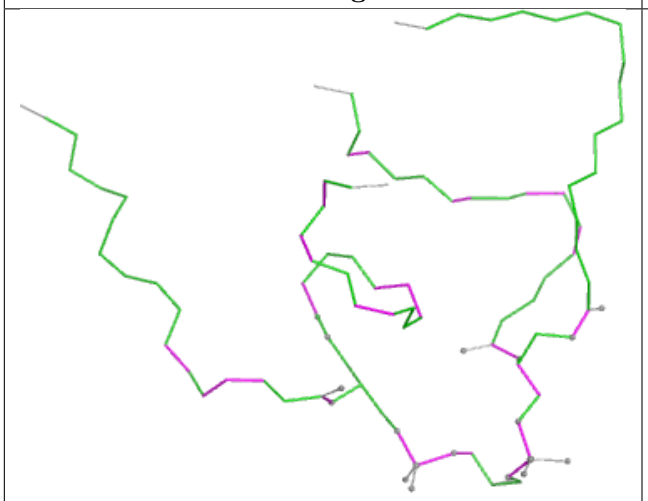
Ligand CDL Ds 406



Bond lengths



Bond angles



Torsions

Rings

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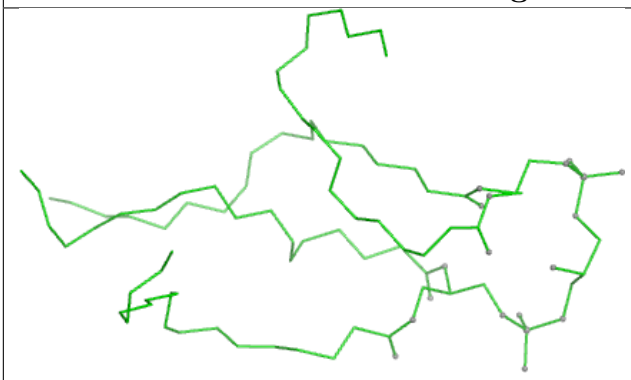
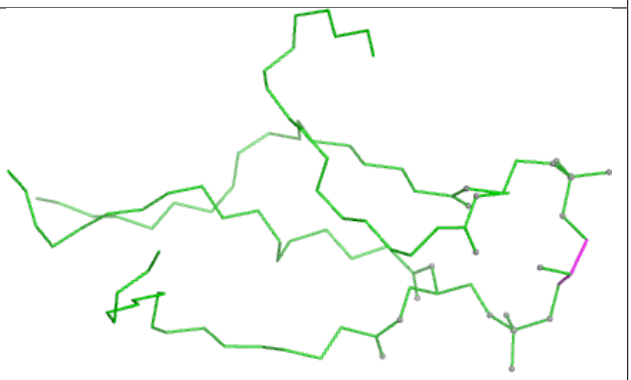
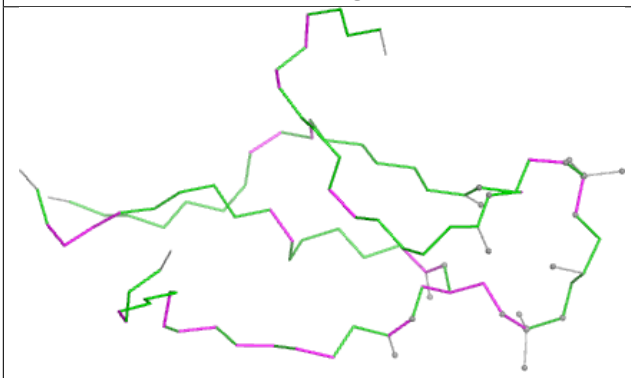
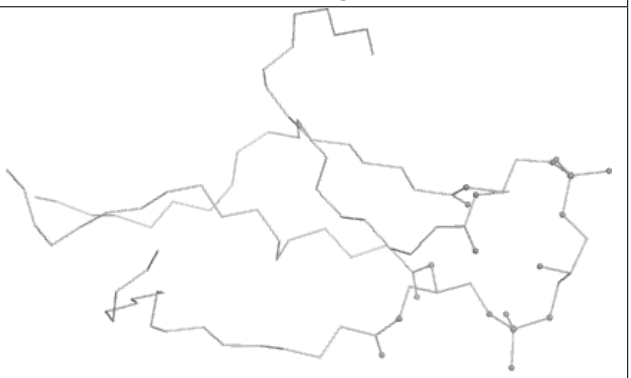
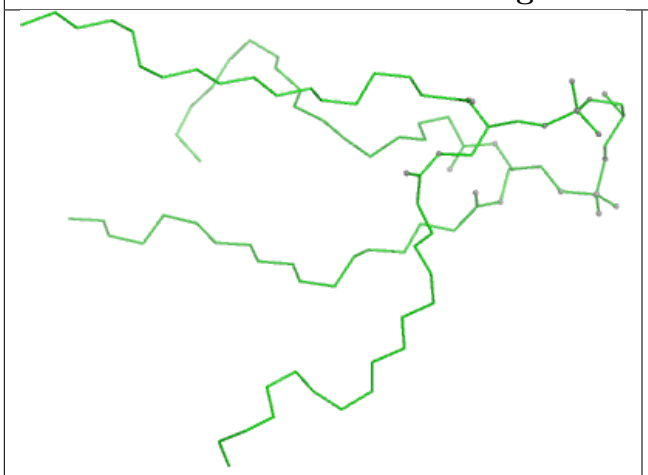
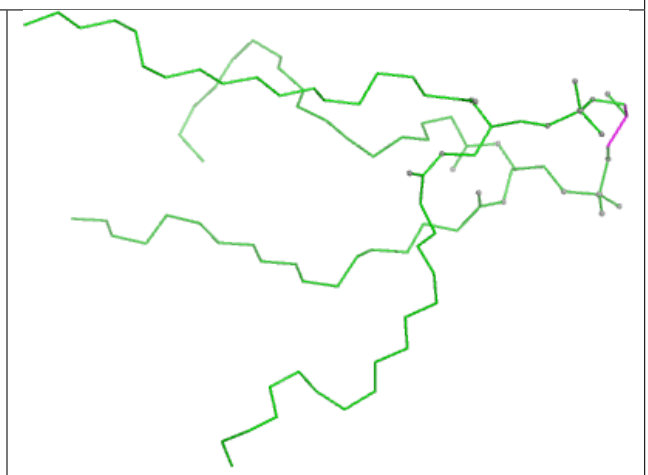
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Dc 601



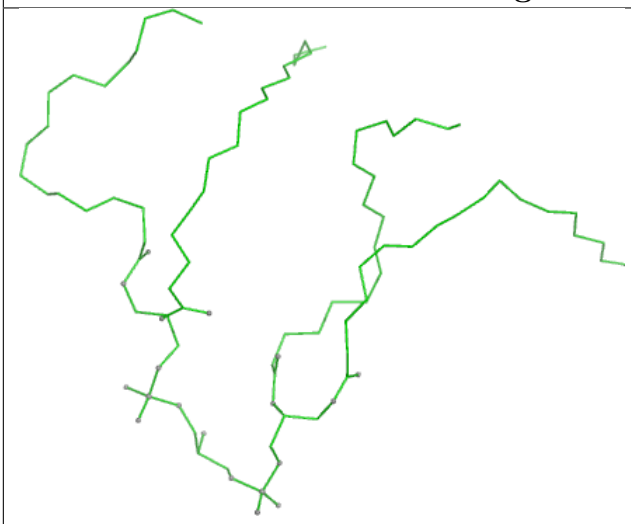
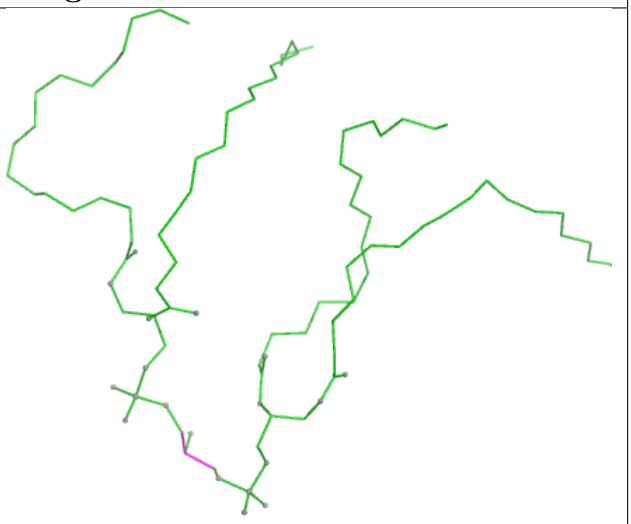
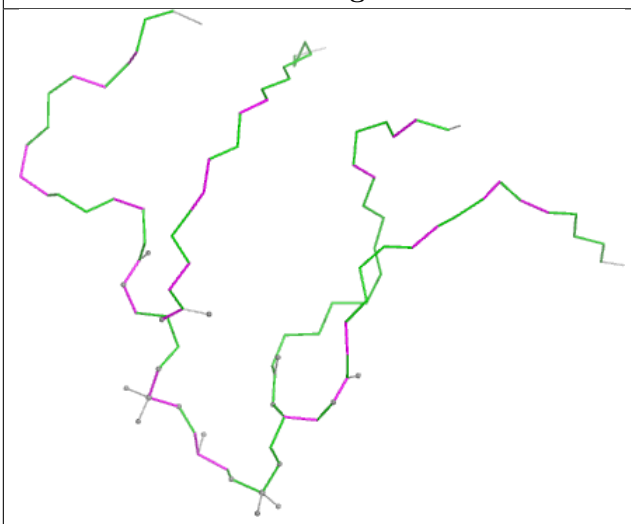
Bond lengths



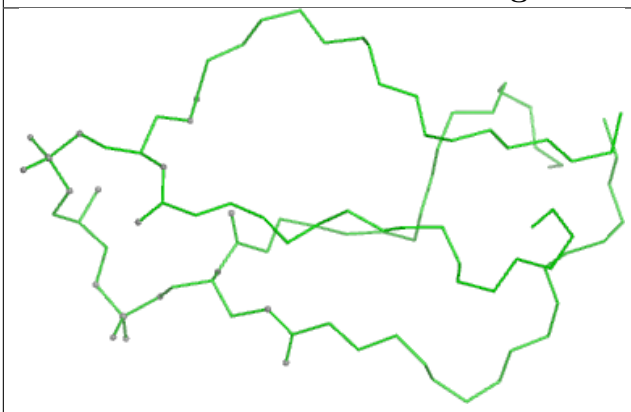
Bond angles

Torsions

Rings

Ligand CDL Dg 202	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL DX 301



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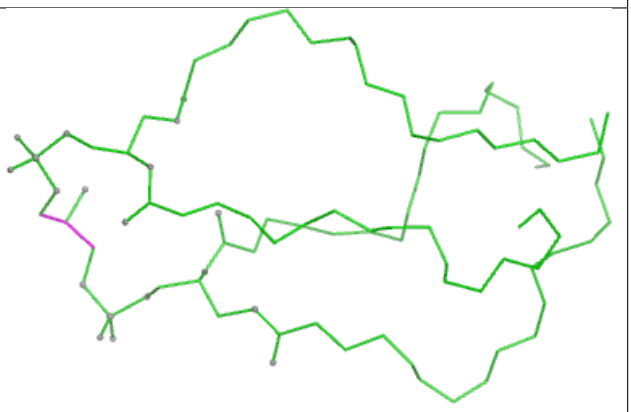

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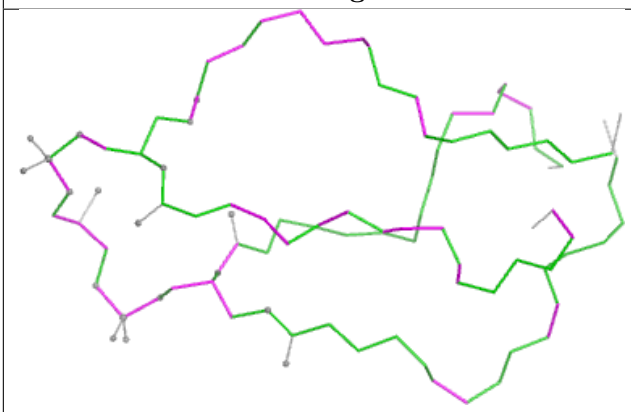

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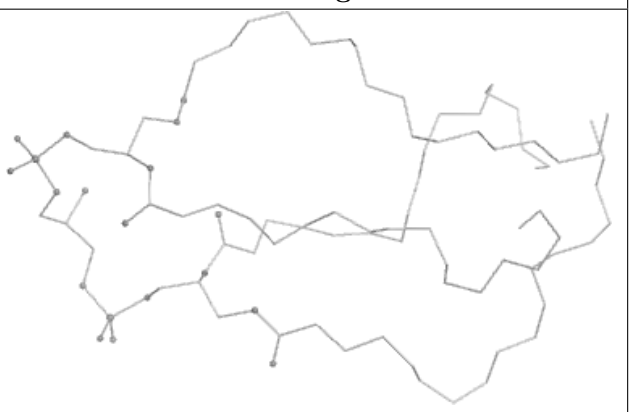

Rings

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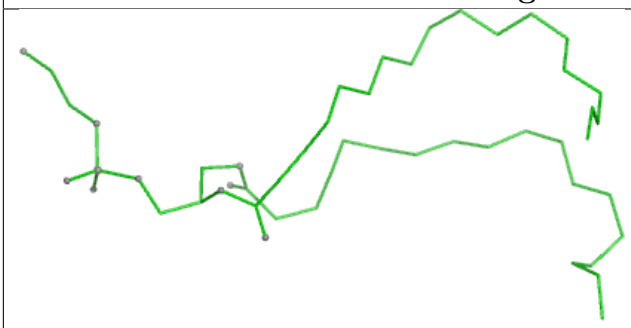

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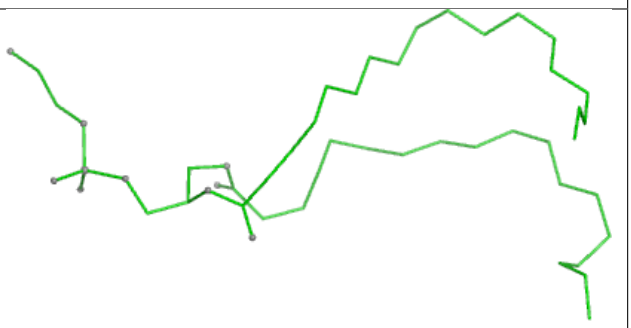

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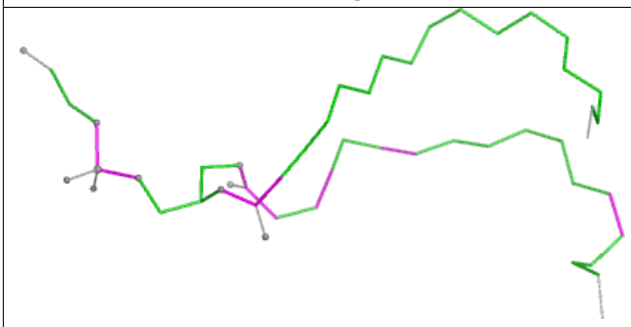
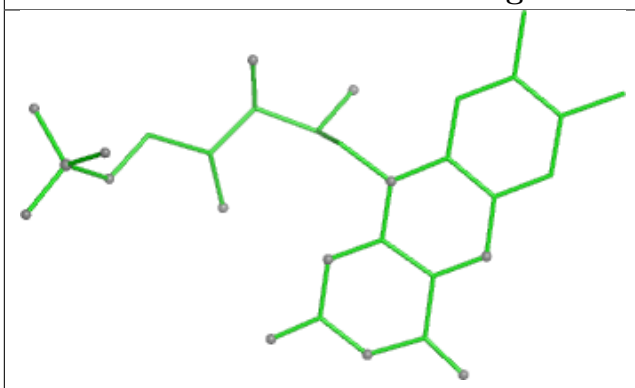
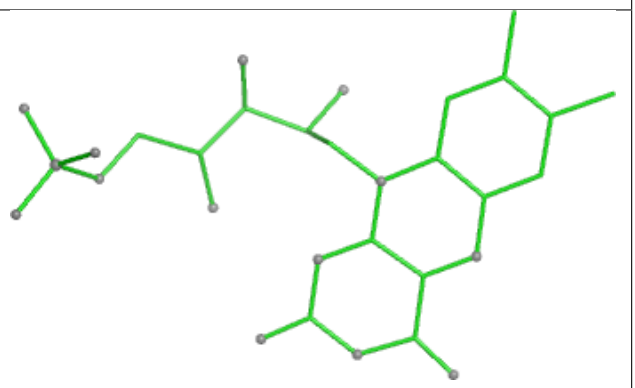
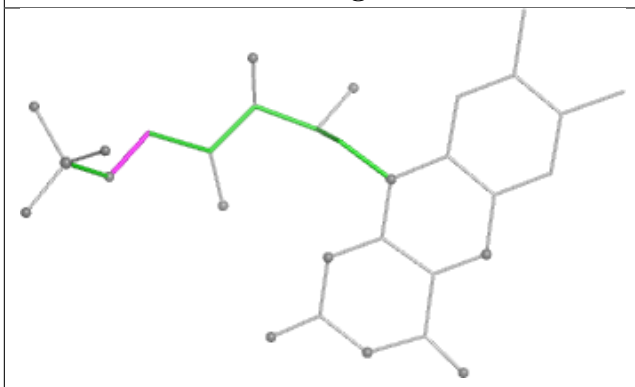
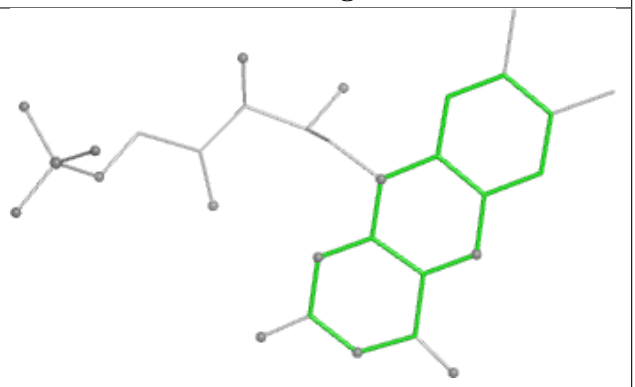
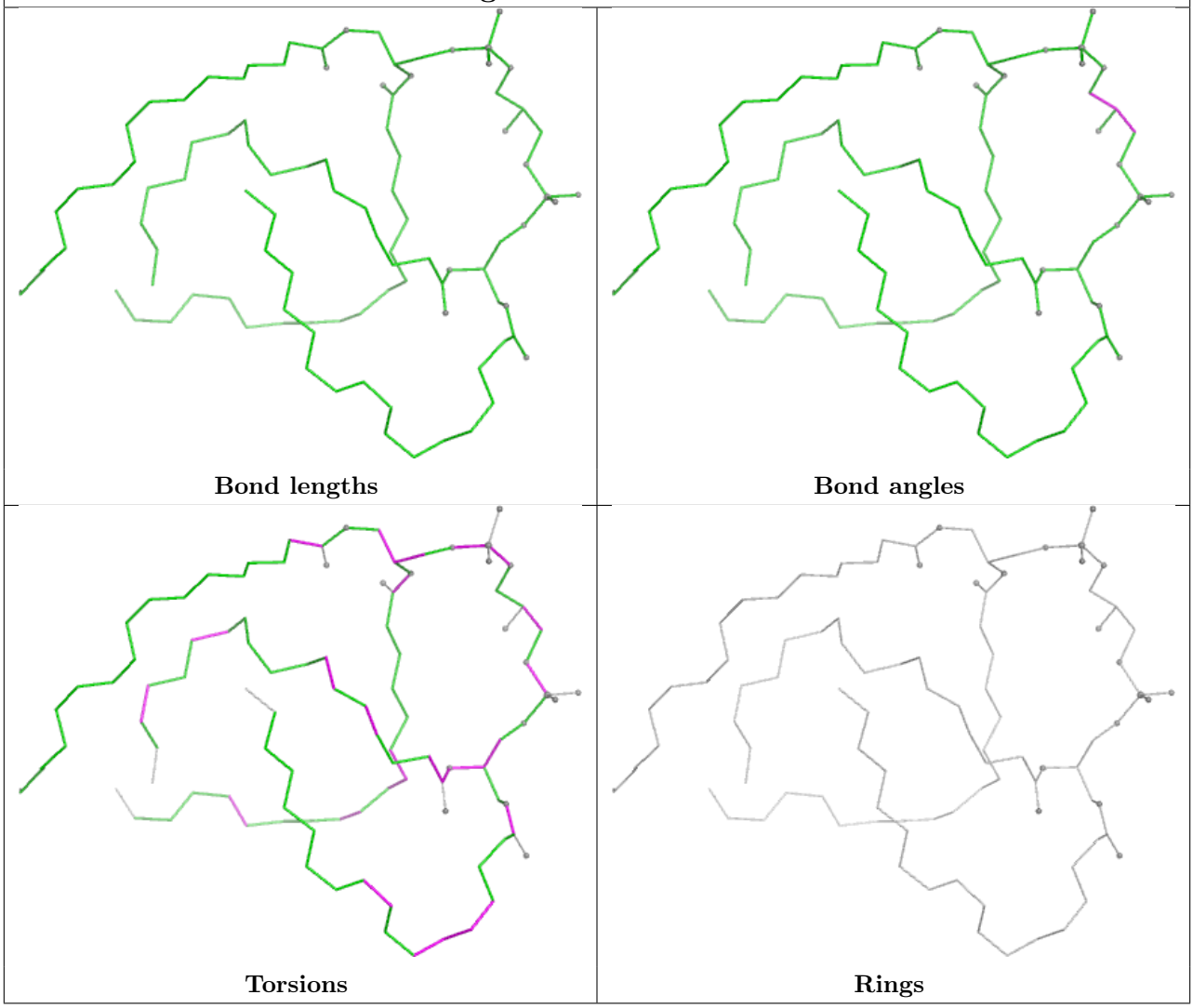


Torsions

Rings

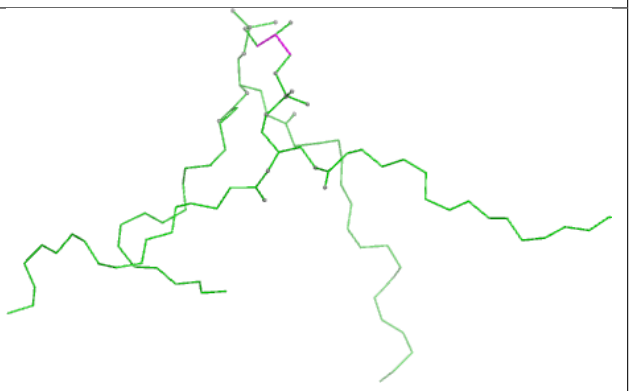
Ligand FMN AD 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Eb 302

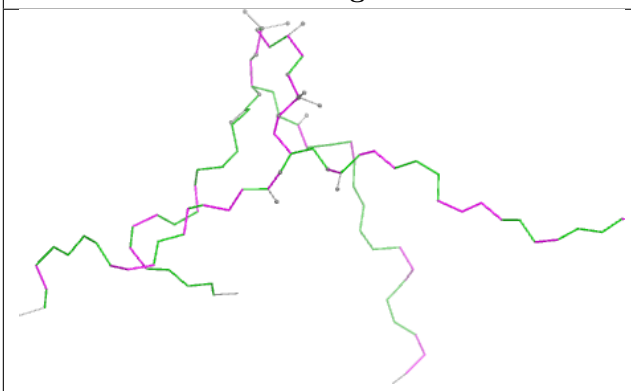


Ligand CDL ES 1101

Bond lengths



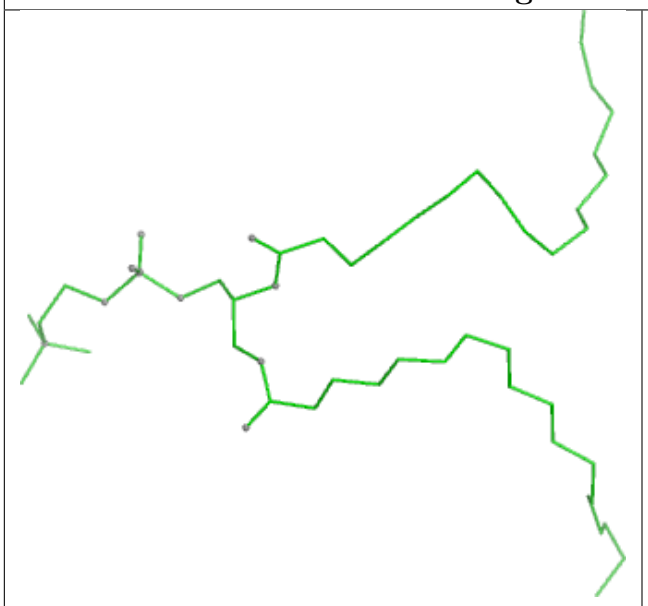
Bond angles



Torsions

Rings

Ligand PC1 AC 804



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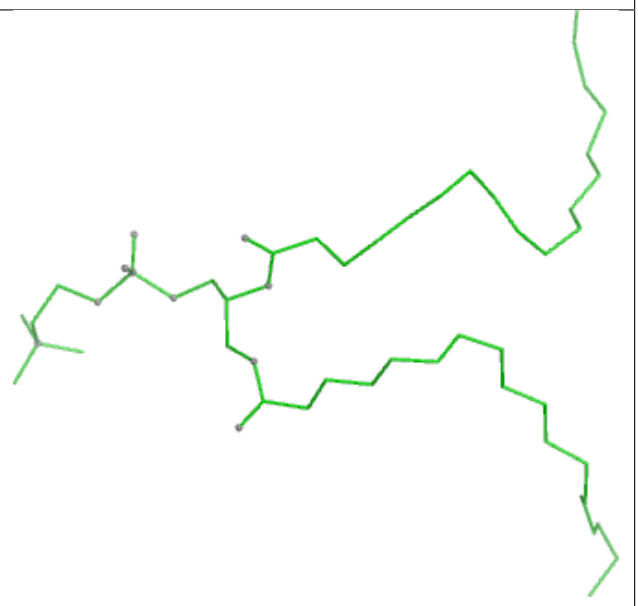

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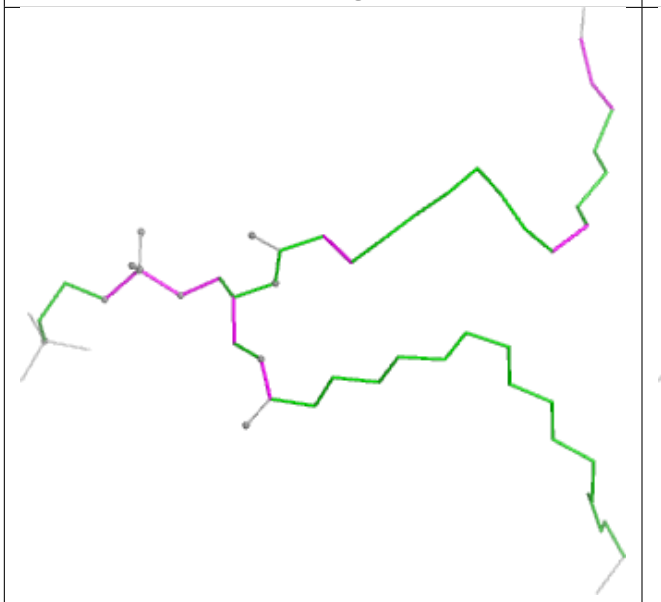

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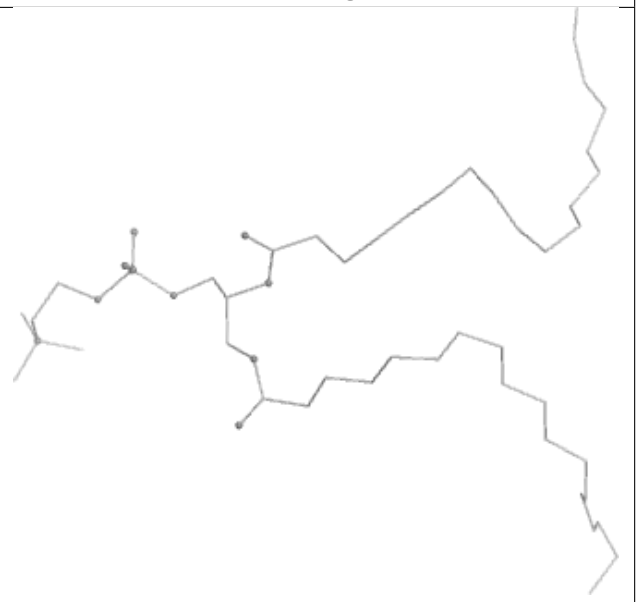
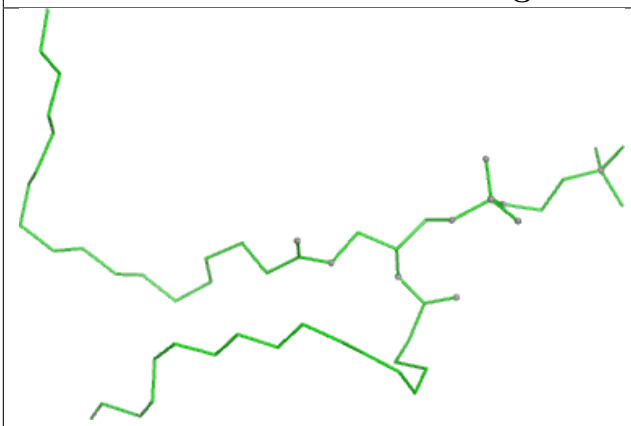
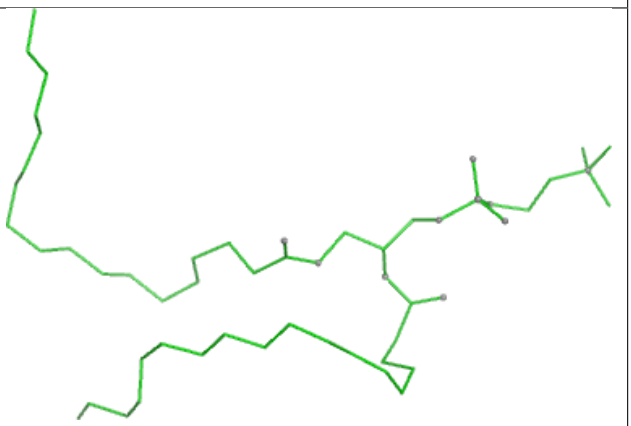
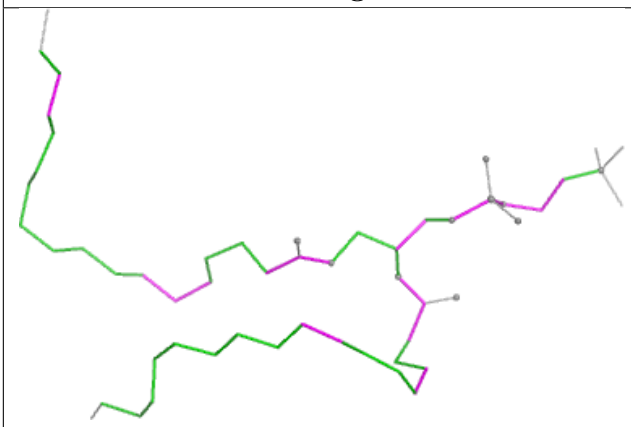
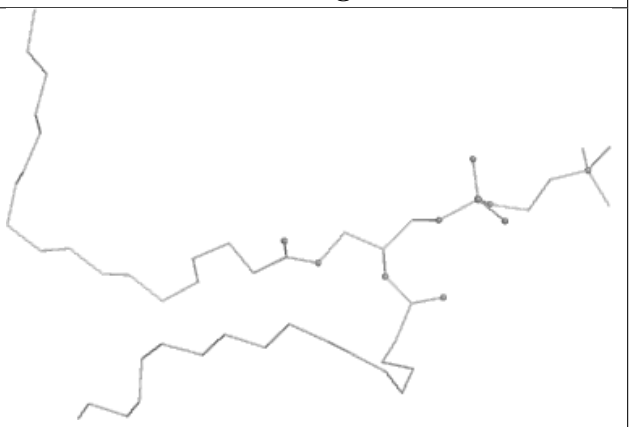
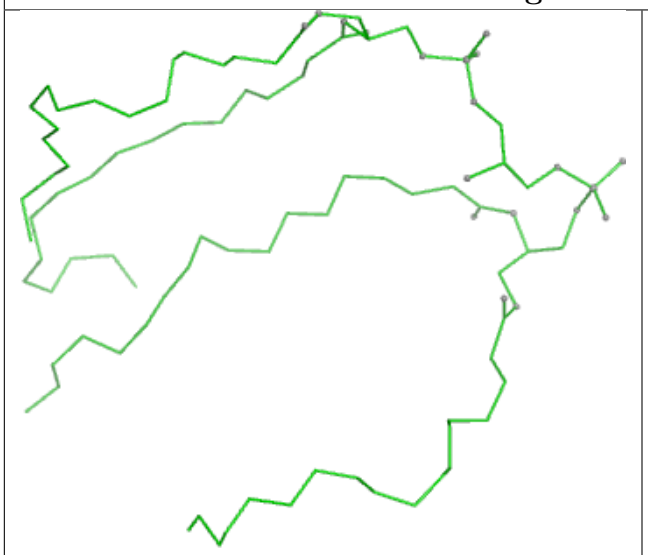


Rings

Ligand PC1 BG 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL C 505



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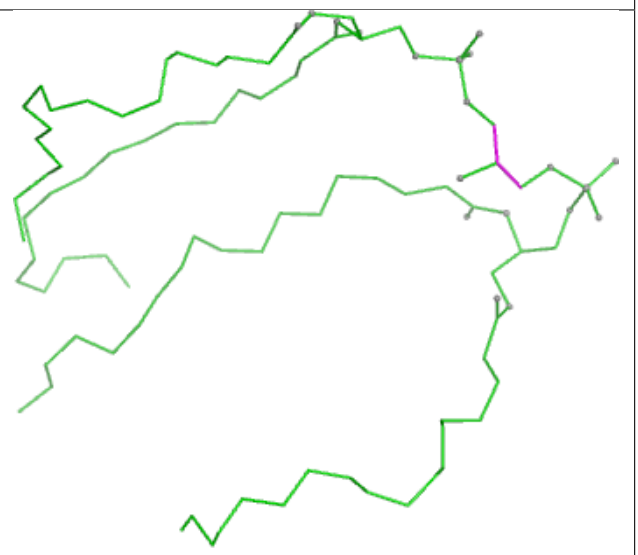

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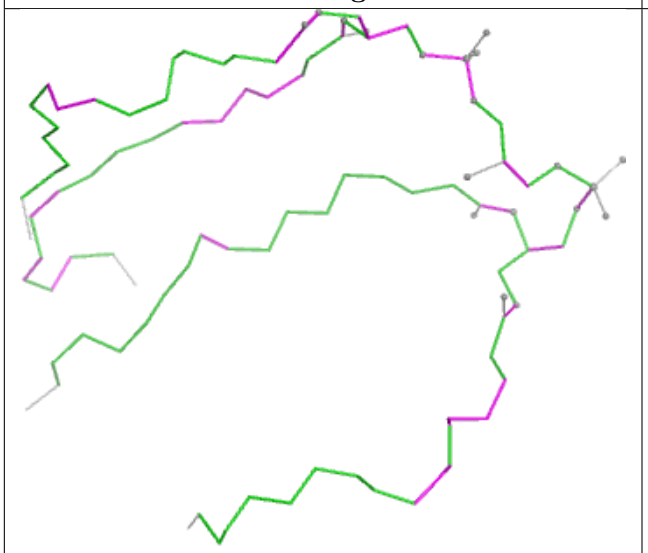
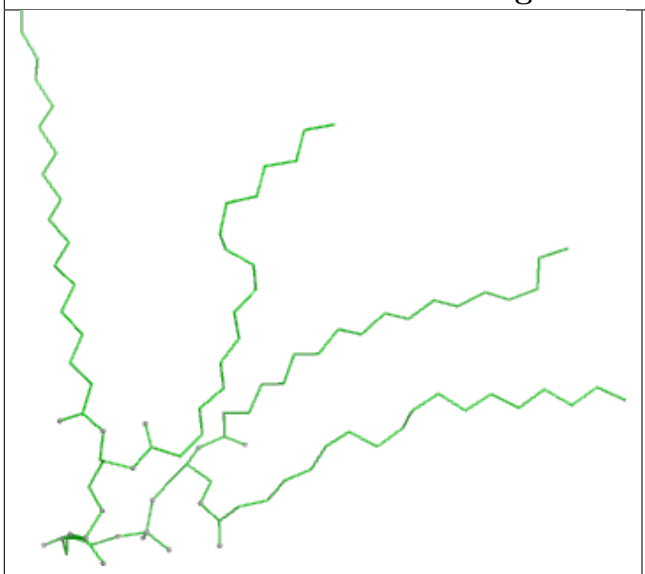


Torsions

Rings

Ligand CDL H 1302



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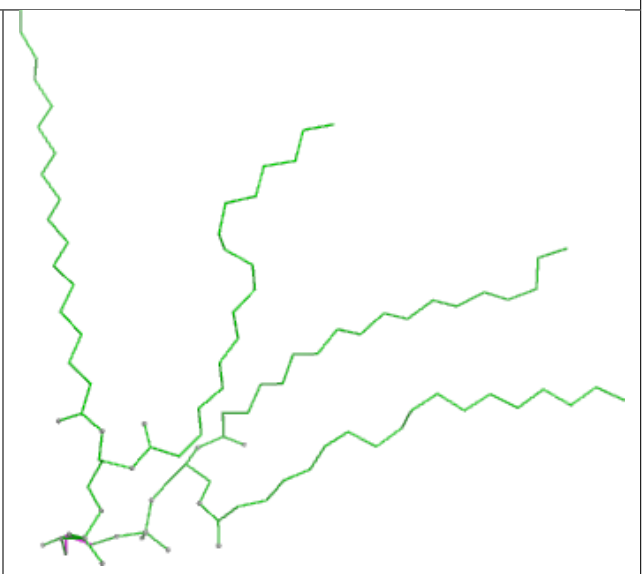
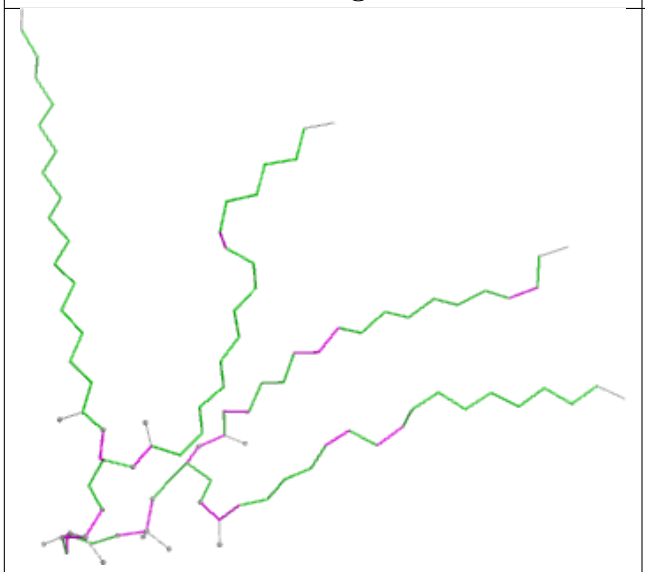
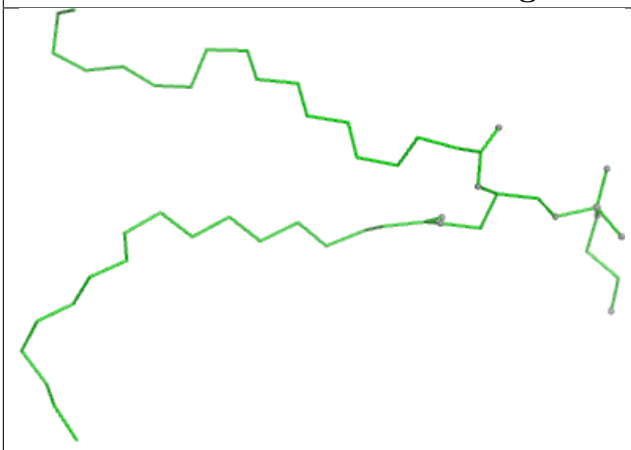
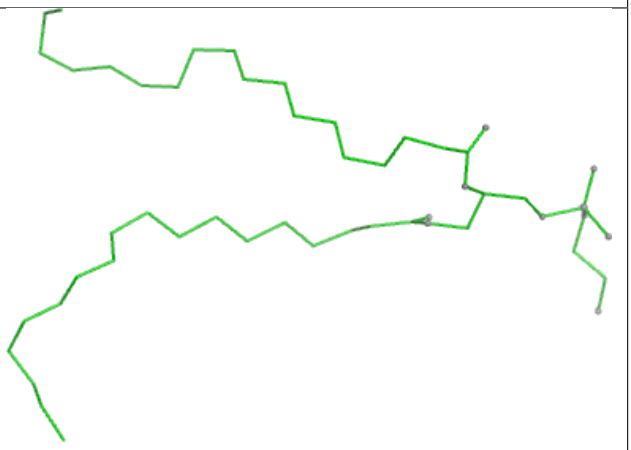
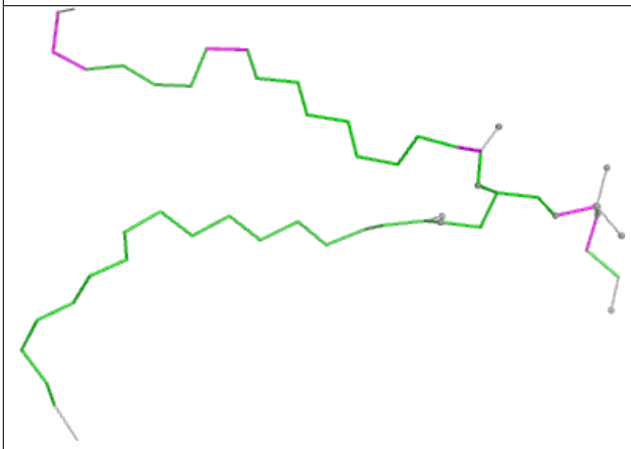
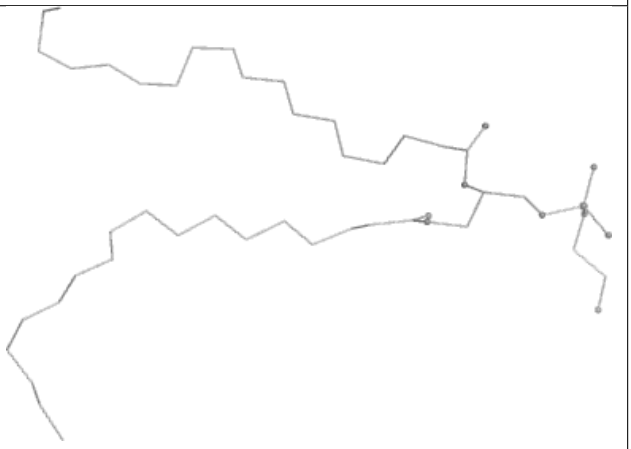


Bond angles

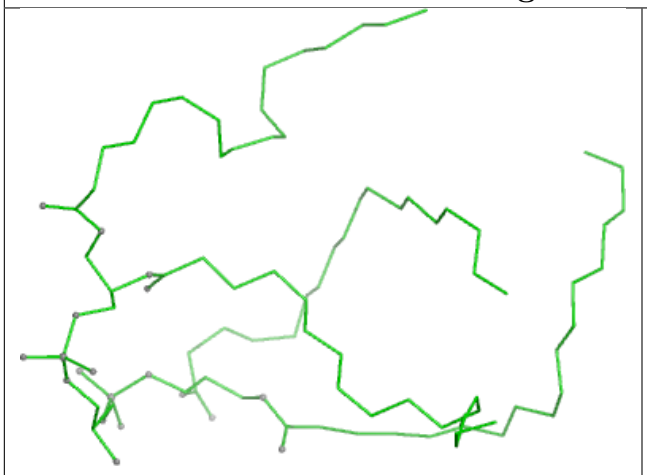


Torsions

Rings

Ligand 3PE A9 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Ea 502



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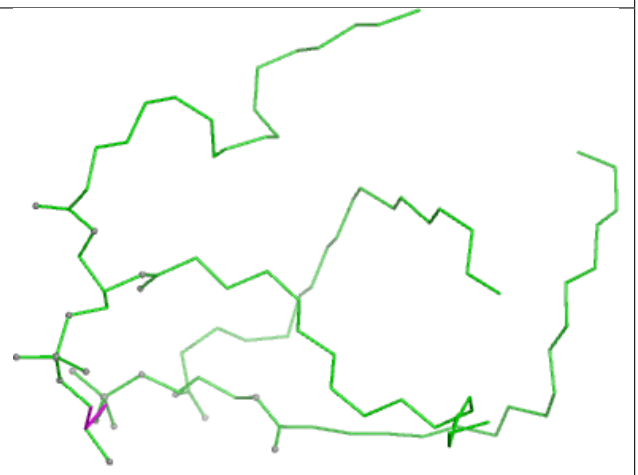
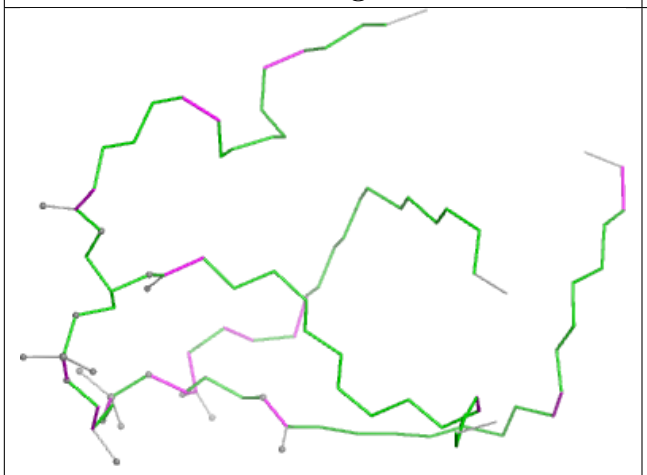


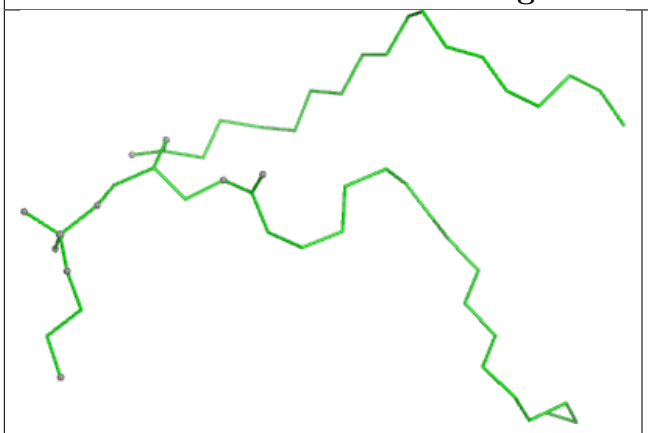
Bond angles



Torsions

Rings

Ligand 3PE BT 201



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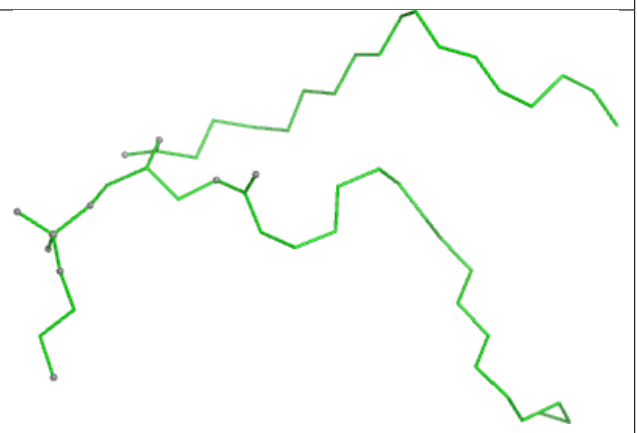
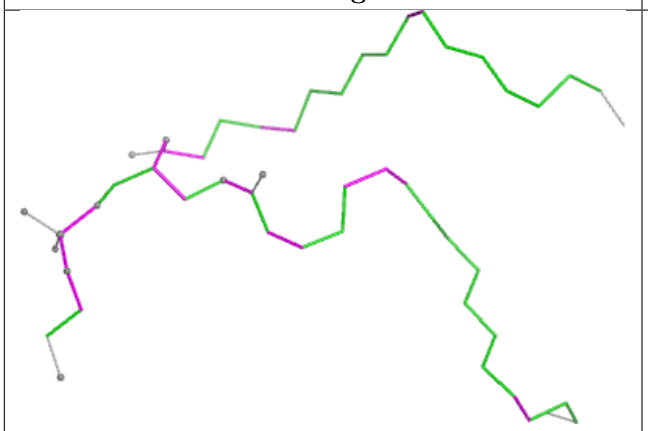


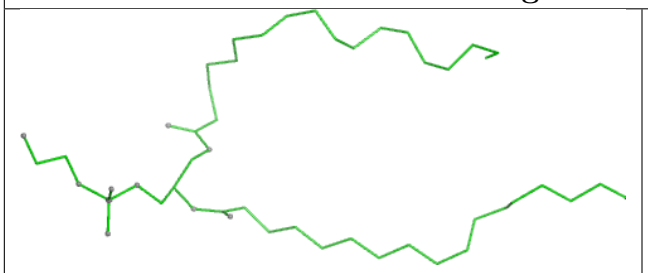
Bond angles



Torsions

Rings

Ligand 3PE Eo 203



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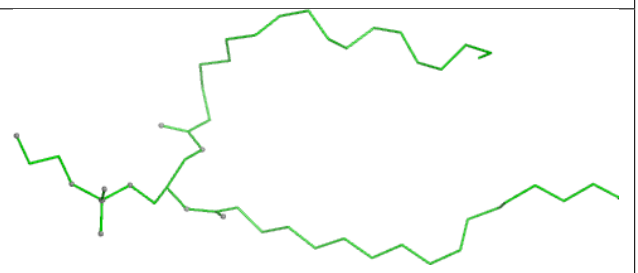

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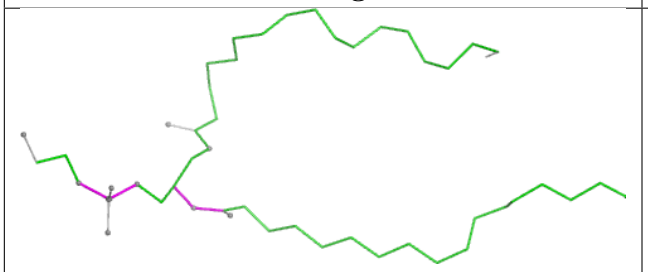

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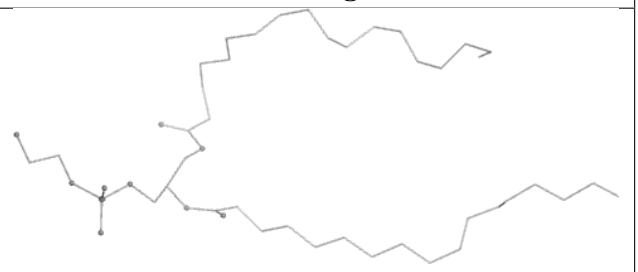
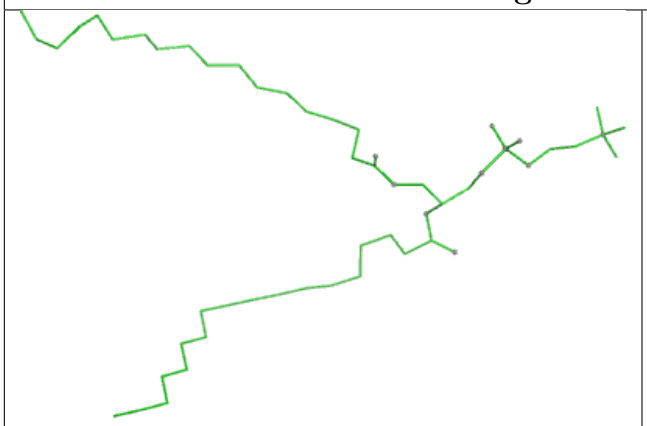


Rings

Ligand PC1 AU 202



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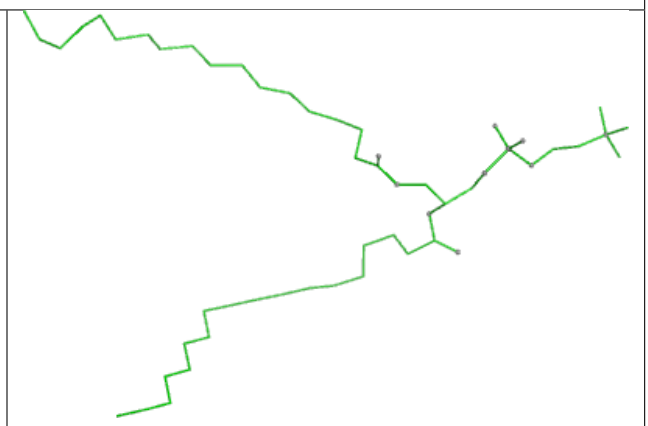
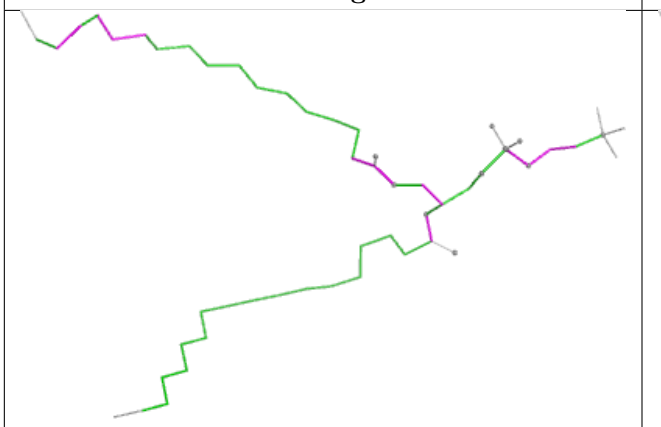
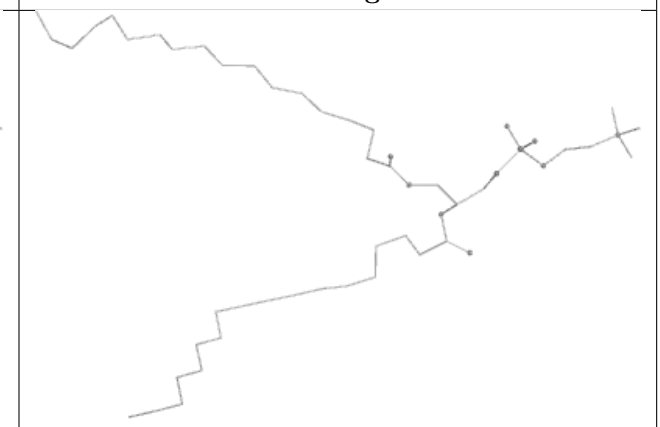


Bond angles

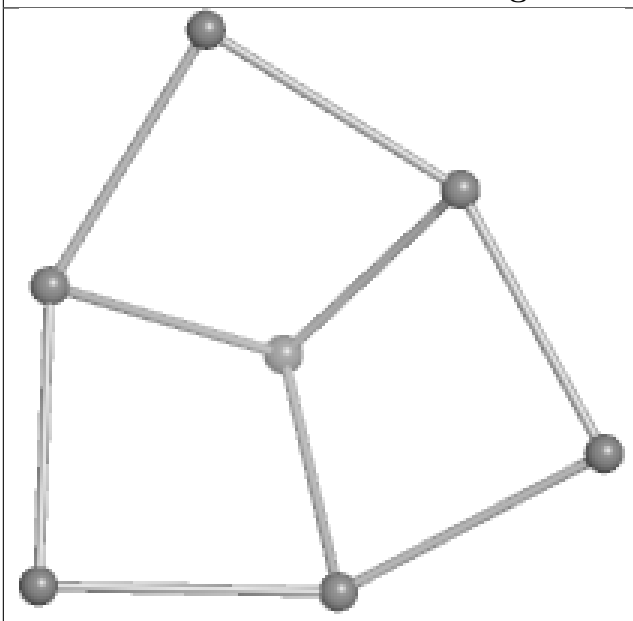


Torsions



Rings

Ligand F3S CB 1002



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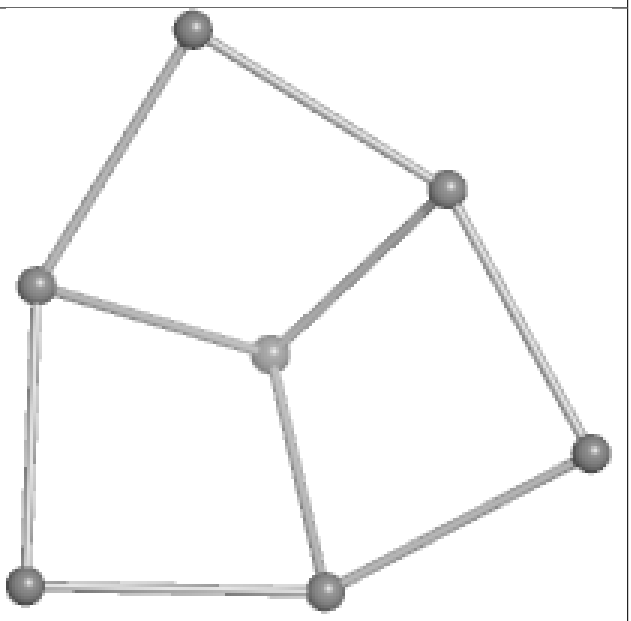
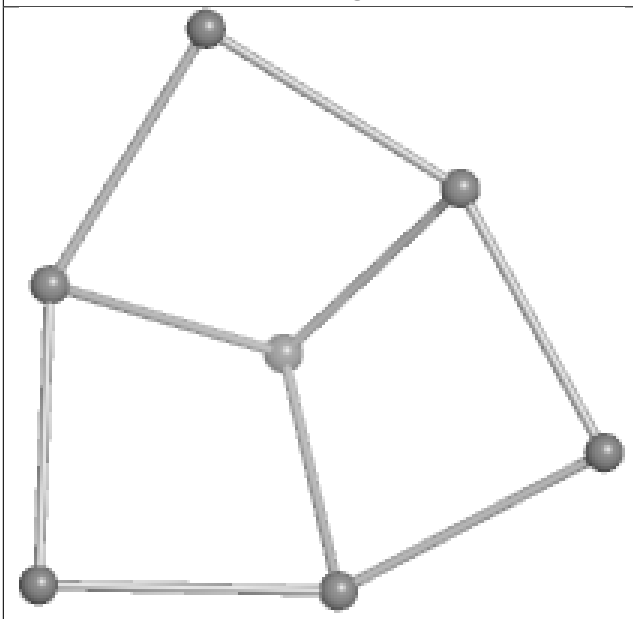
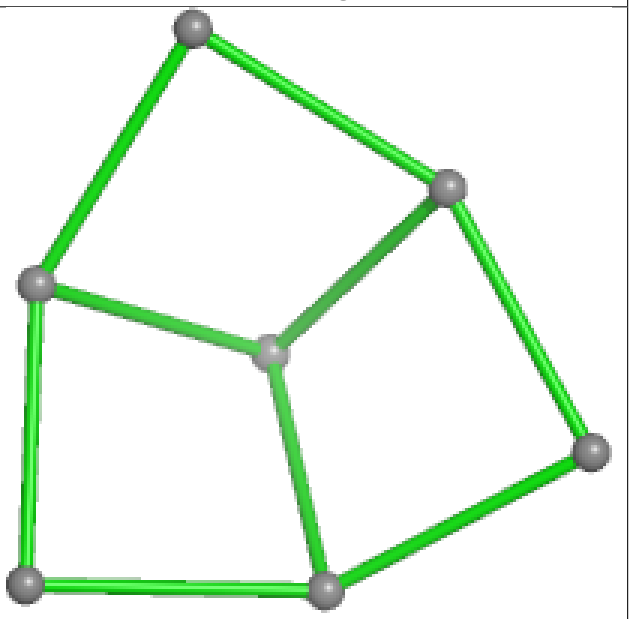


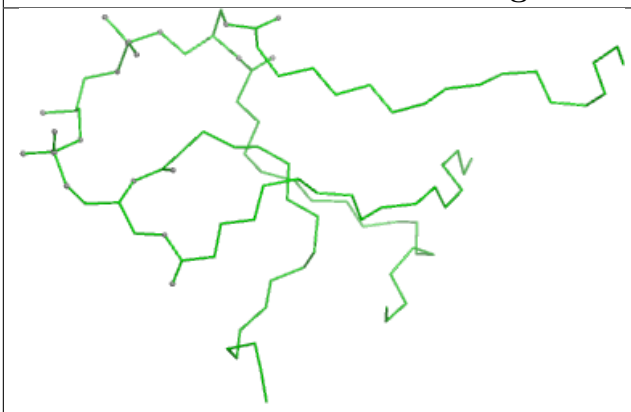
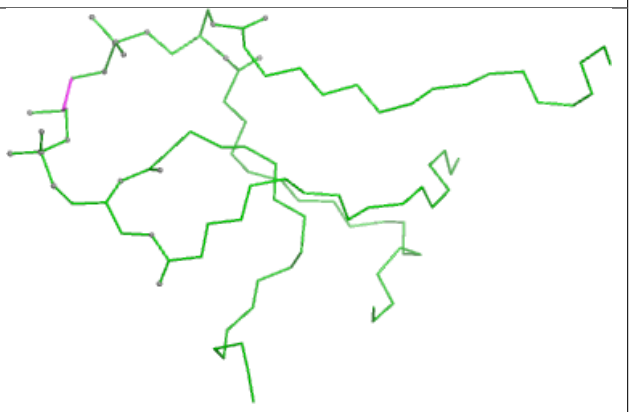
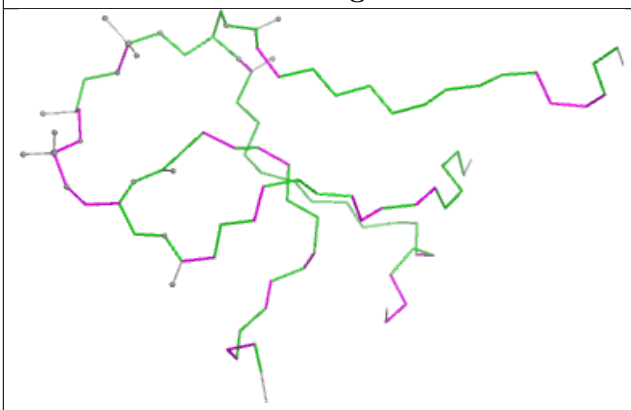
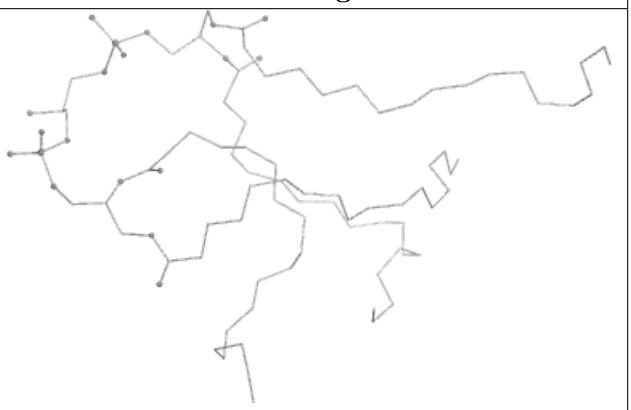
Bond angles



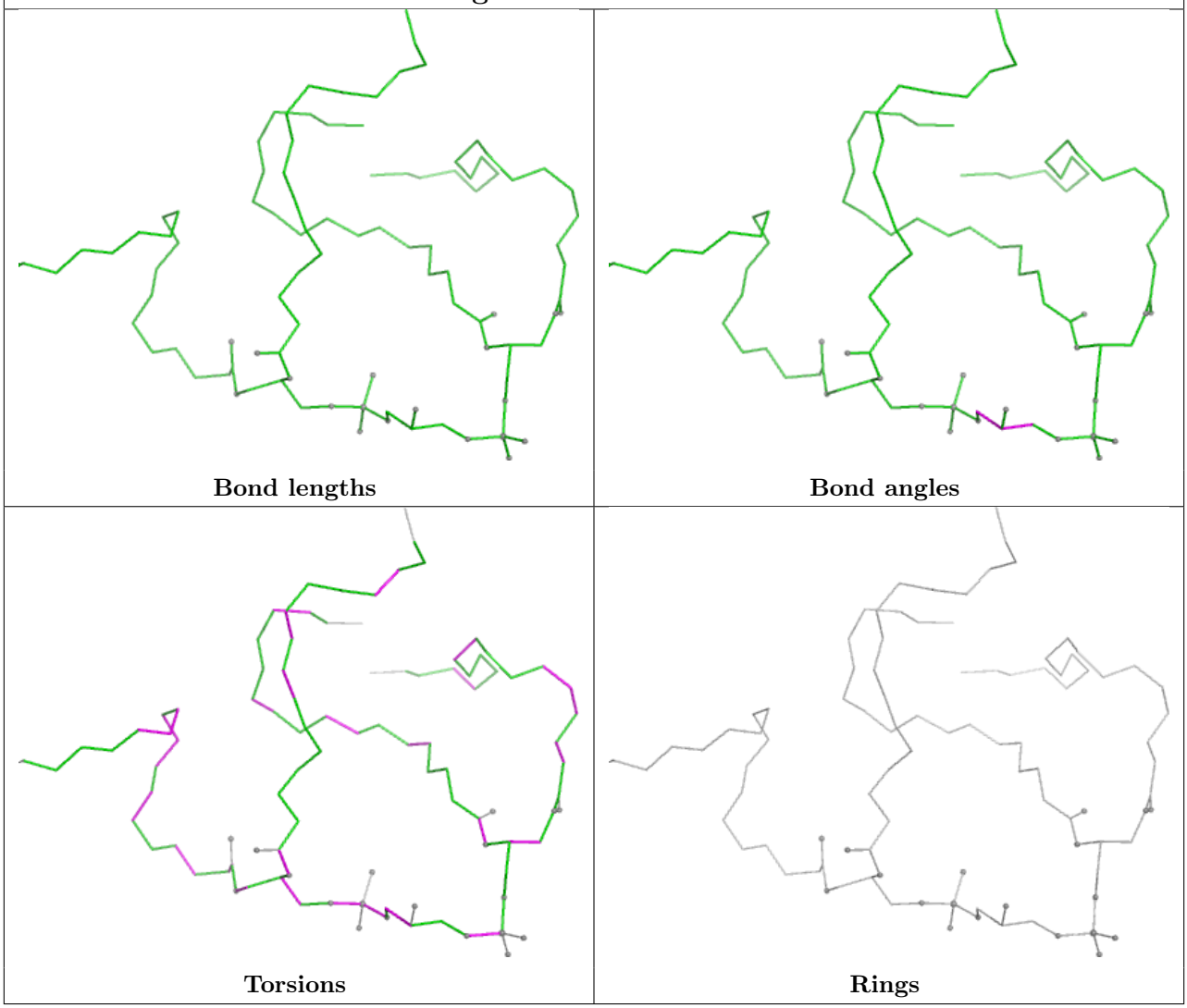
Torsions



Rings

Ligand CDL AA 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Di 1103



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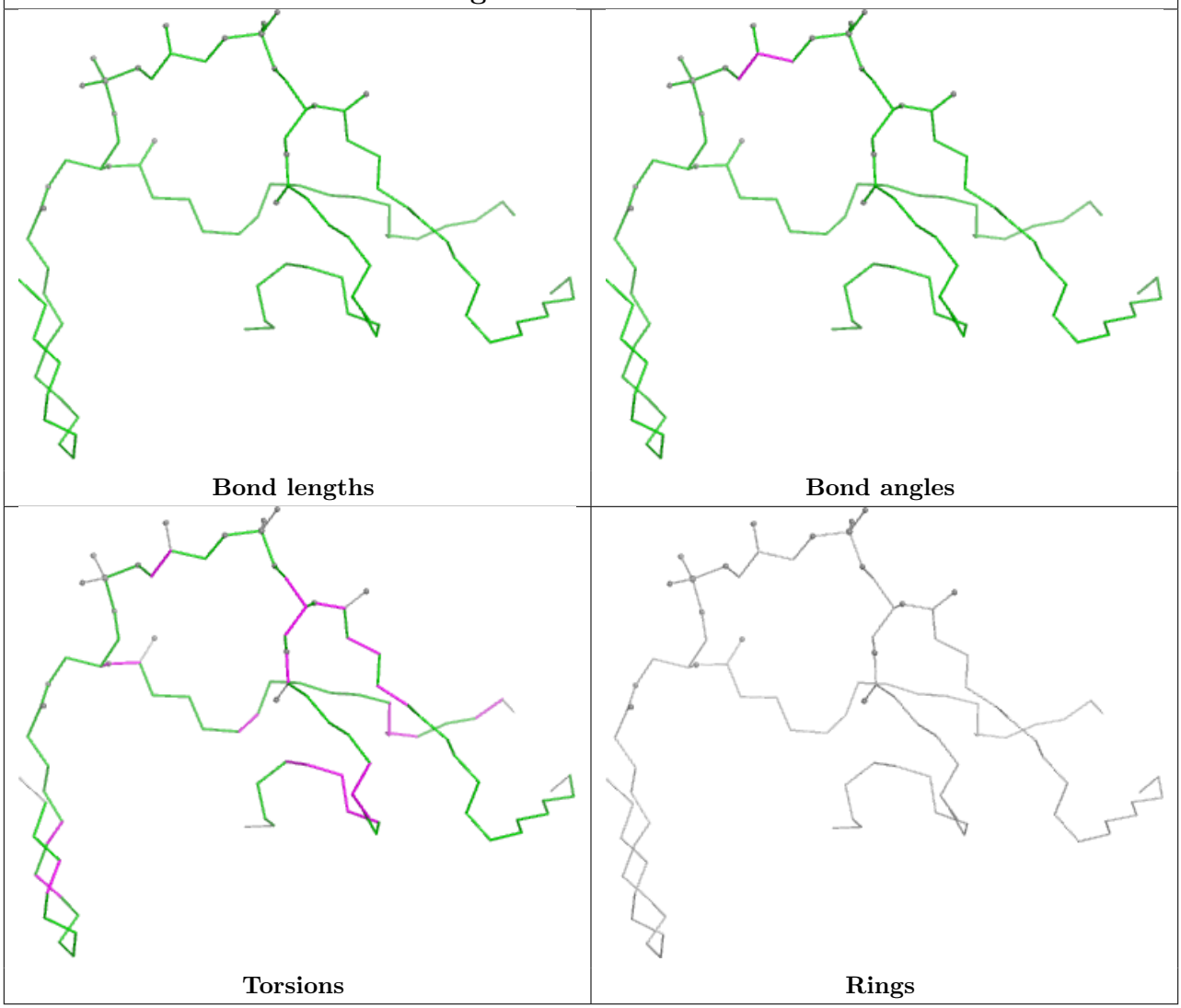
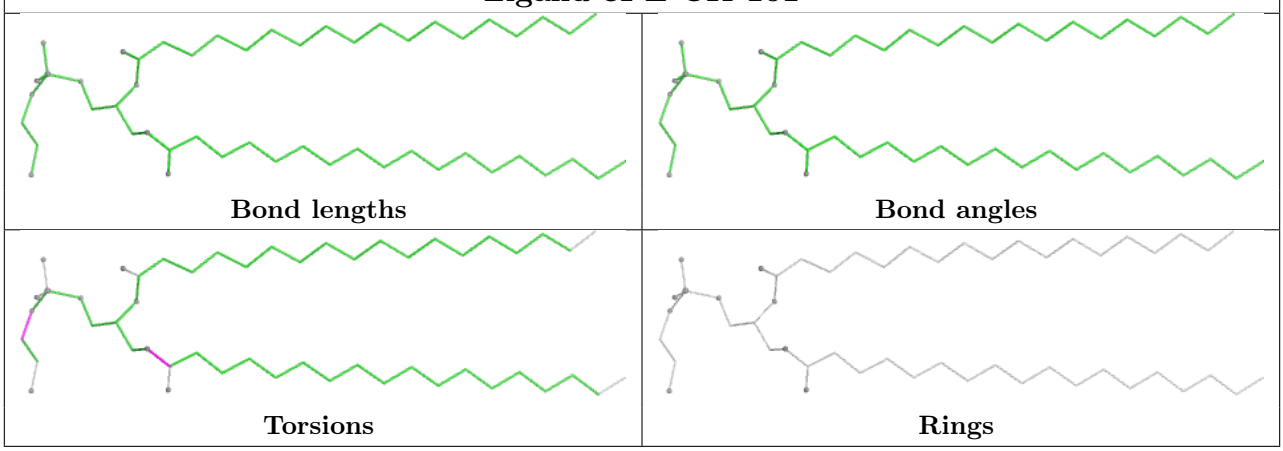


Ligand 3PE CK 101



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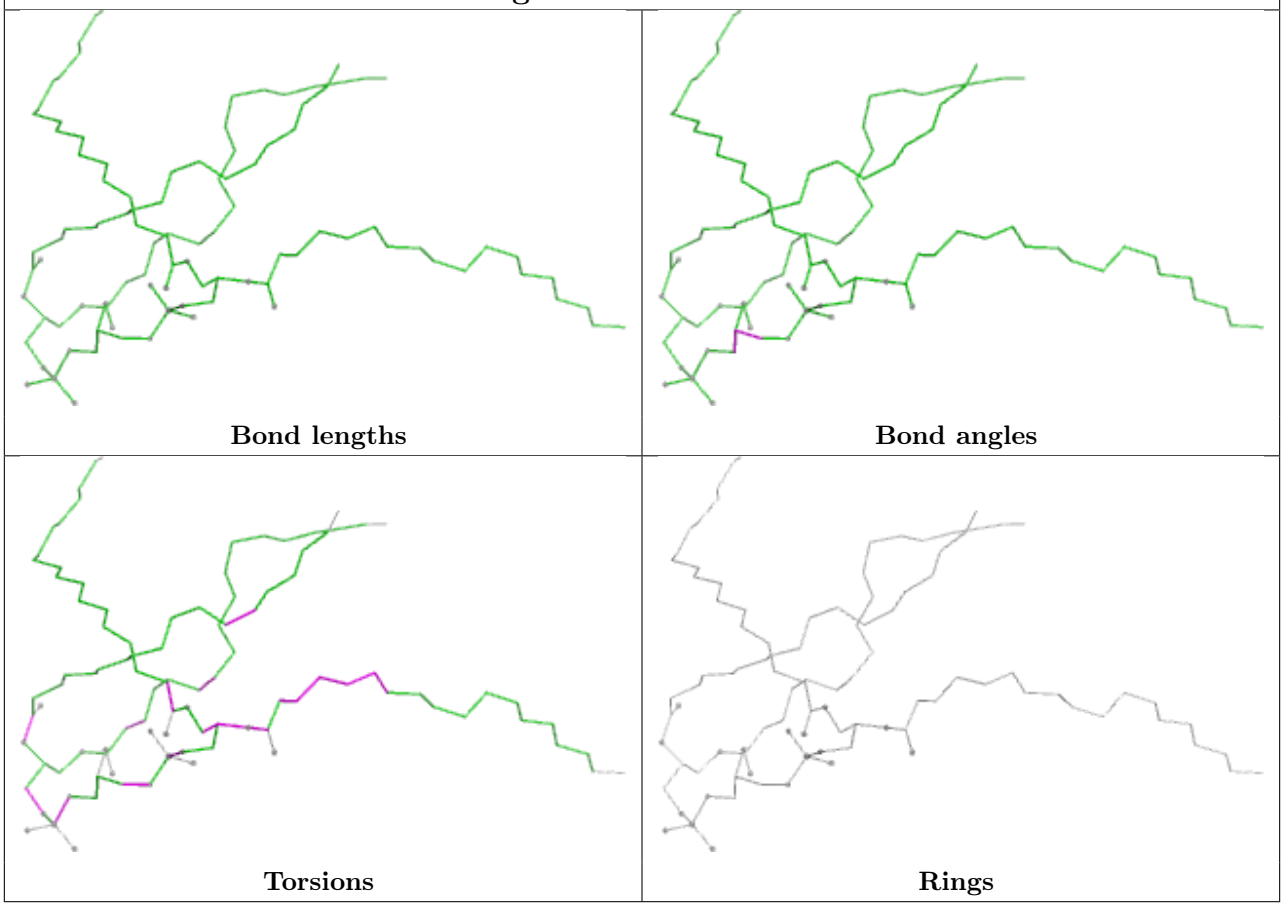

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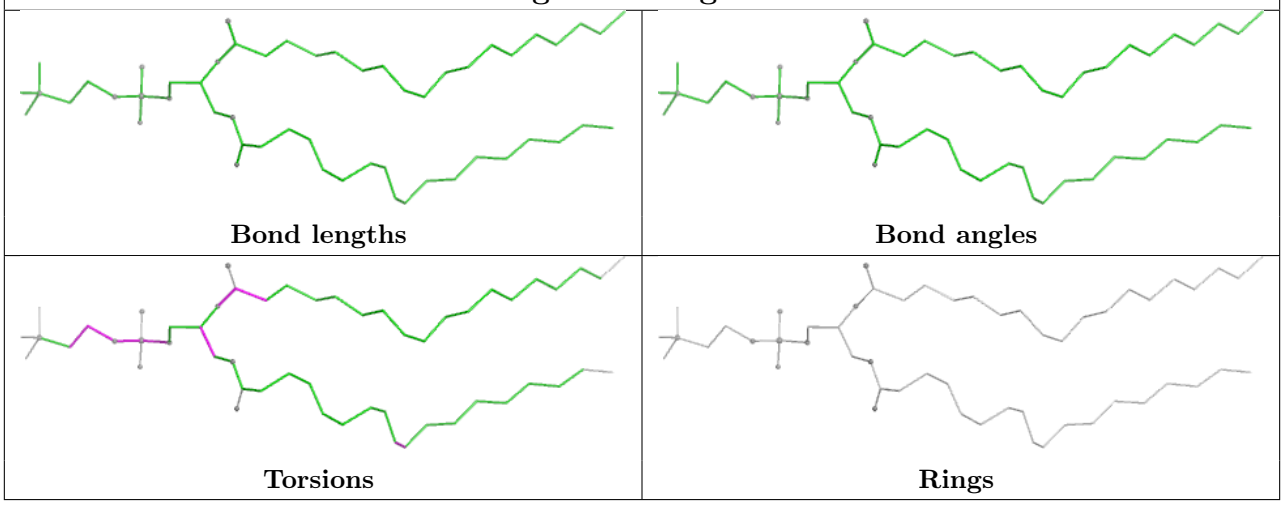

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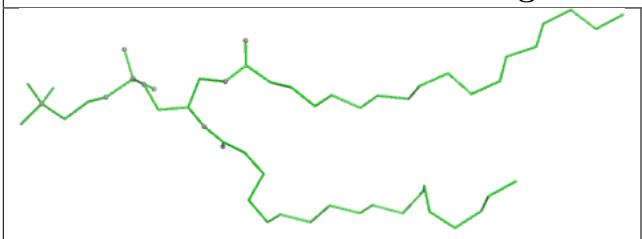
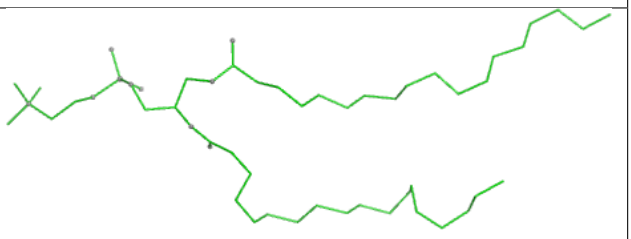
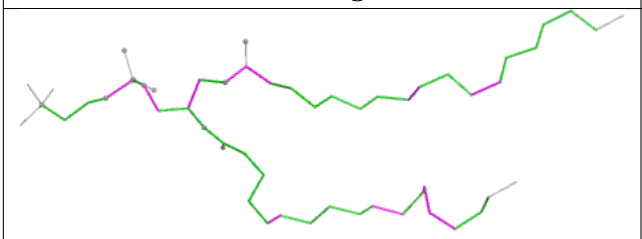
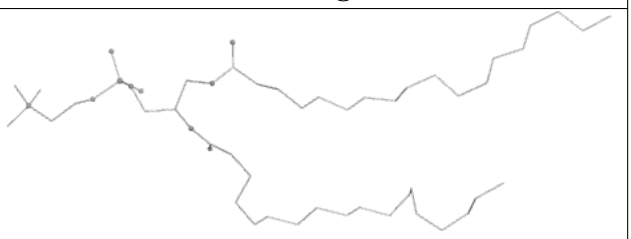
 Bond lengths	 Bond angles
 Torsions	 Rings

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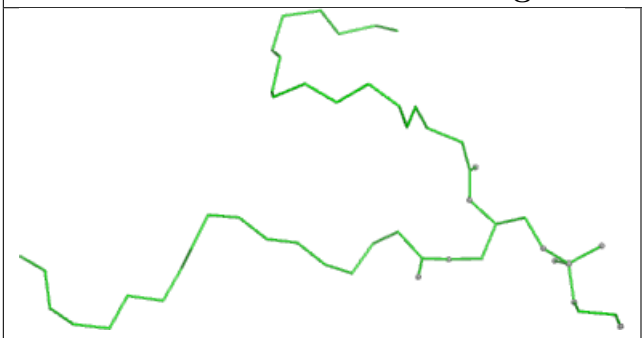
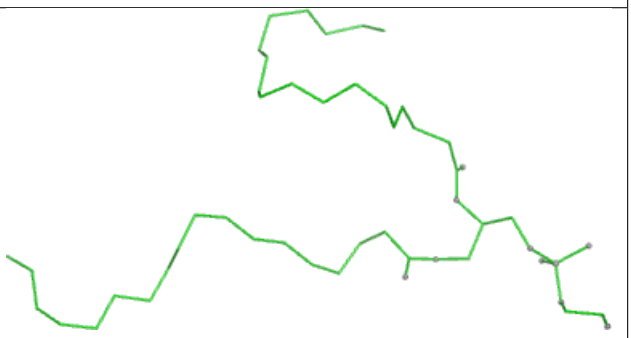
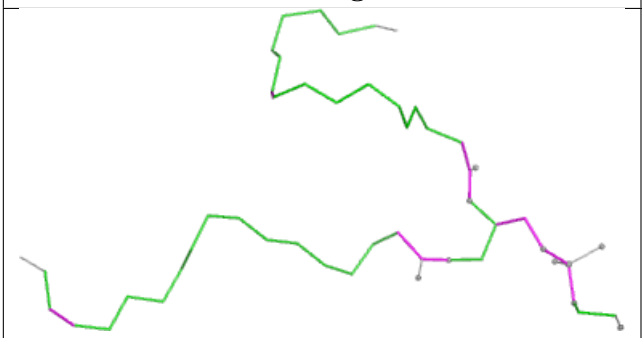
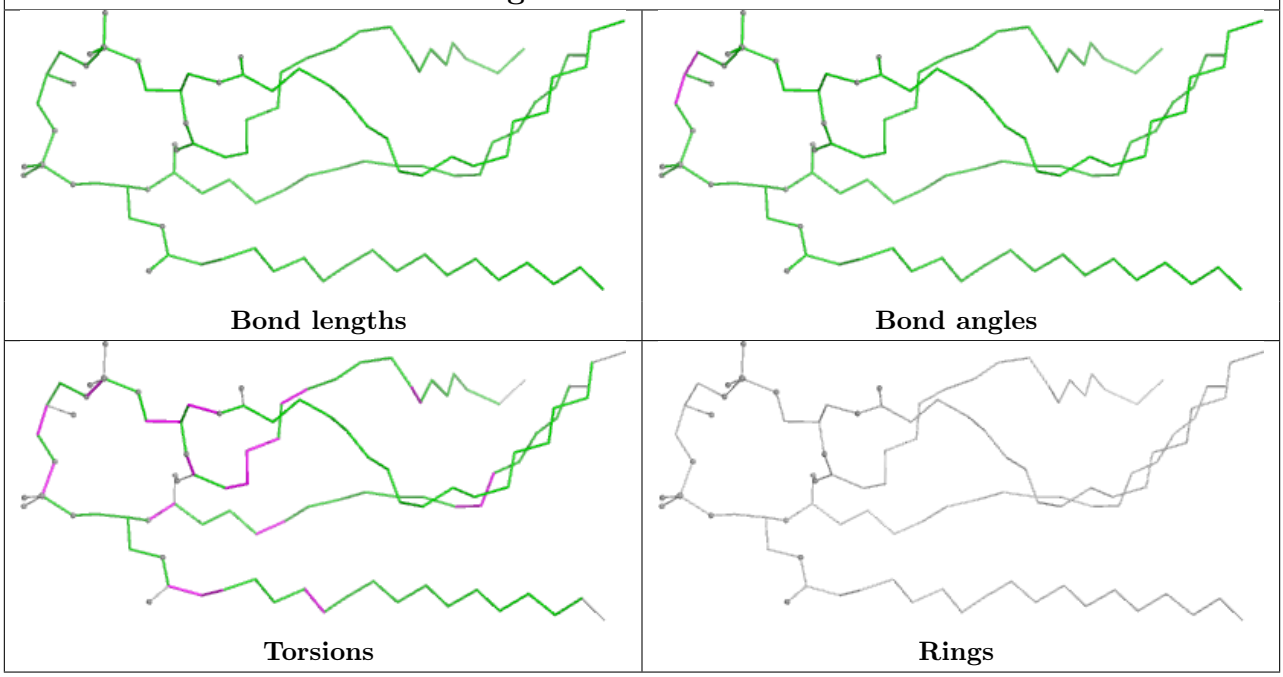
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL DM 502



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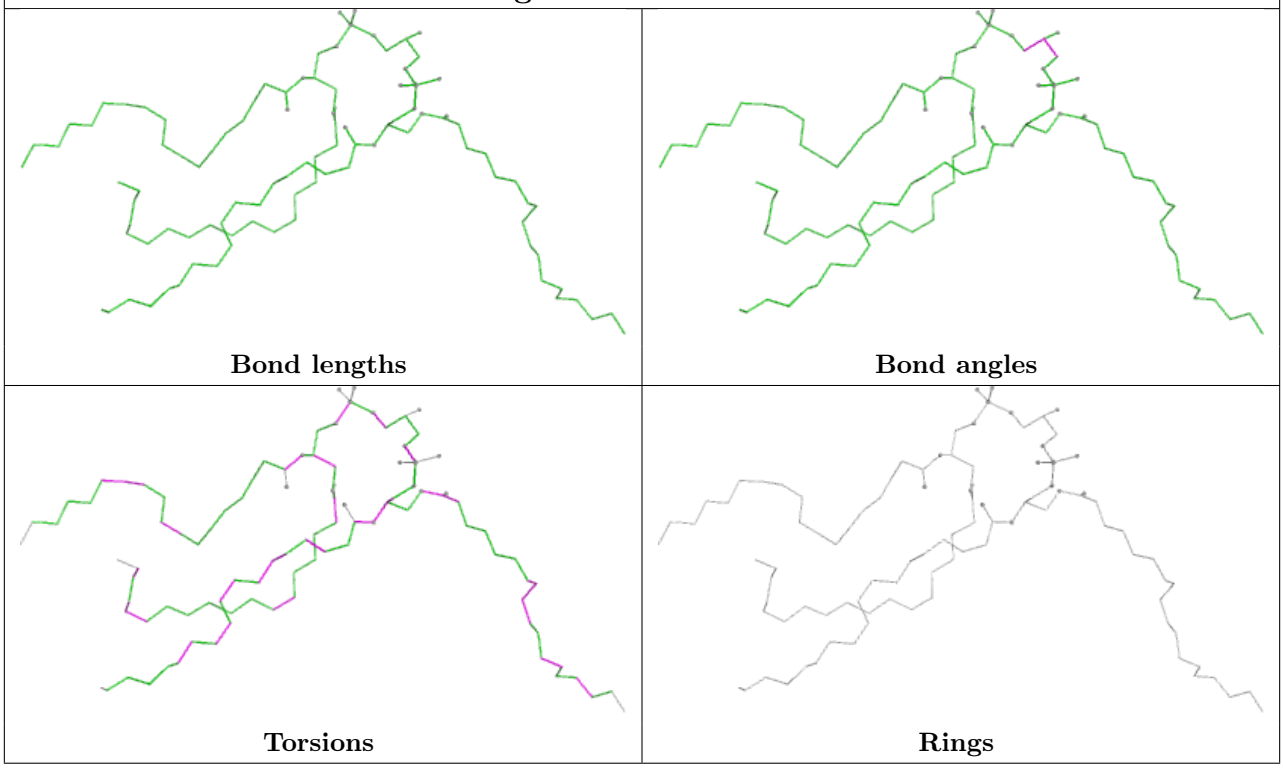

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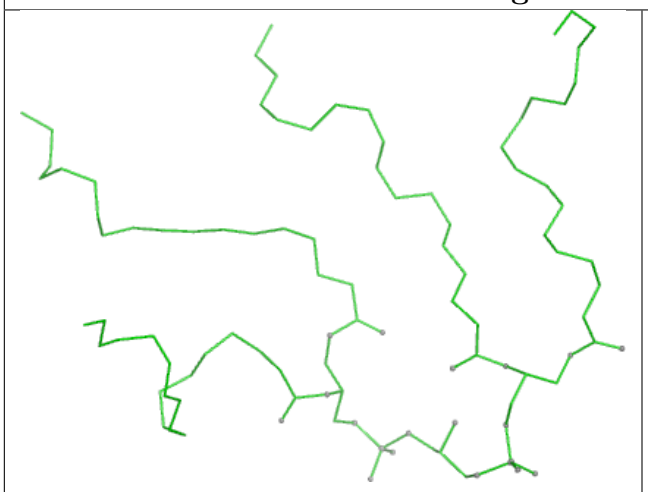
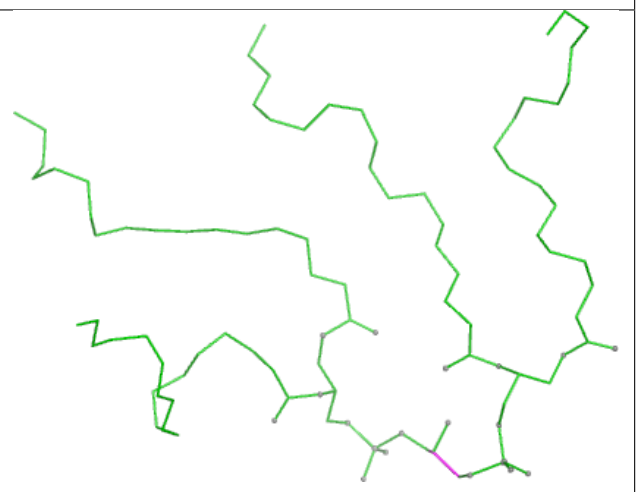
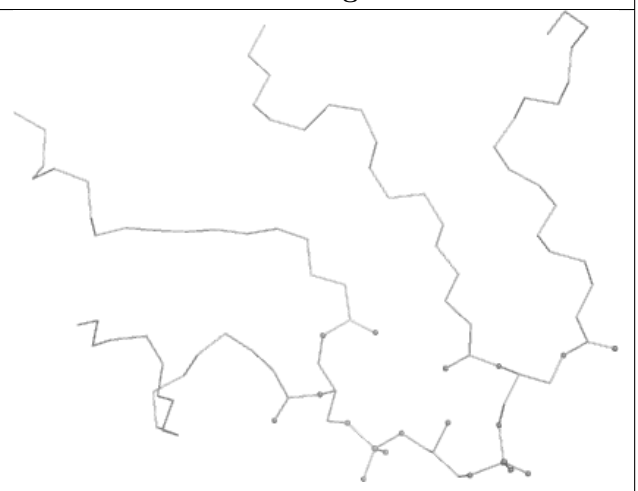


Bond lengths



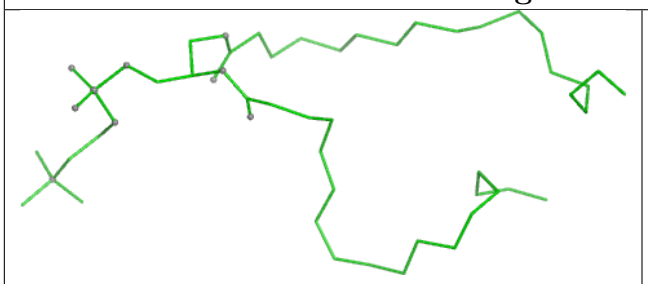
Bond angles

Torsions



Rings

Ligand PC1 DB 702



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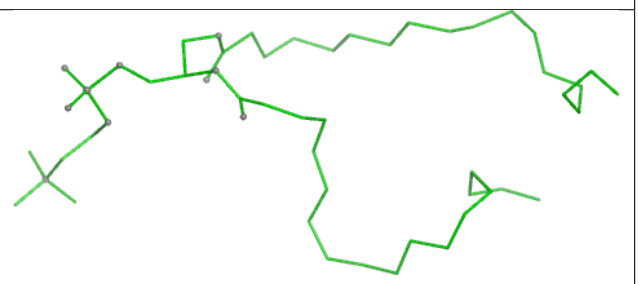

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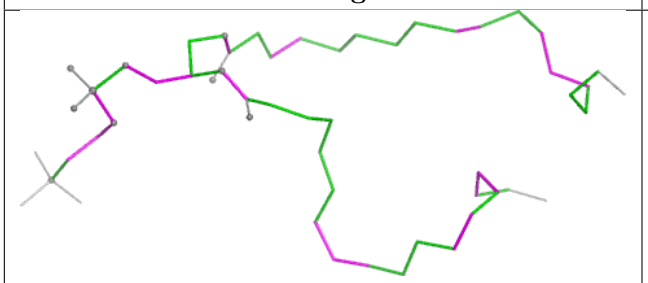

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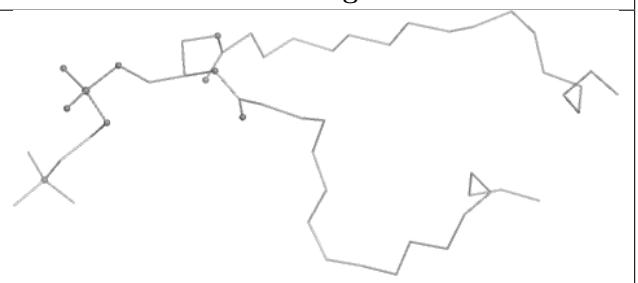
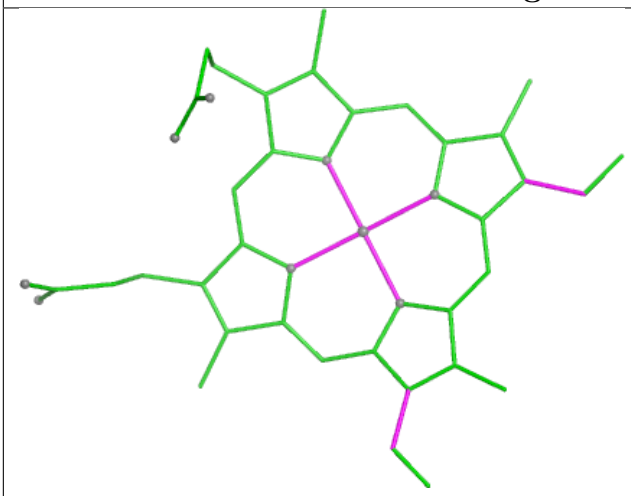


Rings

Ligand HEM c 505



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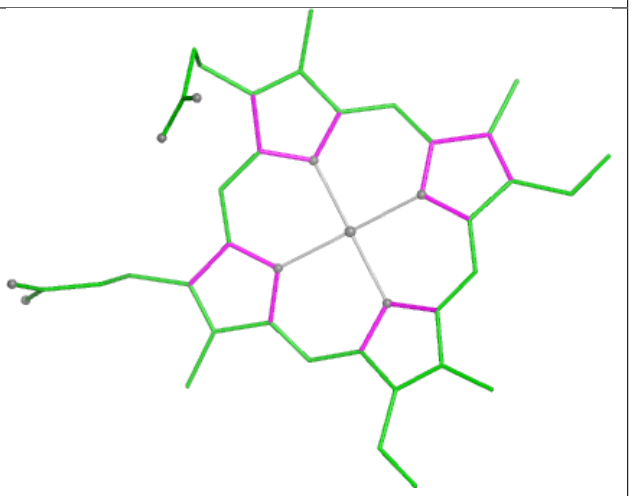

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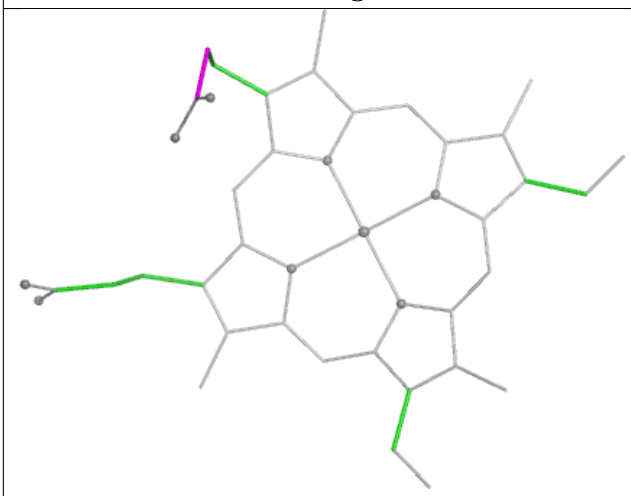

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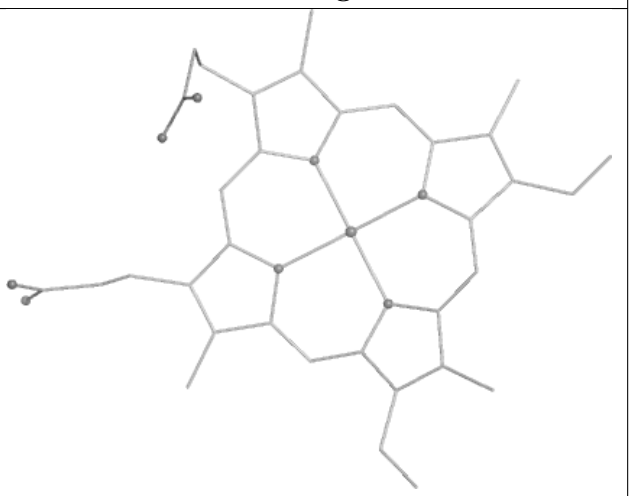
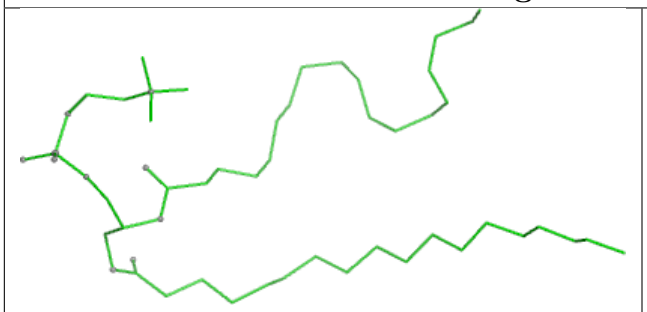


Rings

Ligand PC1 AQ 202



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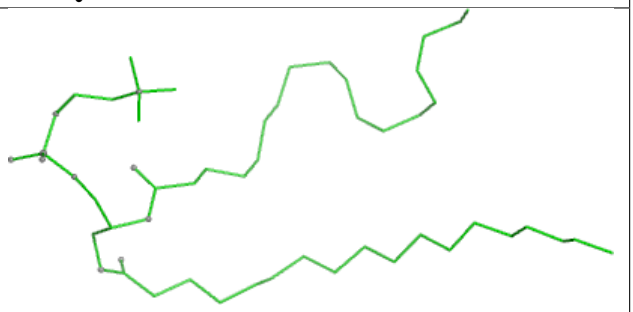

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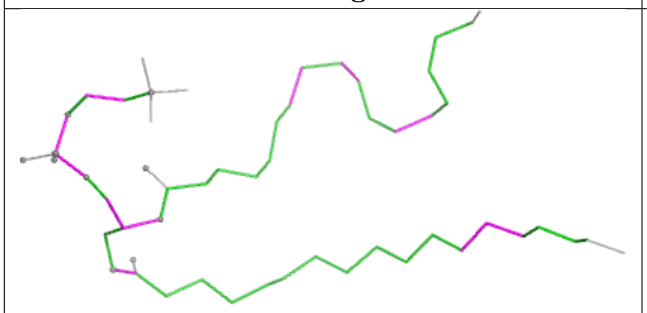

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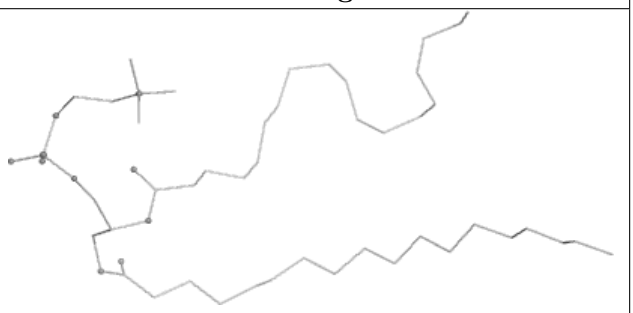
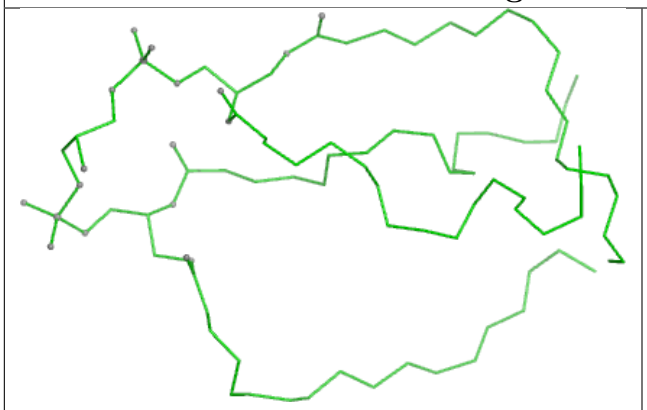


Rings

Ligand CDL Dx 1204



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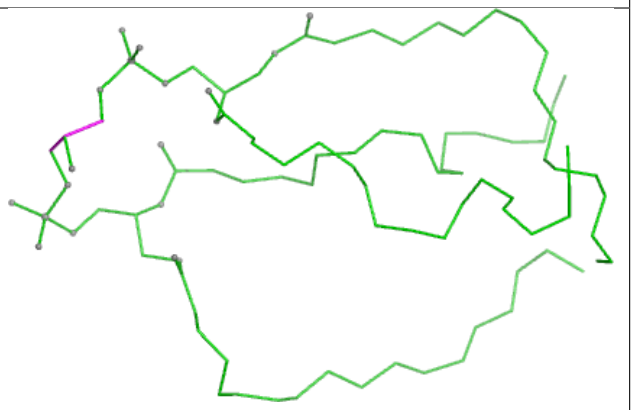

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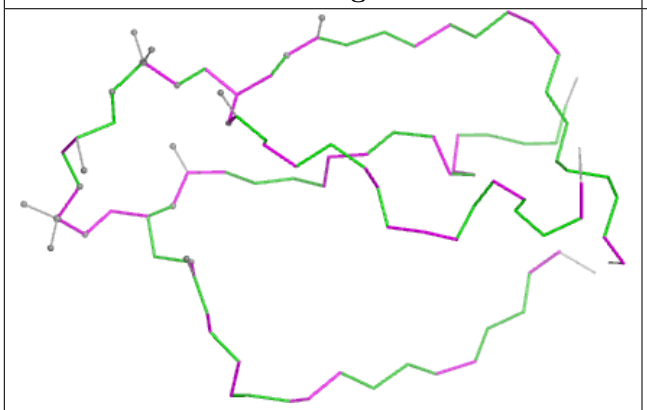

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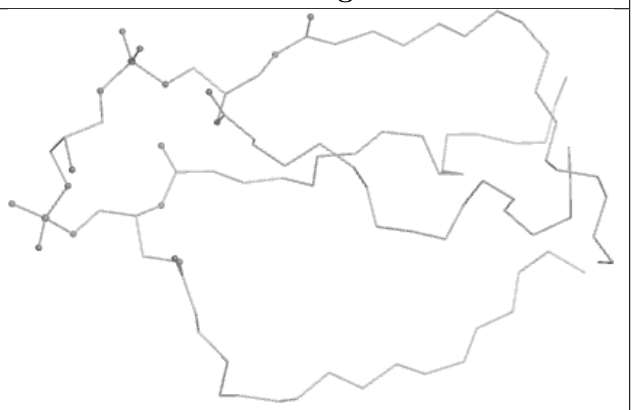
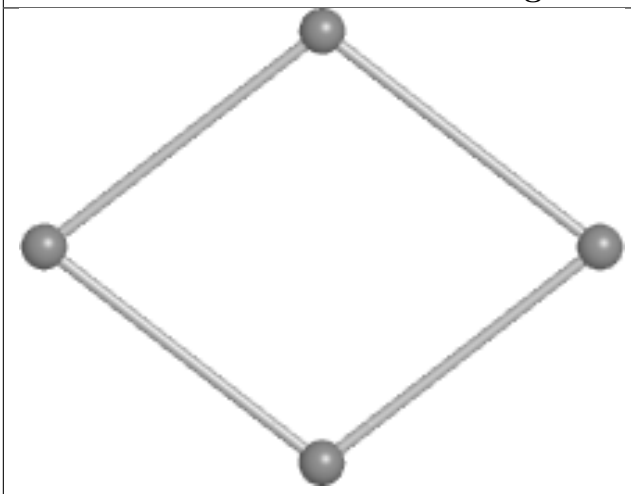


Rings

Ligand FES Ef 502



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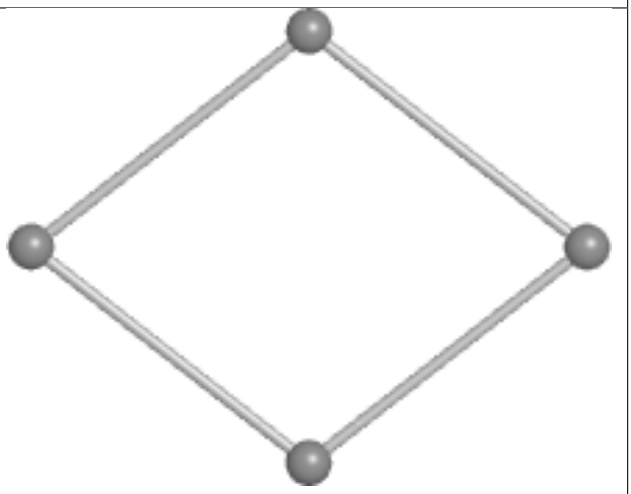

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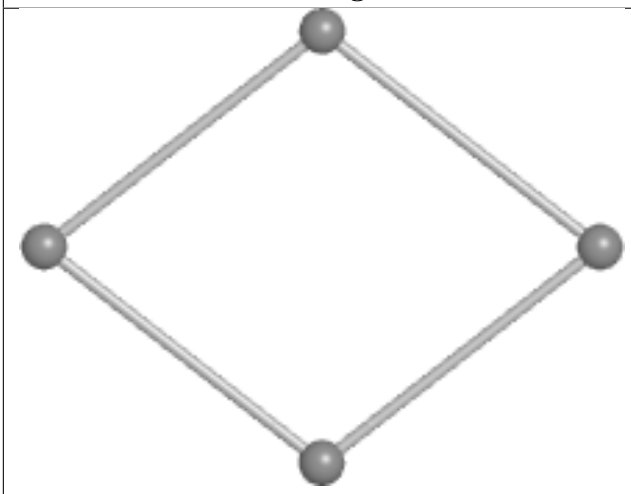

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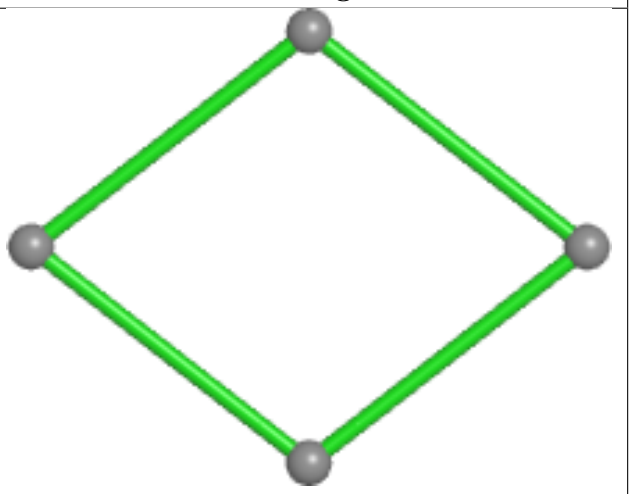
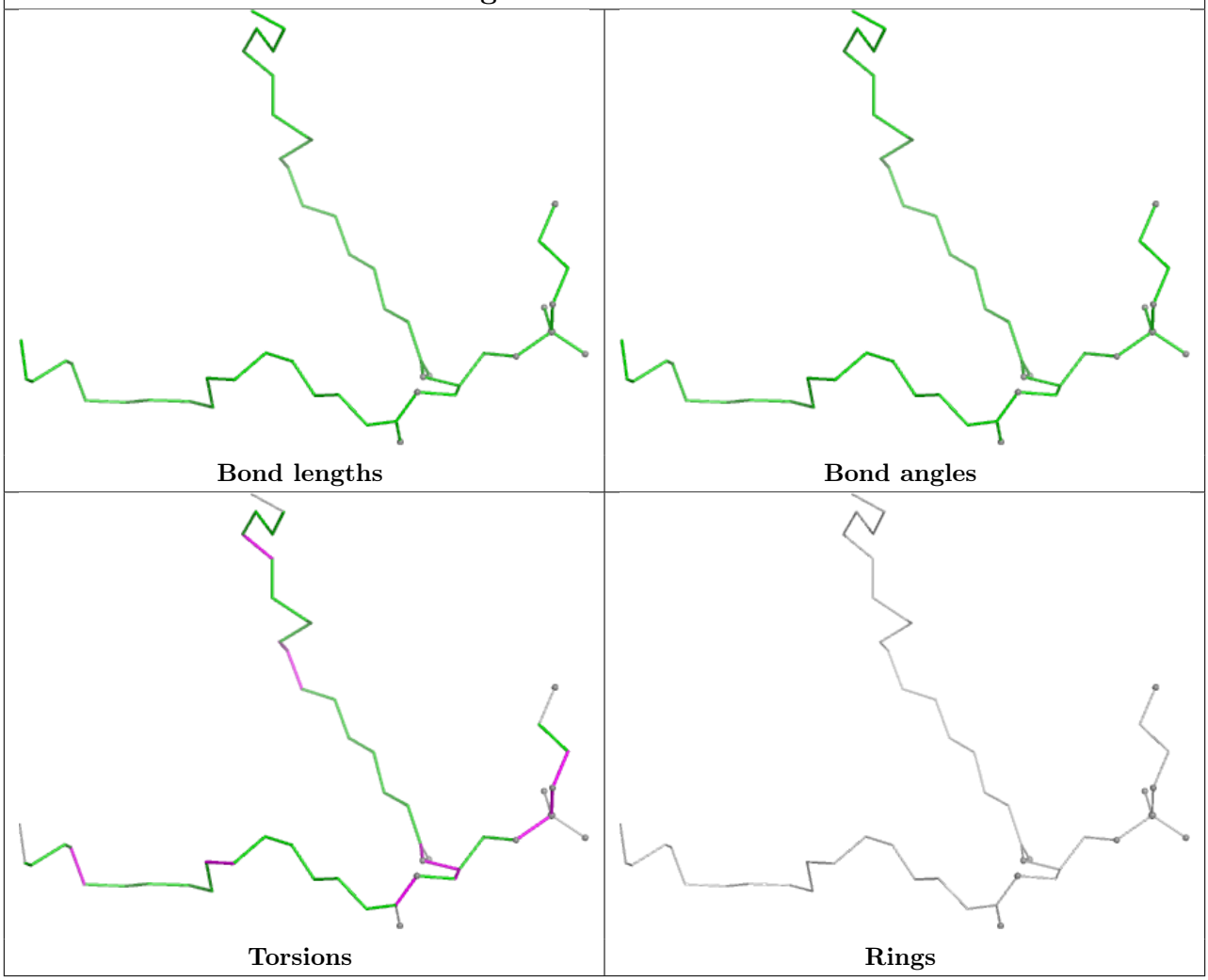


Rings

Ligand 3PE Dx 1202



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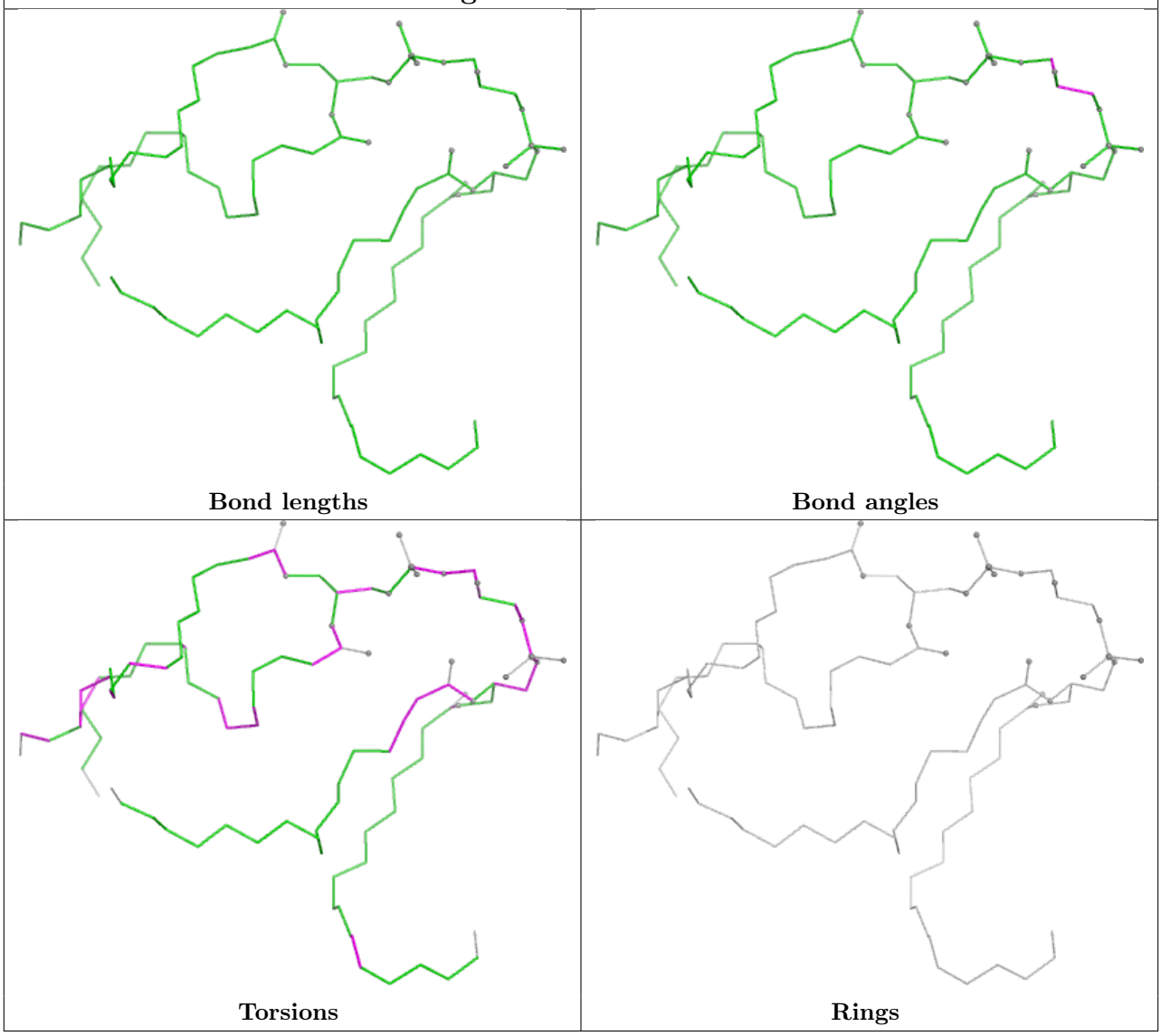
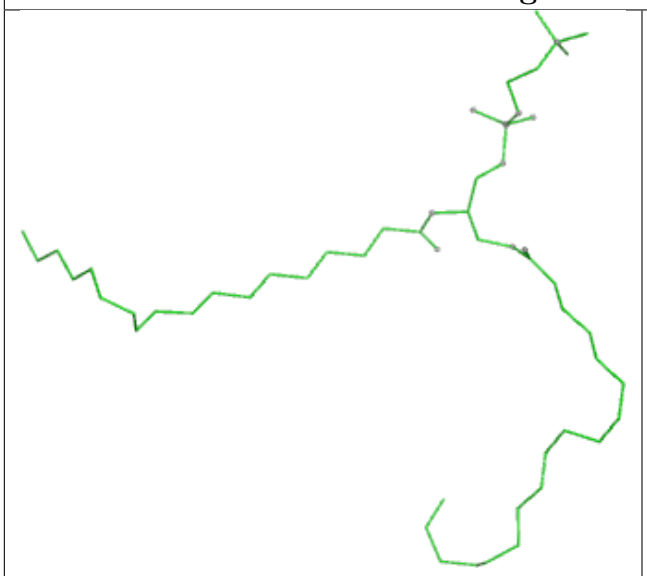


Ligand PC1 Dc 603



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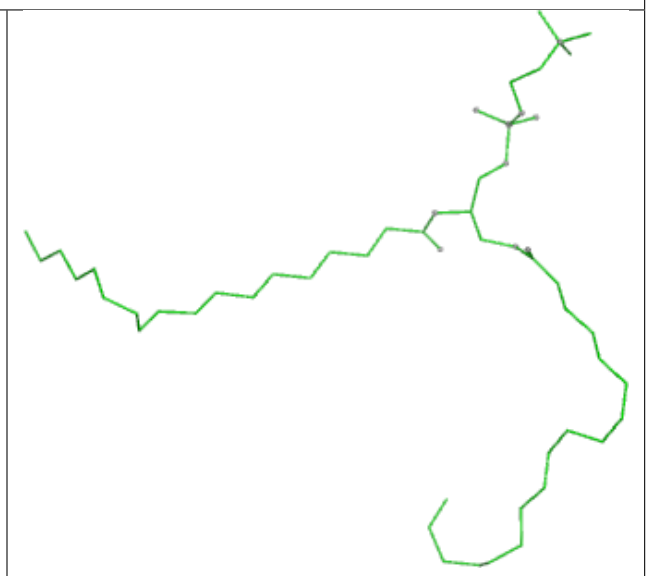

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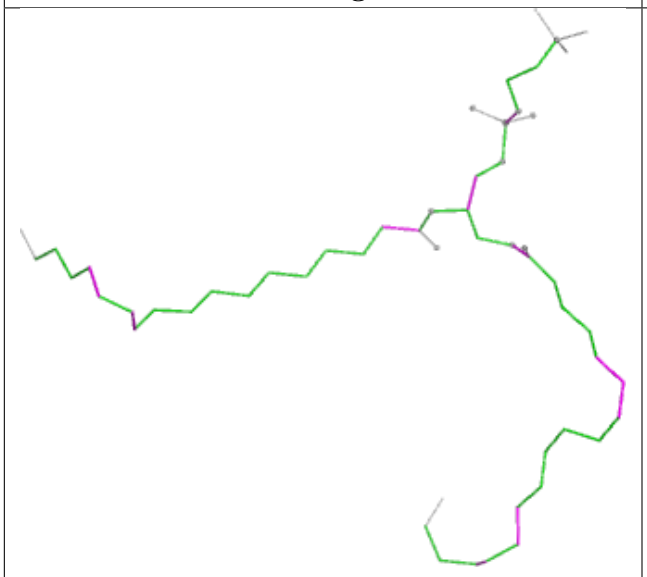


Torsions

Rings

Ligand CDL A0 602

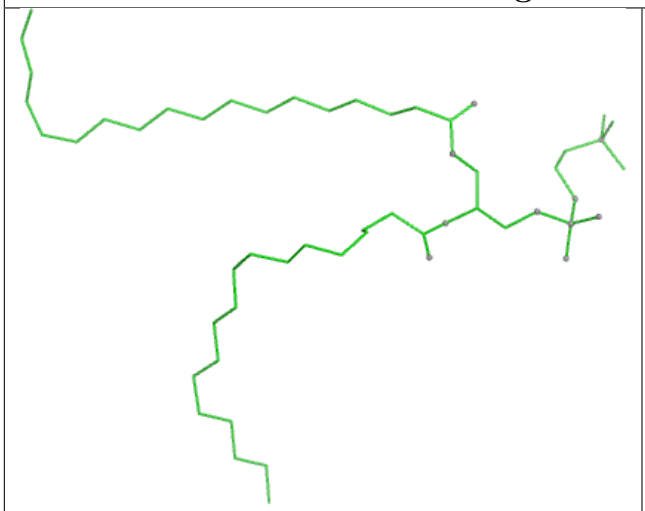
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 DX 305



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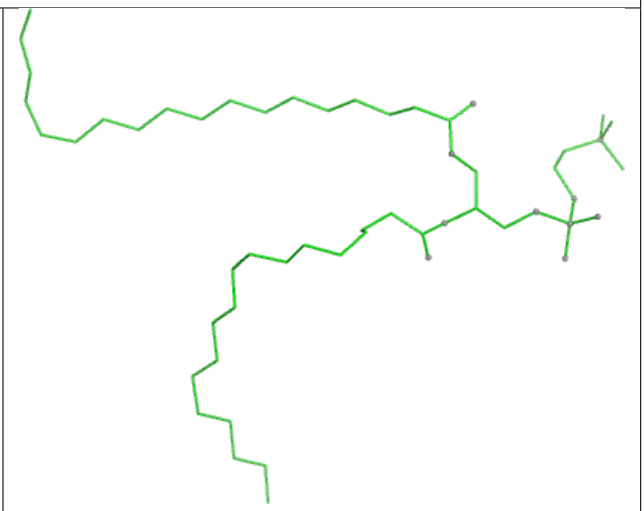

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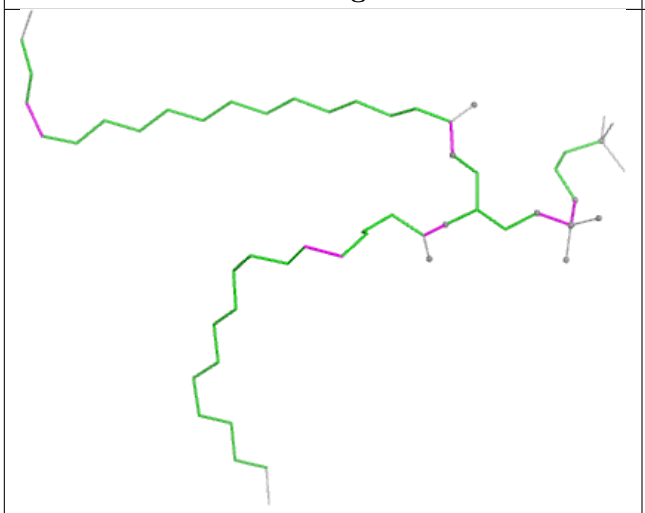

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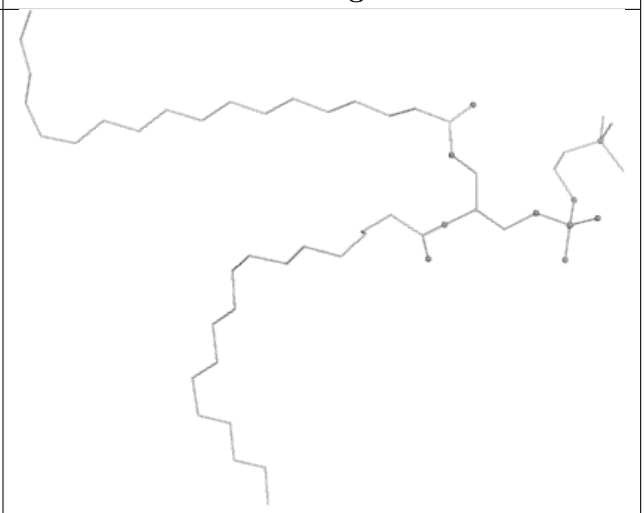
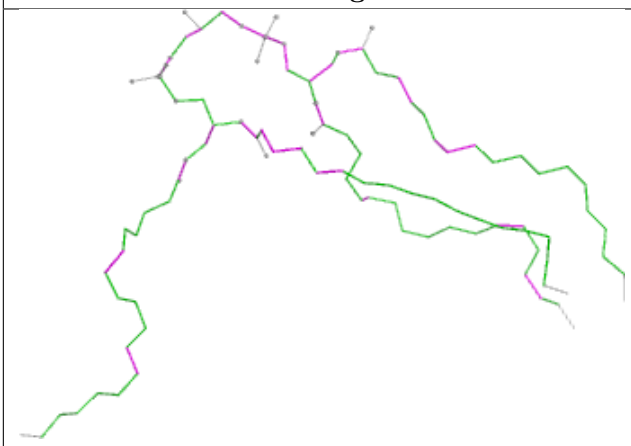


Rings

Ligand CDL BG 201

Bond lengths

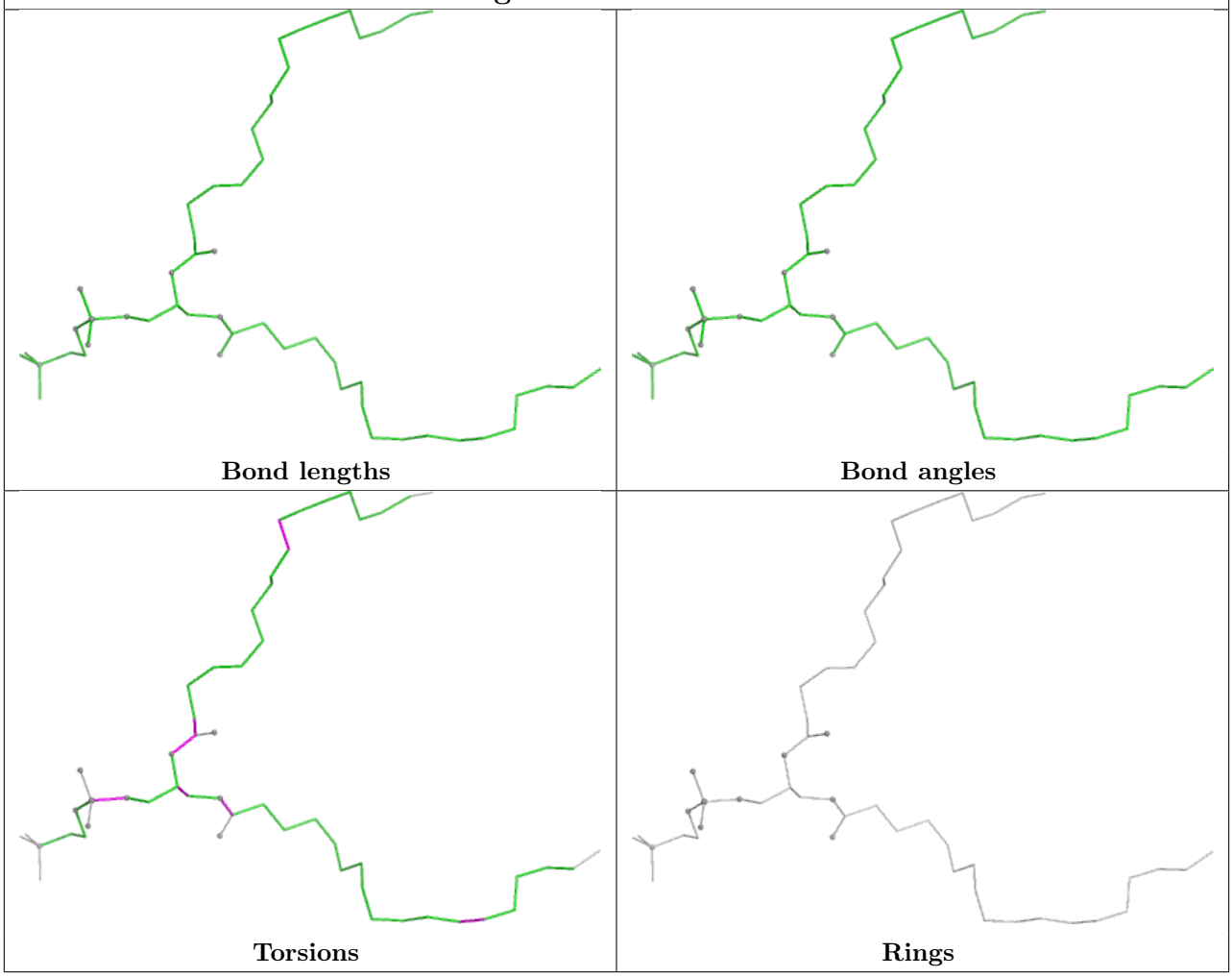
Bond angles



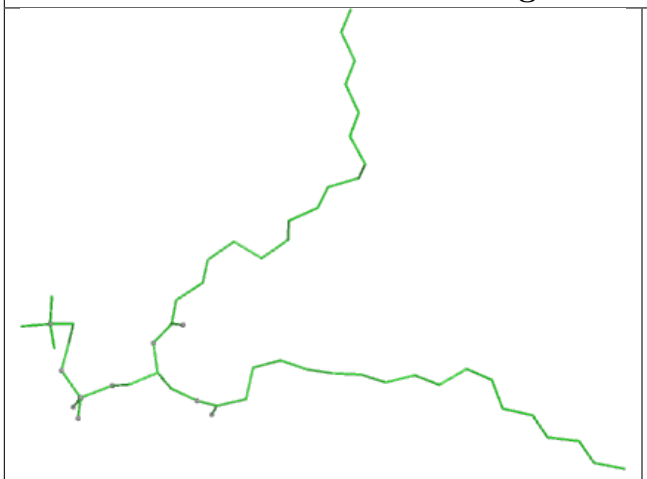
Torsions

Rings

Ligand PC1 DC 605



Ligand PC1 A6 303



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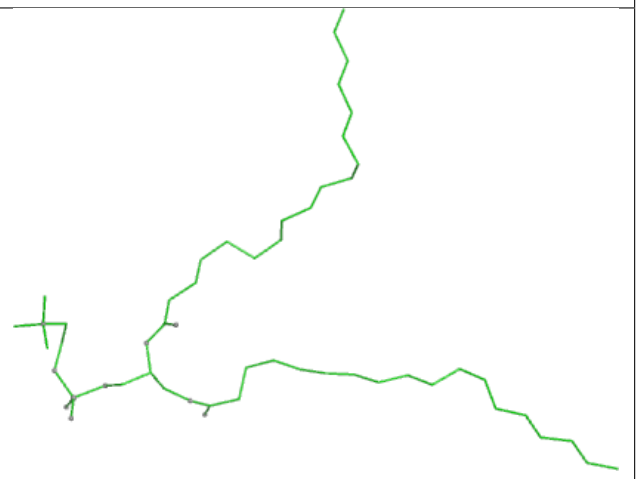
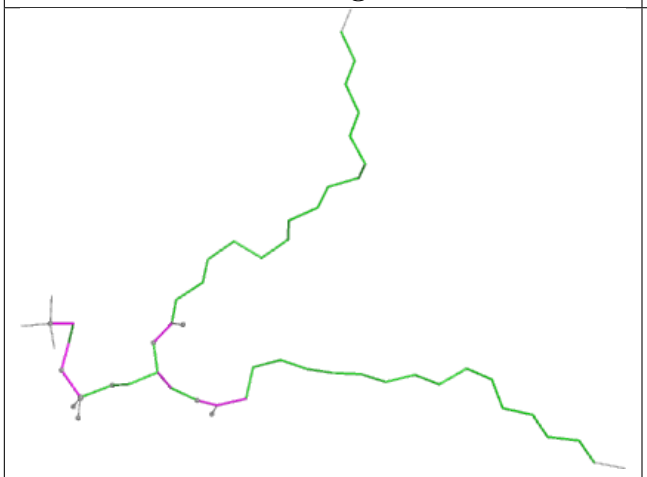


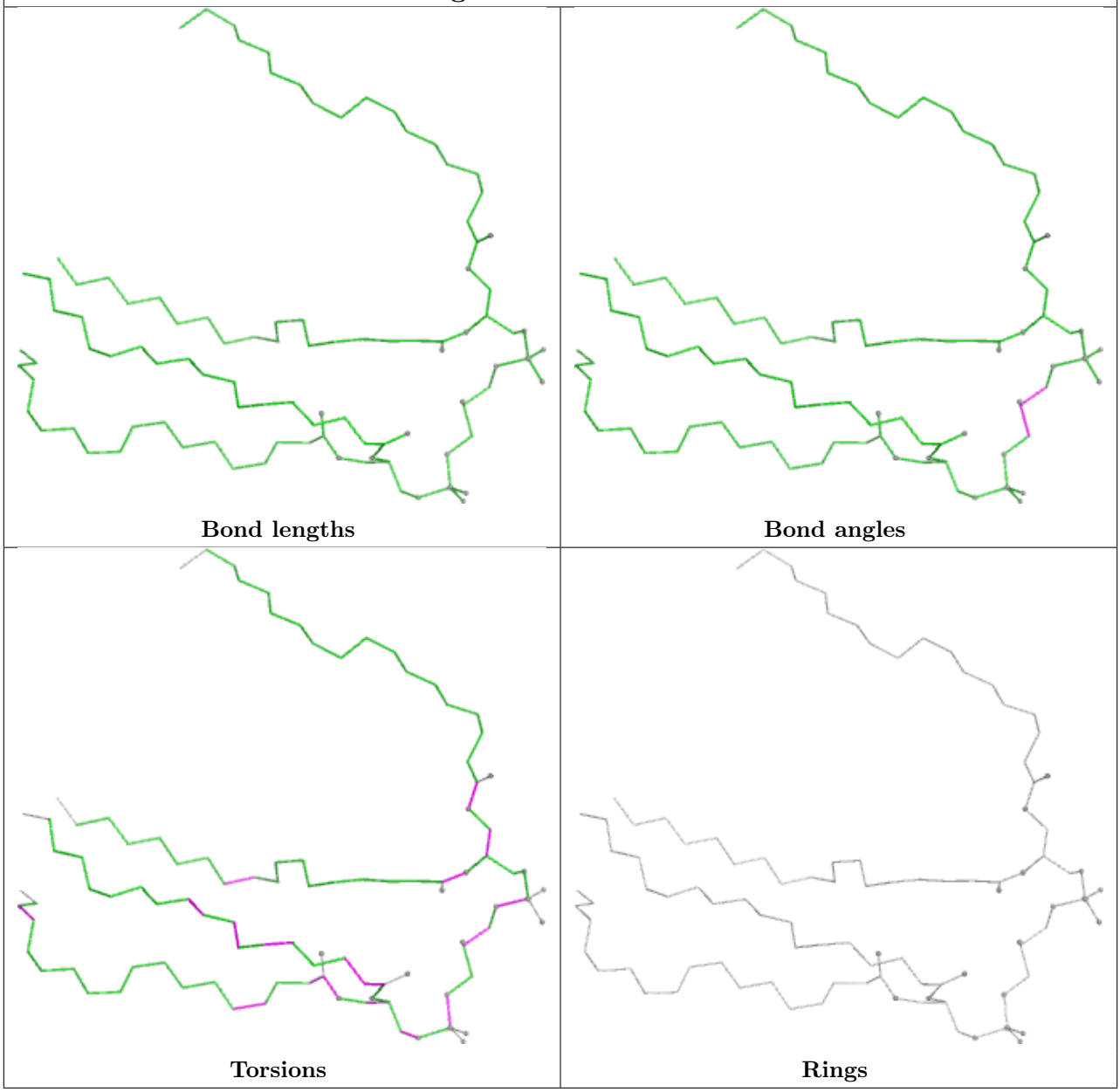
Bond angles

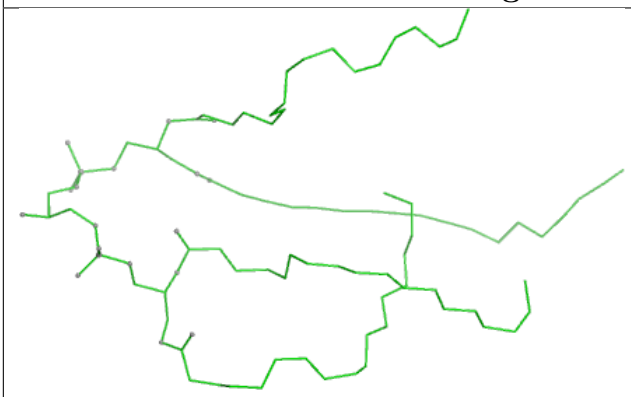
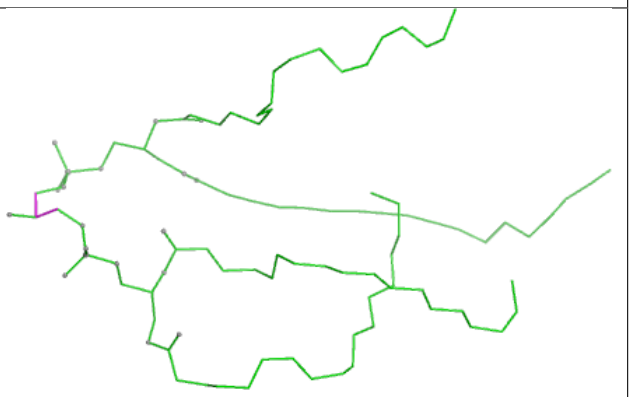
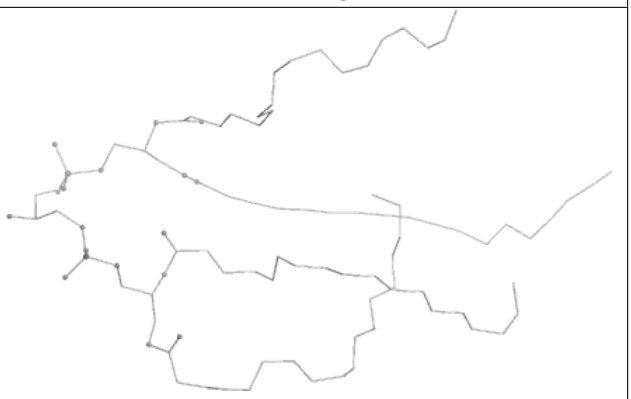


Torsions

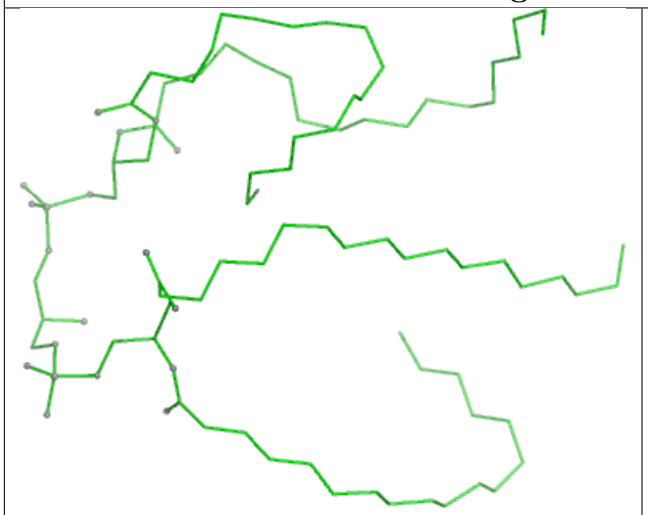
Rings

Ligand CDL B0 102



Ligand CDL EN 1202	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CDL DN 503



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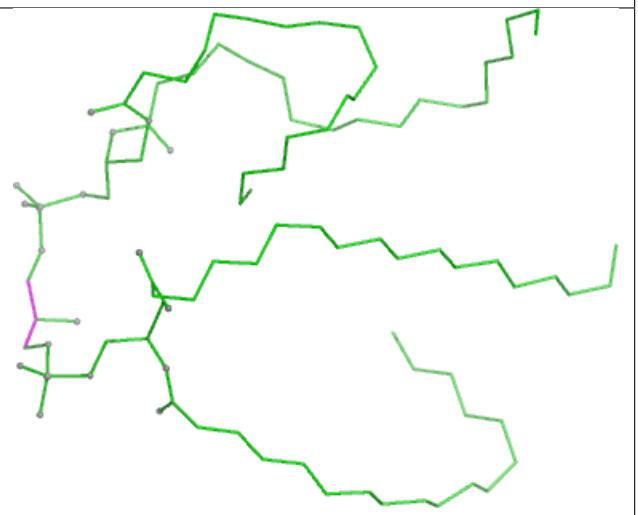

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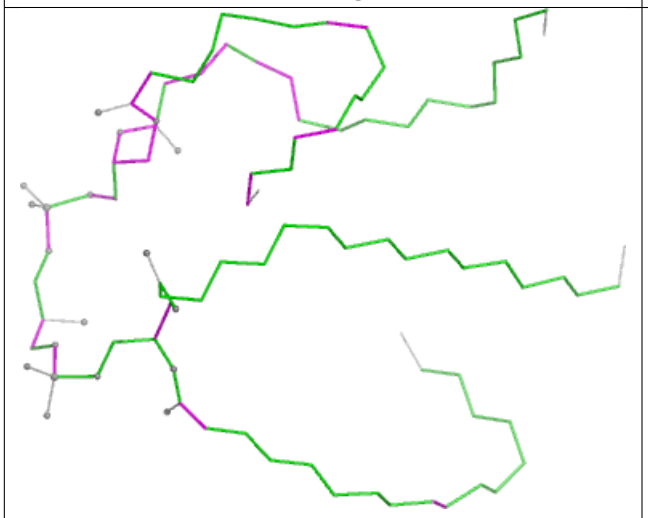
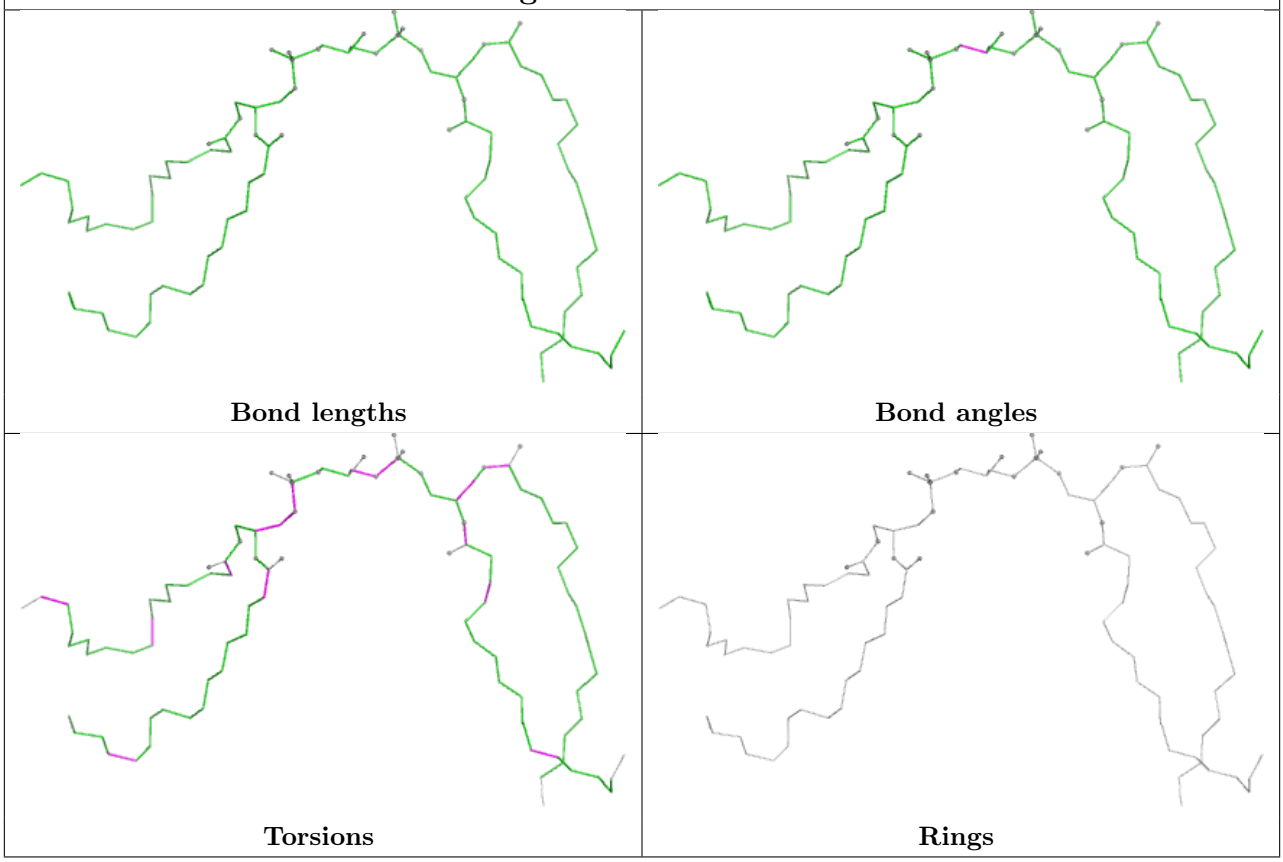


Torsions

Rings

Ligand CDL EI 401



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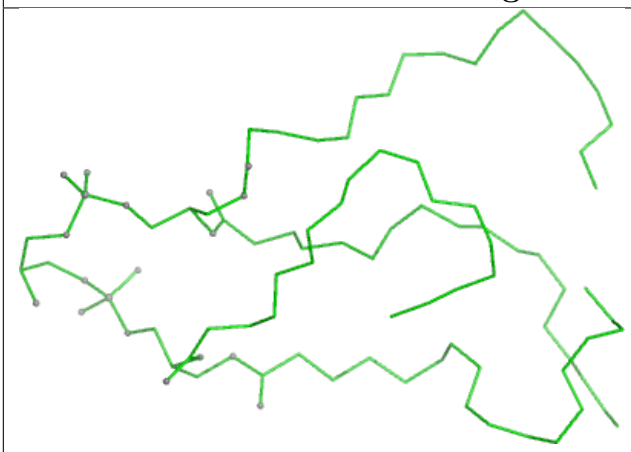
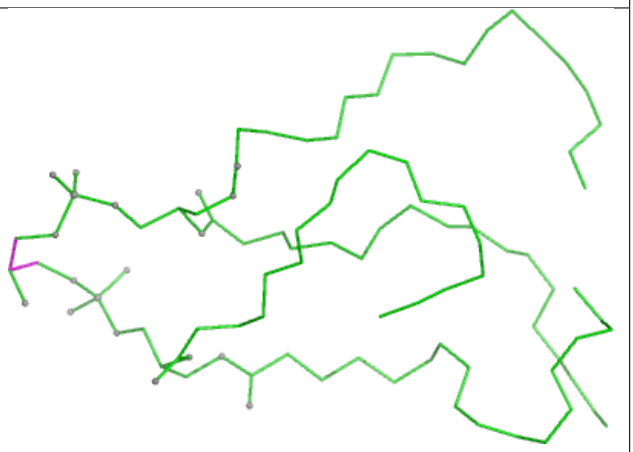
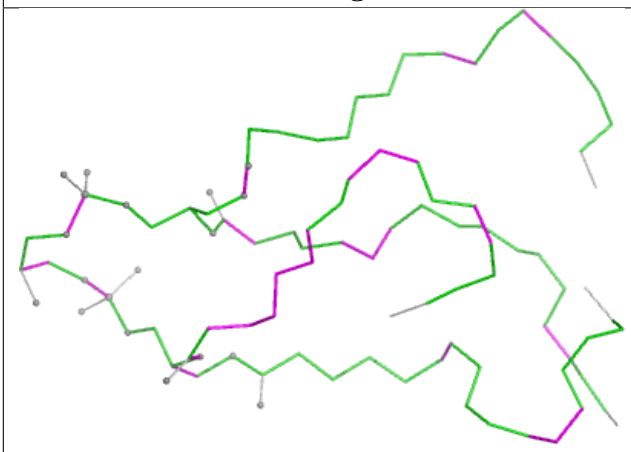
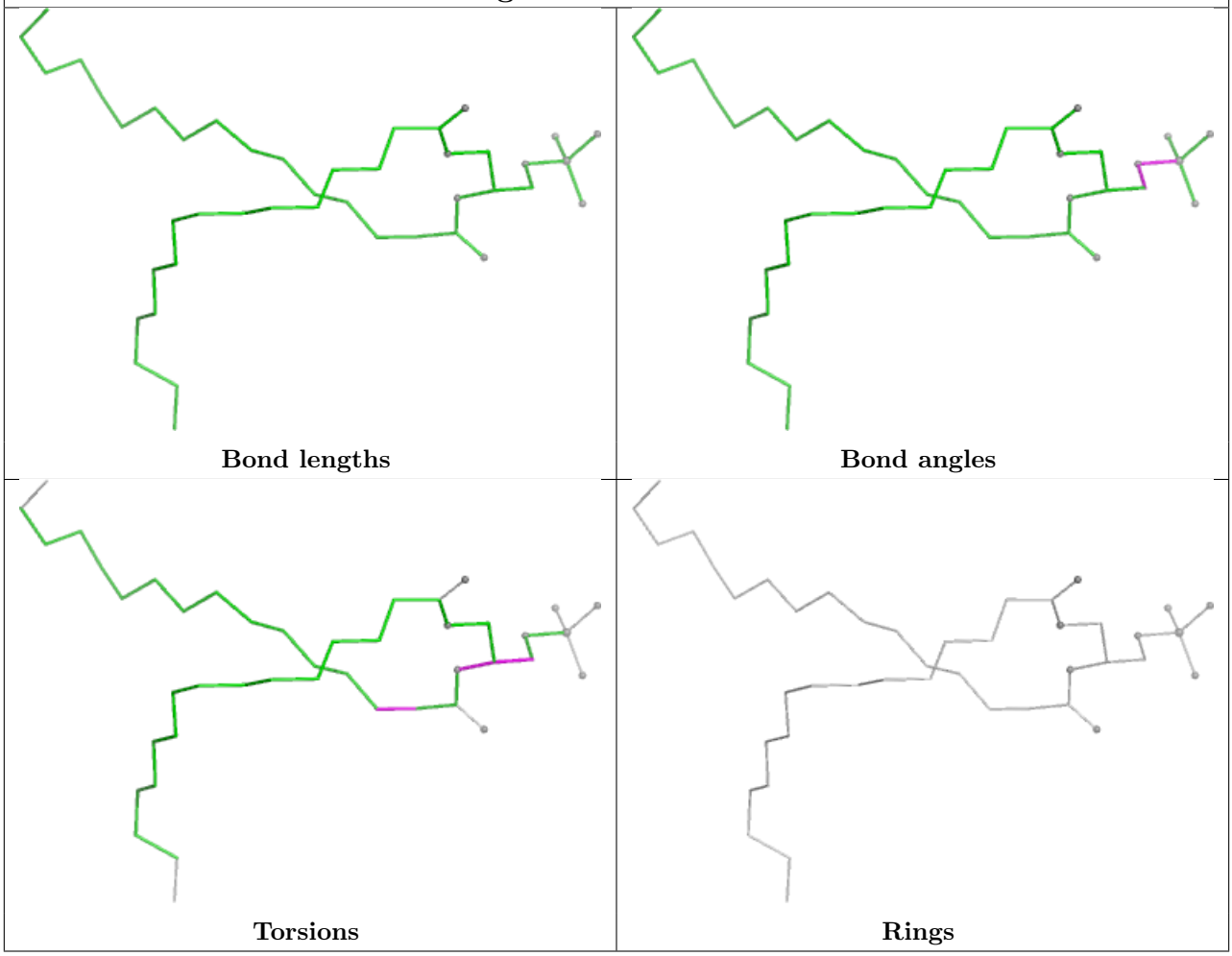
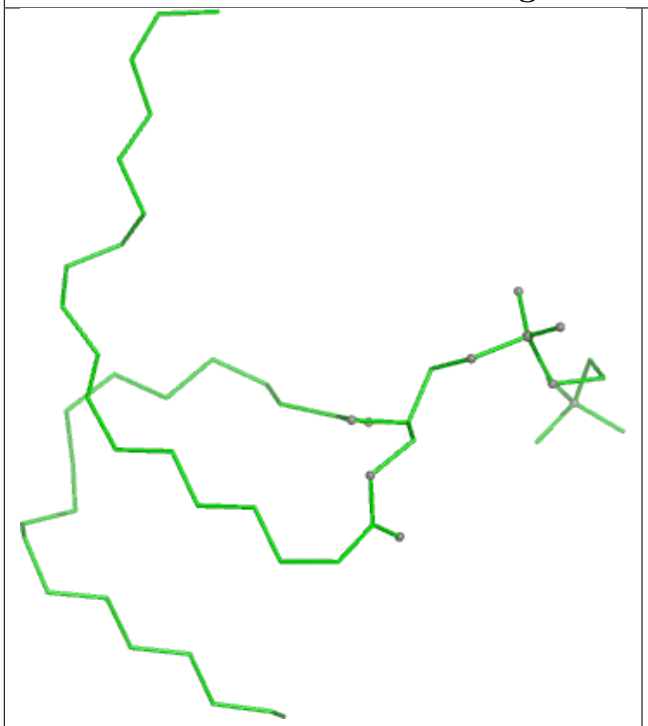
 Bond lengths	 Bond angles
 Torsions	Rings

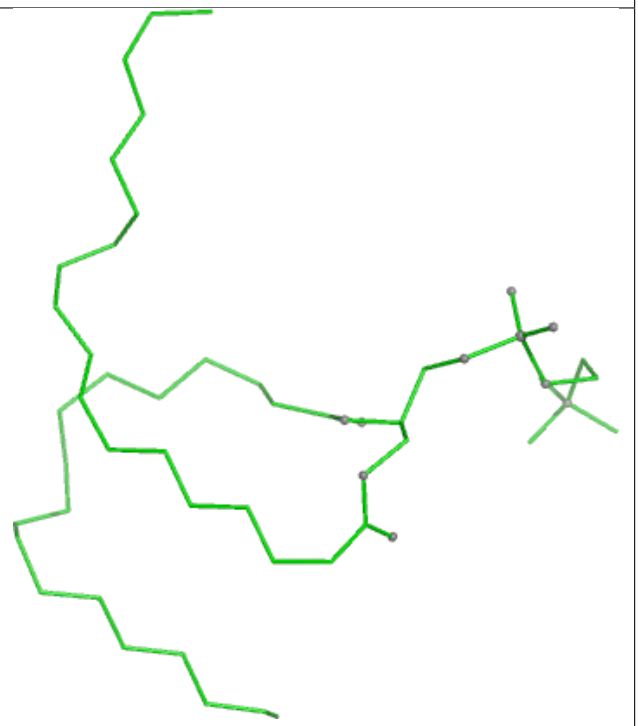
Ligand LPP A6 301



Ligand PC1 A6 302



Bond lengths



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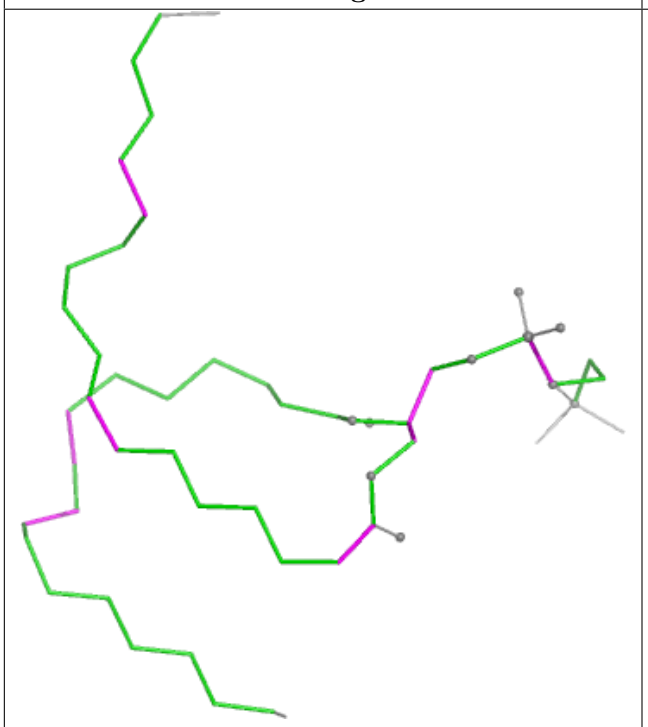

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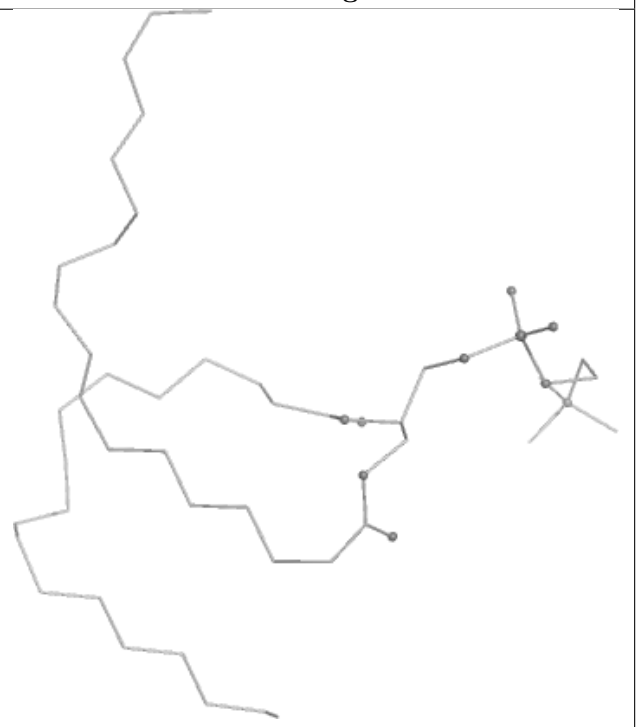

Rings

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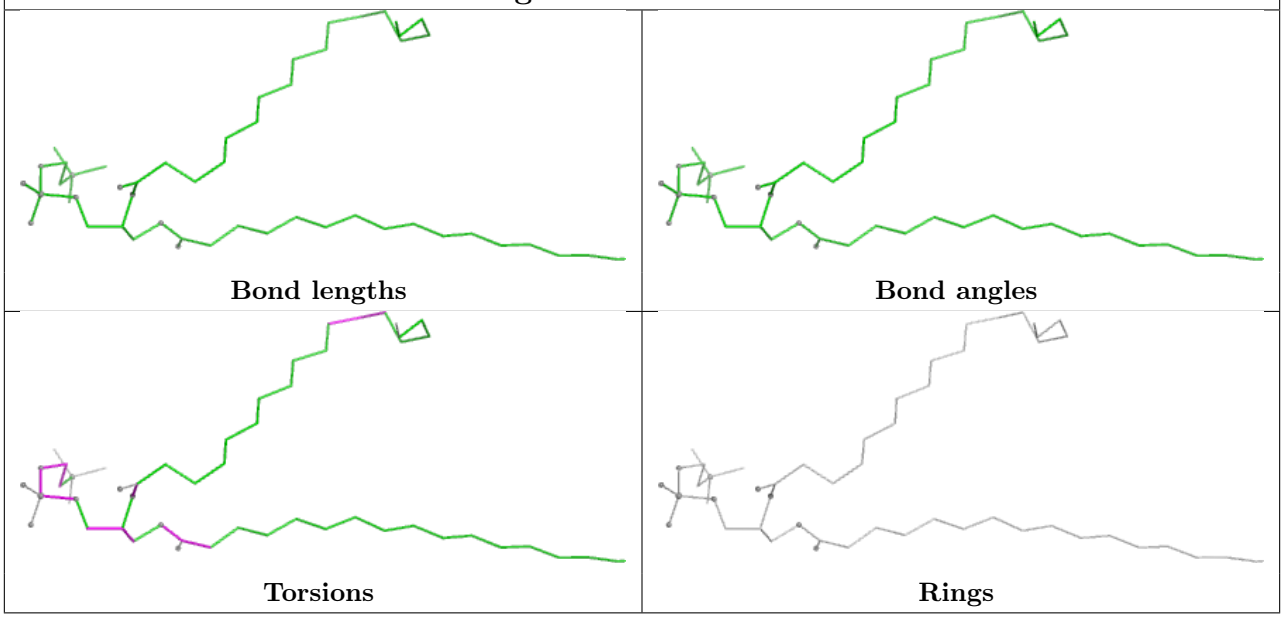
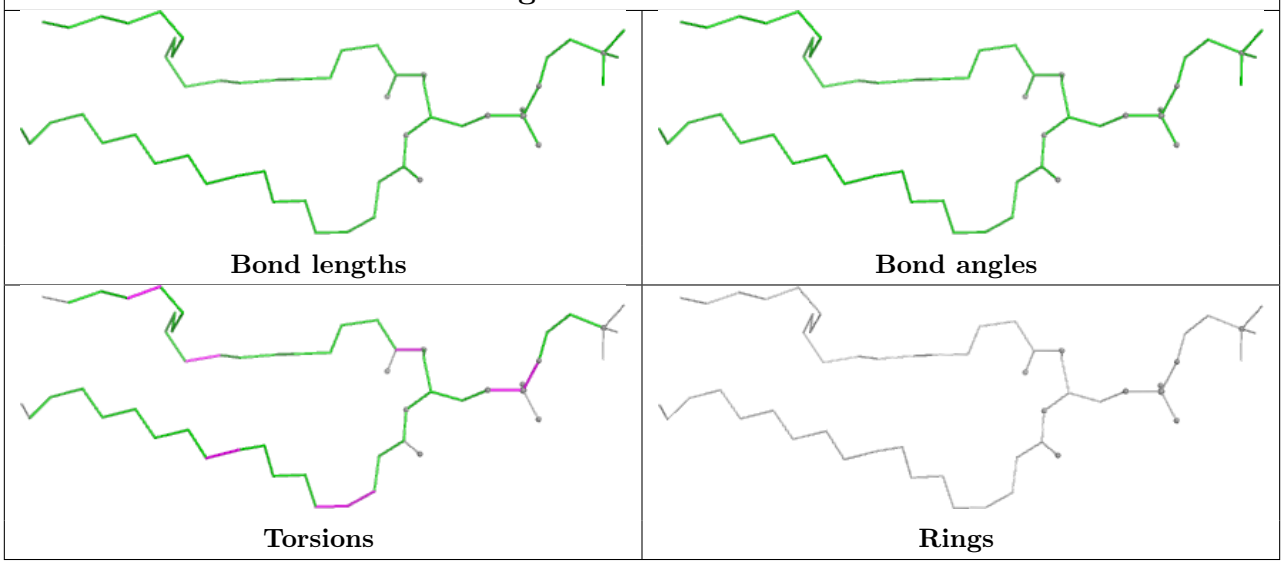


Ligand PC1 DJ 306



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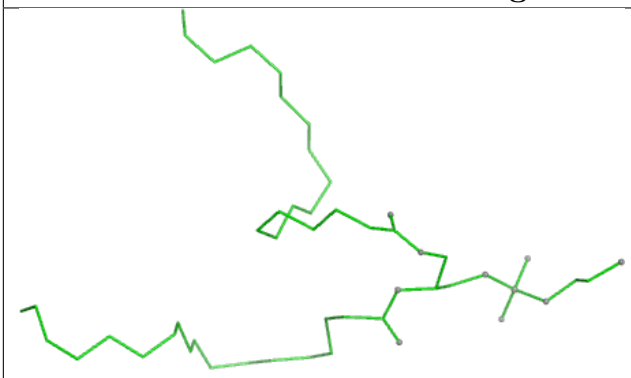
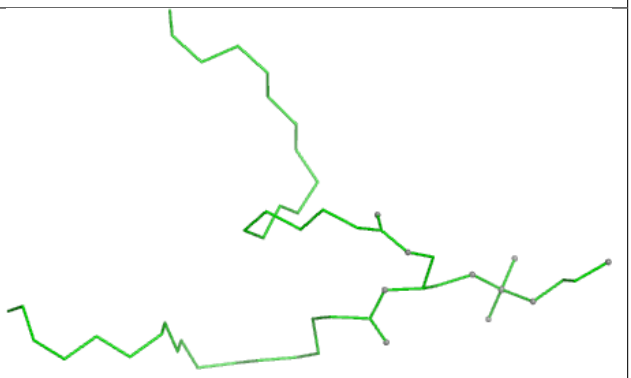
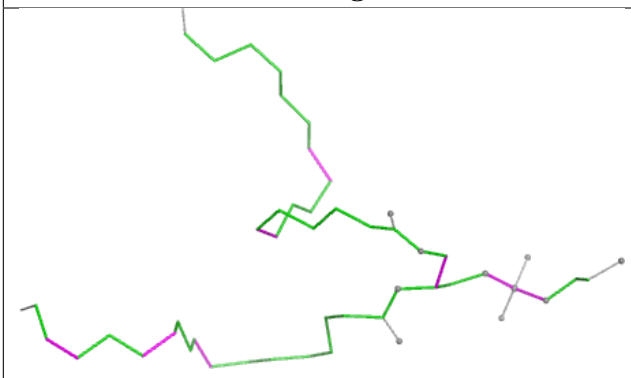
 Bond lengths	 Bond angles
 Torsions	Rings

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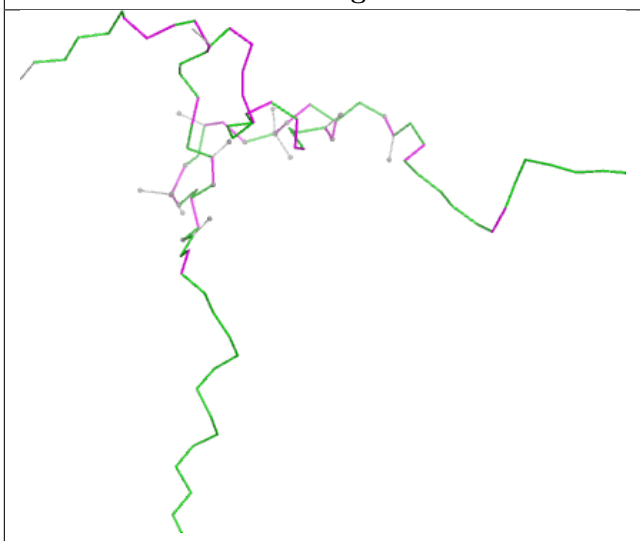
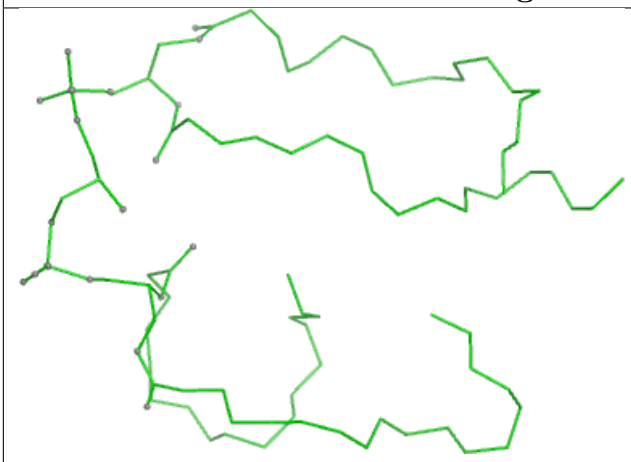
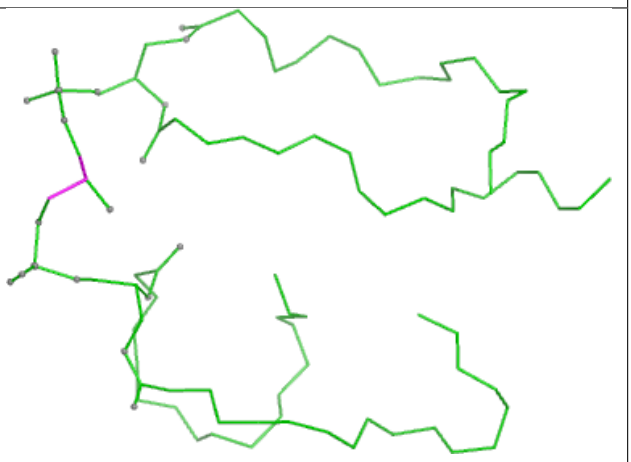
Bond lengths	**Bond angles**
 **Torsions**	**Rings**

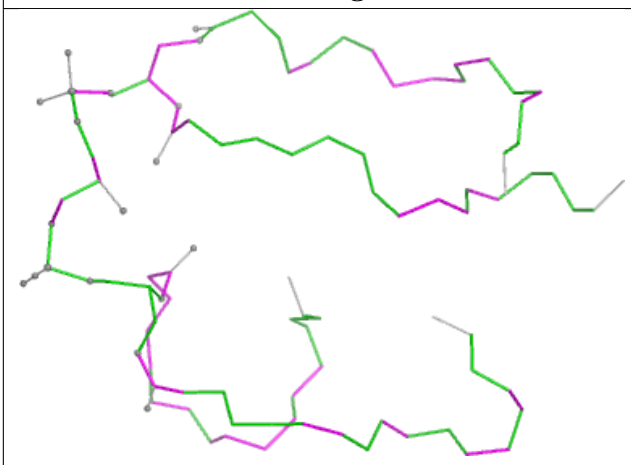
Ligand CDL Ds 405



Bond lengths



Bond angles



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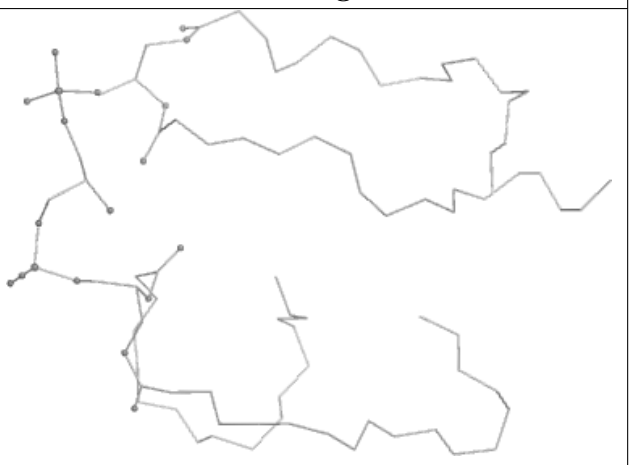

Rings

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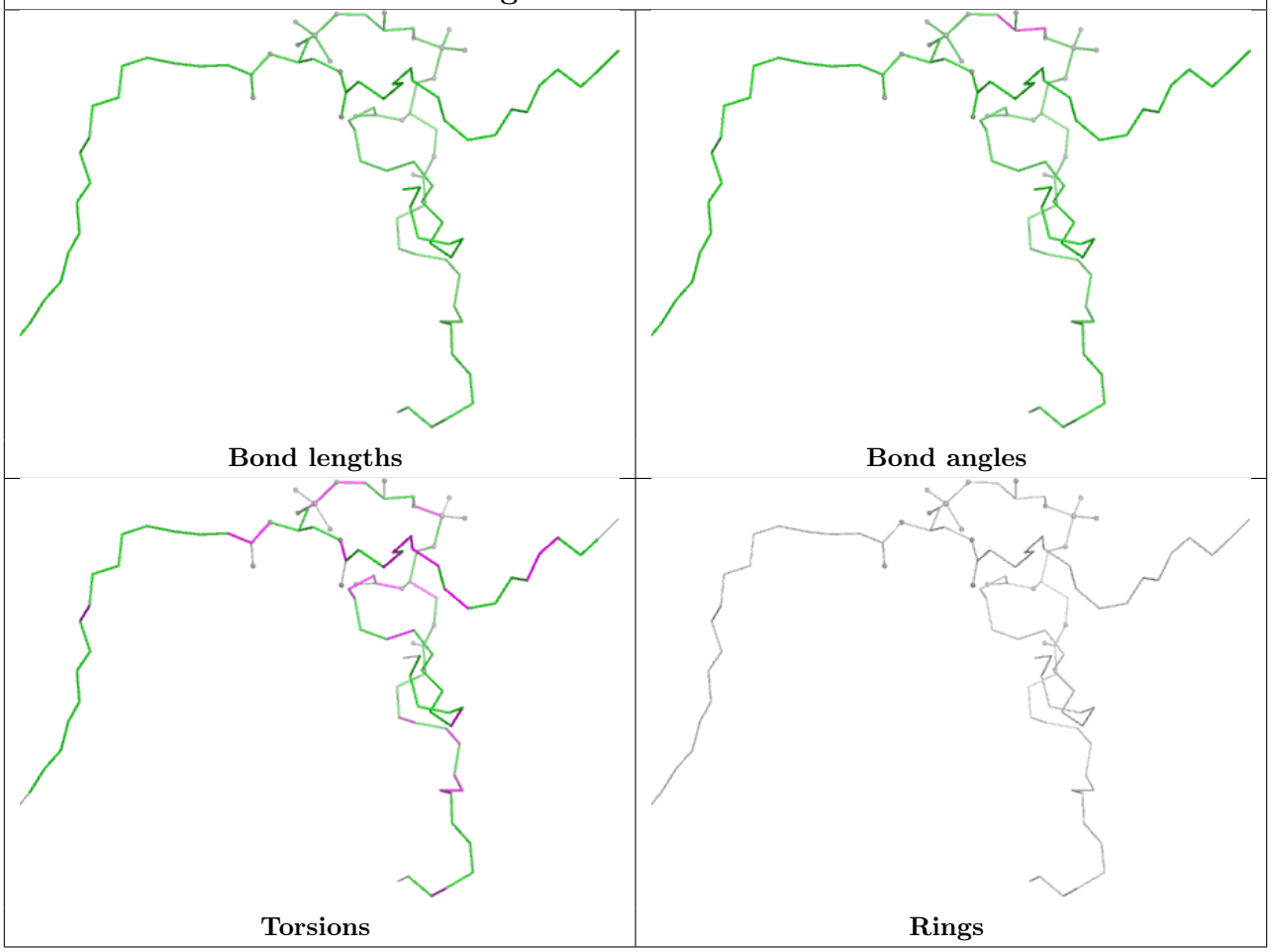

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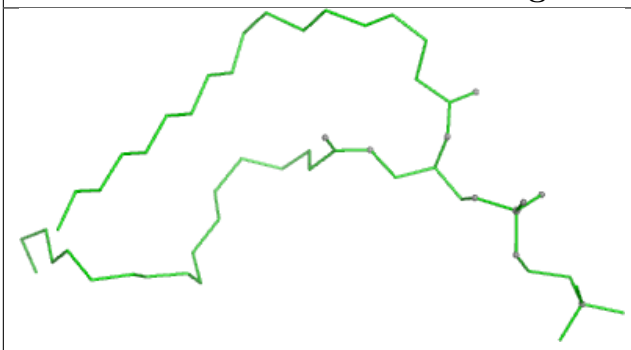
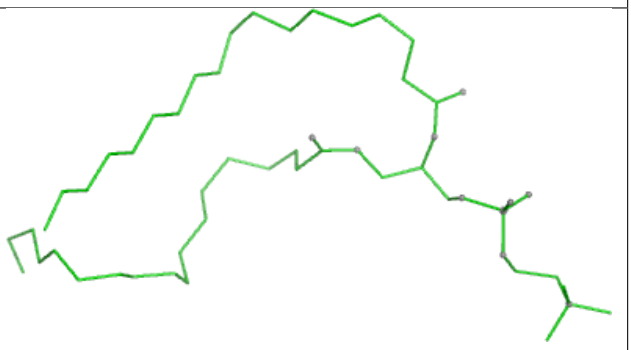
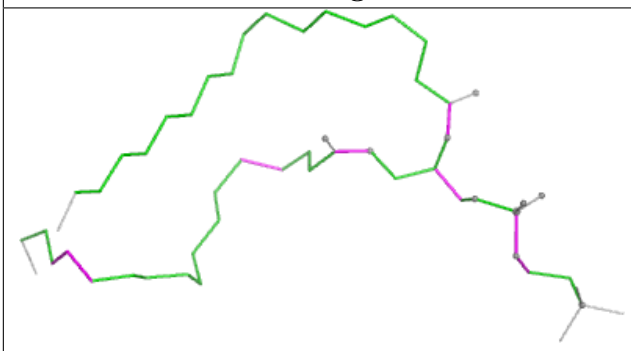
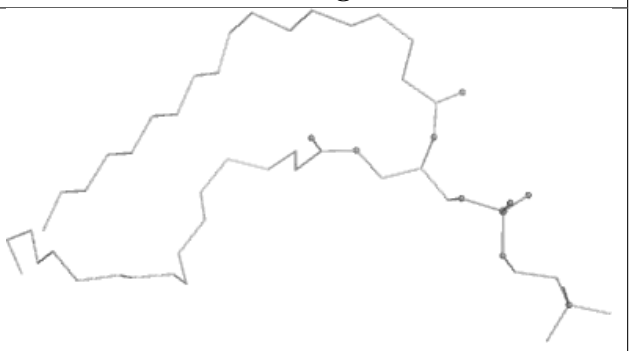
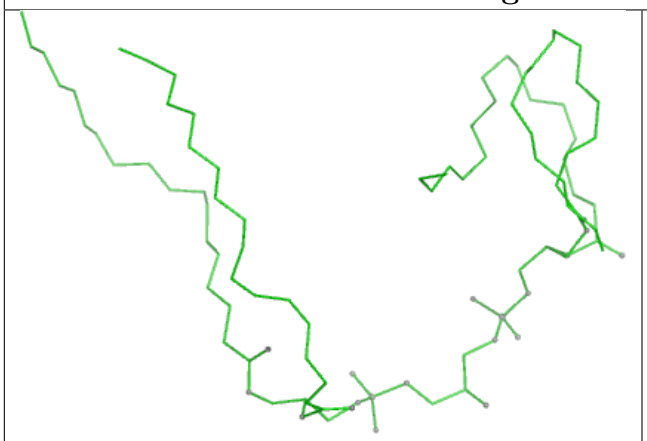
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL DQ 1504



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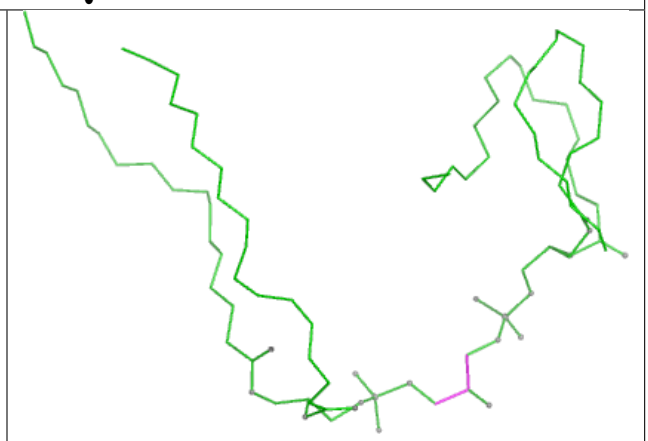

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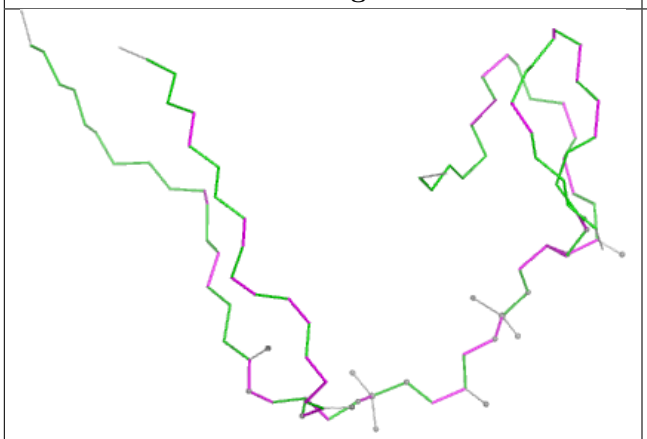

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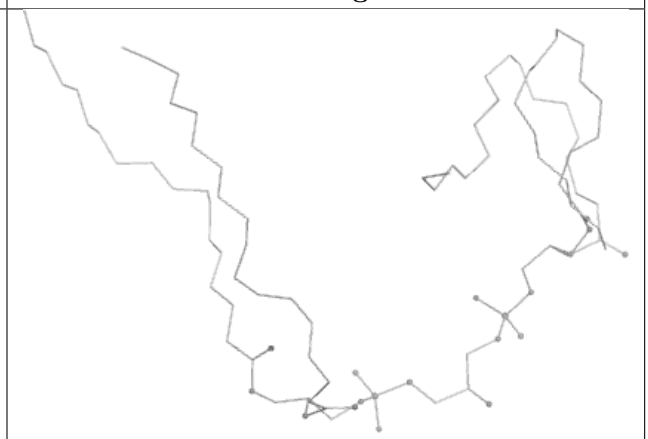
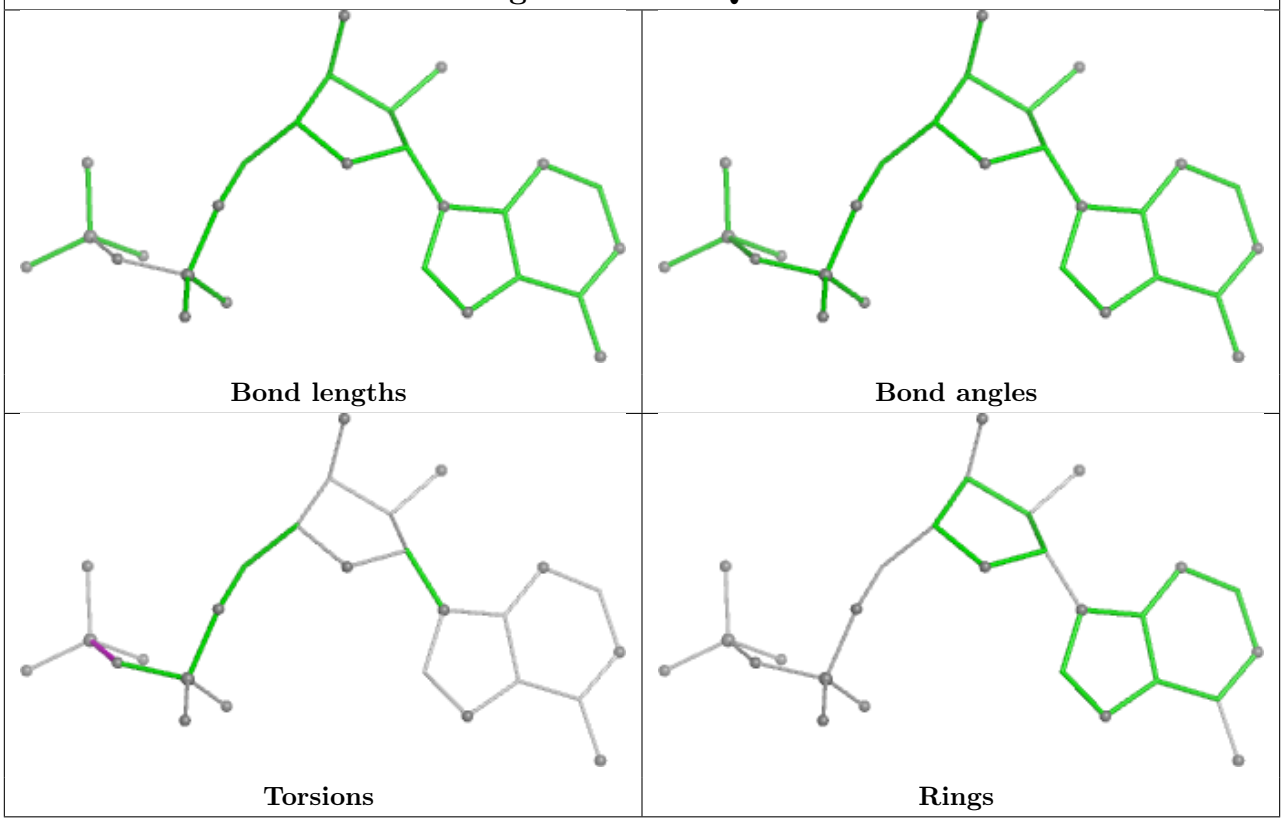


Rings

Ligand ADP AQ 201



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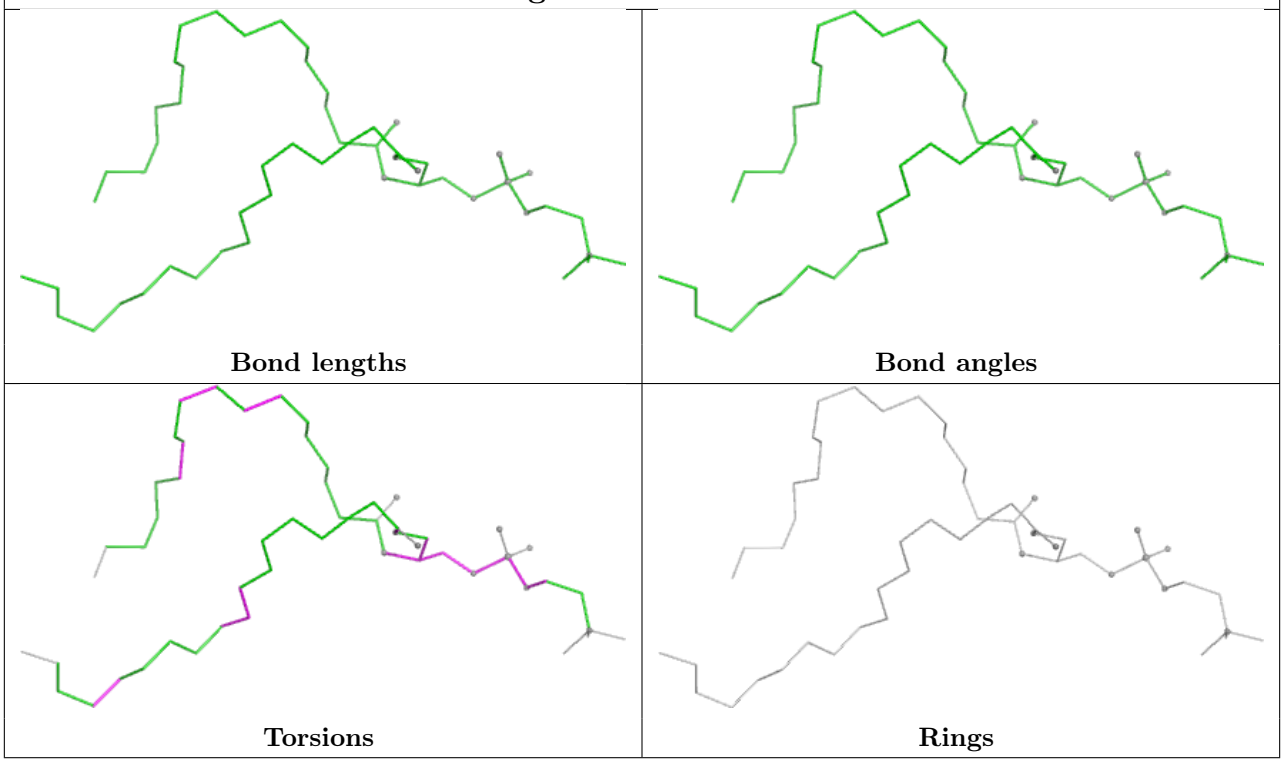

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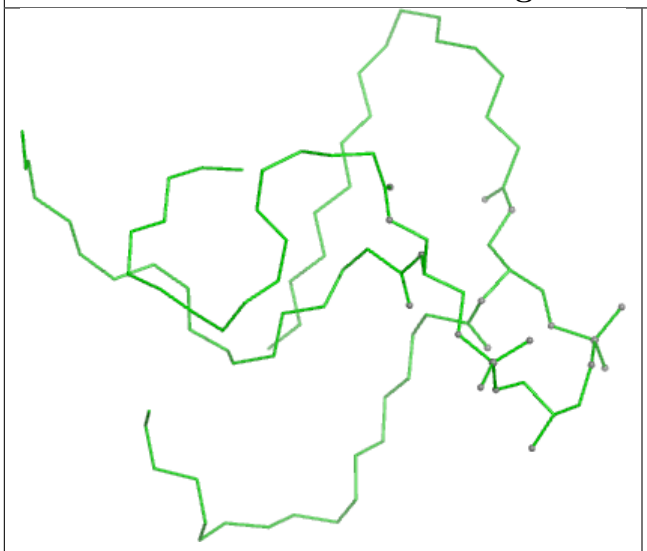

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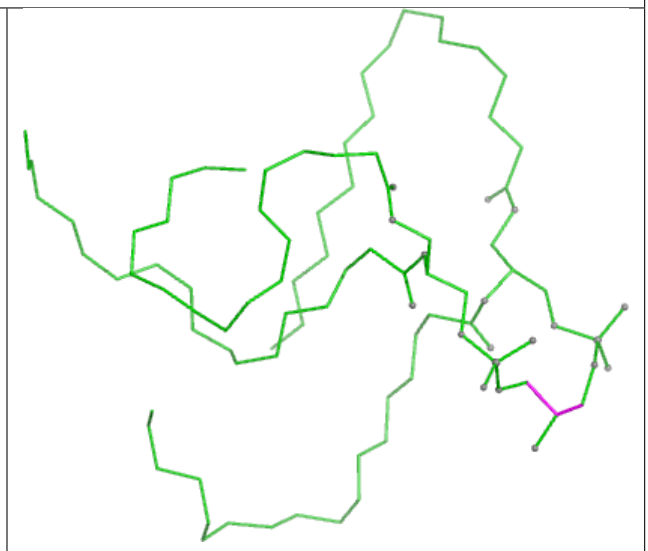

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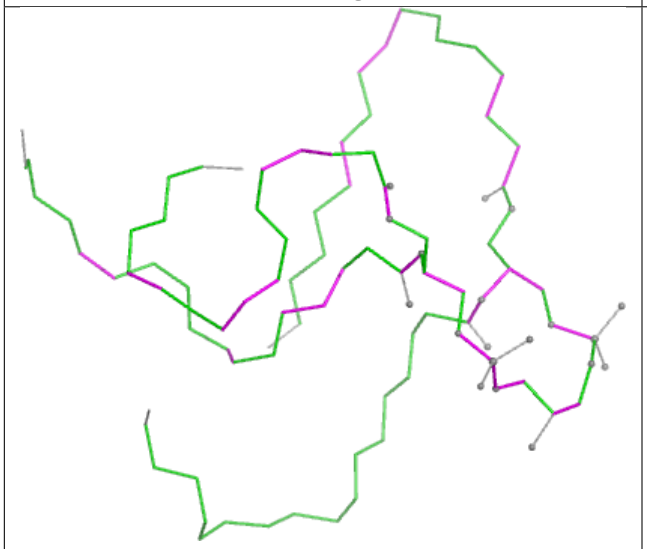
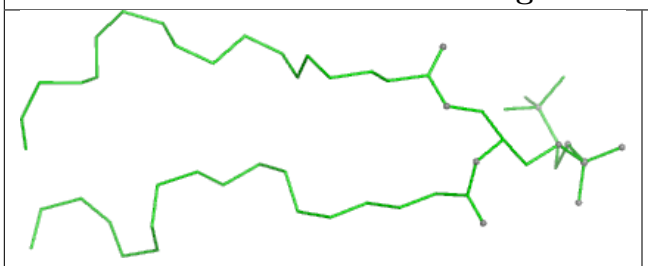


Torsions

Rings

Ligand PC1 EO 205



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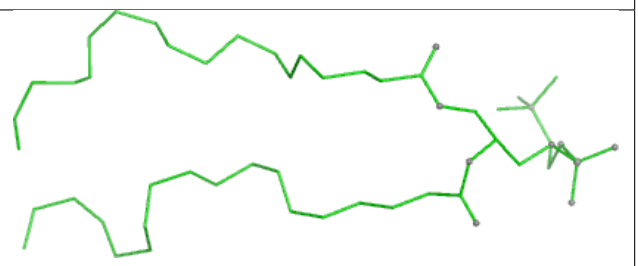

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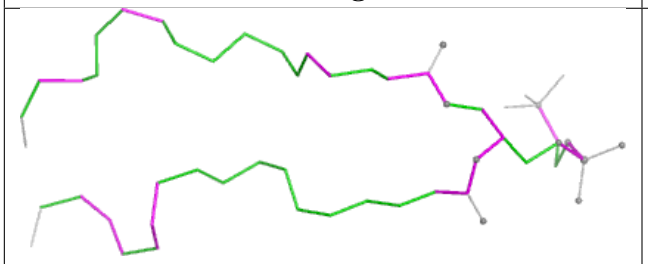

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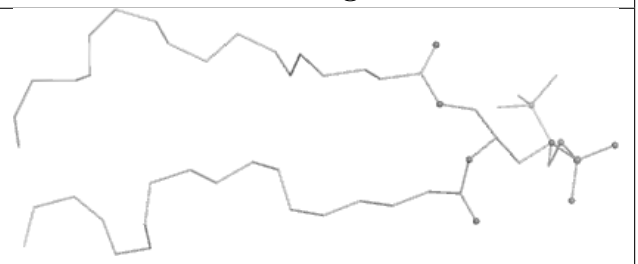
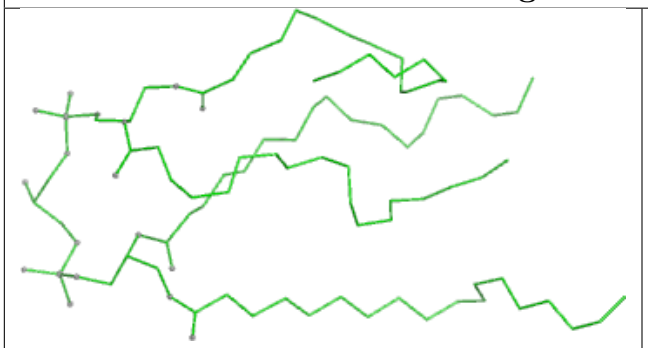


Rings

Ligand CDL Dj 405



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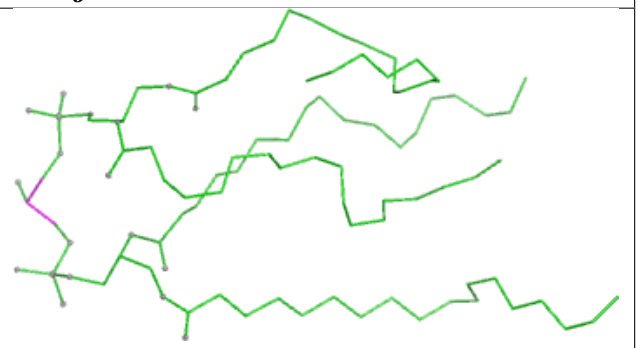

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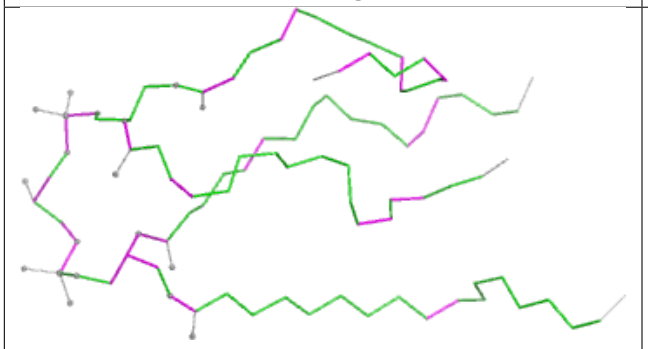
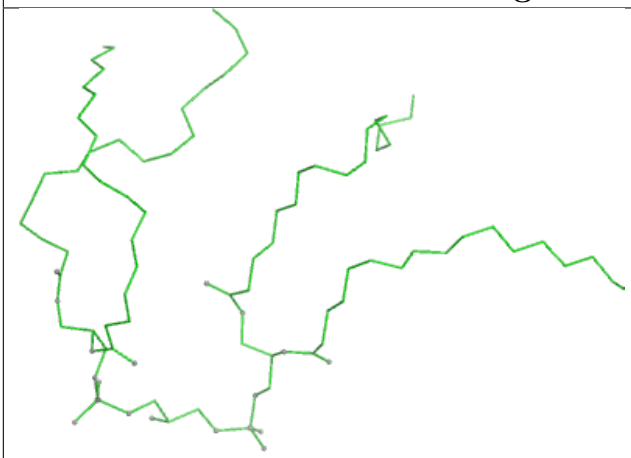
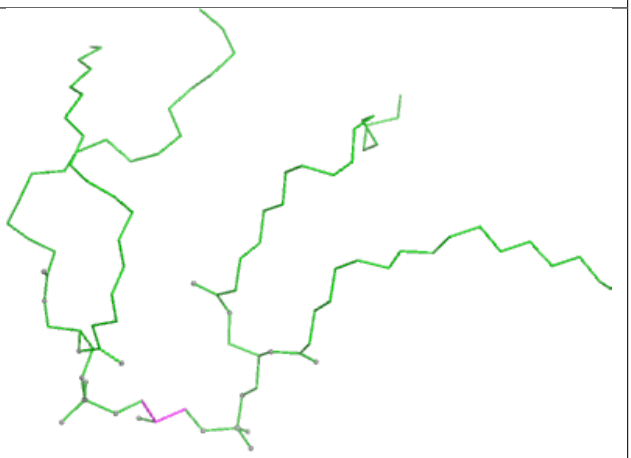


Torsions

Rings

Ligand CDL H 1301	
 Bond lengths	 Bond angles
Torsions	Rings

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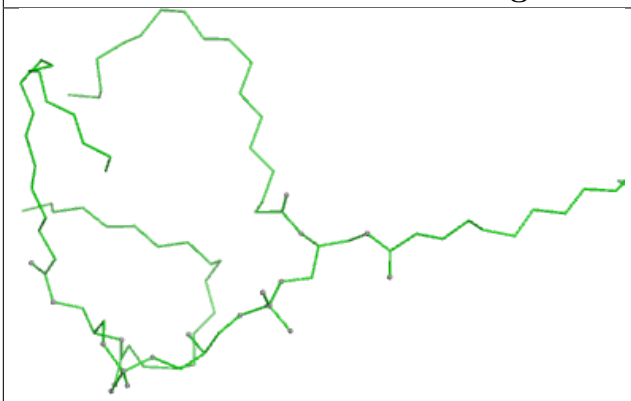
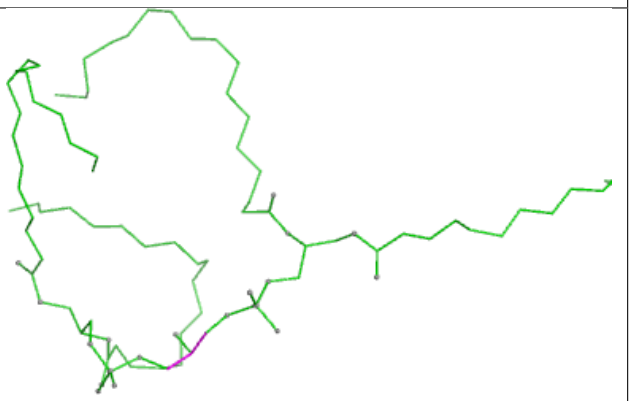
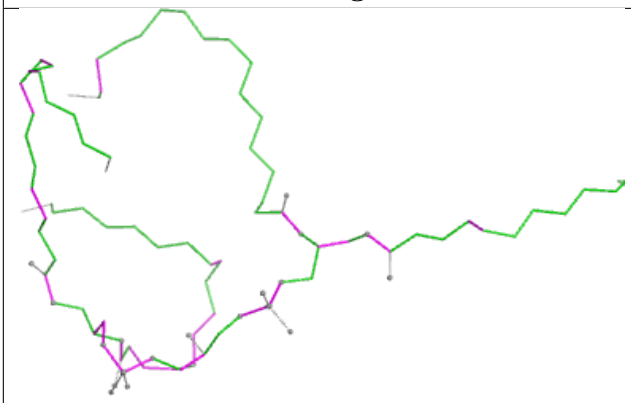
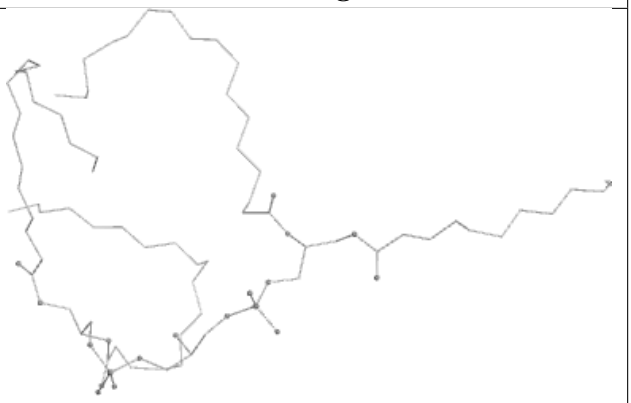
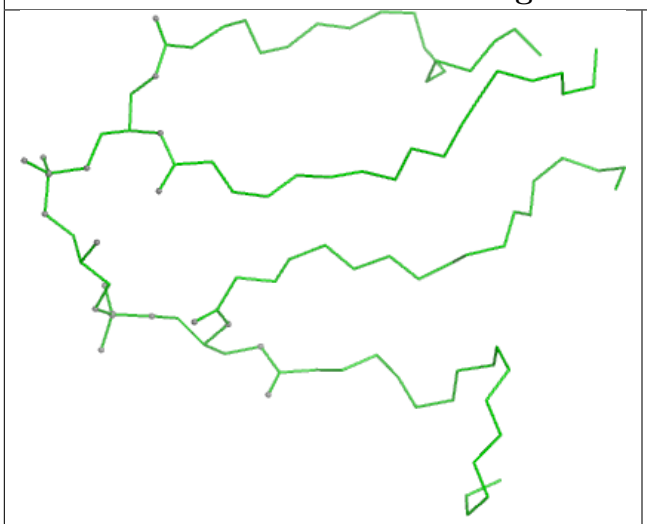
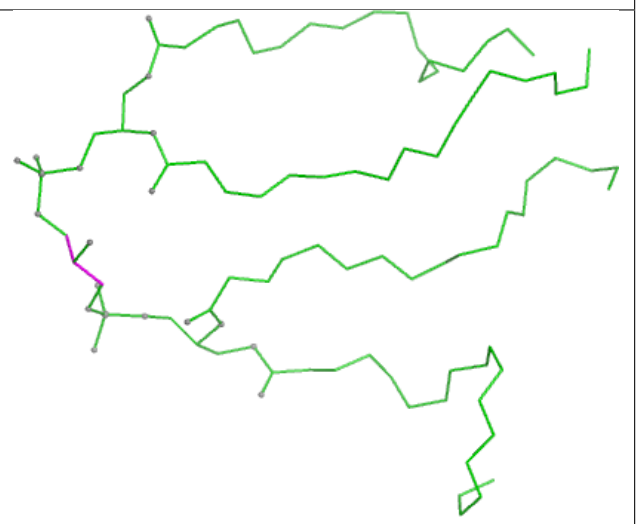
 Bond lengths	 Bond angles
 Torsions	 Rings

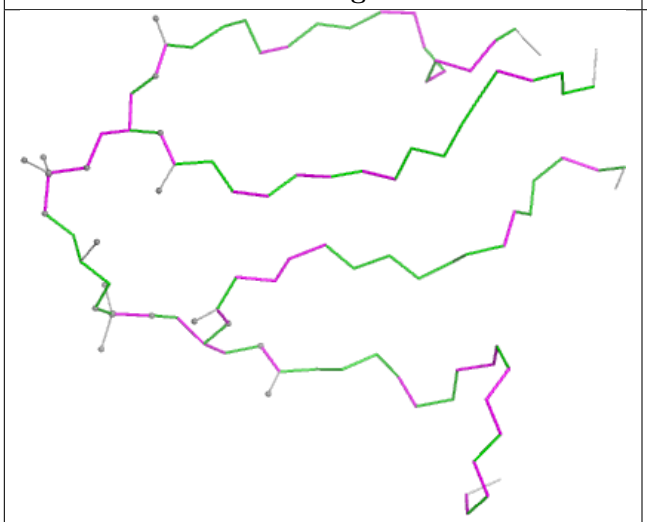
Ligand CDL EL 901



Bond lengths



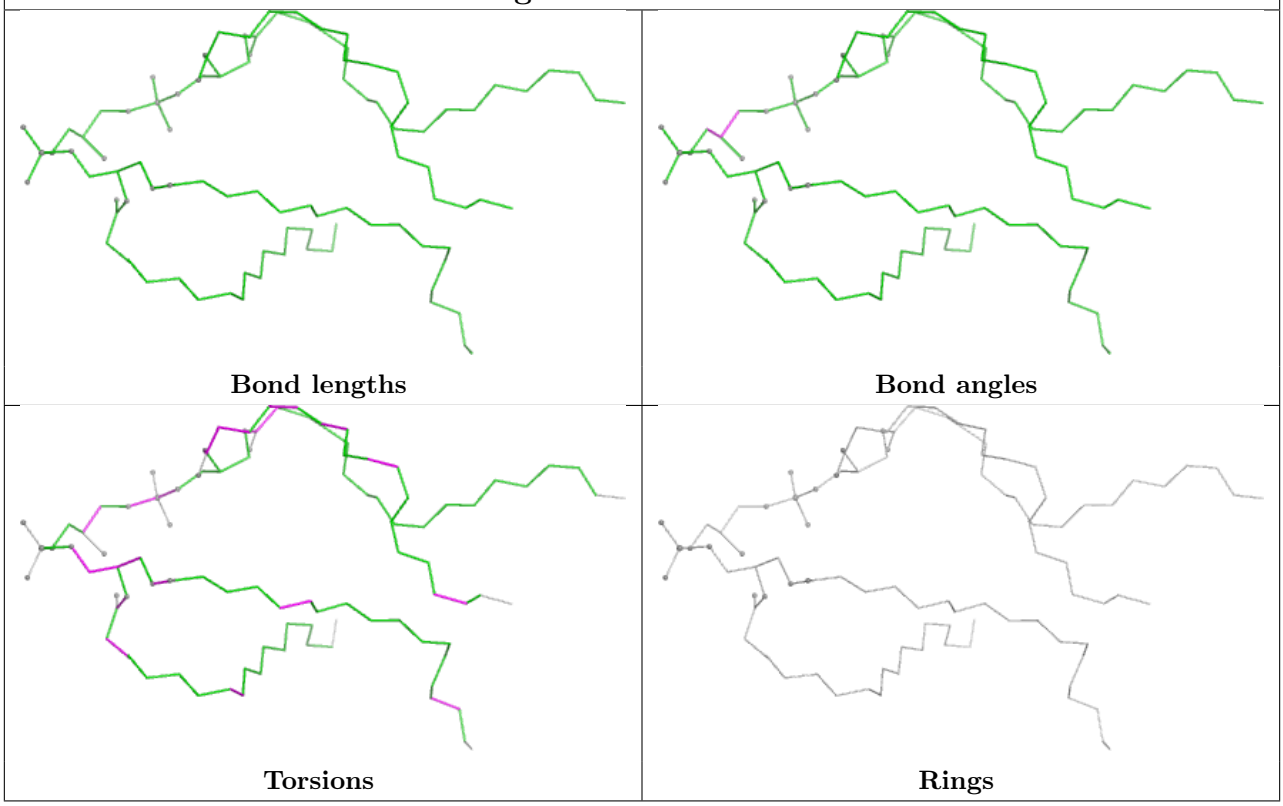
Bond angles



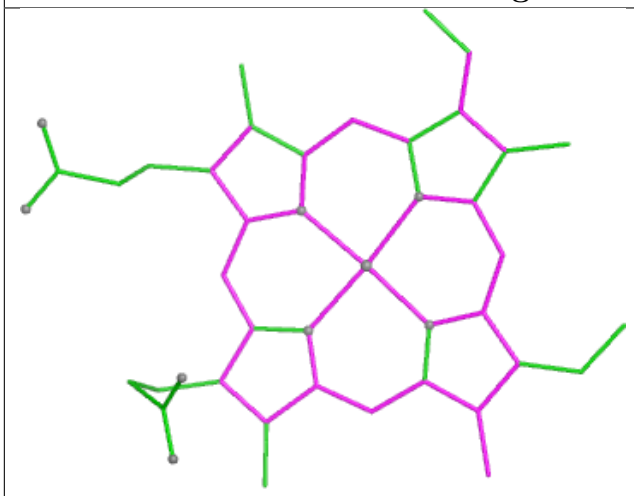
Torsions

Rings

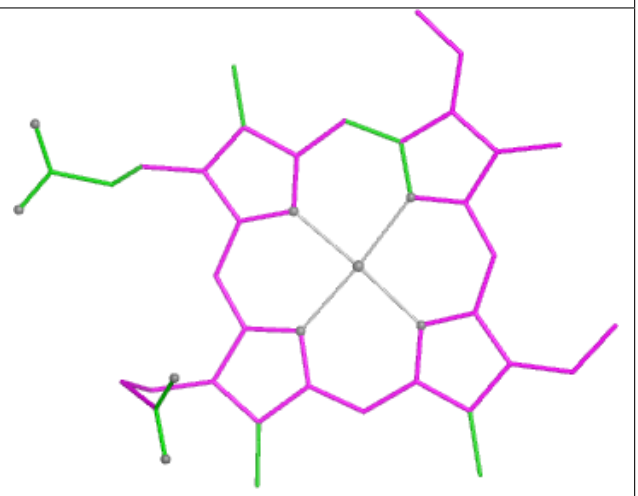
Ligand CDL Dn 503



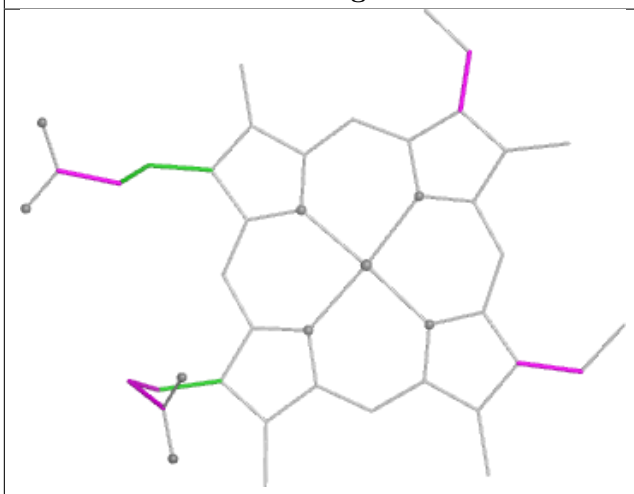
Ligand HEC CE 401



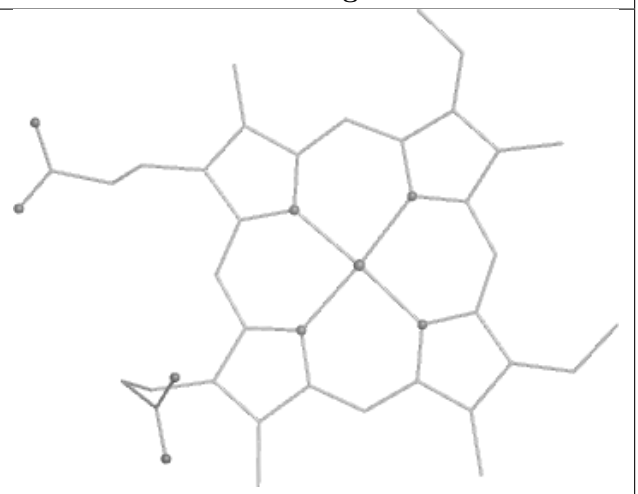
Bond lengths



Bond angles

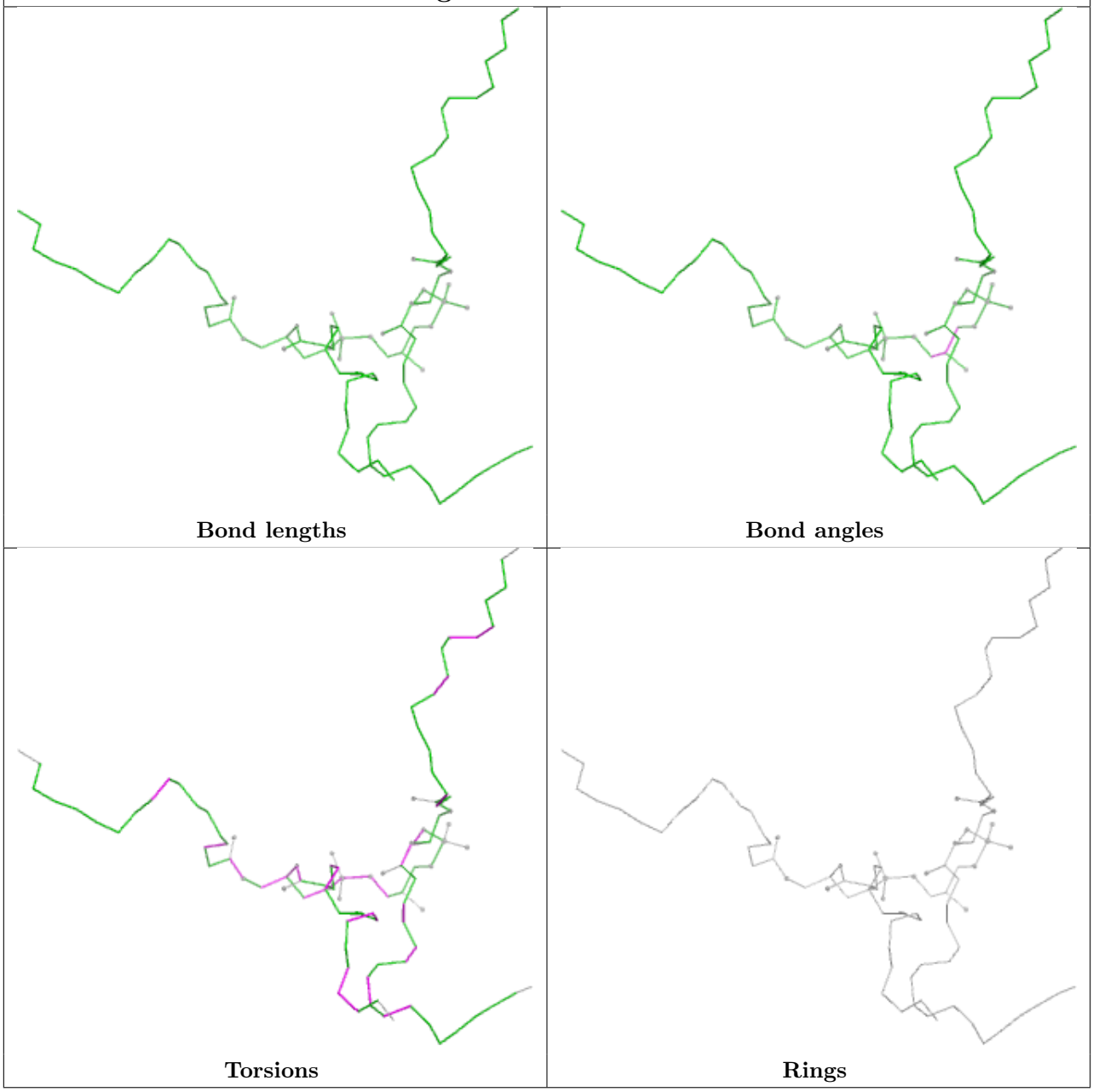


Torsions

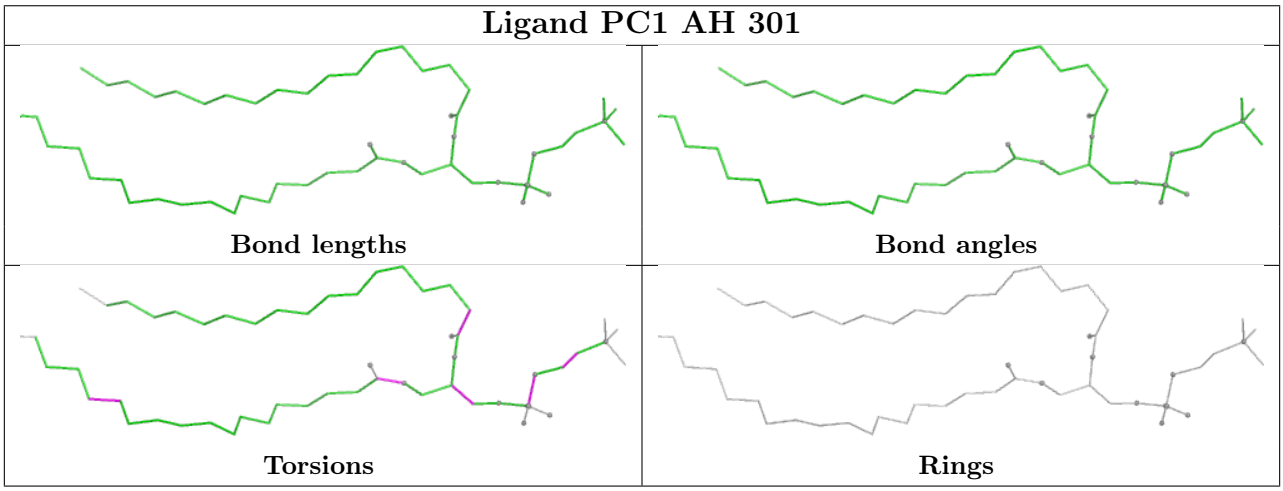


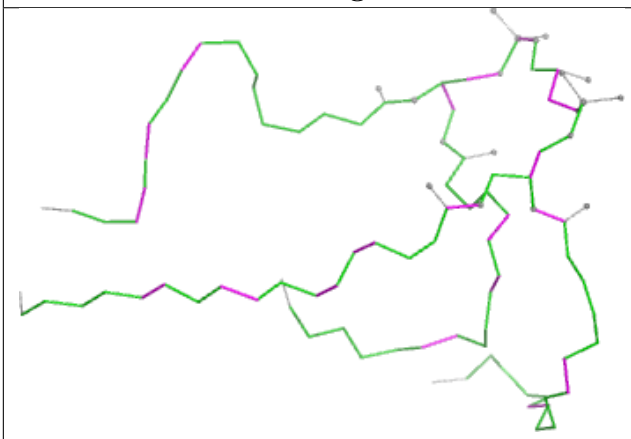
Rings

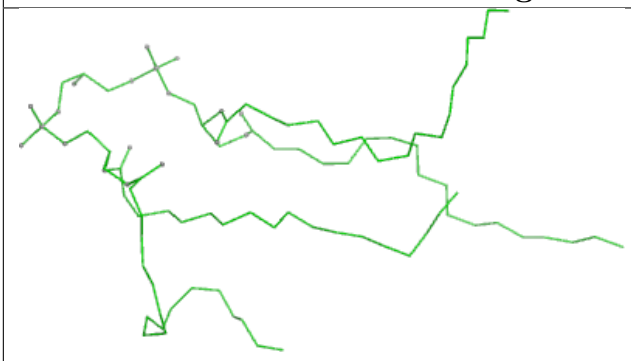
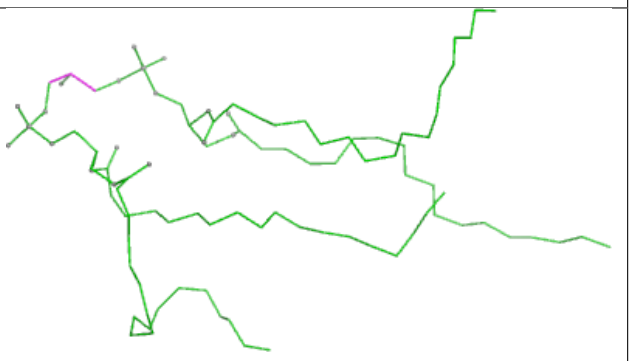
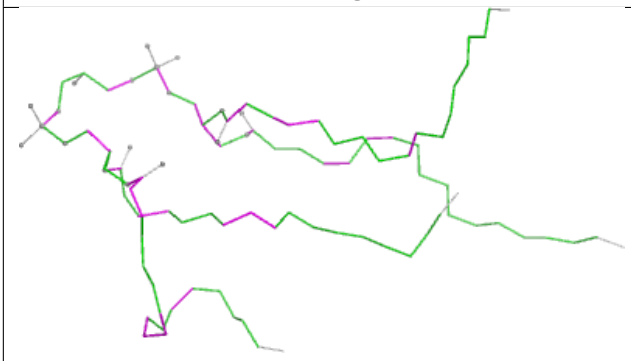
Ligand CDL EO 202



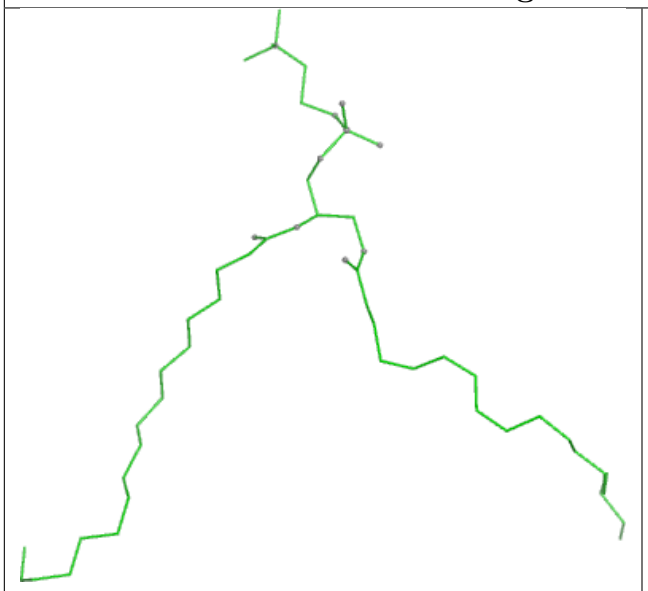
Ligand PC1 AH 301



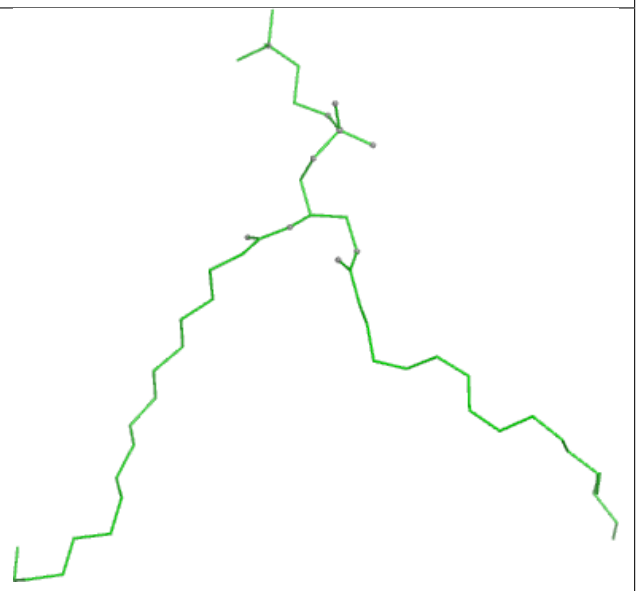
Ligand CDL c 502	
Bond lengths	Bond angles
 Torsions	Rings

Ligand CDL B1 402	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand PC1 EB 303

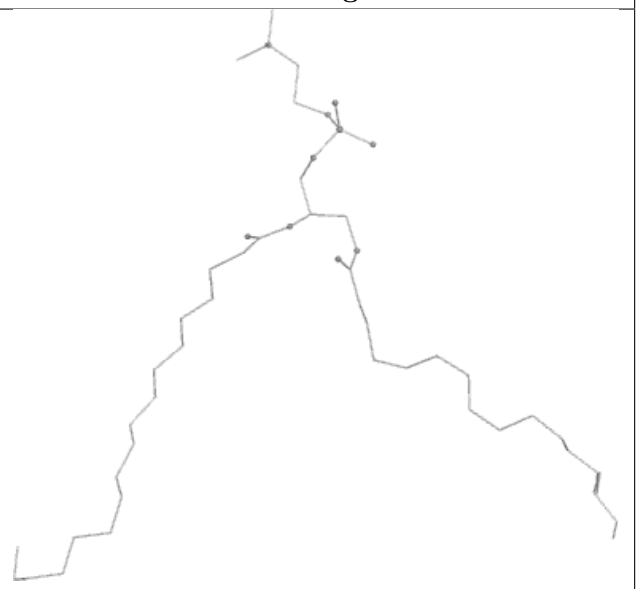


Bond lengths



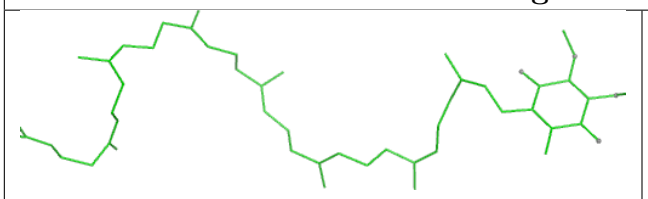
Bond angles

Torsions

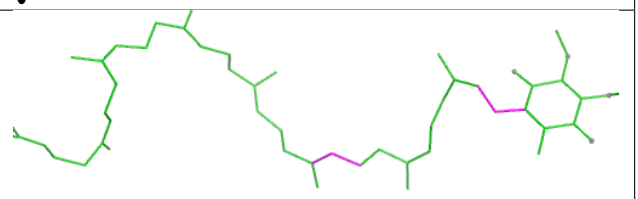


Rings

Ligand UQ8 c 510

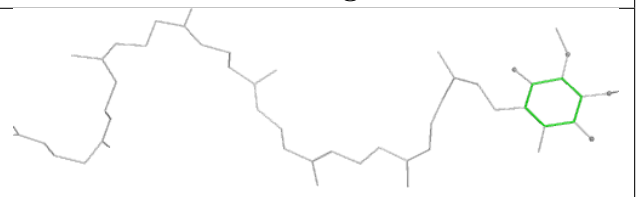


Bond lengths



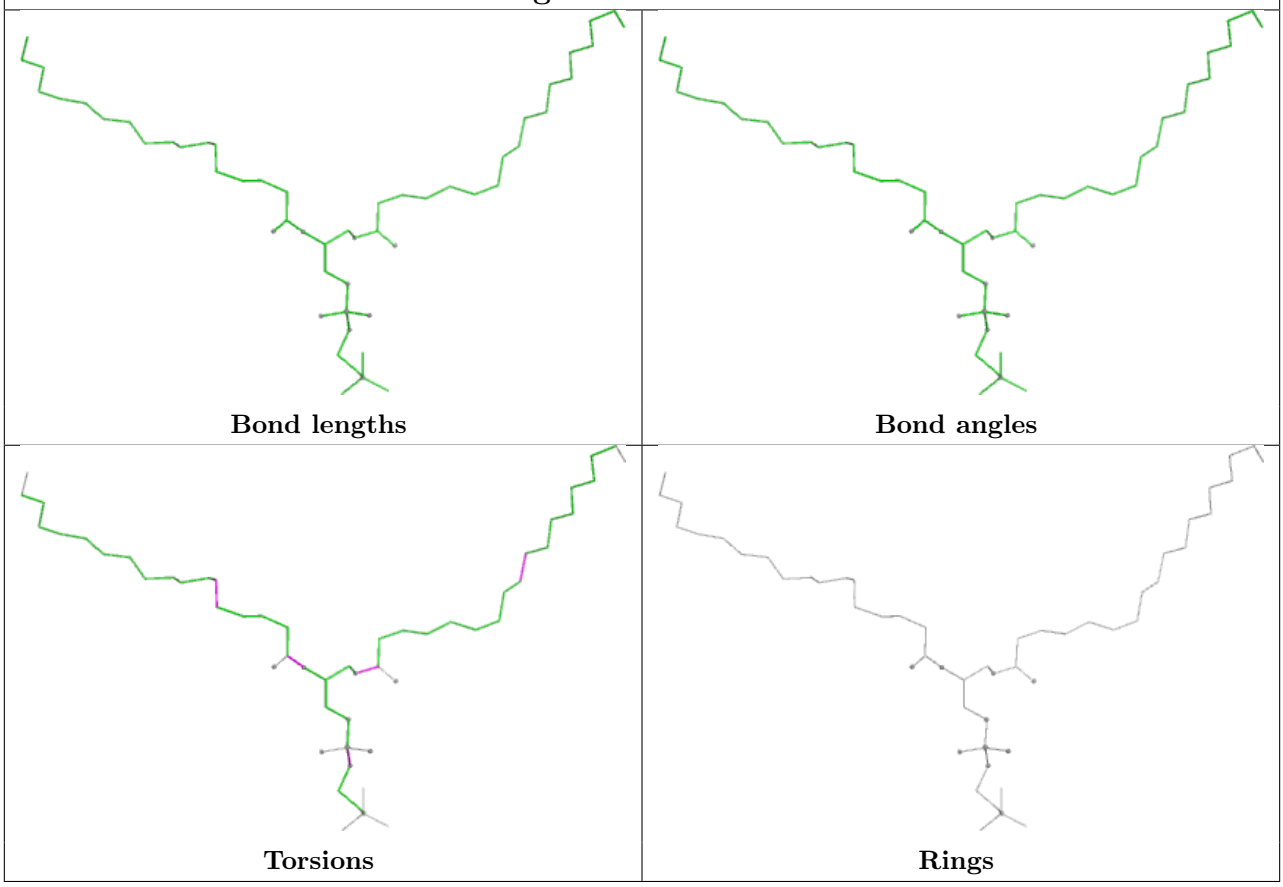
Bond angles

Torsions

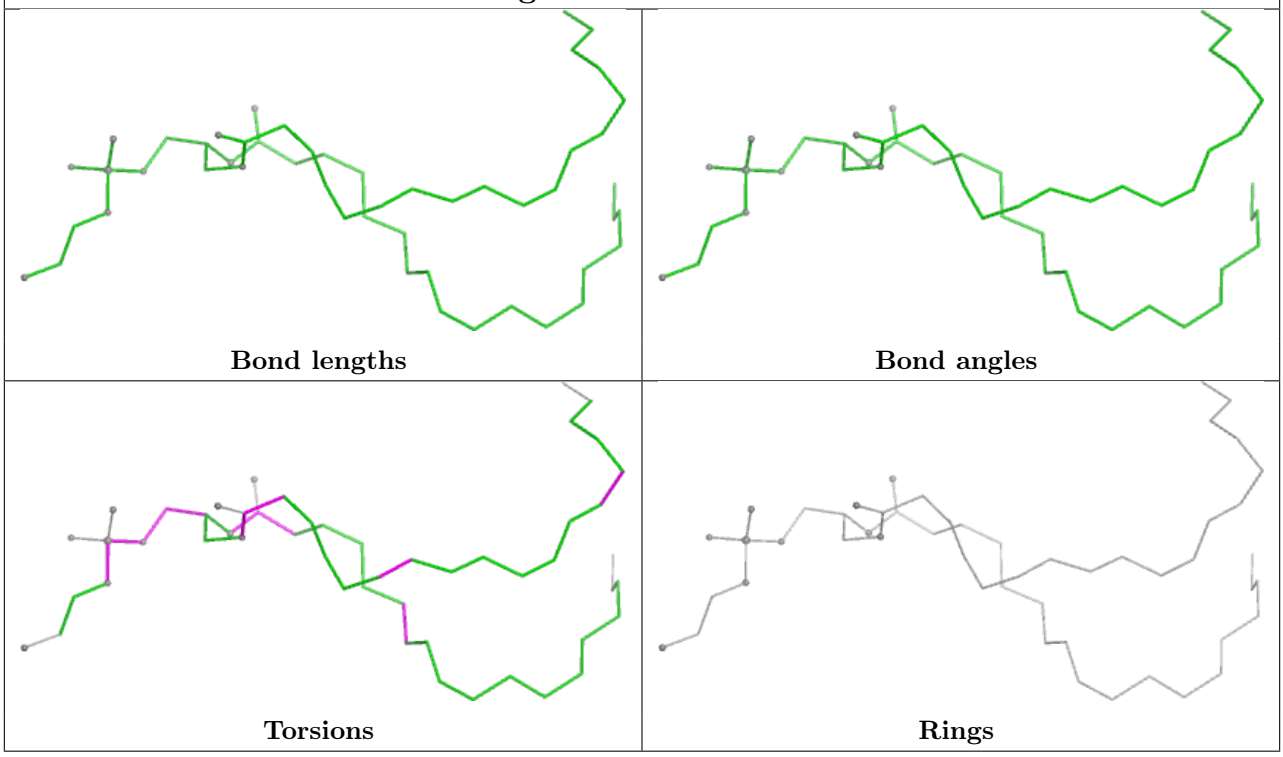


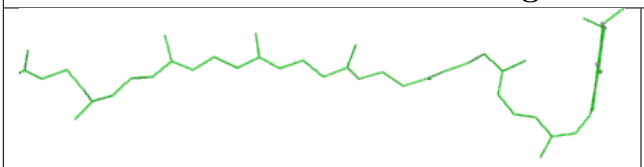
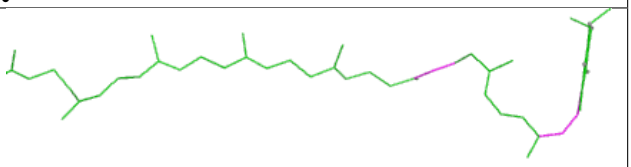
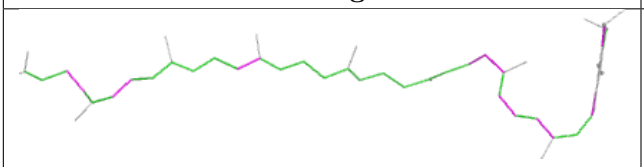
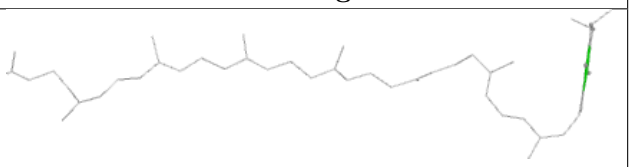
Rings

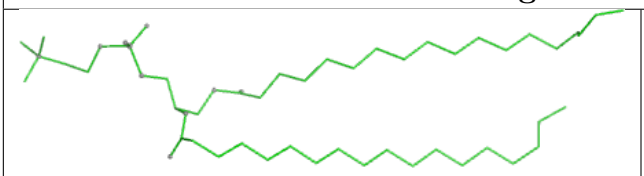
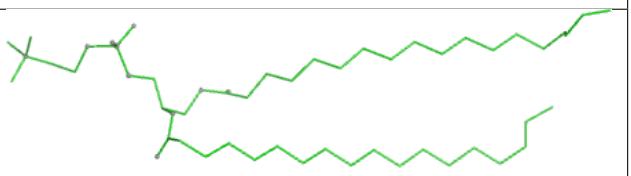
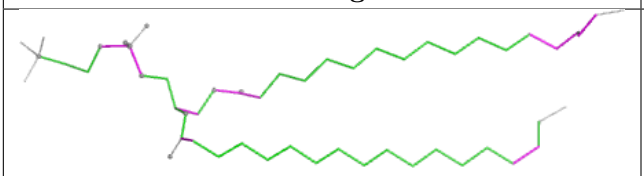
Ligand PC1 c 508

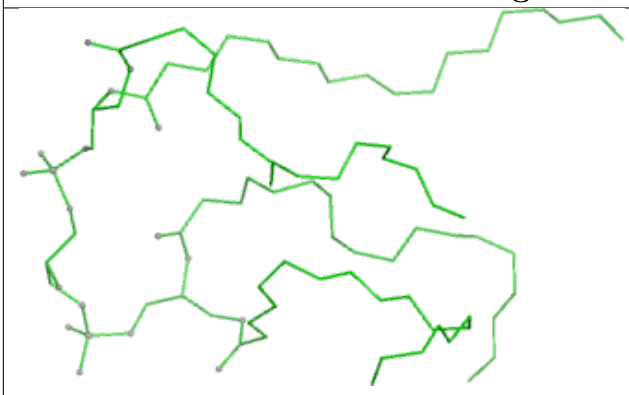
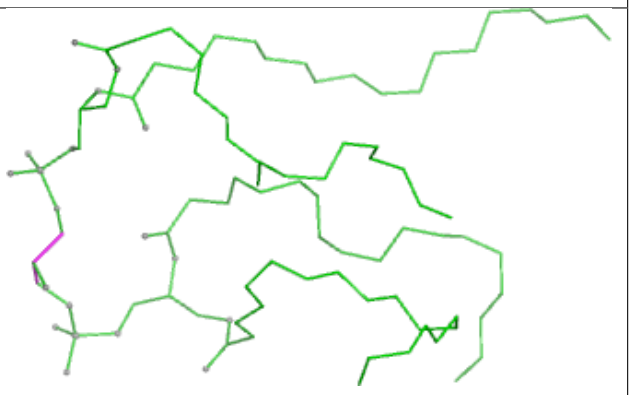
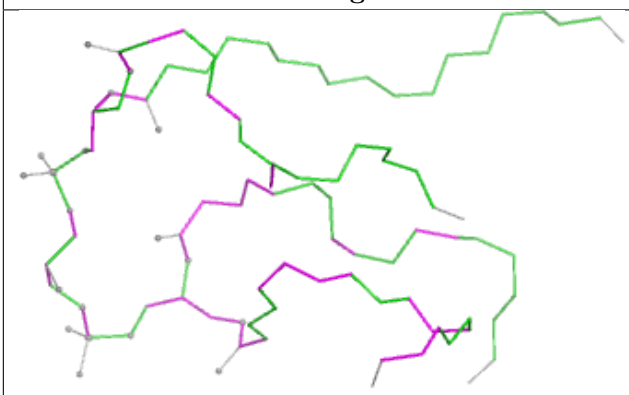
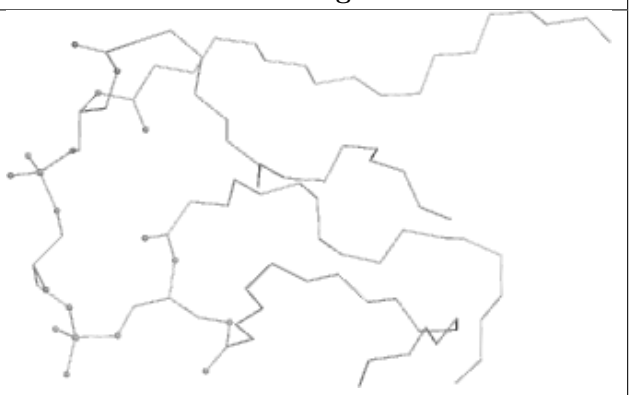


Ligand 3PE Dd 703

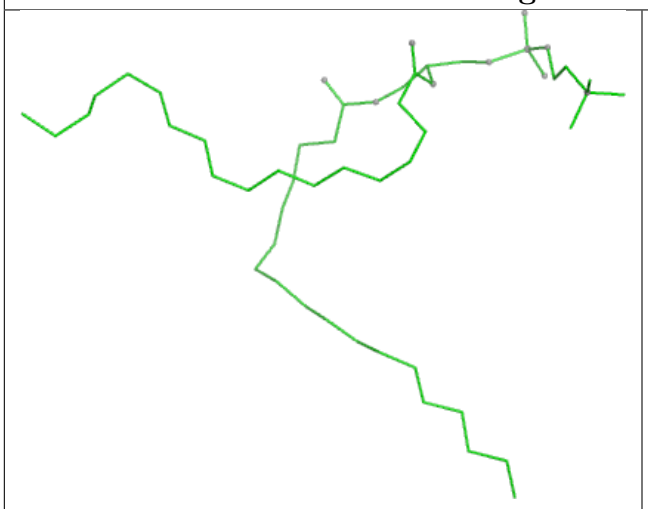


Ligand UQ8 El 906	
 Bond lengths	 Bond angles
 Torsions	 Rings

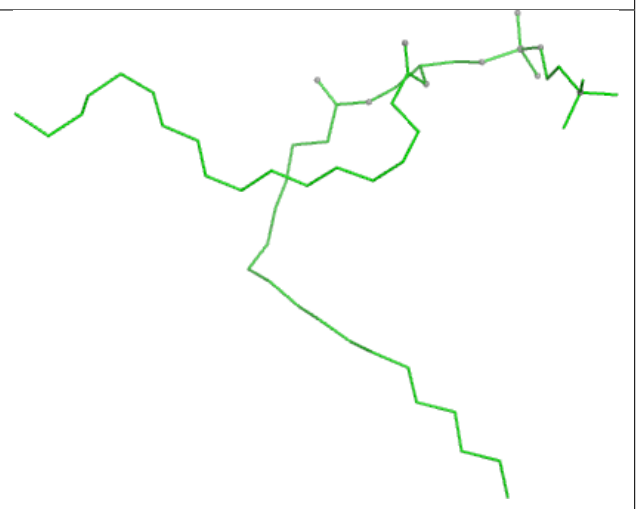
Ligand PC1 Dc 602	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL DZ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 A9 601



Bond lengths

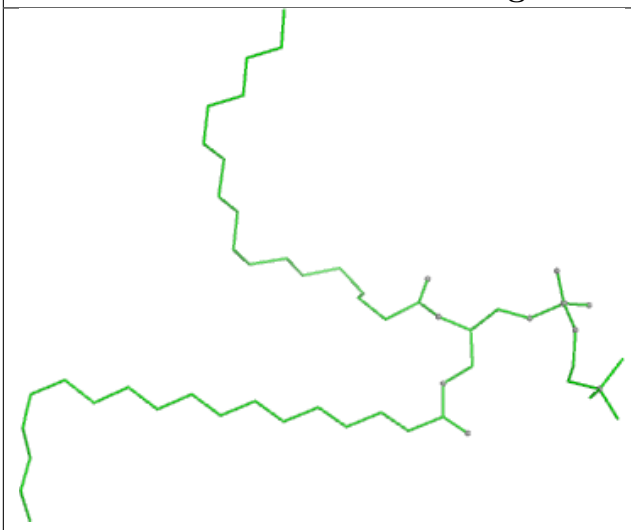


Bond angles

Torsions

Rings

Ligand PC1 Dx 1209



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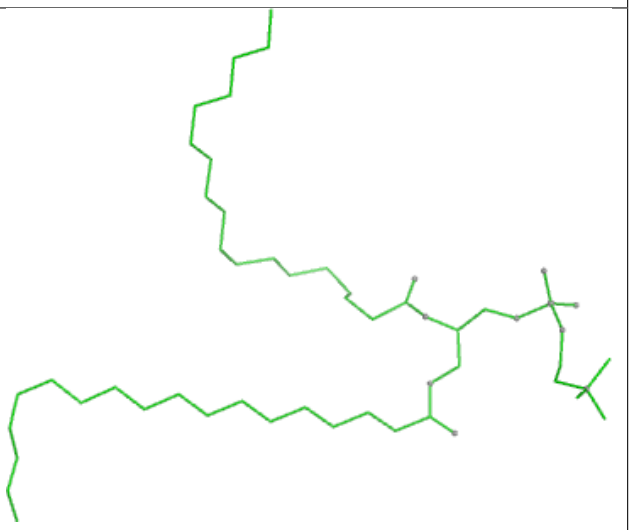
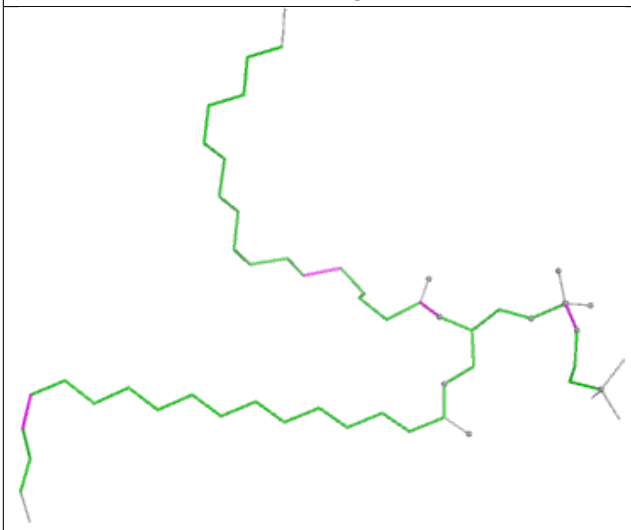
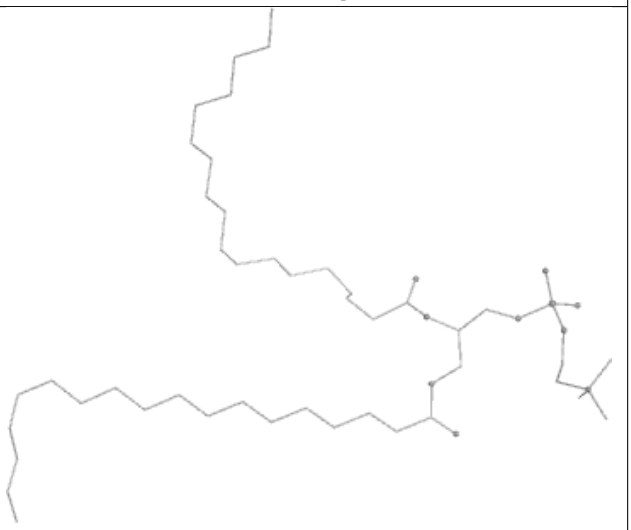


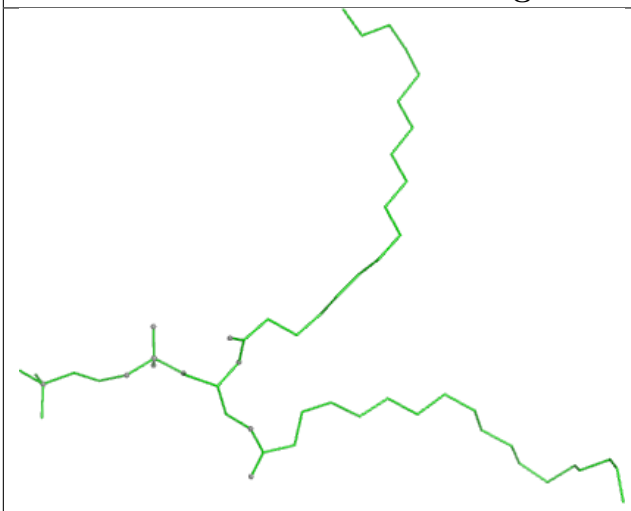
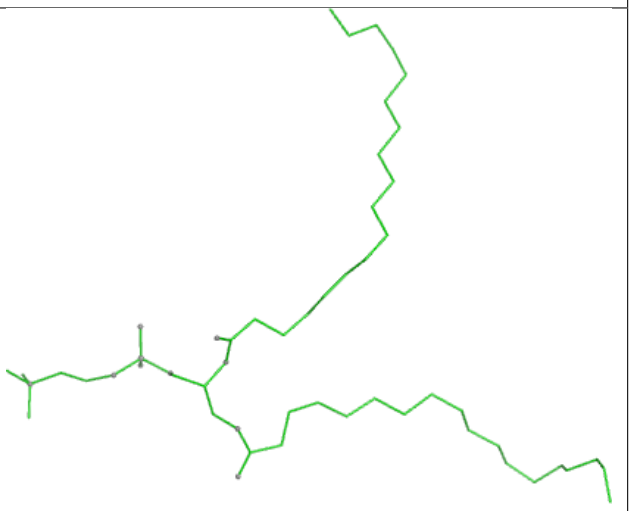
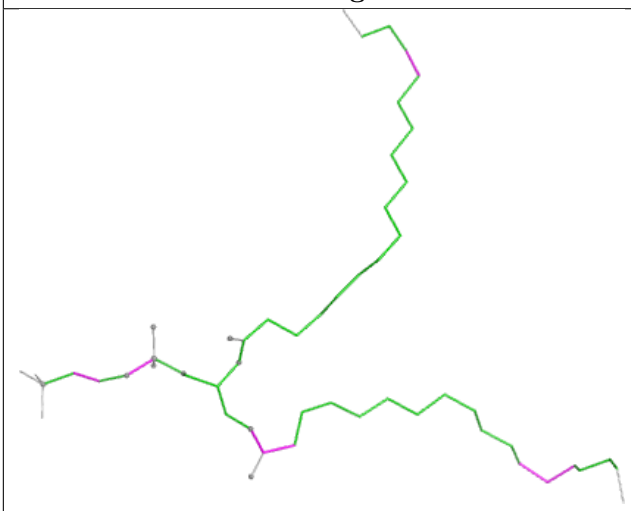
Bond angles



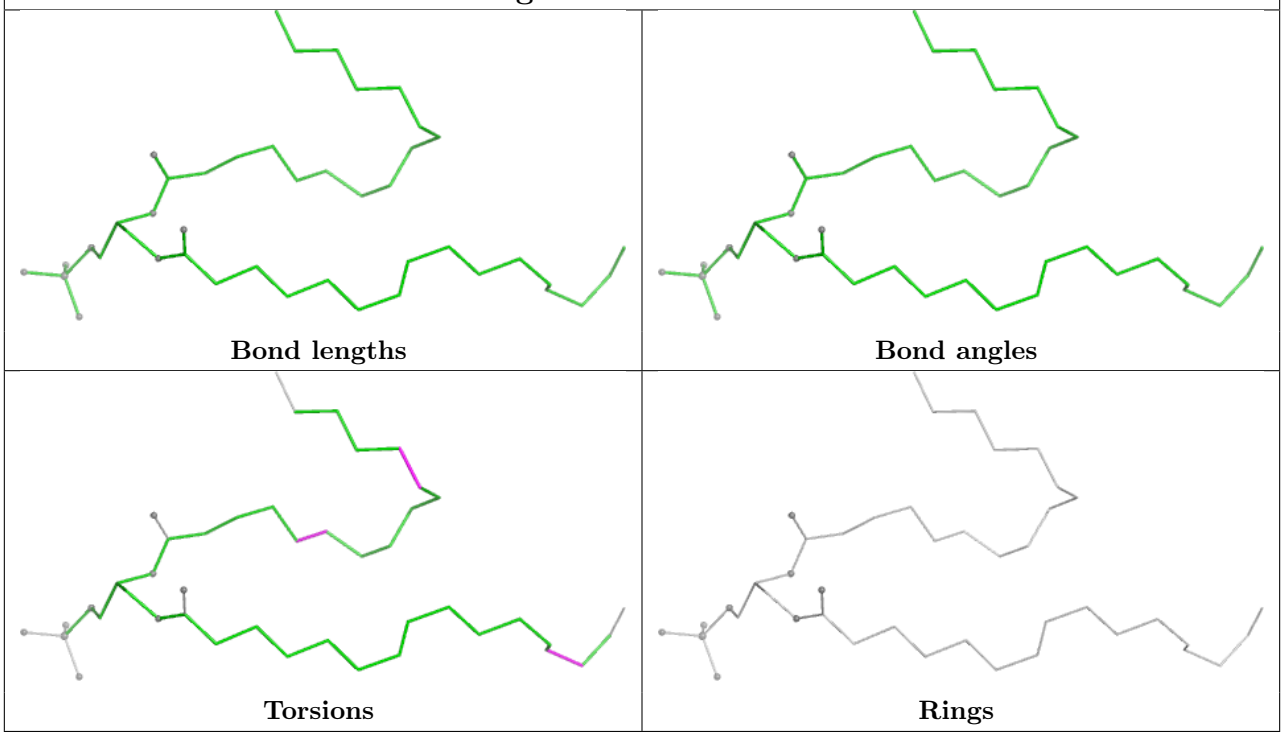
Torsions



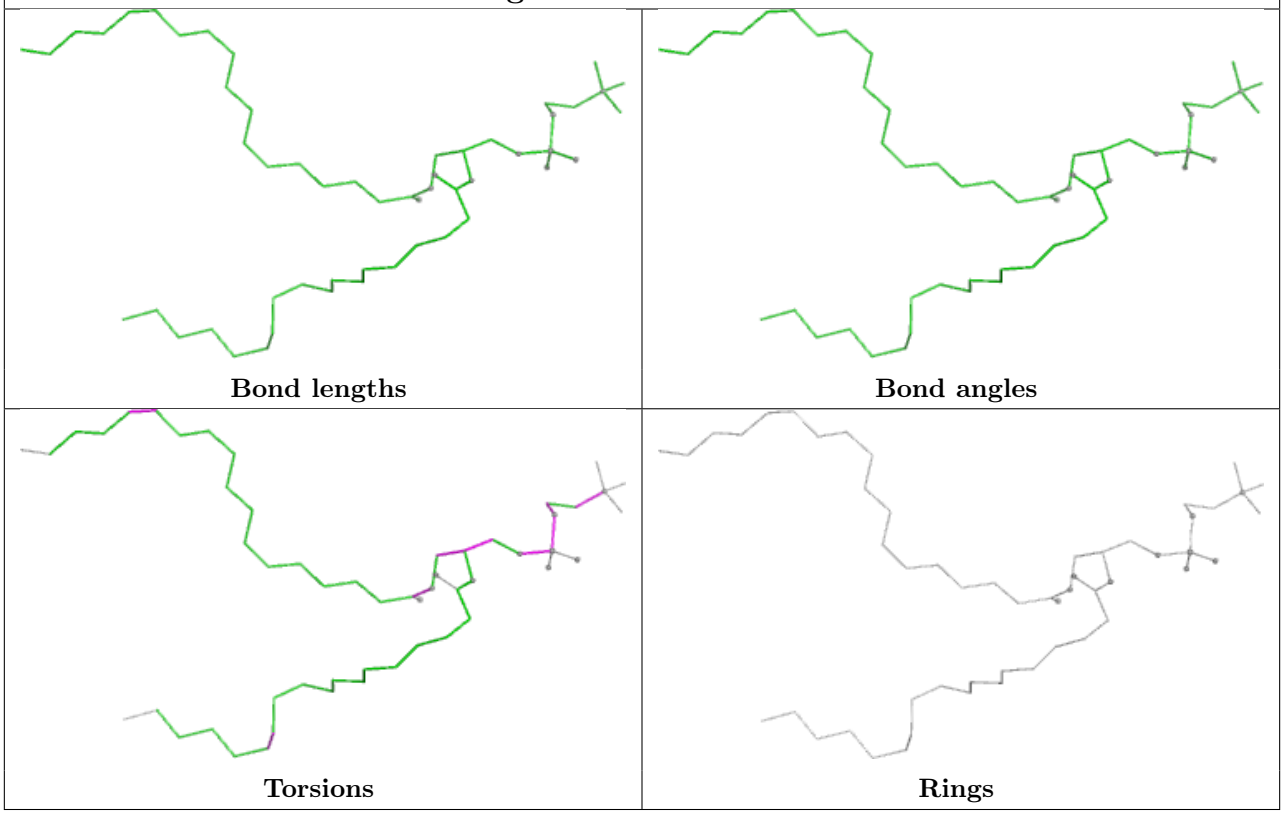
Rings

Ligand PC1 DV 405	
 Bond lengths	 Bond angles
 Torsions	Rings

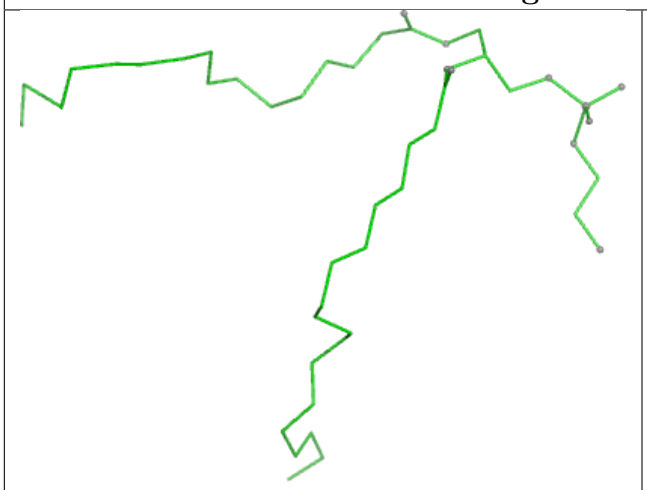
Ligand LPP AL 304



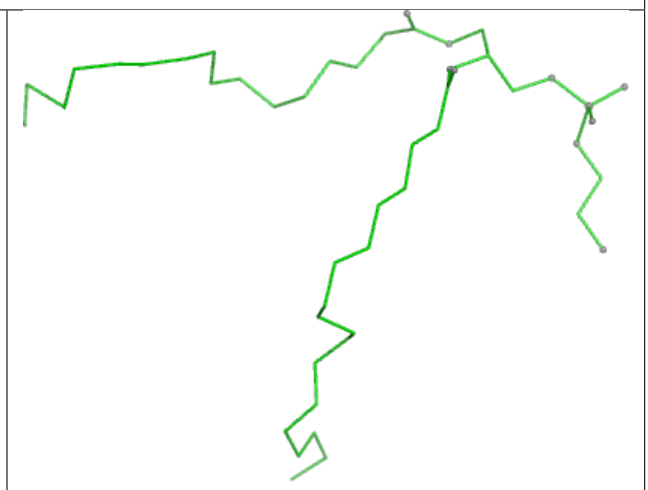
Ligand PC1 EN 1203



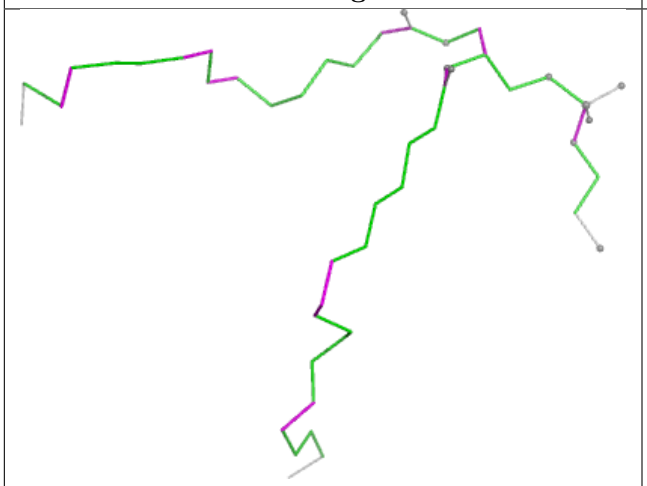
Ligand 3PE Eo 202



Bond lengths



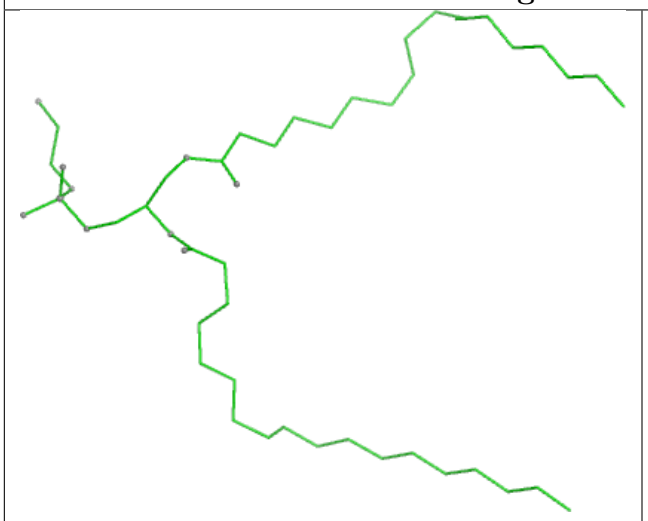
Bond angles



Torsions

Rings

Ligand 3PE BP 201



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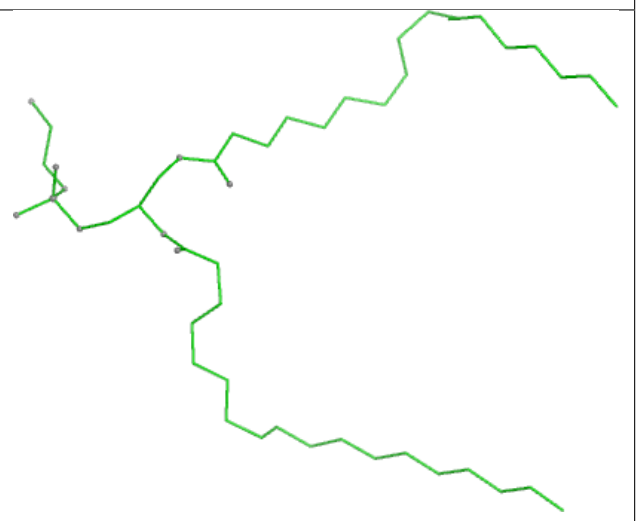
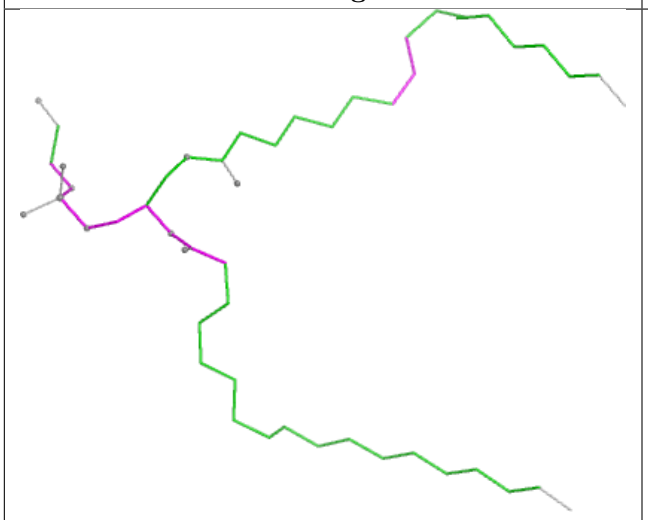
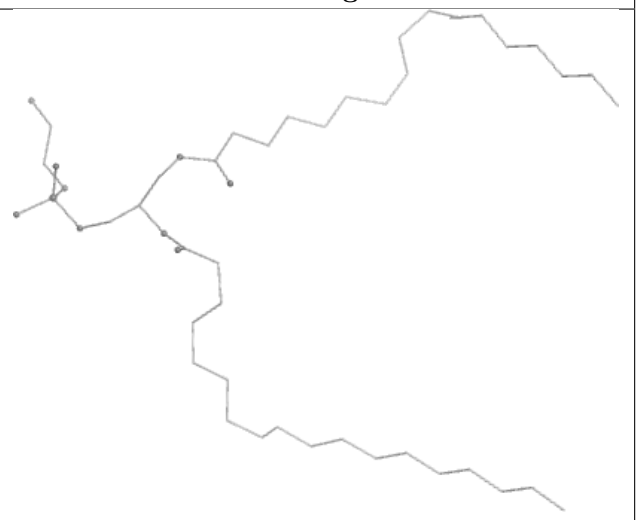


Bond angles

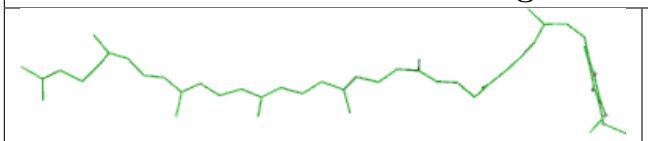


Torsions

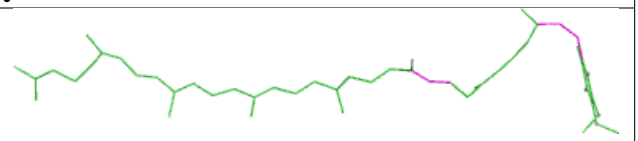


Rings

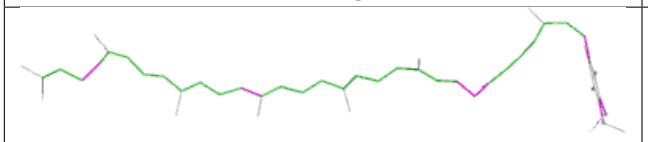
Ligand UQ8 EL 905



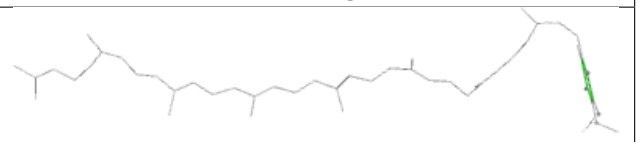
Bond lengths



Bond angles

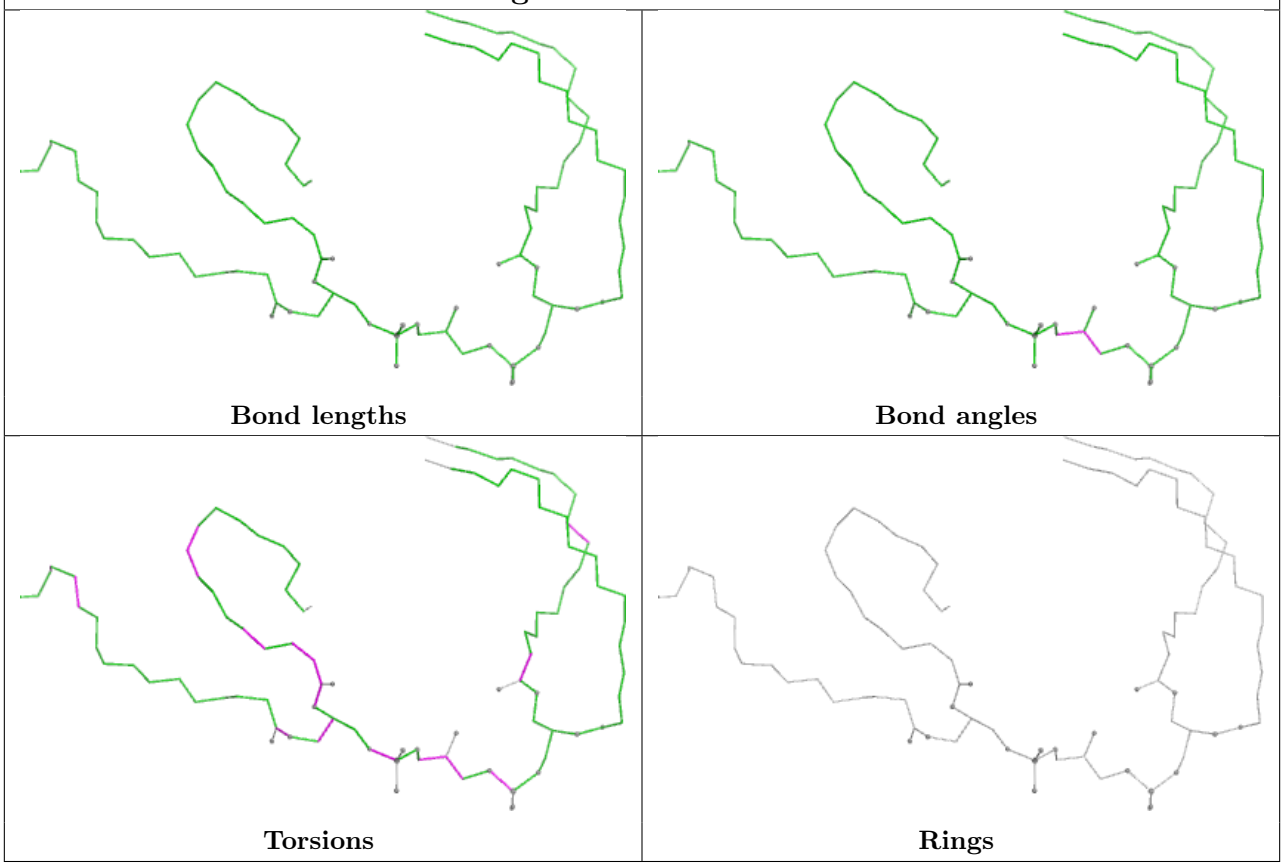


Torsions

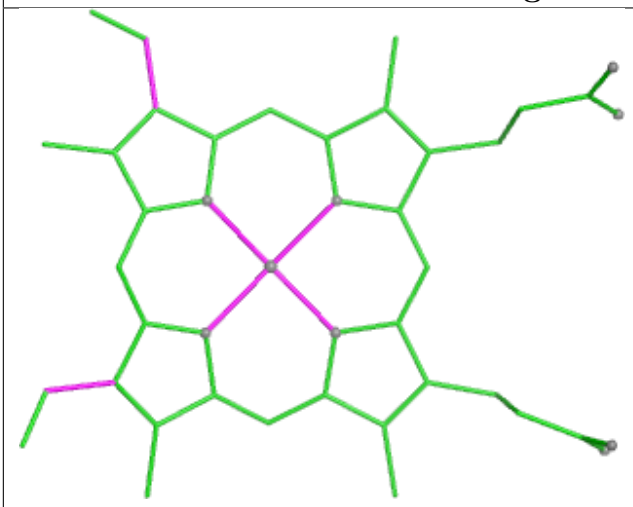


Rings

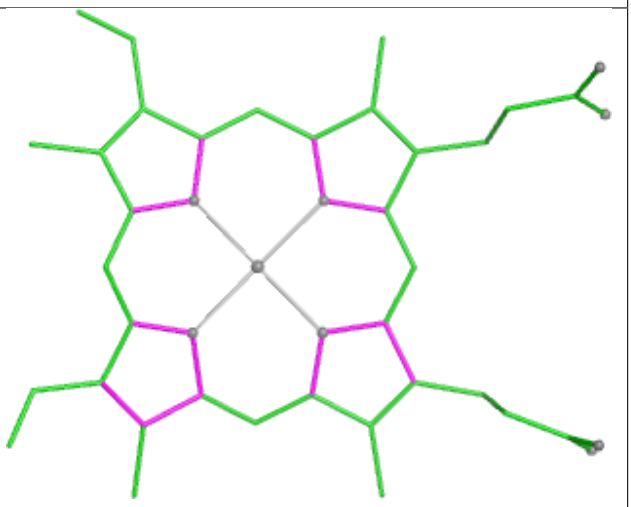
Ligand CDL DA 709



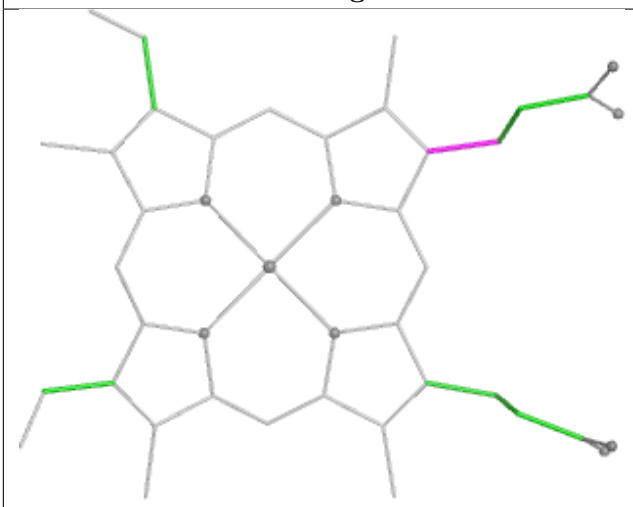
Ligand HEM c 504



Bond lengths



Bond angles



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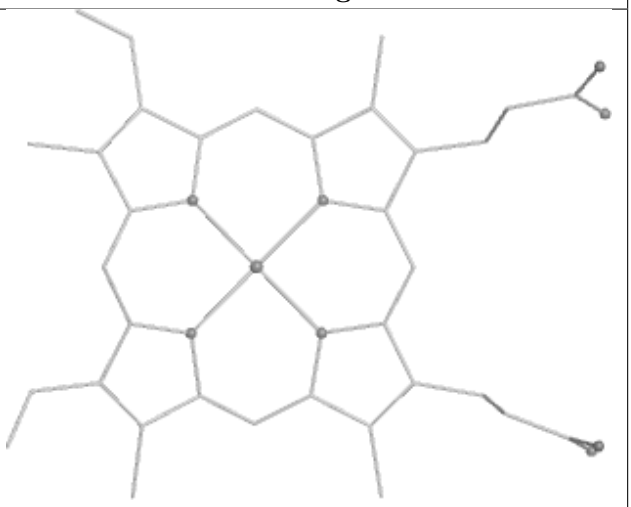


Rings

Ligand CDL DU 402

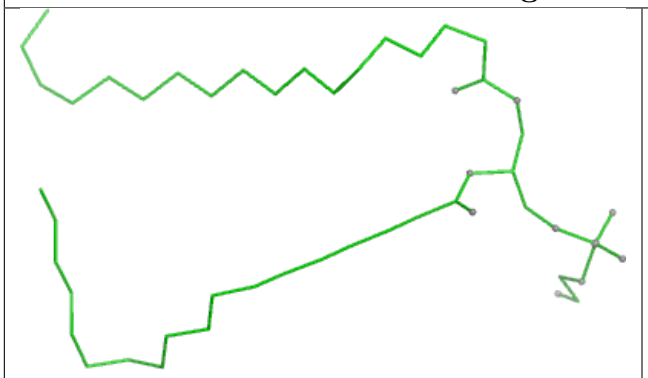
Bond lengths

Bond angles

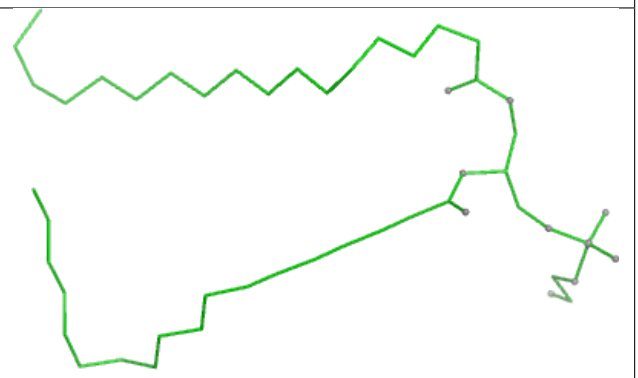
Torsions

Rings

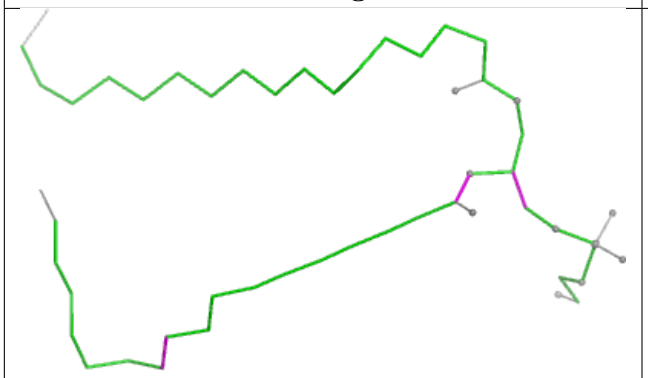
Ligand 3PE Dc 606



Bond lengths



Bond angles



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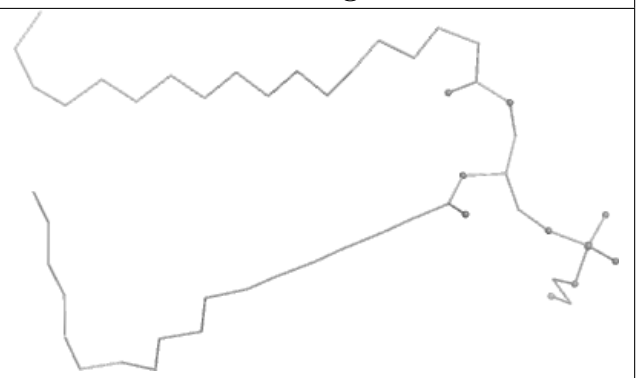
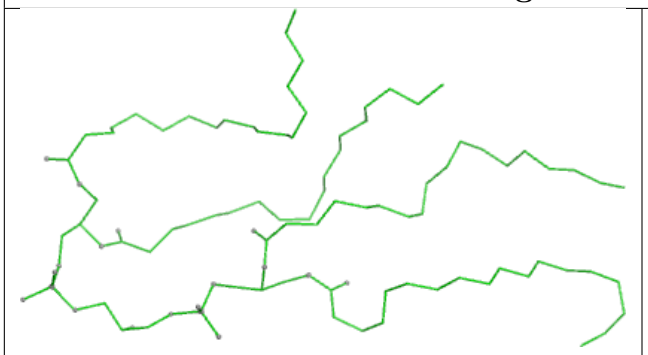


Rings

Ligand CDL A1 402



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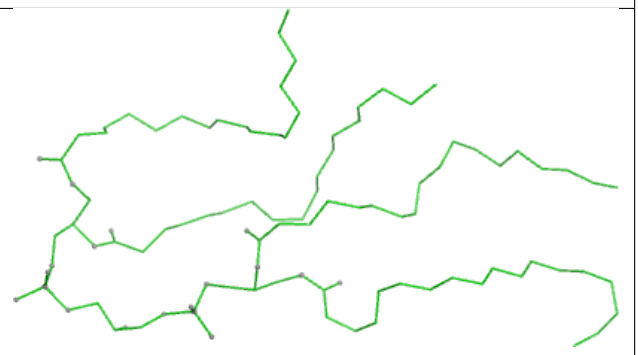

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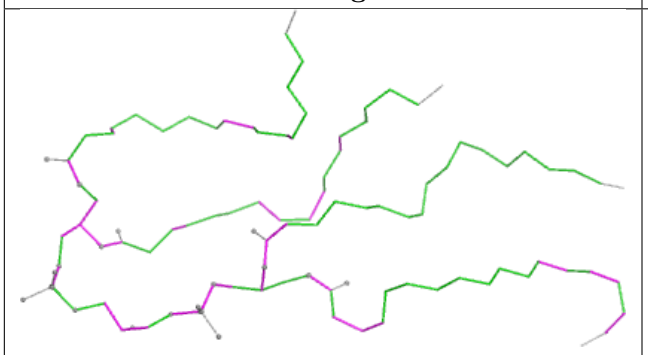

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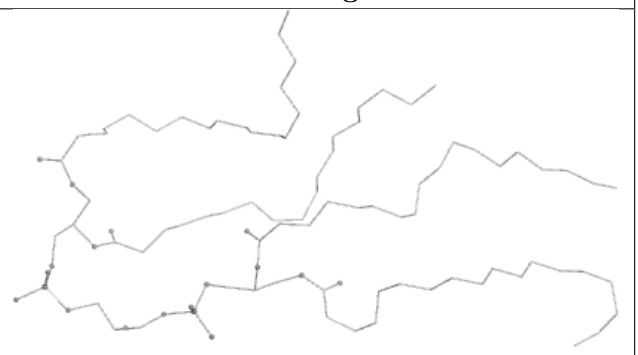
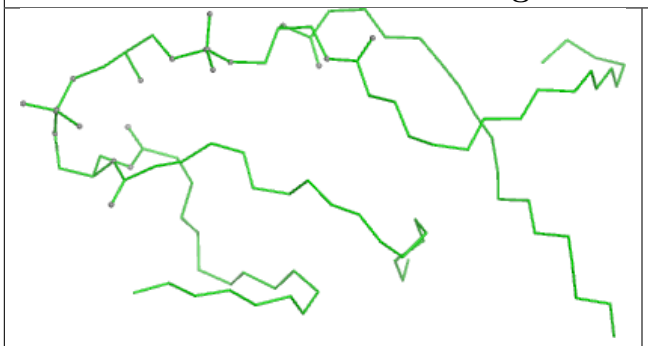


Rings

Ligand CDL AC 802



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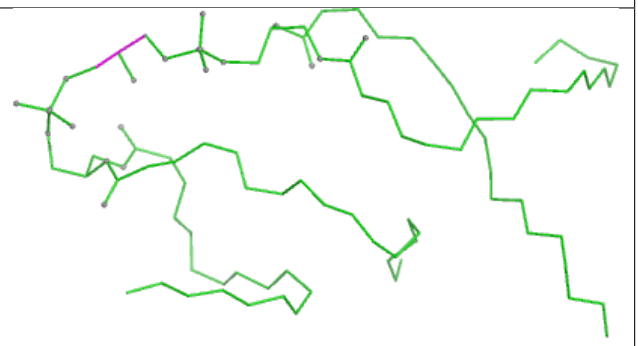

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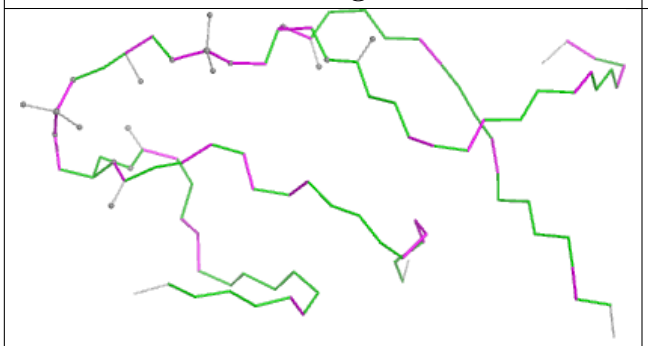
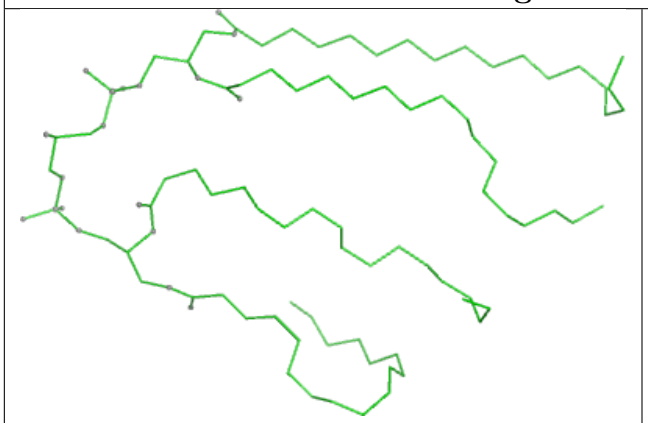


Torsions

Rings

Ligand CDL Dd 705



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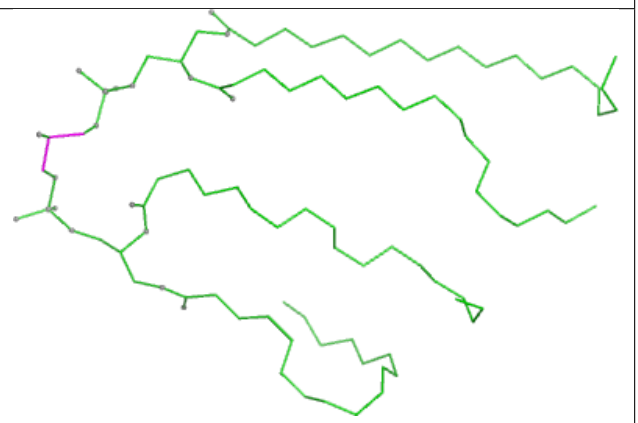

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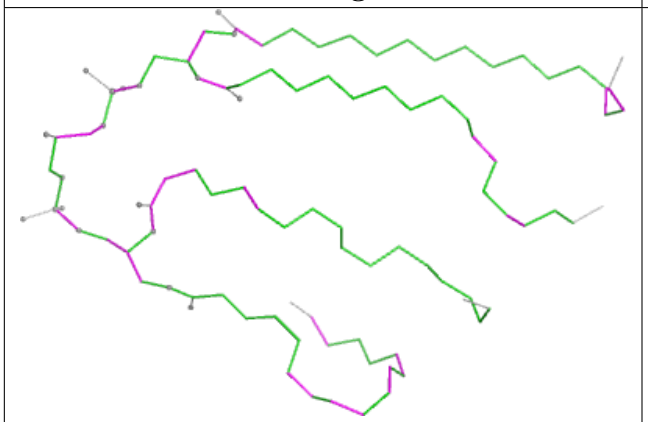

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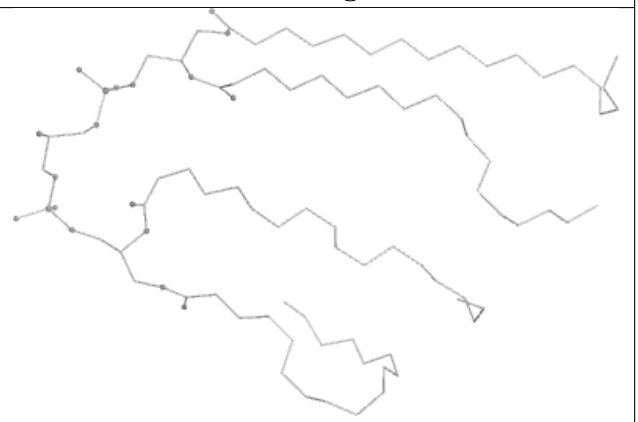
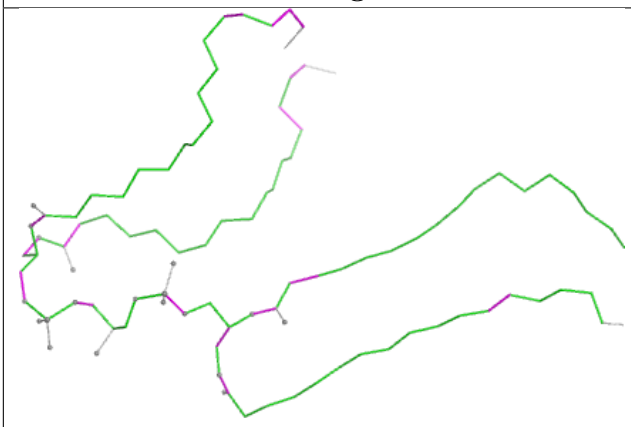
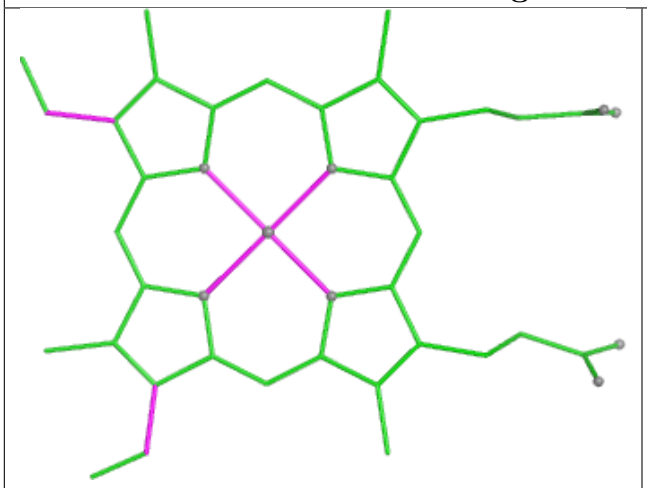


Rings

Ligand CDL AF 401	
Bond lengths	Bond angles
 Torsions	Rings

Ligand HEM Ed 201



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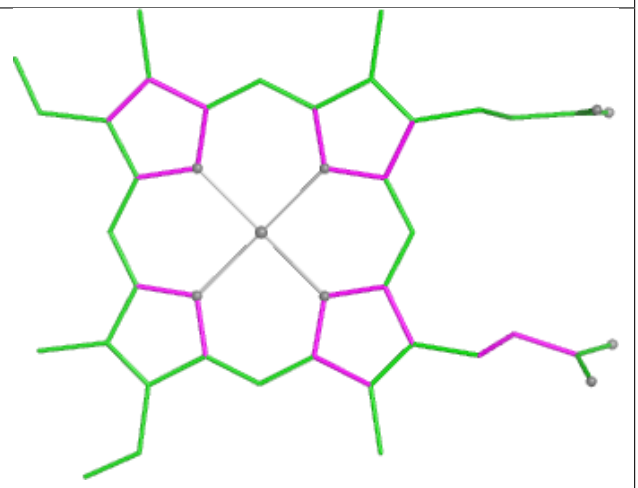

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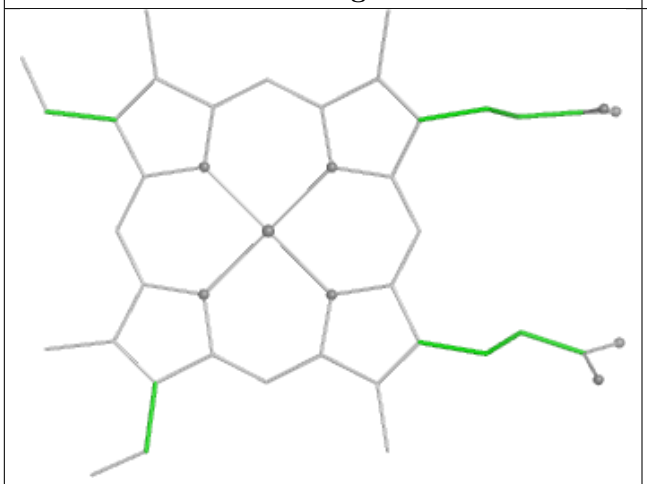

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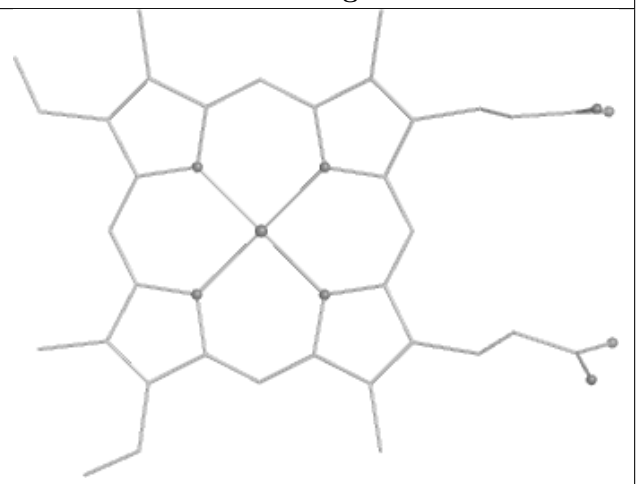
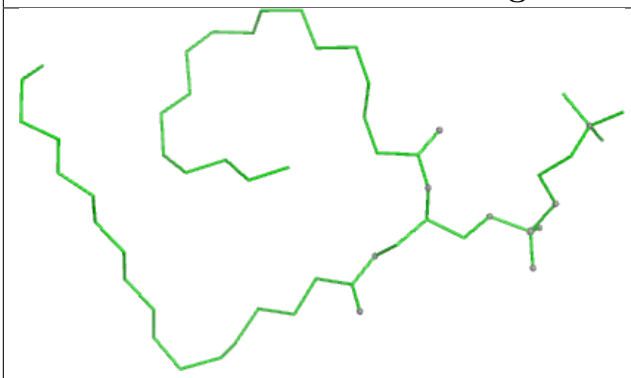
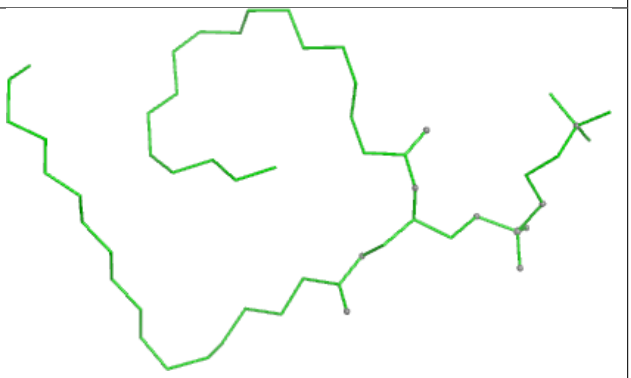
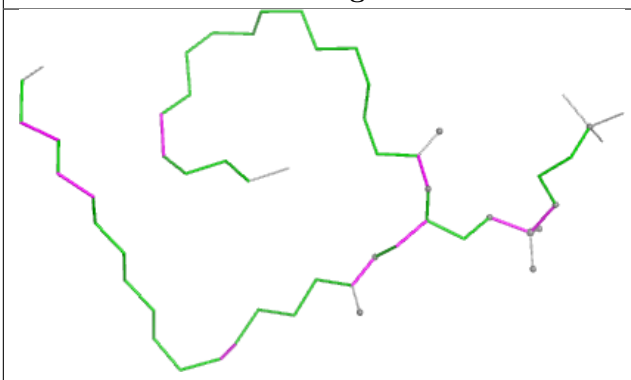
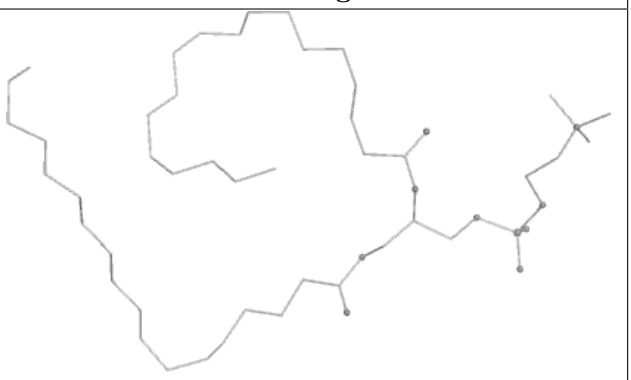
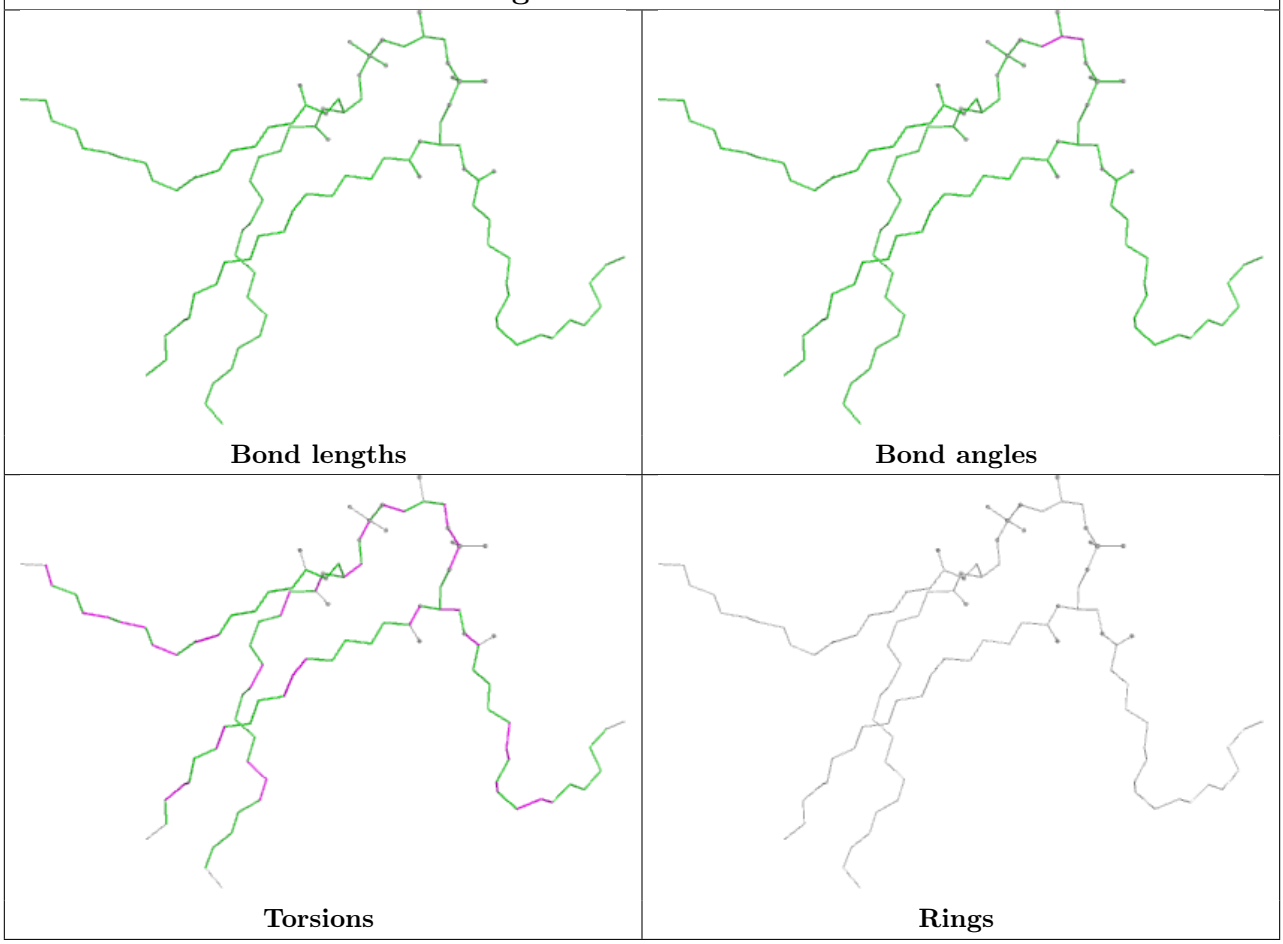


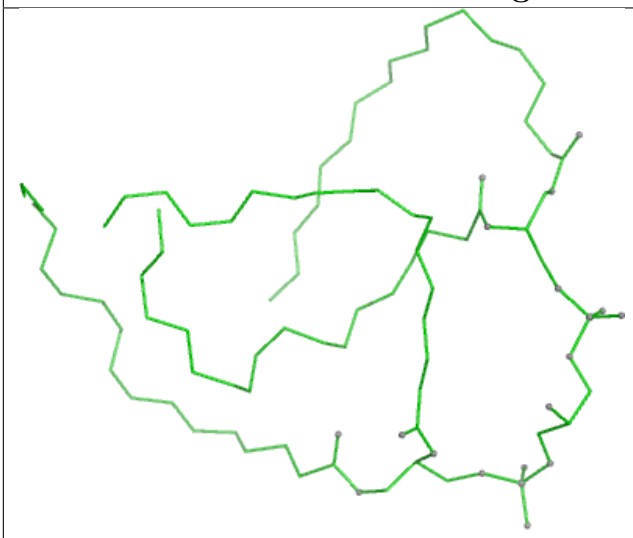
Rings

Ligand PC1 BS 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL AC 801



Ligand CDL EB 302



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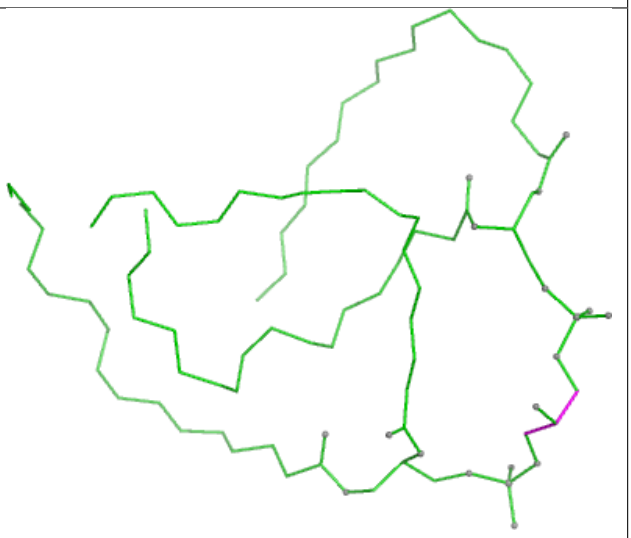

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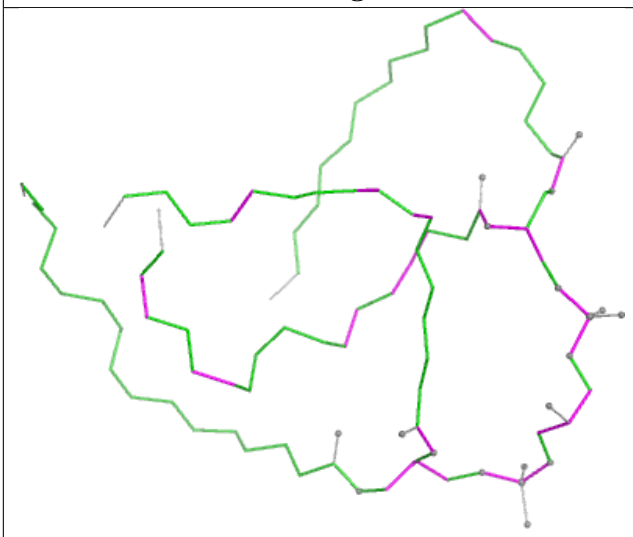

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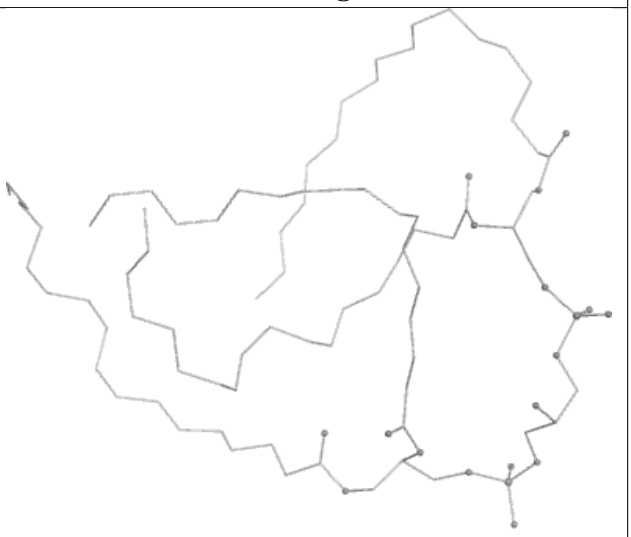

Rings

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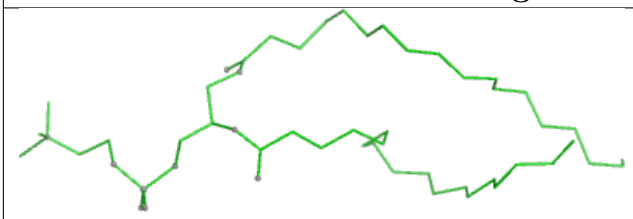

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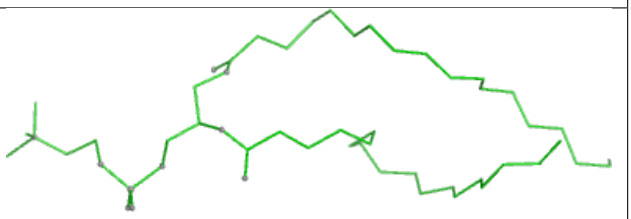

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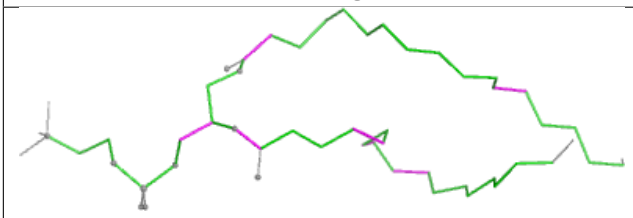

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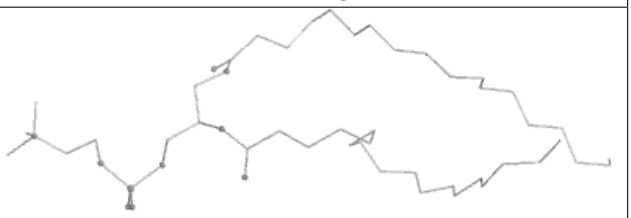
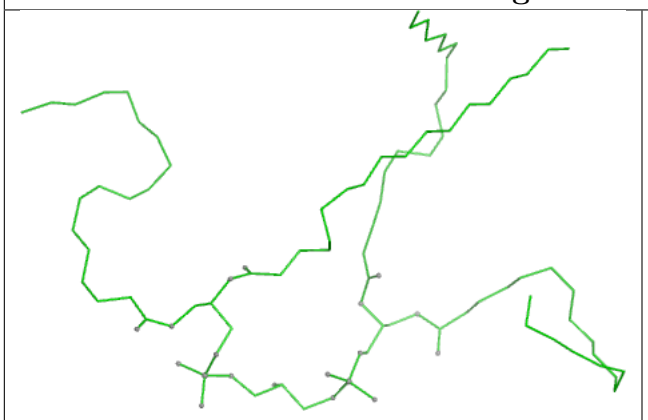


Rings

Ligand CDL EK 201



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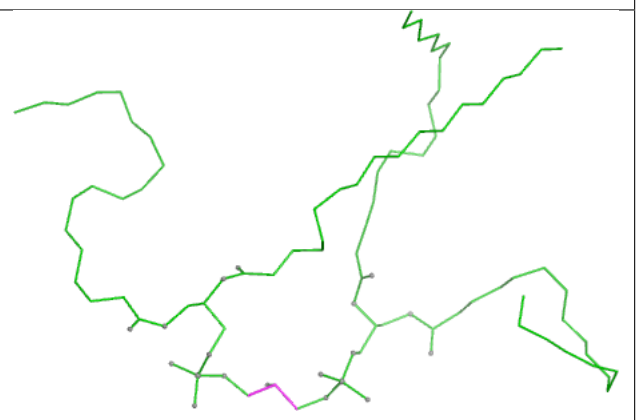

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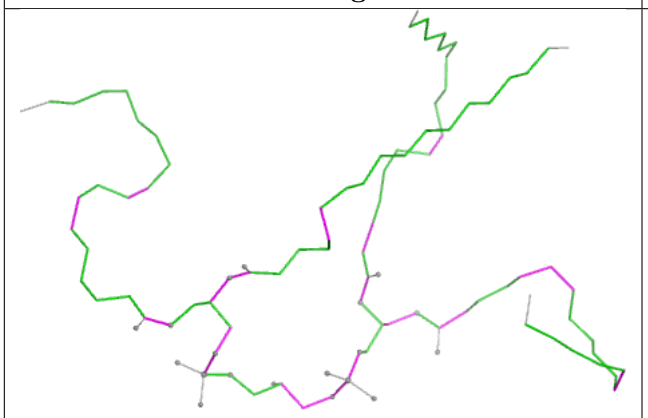

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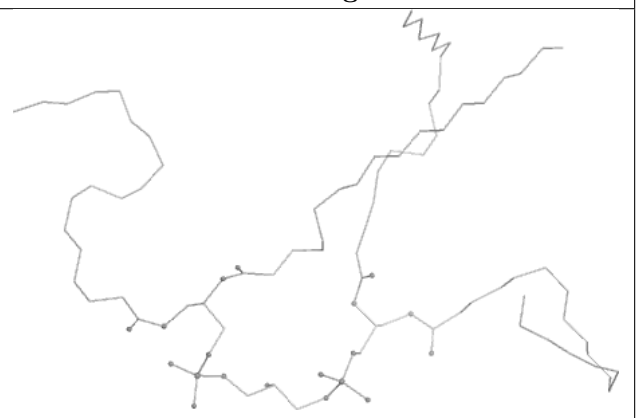
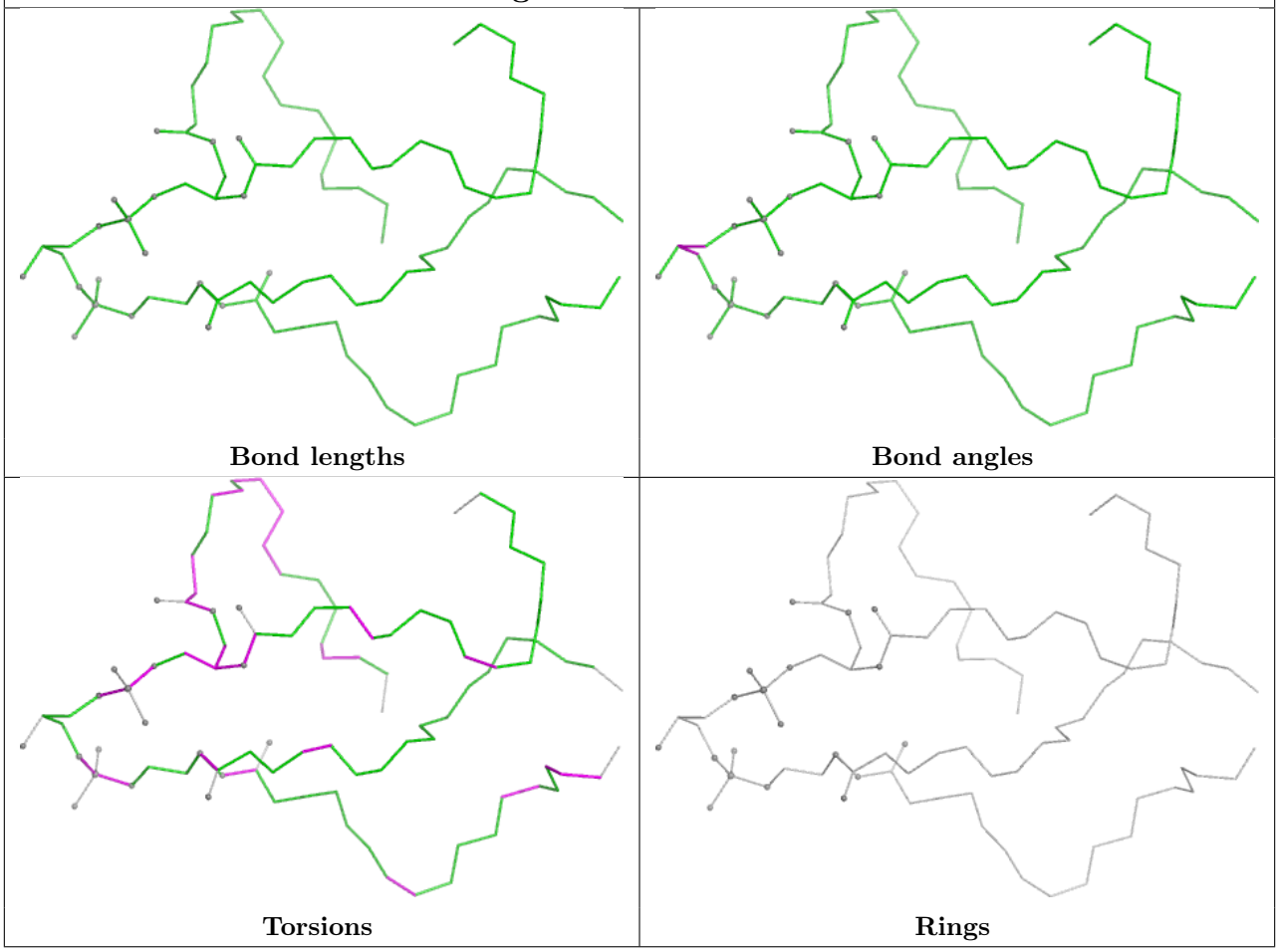


Rings

Ligand CDL Dn 501



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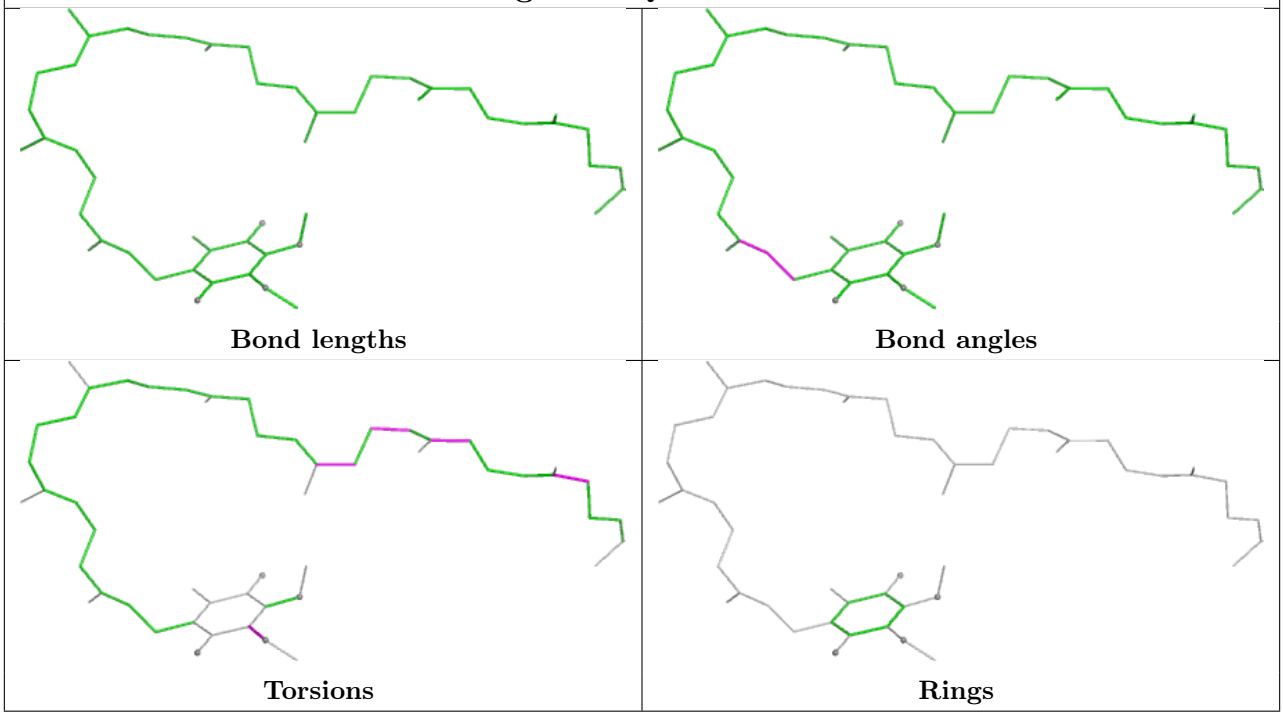
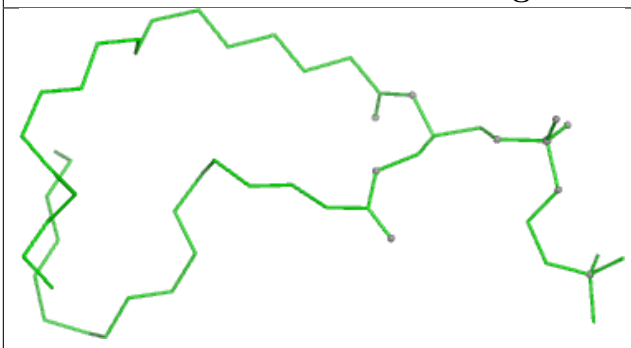


Ligand PC1 Di 1104



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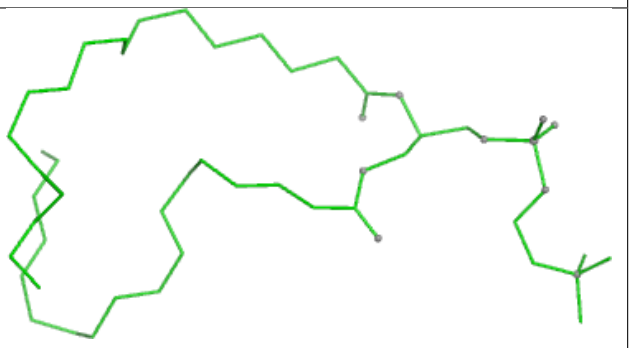
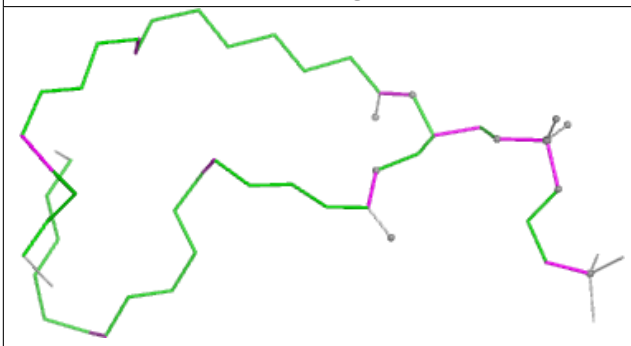


Bond angles



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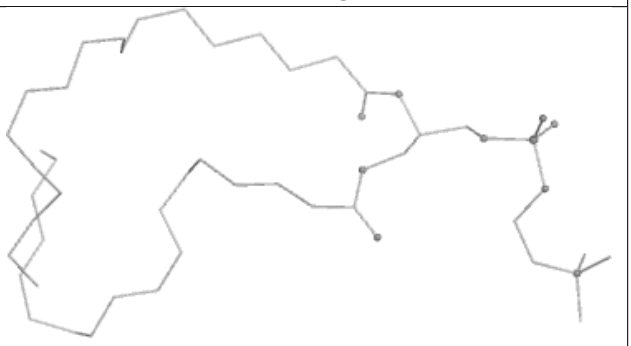

Rings

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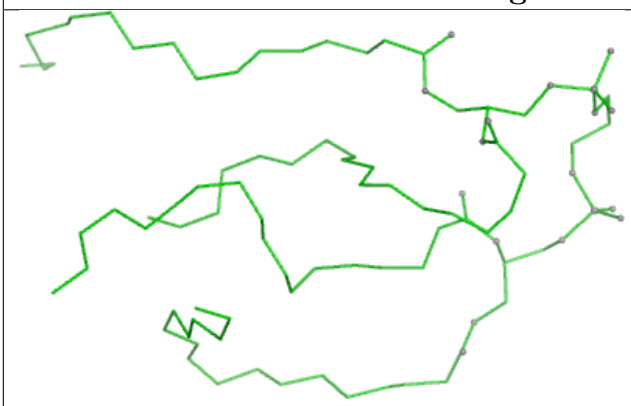

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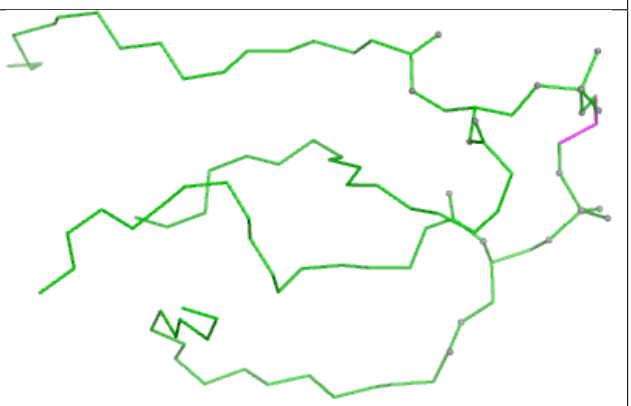

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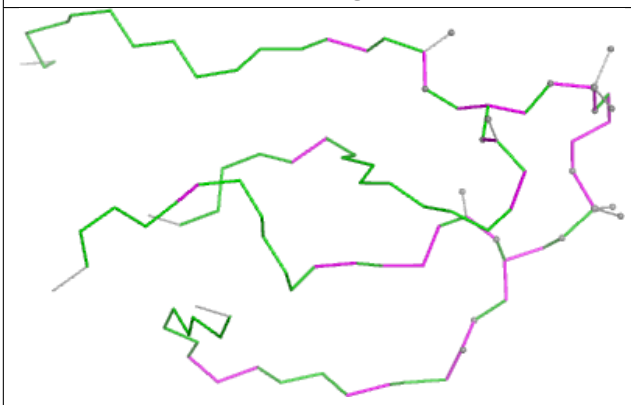

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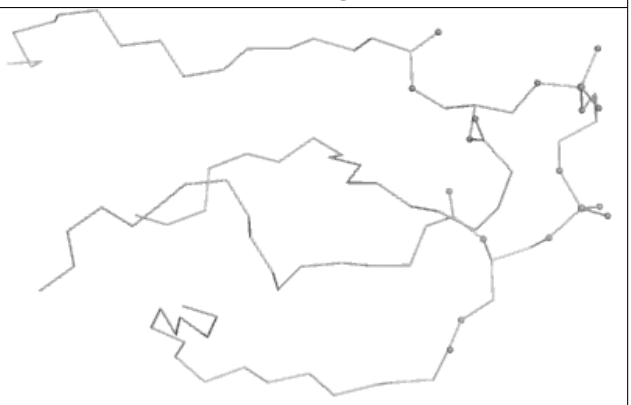

Rings

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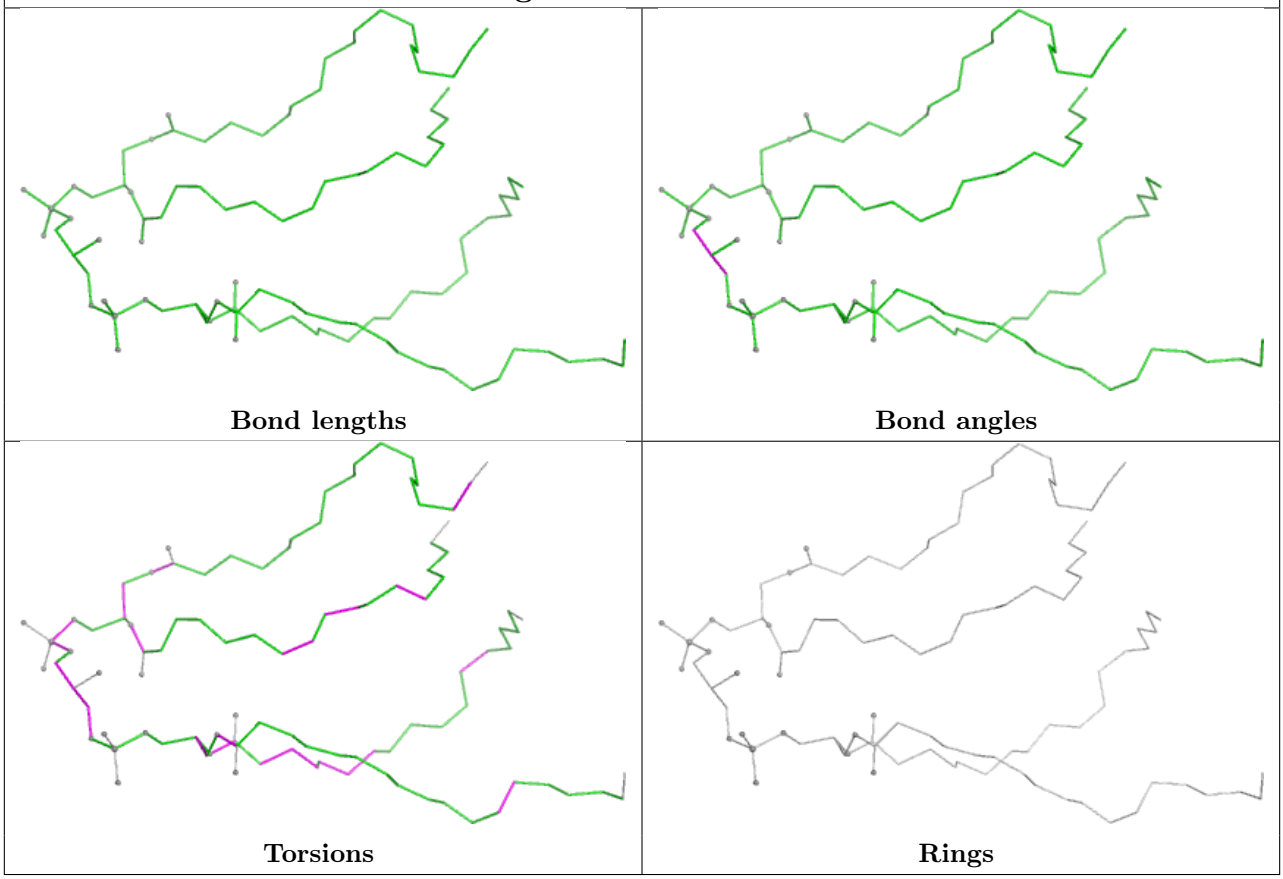
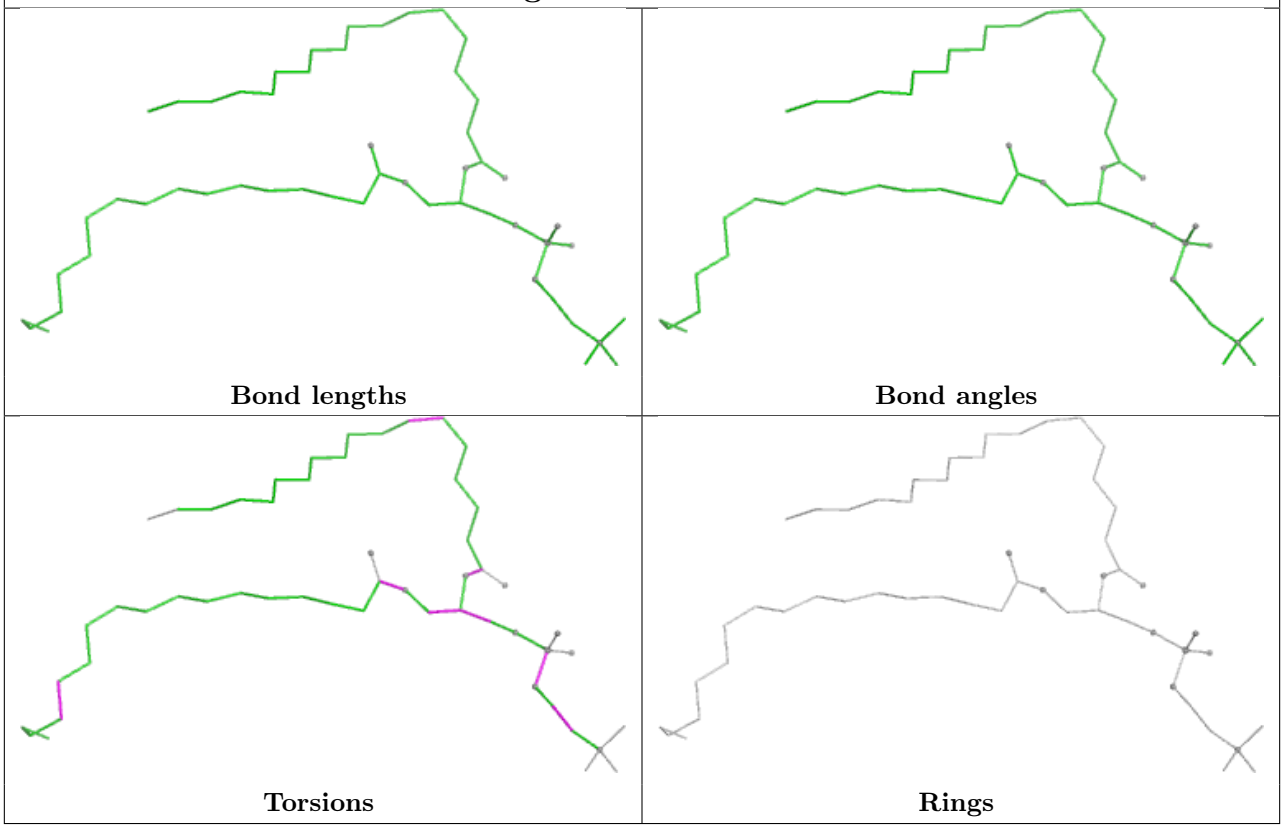


Ligand PC1 e 1101



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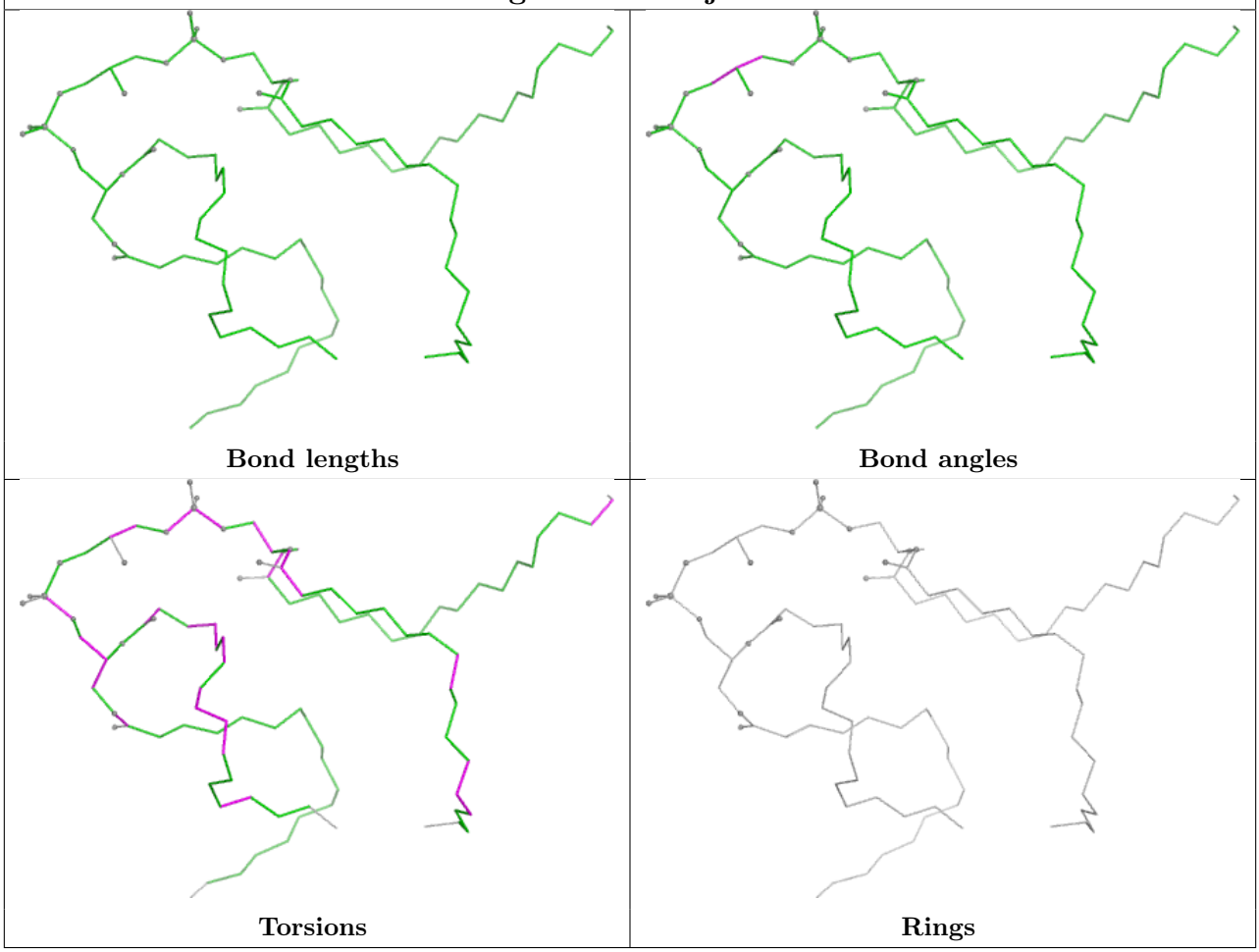
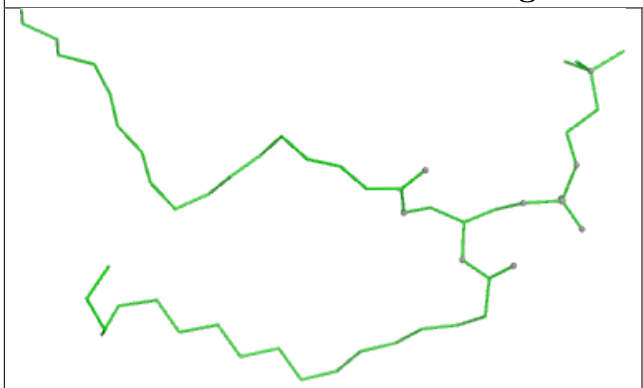
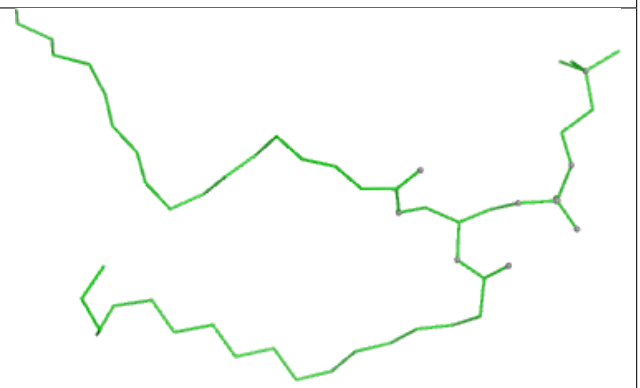
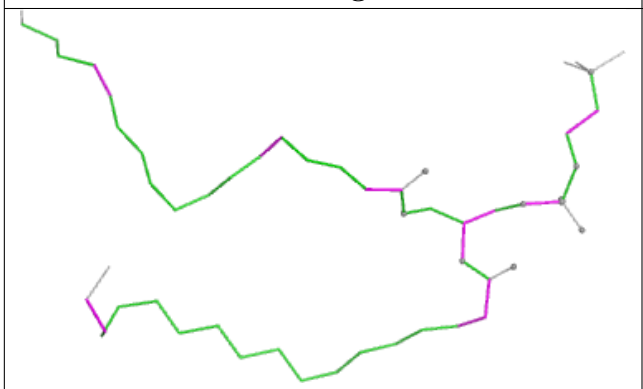
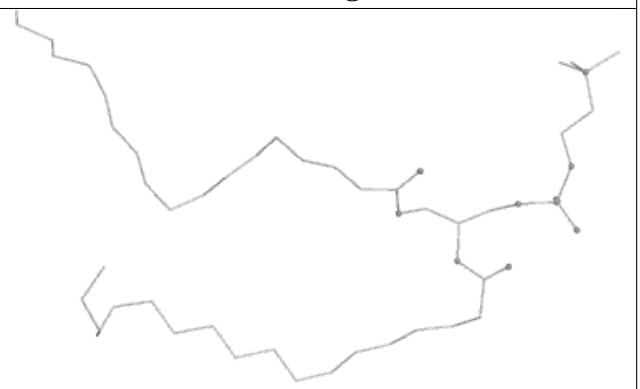
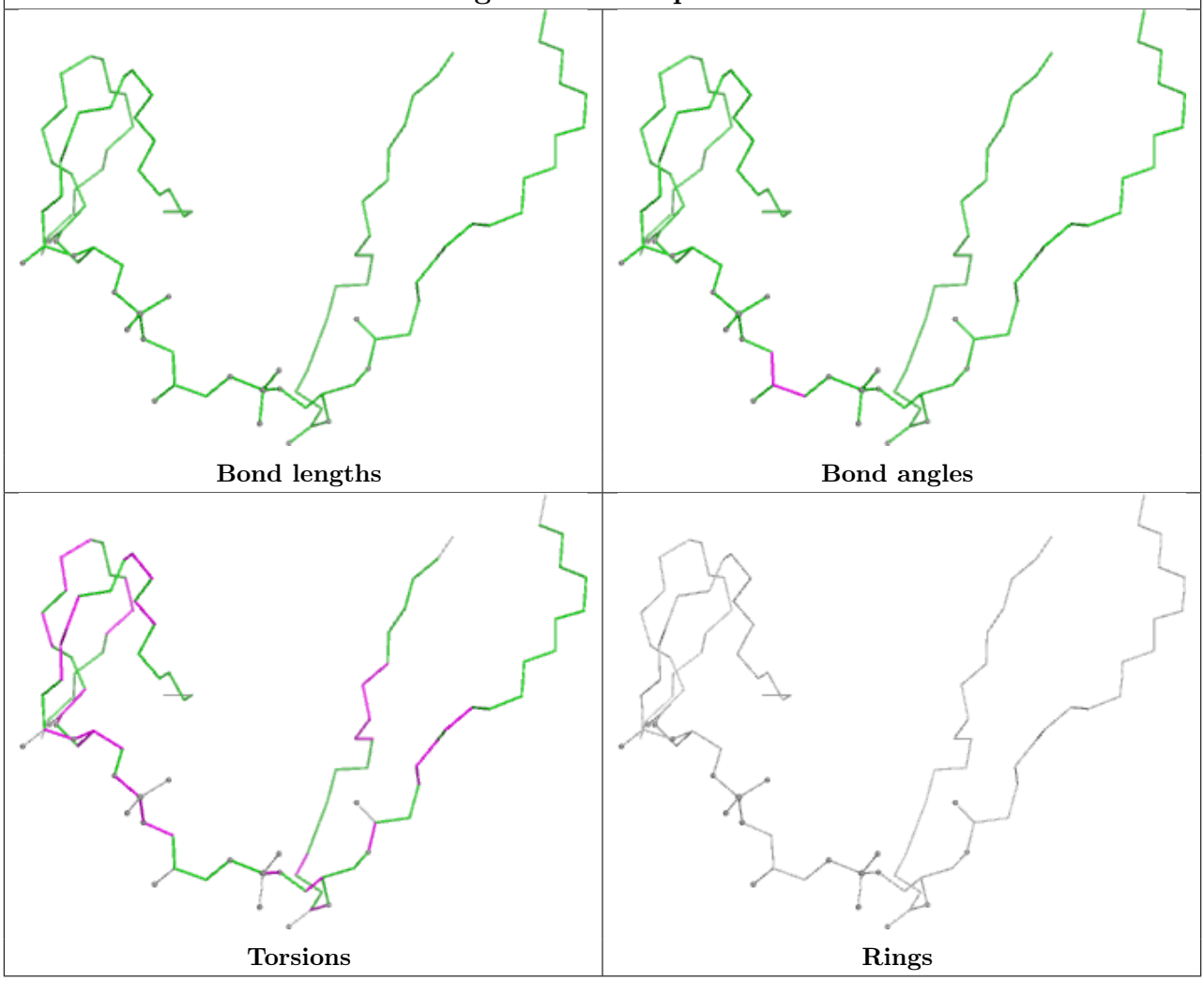


Ligand PC1 AJ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Dq 1401



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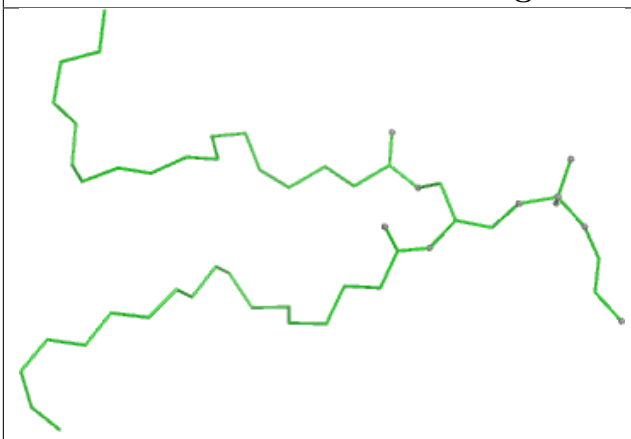
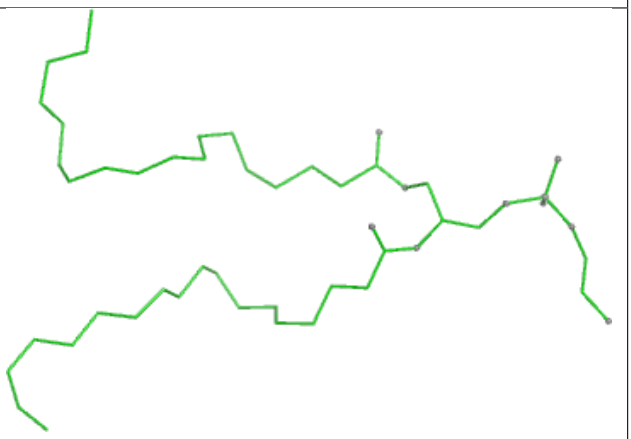
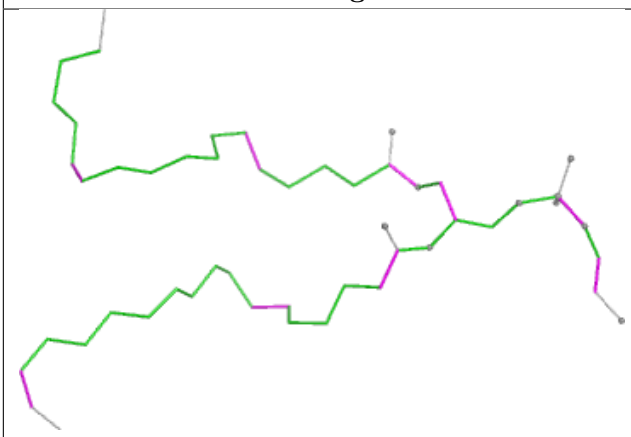
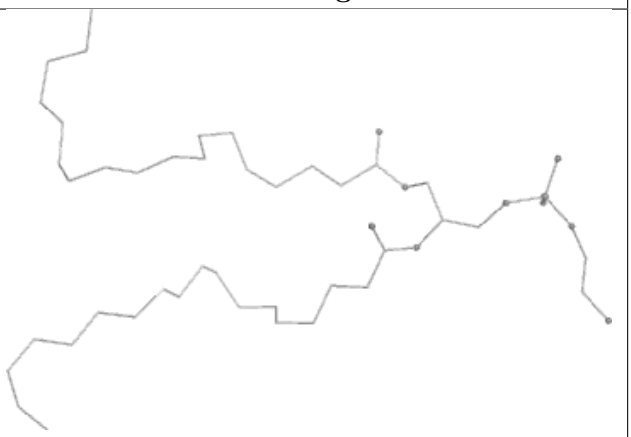
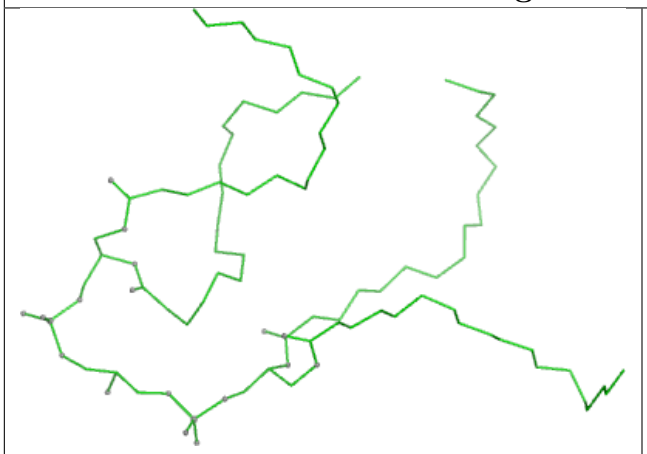
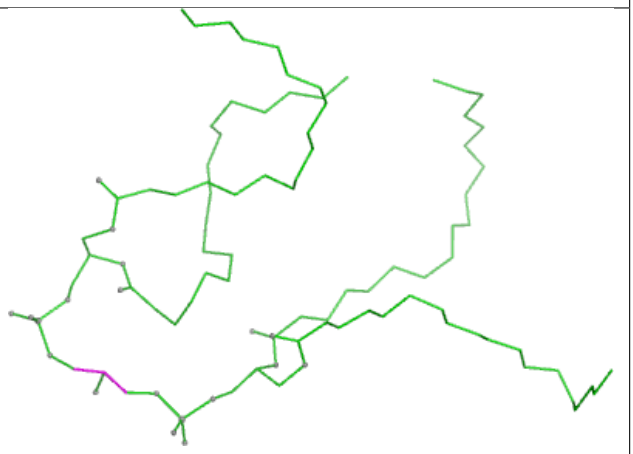
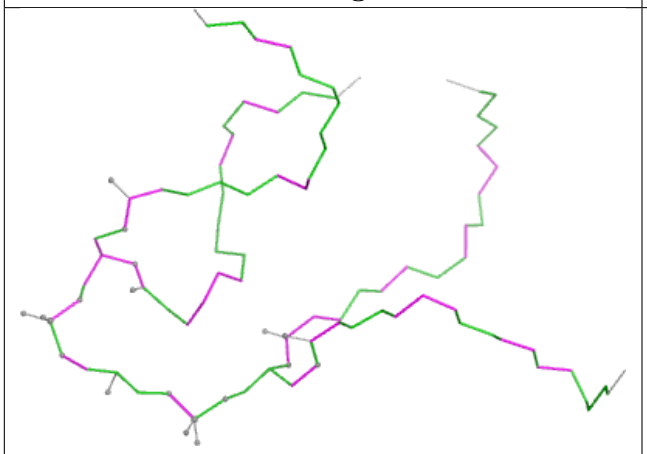
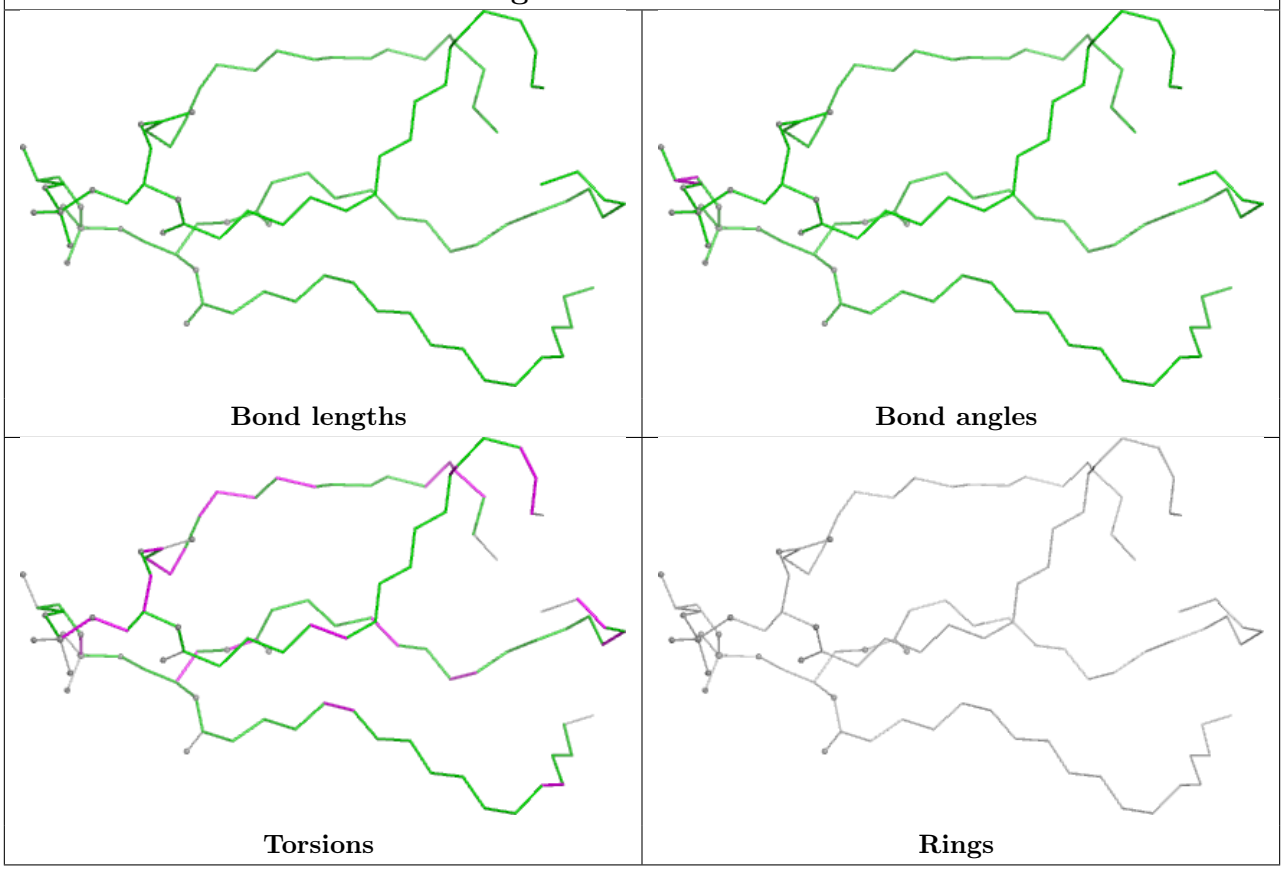
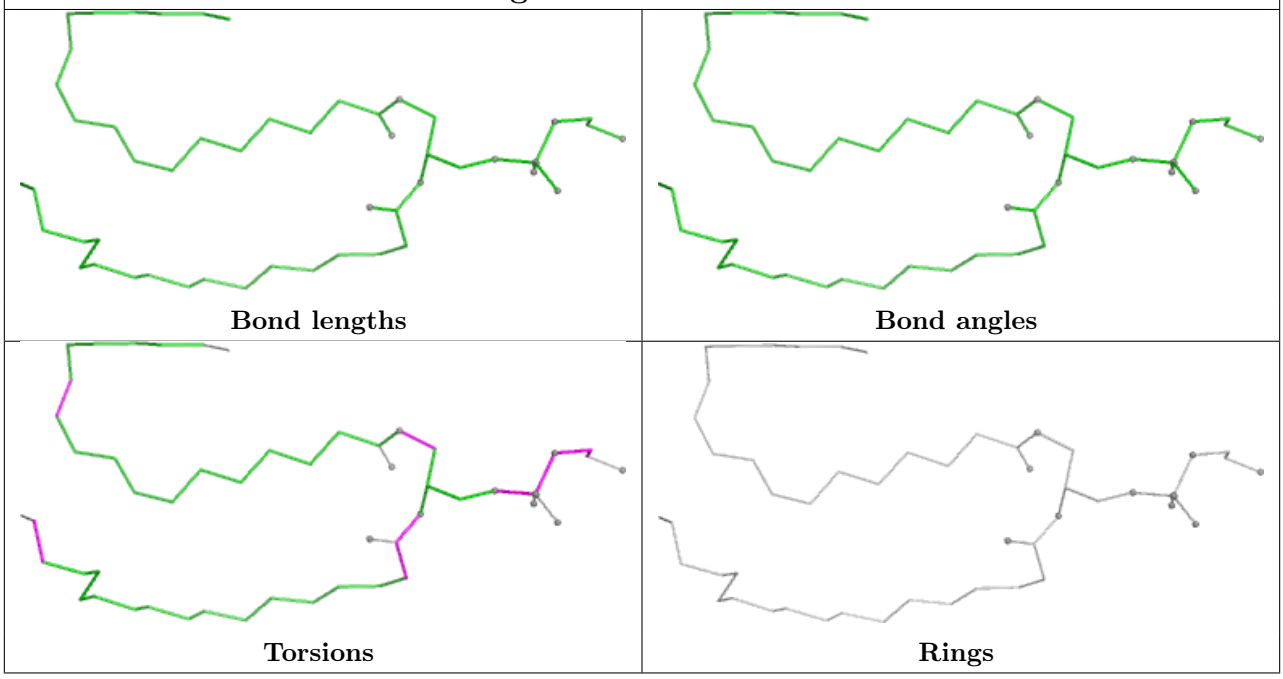
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL DJ 304	
 Bond lengths	 Bond angles
 Torsions	Rings

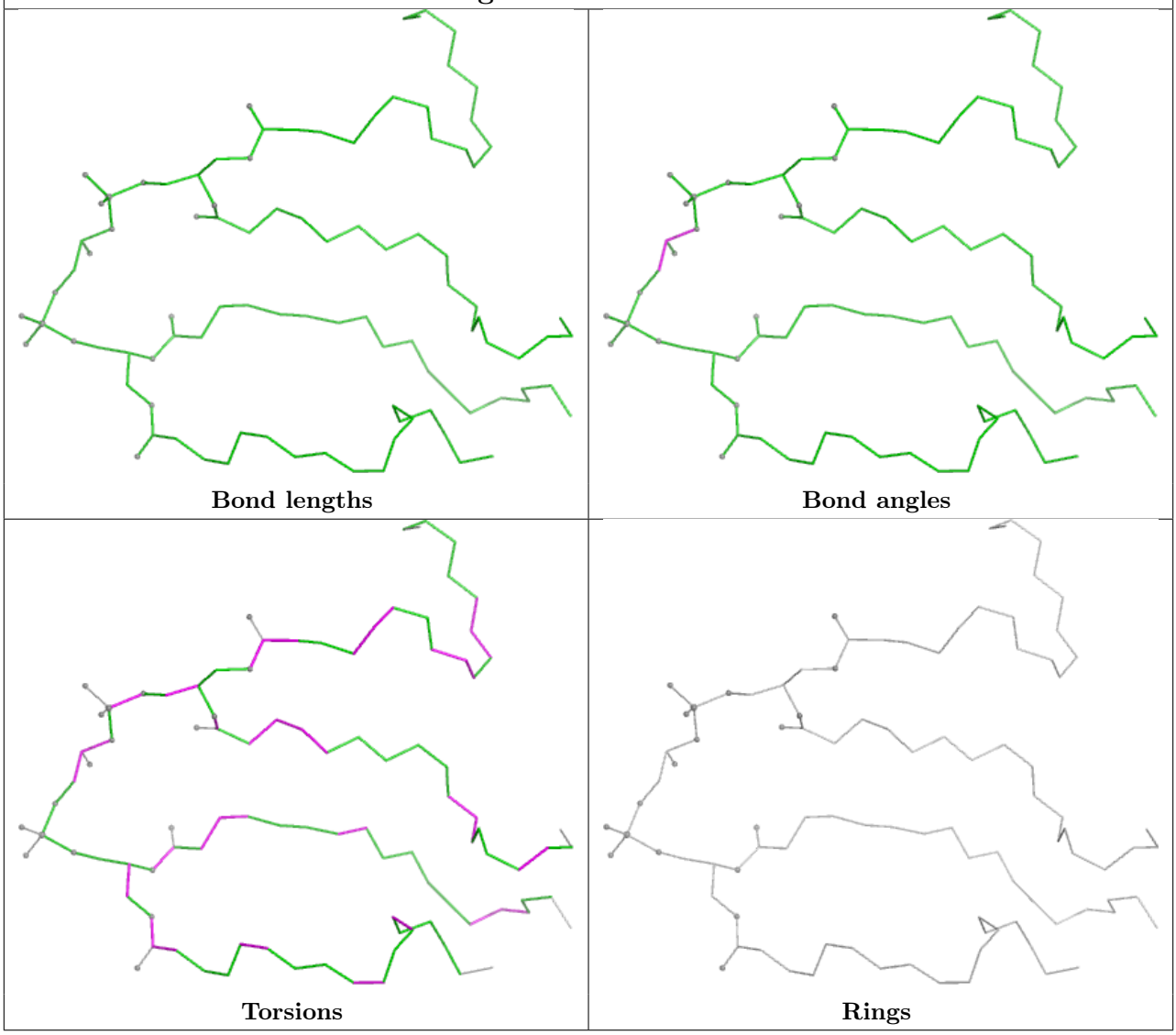
Ligand CDL DR 402



Ligand 3PE Dx 1206



Ligand CDL El 901



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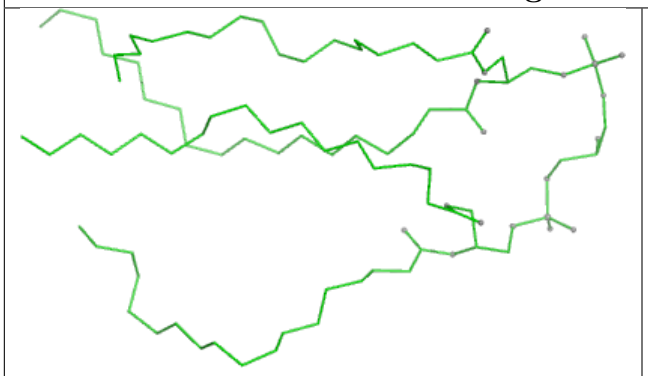
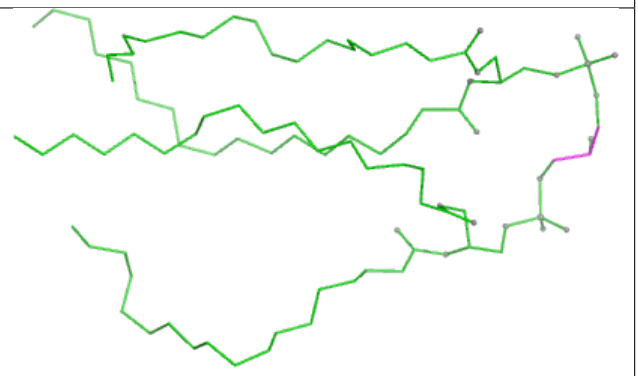
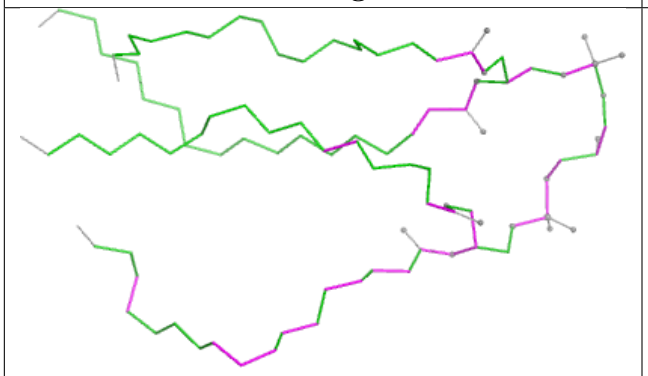


Bond lengths



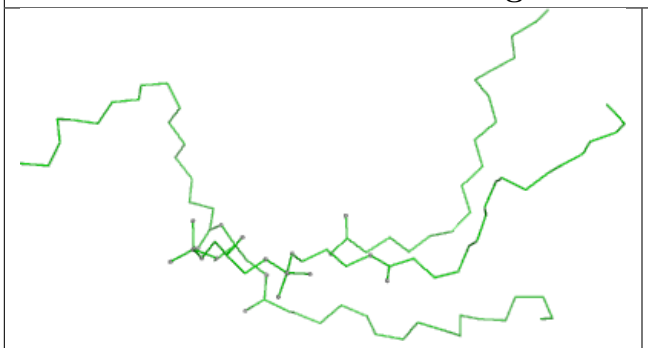
Bond angles



Torsions

Rings

Ligand CDL Dq 1403



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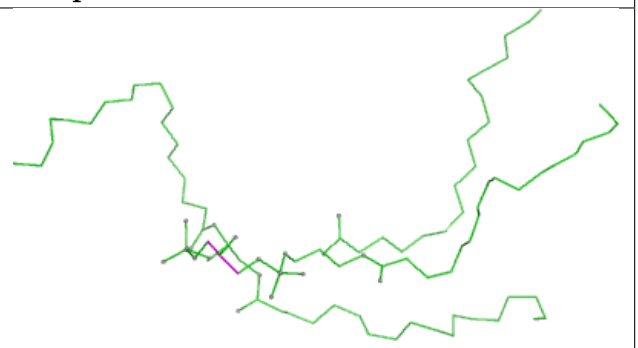

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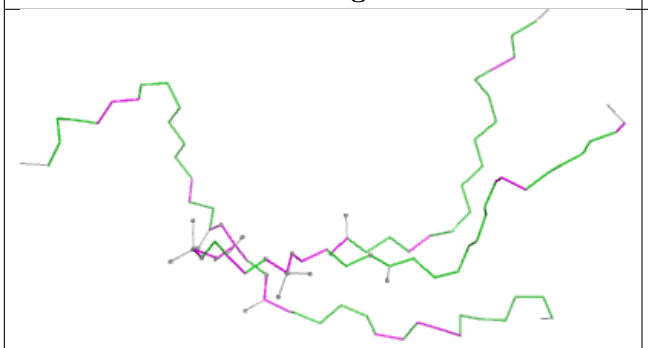

Torsions

Rings

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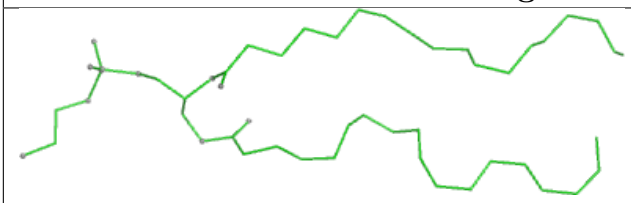
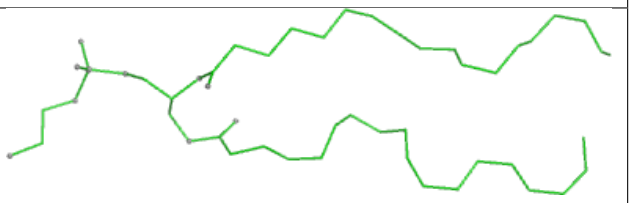
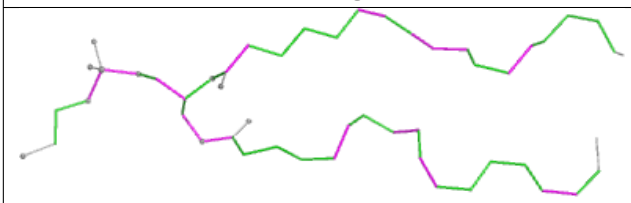
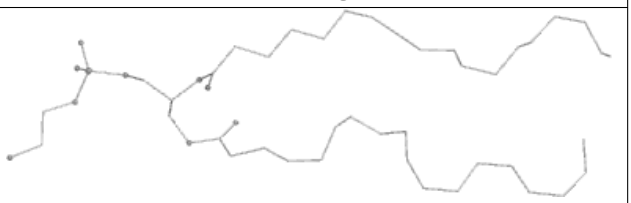
 Bond lengths	 Bond angles
 Torsions	 Rings

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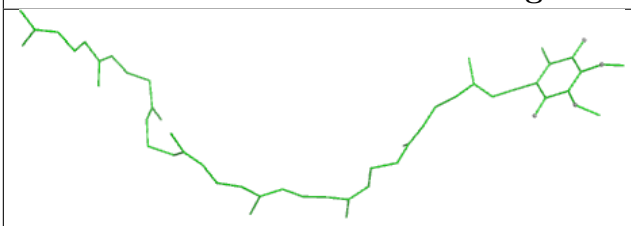
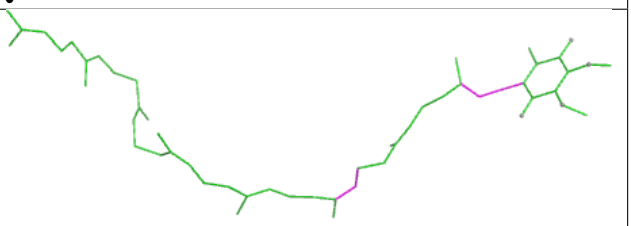
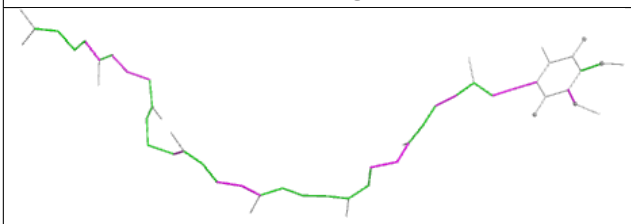
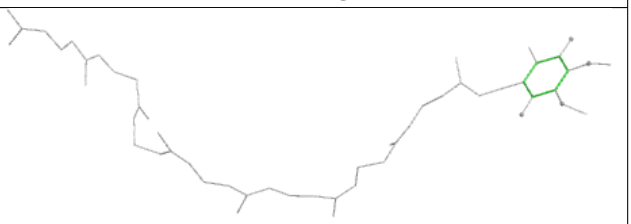
 Bond lengths	 Bond angles
 Torsions	 Rings

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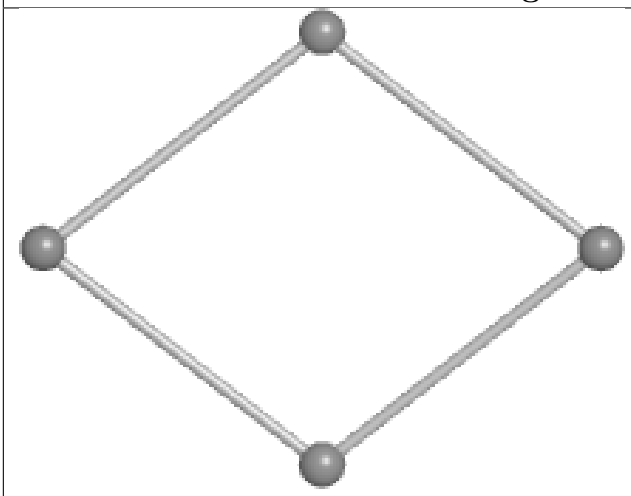
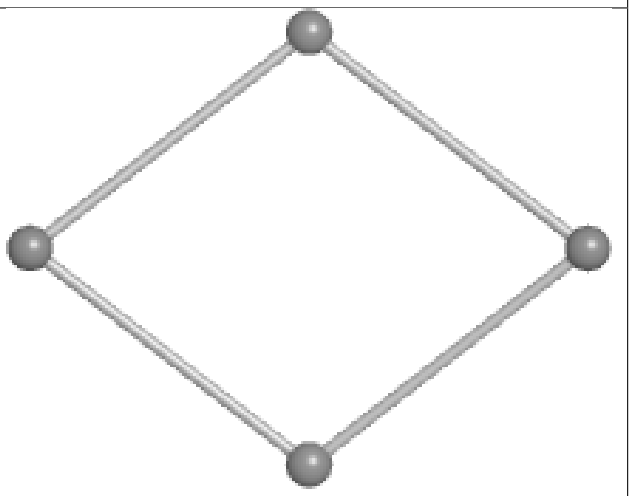
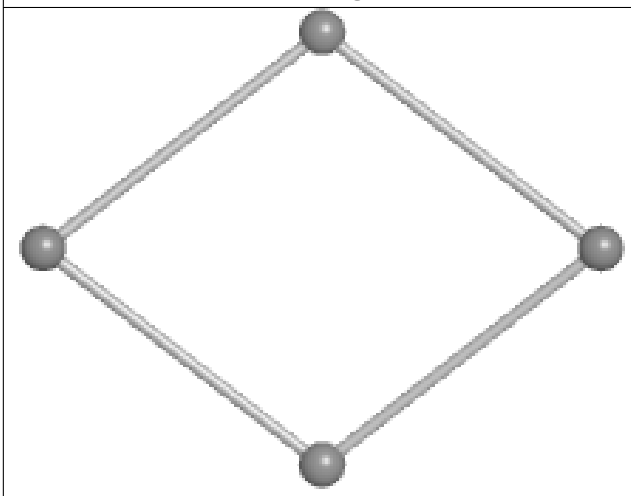
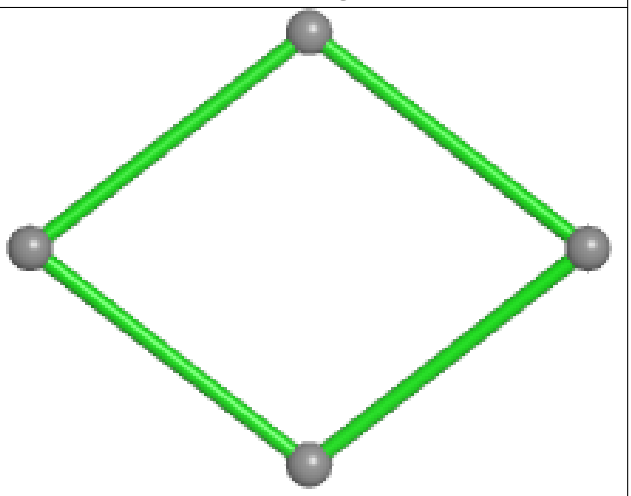
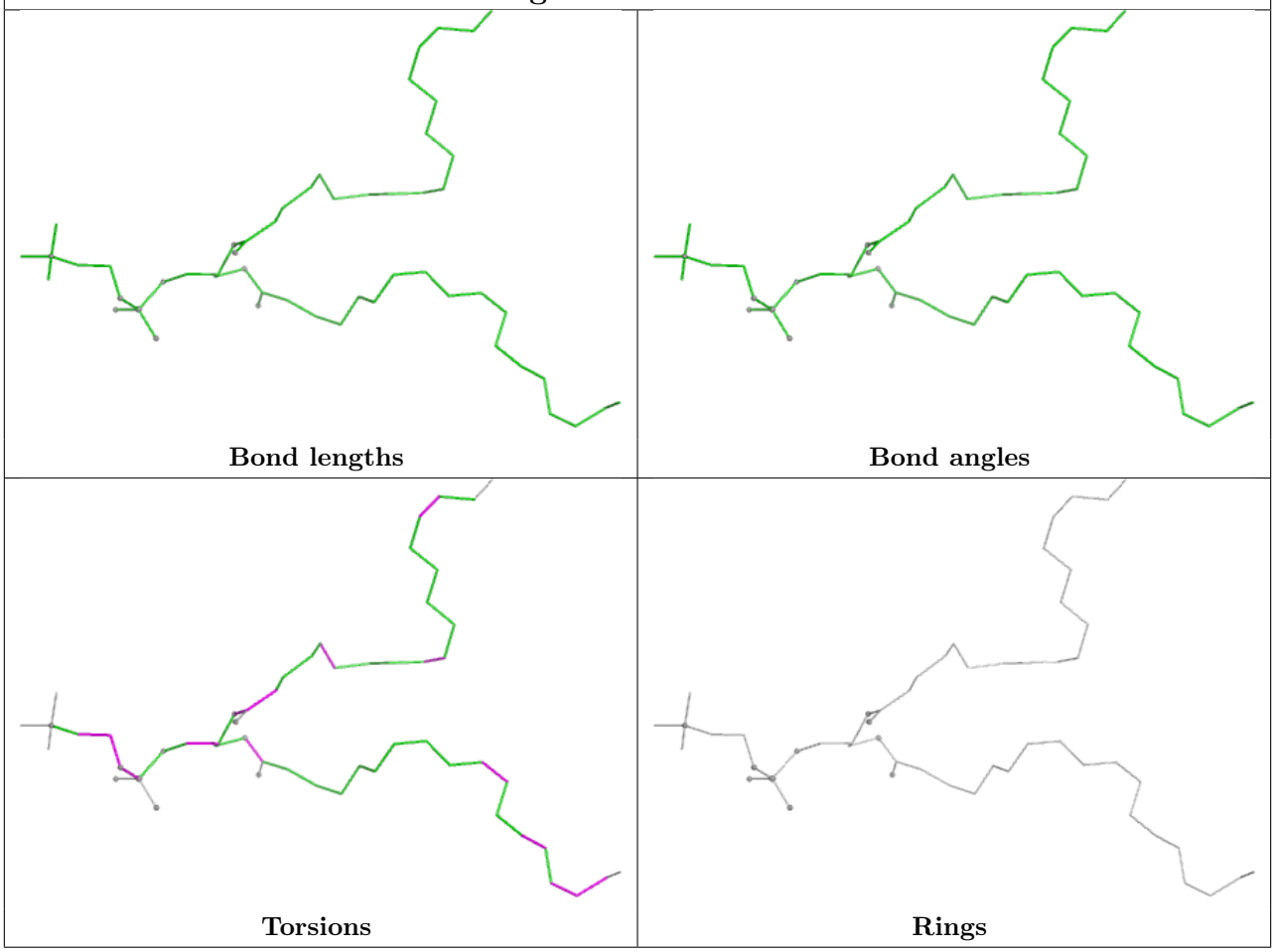
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 c 507



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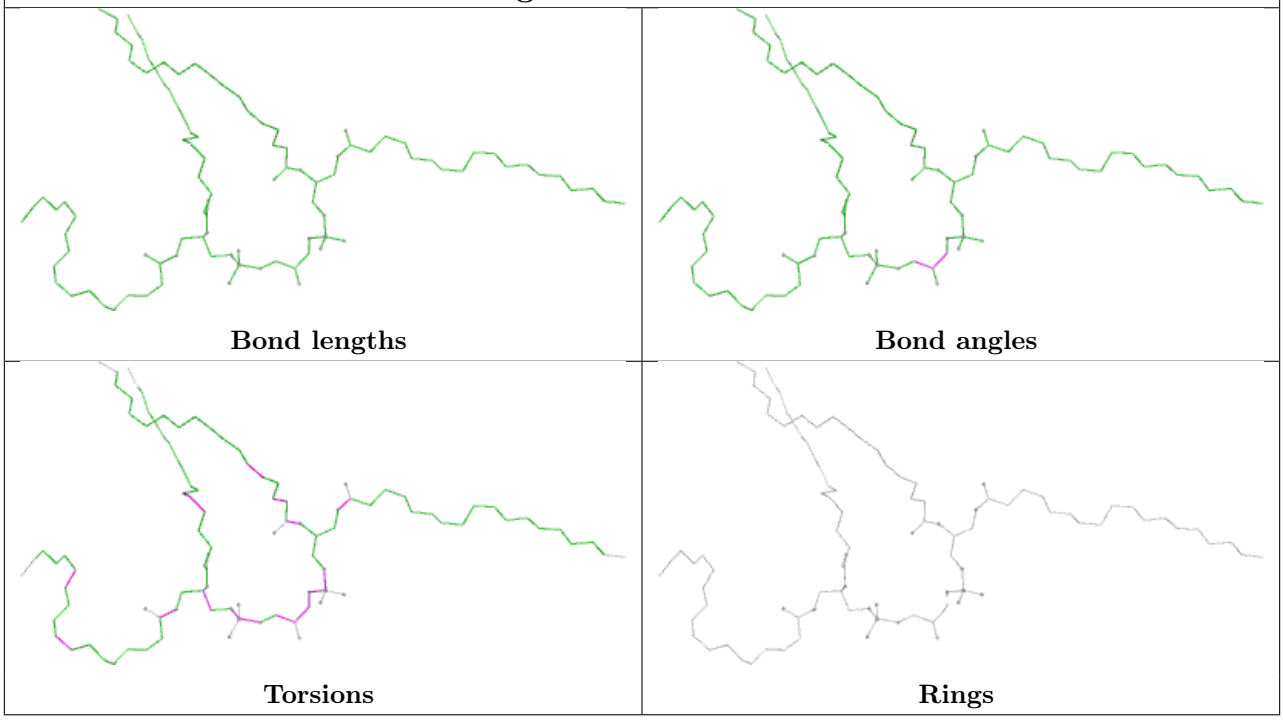

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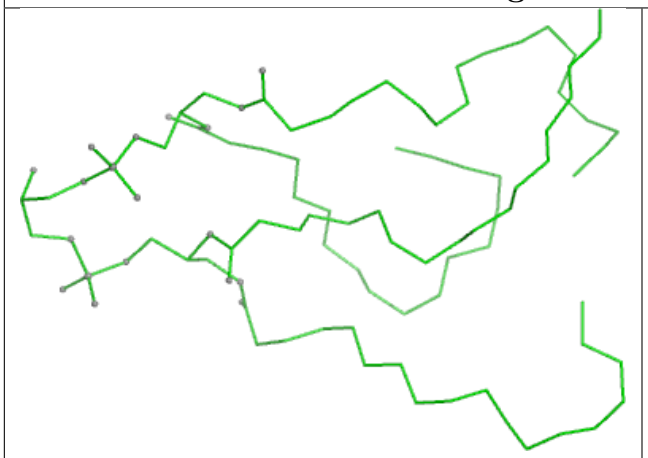

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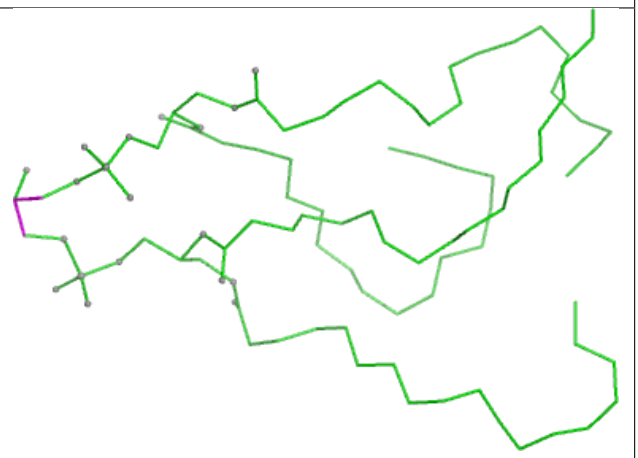
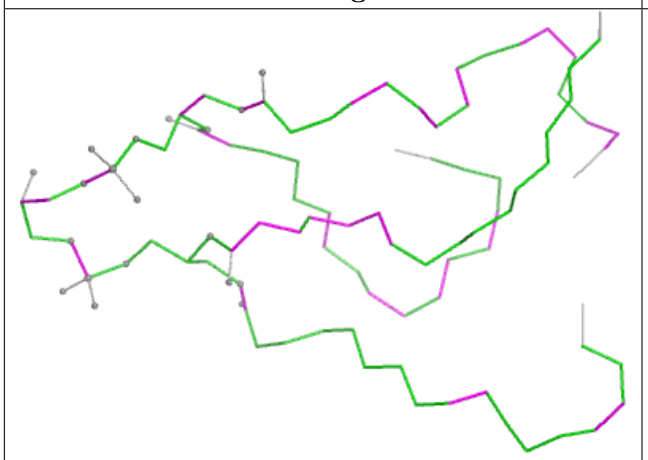


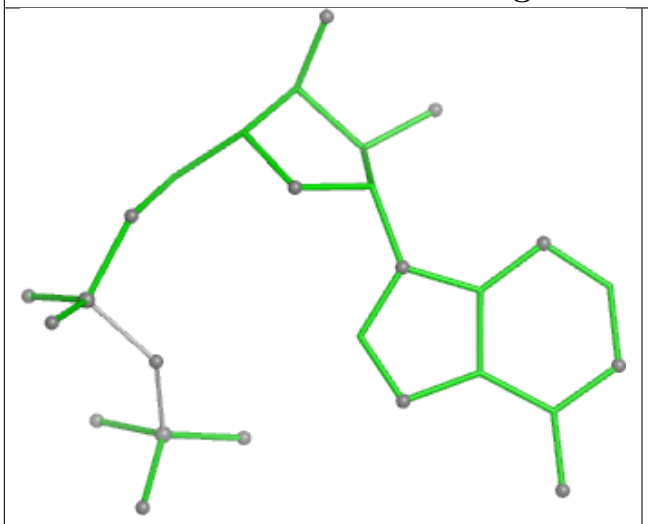
Bond angles



Torsions

Rings

Ligand ADP A8 401



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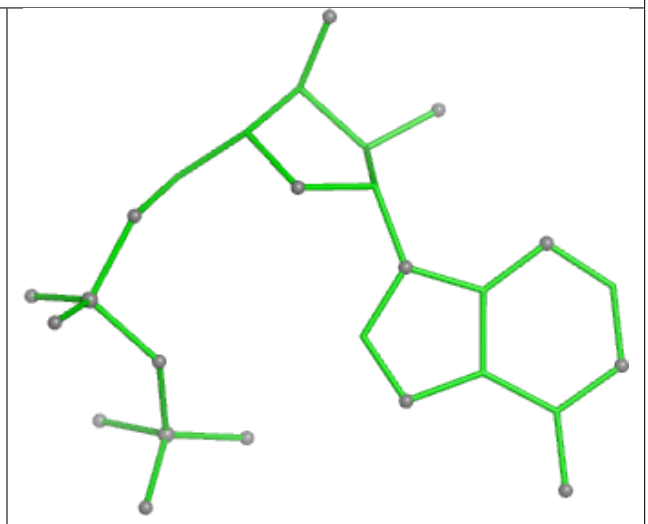
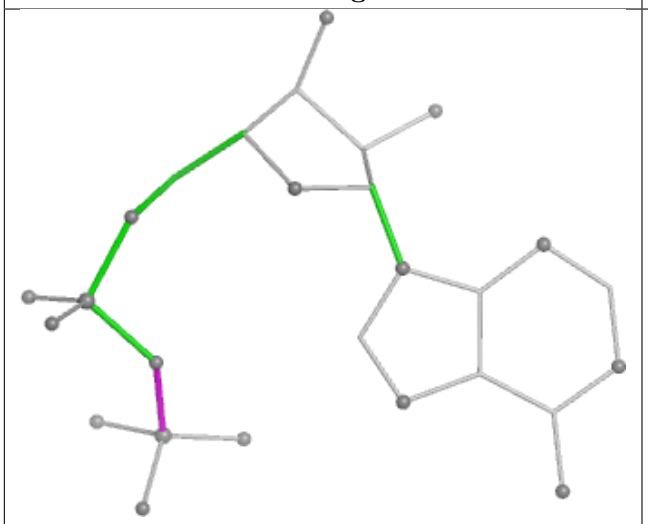
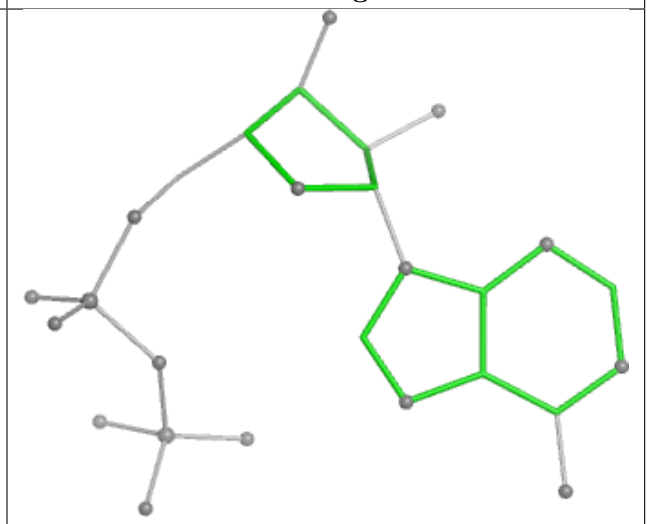


Bond angles



Torsions

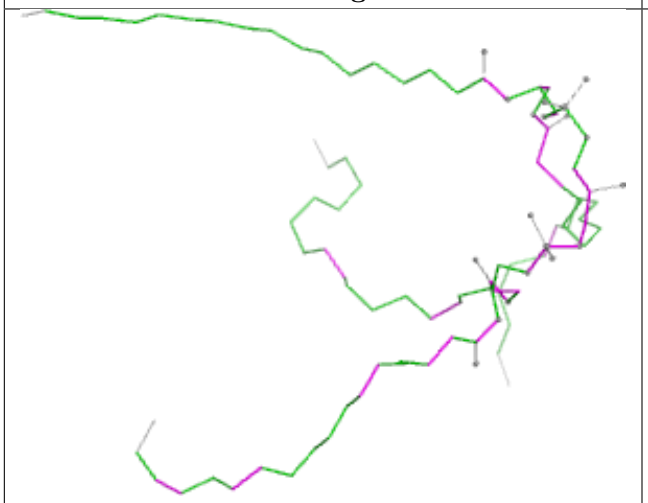


Rings

Ligand CDL Dd 702

Bond lengths

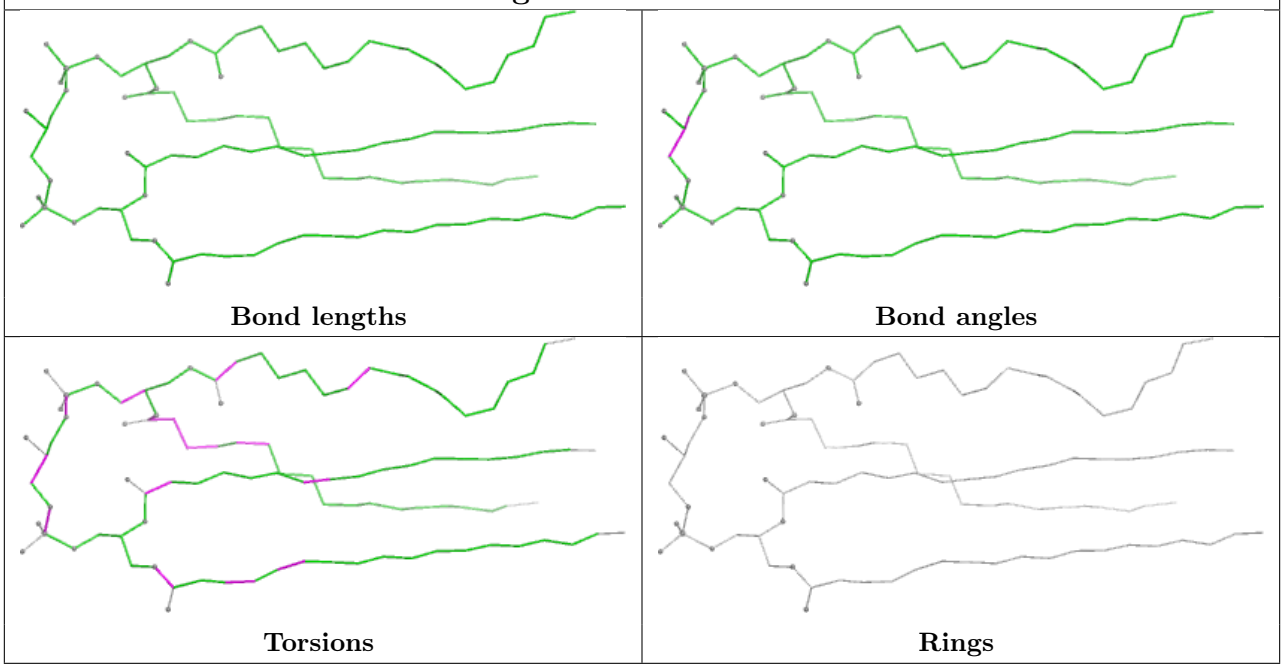
Bond angles



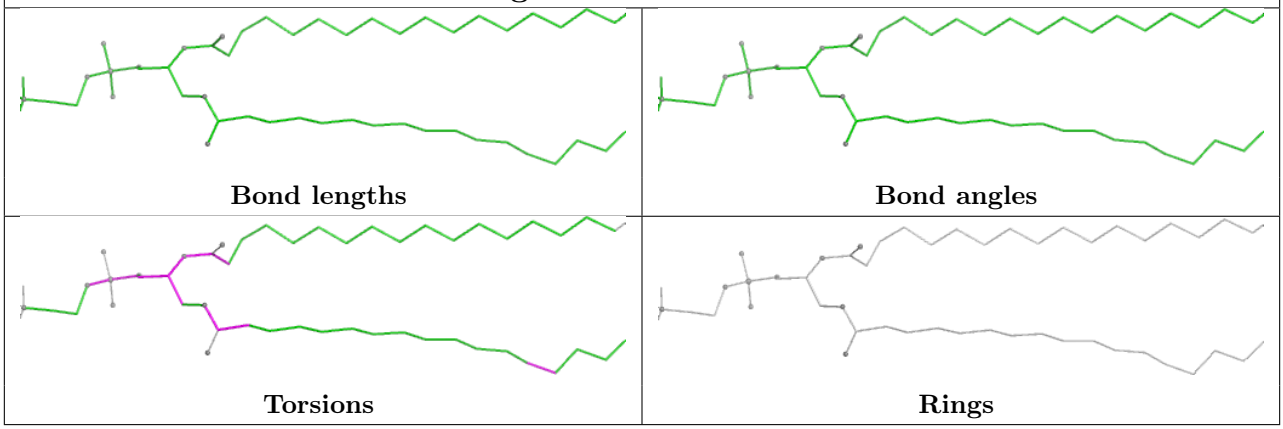
Torsions

Rings

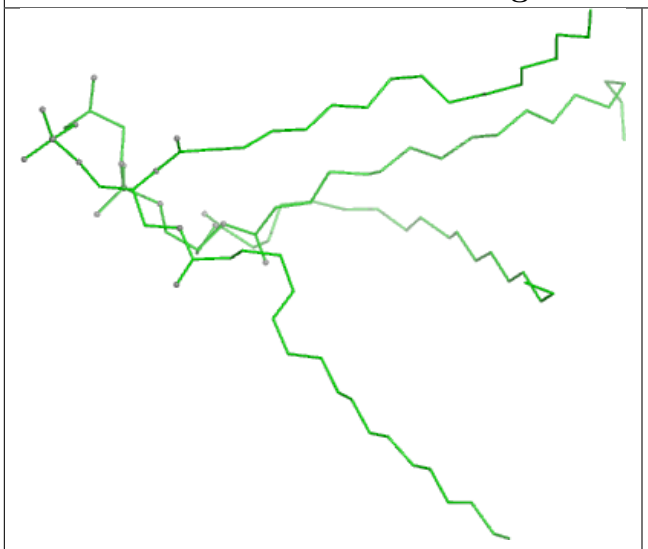
Ligand CDL BC 301



Ligand PC1 AM 302



Ligand CDL CG 301



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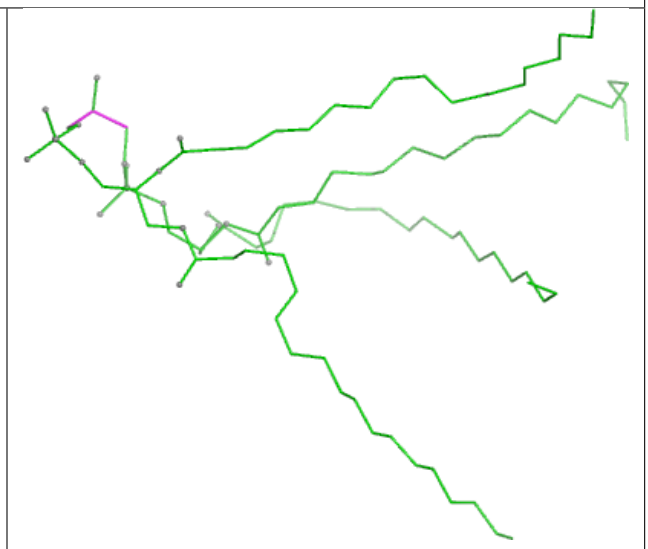
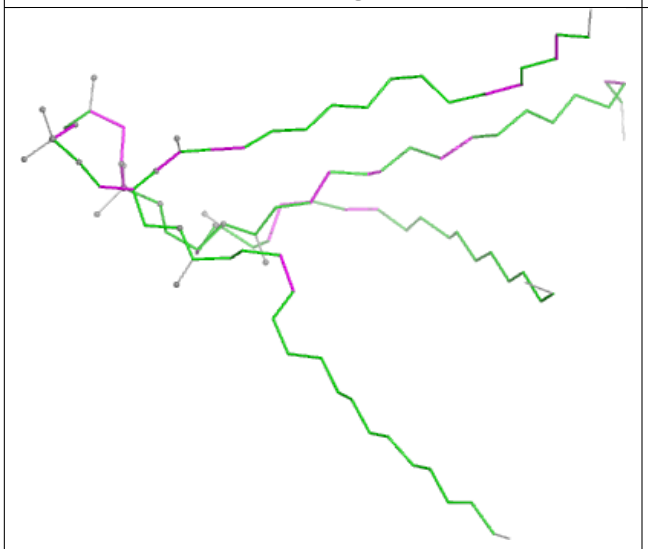
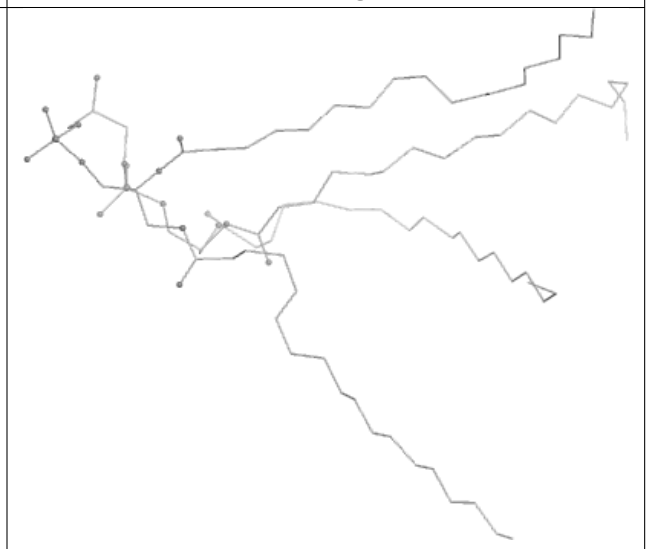


Bond angles

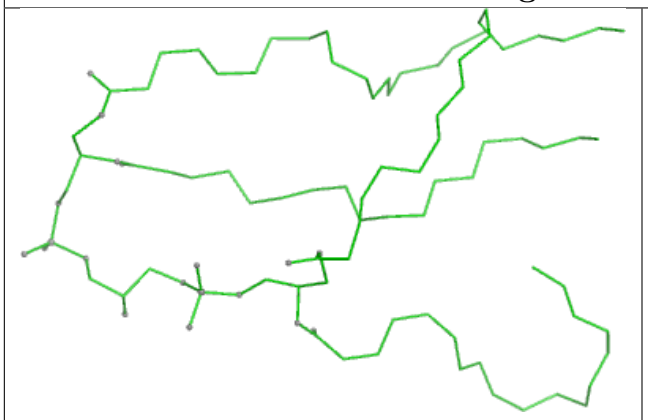


Torsions



Rings

Ligand CDL Dj 401



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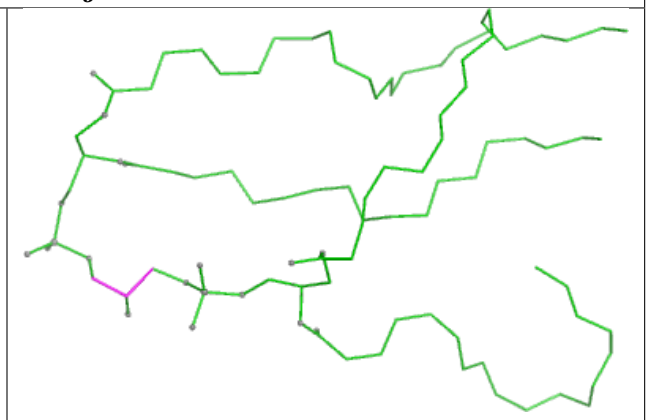
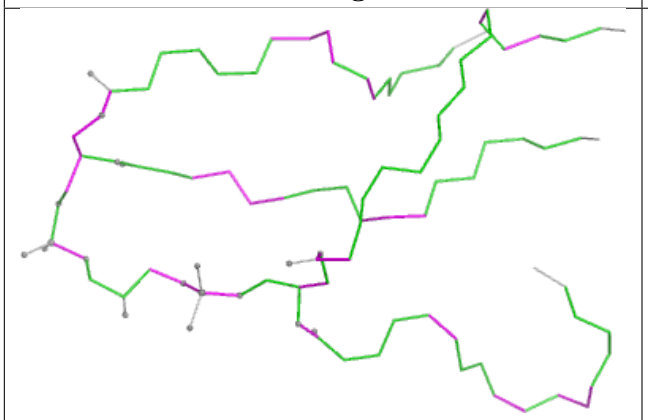


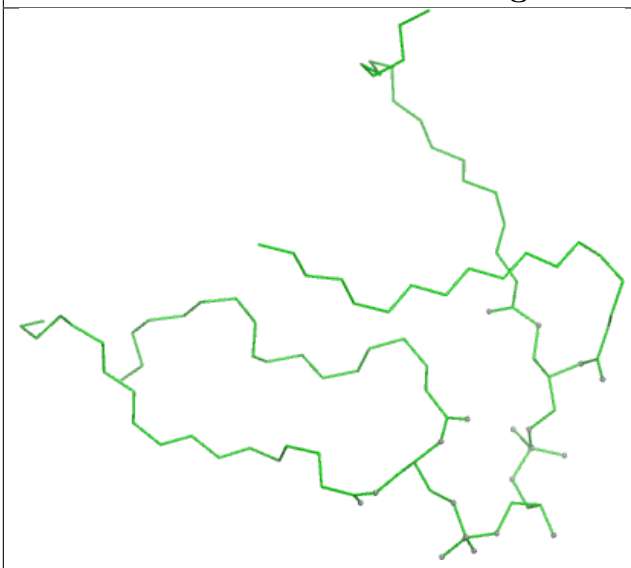
Bond angles



Torsions

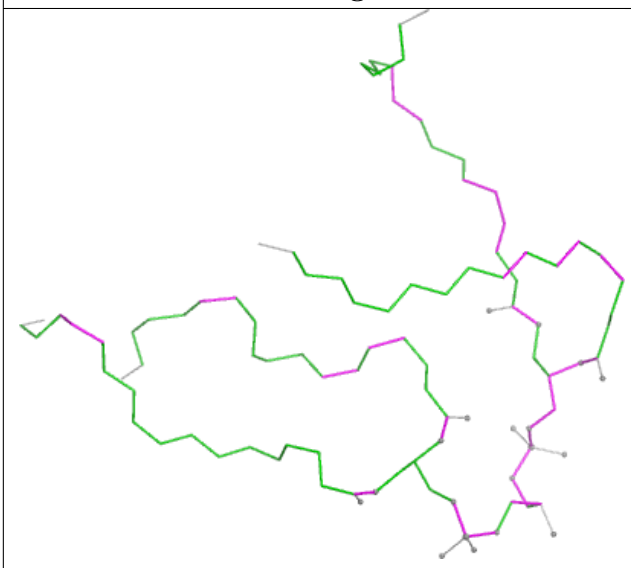
Rings

Ligand CDL CG 302



Bond lengths

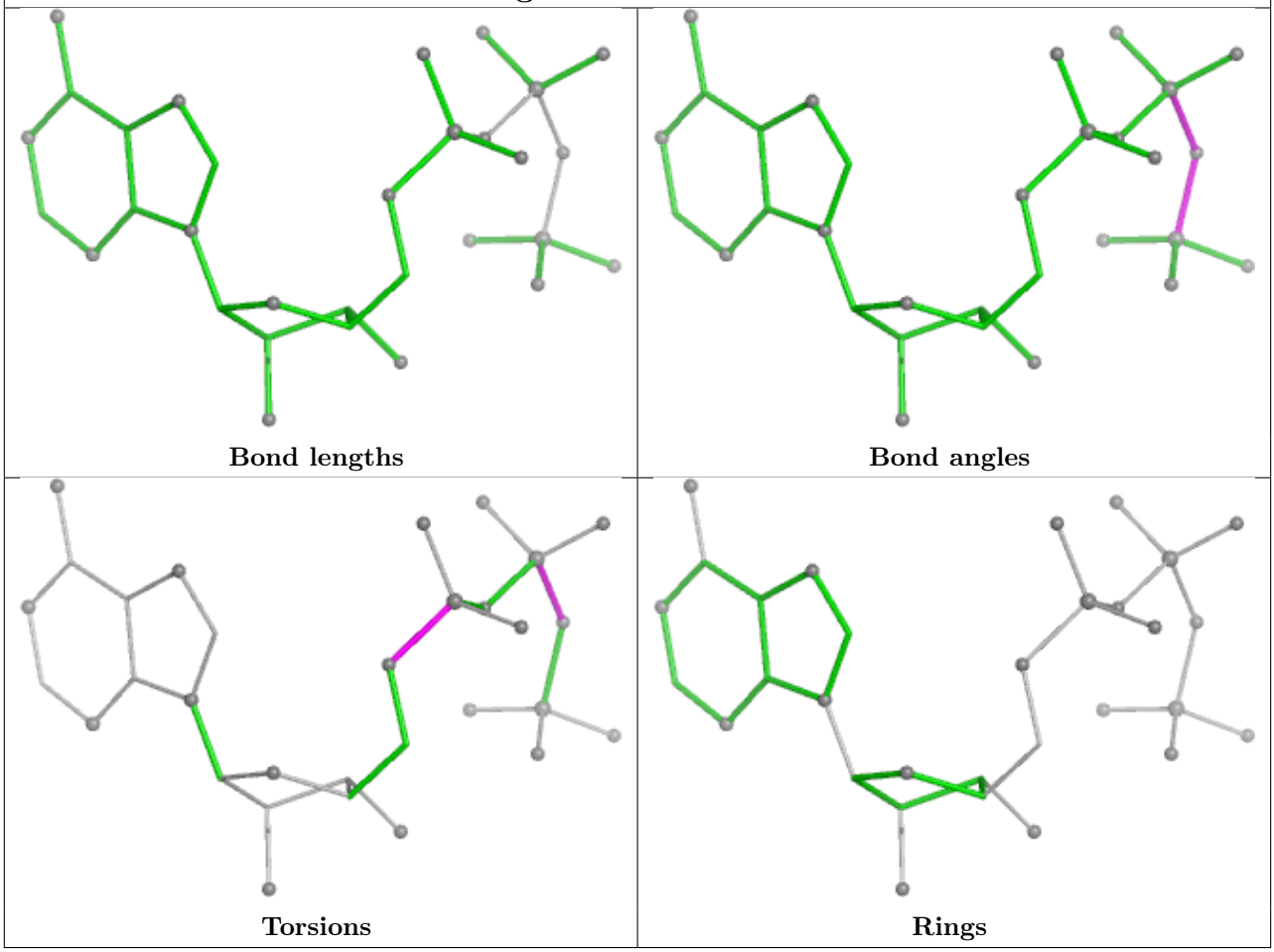
Bond angles



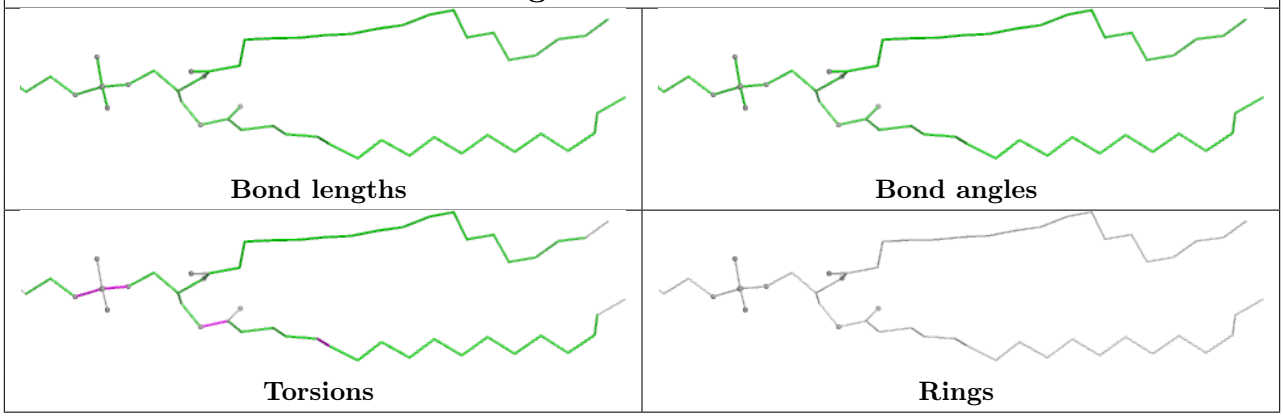
Torsions

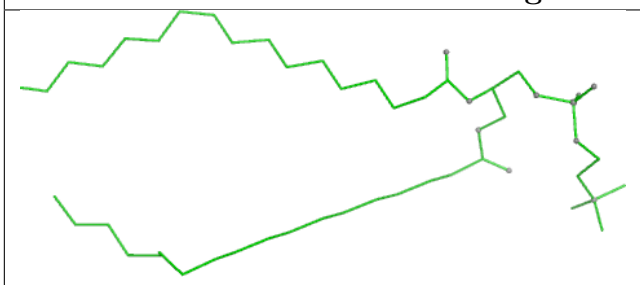
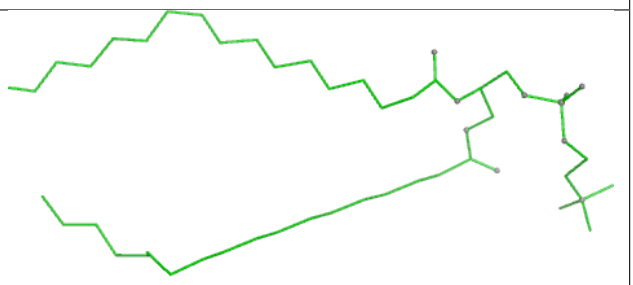
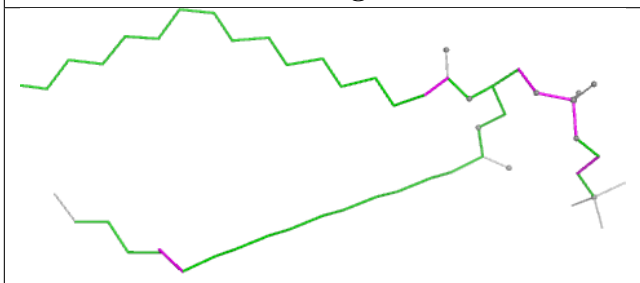
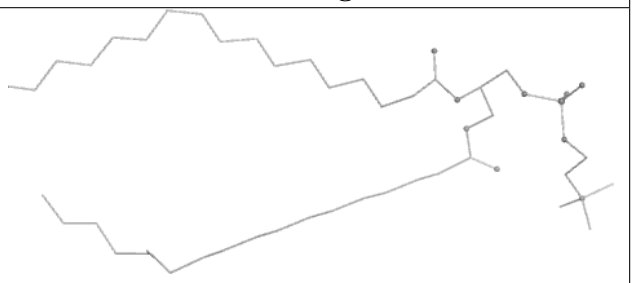
Rings

Ligand ATP Er 201



Ligand 3PE G 401



Ligand PC1 El 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

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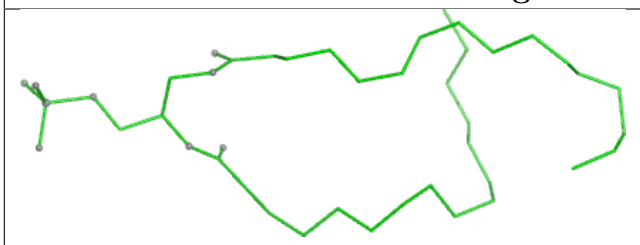
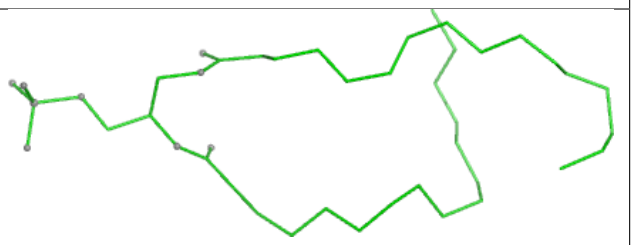
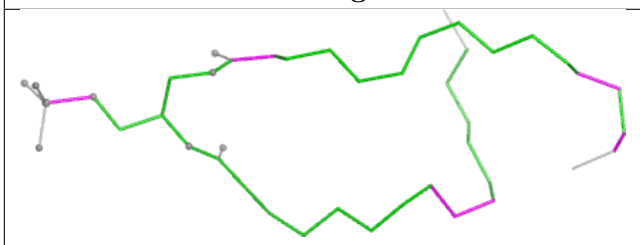
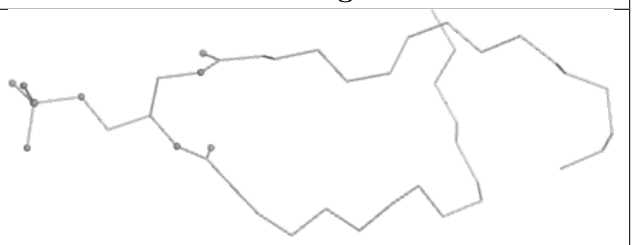
 Bond lengths	 Bond angles
 Torsions	 Rings

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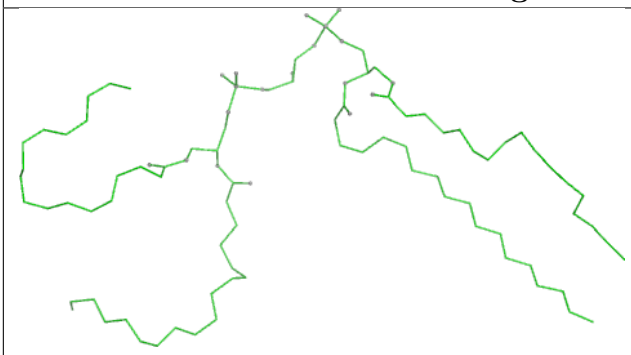
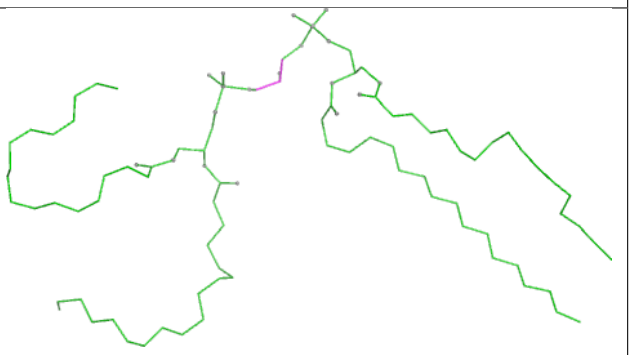
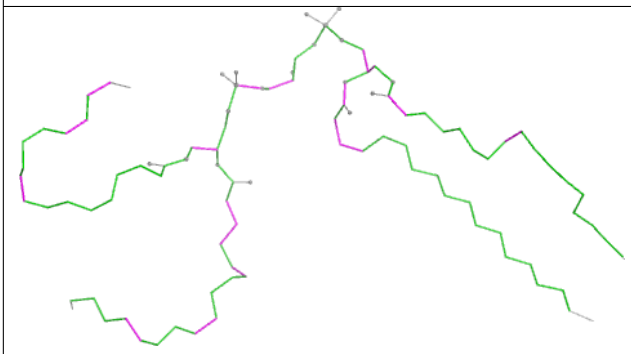
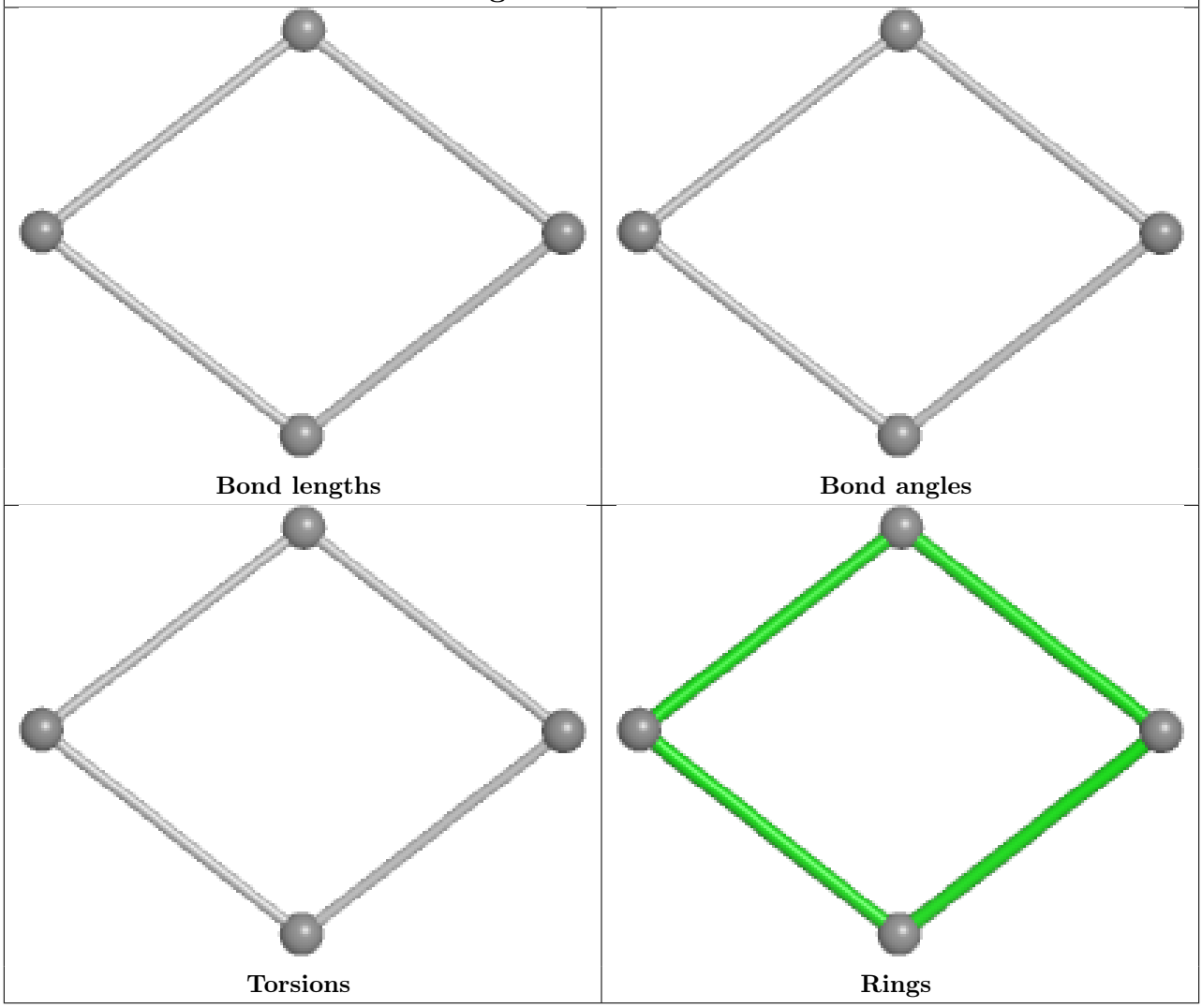
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand FES AI 301



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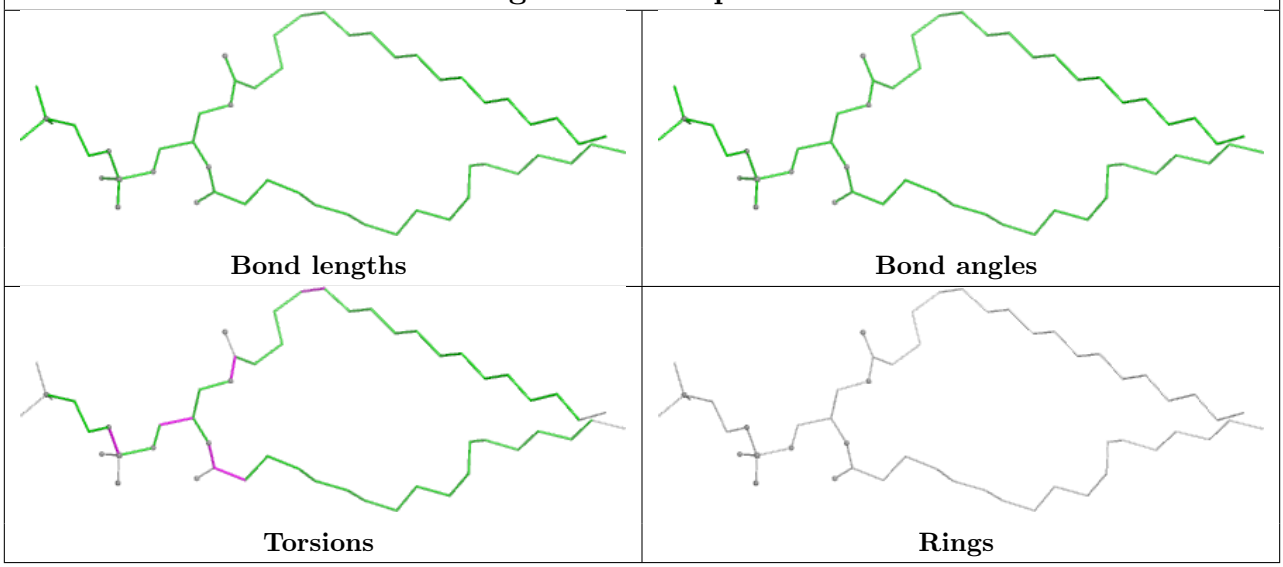

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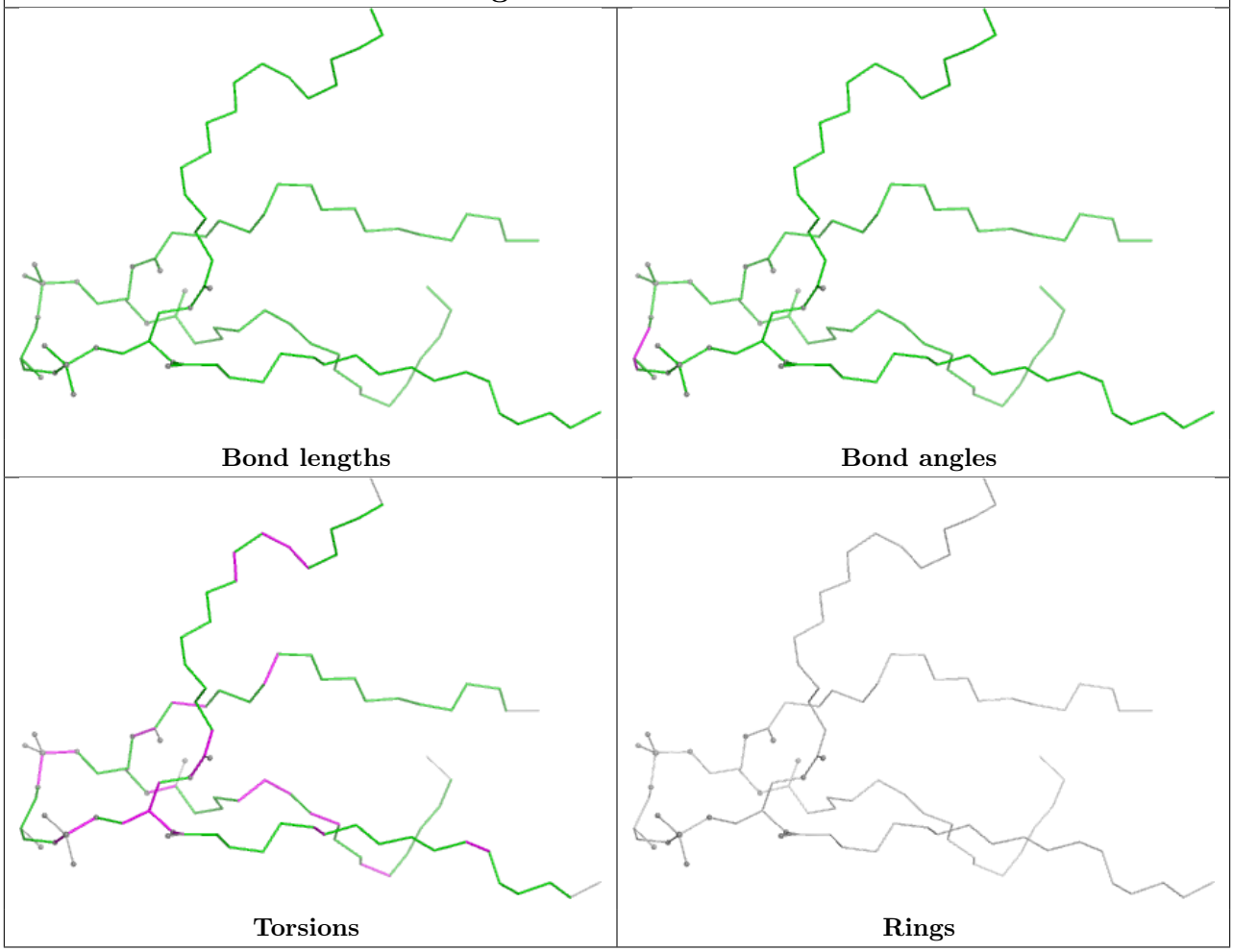

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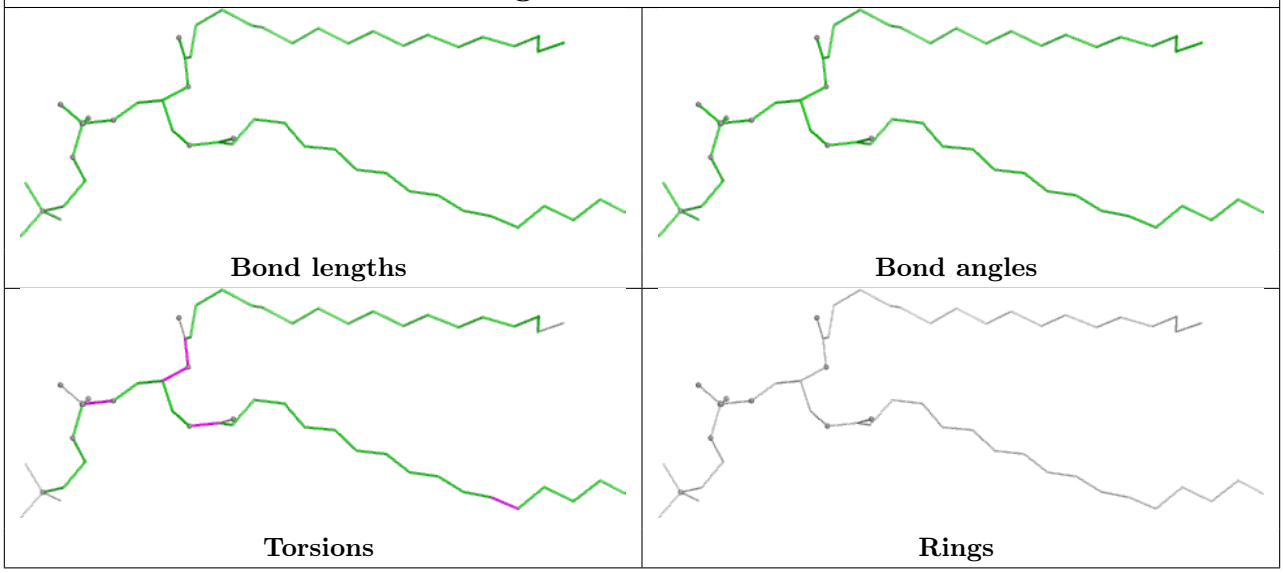

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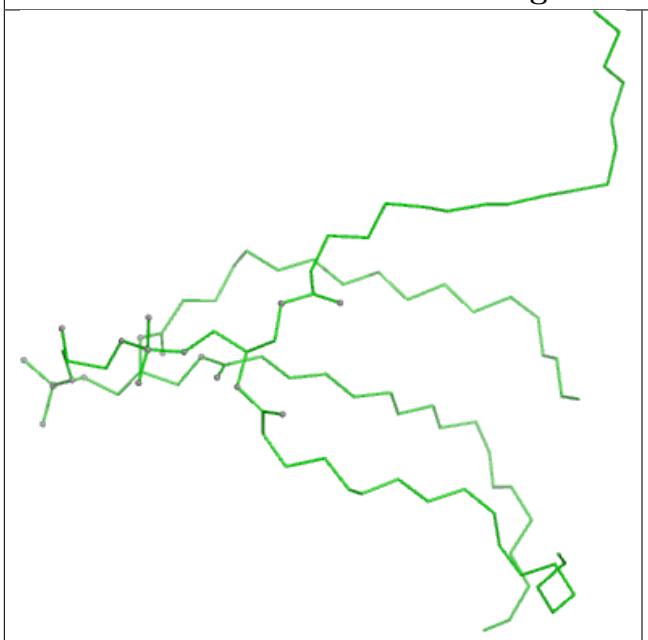
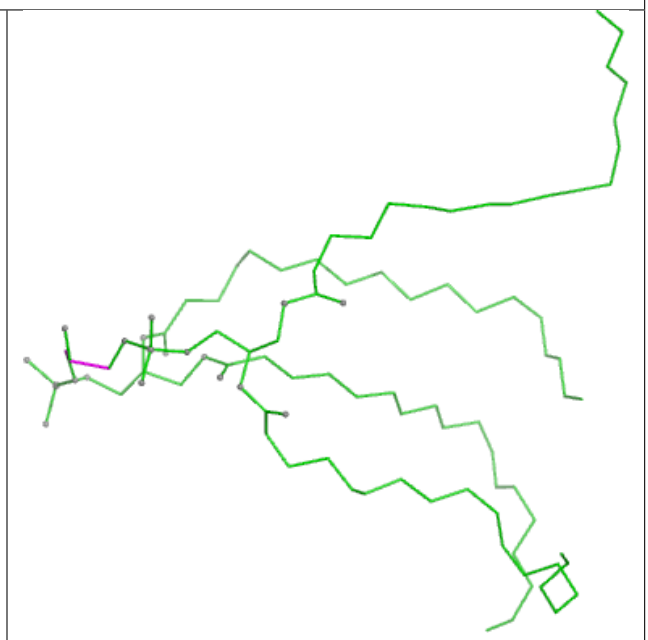
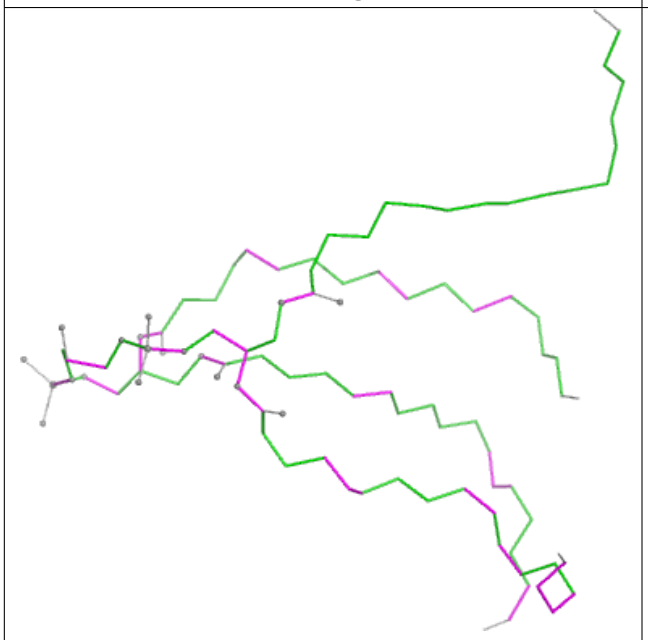


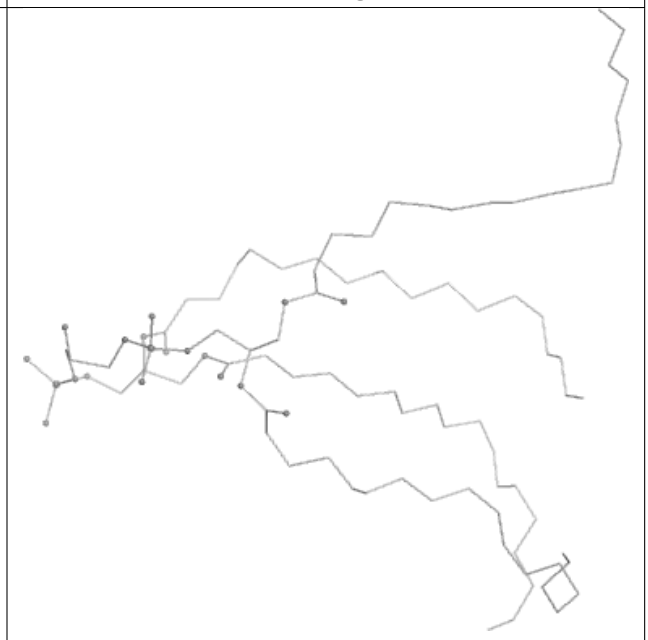
Bond lengths



Bond angles



Torsions



Rings

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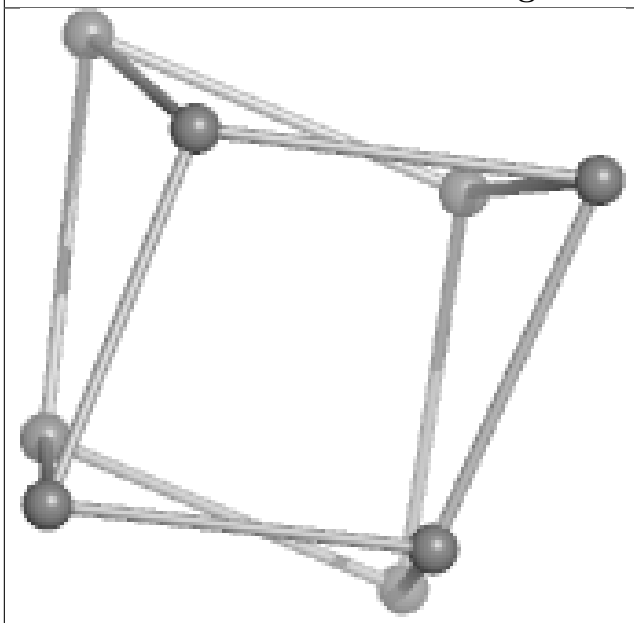

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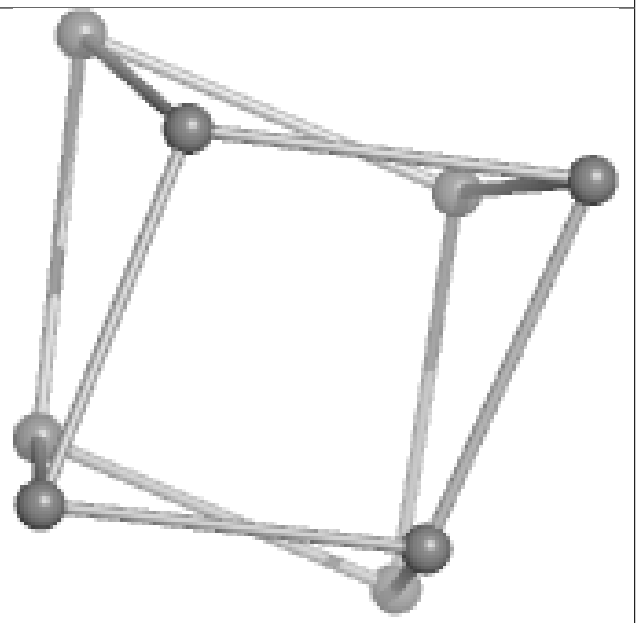

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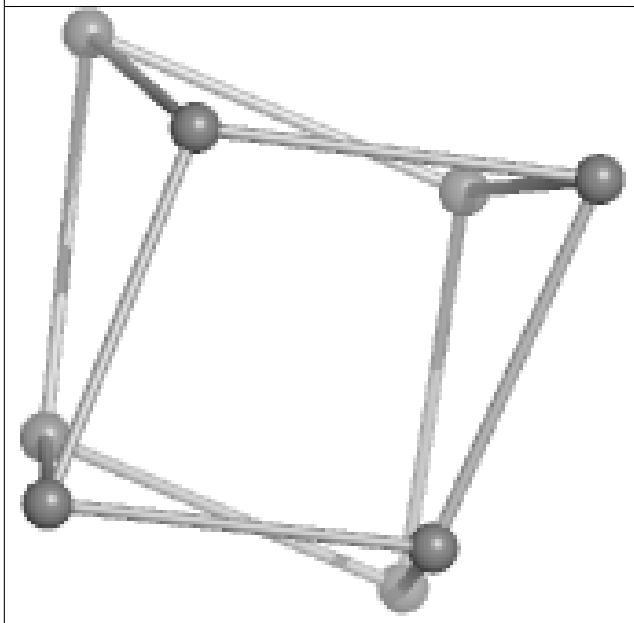

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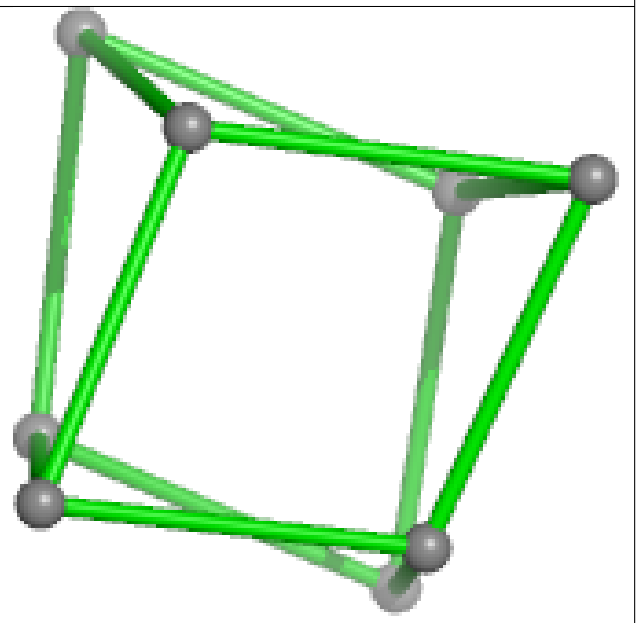

Rings

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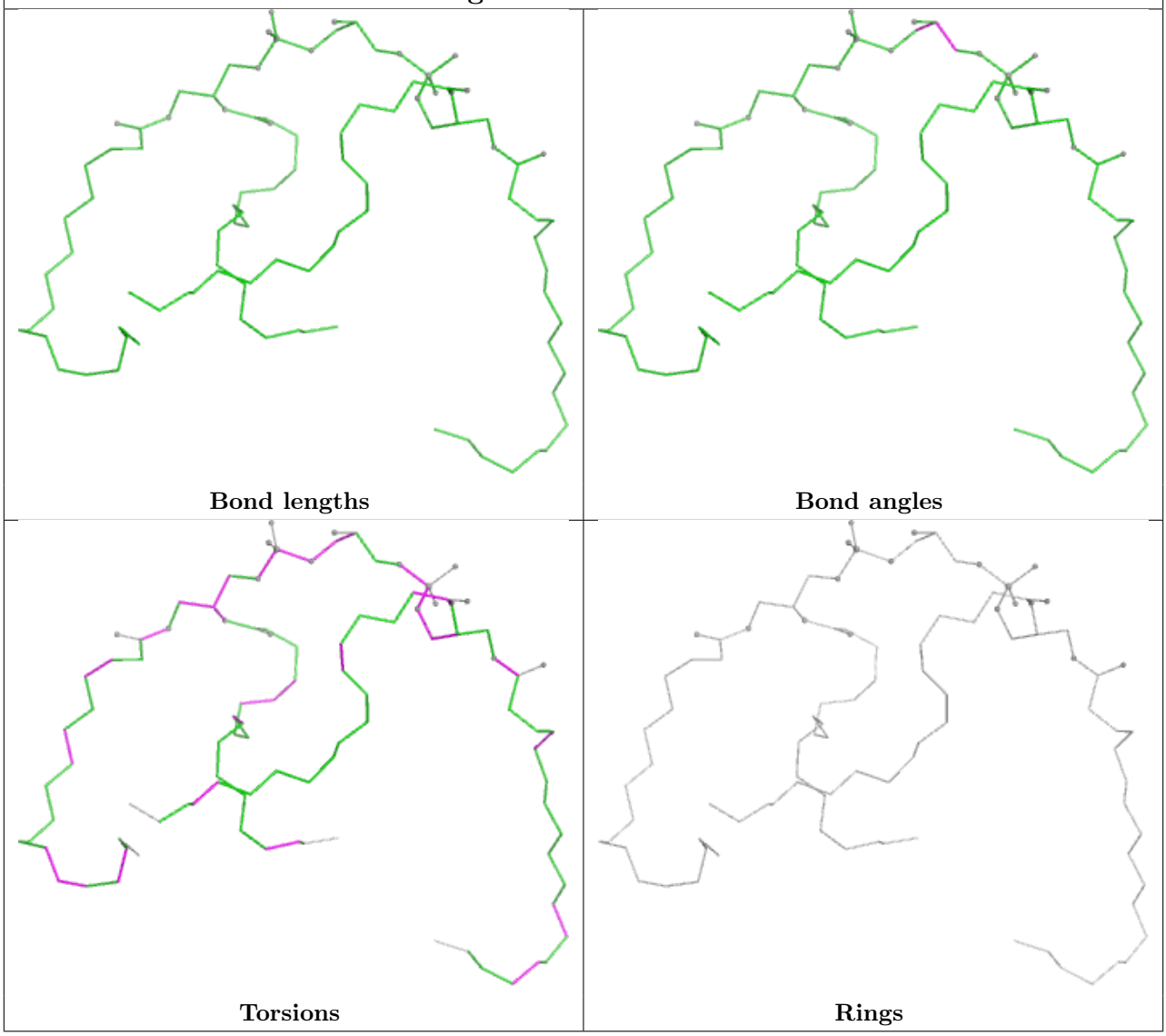

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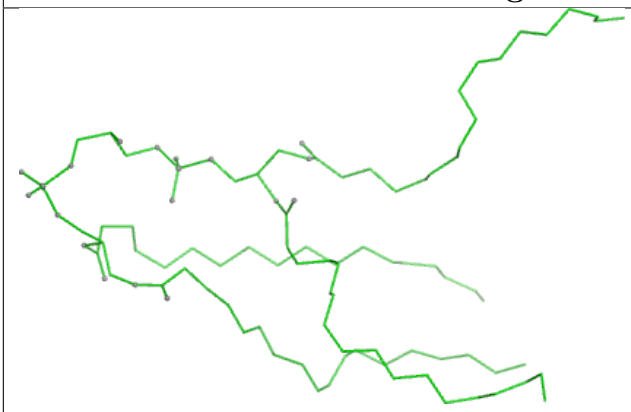
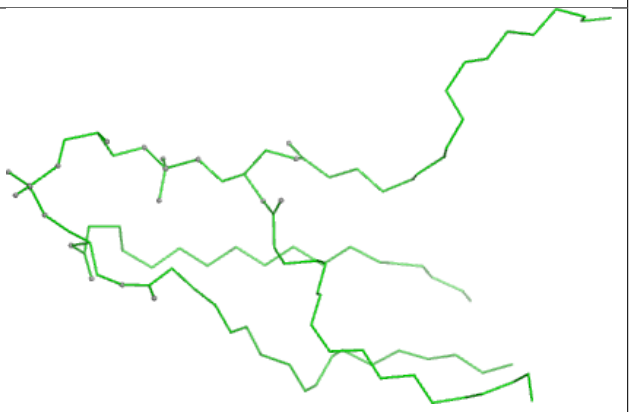
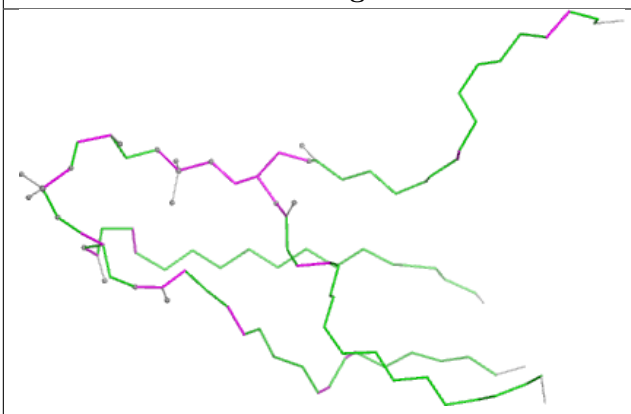
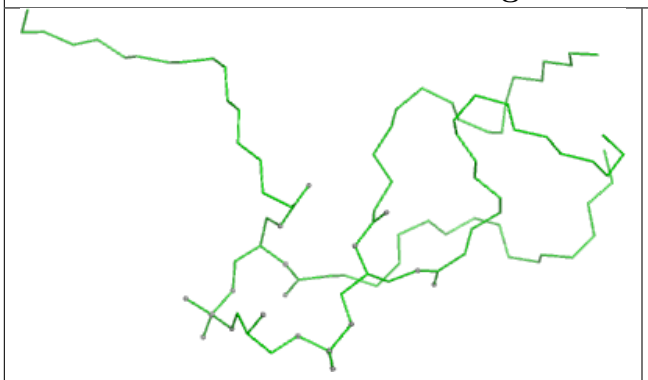
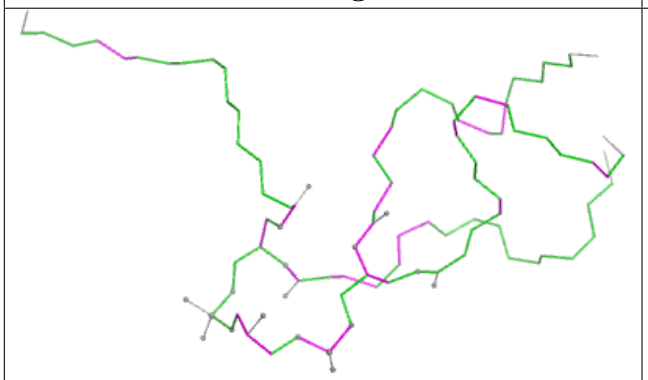
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL DQ 1501

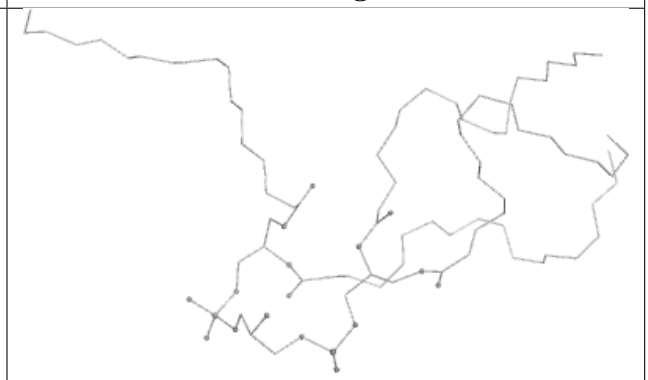


Bond lengths

Bond angles

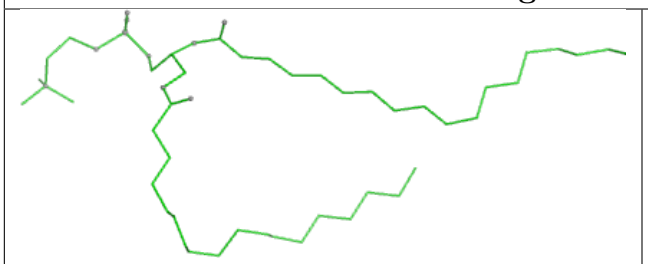


Torsions



Rings

Ligand PC1 A 1201



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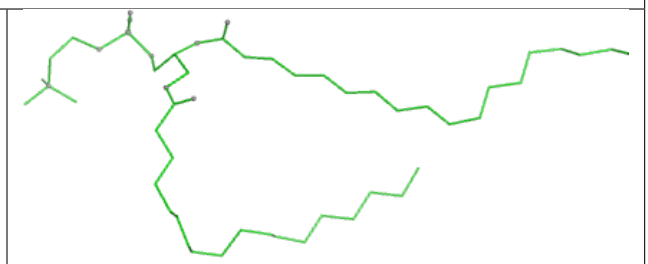

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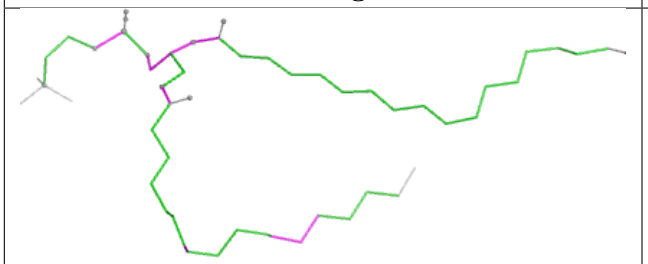
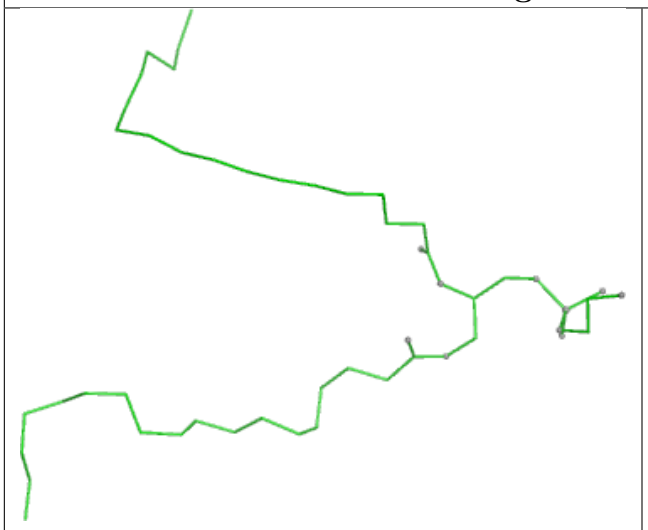


Torsions

Rings

Ligand 3PE DG 204



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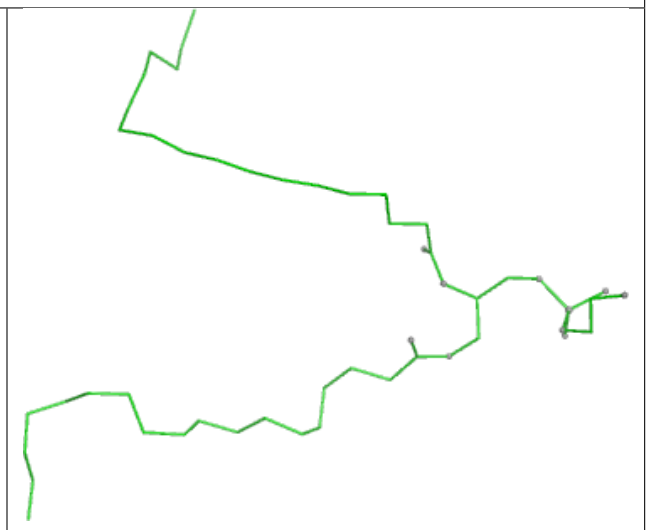
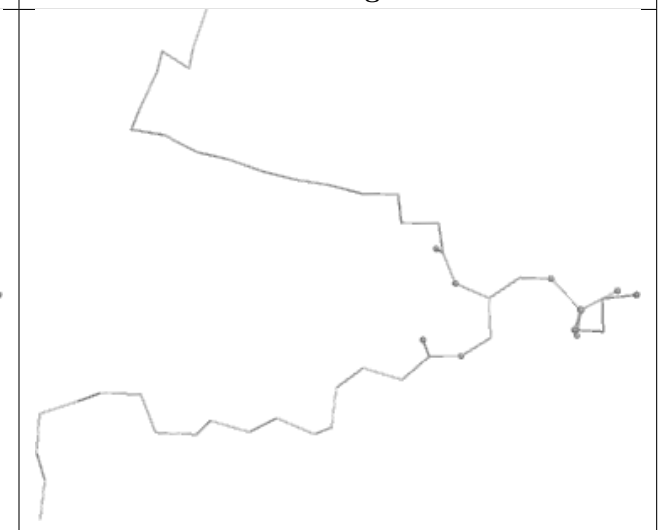


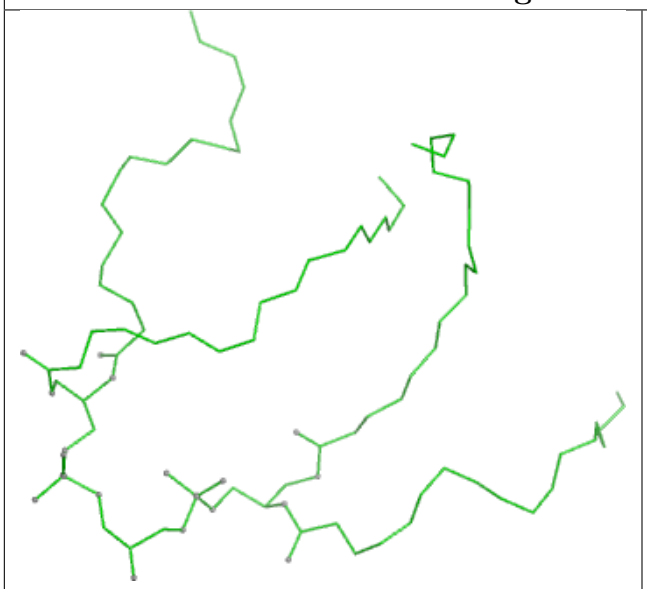
Bond angles

Torsions



Rings

Ligand CDL Dh 201



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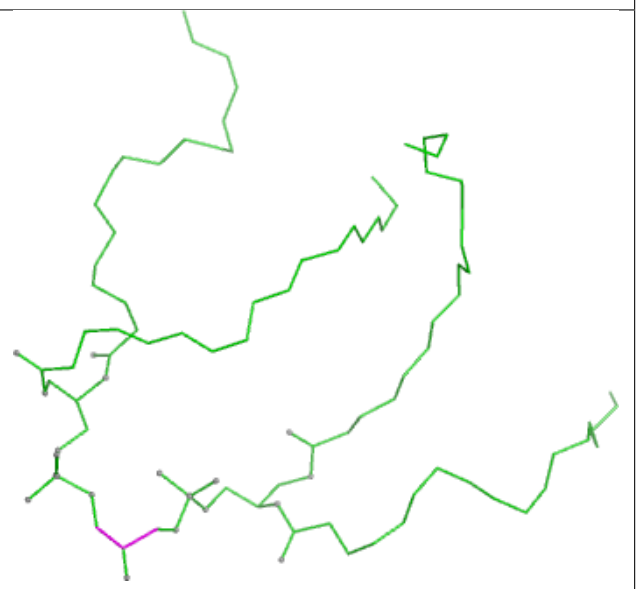

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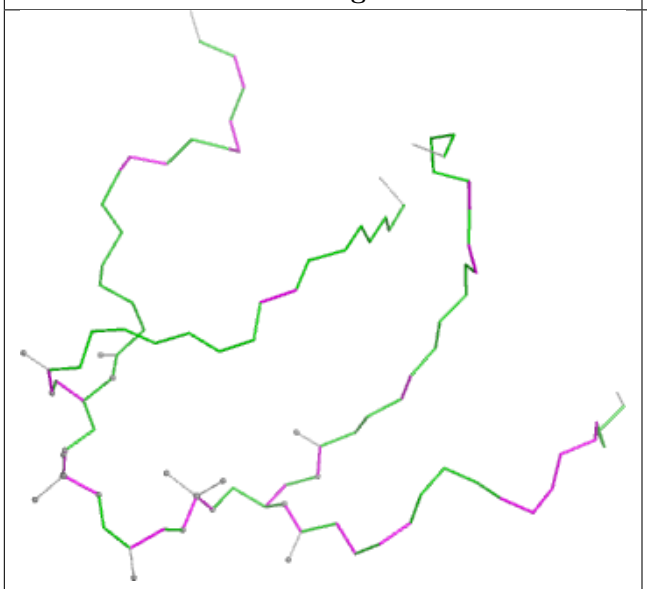

Torsions

Rings

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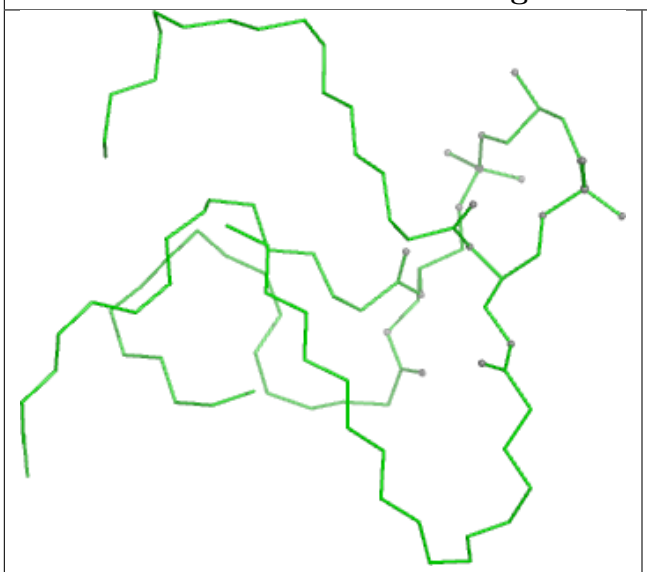

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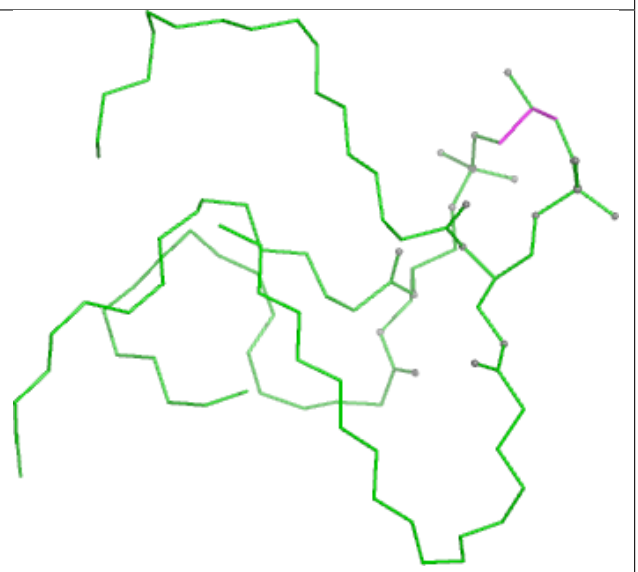

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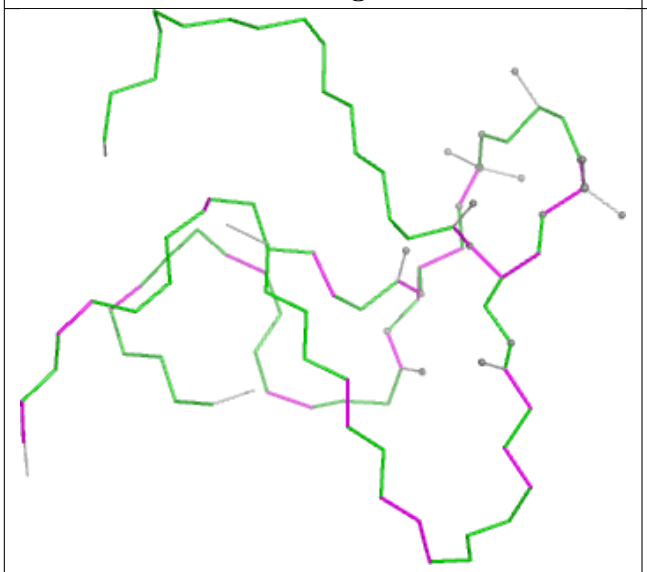
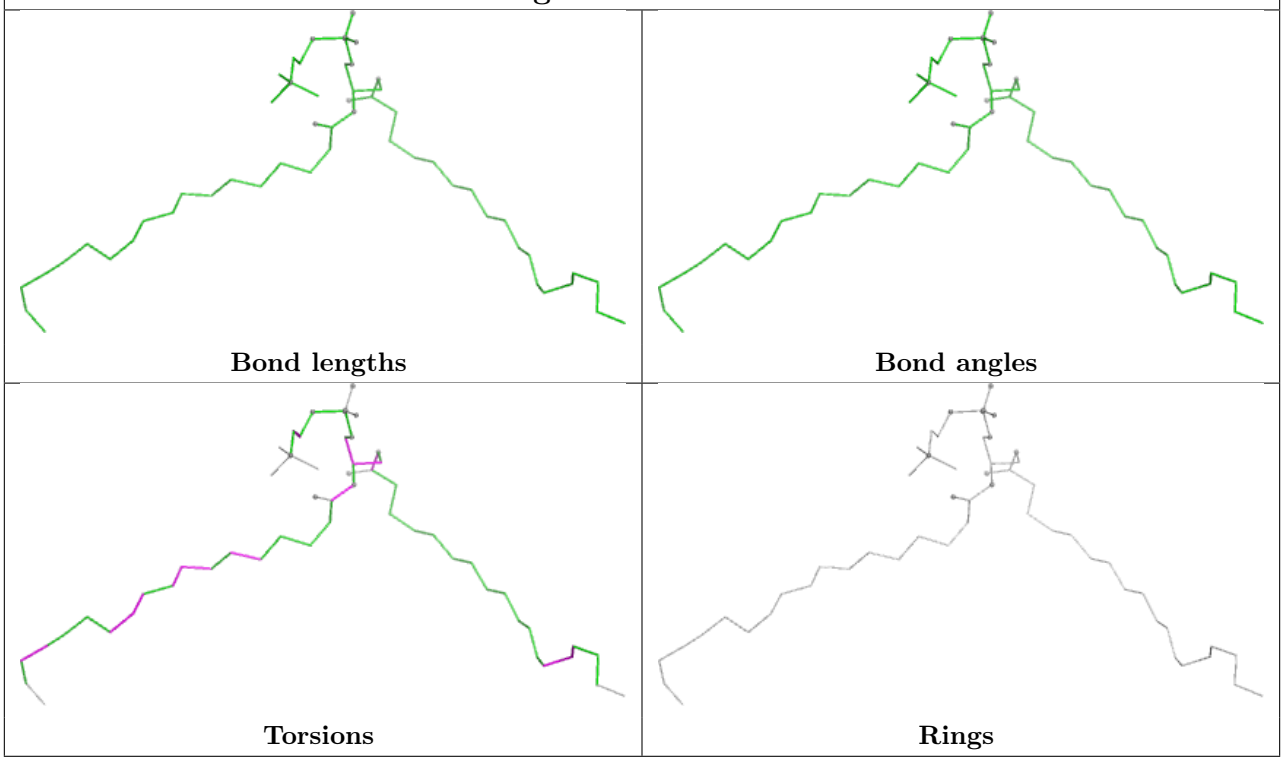


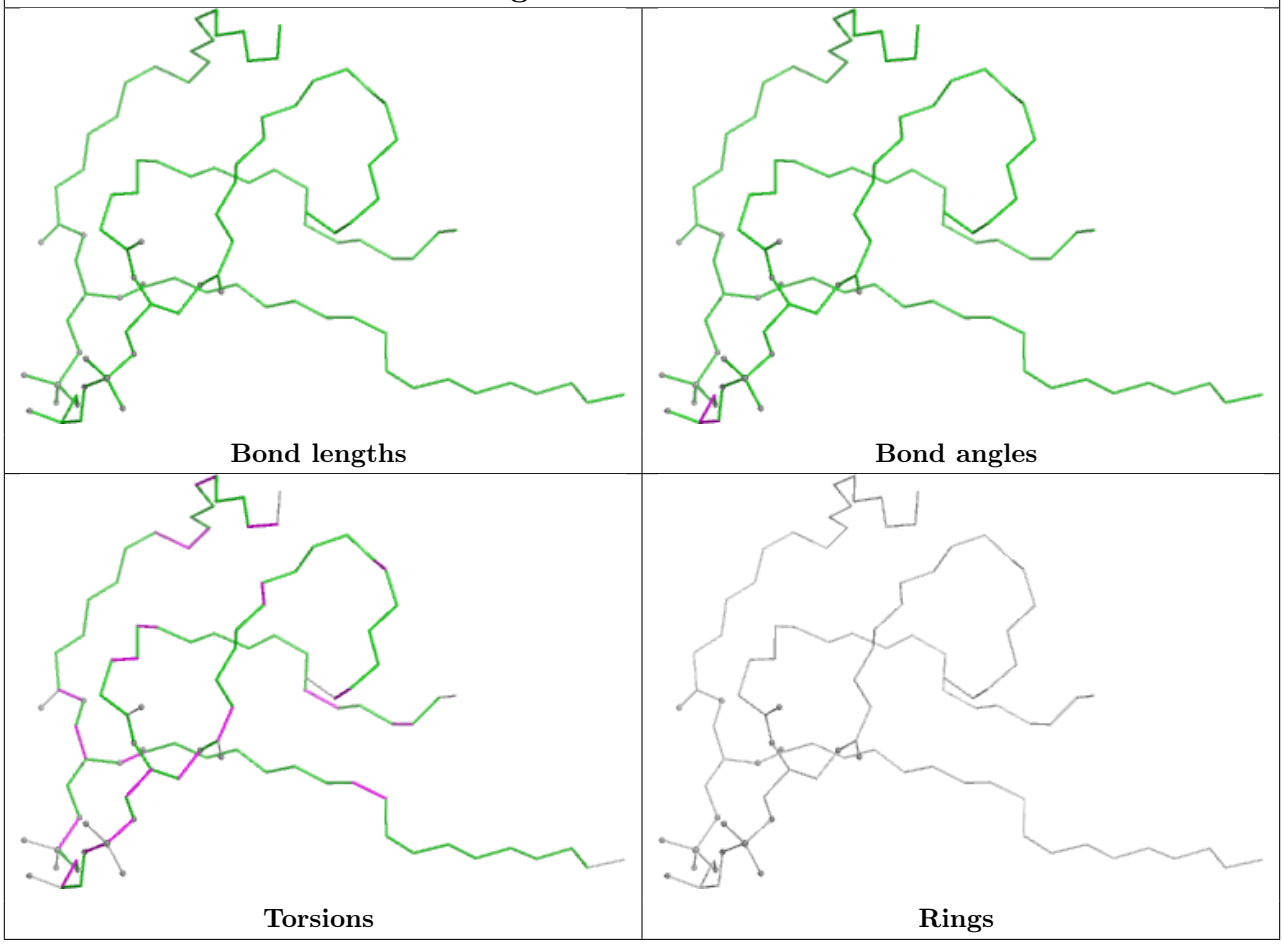
Torsions

Rings

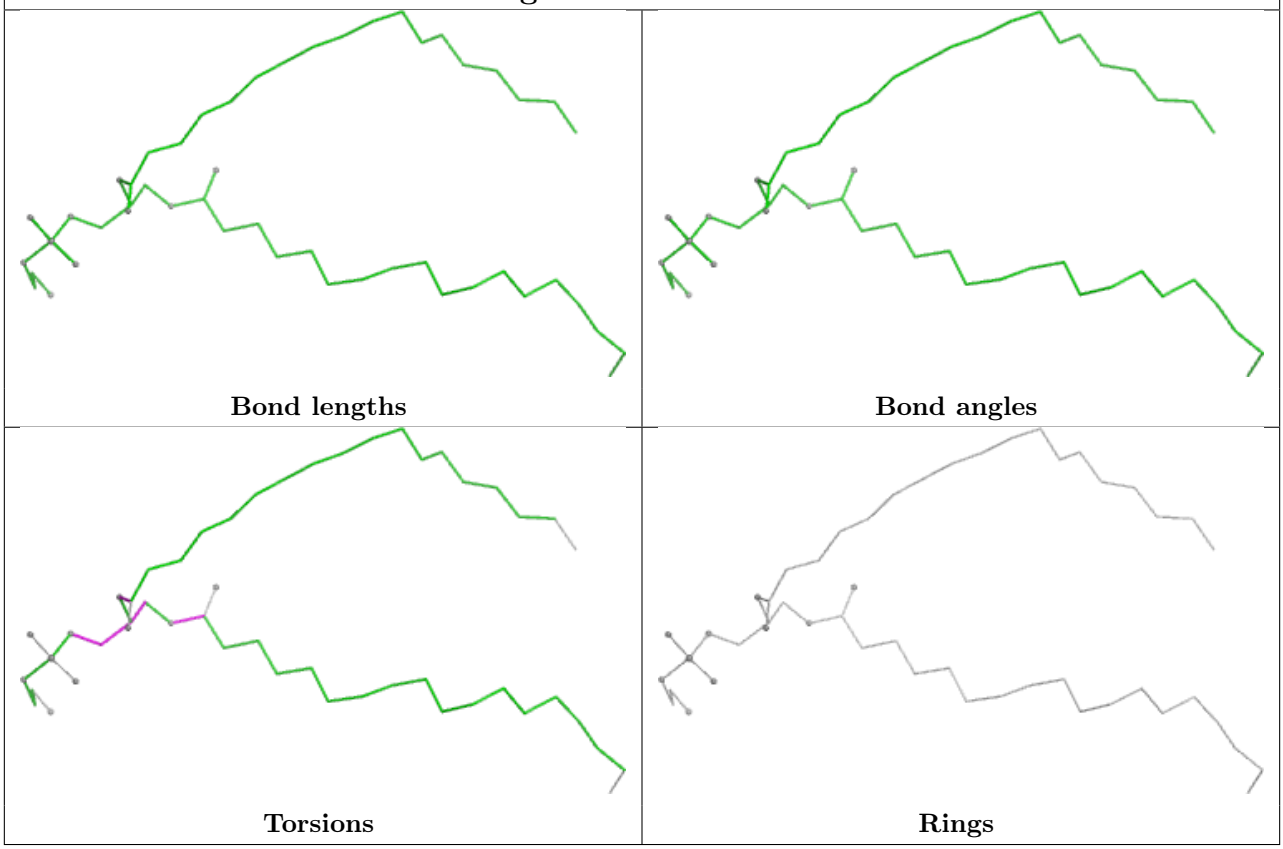
Ligand PC1 c 503



Ligand CDL DD 706



Ligand 3PE A2 401



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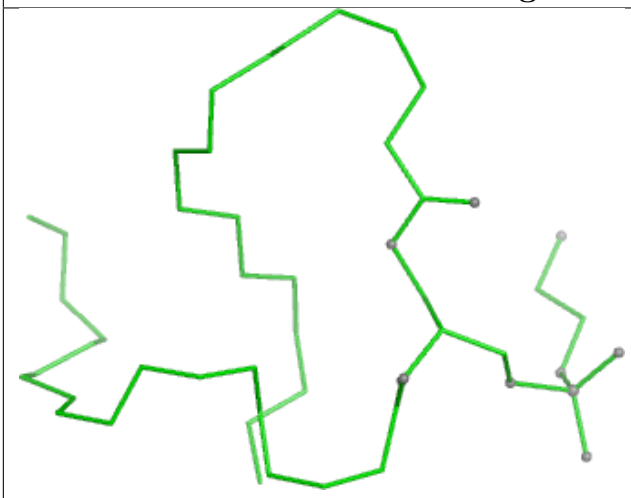

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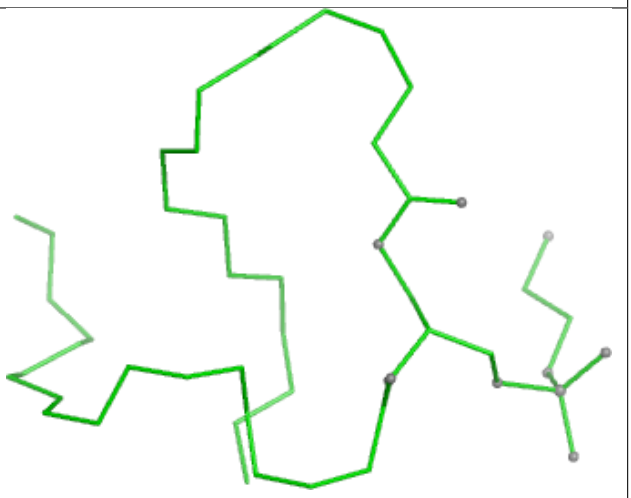
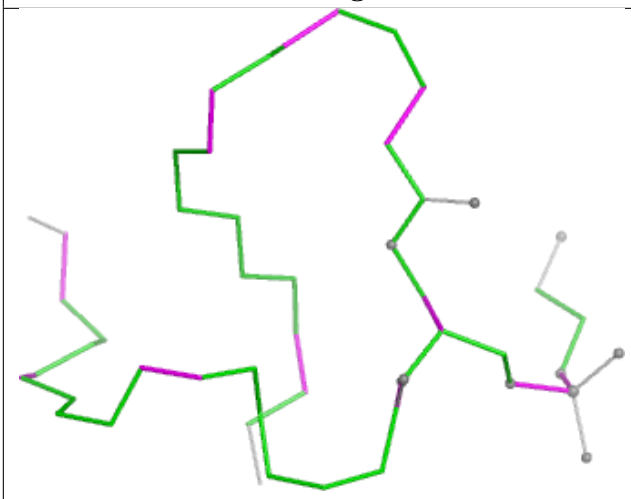
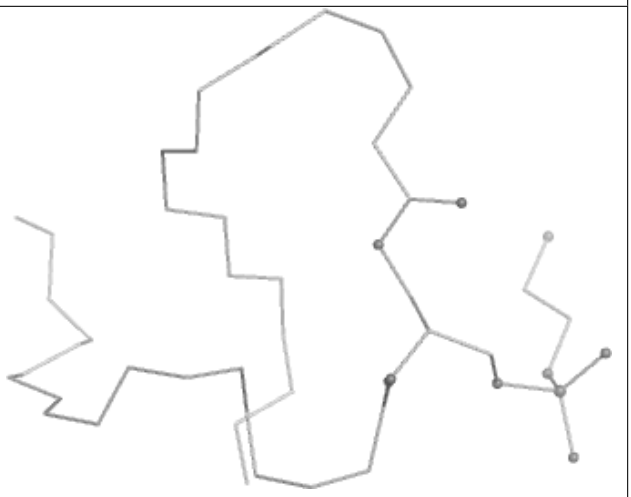


Bond angles

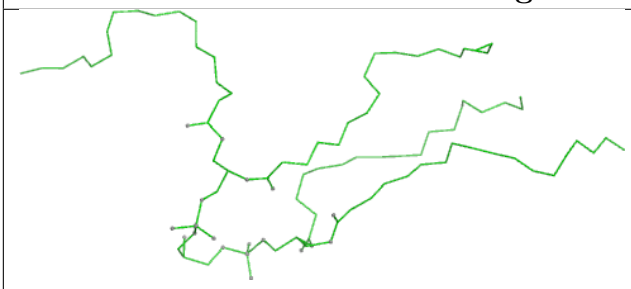


Torsions



Rings

Ligand CDL B0 101



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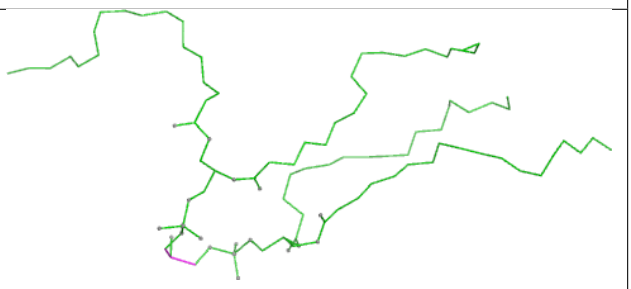
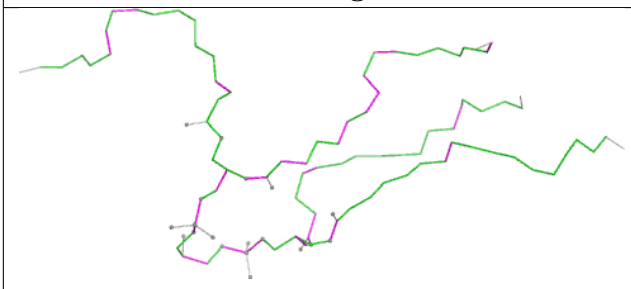


Bond angles



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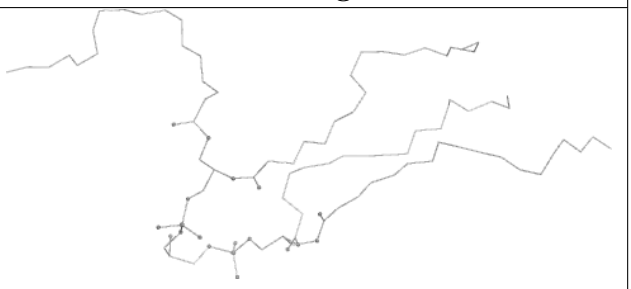
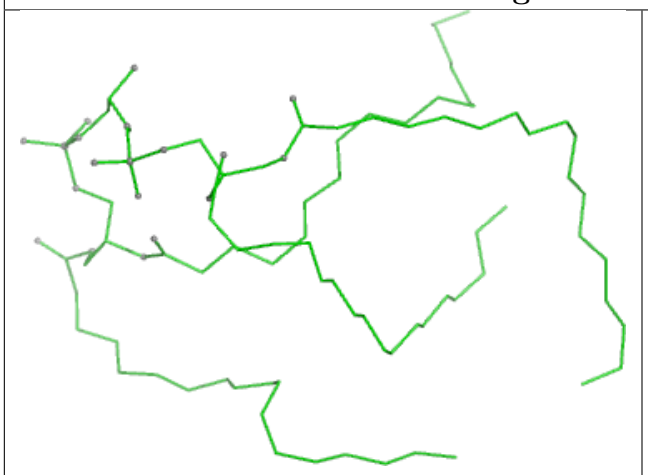


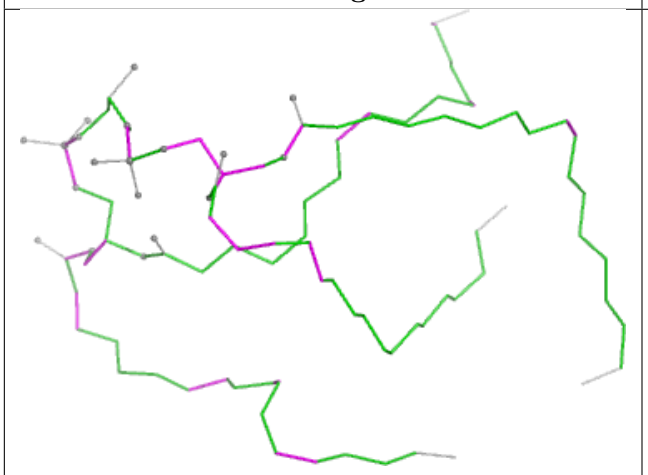
Rings

Ligand CDL EA 301



Bond lengths

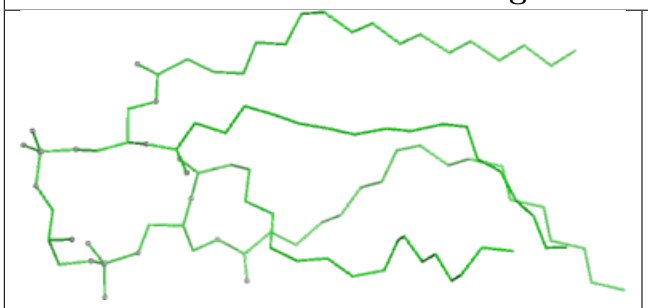
Bond angles



Torsions

Rings

Ligand CDL Dm 502



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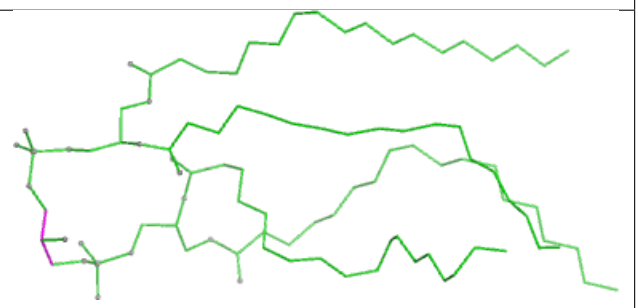
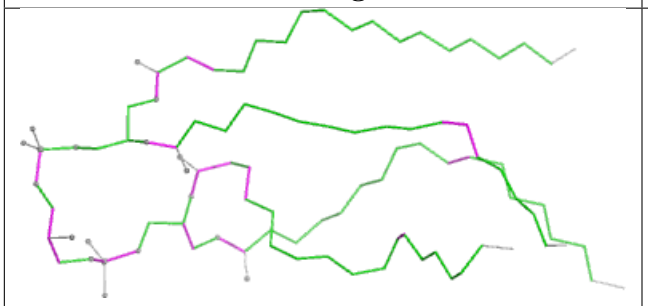


Bond angles



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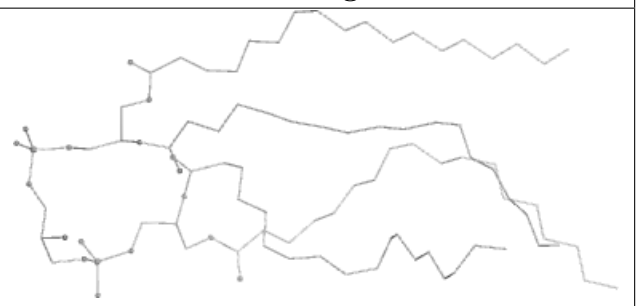
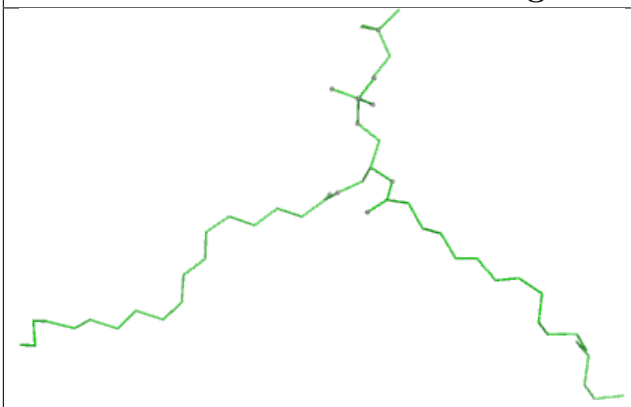
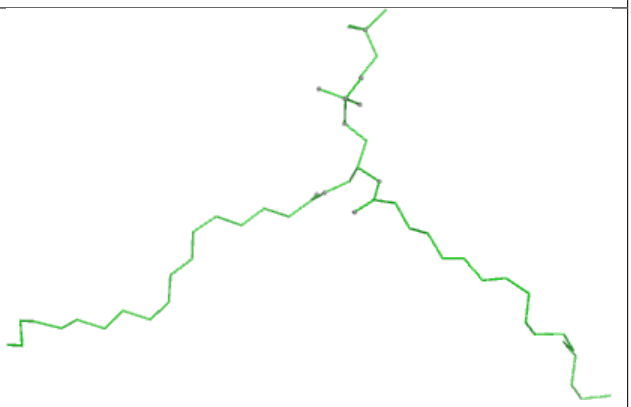
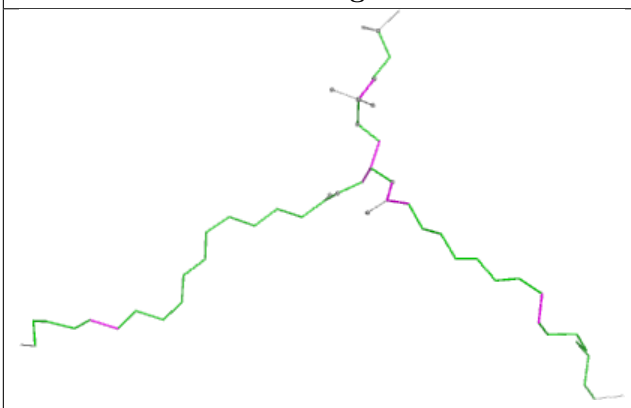
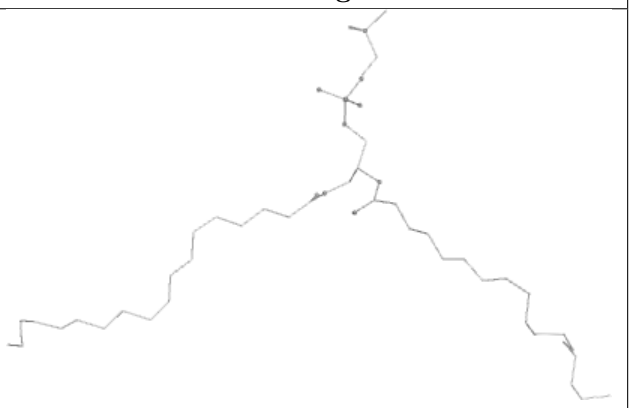
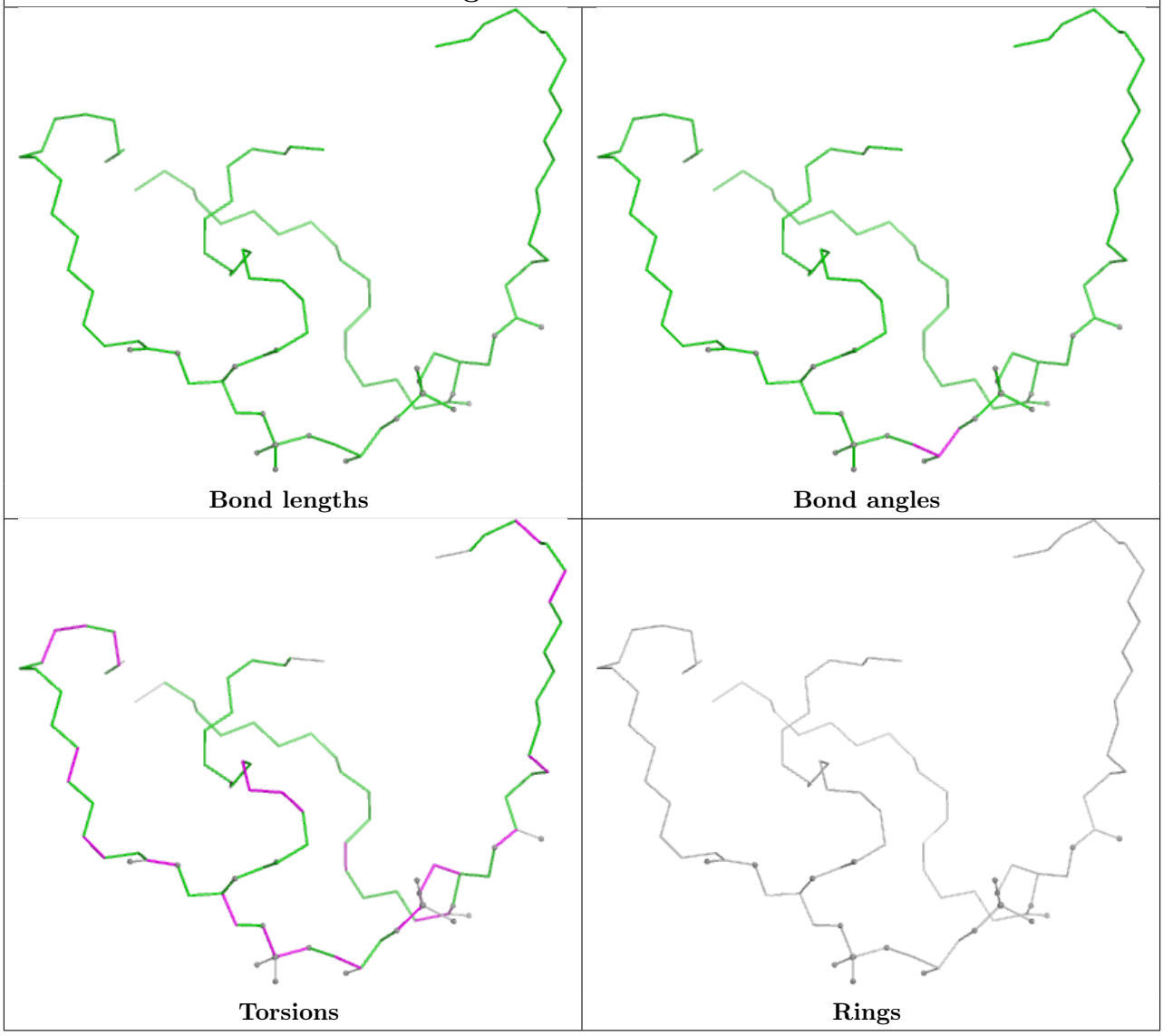


Rings

Ligand PC1 C 510	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CDL DV 403



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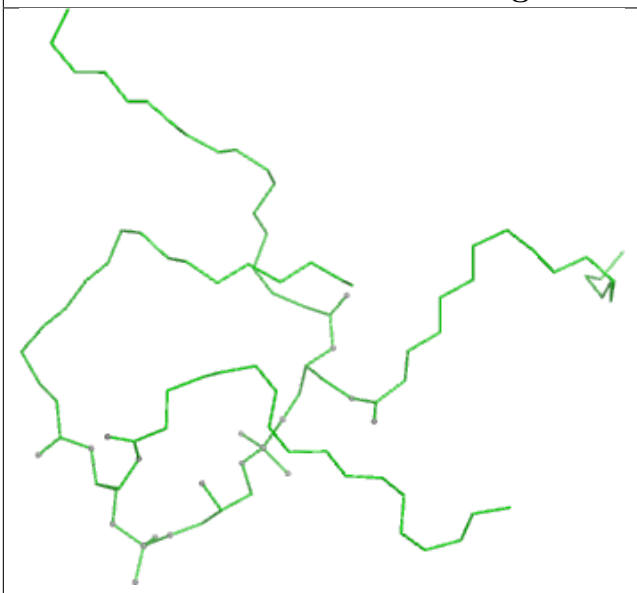
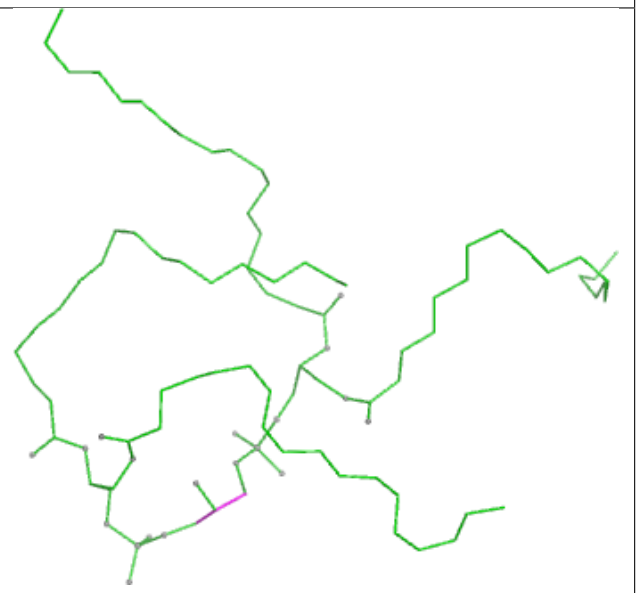
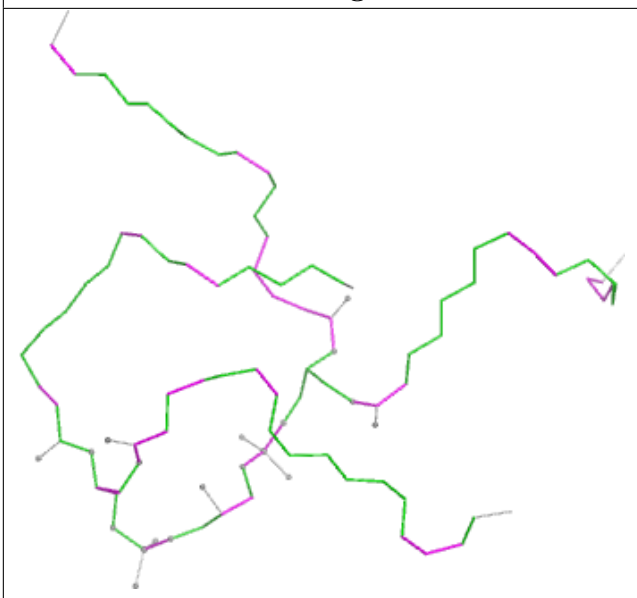
 Bond lengths	 Bond angles
 Torsions	Rings

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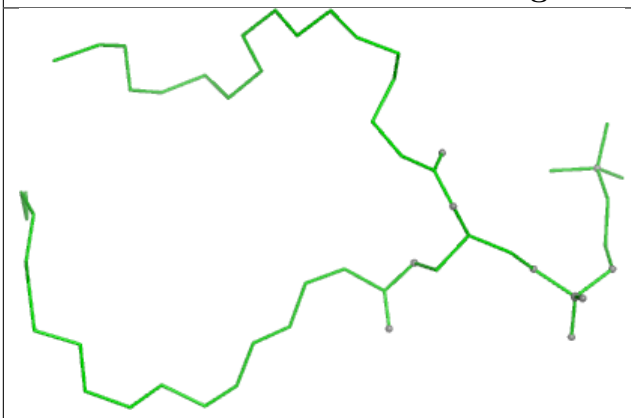
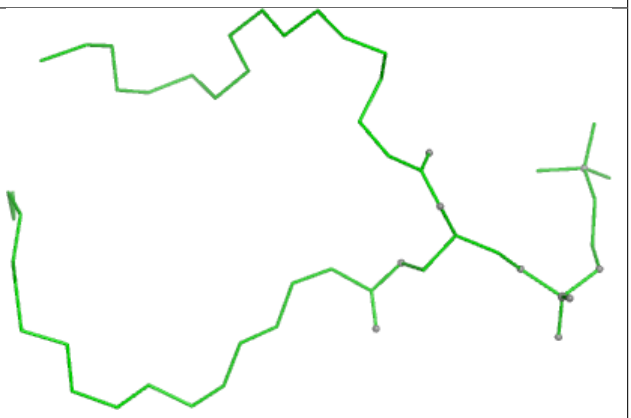
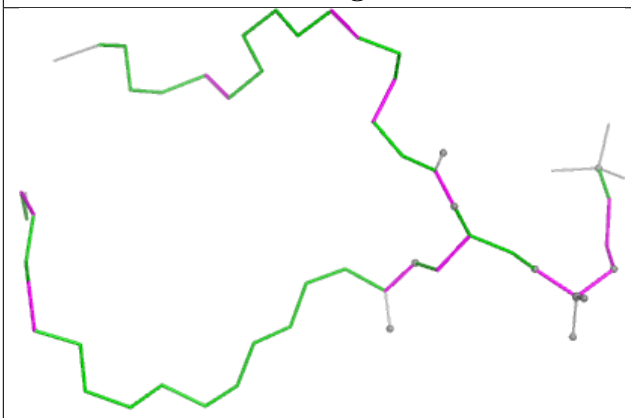
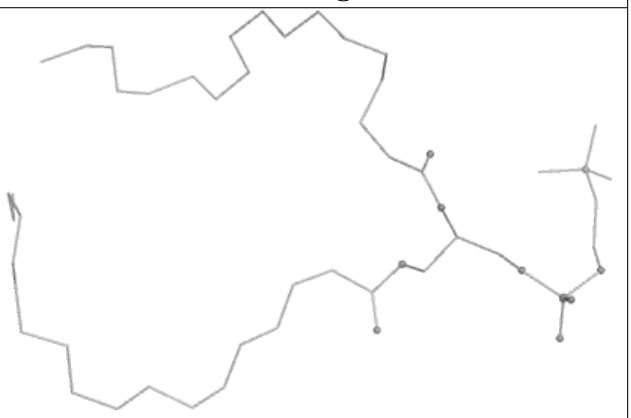
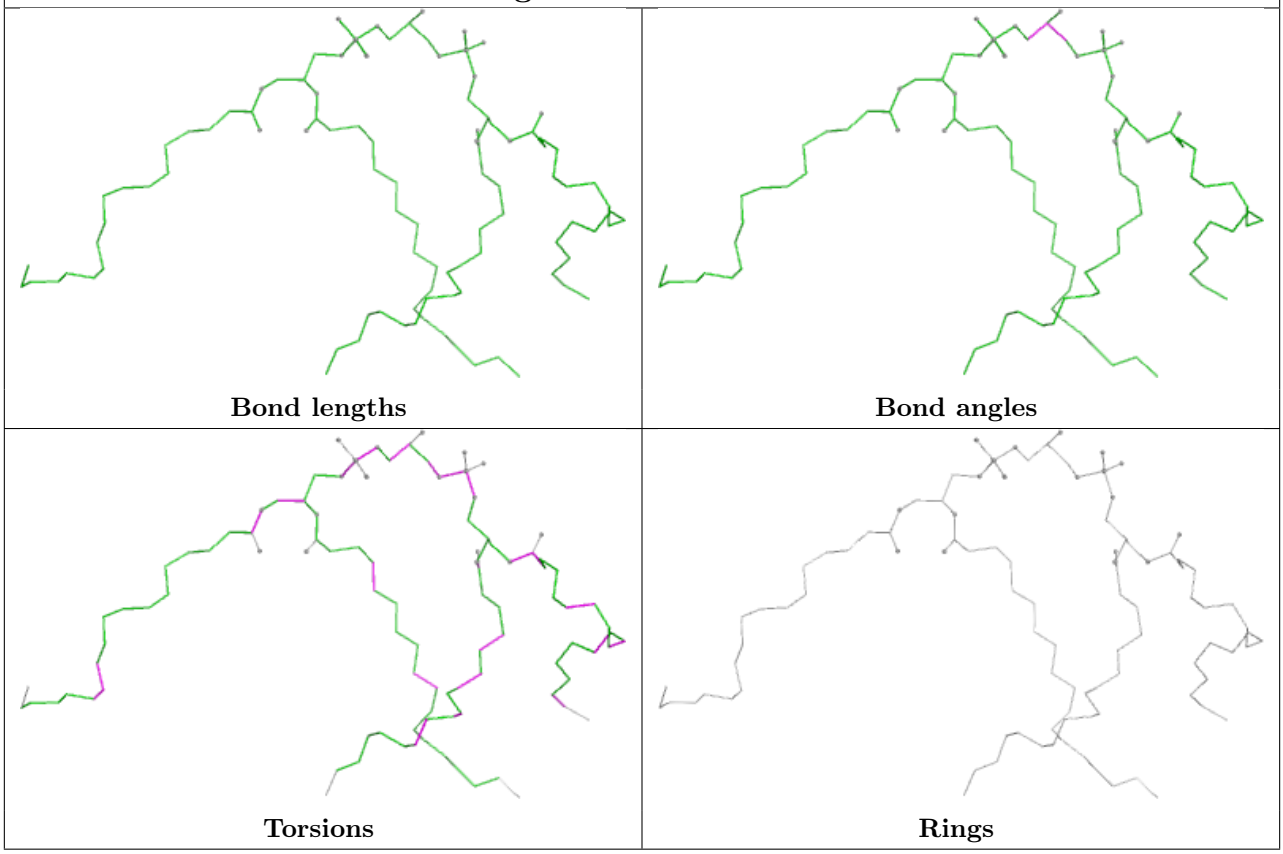
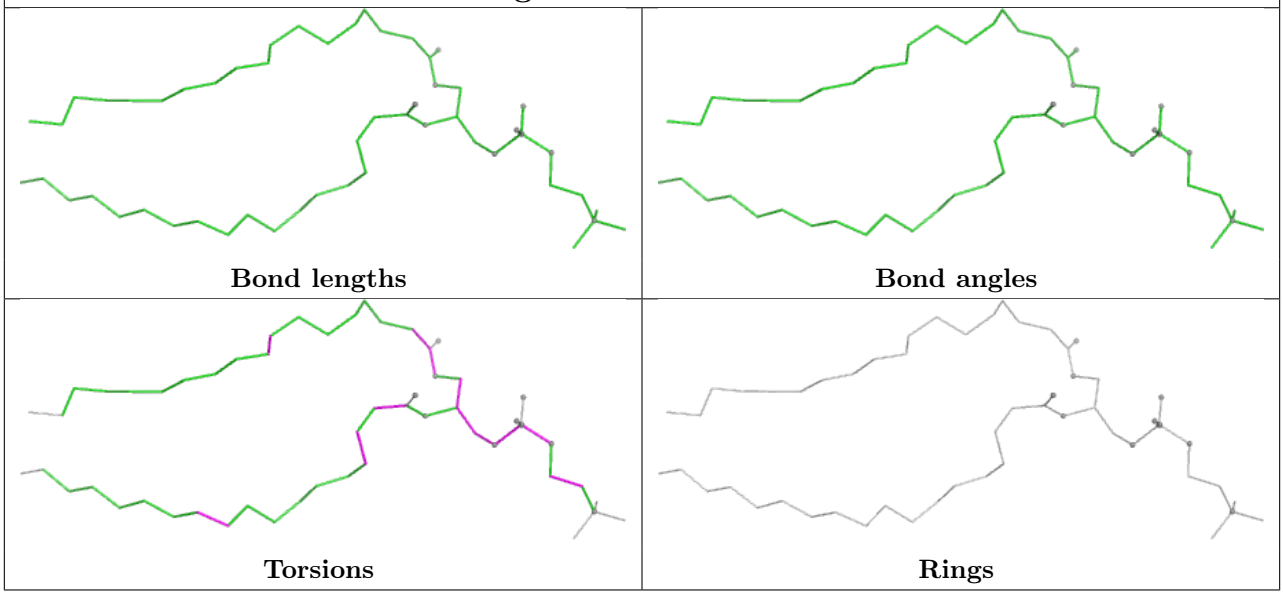
 Bond lengths	 Bond angles
 Torsions	 Rings

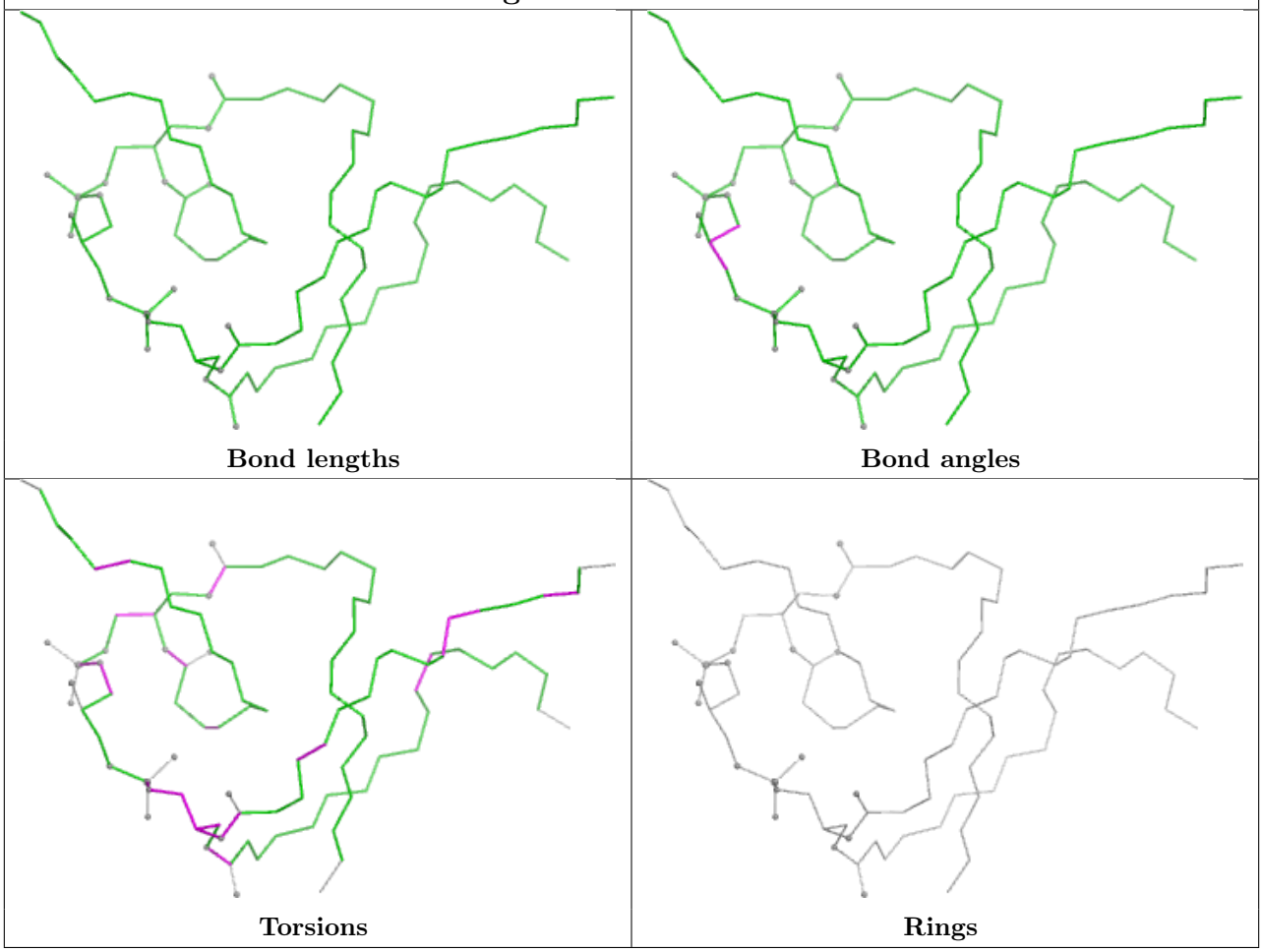
Ligand CDL Du 402



Ligand PC1 AA 907



Ligand CDL CD 302



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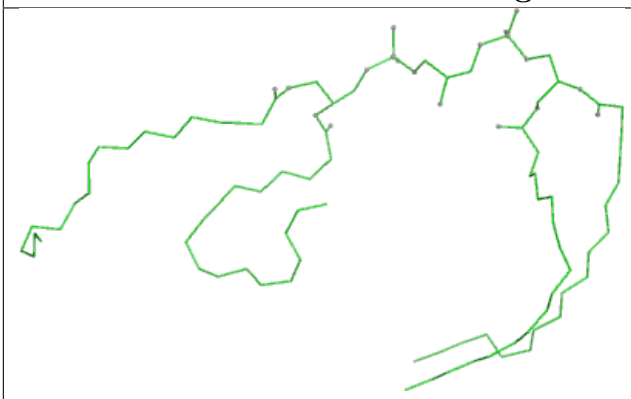
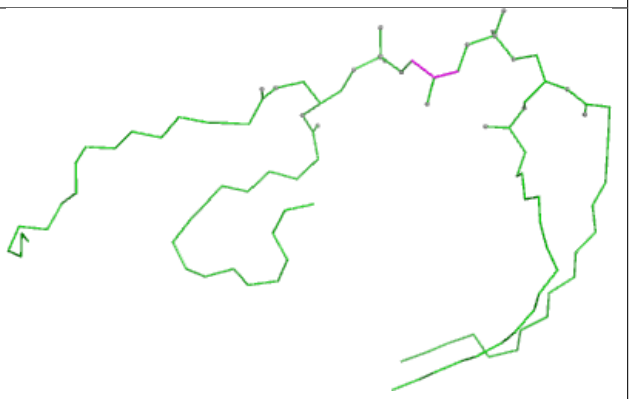
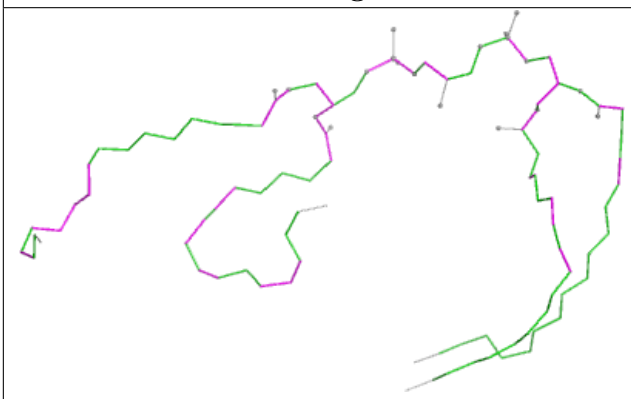
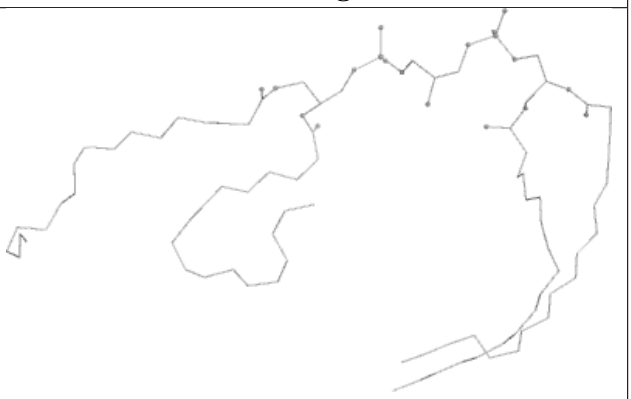
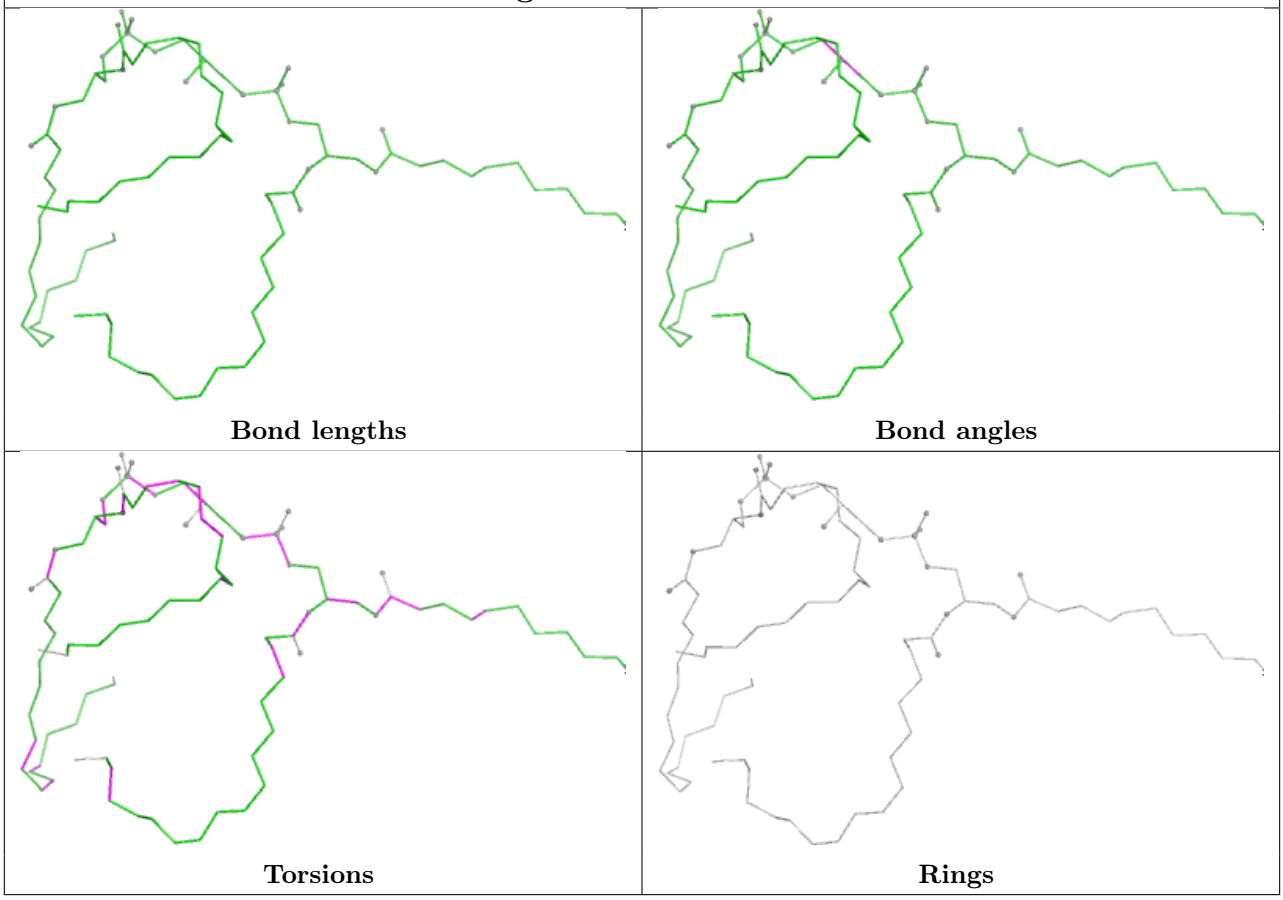
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Eu 101



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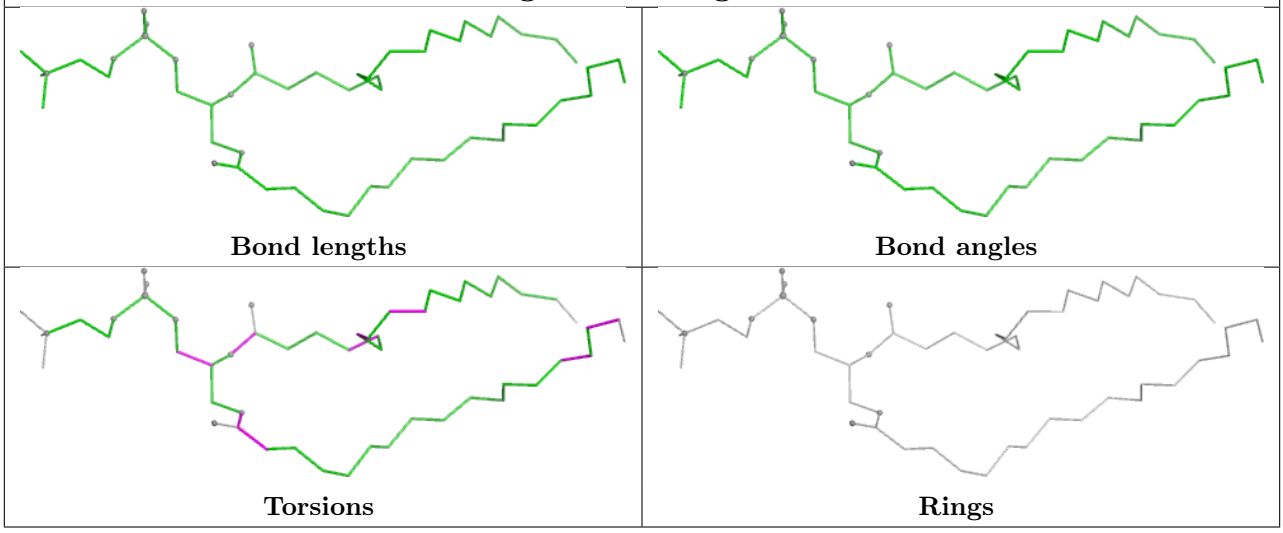

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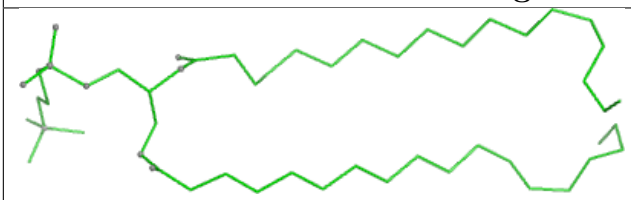
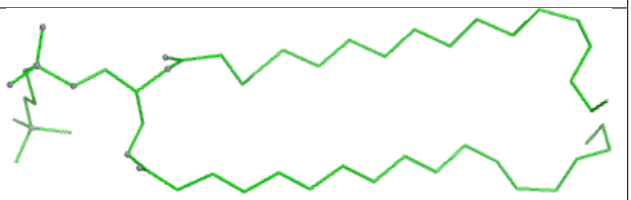
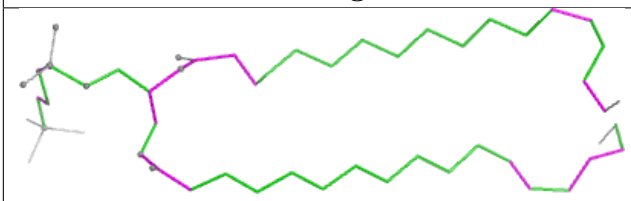
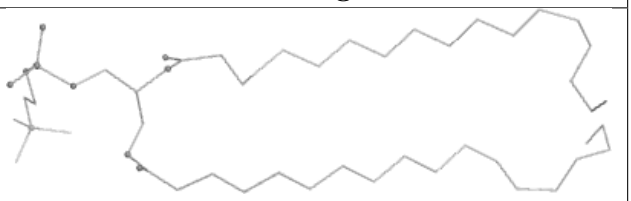
 Bond lengths	 Bond angles
 Torsions	 Rings

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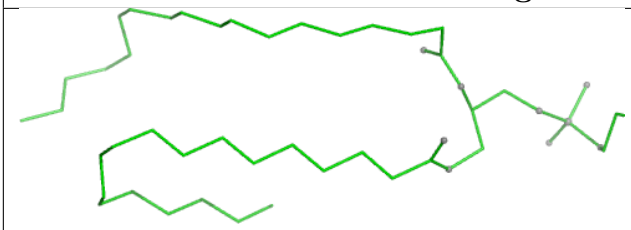
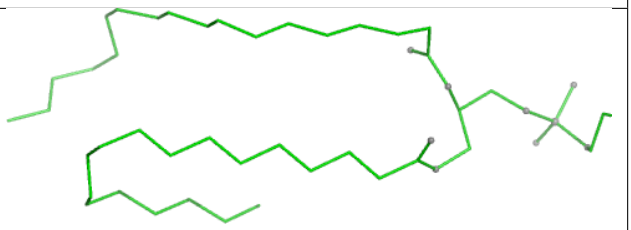
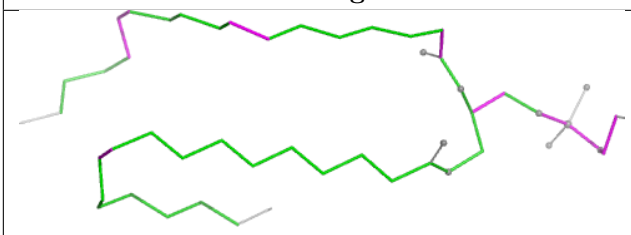
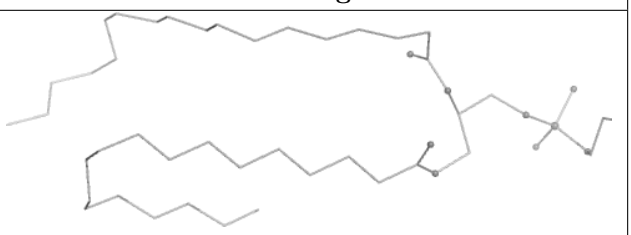
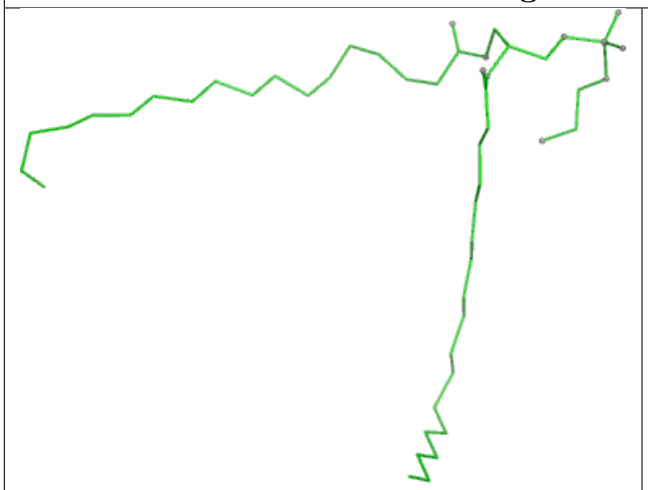
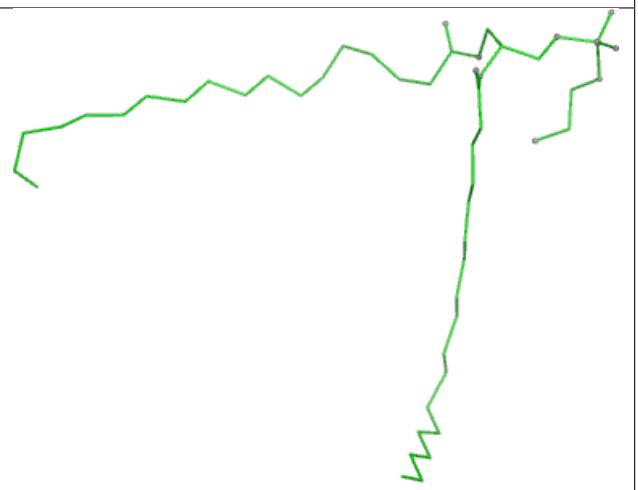
 Bond lengths	 Bond angles
 Torsions	 Rings

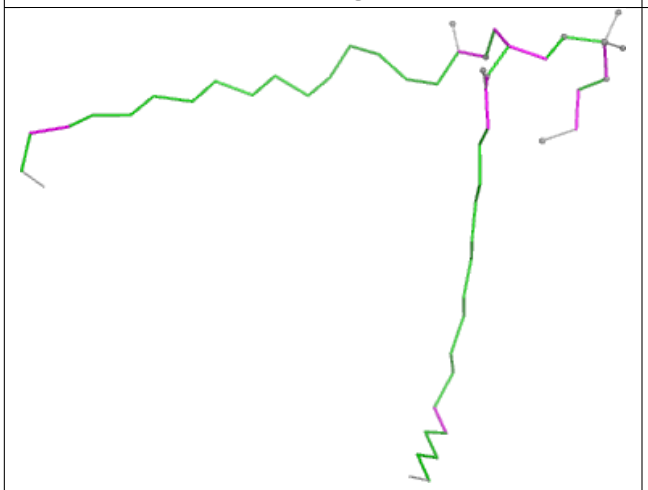
Ligand 3PE AJ 502



Bond lengths



Bond angles



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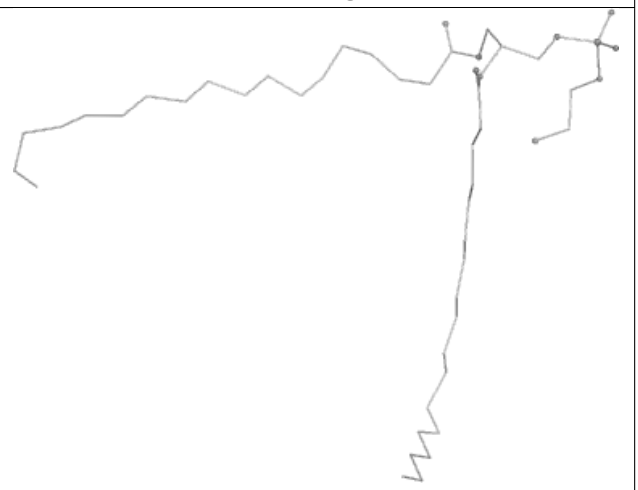
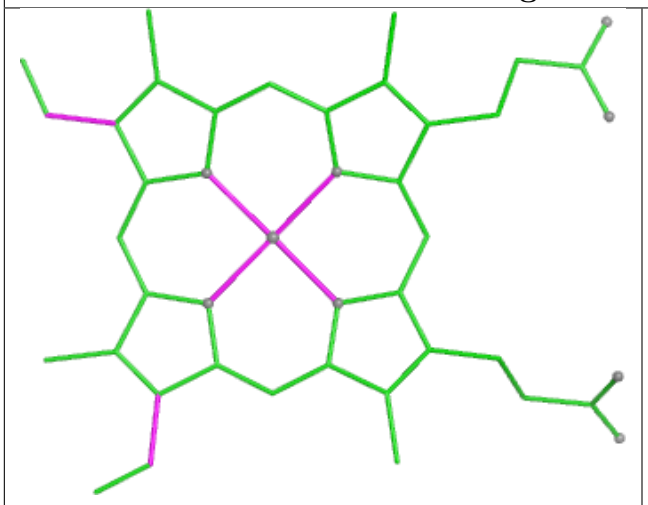


Rings

Ligand HEM C 501



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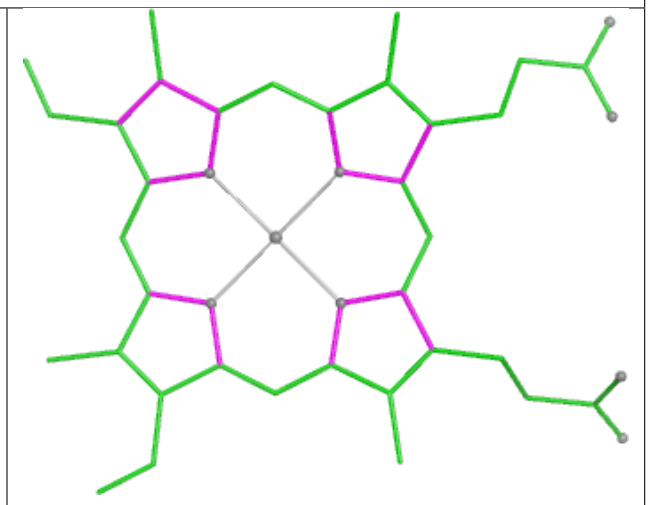

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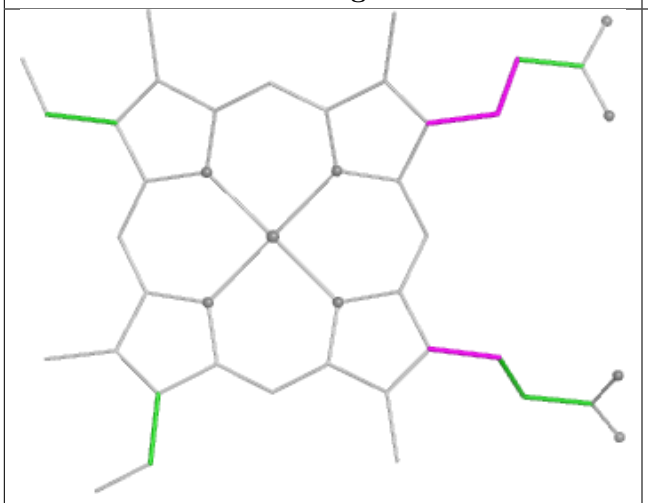

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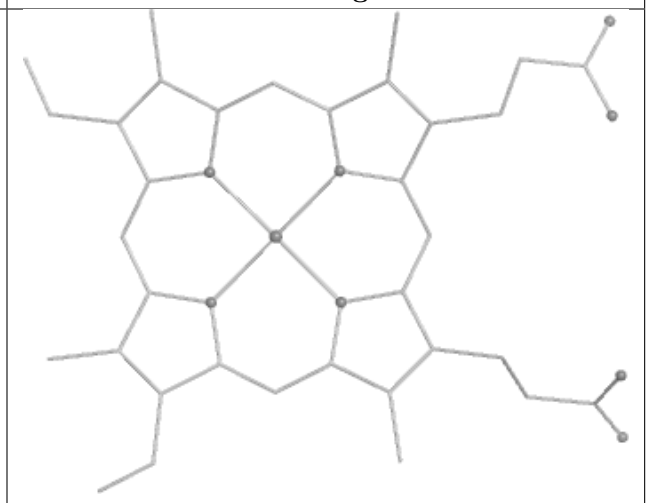
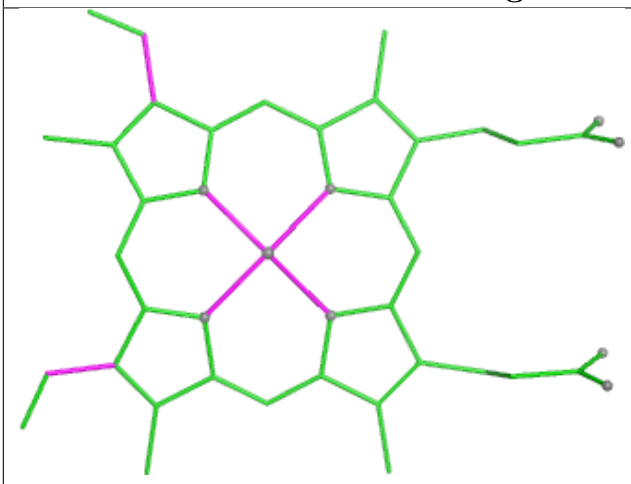
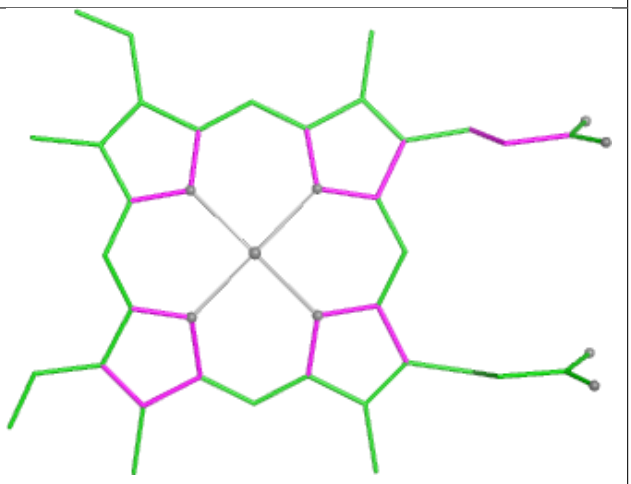
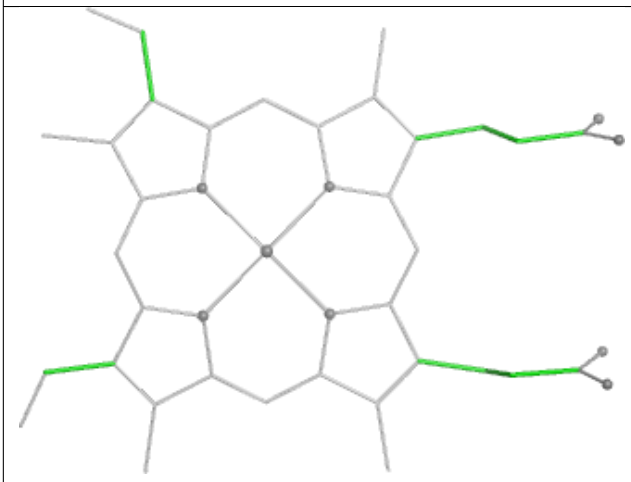
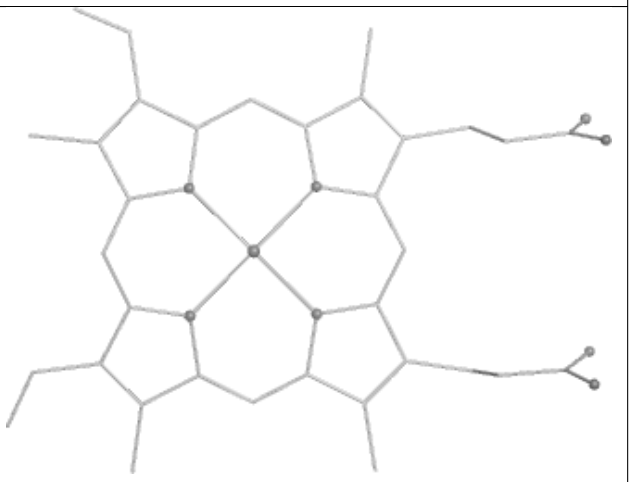


Rings

Ligand HEM ED 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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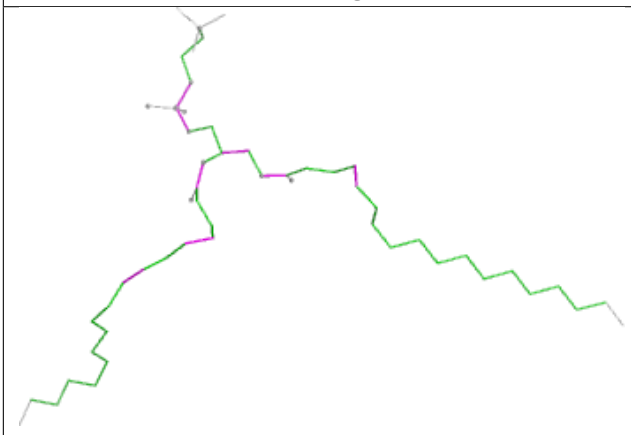
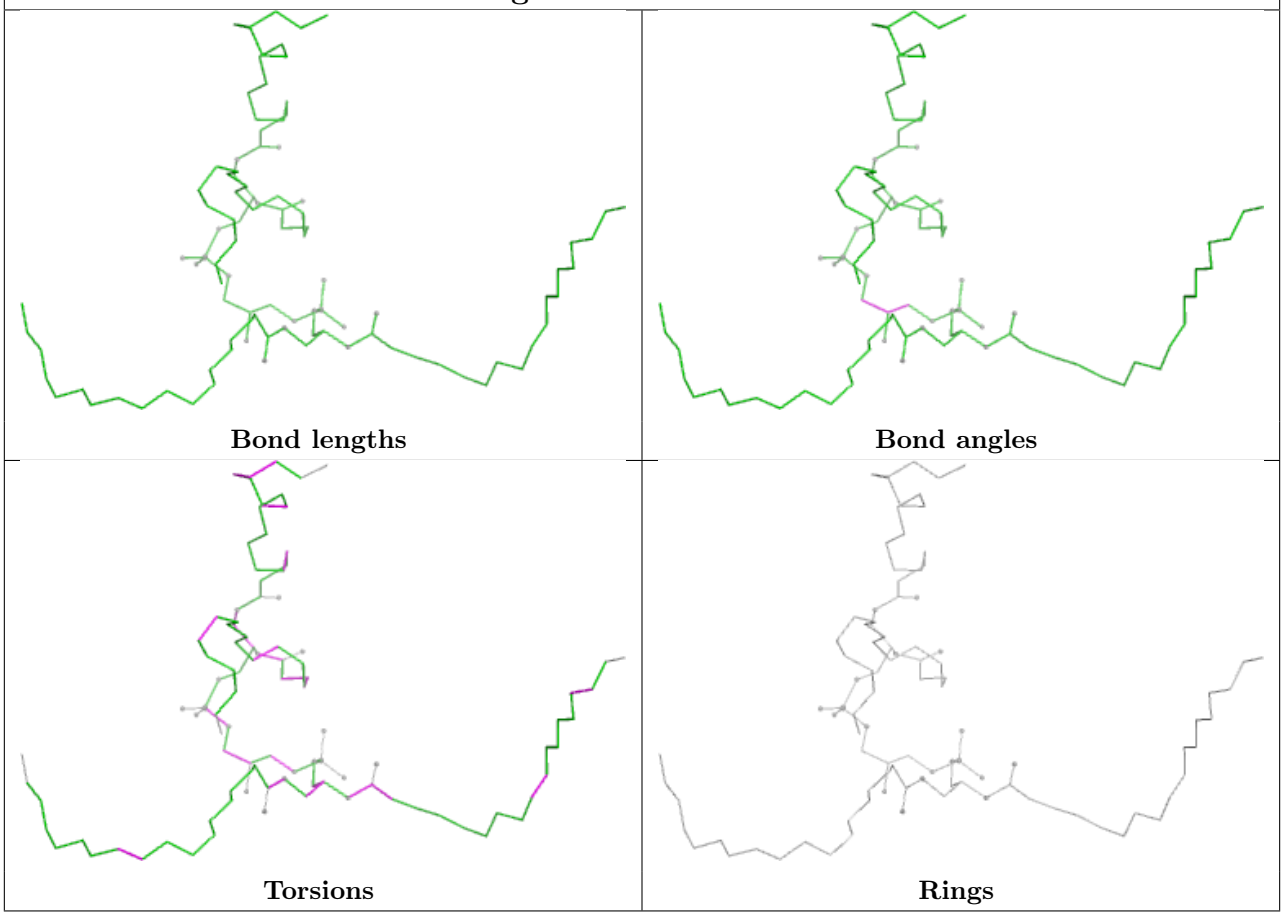
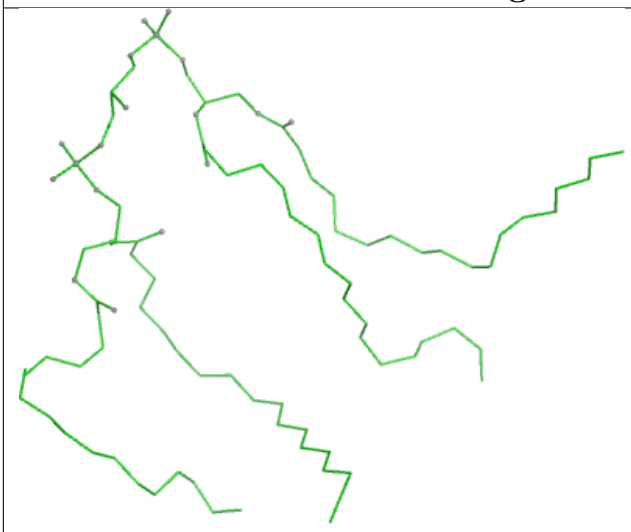
Bond lengths	**Bond angles**
 **Torsions**	**Rings**

Ligand CDL DX 307

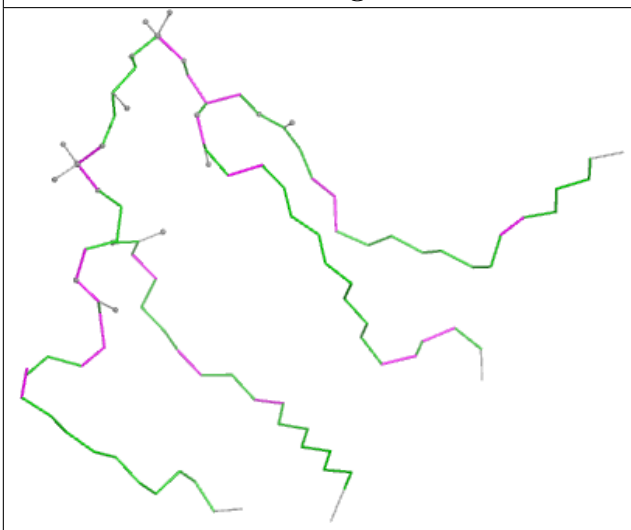


Ligand CDL DG 202



Bond lengths

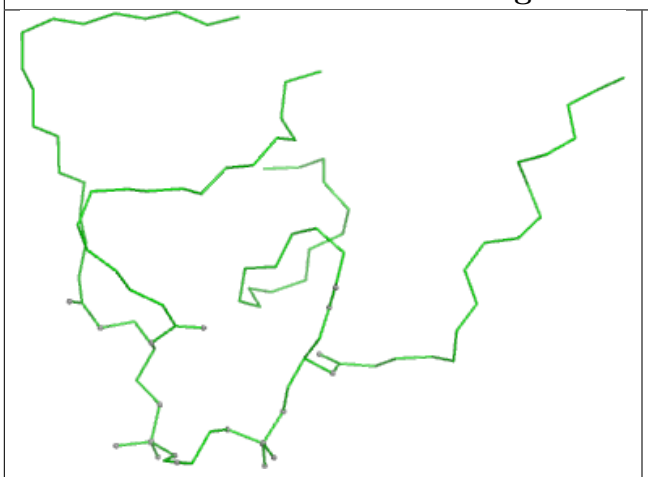
Bond angles



Torsions

Rings

Ligand CDL DS 405



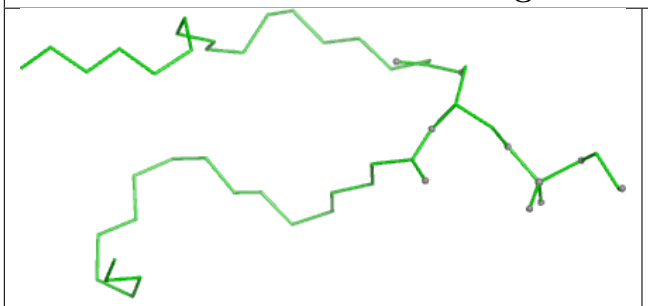
Bond lengths

Bond angles

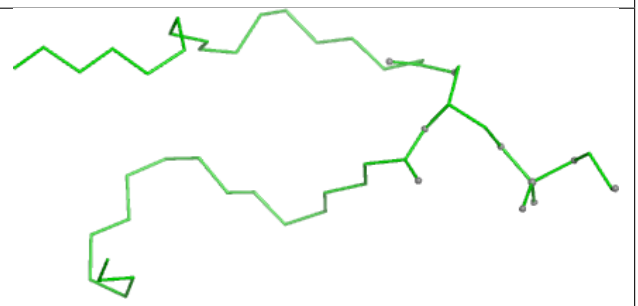
Torsions

Rings

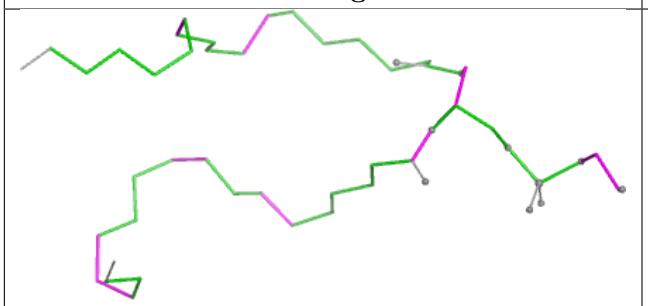
Ligand 3PE DN 501



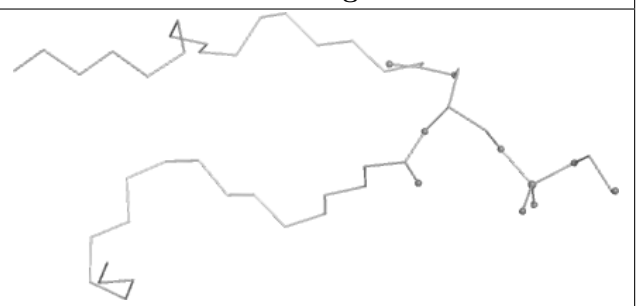
Bond lengths



Bond angles



Torsions



Rings

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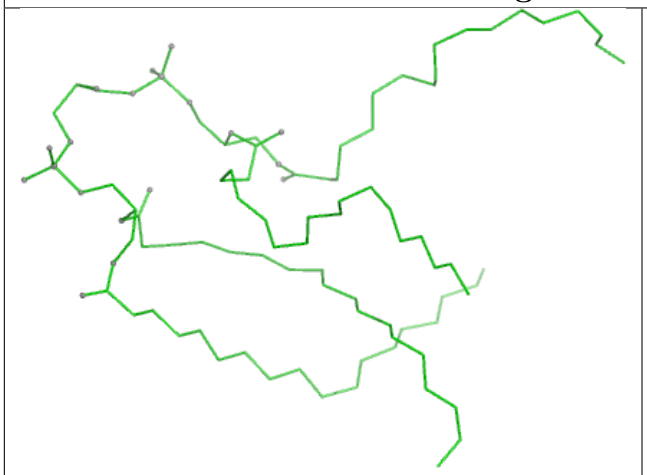
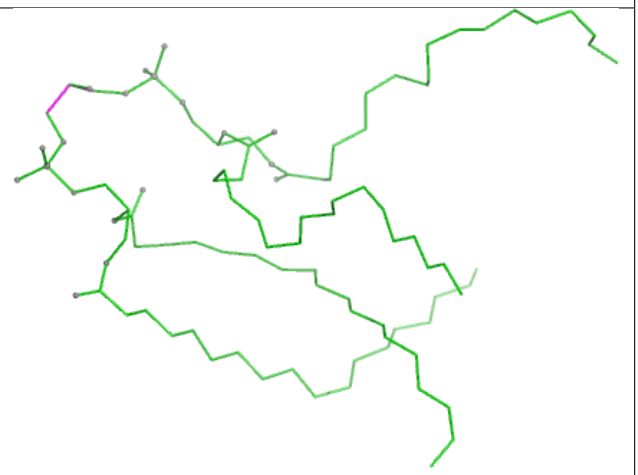
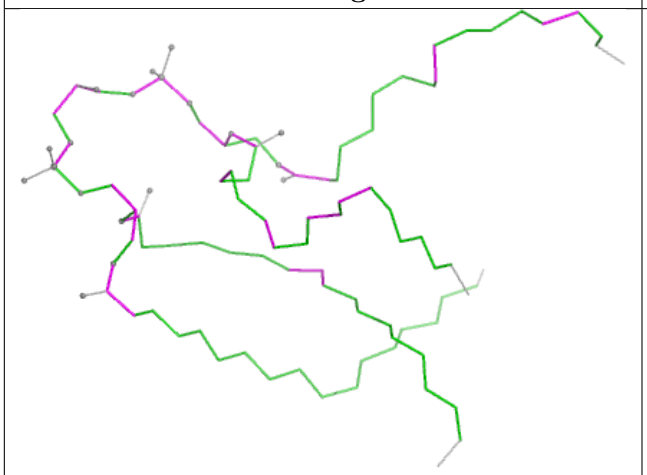


Bond lengths



Bond angles



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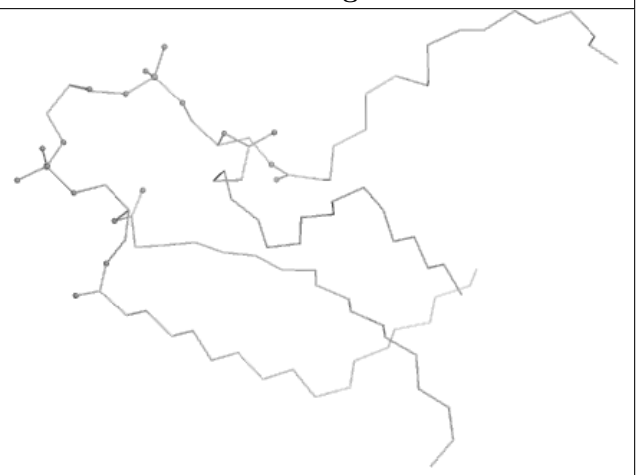
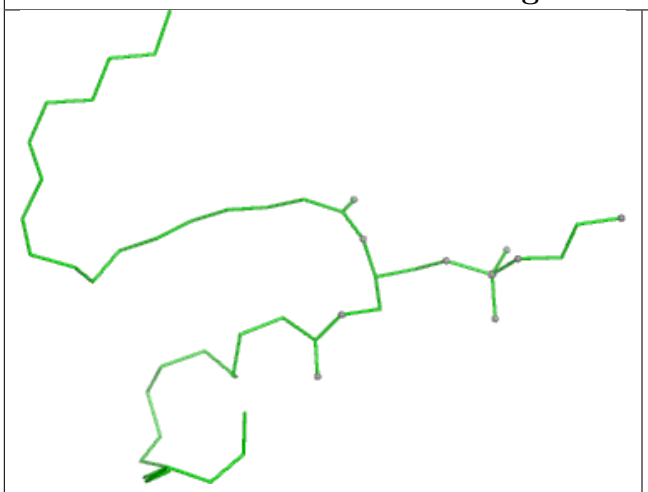
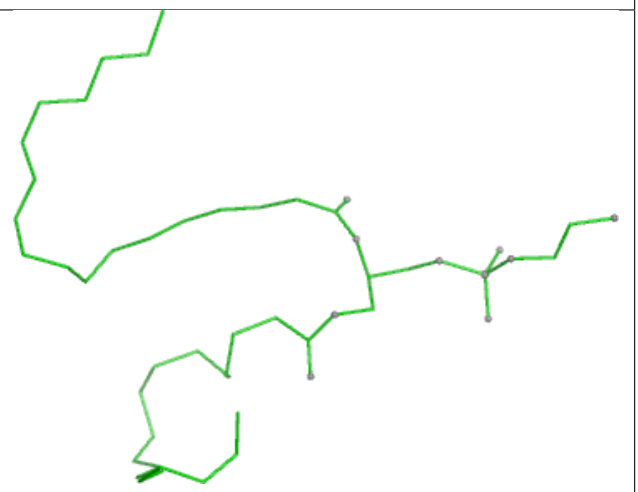


Rings

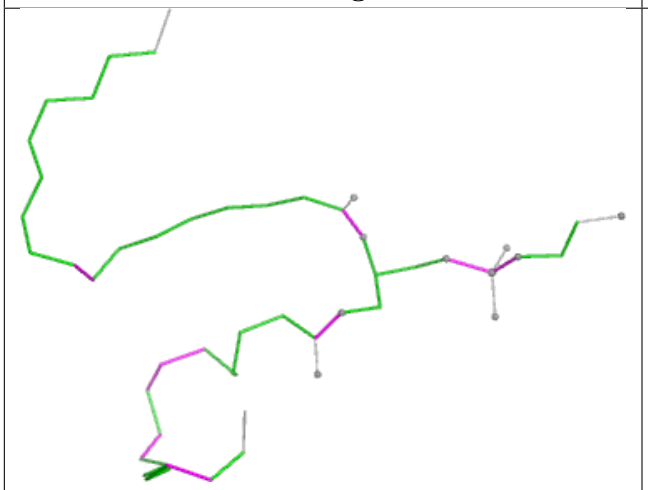
Ligand 3PE Ds 408



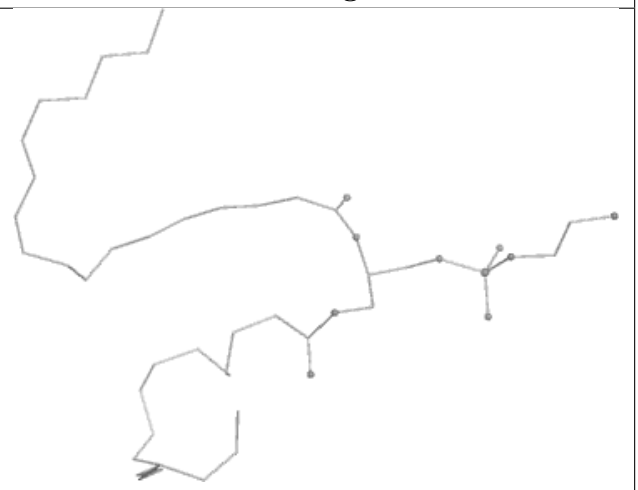
Bond lengths



Bond angles

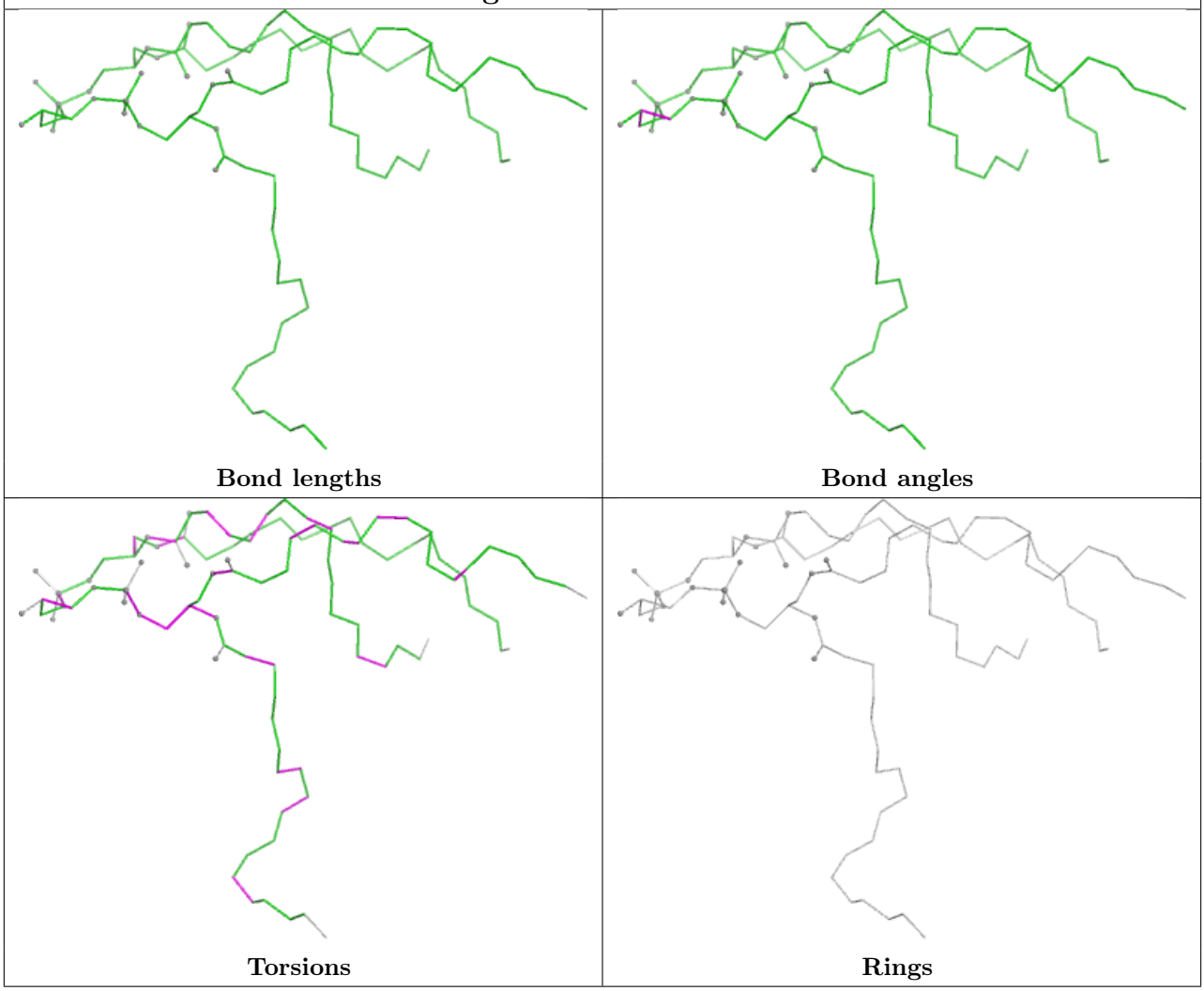


Torsions

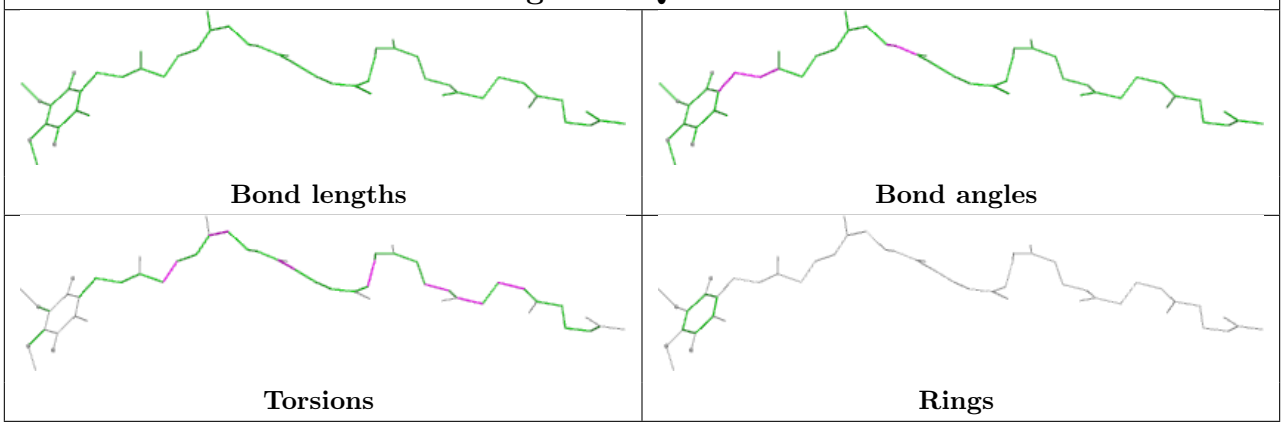


Rings

Ligand CDL DS 401



Ligand UQ8 C 512



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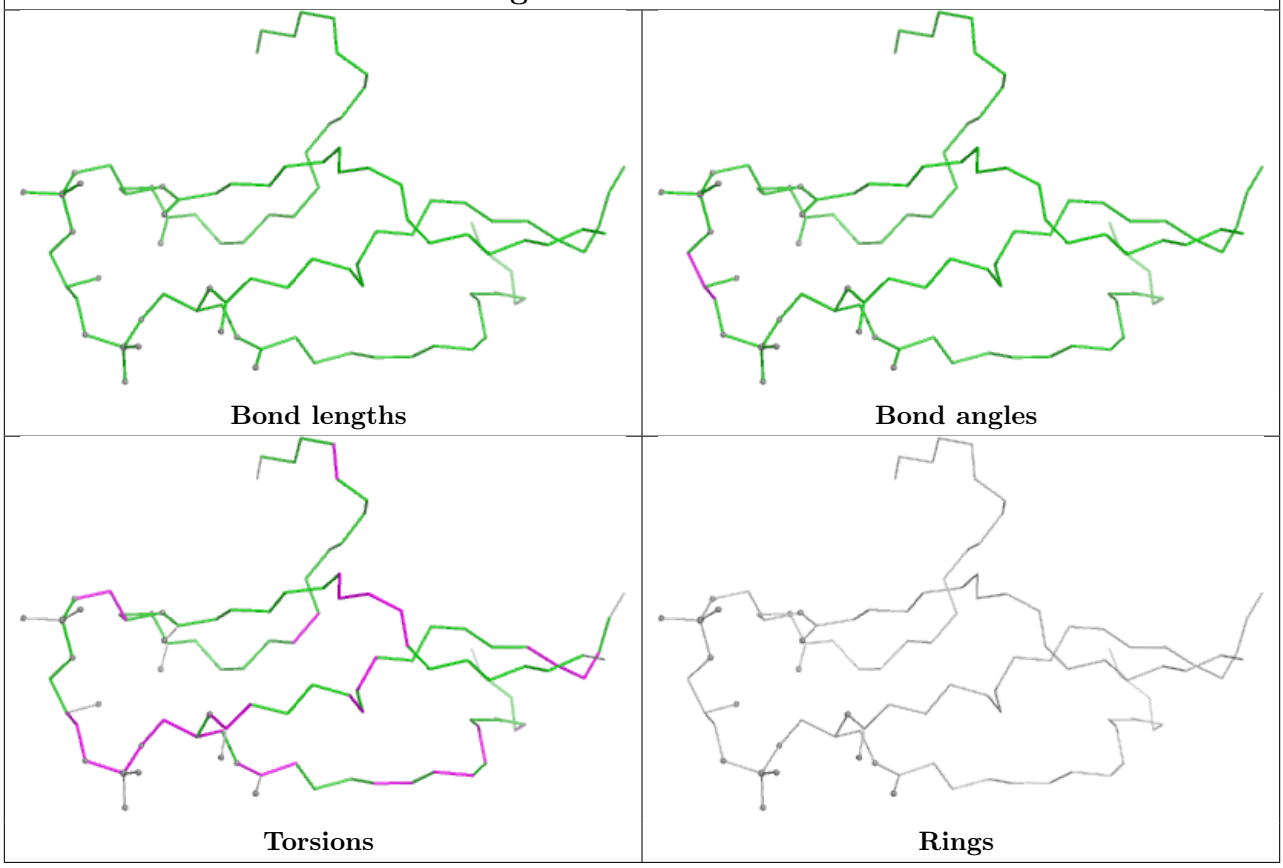

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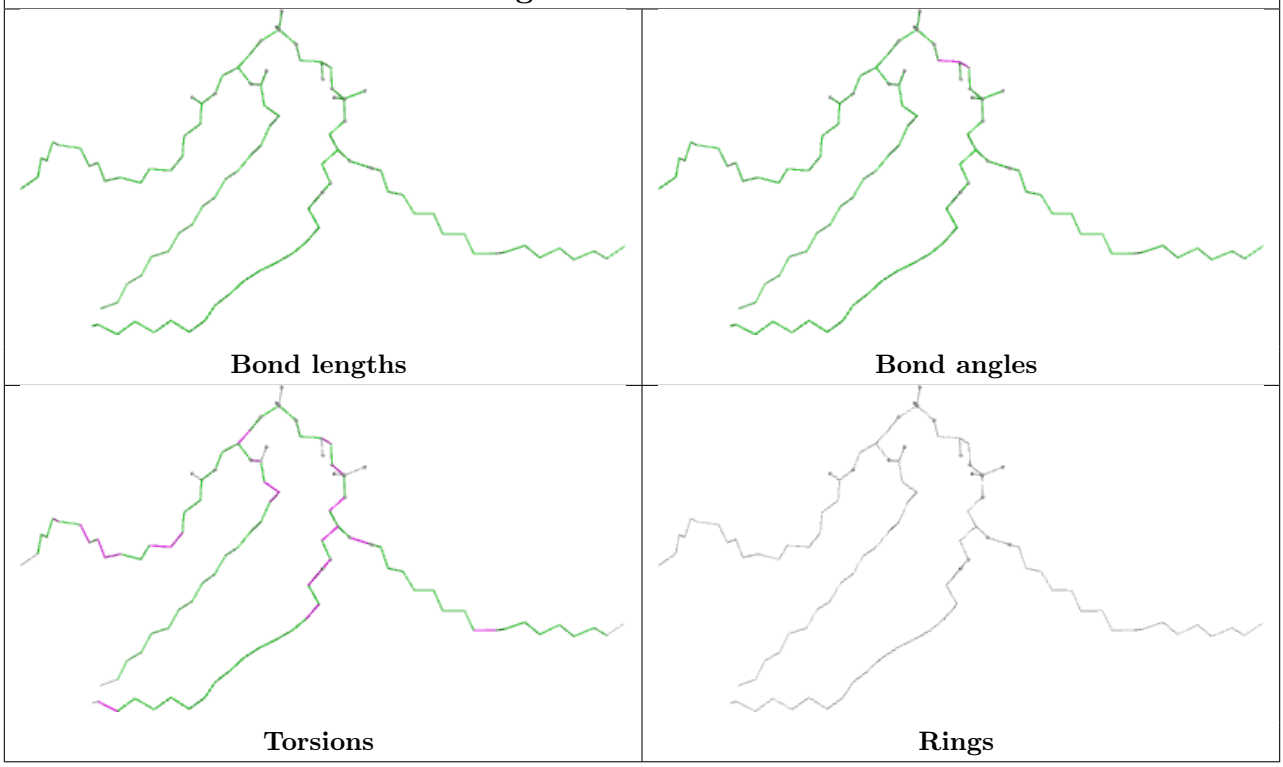

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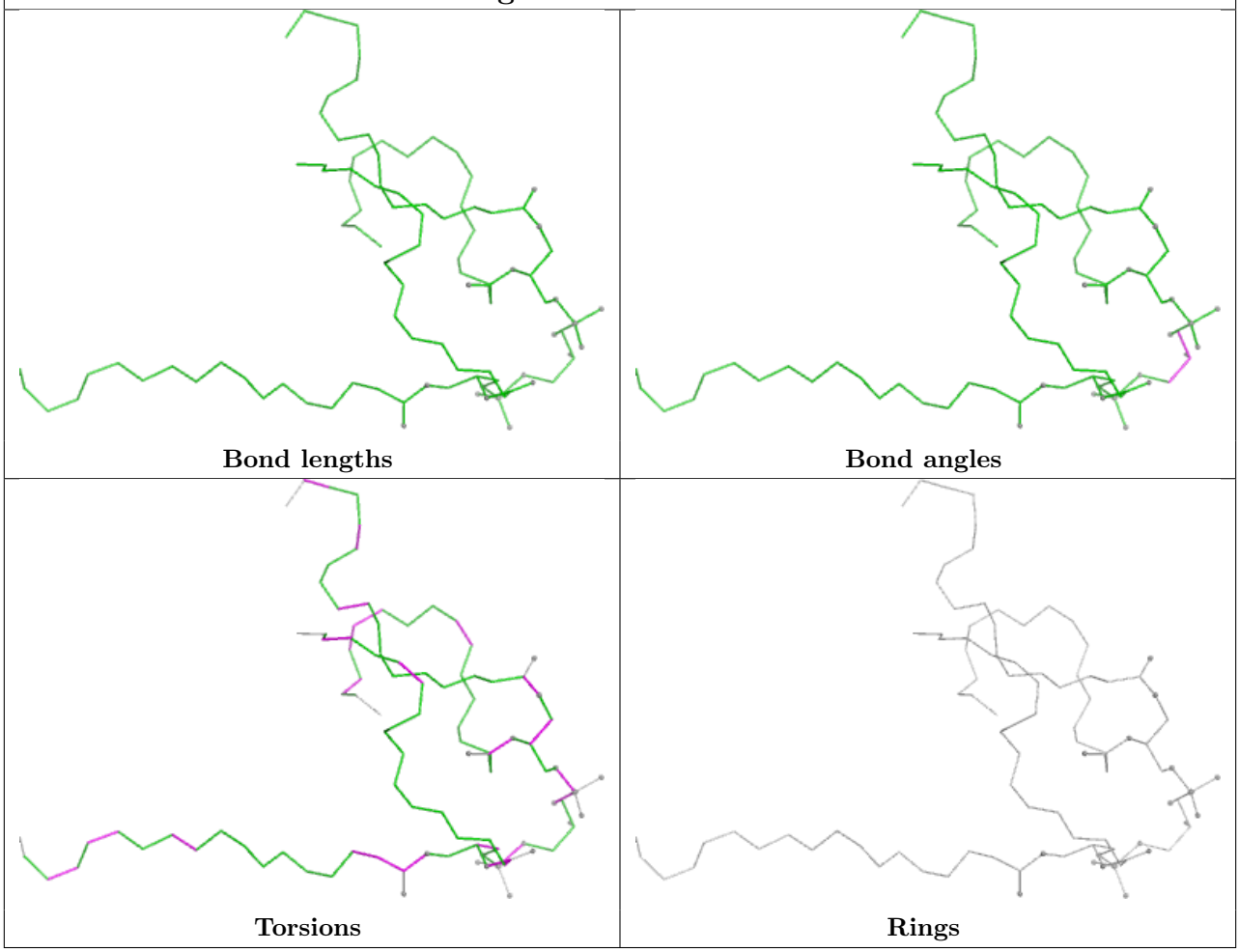
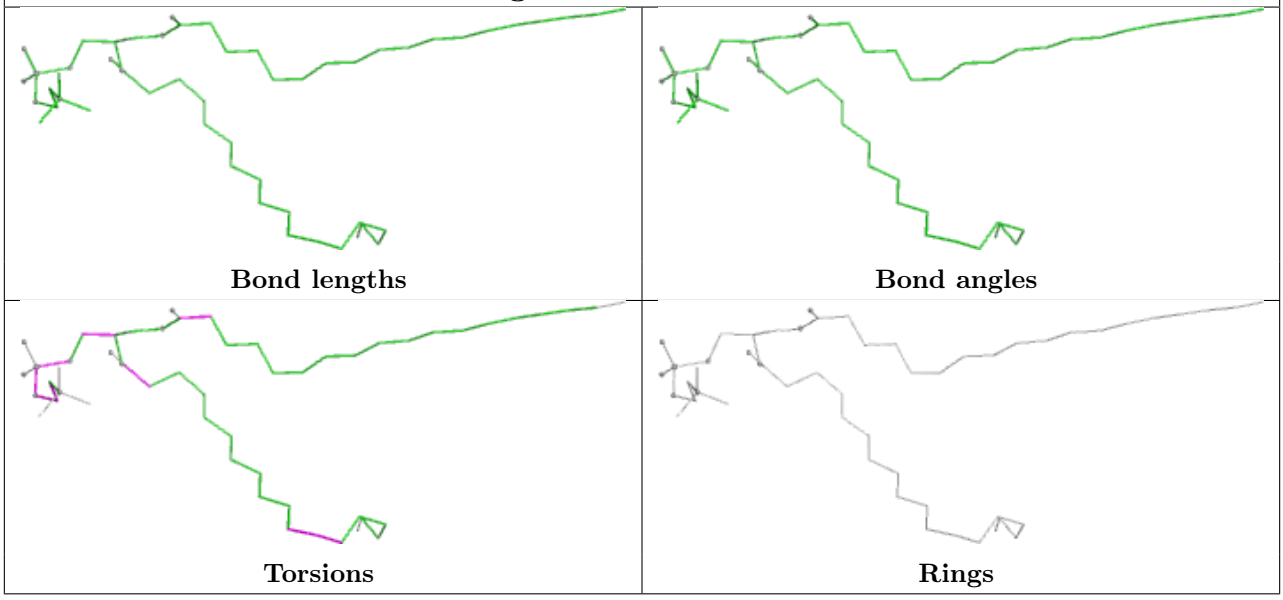
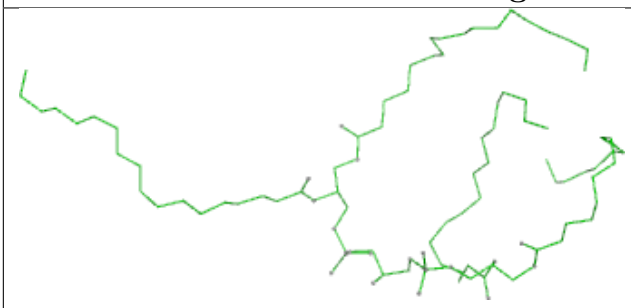
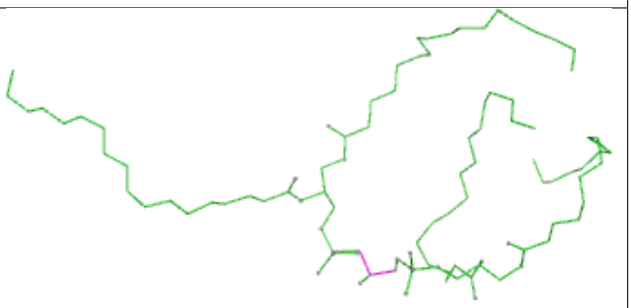
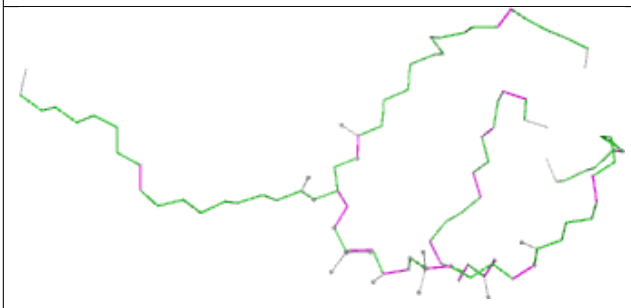
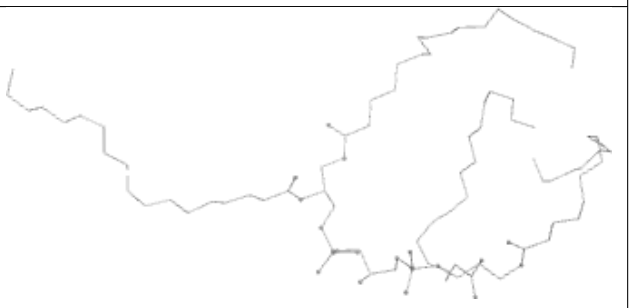
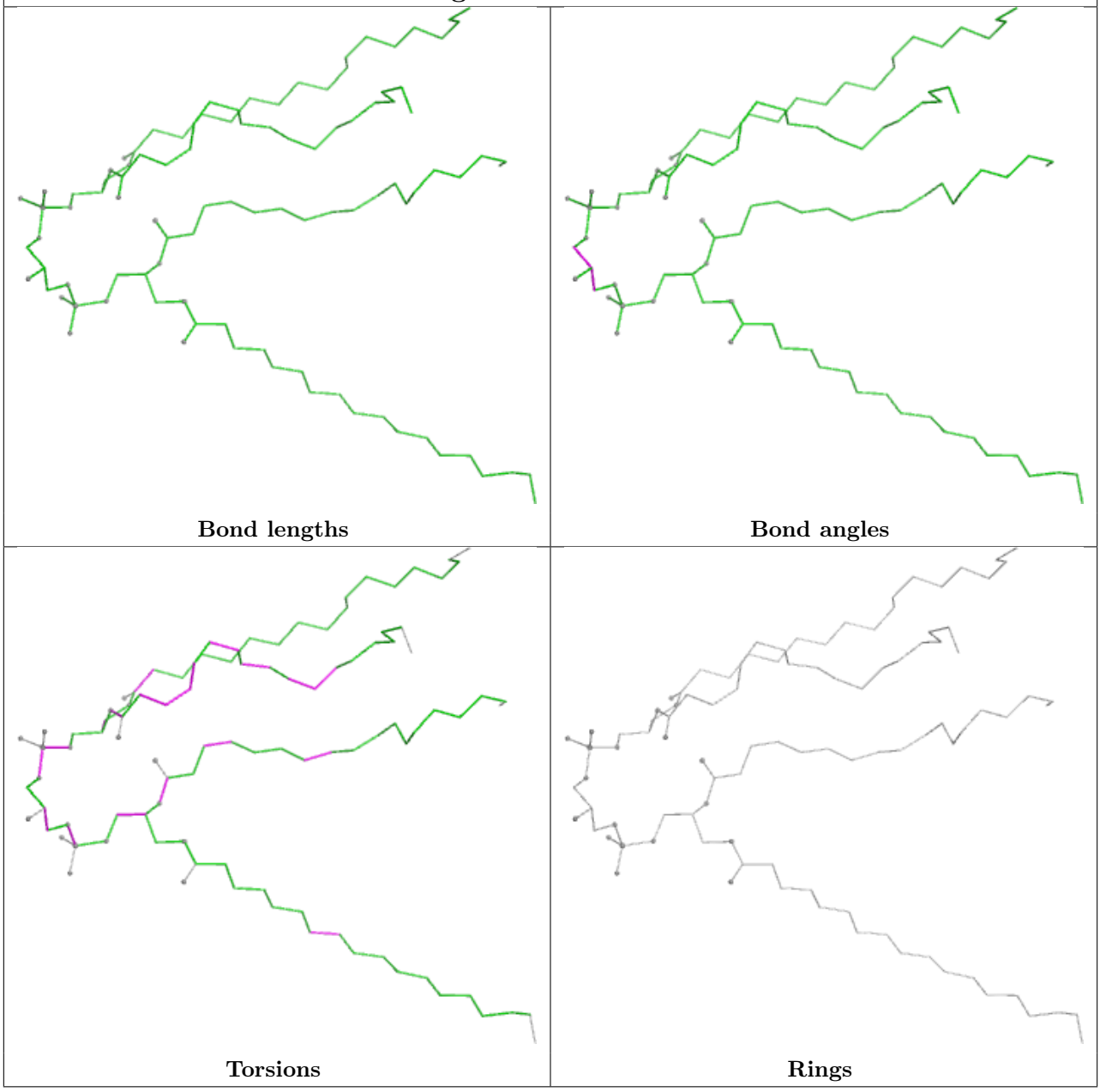


Ligand PC1 Dx 1203

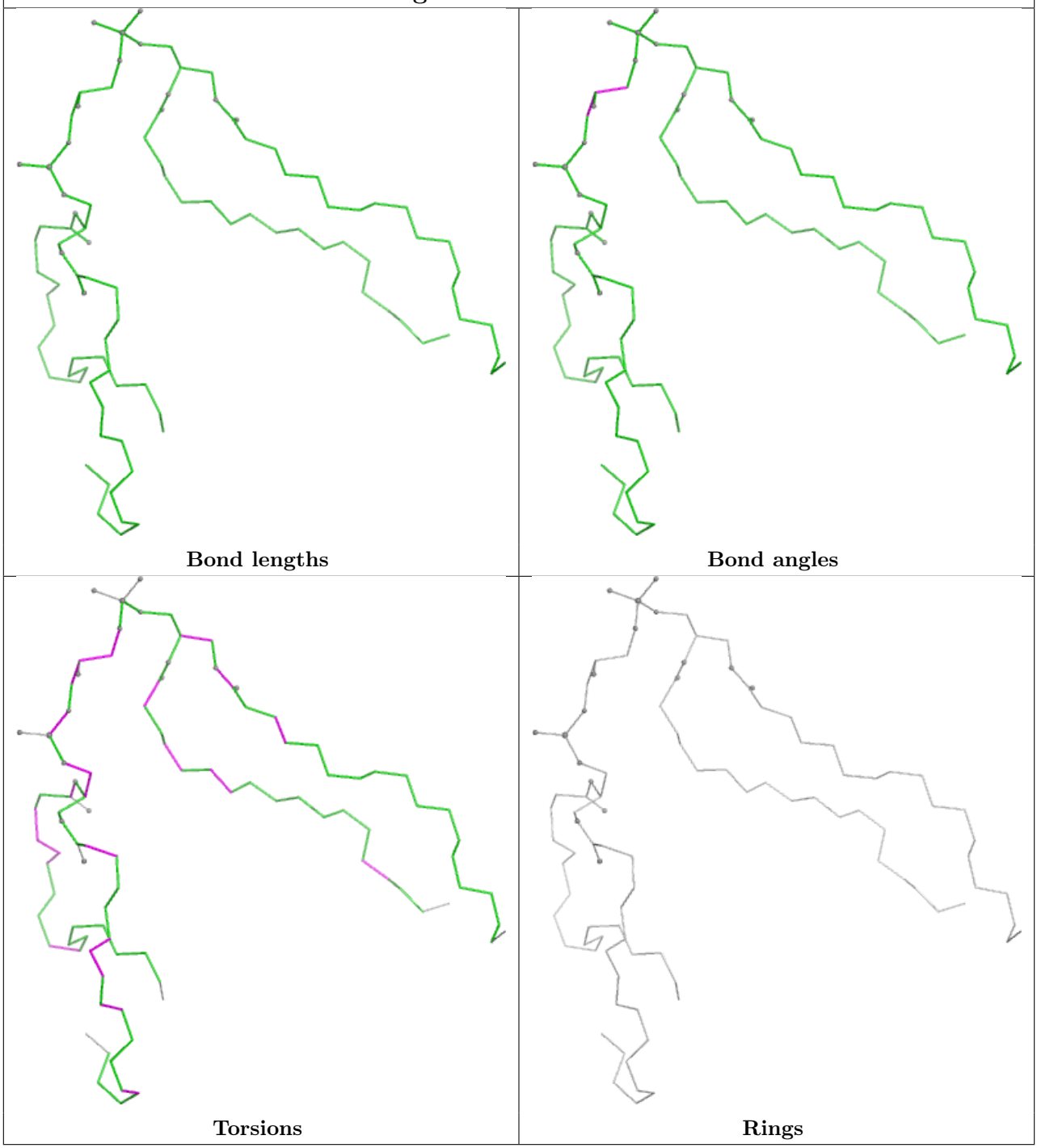


Ligand CDL DU 404	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CDL E 301



Ligand CDL DR 403



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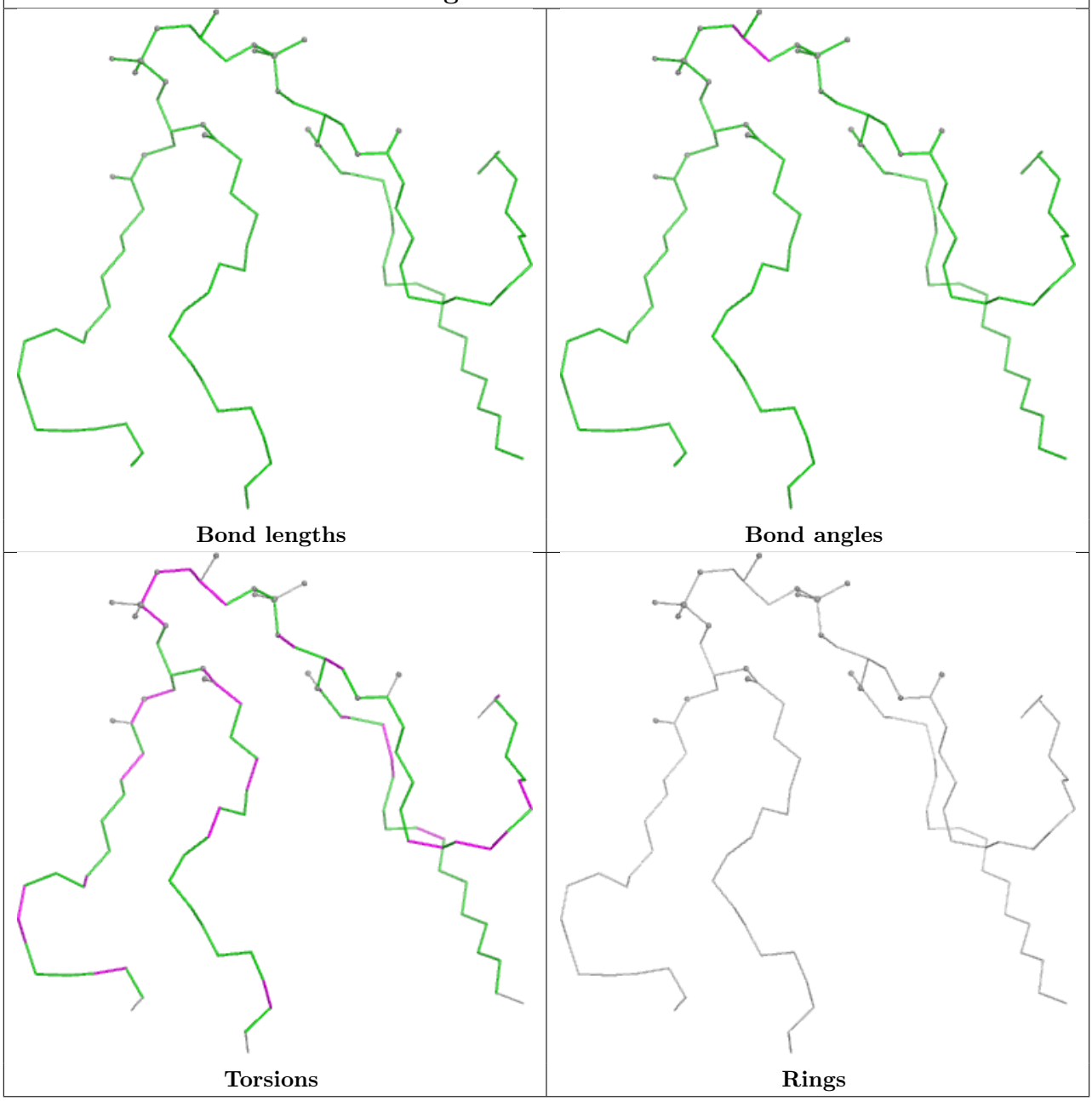
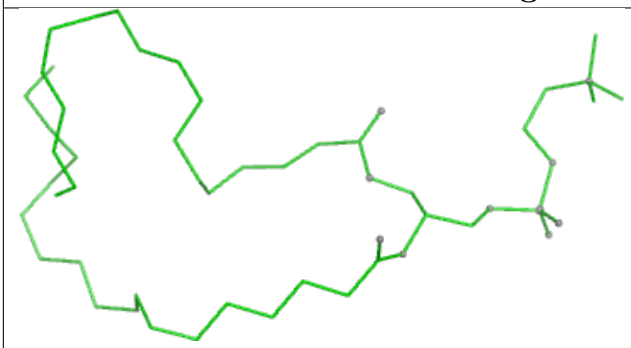
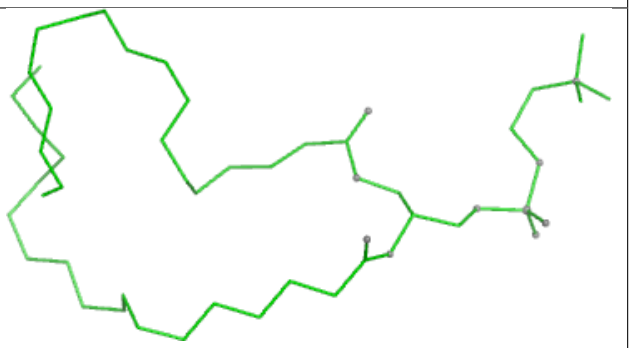


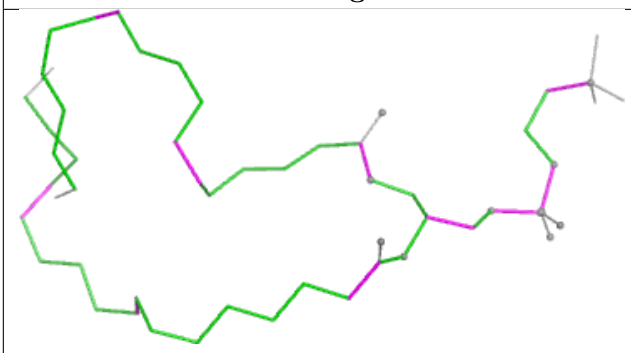
Ligand PC1 DI 303



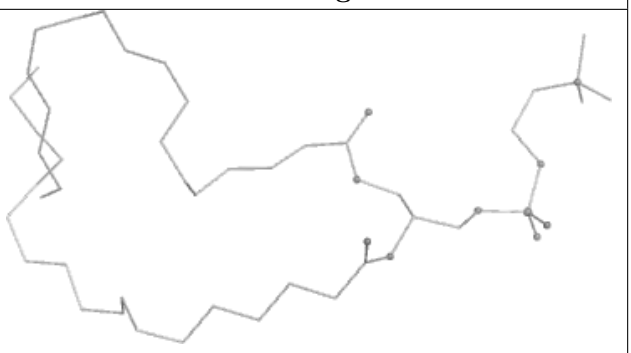
Bond lengths



Bond angles

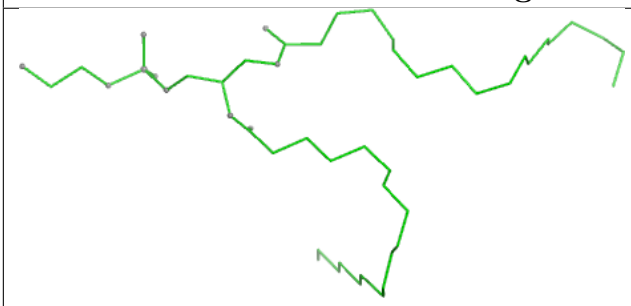


Torsions



Rings

Ligand 3PE DX 303



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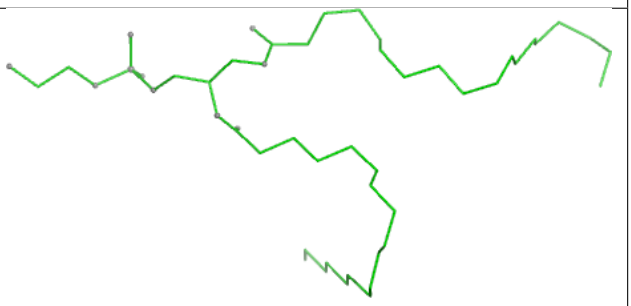
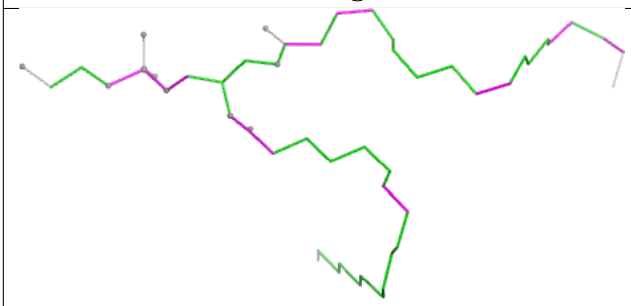


Bond angles



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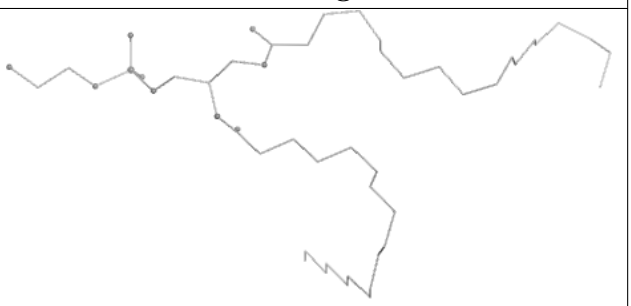
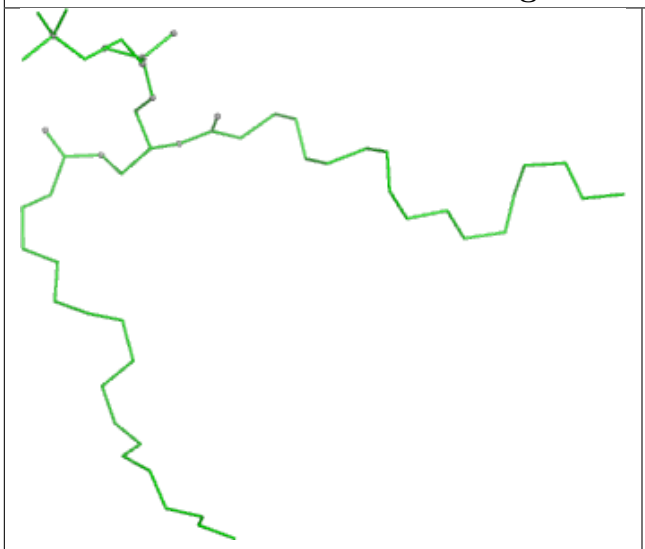


Rings

Ligand PC1 B1 403



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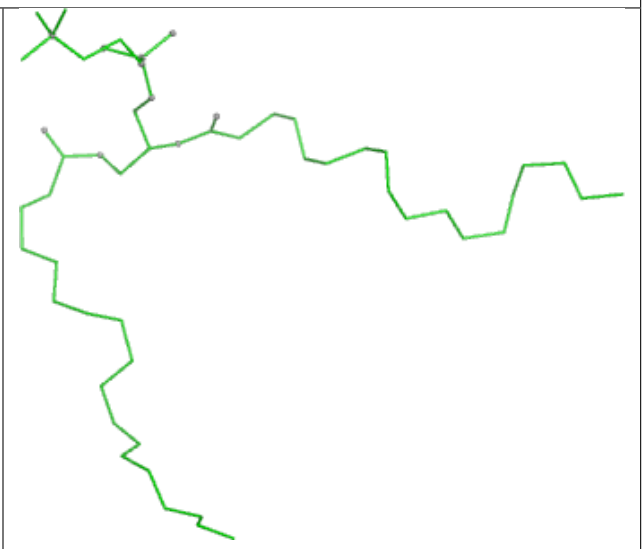
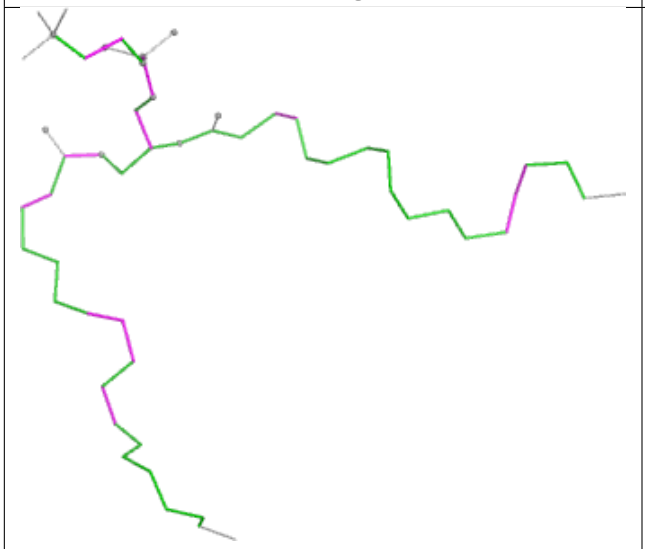


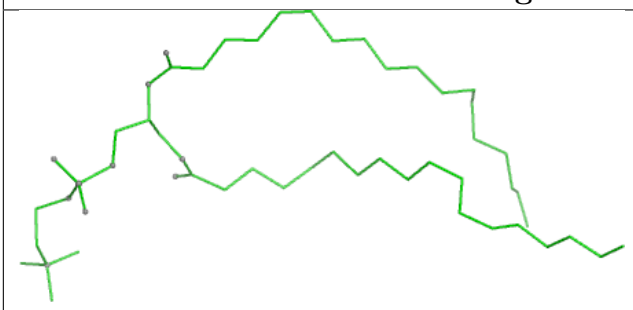
Bond angles



Torsions

Rings

Ligand PC1 BT 203



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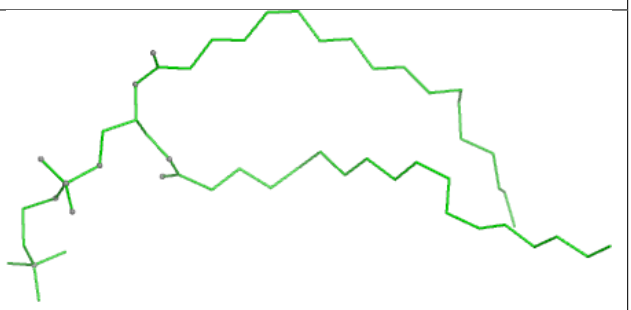
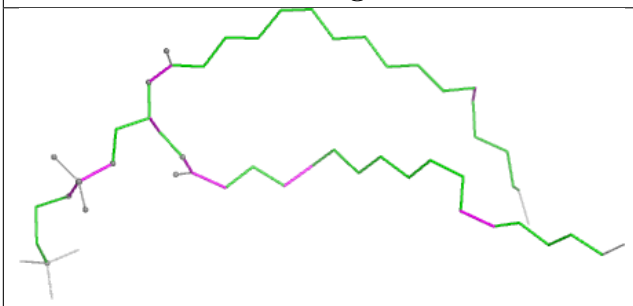


Bond angles



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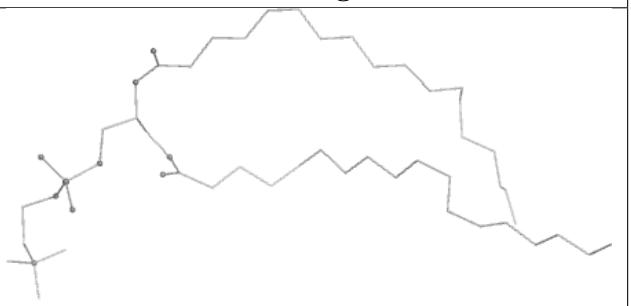
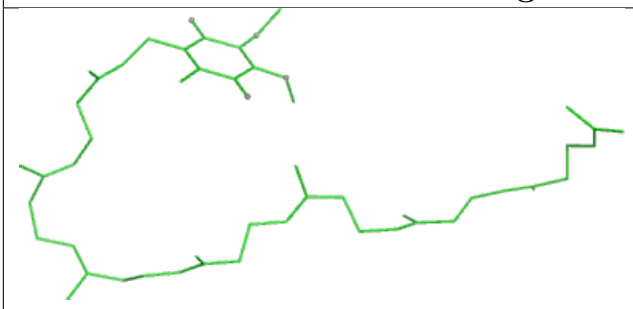


Rings

Ligand UQ8 Ds 404



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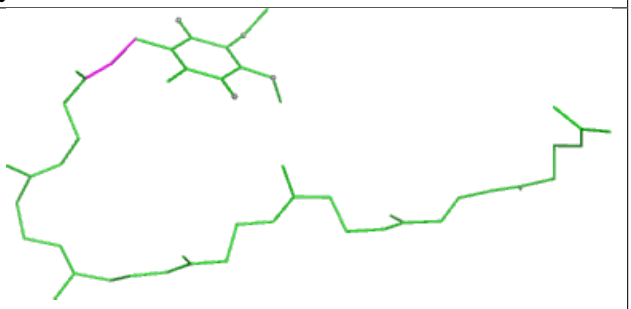

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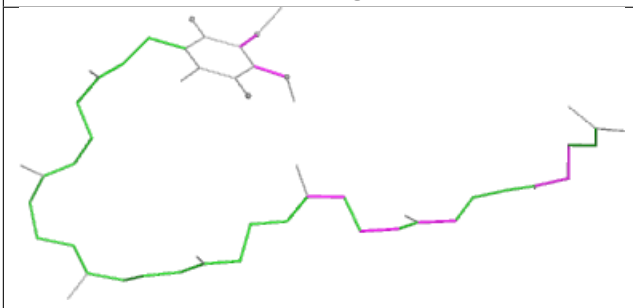

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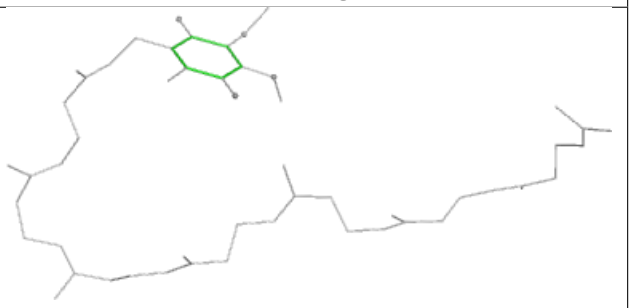
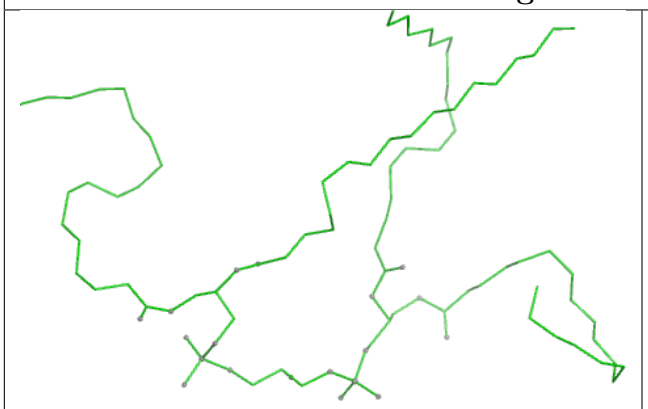


Rings

Ligand CDL Ek 201



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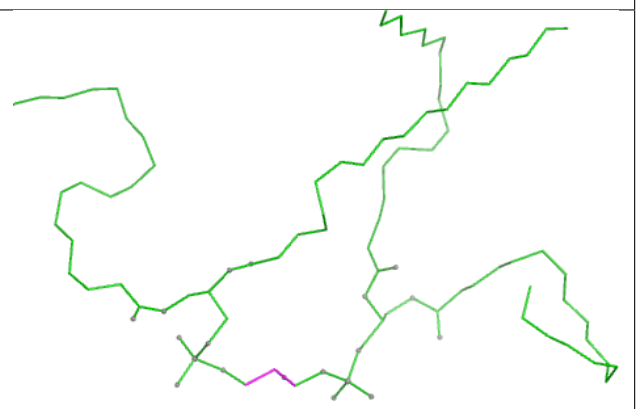

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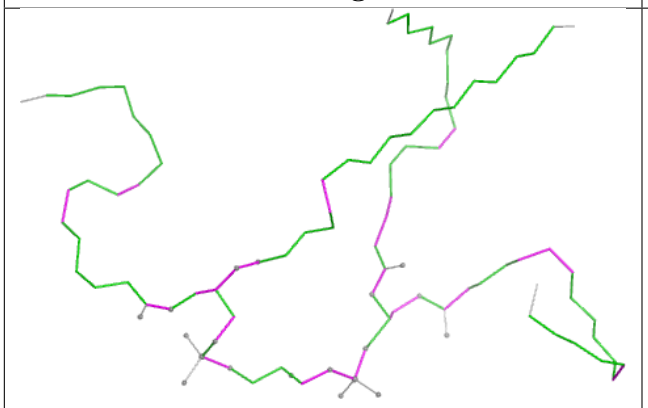

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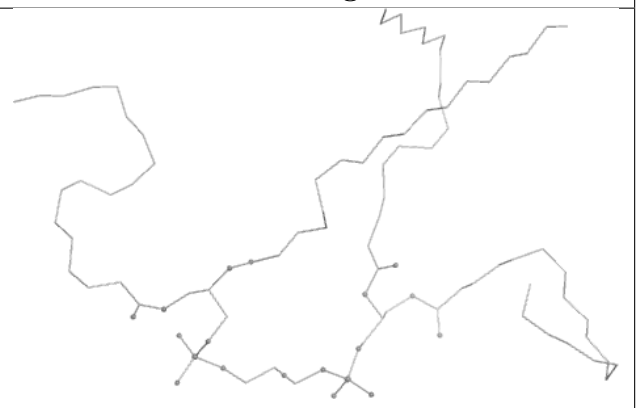
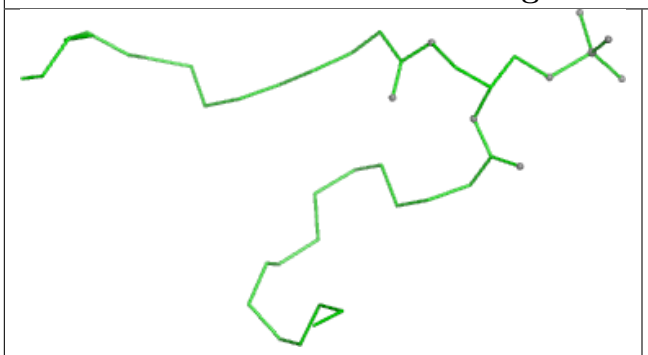


Rings

Ligand LPP EI 402



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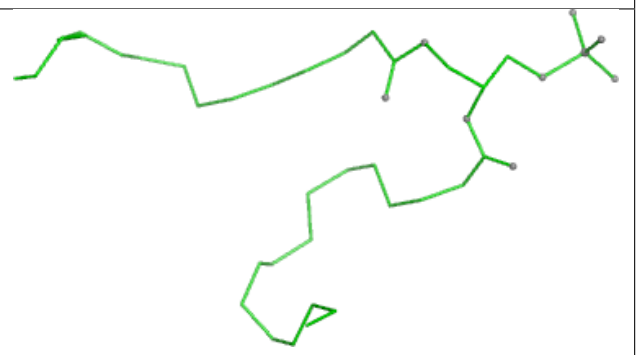
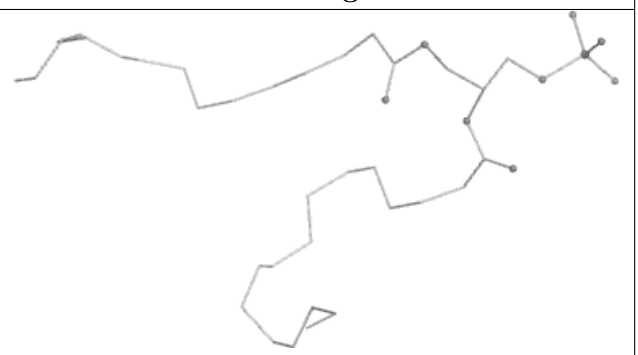


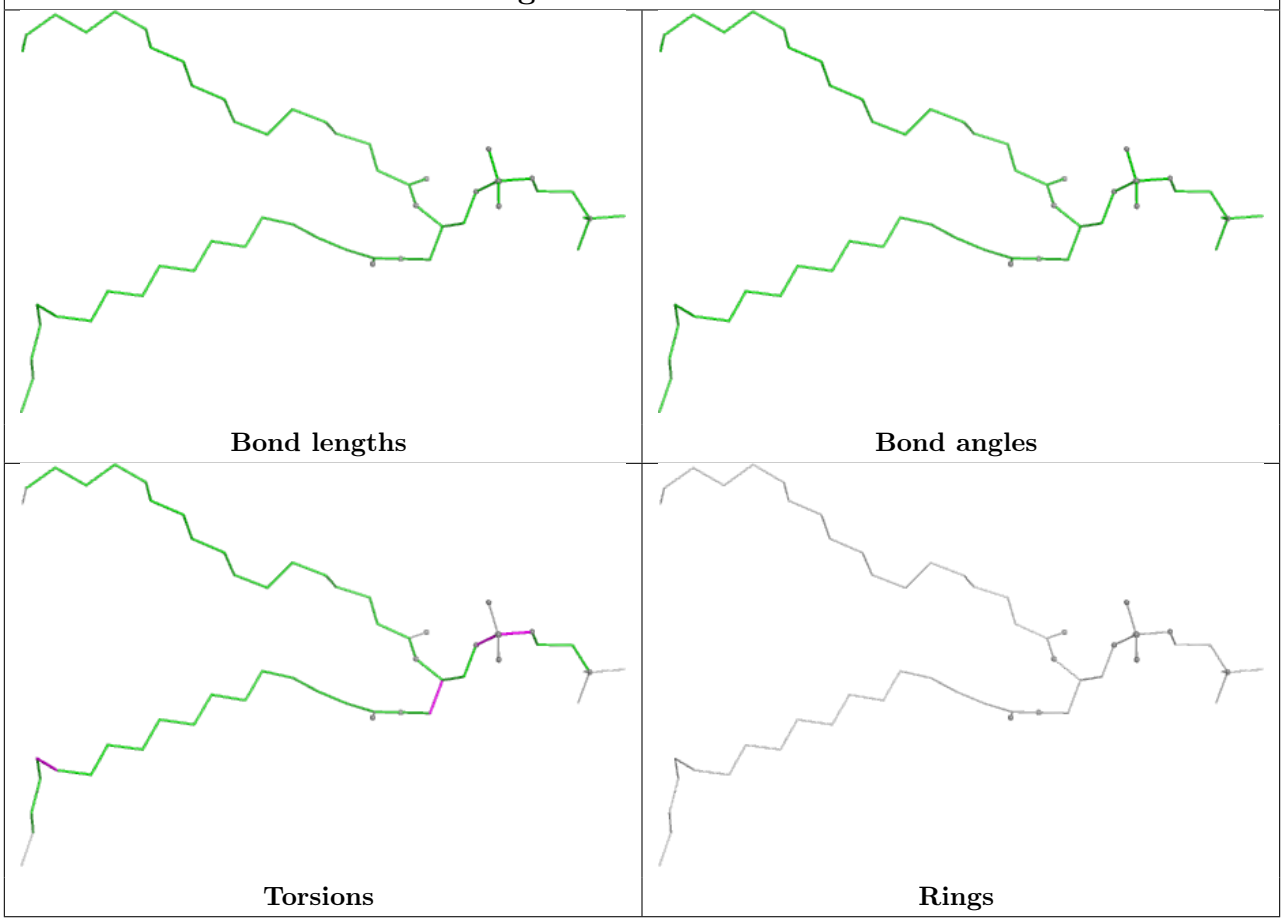
Bond angles

Torsions

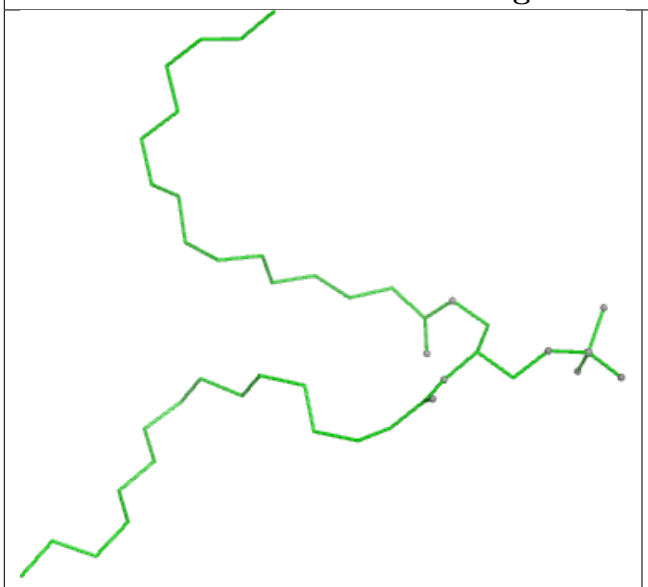


Rings

Ligand PC1 Dv 407



Ligand LPP AA 902



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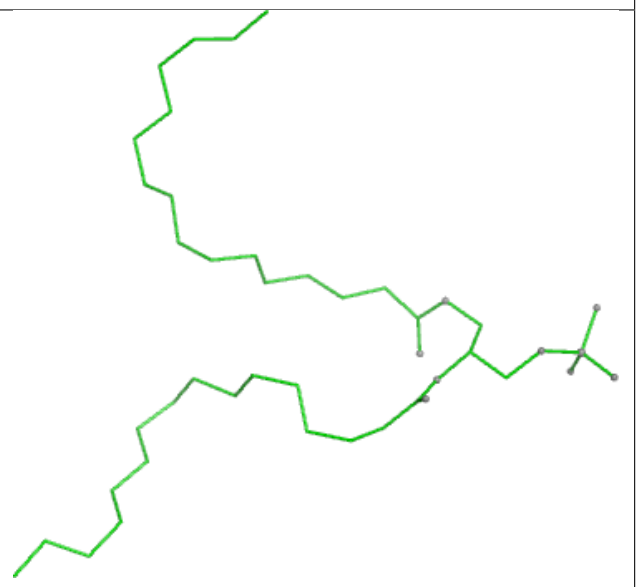
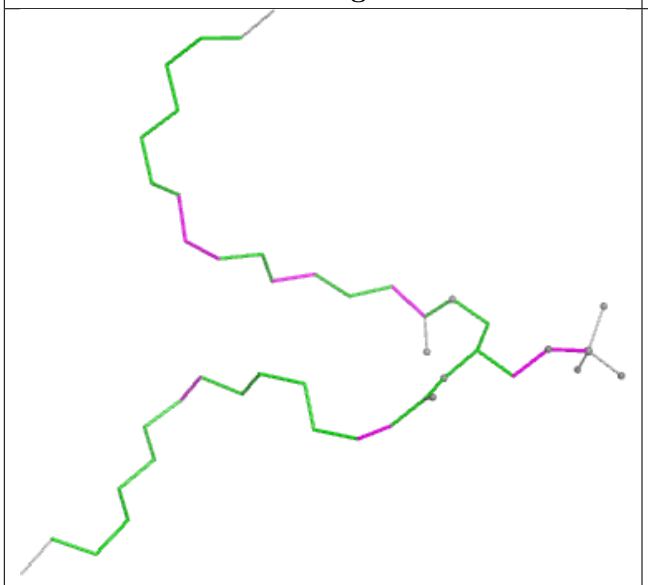


Bond angles



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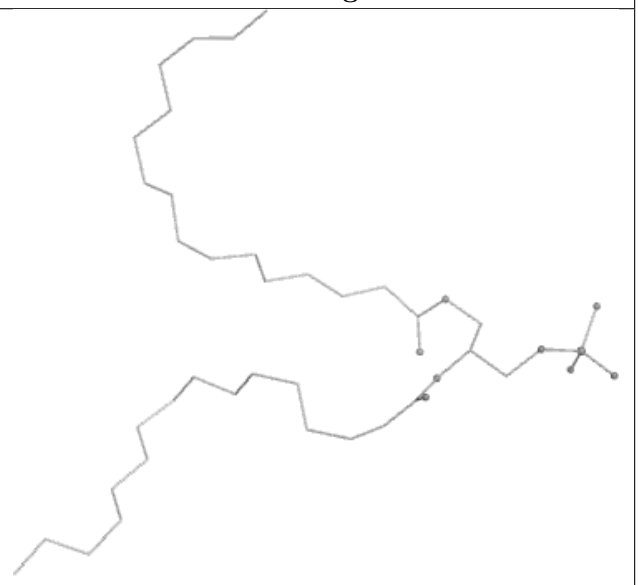
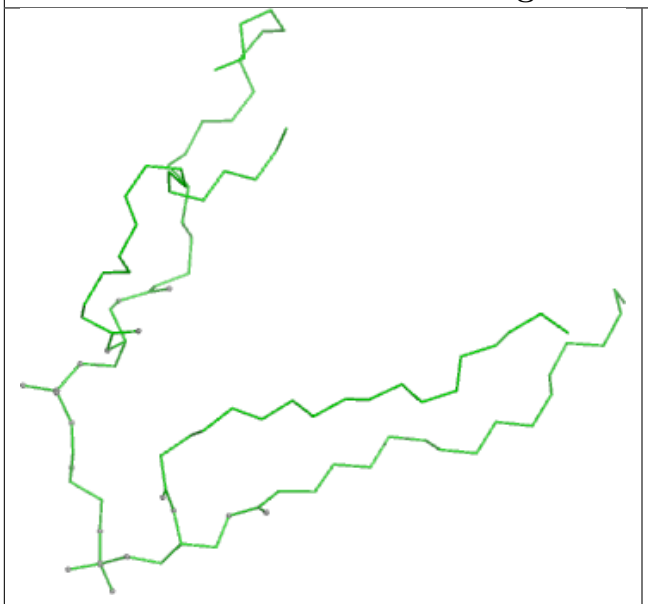


Rings

Ligand CDL Dr 403



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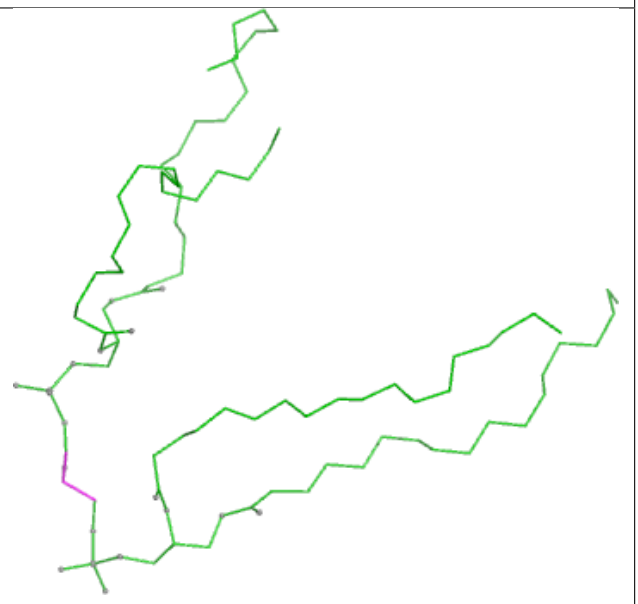
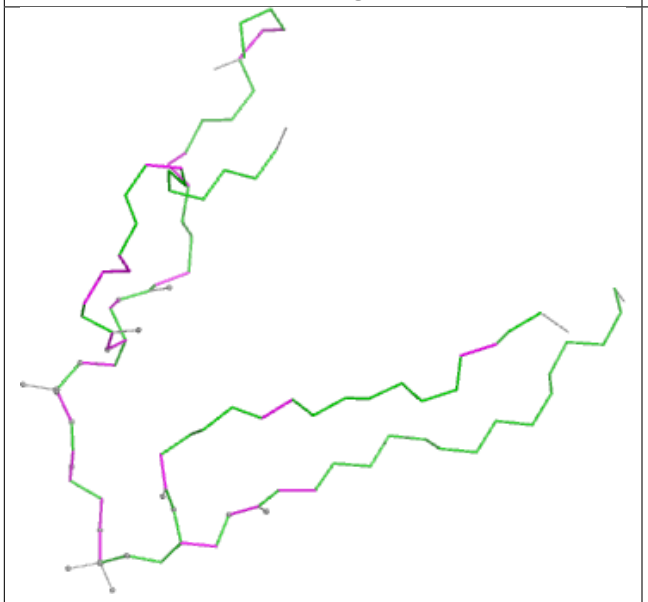


Bond angles



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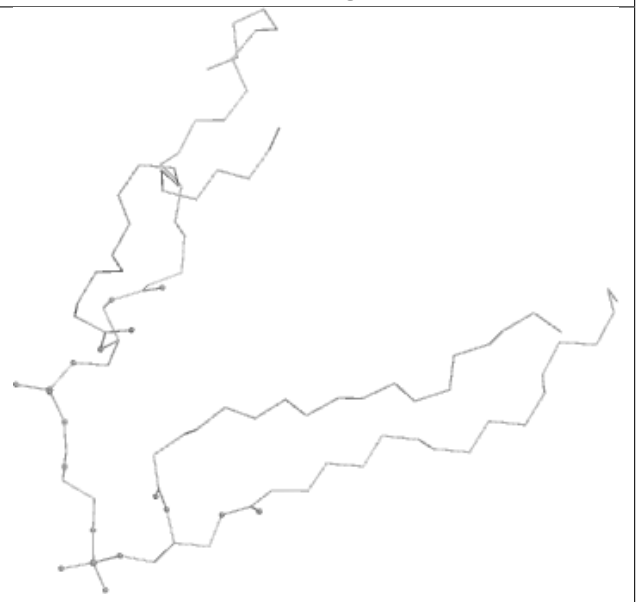
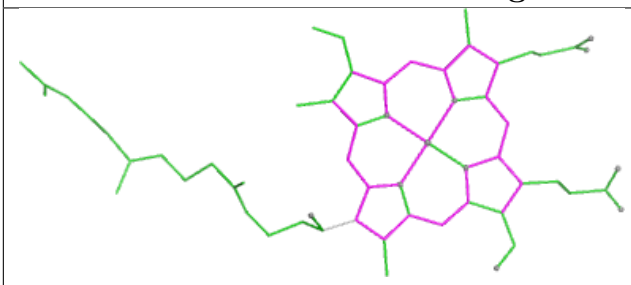
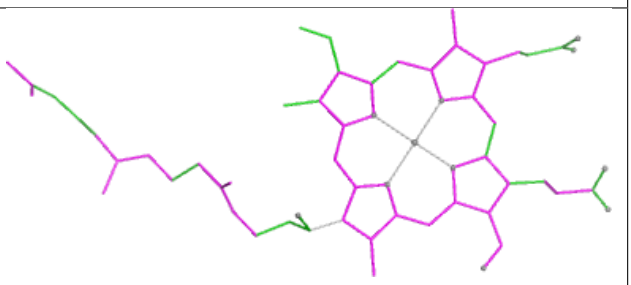
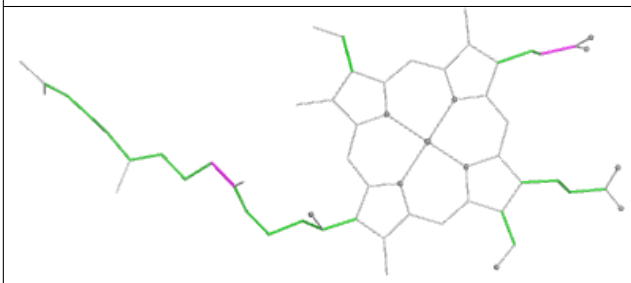
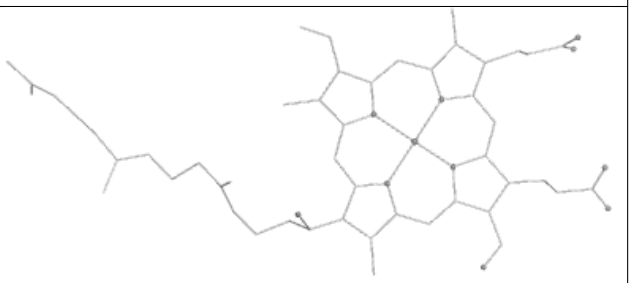
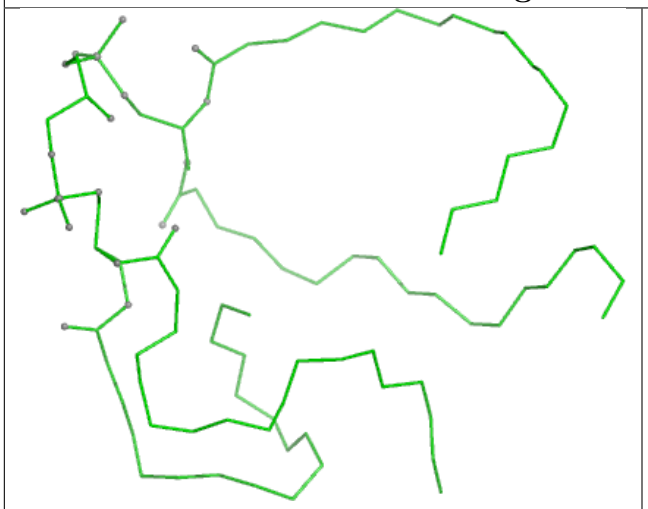


Rings

Ligand HEA DA 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Dn 502

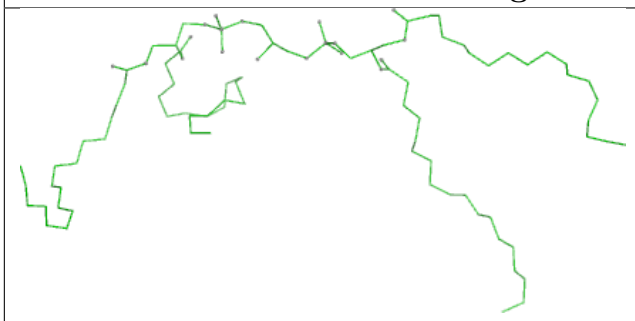
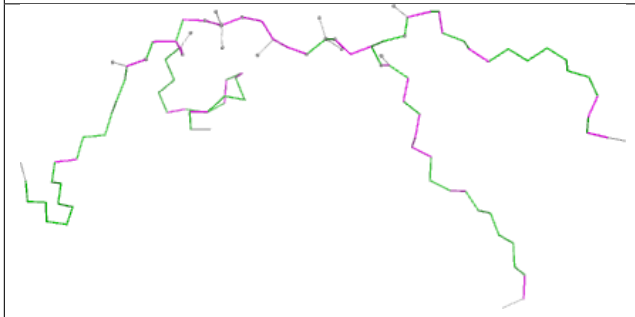


Bond lengths

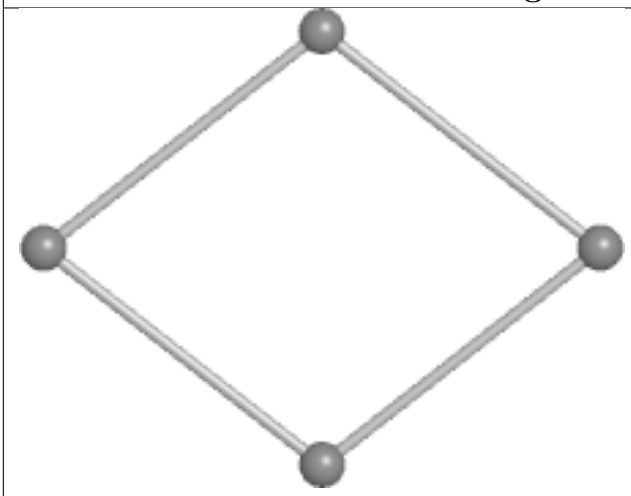
Bond angles

Torsions

Rings

Ligand CDL DG 201	
 Bond lengths	Bond angles
 Torsions	Rings

Ligand FES e 1102



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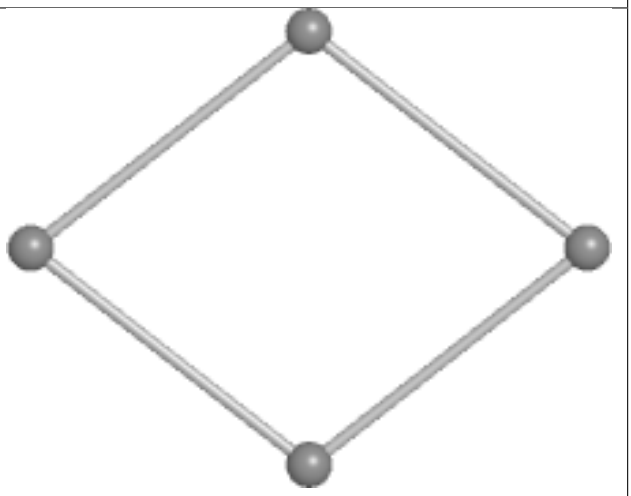
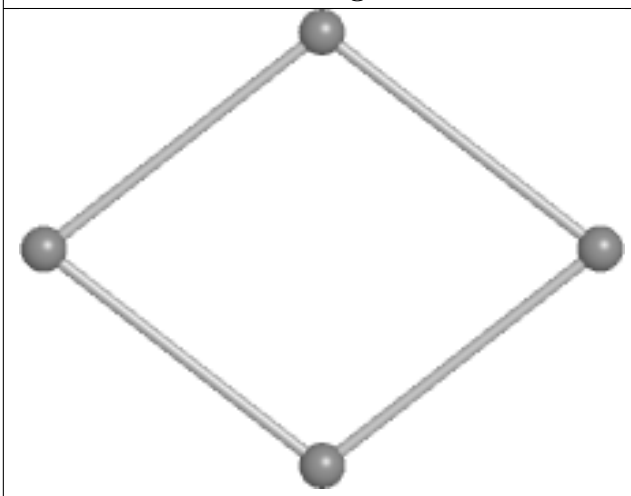


Bond angles



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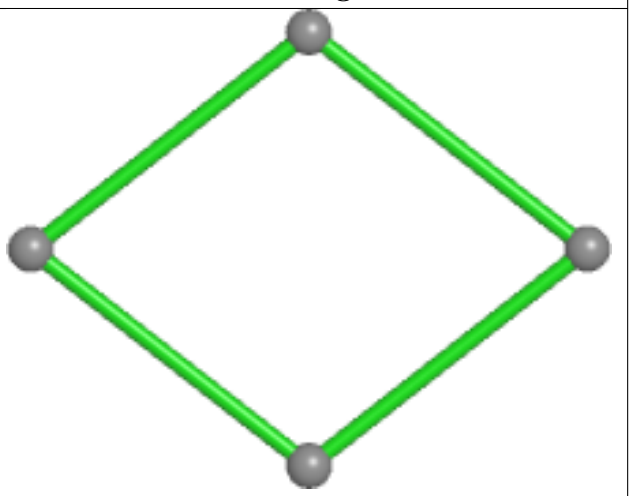
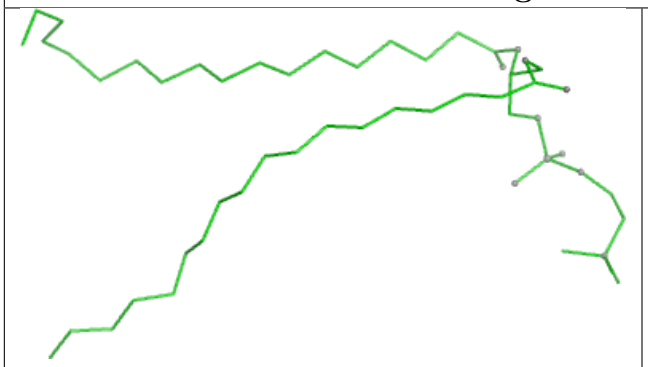


Rings

Ligand PC1 DC 608



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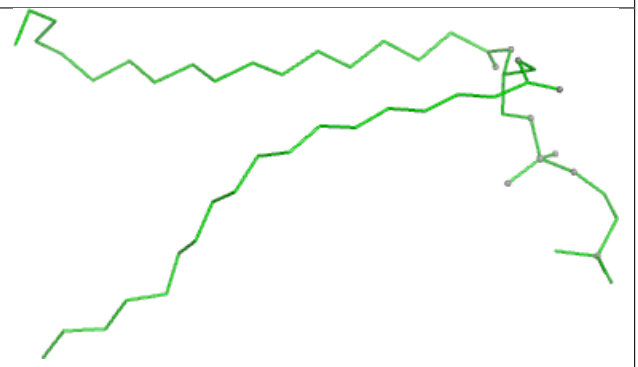

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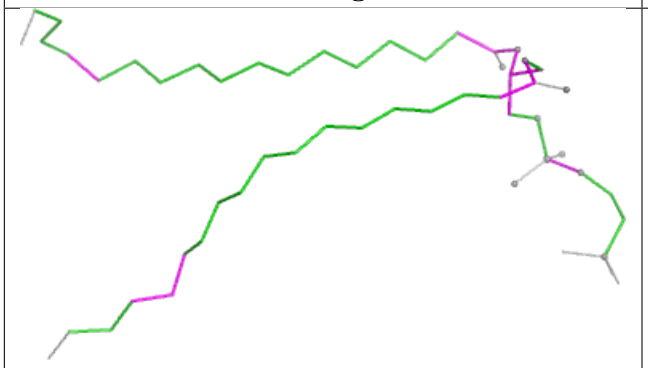

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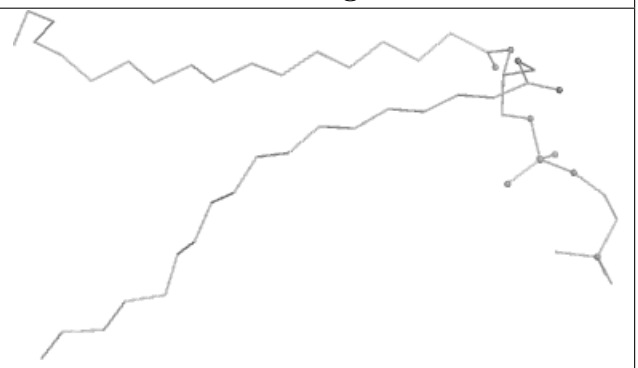
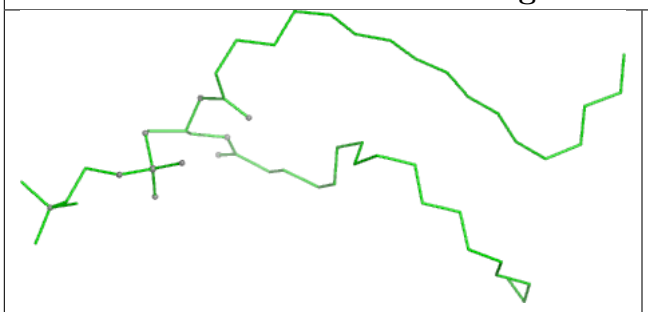


Rings

Ligand PC1 A0 605



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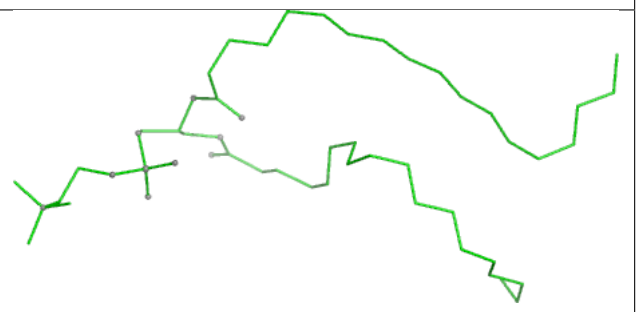

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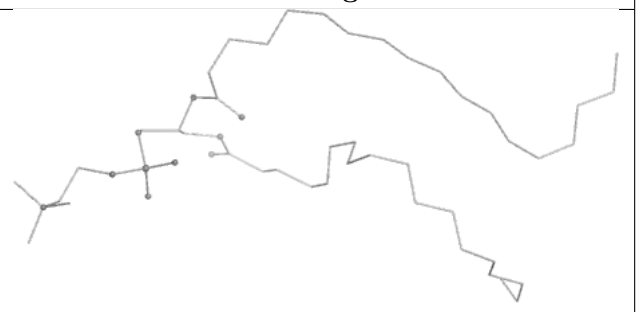
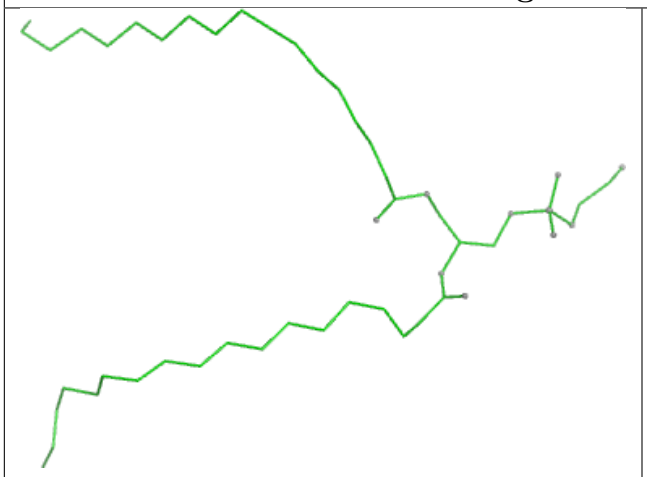
Torsions



Rings

Ligand 3PE CC 301



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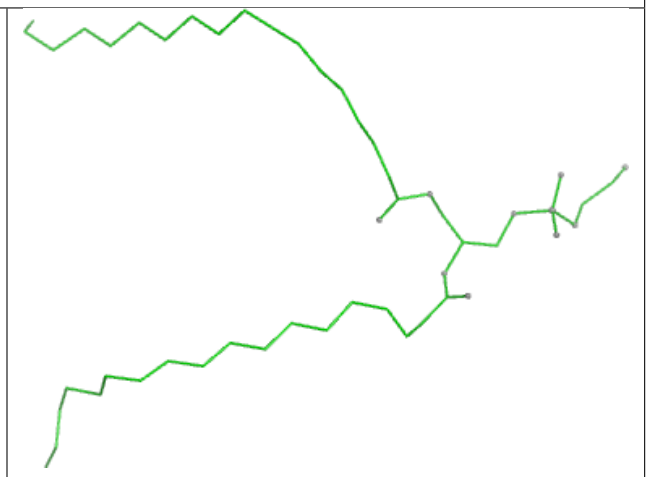

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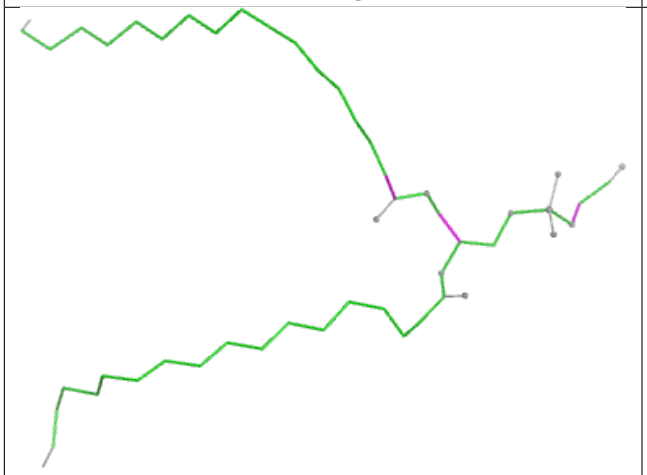

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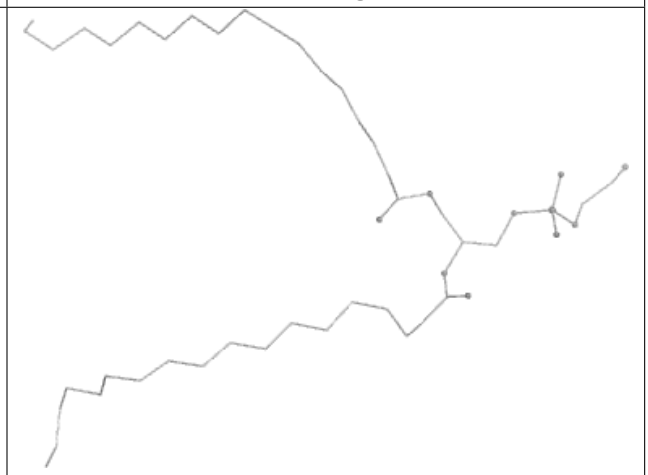


Rings

Ligand CDL DY 301

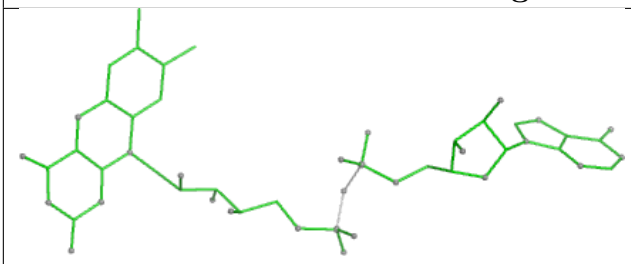
Bond lengths

Bond angles

Torsions

Rings

Ligand FAD CA 702



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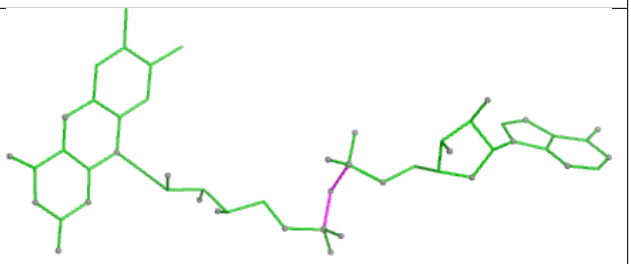
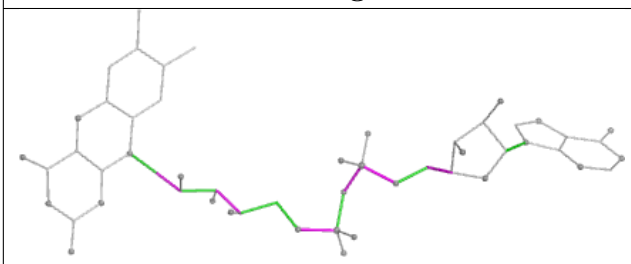


Bond angles



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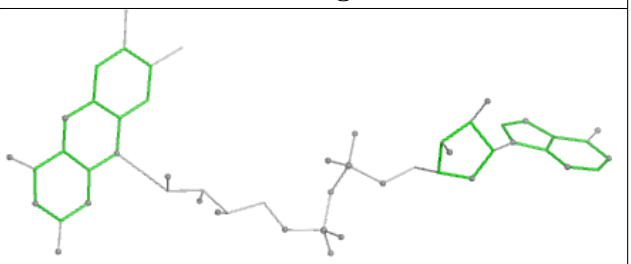
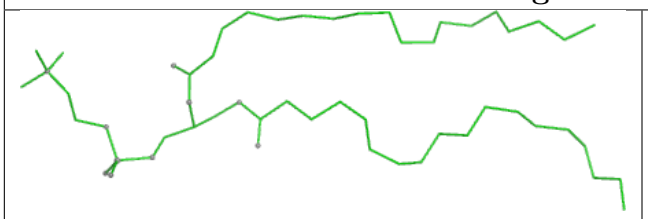


Rings

Ligand PC1 k 301



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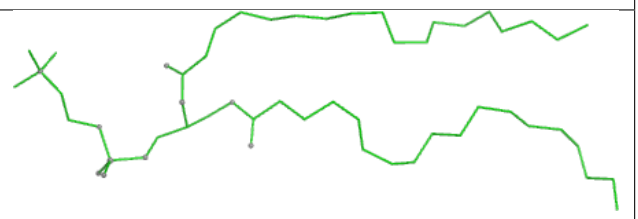

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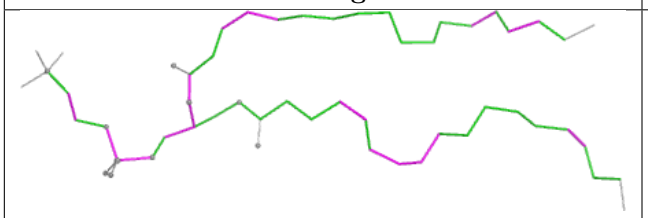

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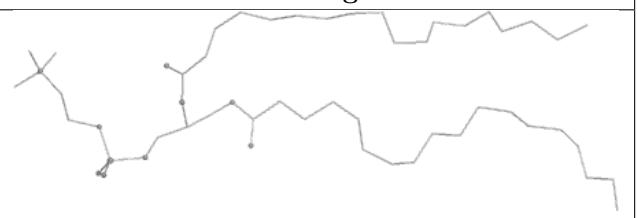
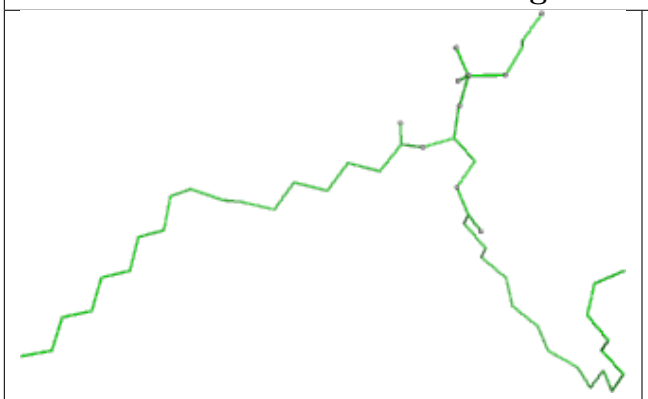


Rings

Ligand 3PE C 513



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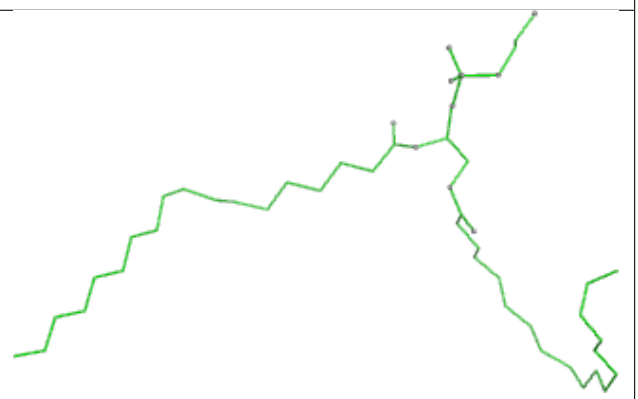

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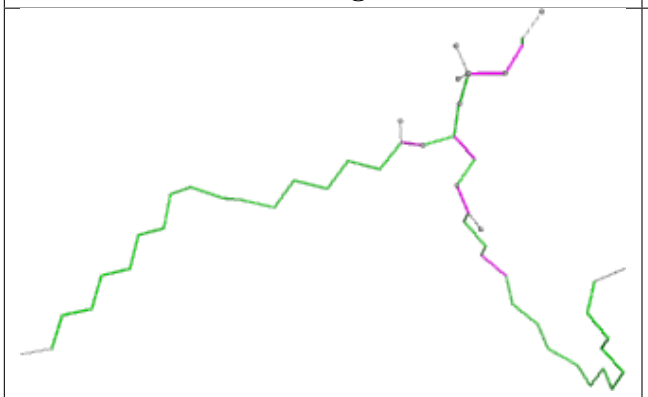
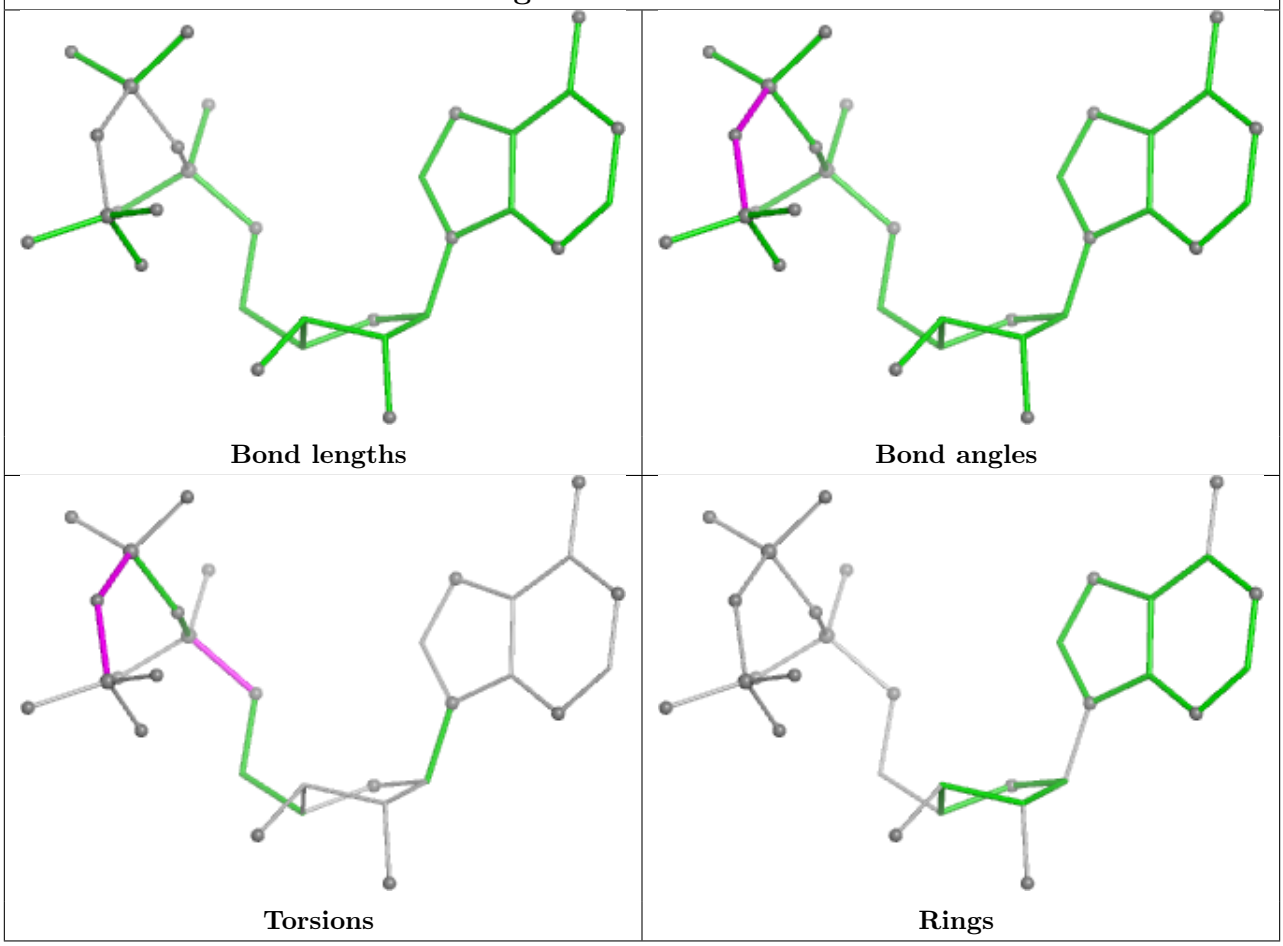
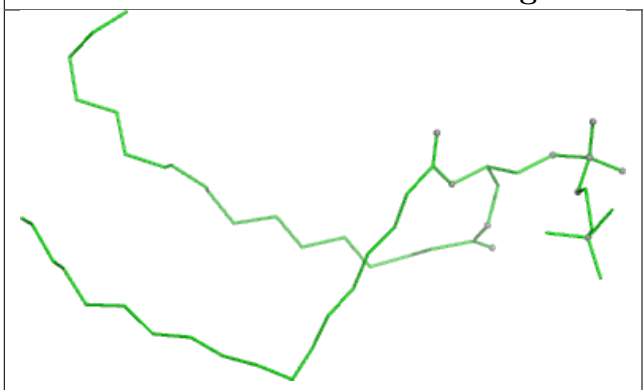
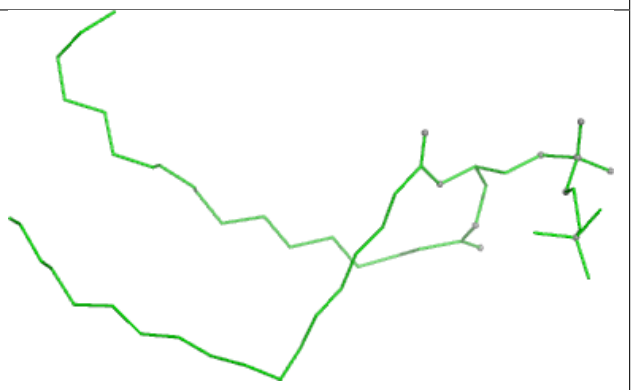
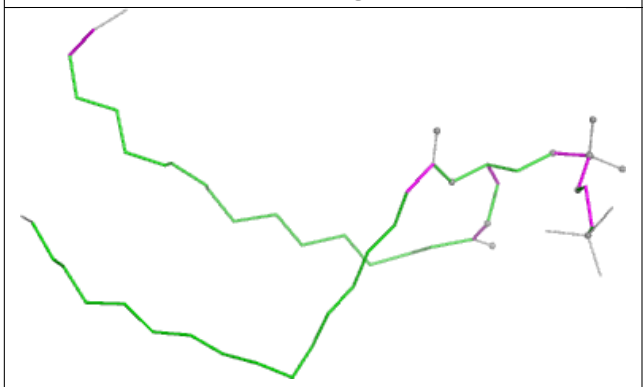


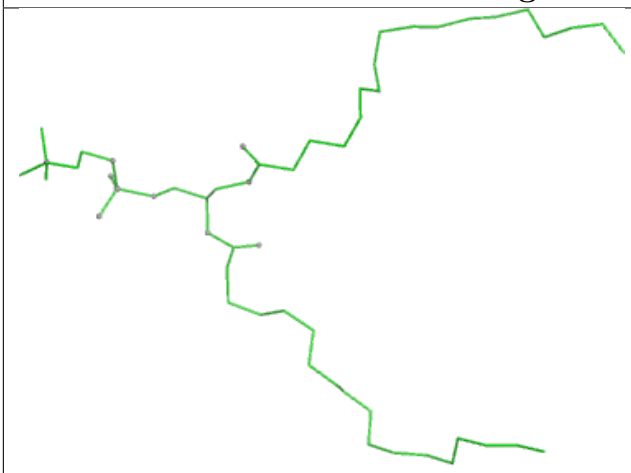
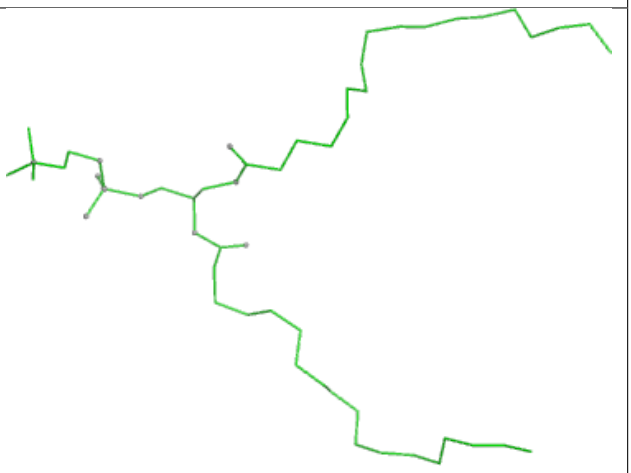
Torsions

Rings

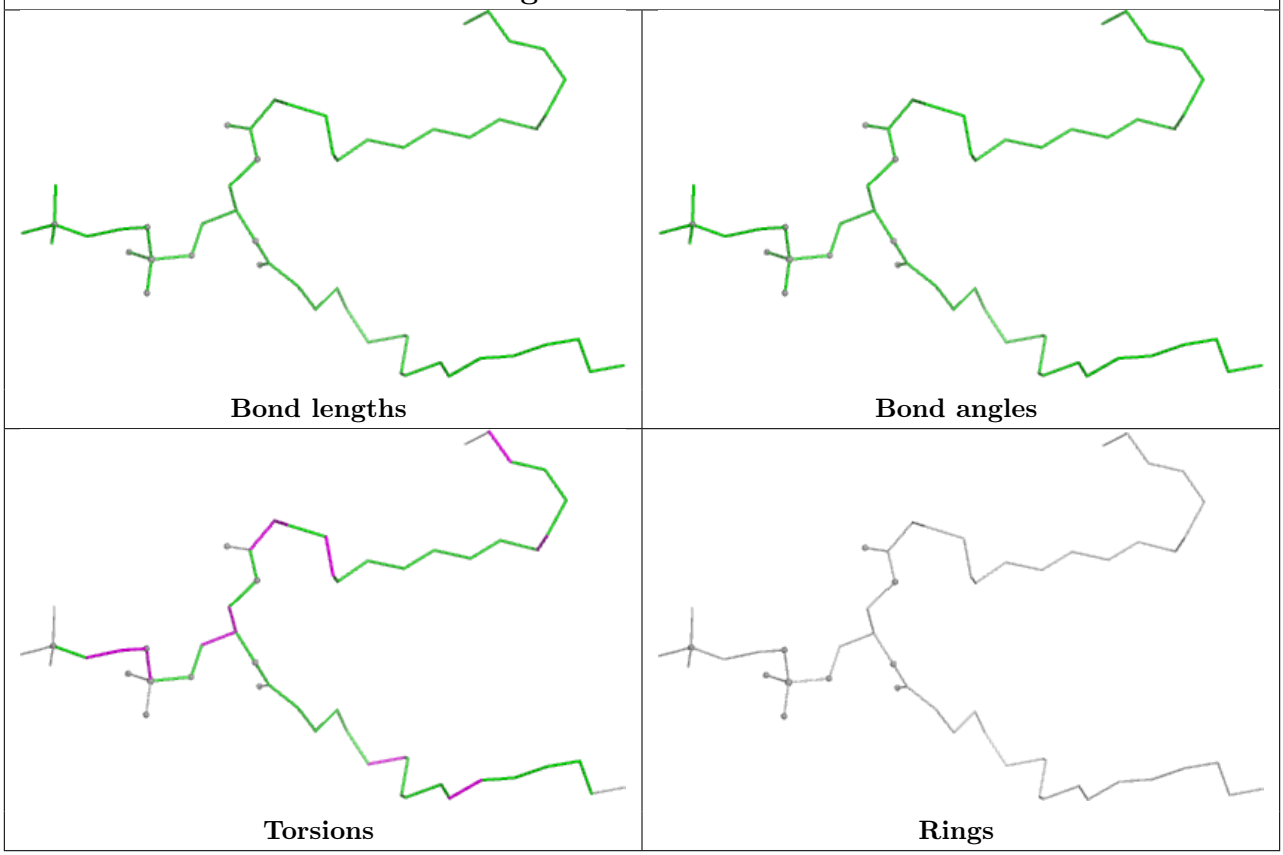
Ligand ATP ER 201



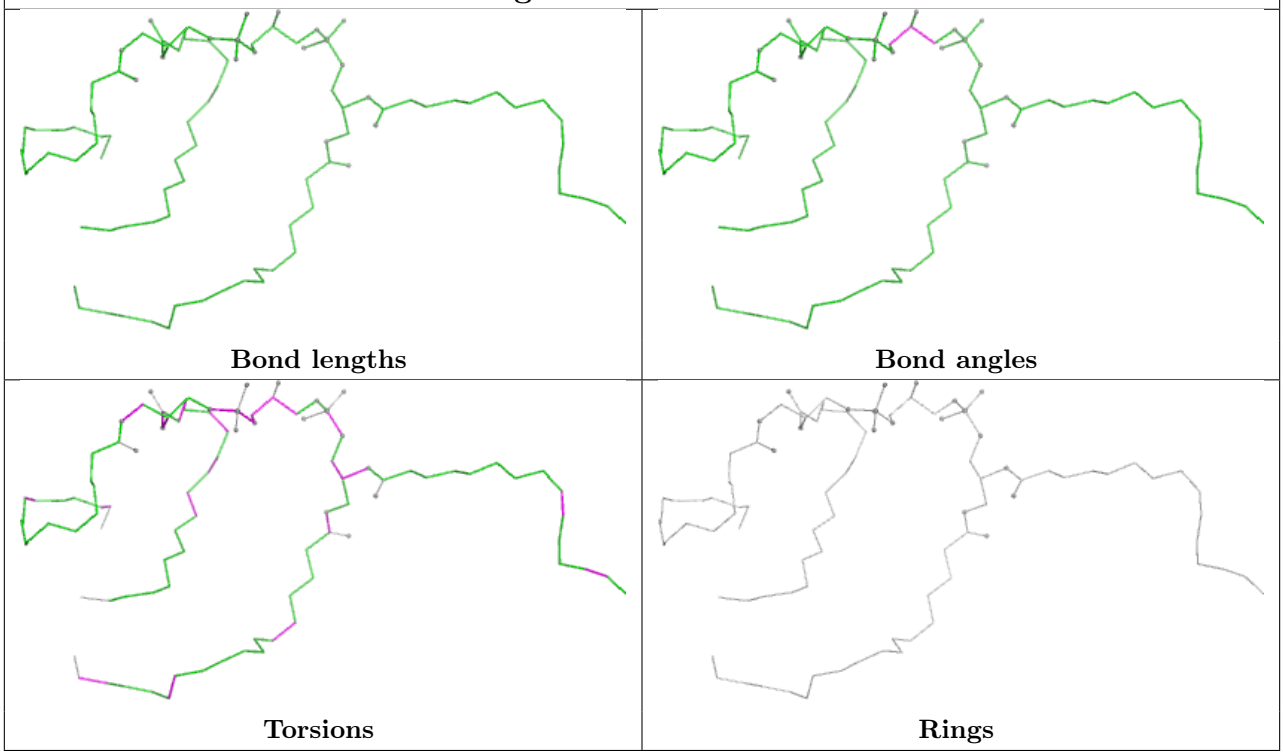
Ligand PC1 Dc 604	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand PC1 Dc 605	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand PC1 Eo 201



Ligand CDL Du 403



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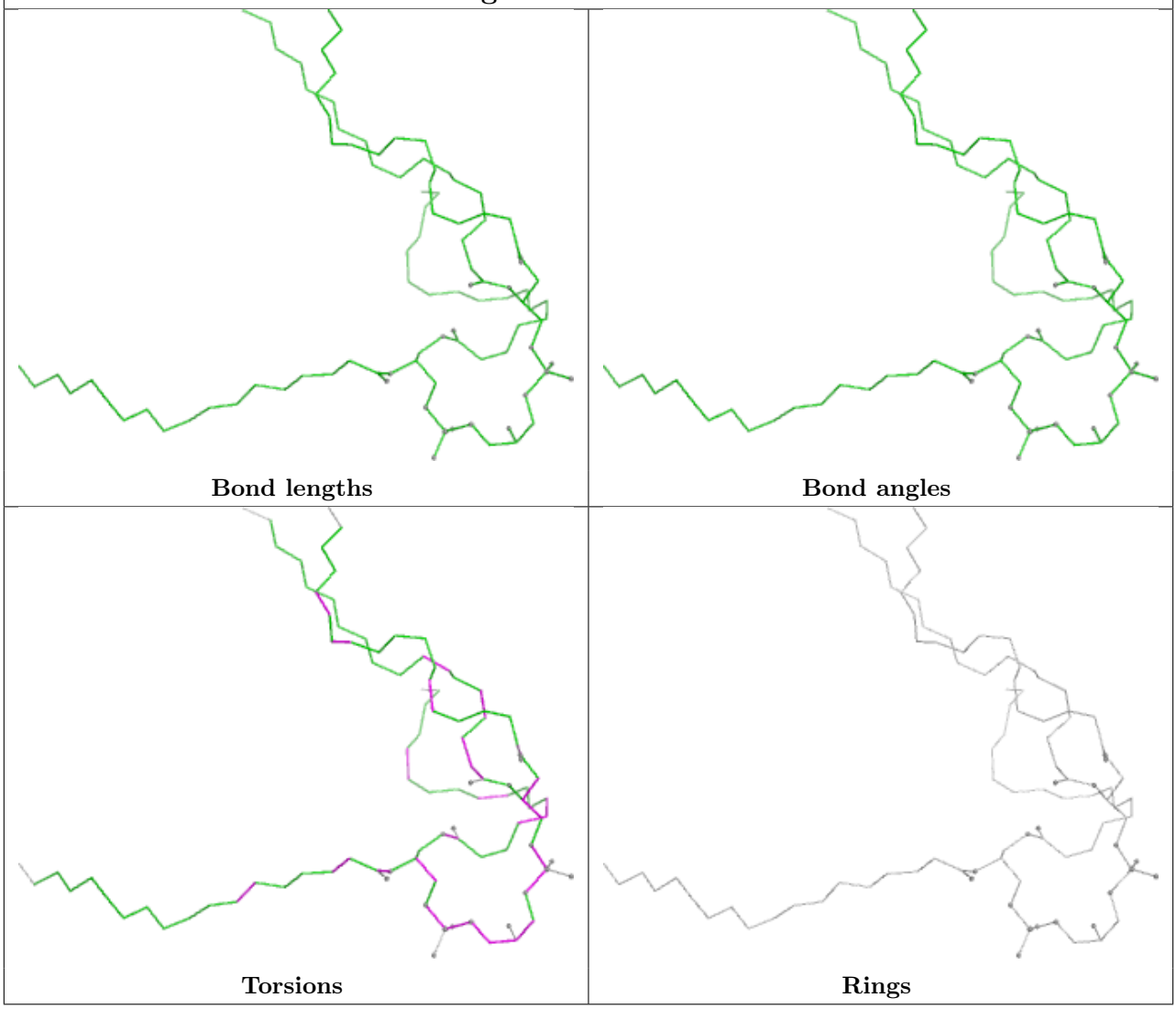

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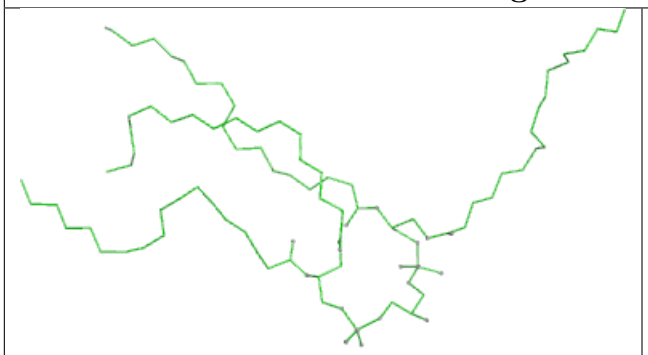

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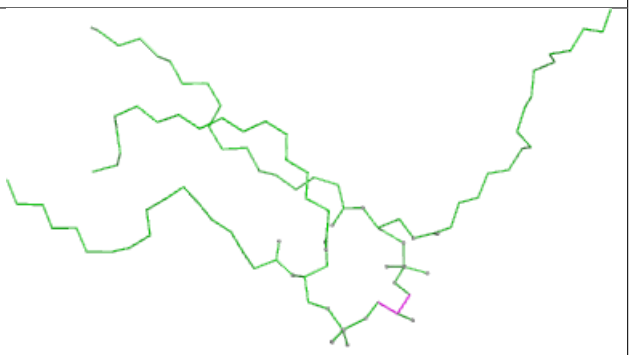
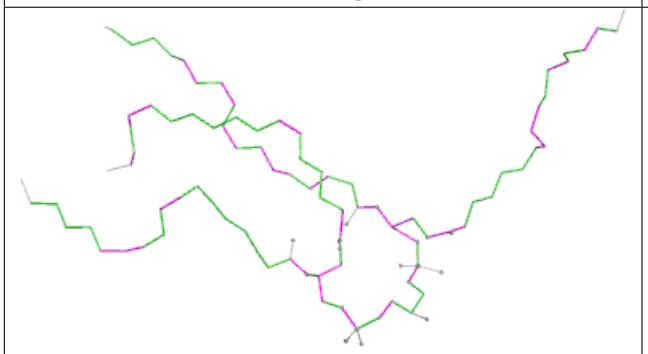


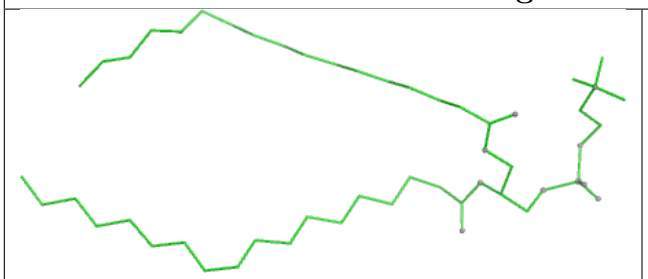
Bond angles



Torsions

Rings

Ligand PC1 EO 204



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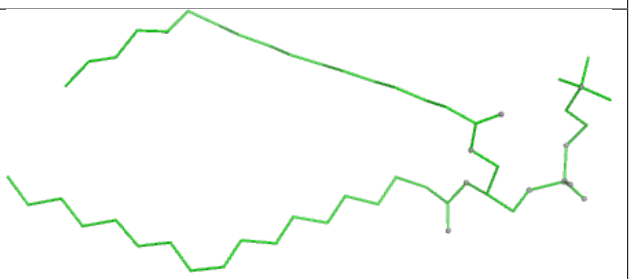

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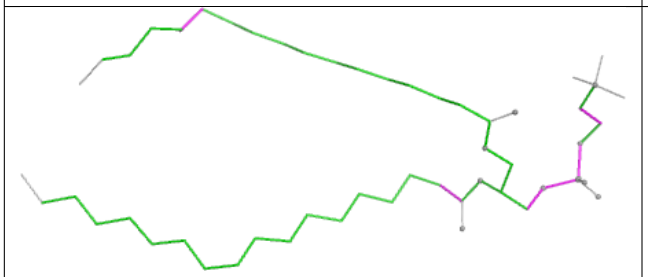

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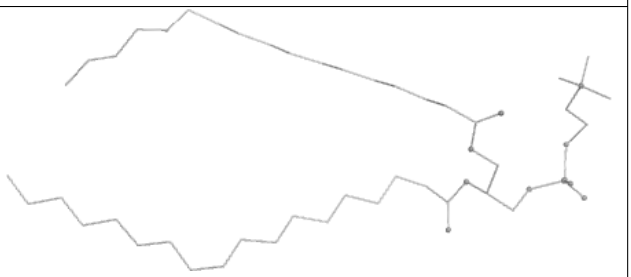
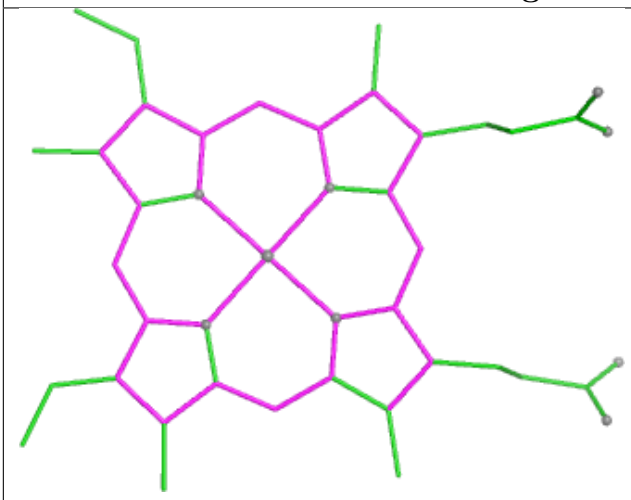


Rings

Ligand HEC D 401



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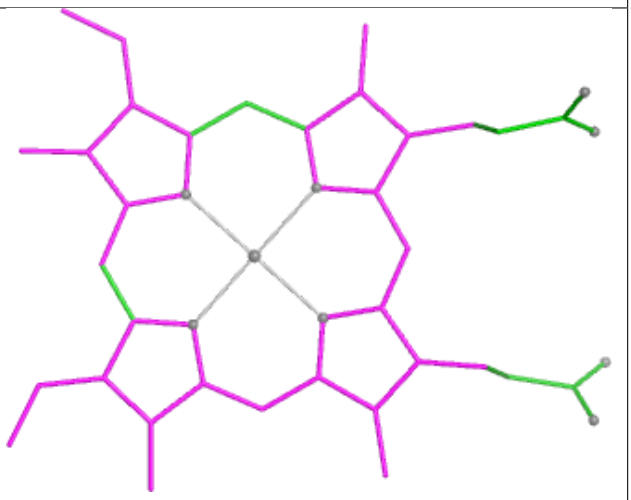
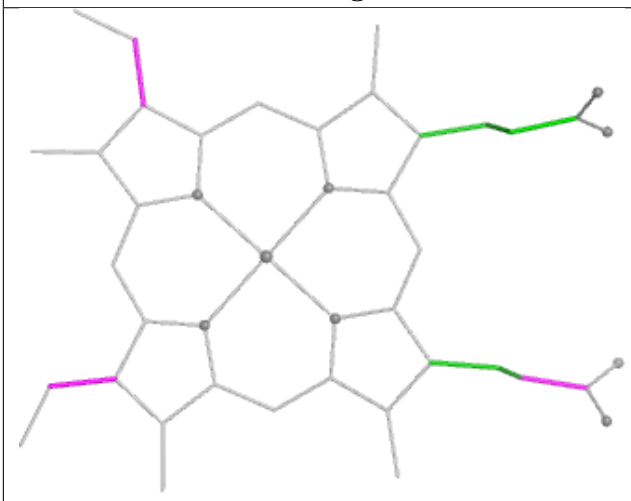


Bond angles



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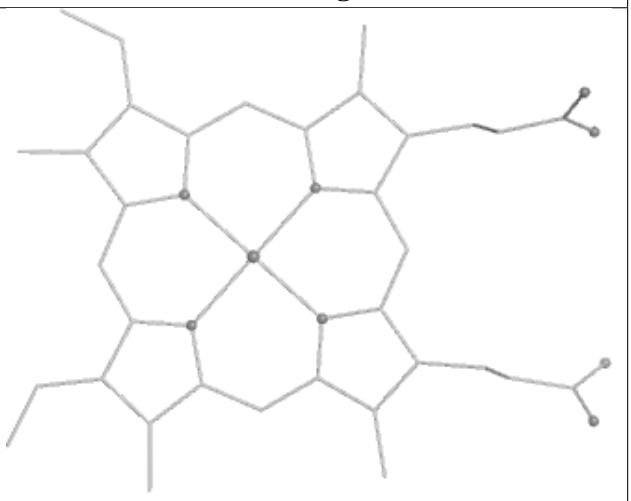
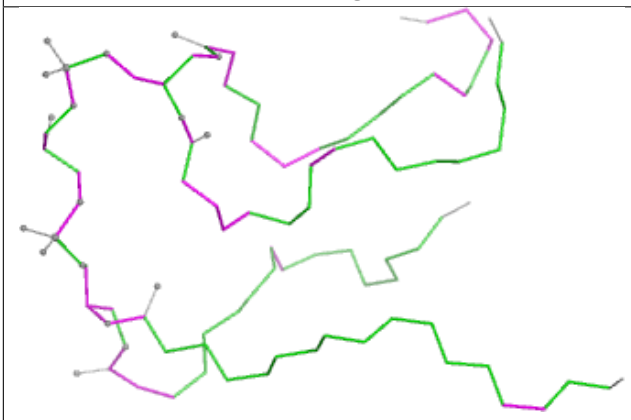
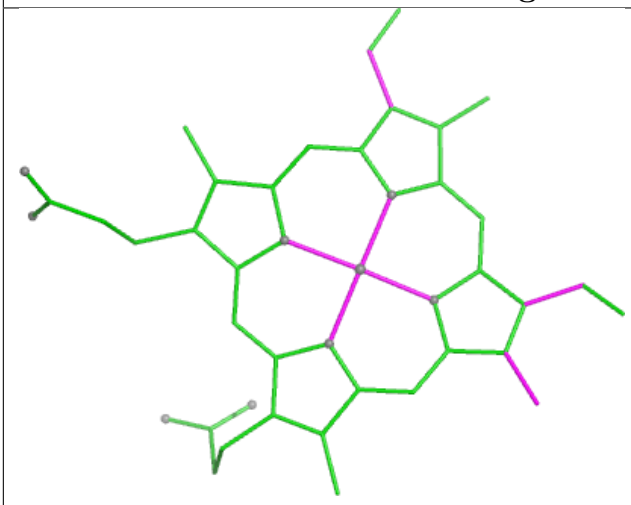
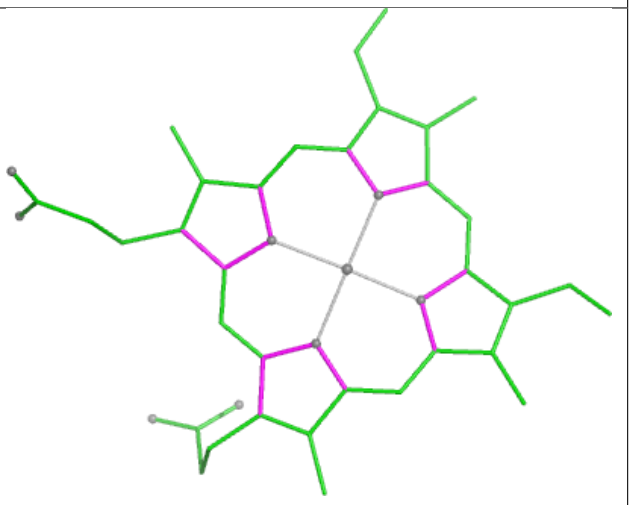
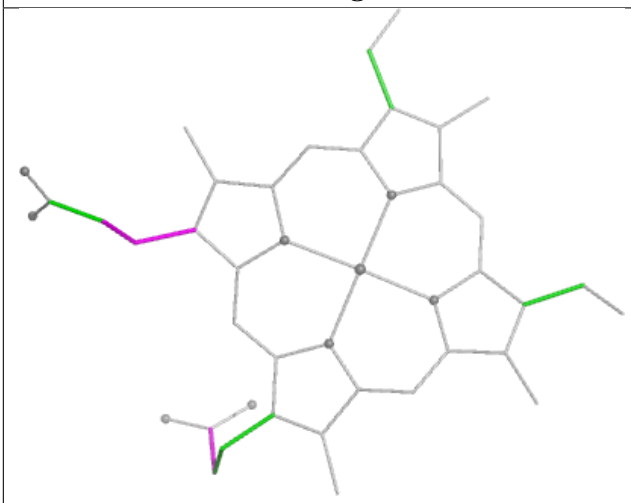
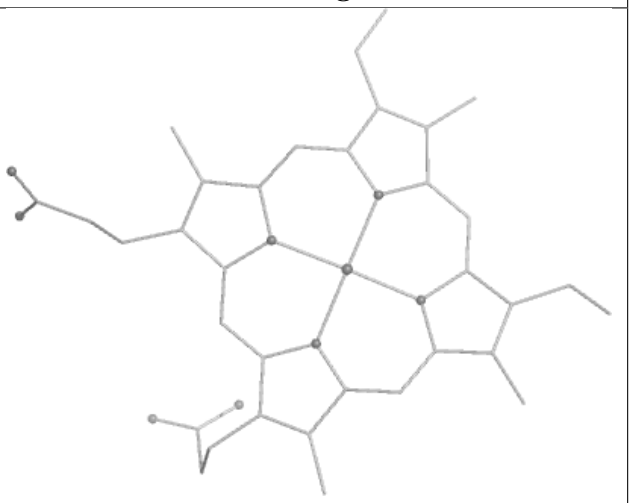


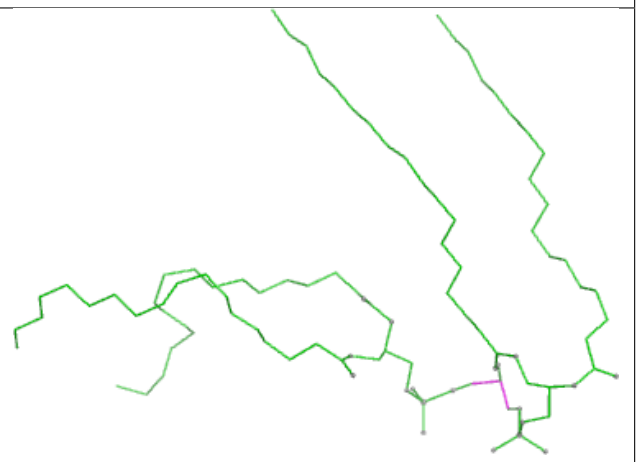
Rings

Ligand CDL Ea 501	
Bond lengths	Bond angles
 Torsions	Rings

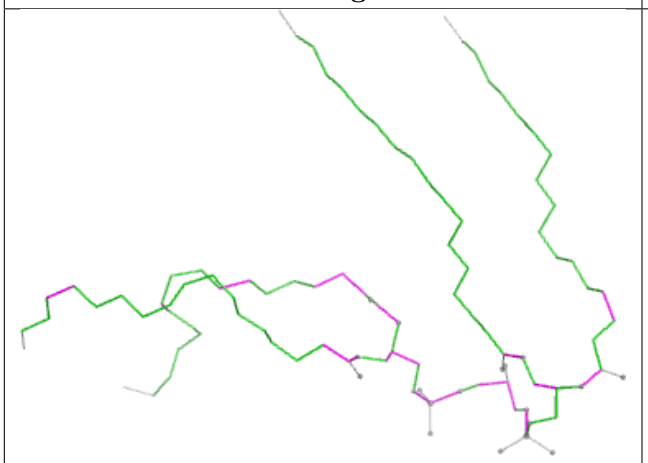
Ligand HEM C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL BE 201

Bond lengths



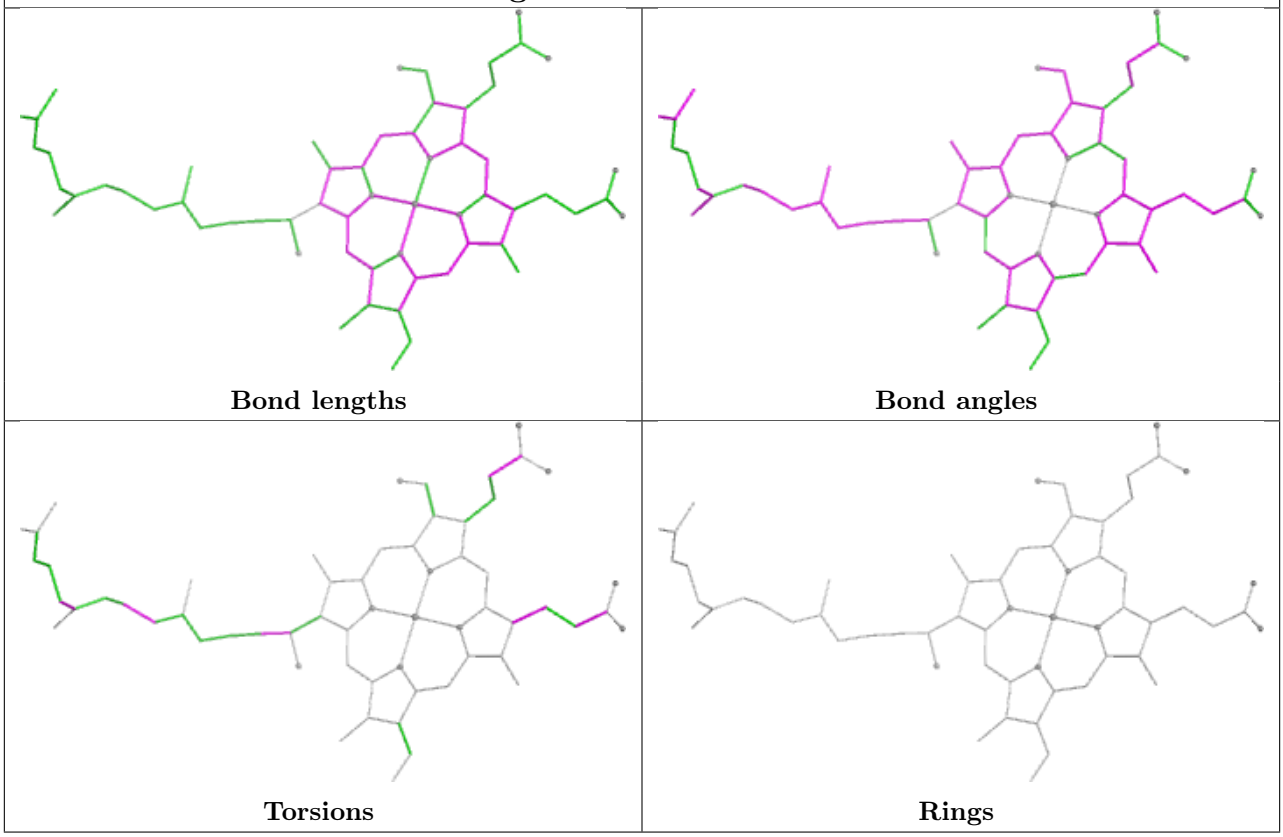
Bond angles



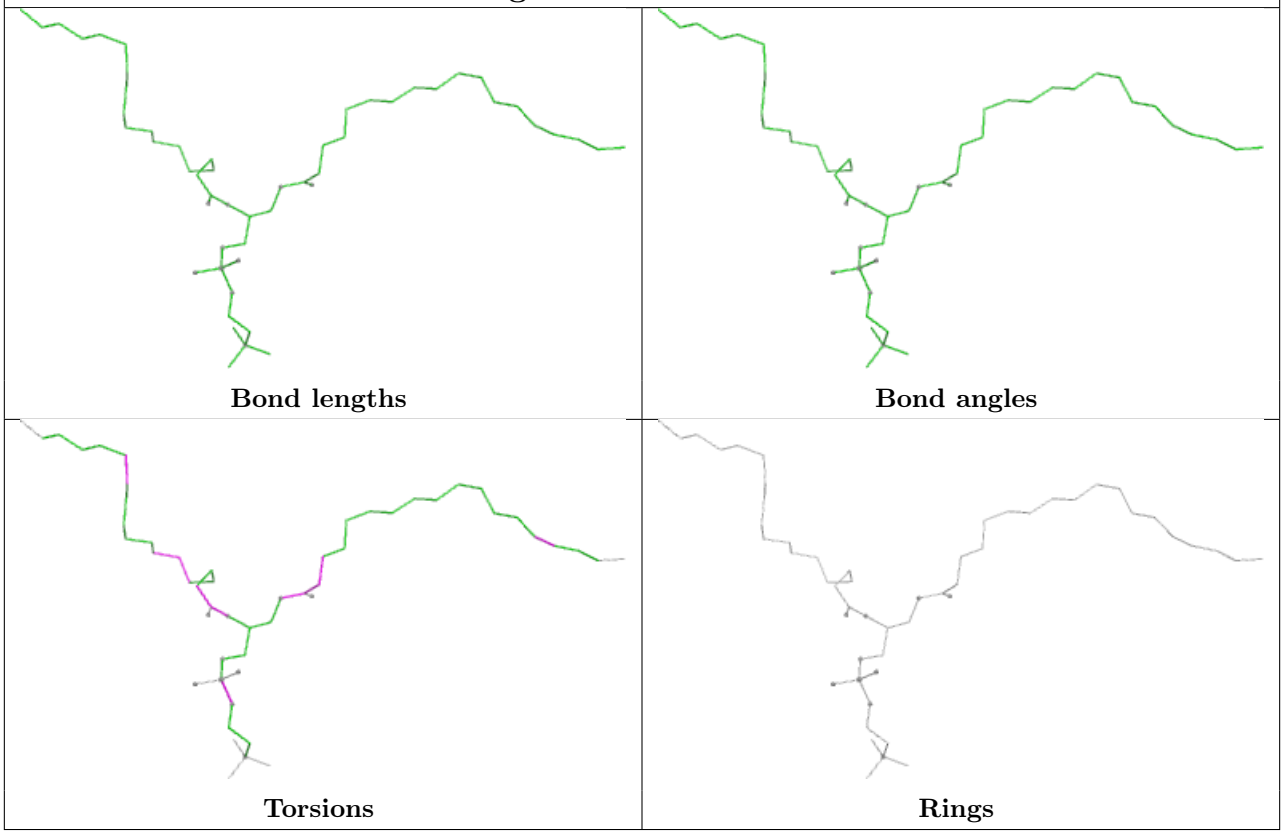
Torsions

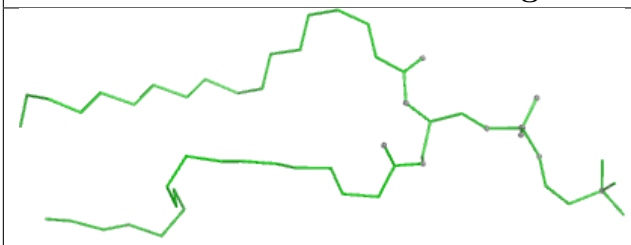
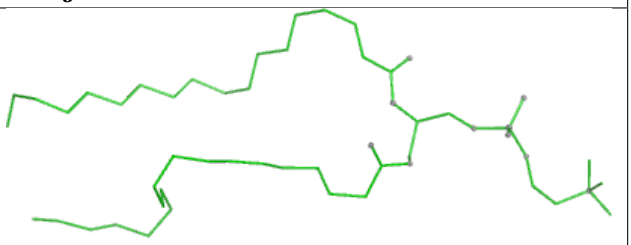
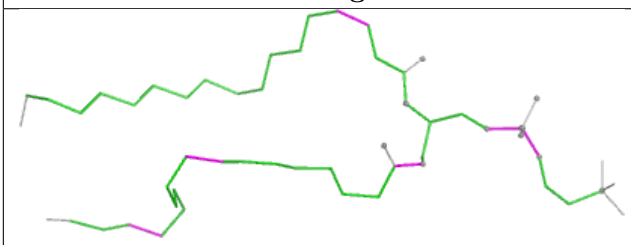
Rings

Ligand HEA DA 703



Ligand PC1 Dx 1205



Ligand PC1 Dj 406	
 Bond lengths	 Bond angles
 Torsions	Rings

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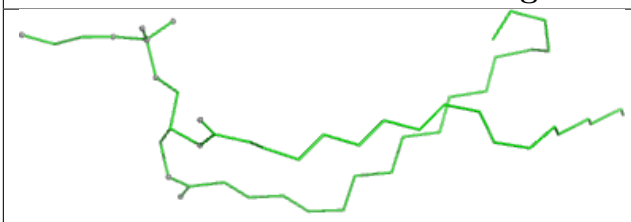
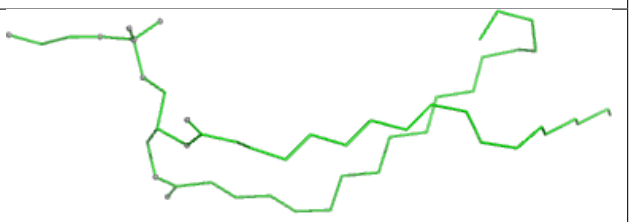
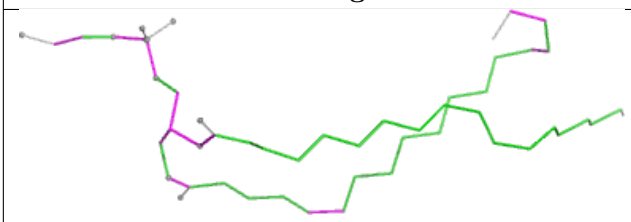
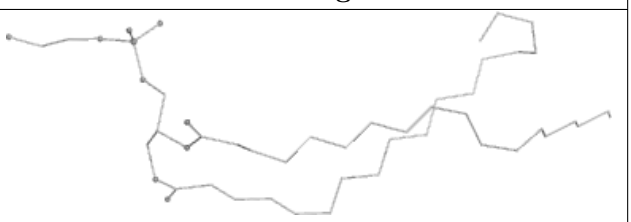
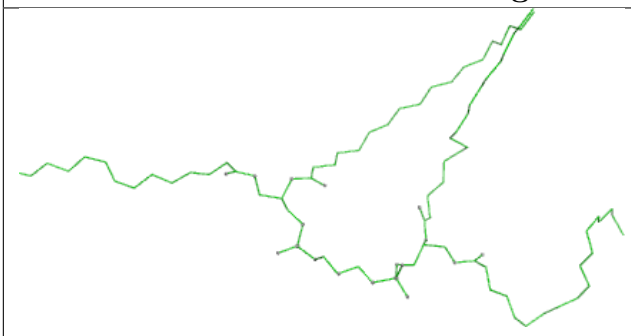
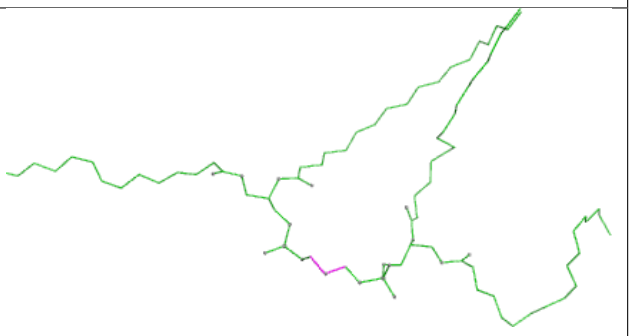
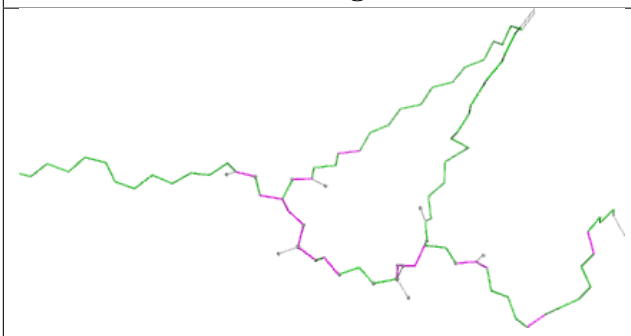
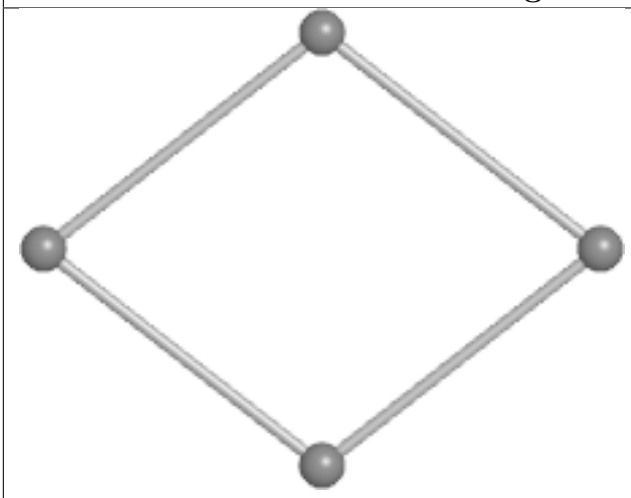
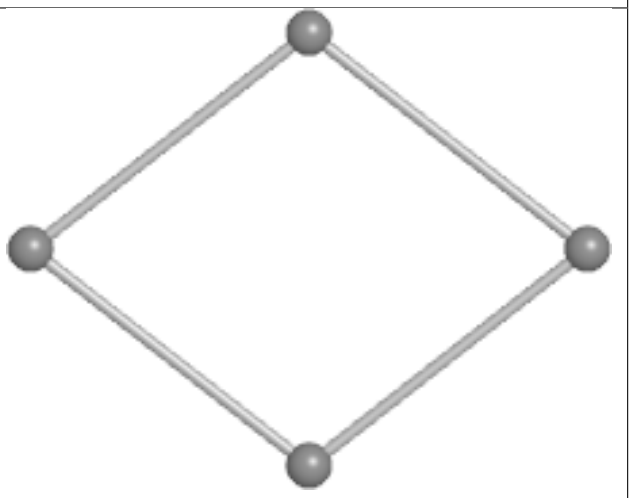
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL ED 604	
 Bond lengths	 Bond angles
 Torsions	Rings

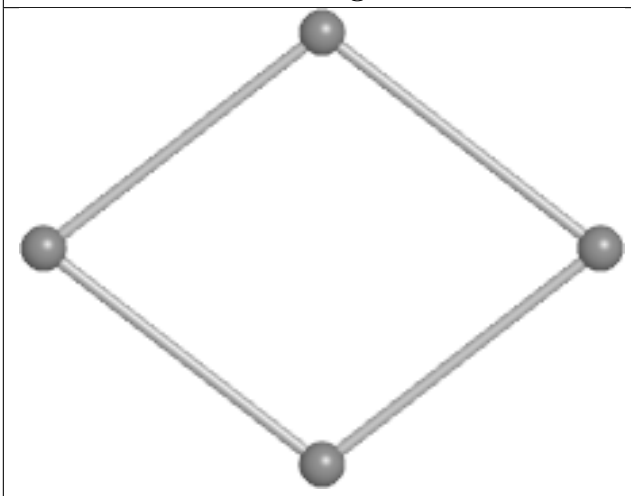
Ligand FES Ef 503



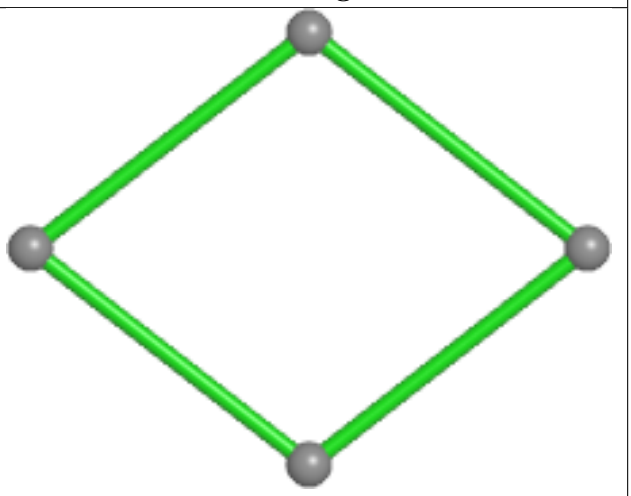
Bond lengths



Bond angles

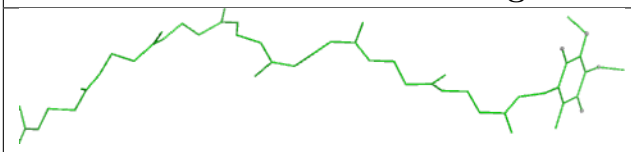


Torsions



Rings

Ligand UQ8 En 1202



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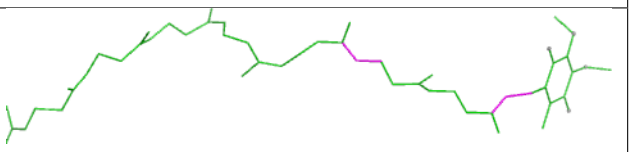

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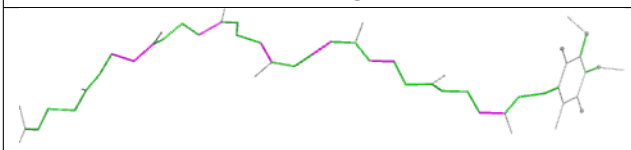

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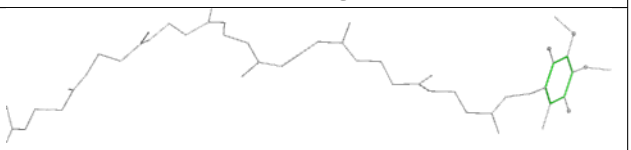
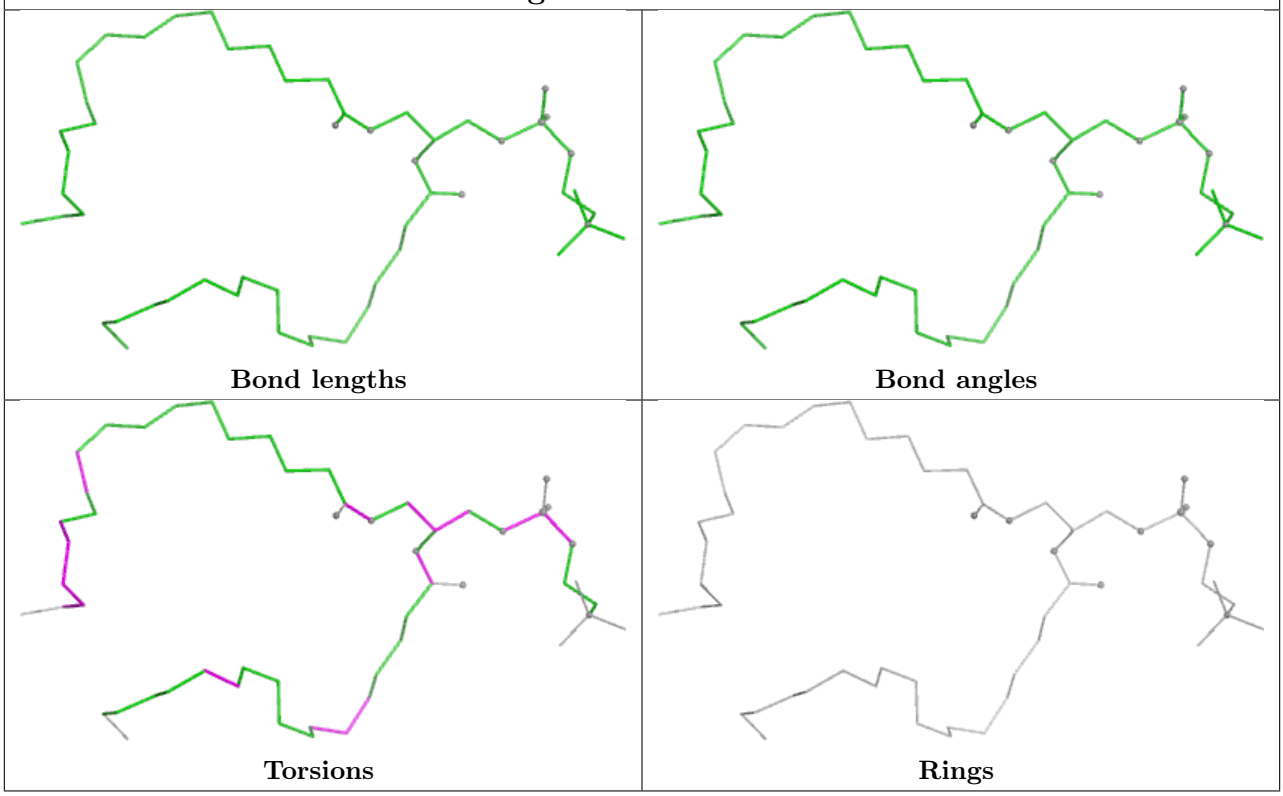
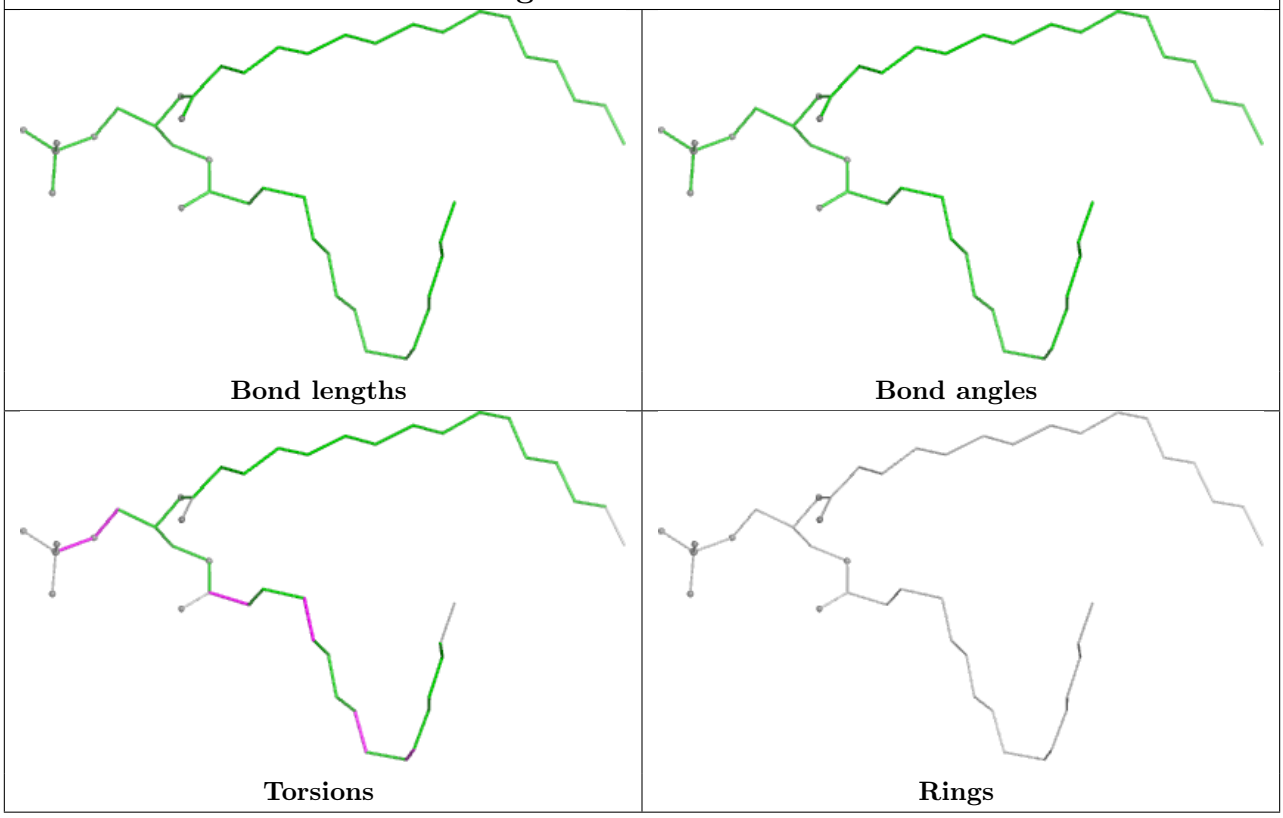


Rings

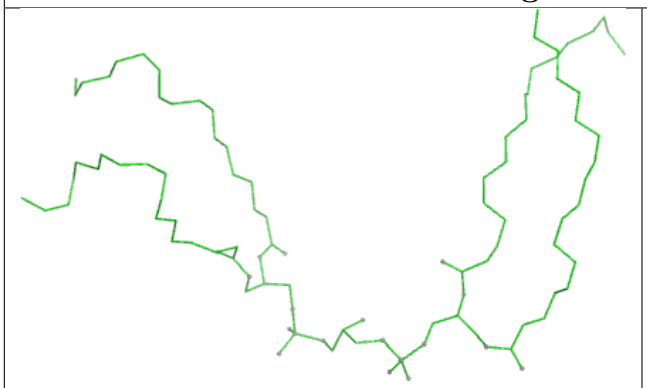
Ligand PC1 D 402



Ligand LPP Dn 504



Ligand CDL Ei 401



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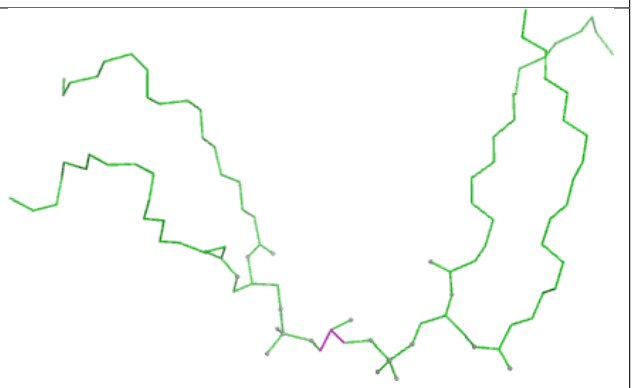

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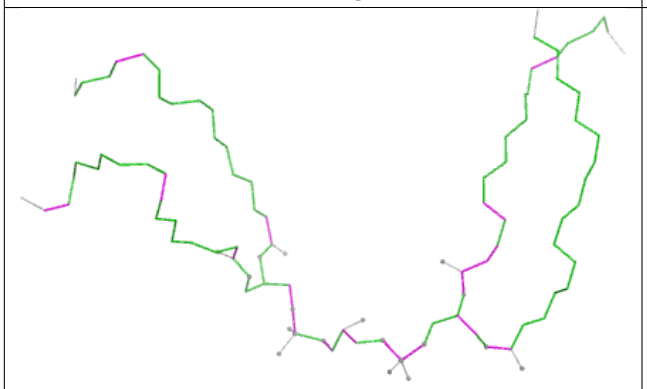

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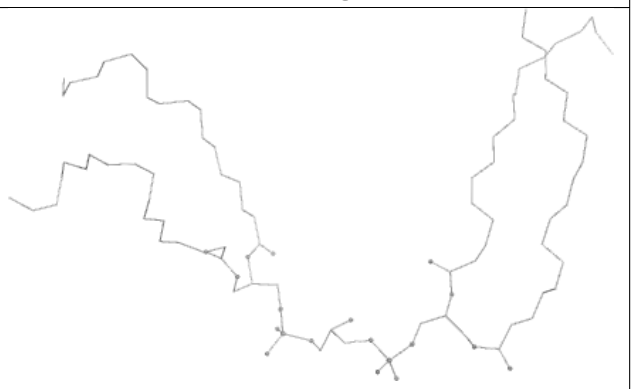
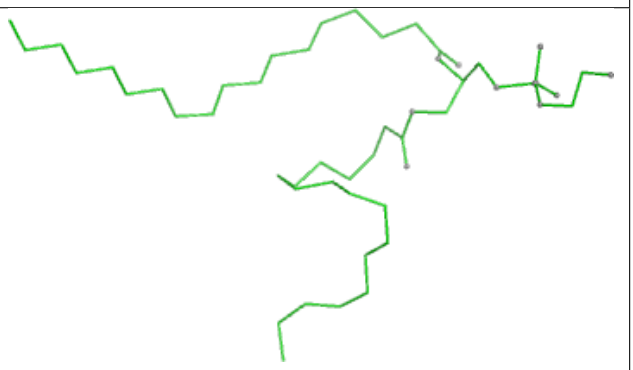


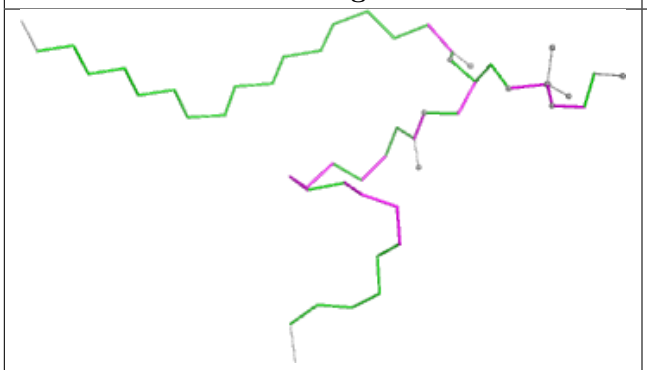
Rings

Ligand 3PE Di 1102

Bond lengths



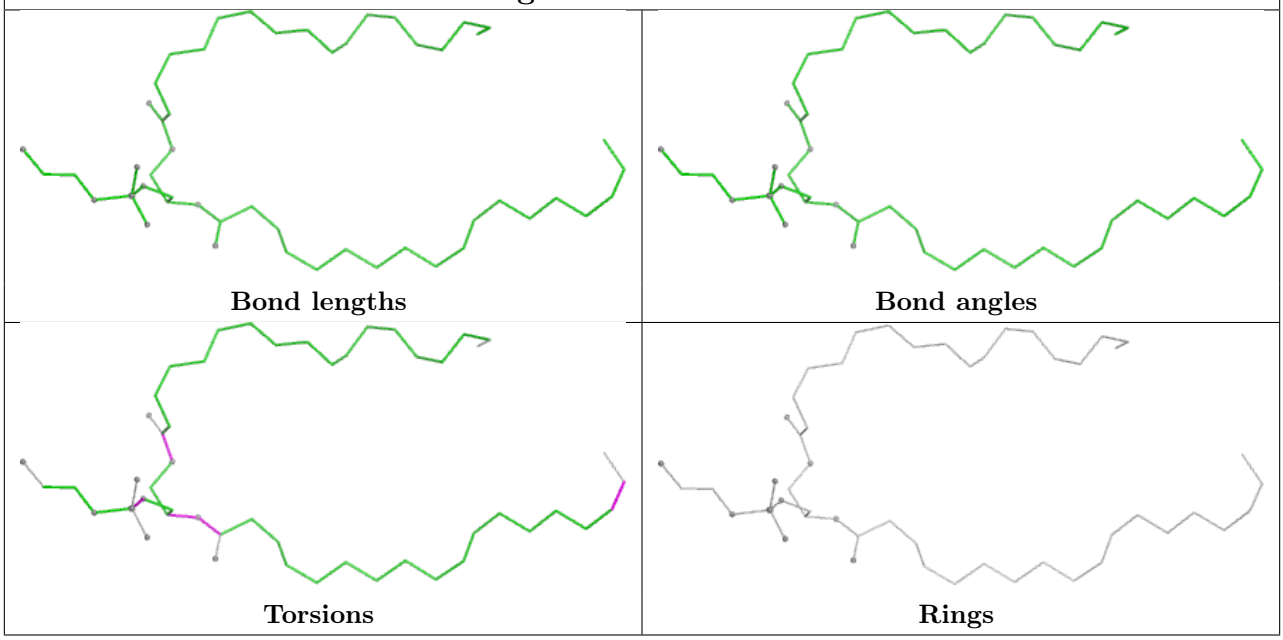
Bond angles



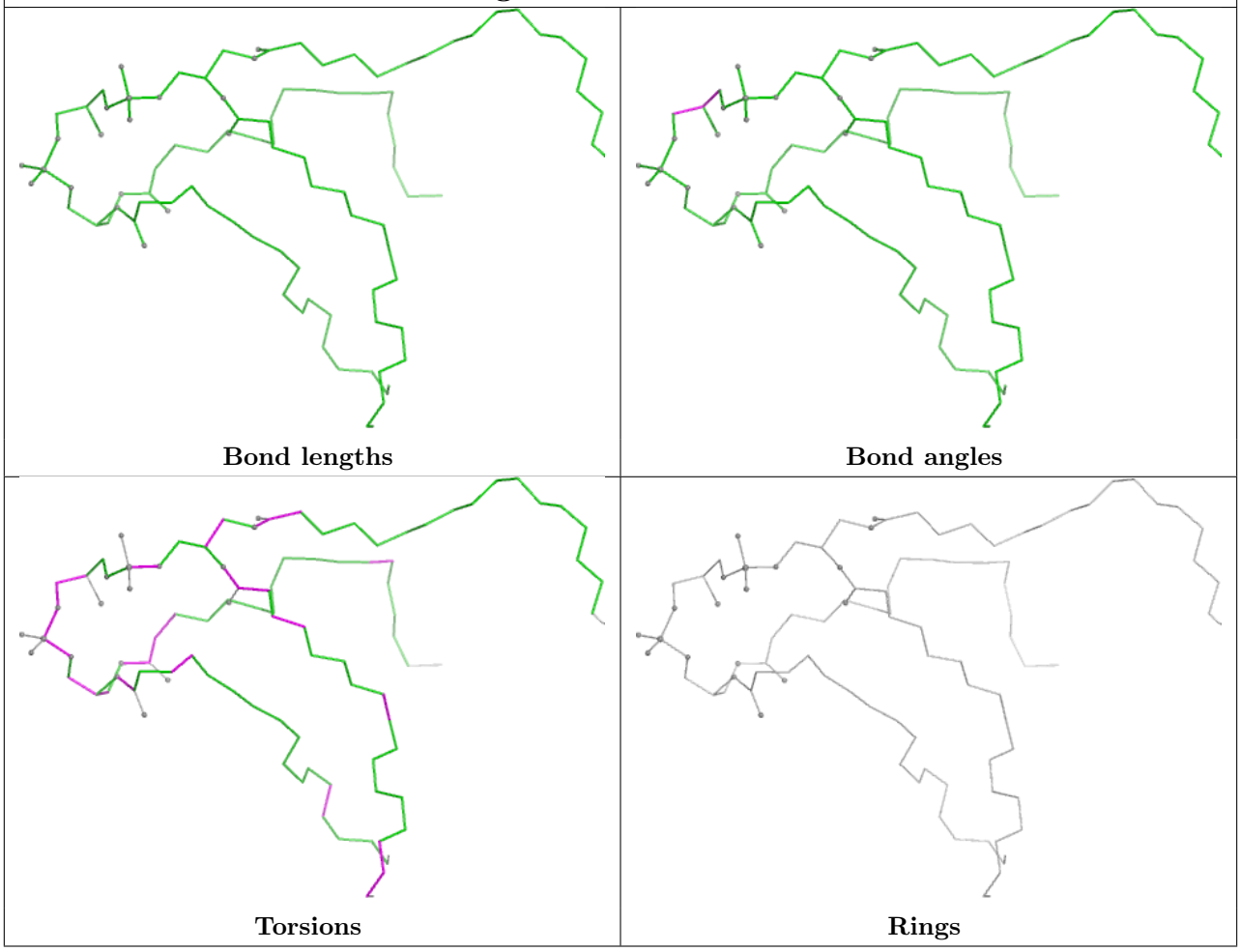
Torsions

Rings

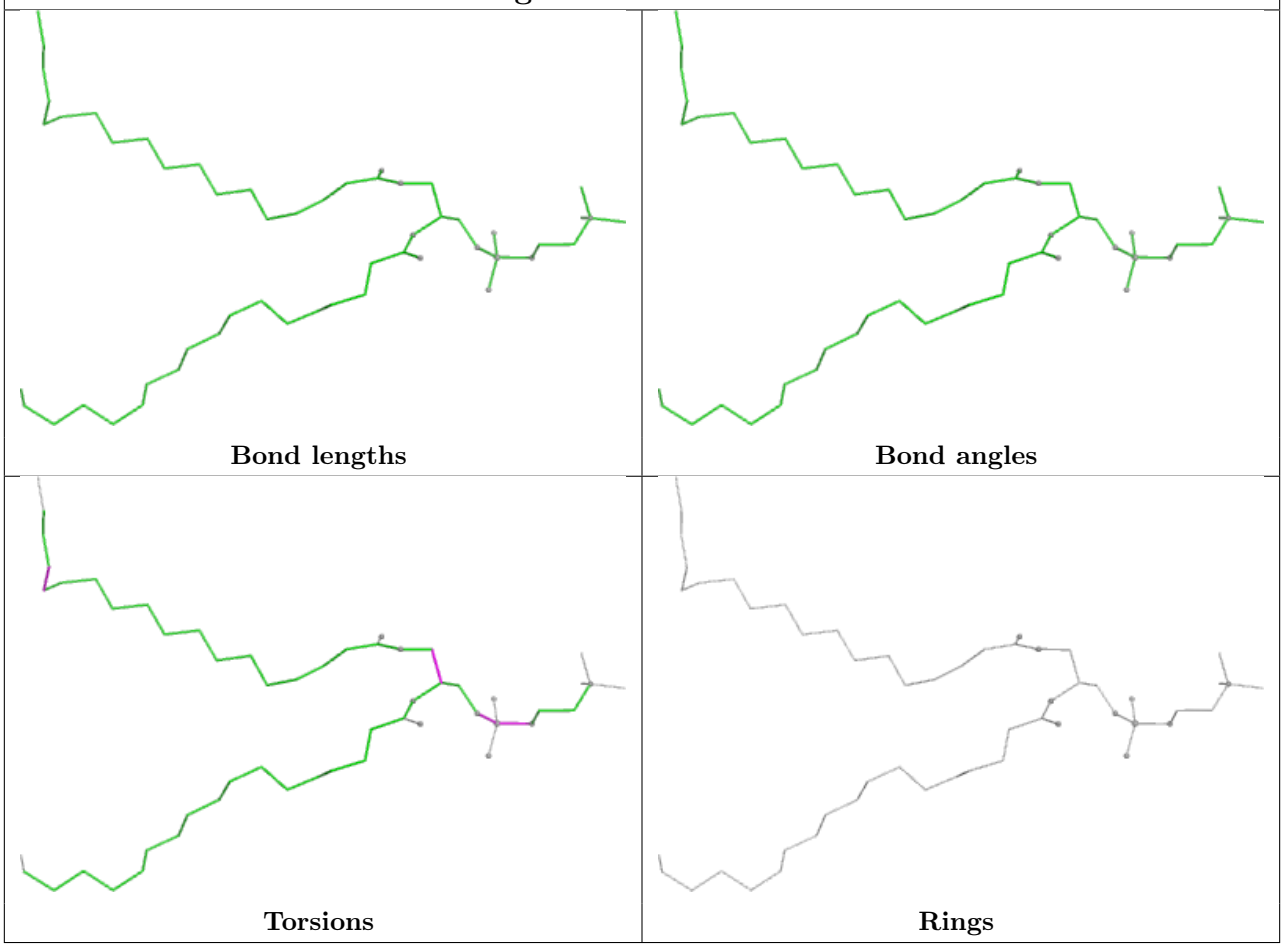
Ligand 3PE EO 203



Ligand CDL ED 605



Ligand PC1 DV 406



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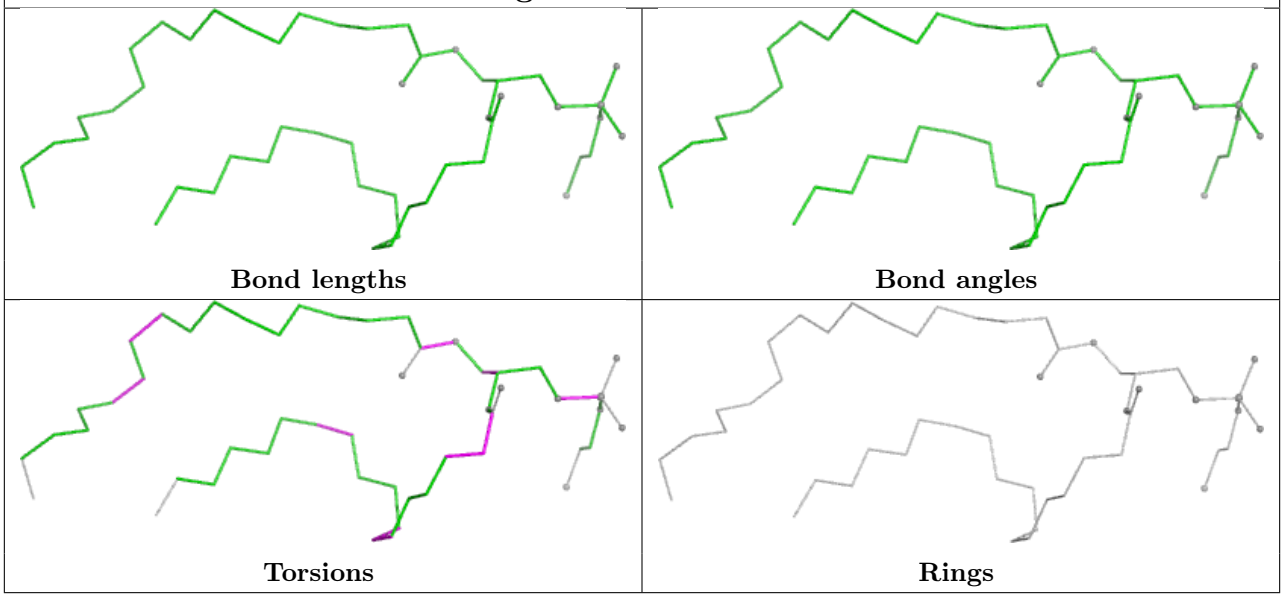

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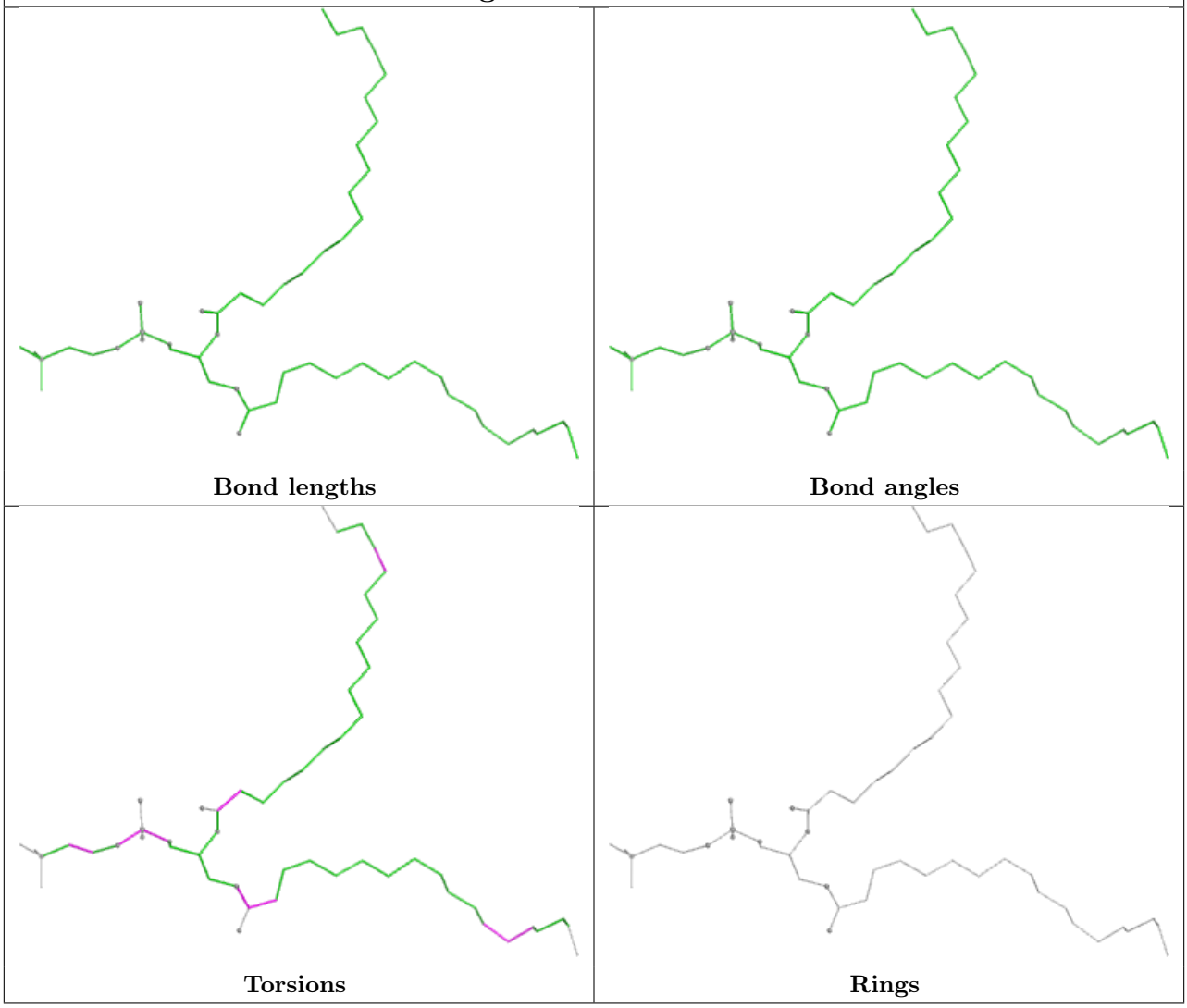
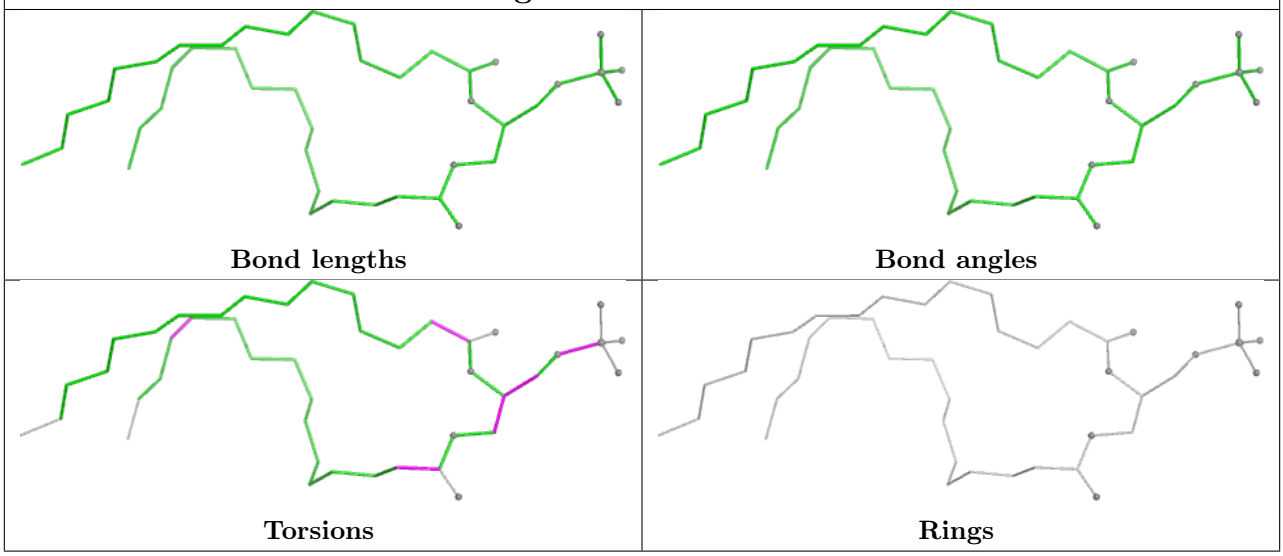


Ligand LPP AC 803



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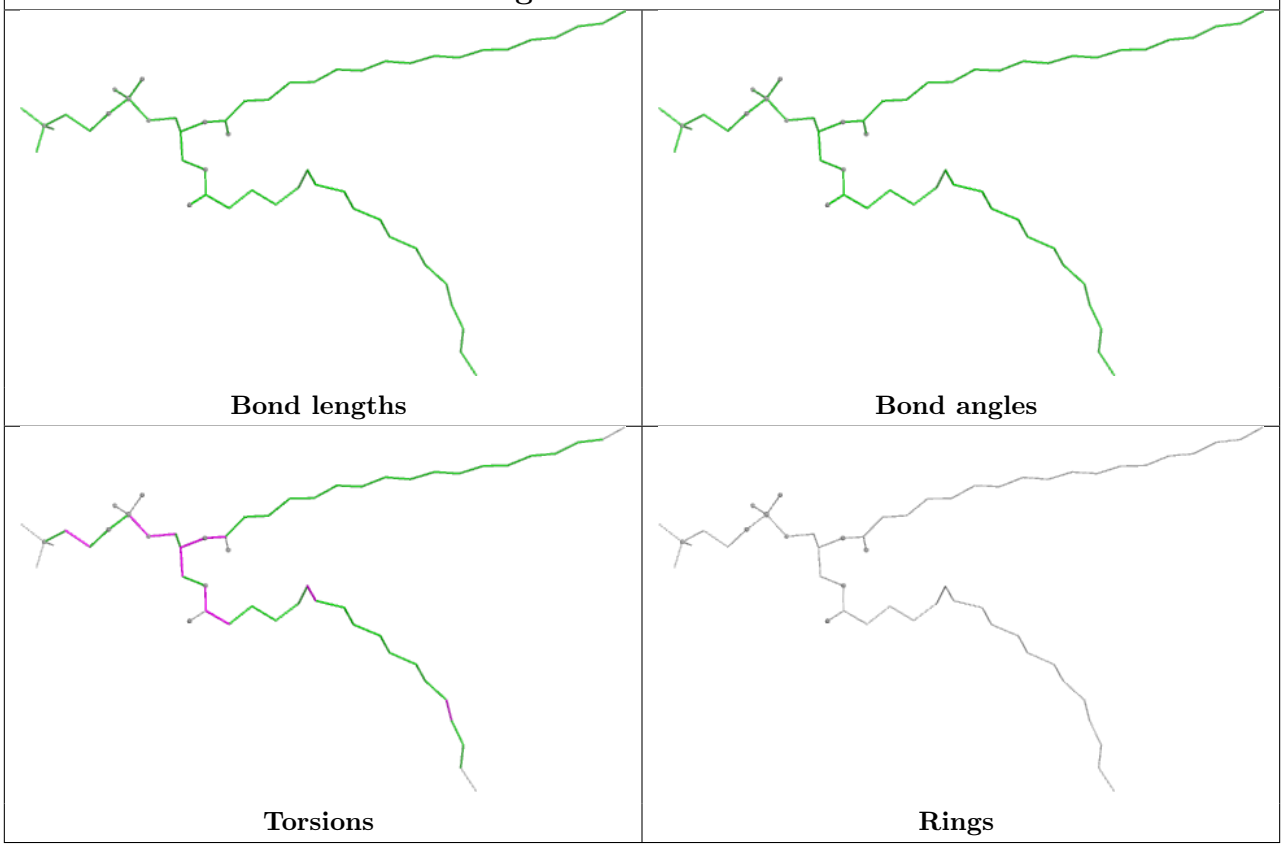

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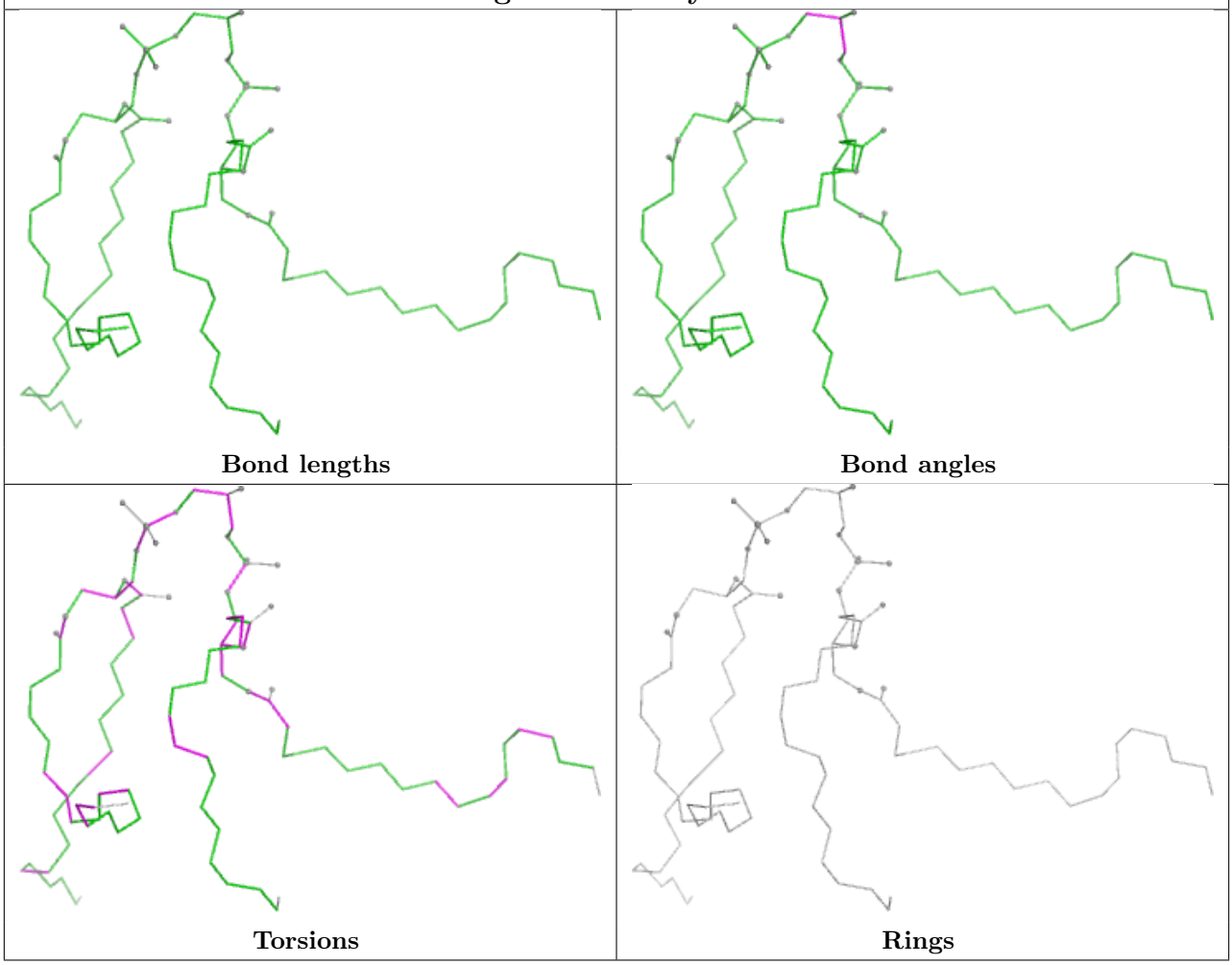

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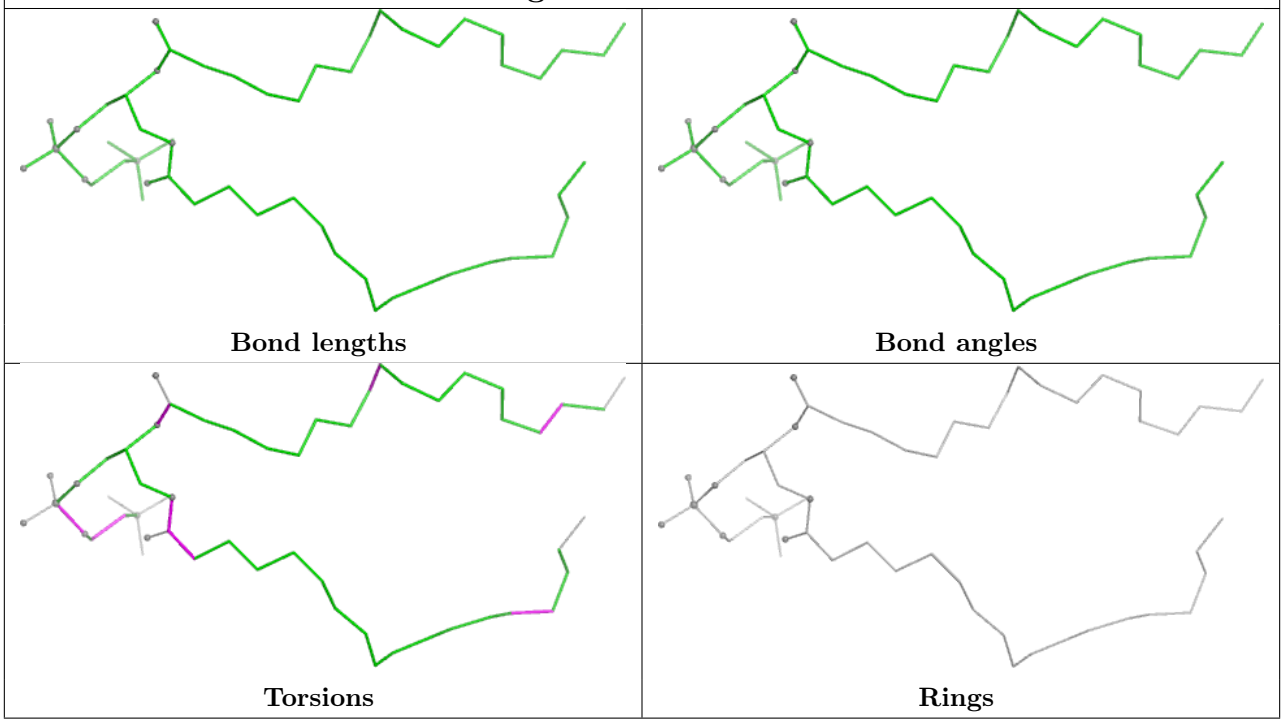

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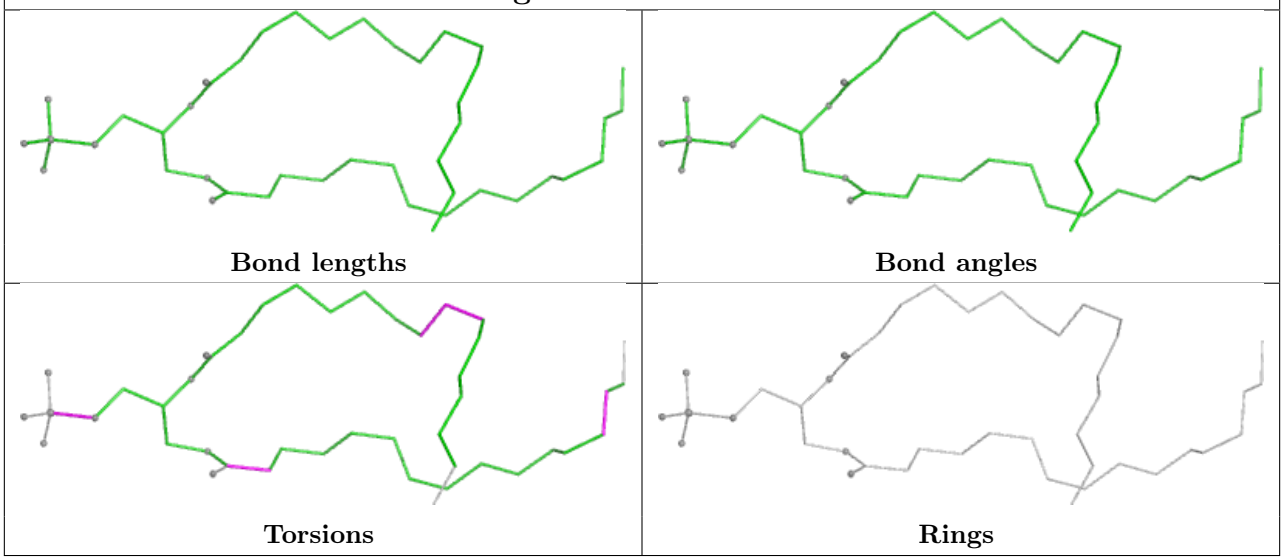

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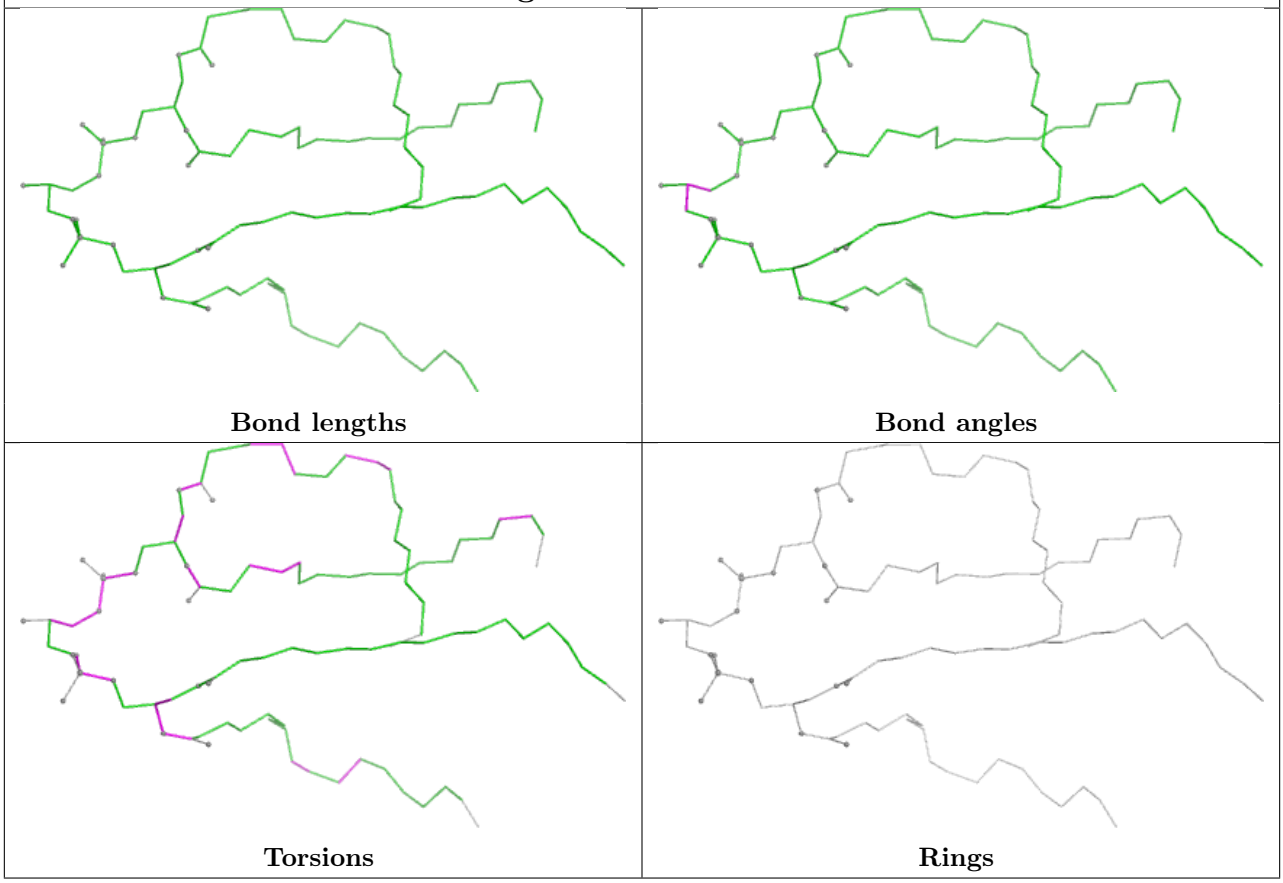

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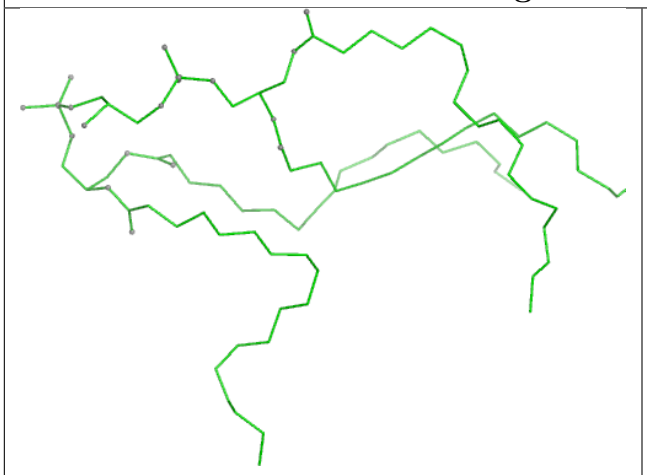
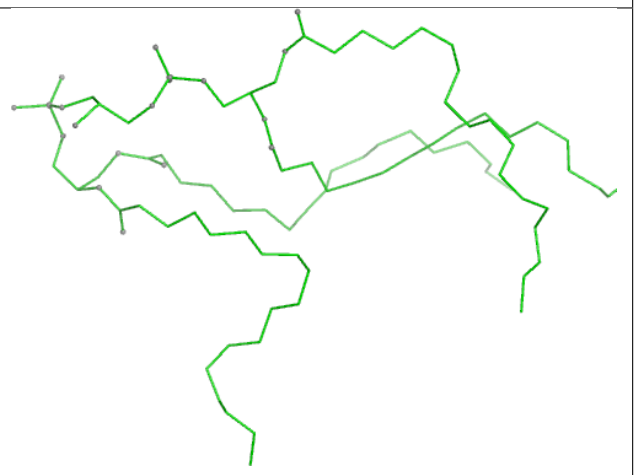
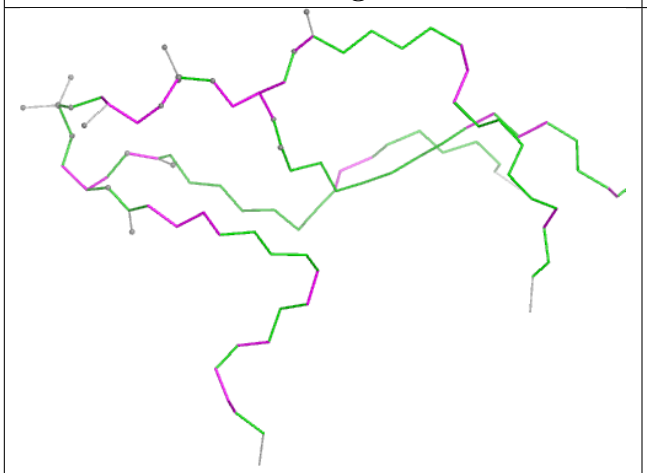


Bond lengths



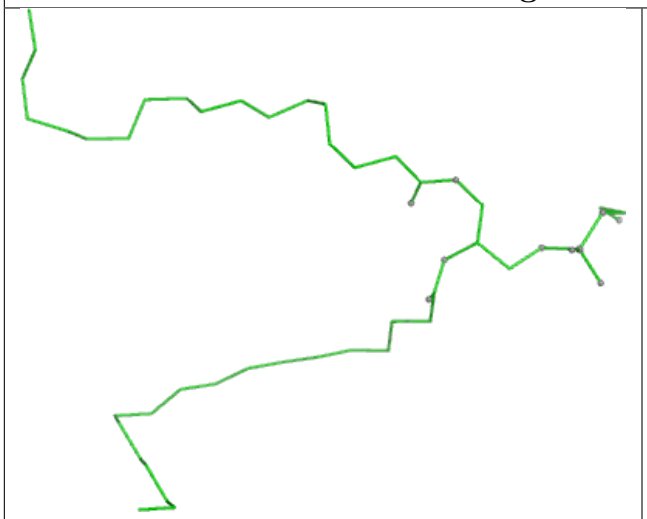
Bond angles



Torsions

Rings

Ligand 3PE Dg 204



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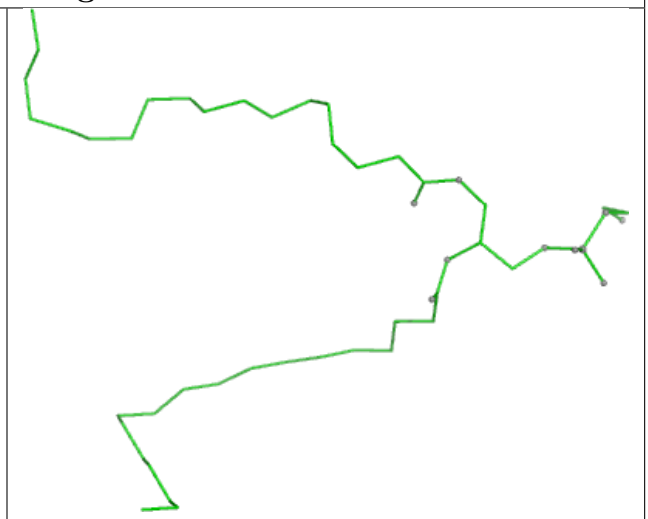
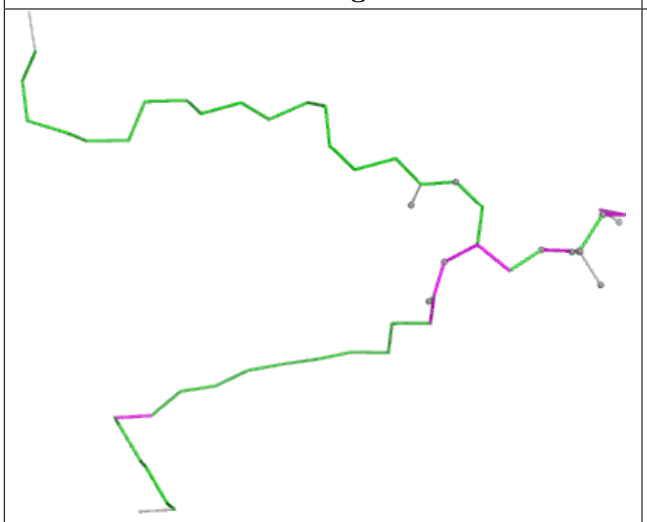
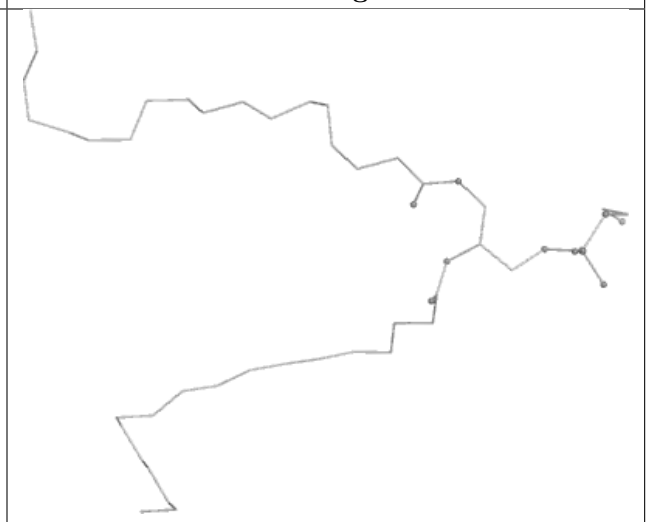


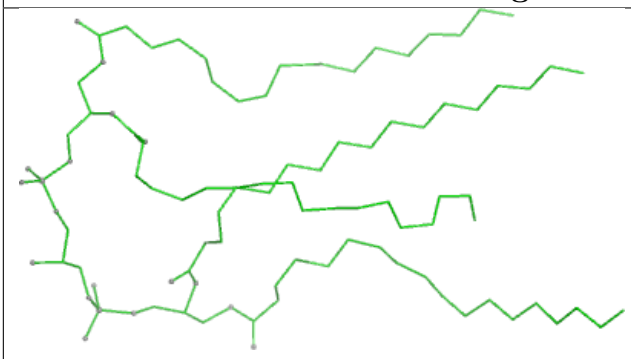
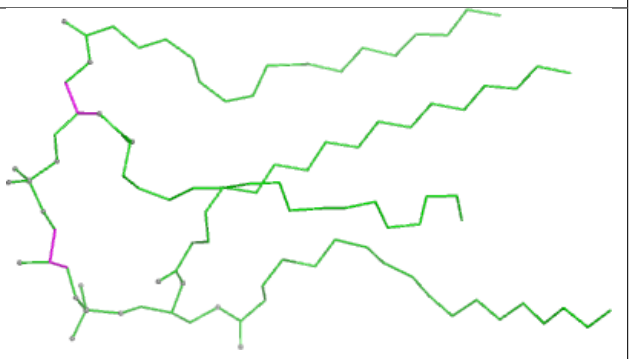
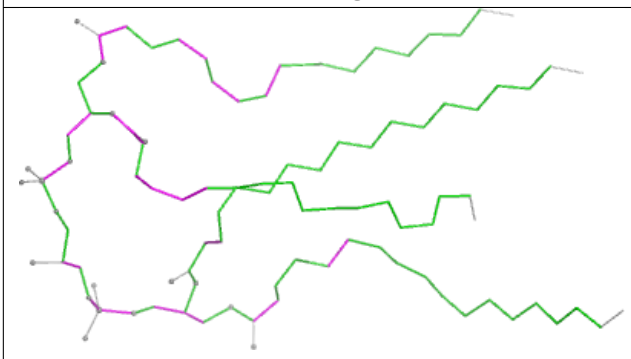
Bond angles



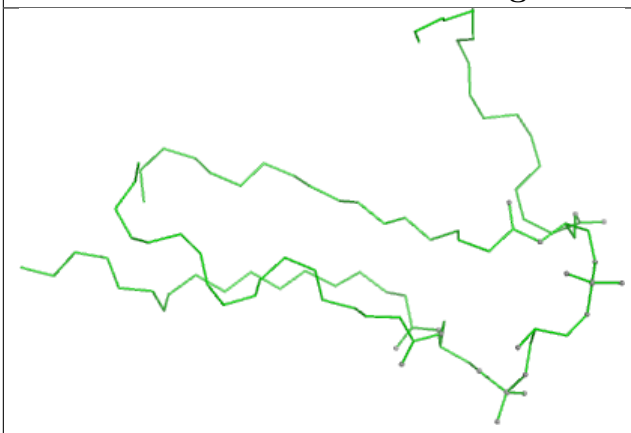
Torsions



Rings

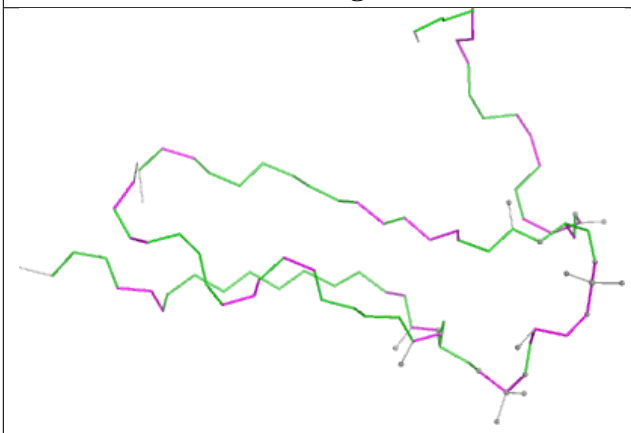
Ligand CDL BC 302	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL DH 202



Bond lengths

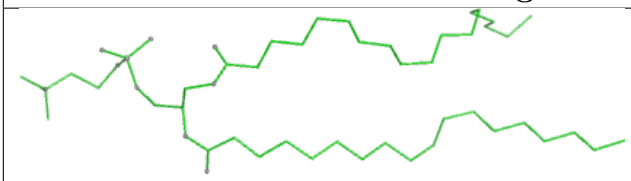
Bond angles



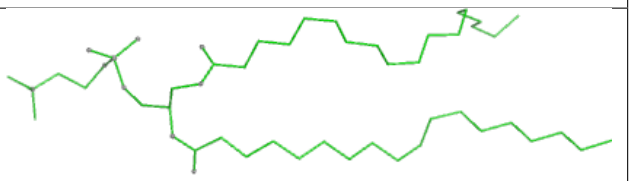
Torsions

Rings

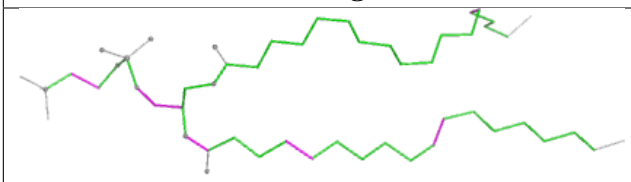
Ligand PC1 AL 303



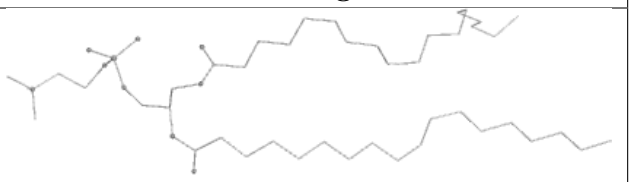
Bond lengths



Bond angles

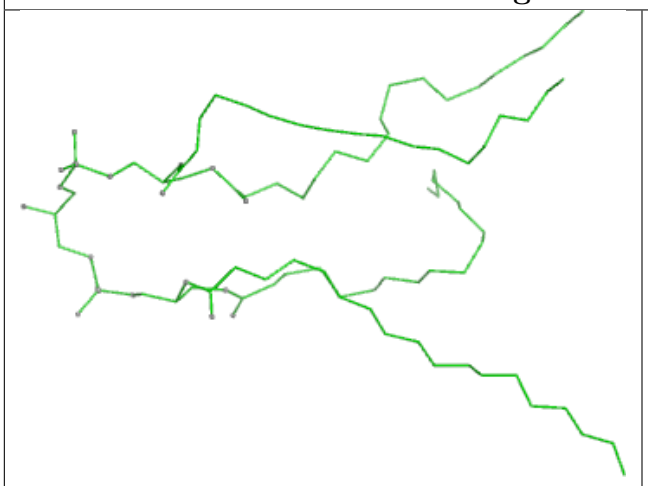


Torsions

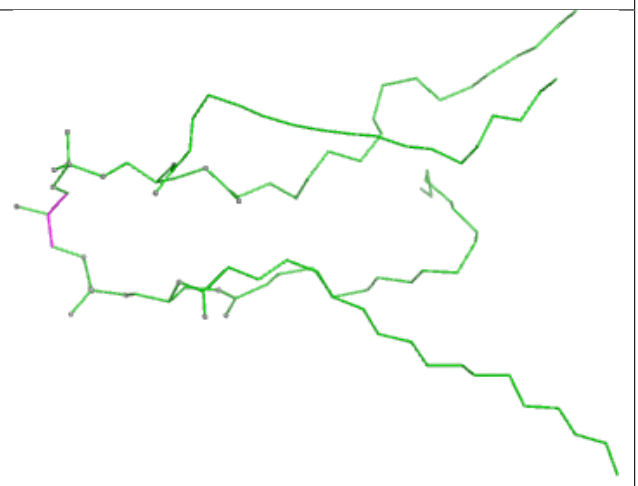


Rings

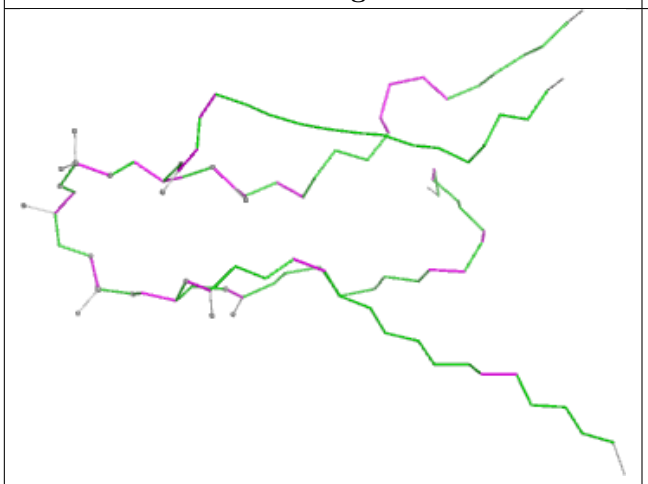
Ligand CDL AF 402



Bond lengths



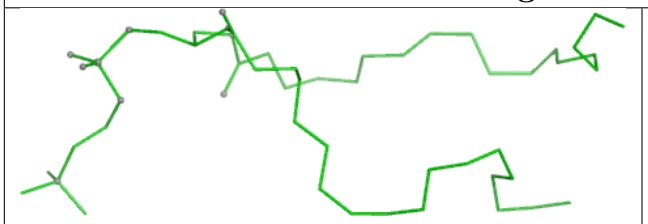
Bond angles



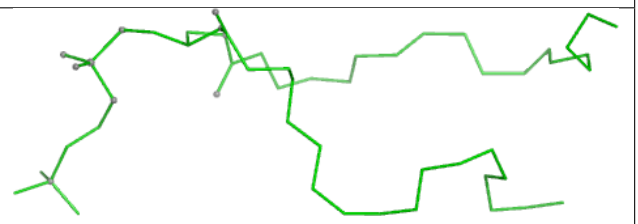
Torsions

Rings

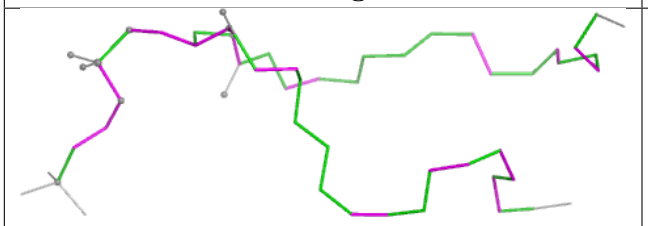
Ligand PC1 Db 702



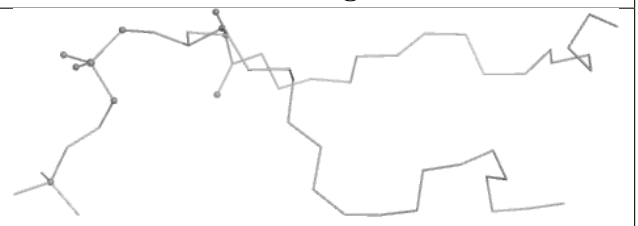
Bond lengths



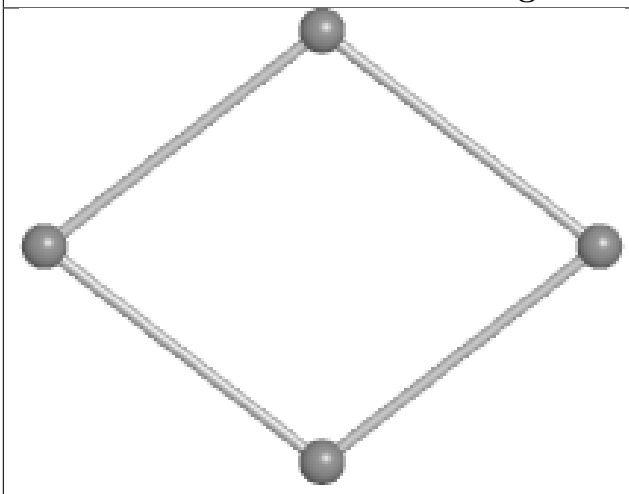
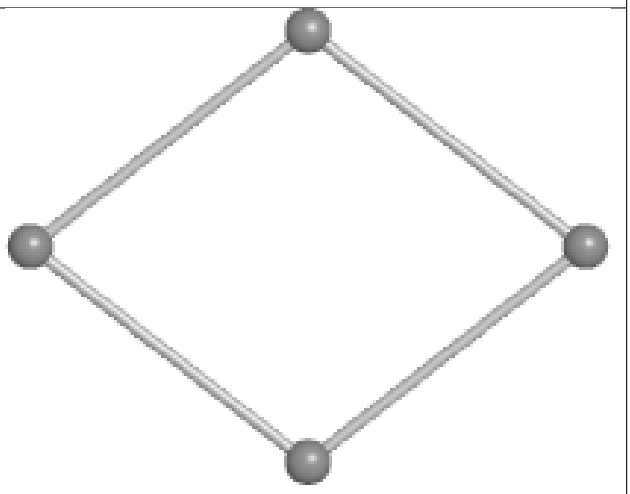
Bond angles



Torsions



Rings

Ligand FES EF 202	
	
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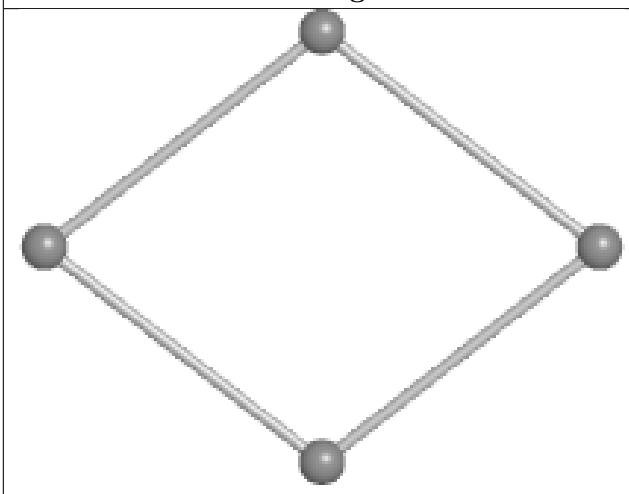
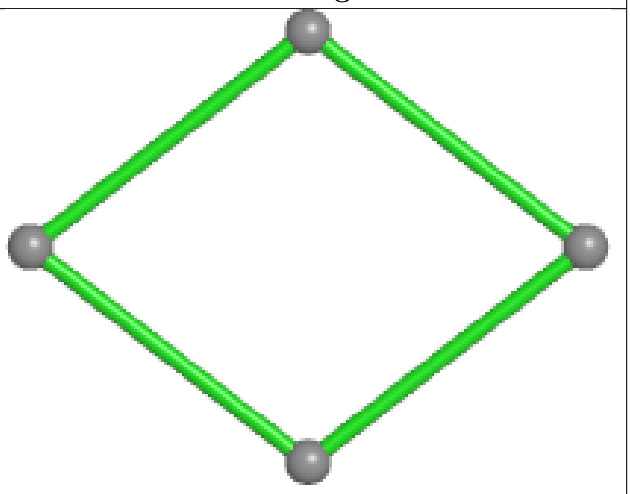
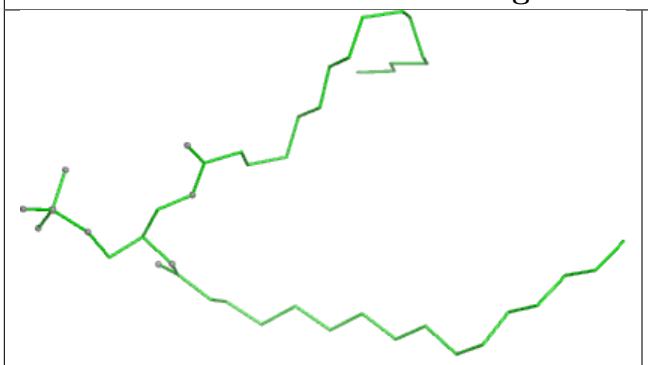
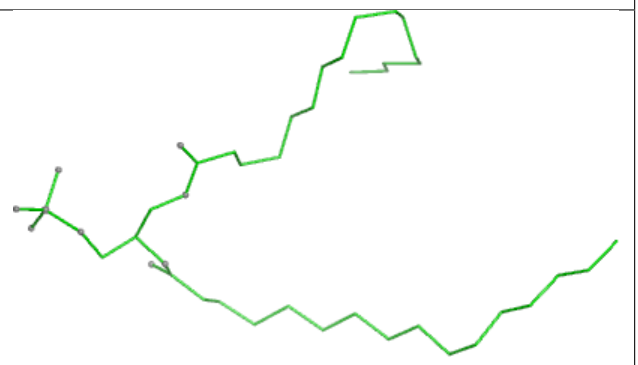
	
Torsions	**Rings**

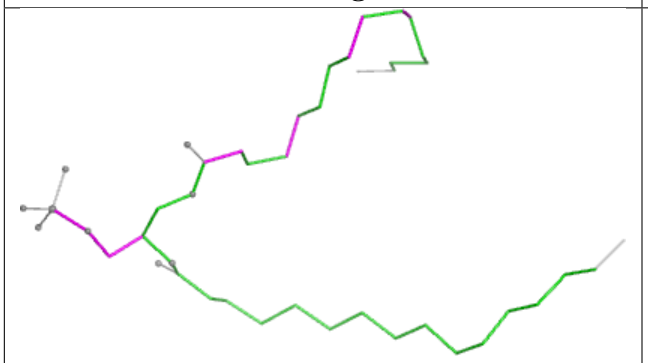
Ligand LPP DN 504



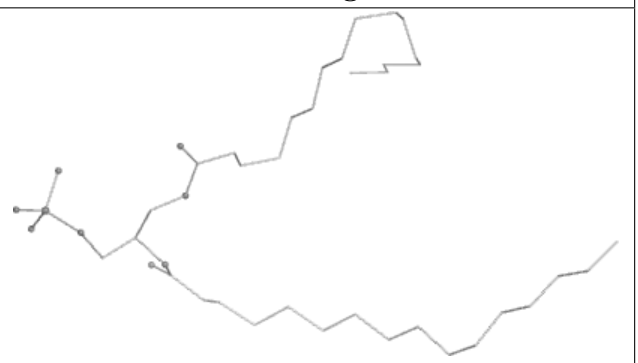
Bond lengths



Bond angles

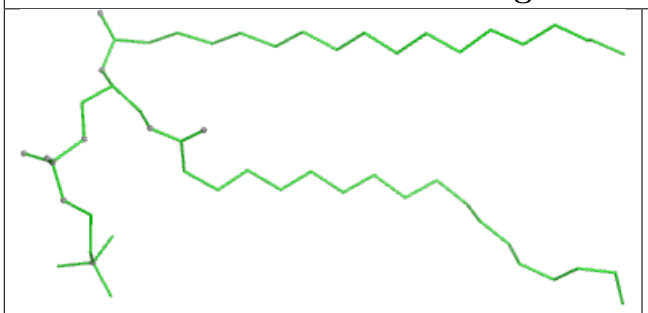


Torsions



Rings

Ligand PC1 AA 904



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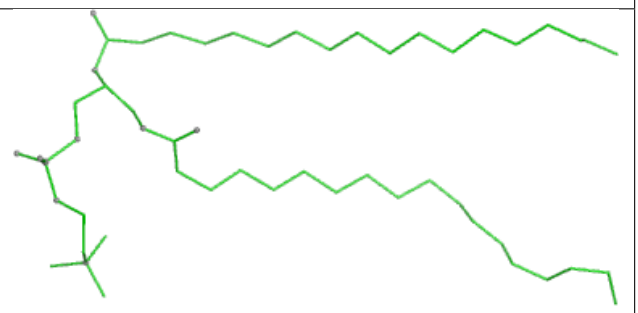
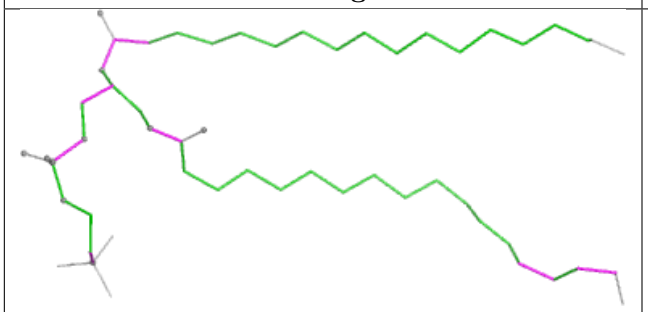


Bond angles



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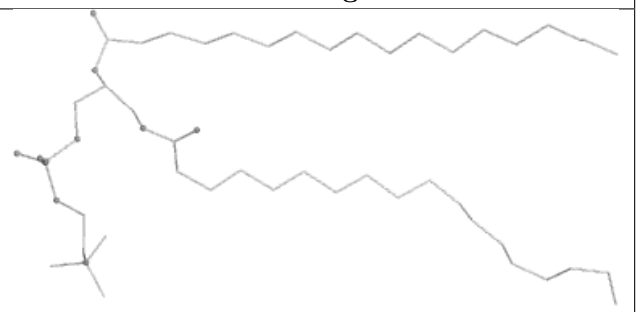
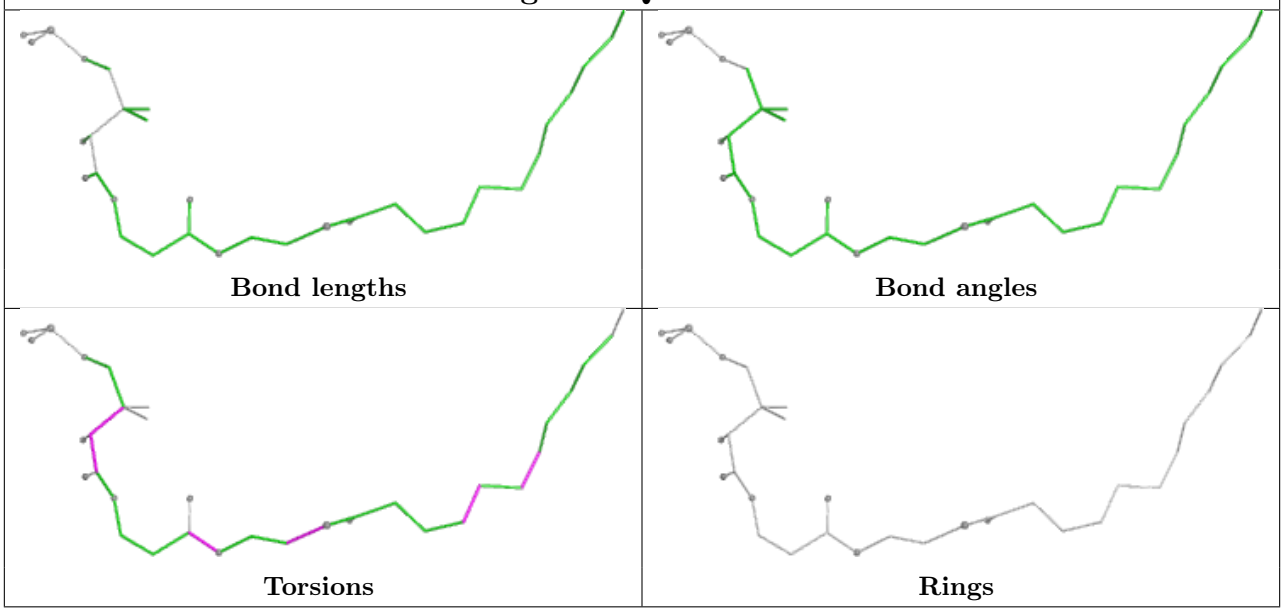
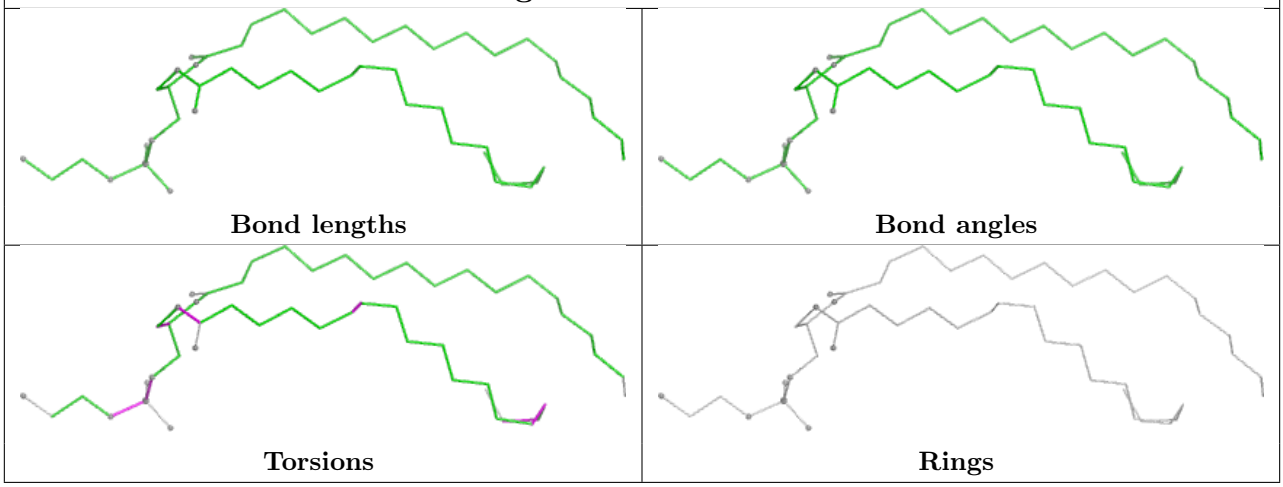


Rings

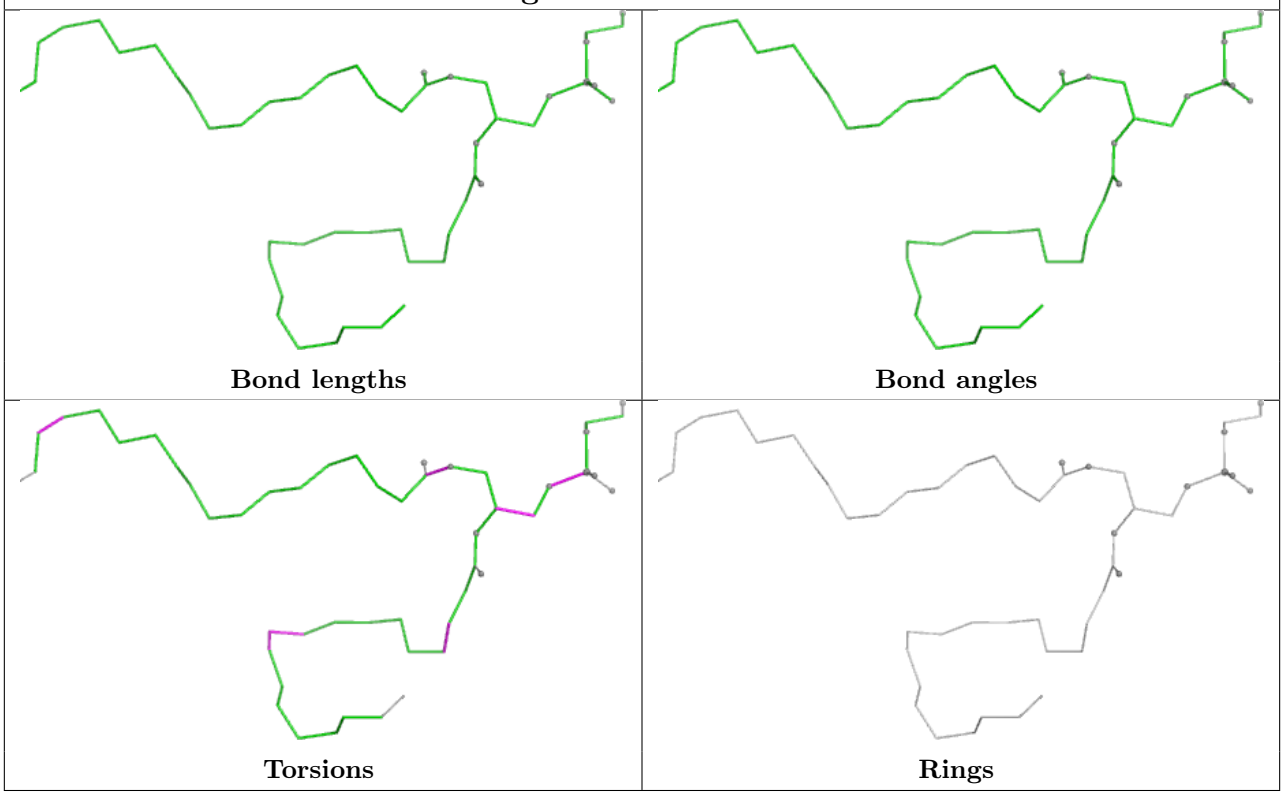
Ligand 8Q1 AS 200



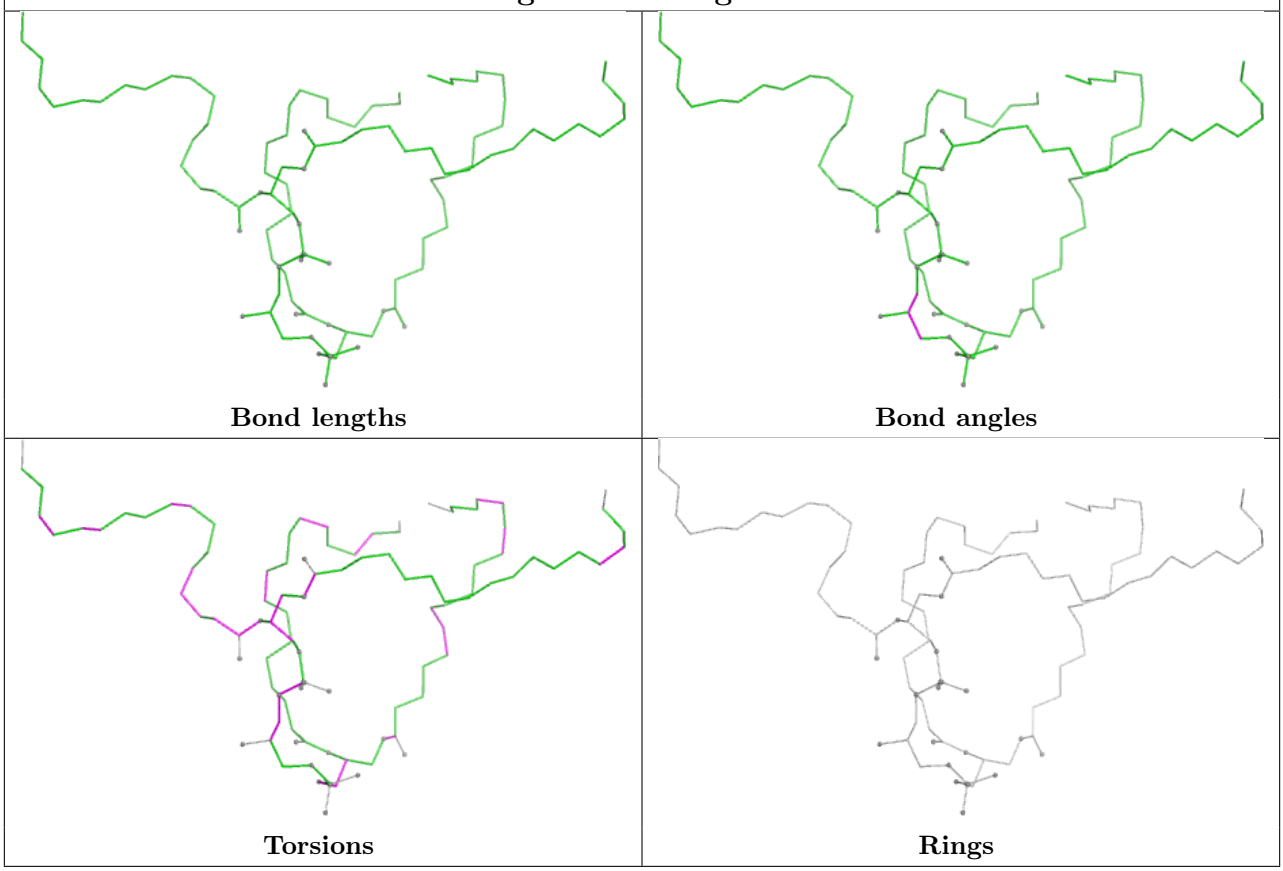
Ligand 3PE DR 401

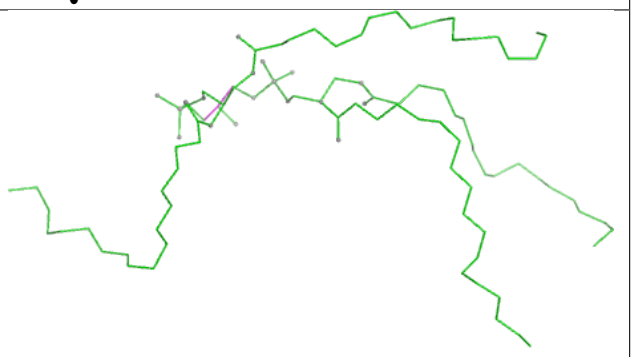
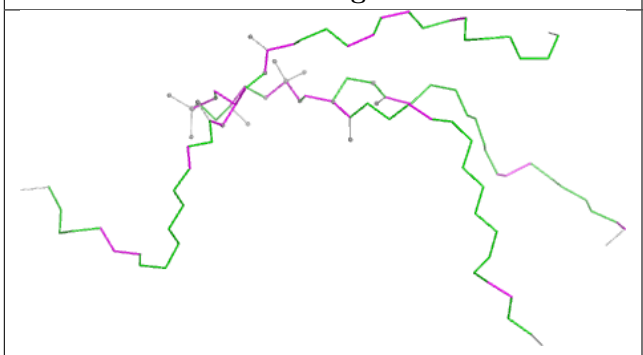


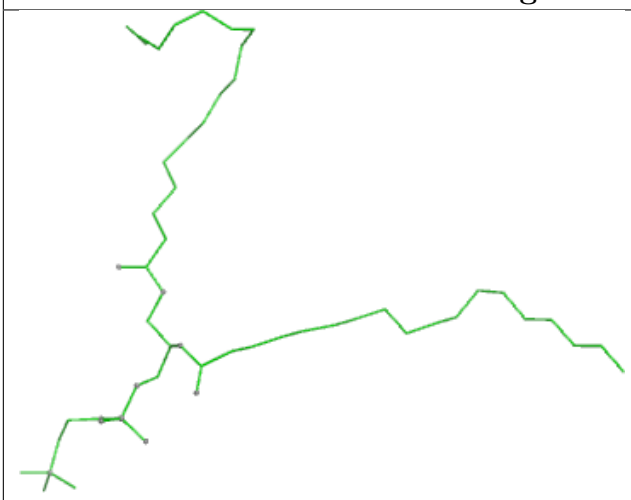
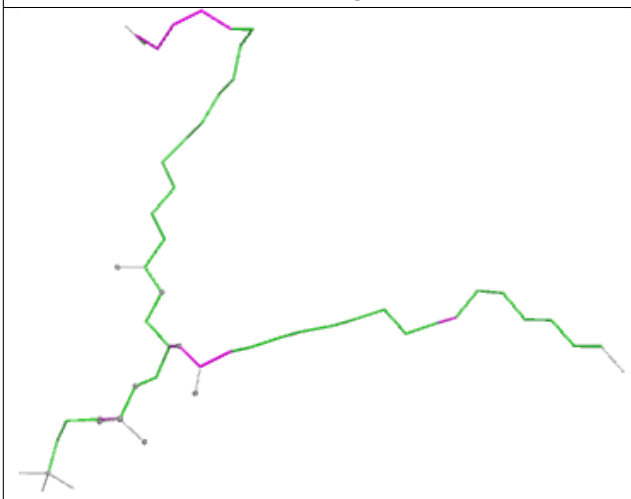
Ligand 3PE Dr 404



Ligand CDL Eg 101



Ligand CDL DQ 1502	
Bond lengths	 Bond angles
 Torsions	Rings

Ligand PC1 Eo 205	
 Bond lengths	Bond angles
 Torsions	Rings

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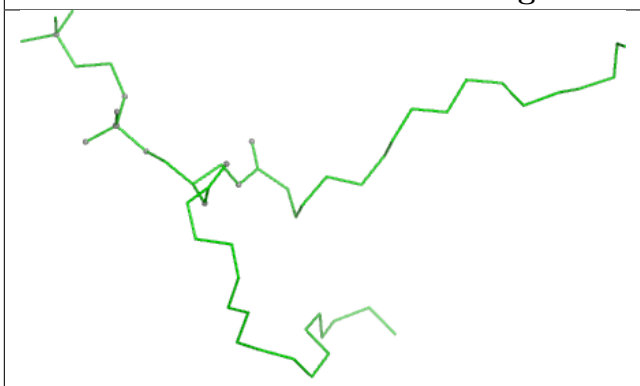
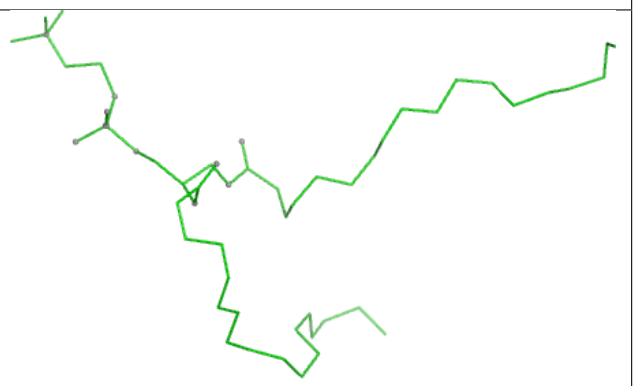
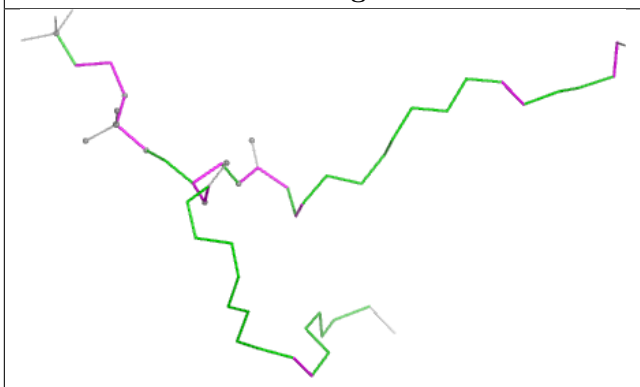
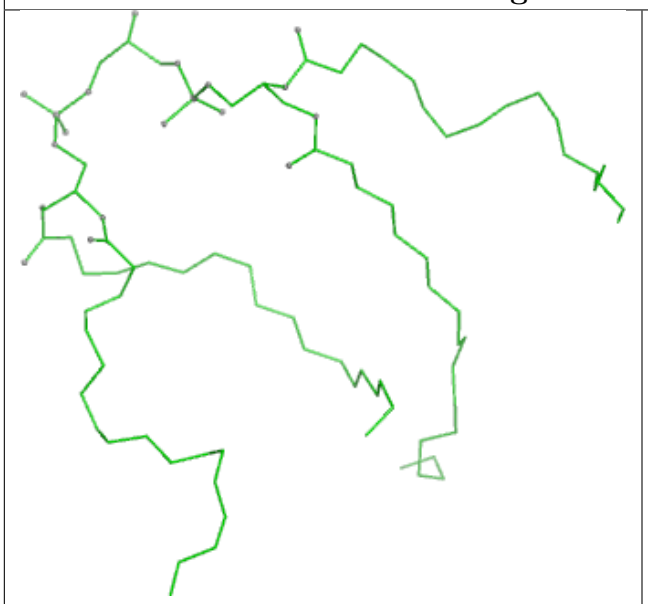
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL DH 201



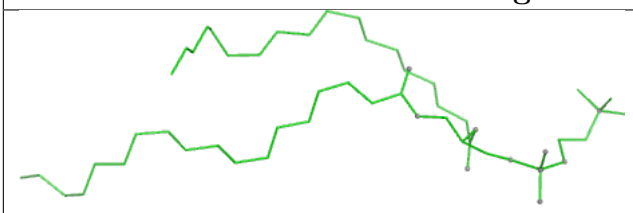
Bond lengths

Bond angles

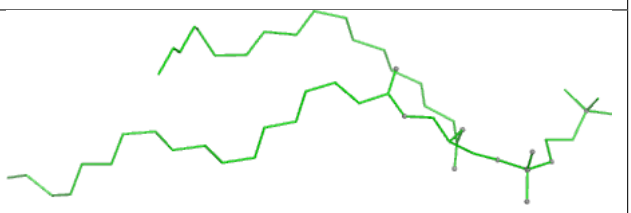
Torsions

Rings

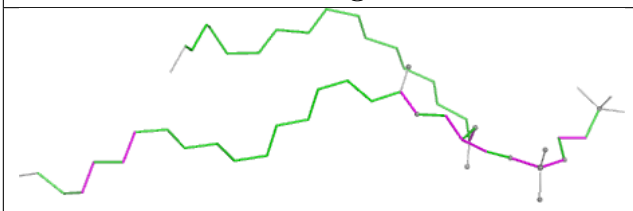
Ligand PC1 AA 905



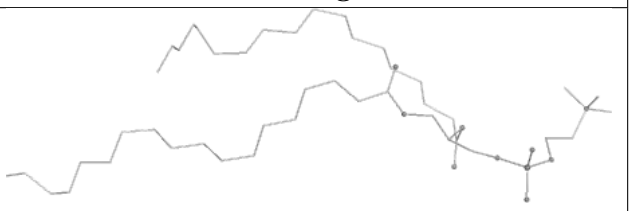
Bond lengths



Bond angles

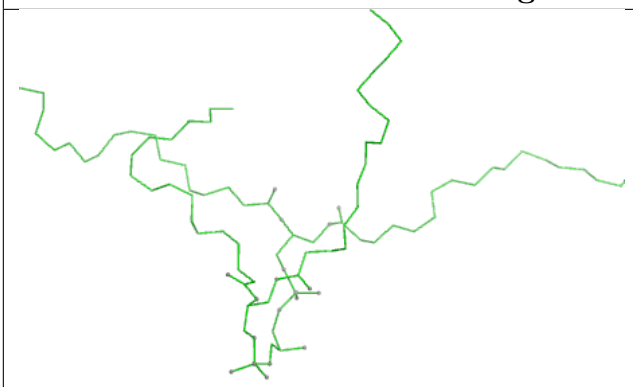


Torsions

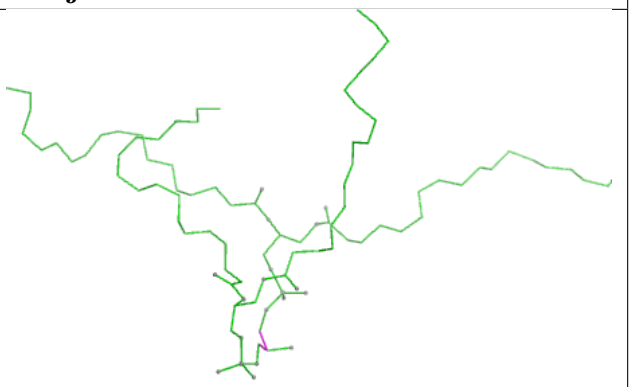


Rings

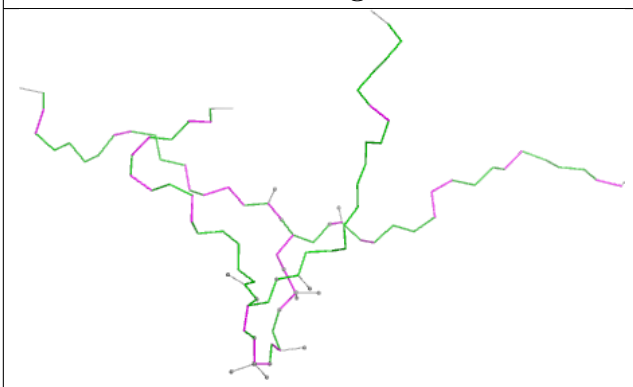
Ligand CDL Dj 403



Bond lengths

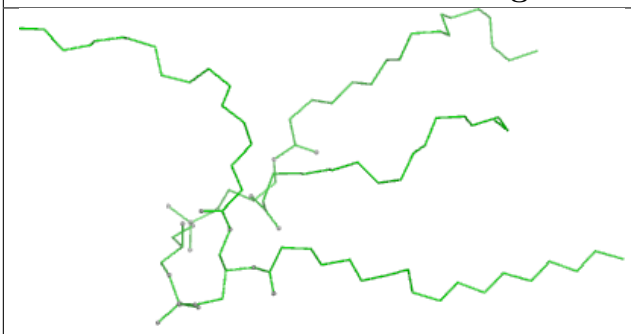
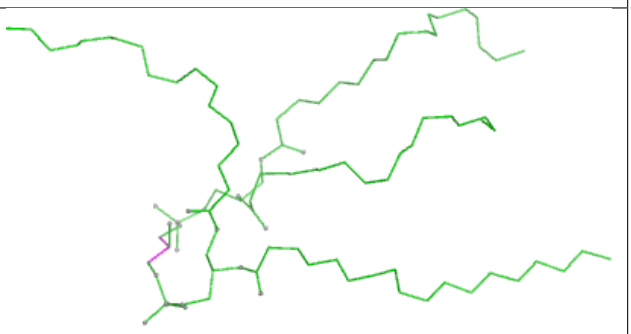
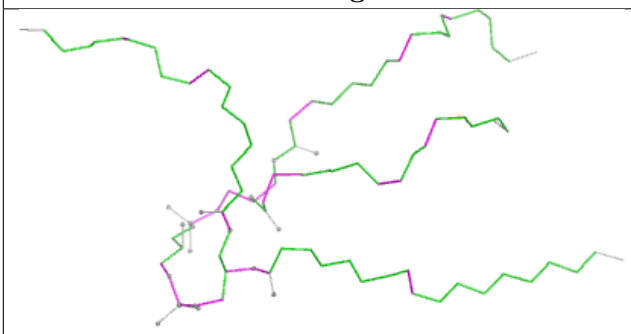


Bond angles

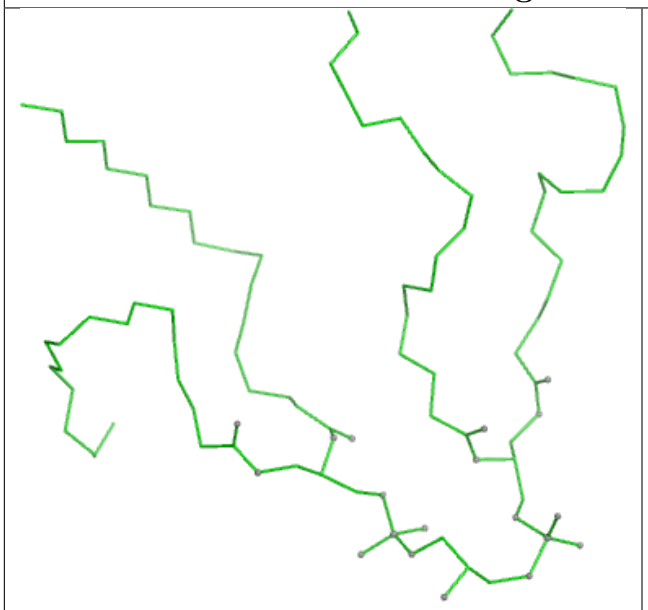


Torsions

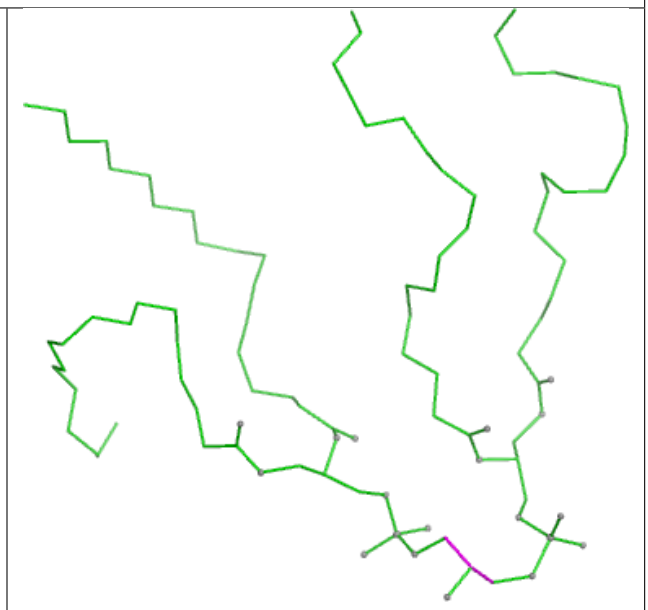
Rings

Ligand CDL BY 201	
 Bond lengths	 Bond angles
 Torsions	Rings

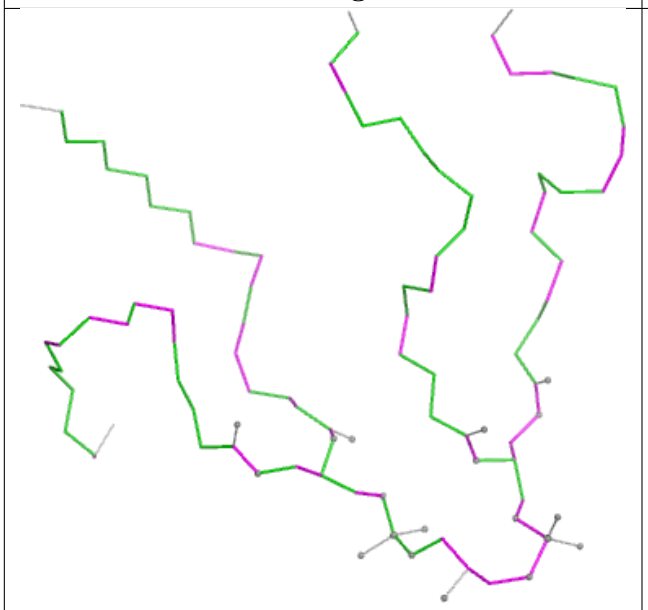
Ligand CDL EL 902



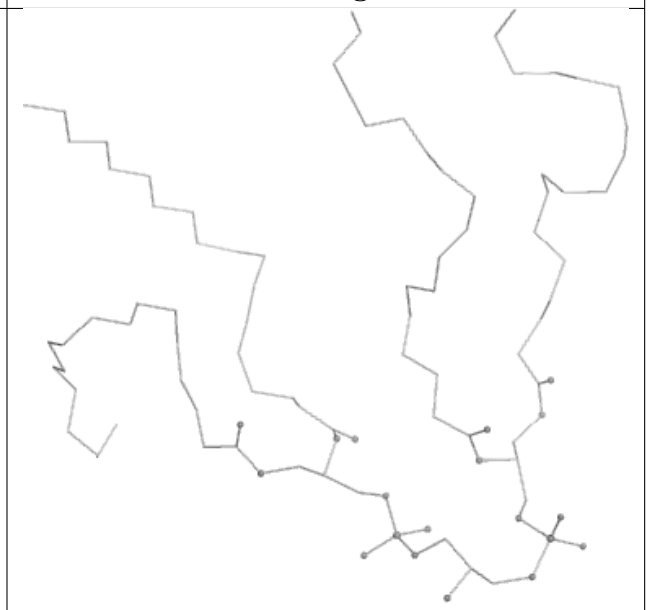
Bond lengths



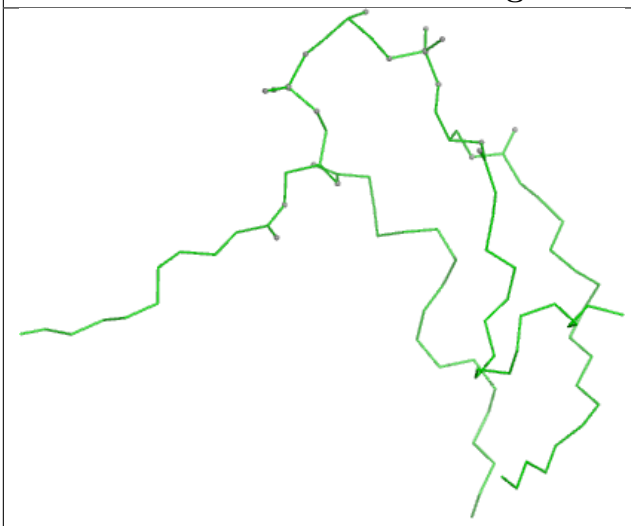
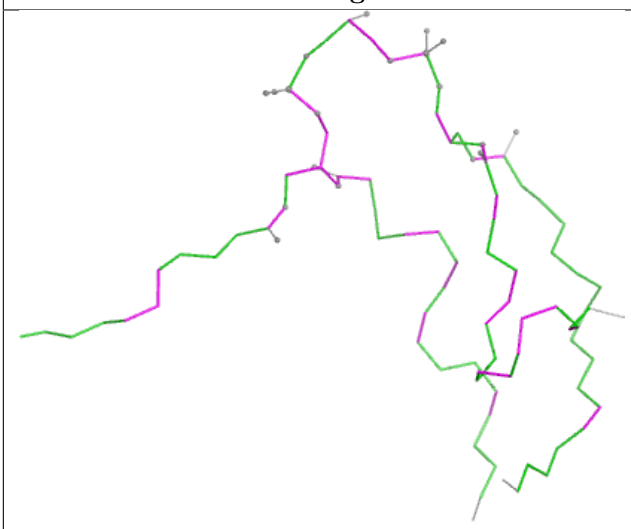
Bond angles



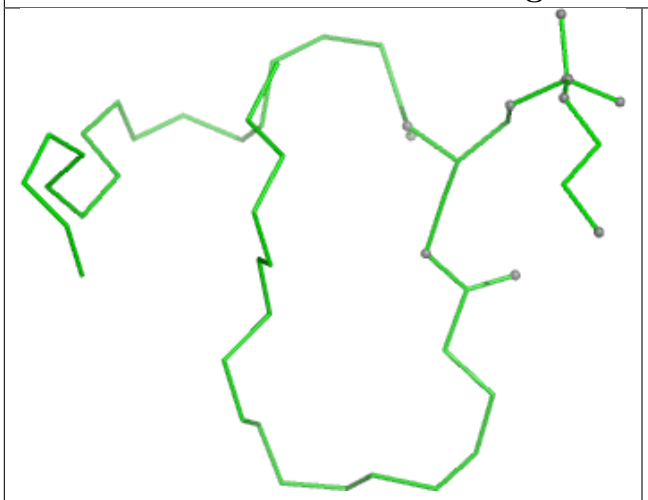
Torsions



Rings

Ligand CDL Eh 1601	
 Bond lengths	Bond angles
 Torsions	Rings

Ligand 3PE El 905



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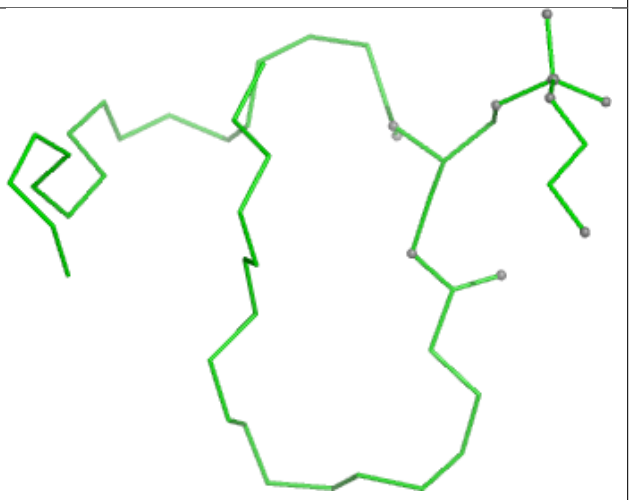
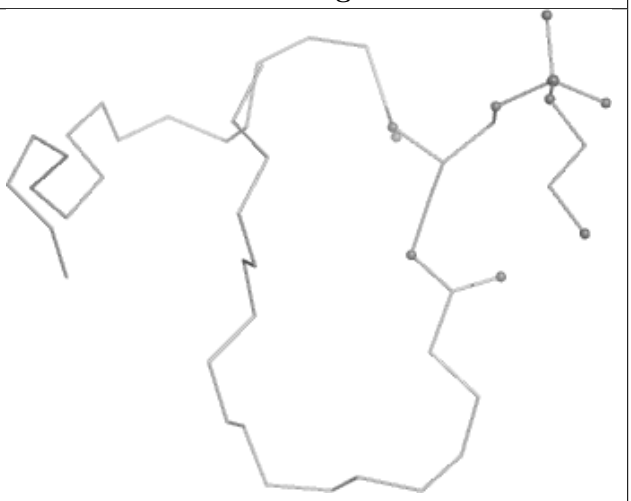


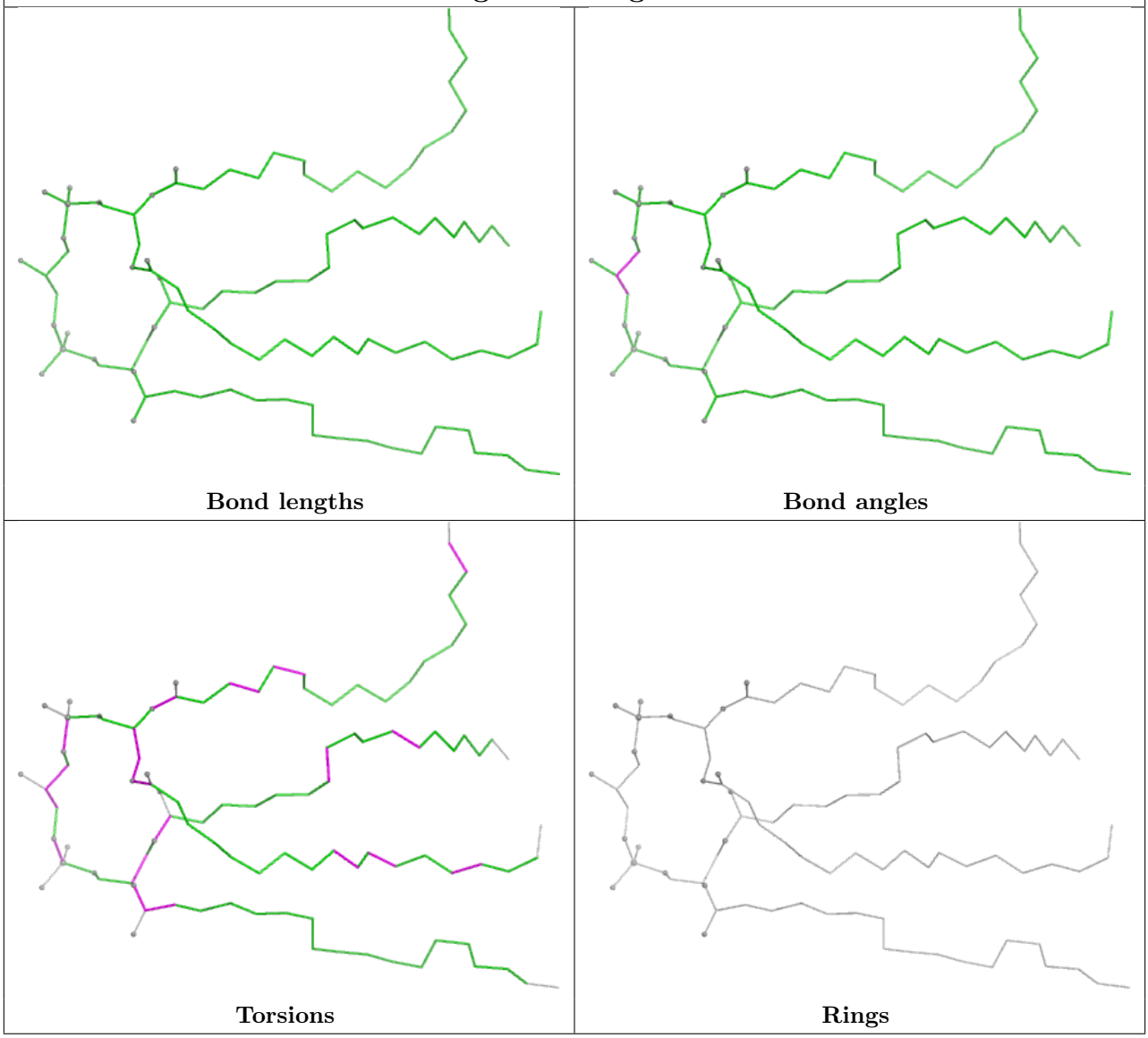
Bond angles

Torsions

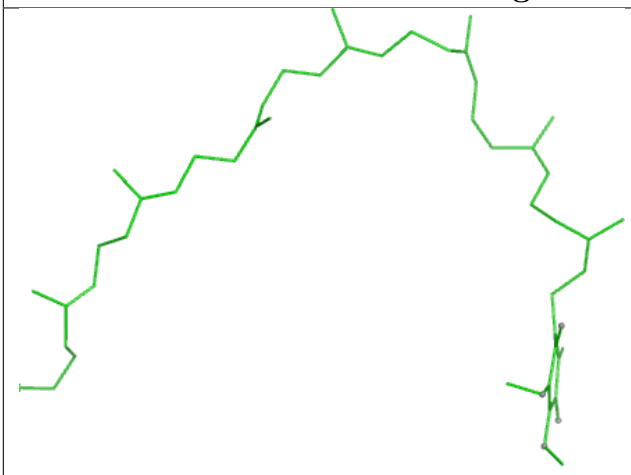


Rings

Ligand CDL g 801



Ligand UQ8 ED 603



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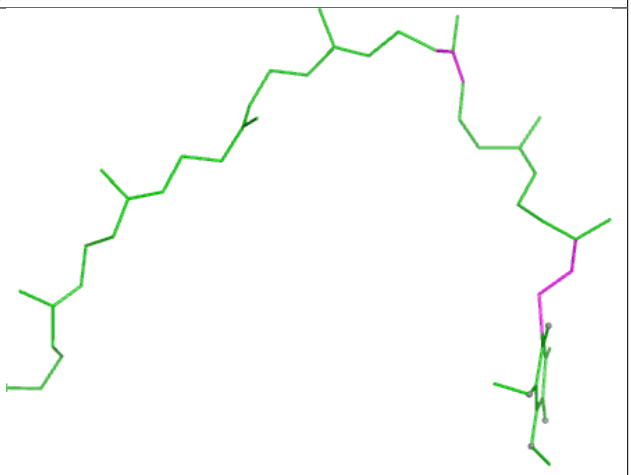
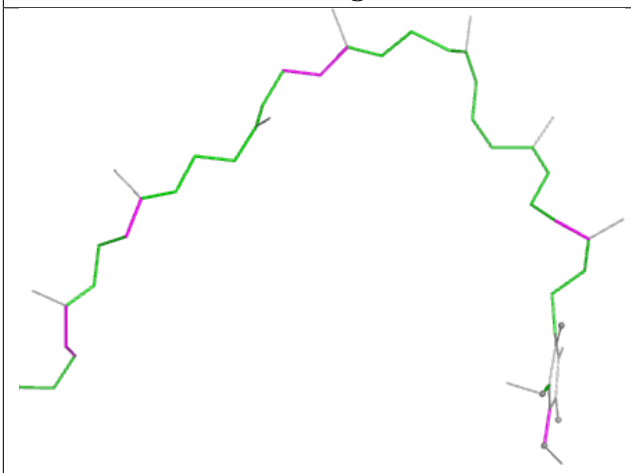


Bond angles



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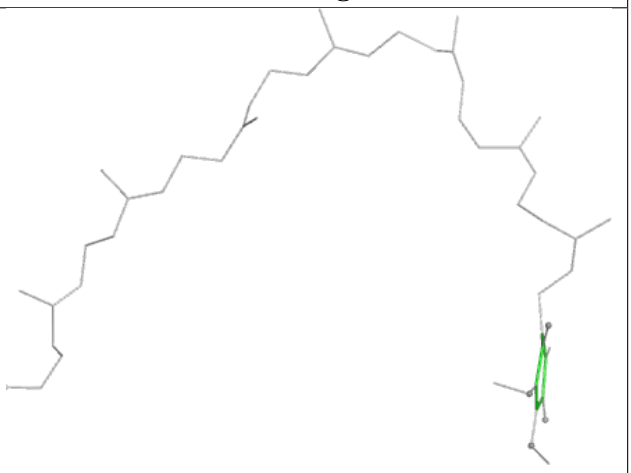
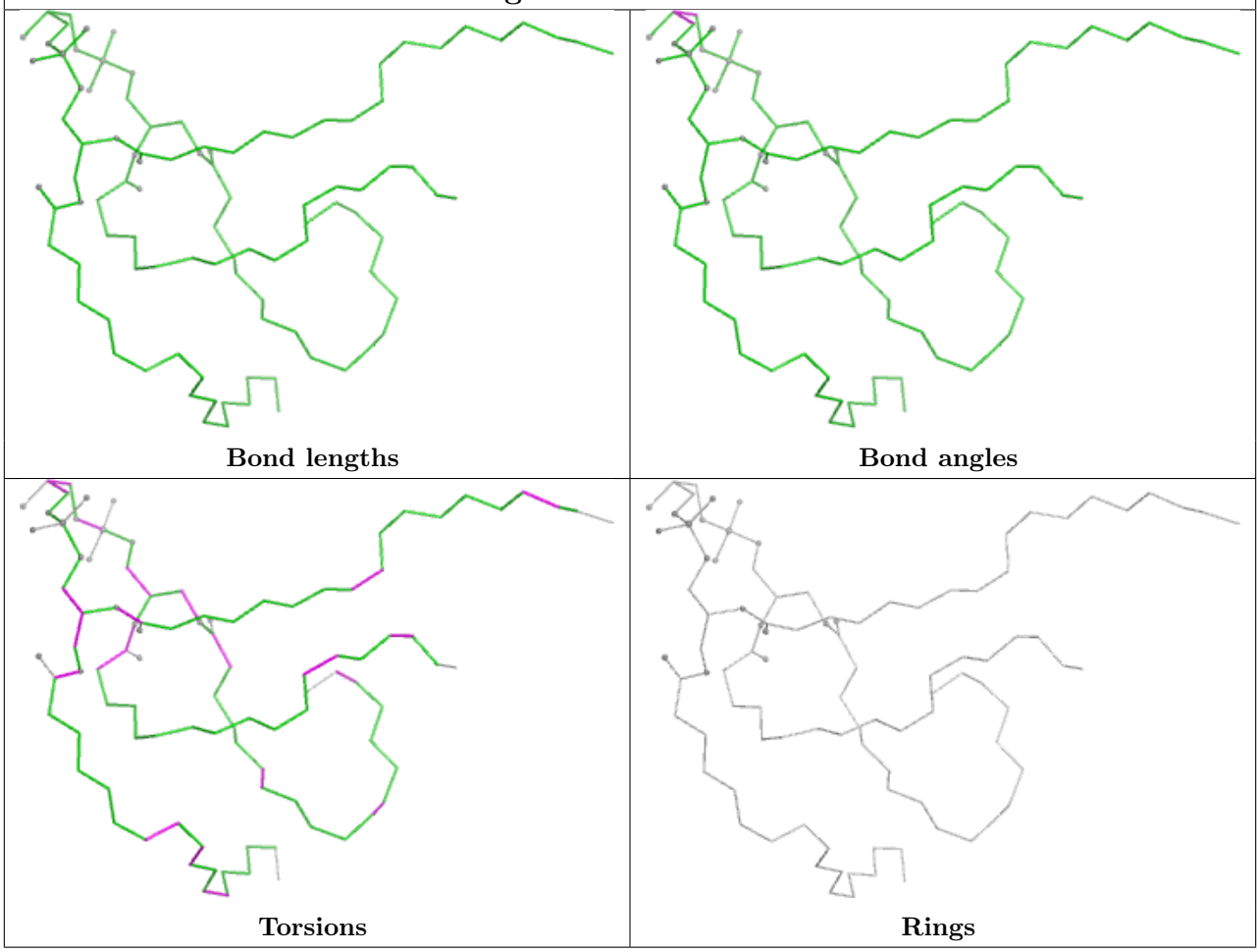
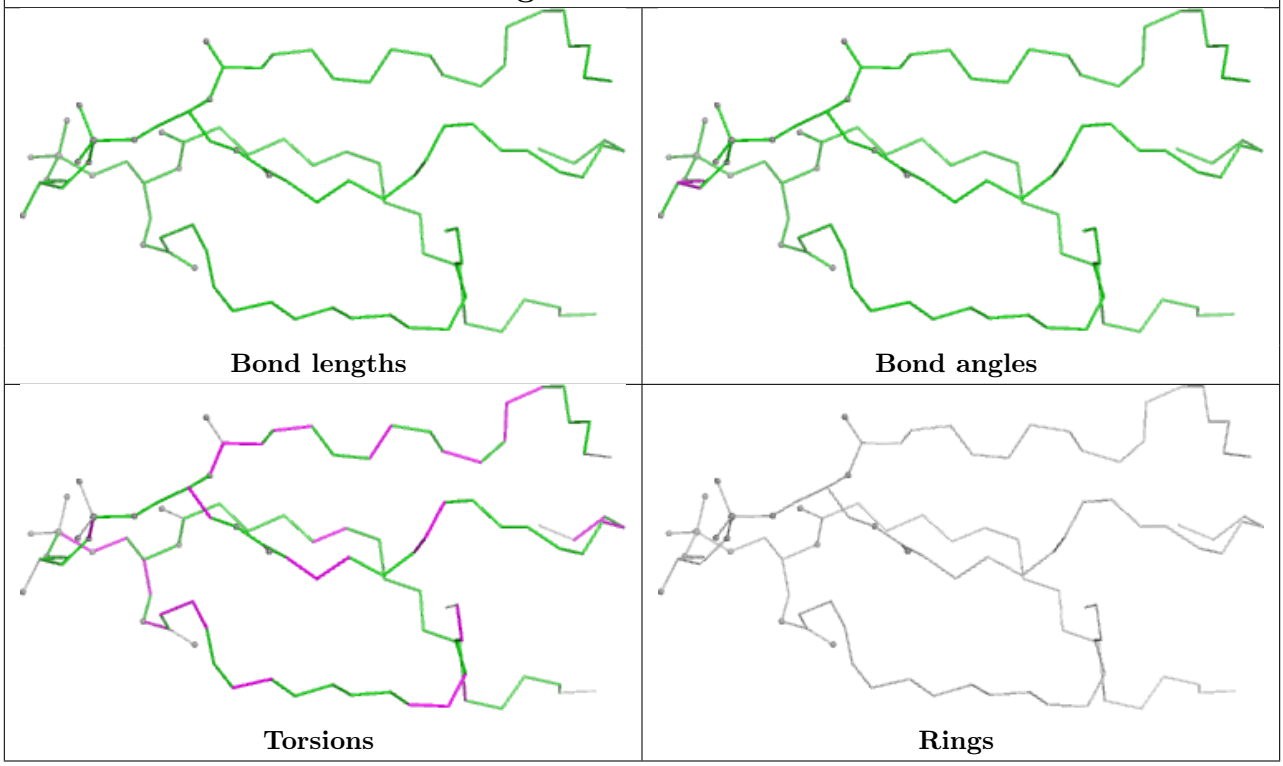


Rings

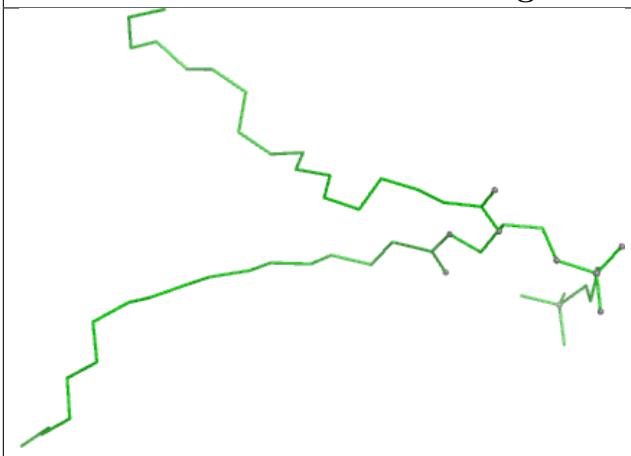
Ligand CDL Dd 706



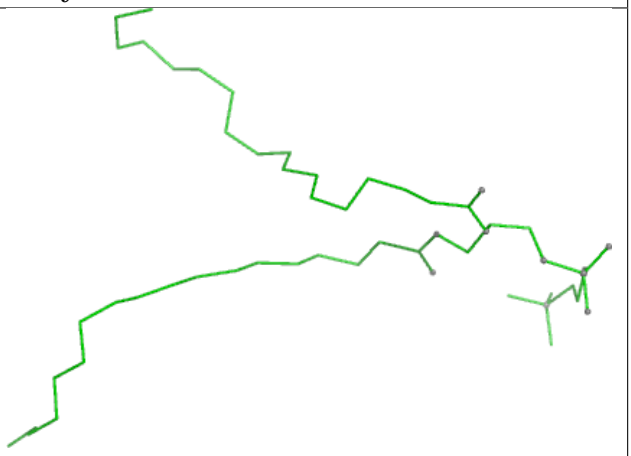
Ligand CDL Dr 402



Ligand PC1 Dy 302

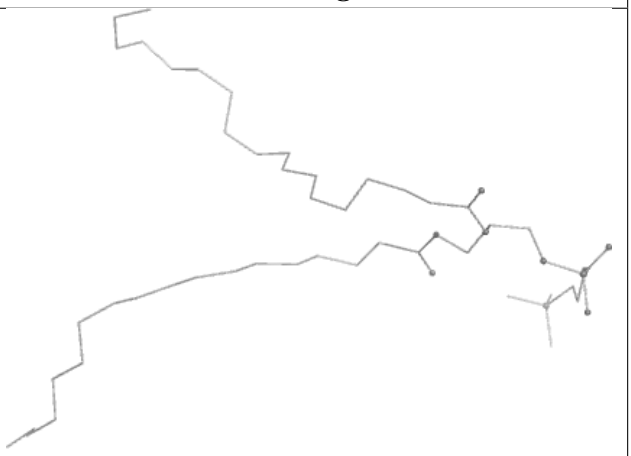


Bond lengths

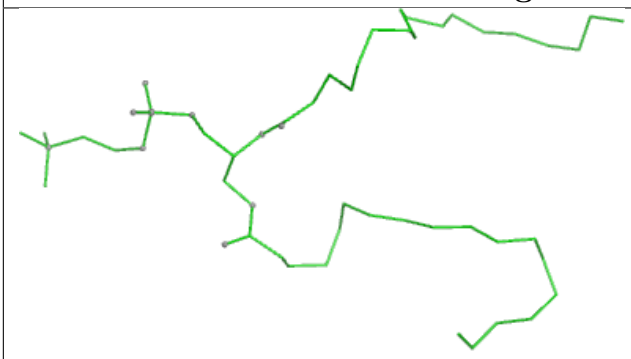
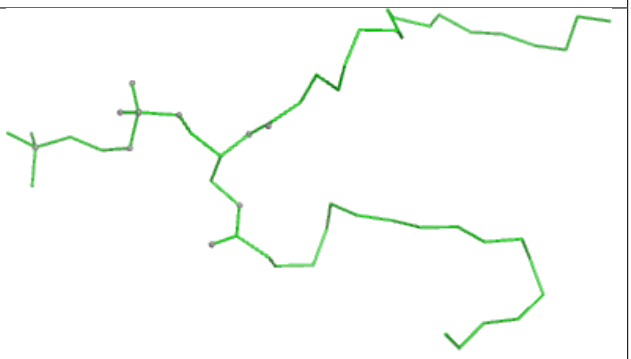
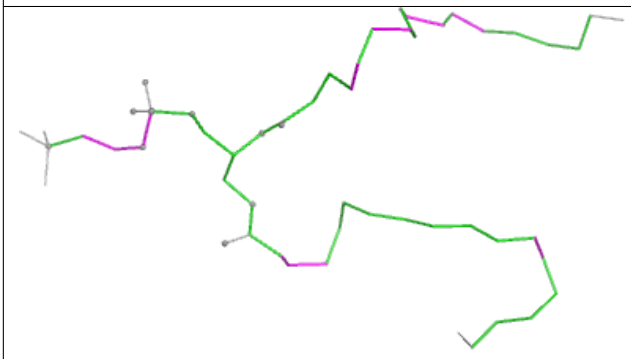


Bond angles

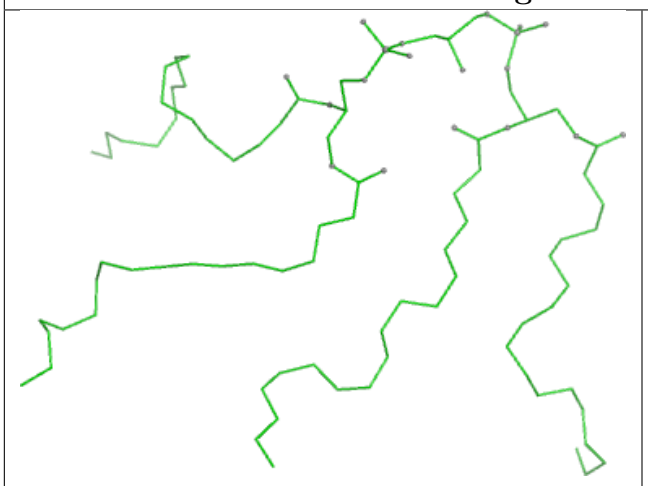
Torsions



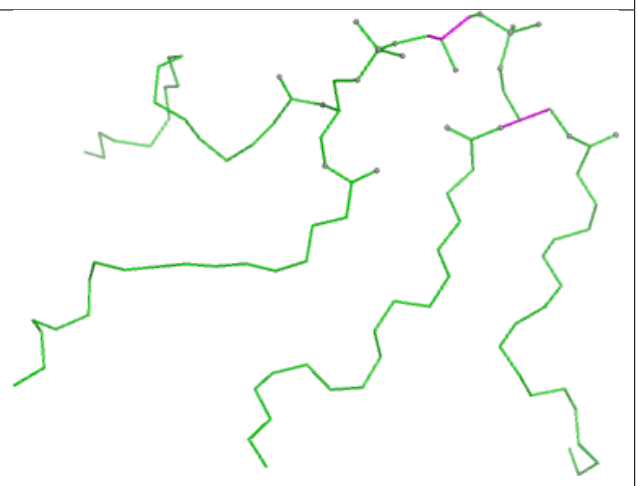
Rings

Ligand PC1 EO 201	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL Dv 401



Bond lengths

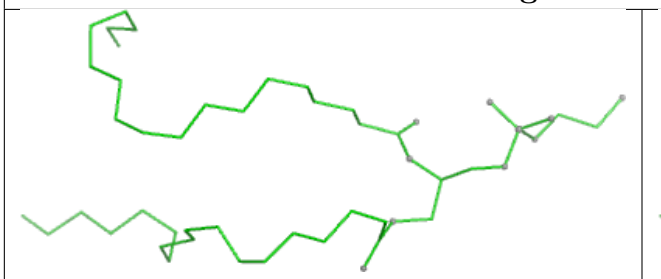


Bond angles

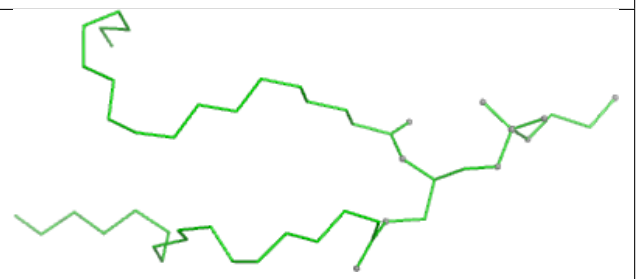
Torsions

Rings

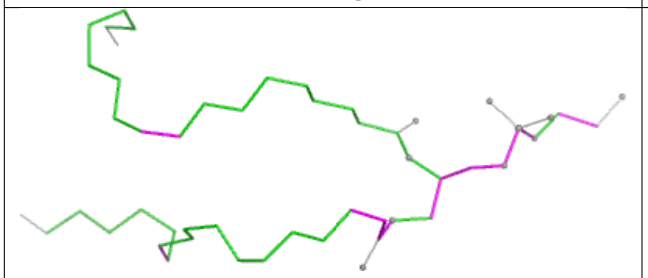
Ligand 3PE Da 708



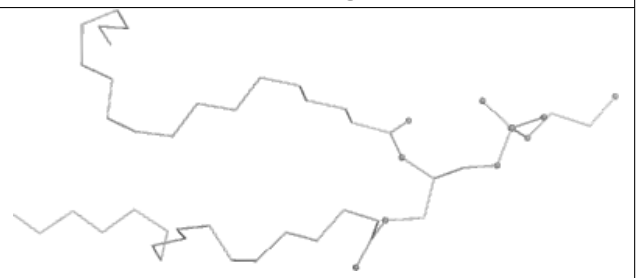
Bond lengths



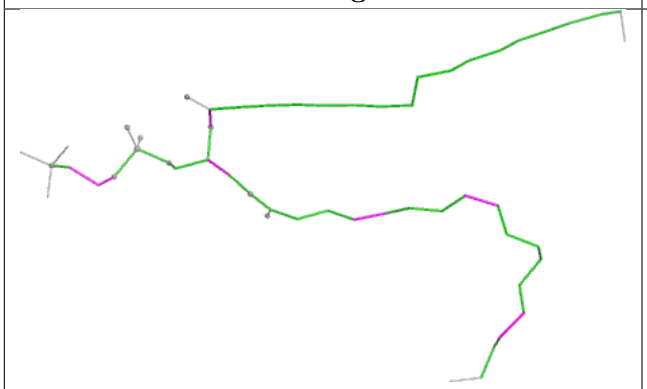
Bond angles



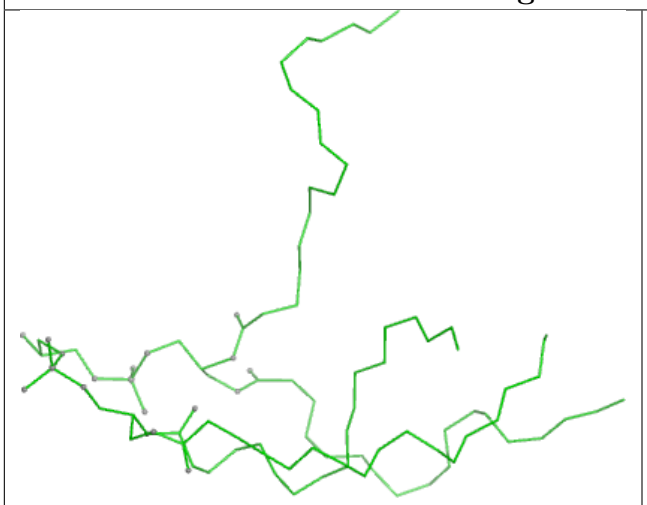
Torsions



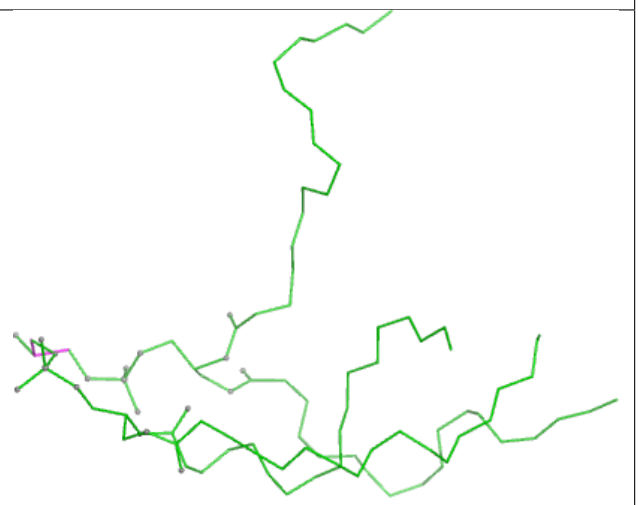
Rings

Ligand PC1 A2 402	
Bond lengths	Bond angles
 Torsions	Rings

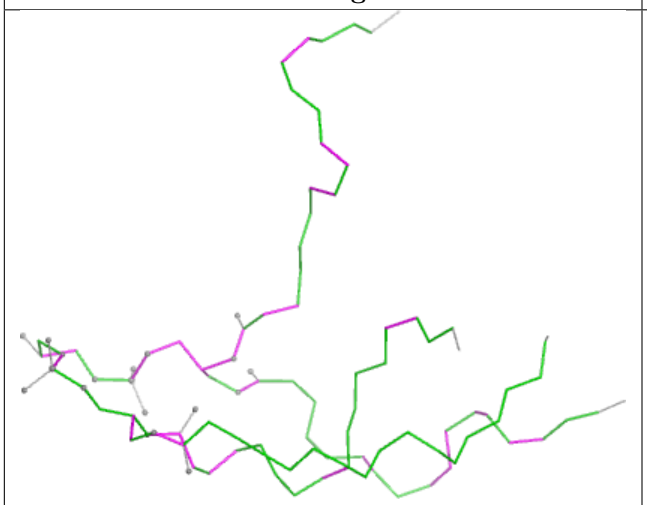
Ligand CDL Ds 402



Bond lengths



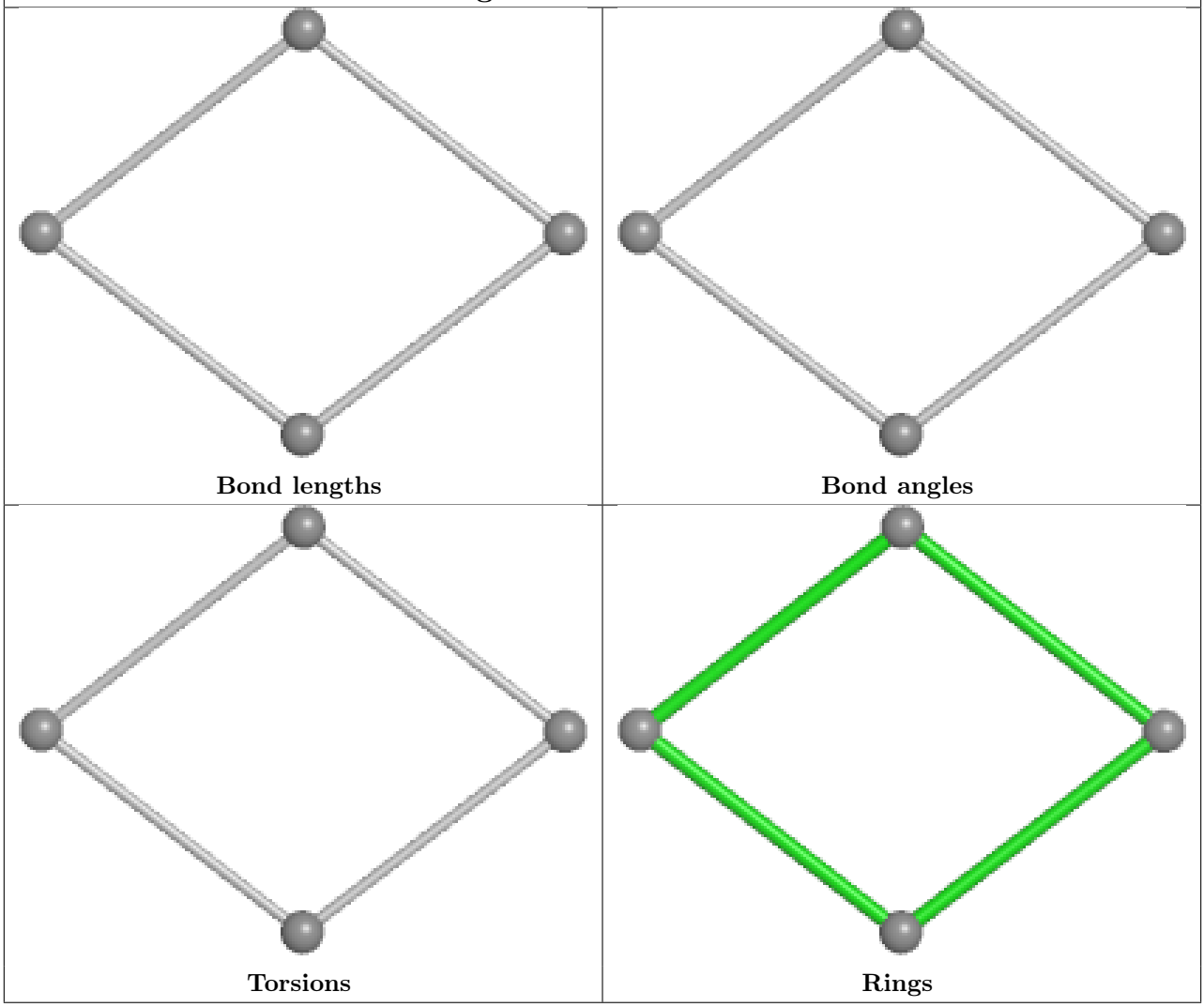
Bond angles



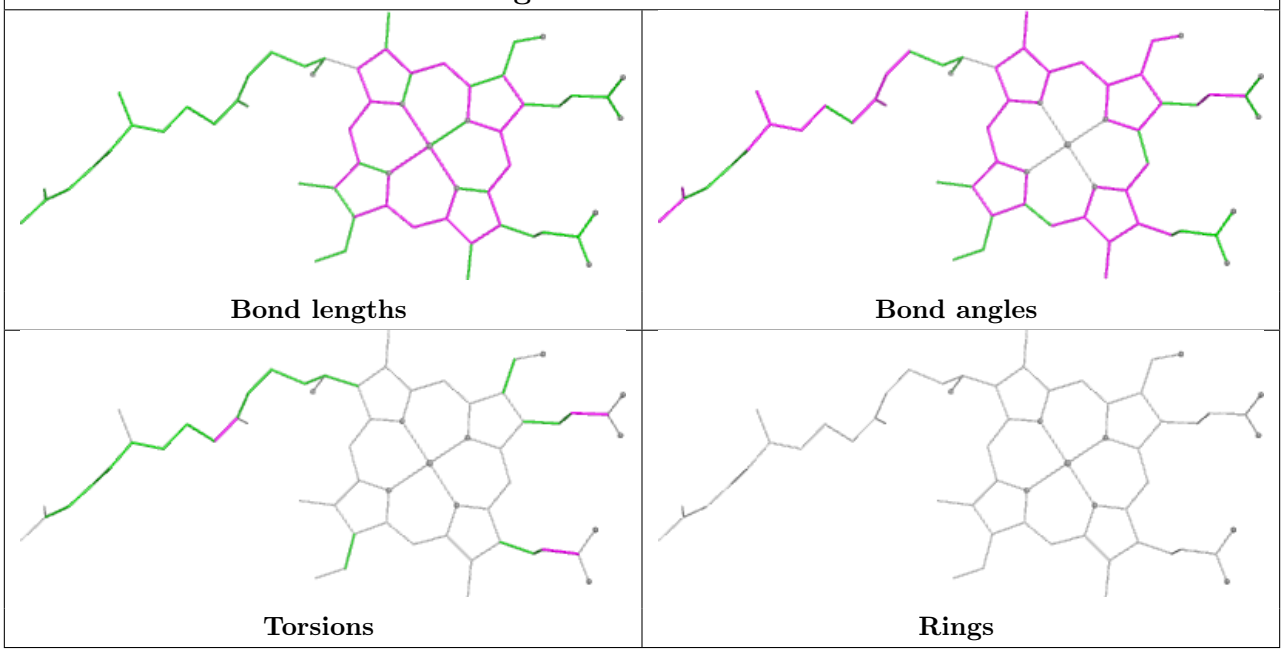
Torsions

Rings

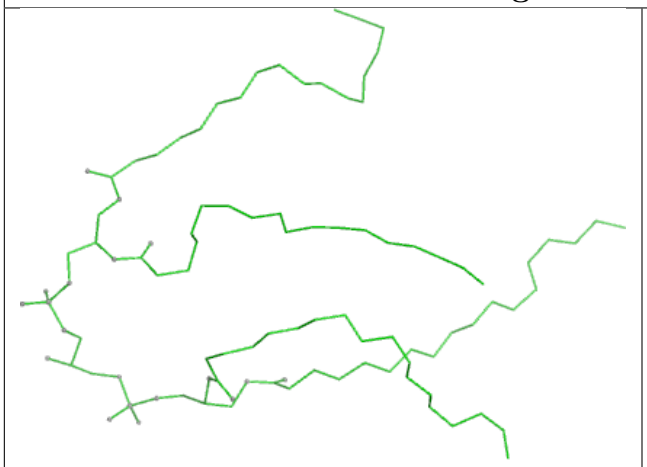
Ligand FES CB 1000



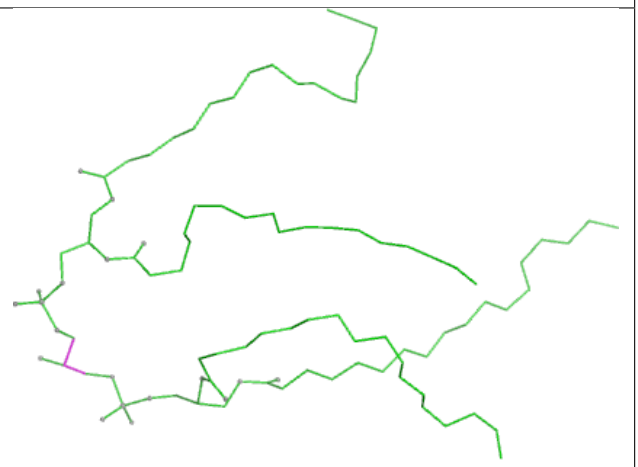
Ligand HEA Da 702



Ligand CDL CC 304



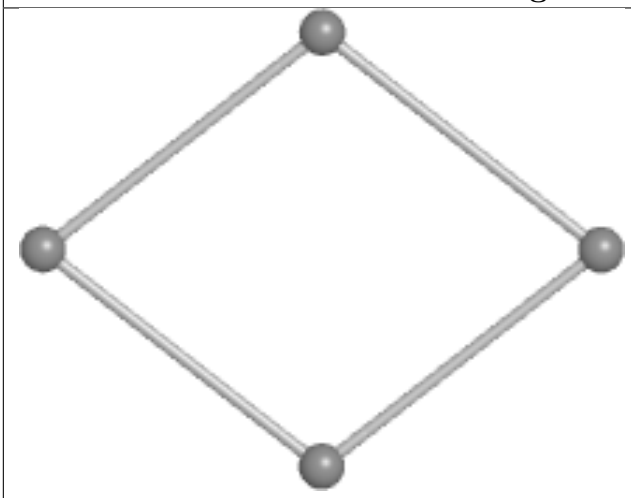
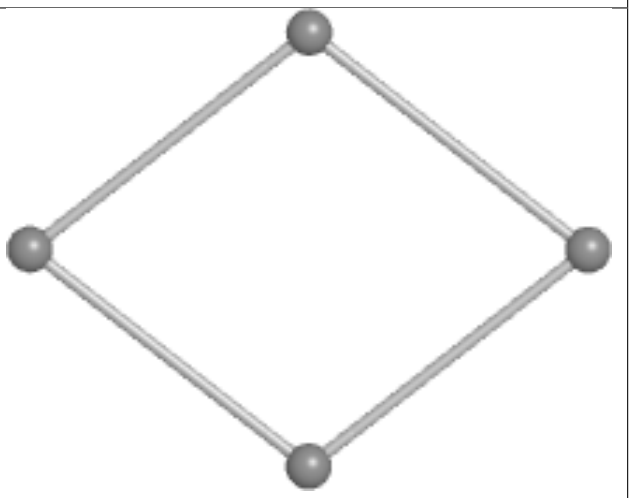
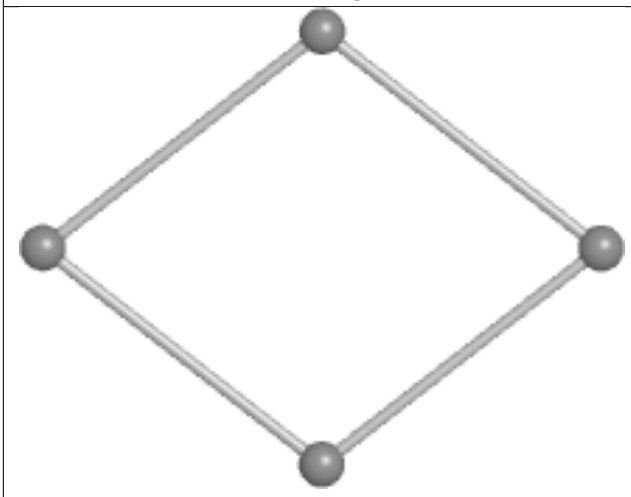
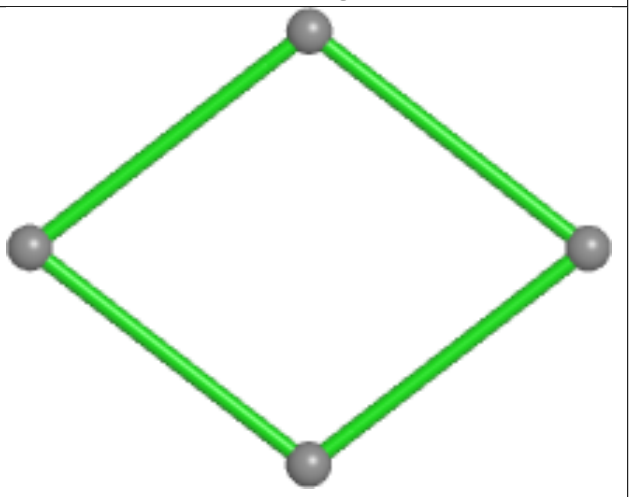
Bond lengths

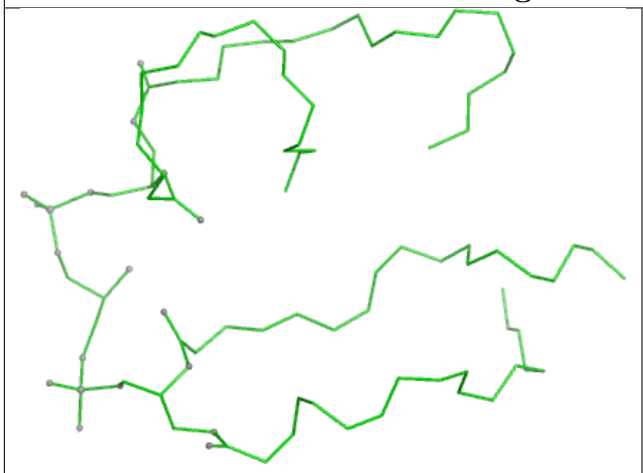
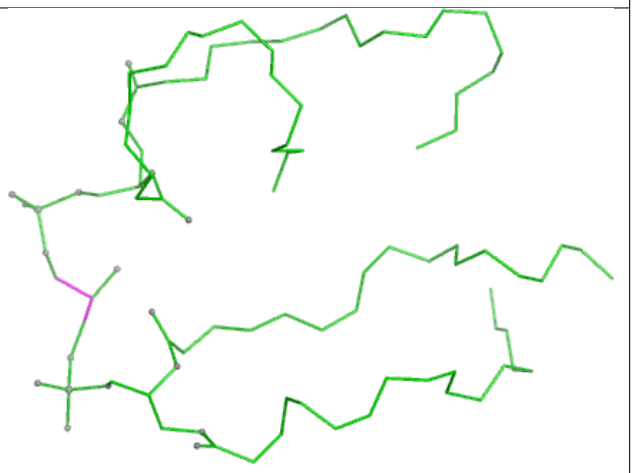
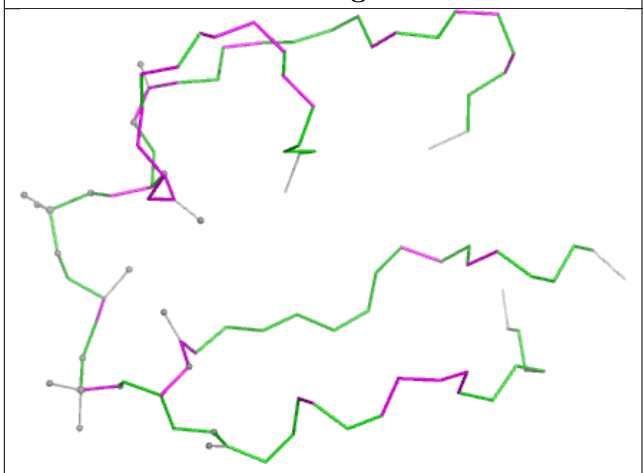


Bond angles

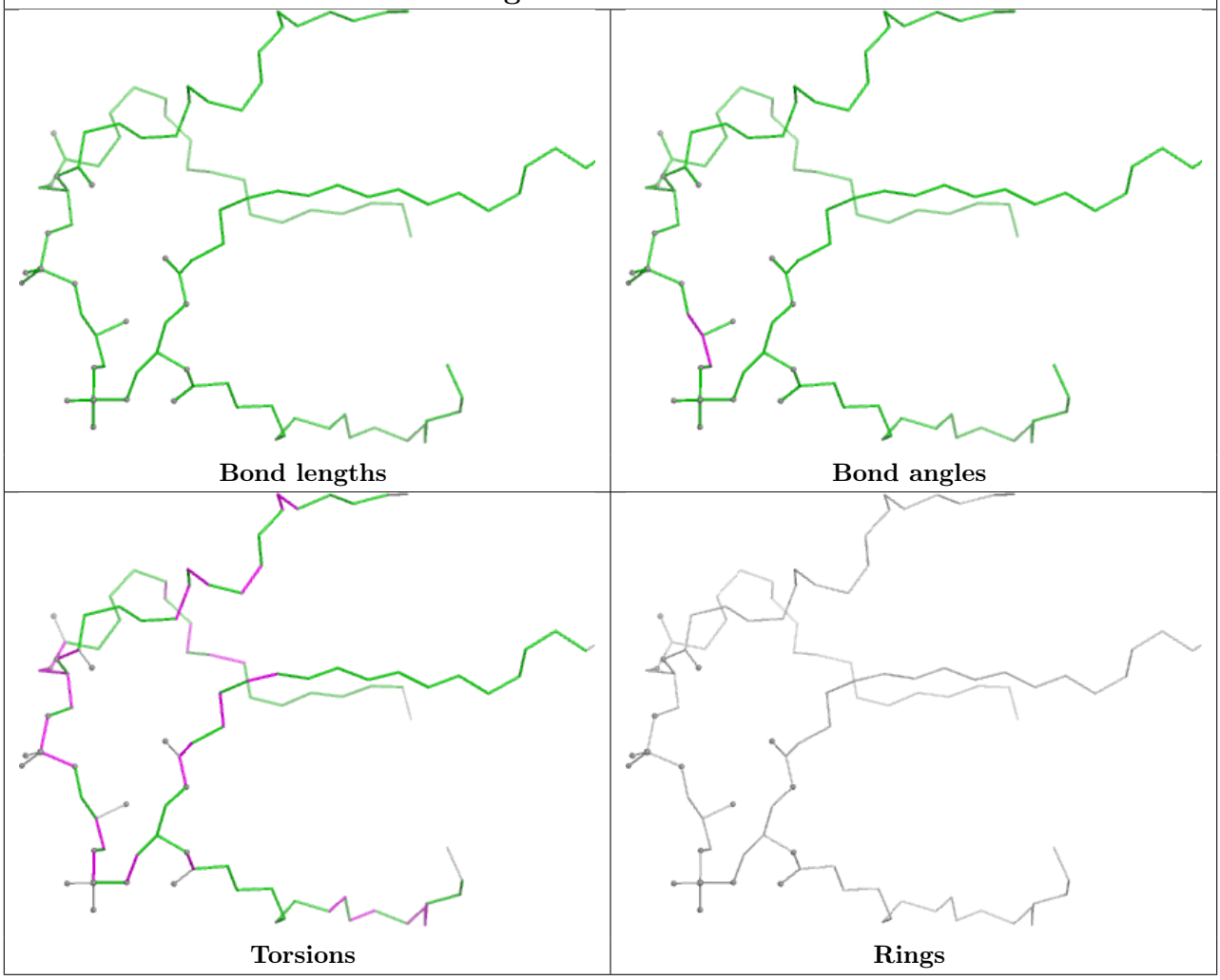
Torsions

Rings

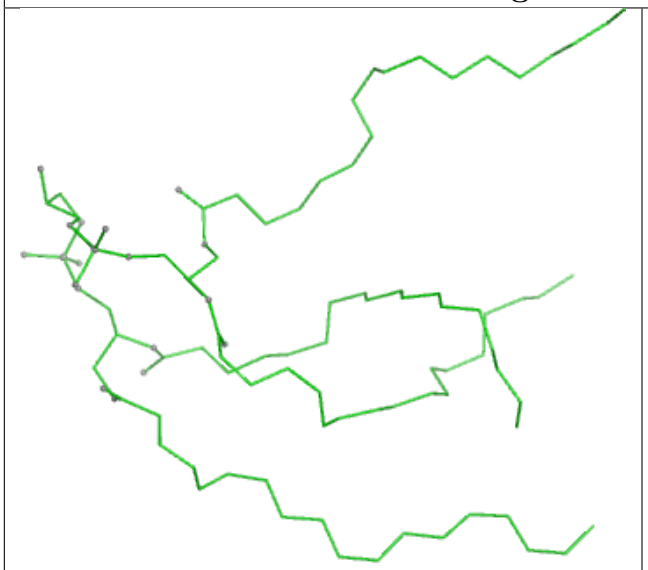
Ligand FES E 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL DS 404	
 Bond lengths	 Bond angles
 Torsions	Rings

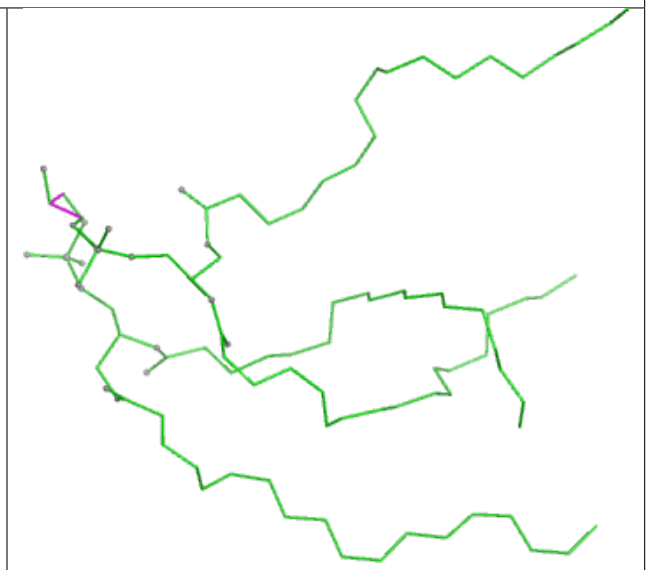
Ligand CDL c 506



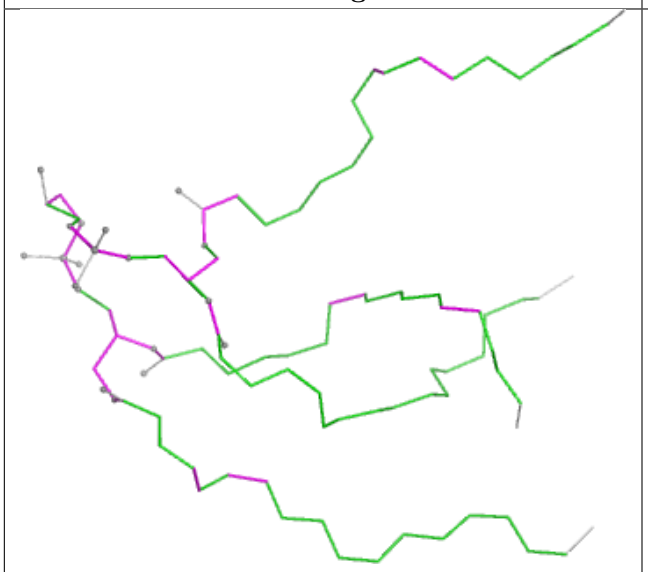
Ligand CDL CD 301



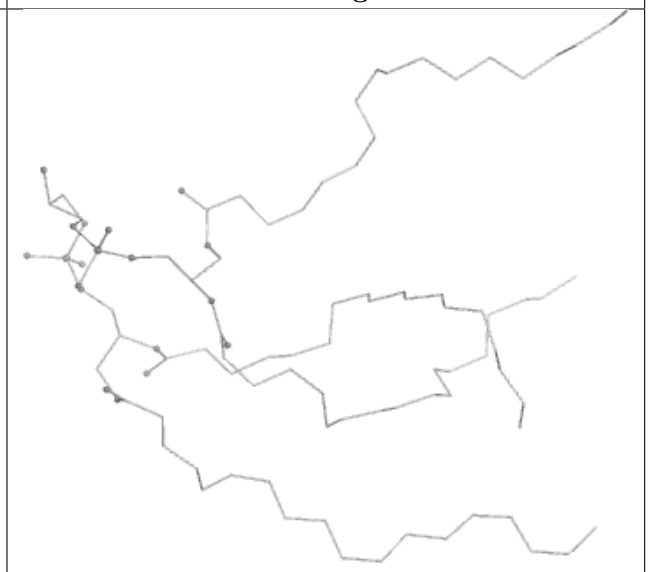
Bond lengths



Bond angles

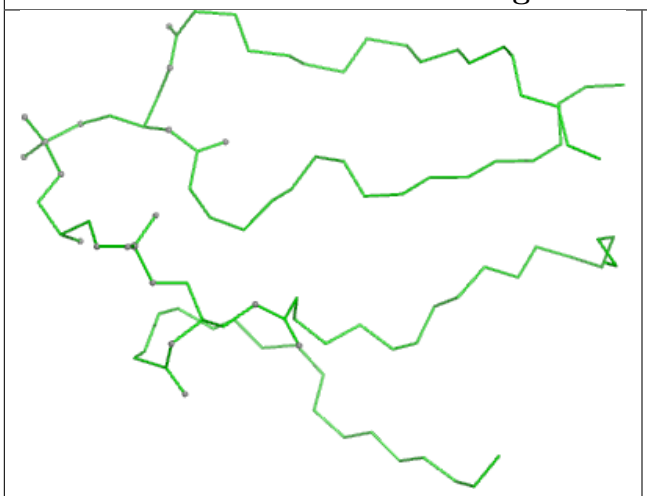


Torsions



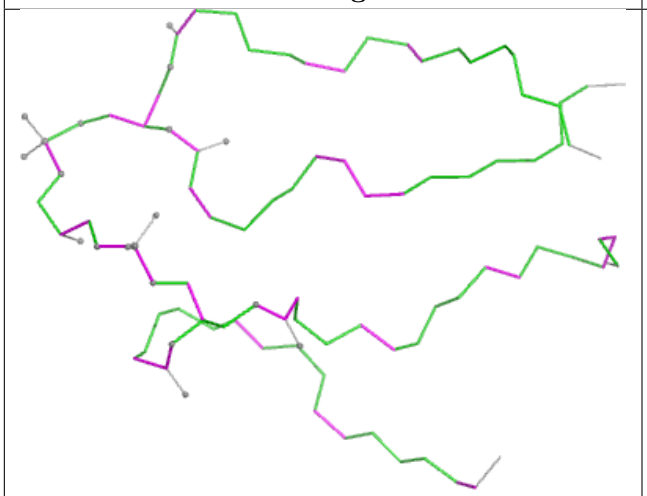
Rings

Ligand CDL BT 202



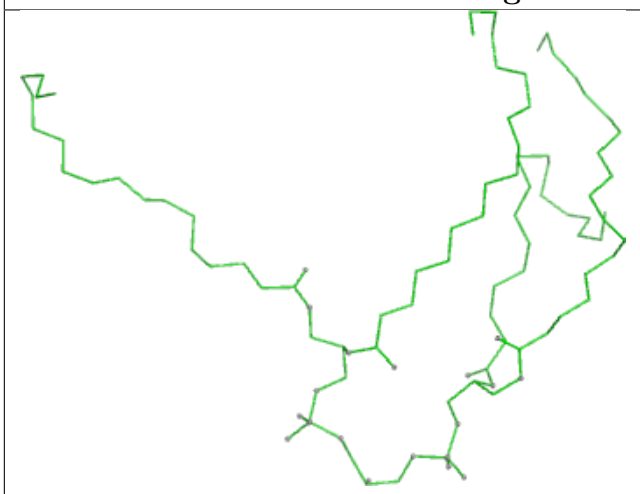
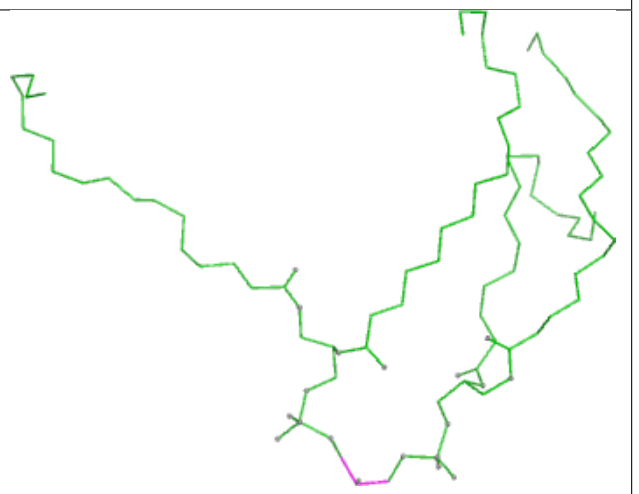
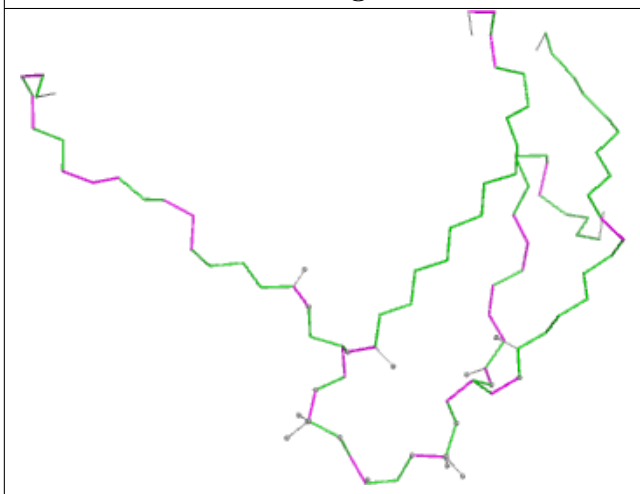
Bond lengths

Bond angles



Torsions

Rings

Ligand CDL EH 1601	
 Bond lengths	 Bond angles
 Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

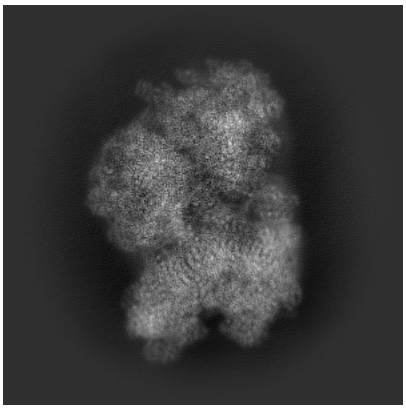
6 Map visualisation (i)

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

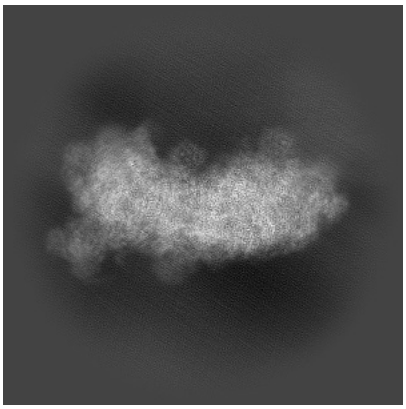
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

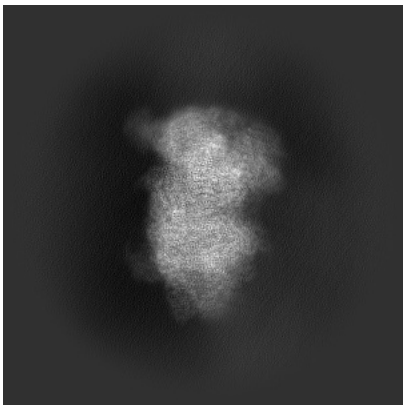
6.1.1 Primary map



X

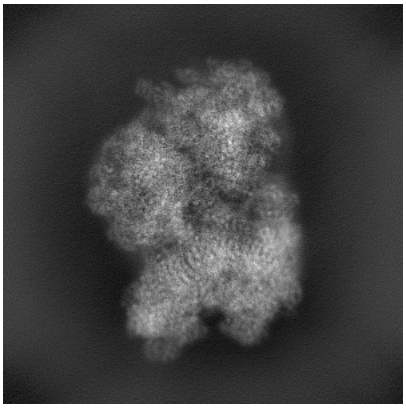


Y

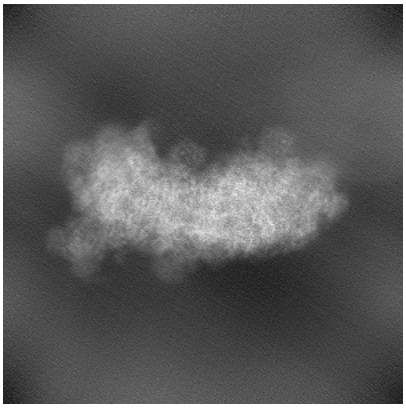


Z

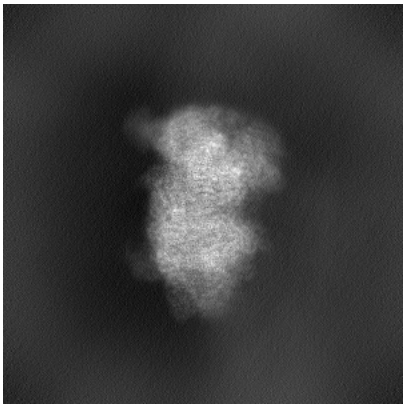
6.1.2 Raw map



X



Y

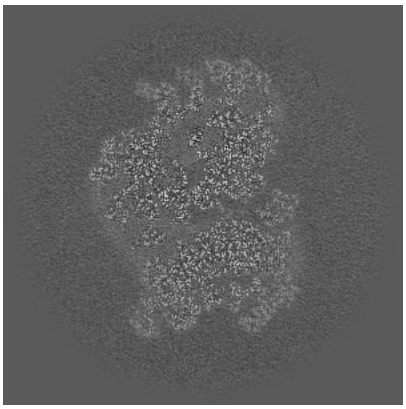


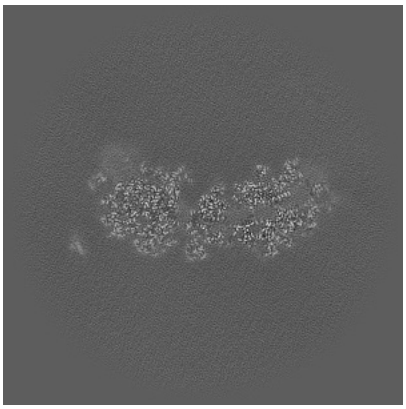
Z

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

6.2 Central slices (i)

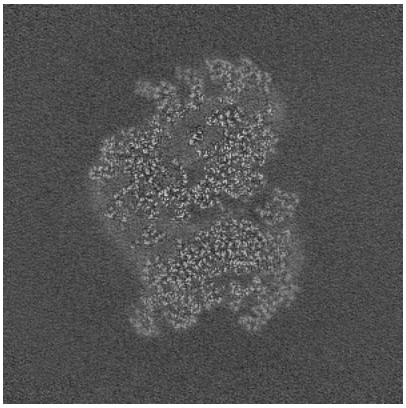
6.2.1 Primary map

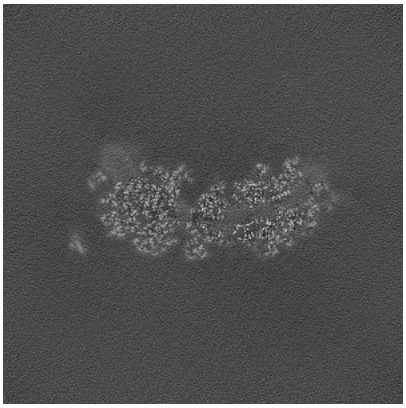

X Index: 240

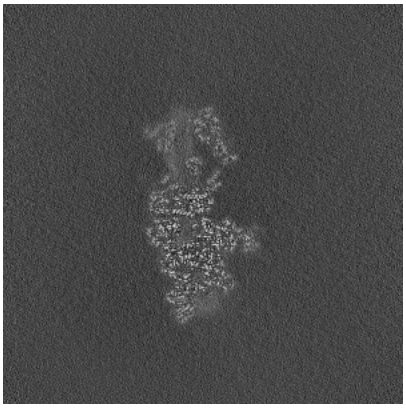

Y Index: 240

Z Index: 240

6.2.2 Raw map


X Index: 240

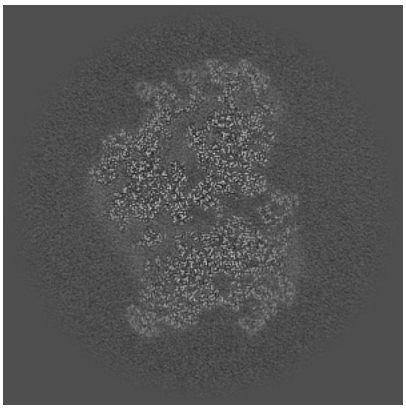

Y Index: 240

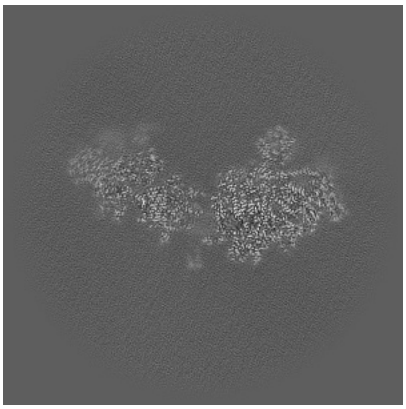

Z Index: 240

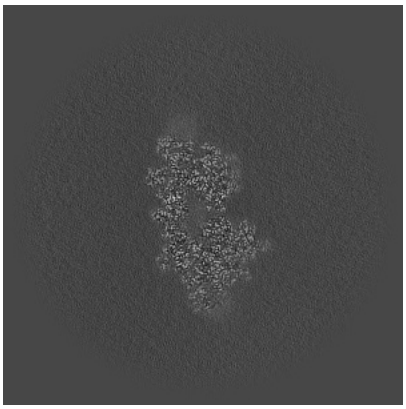
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

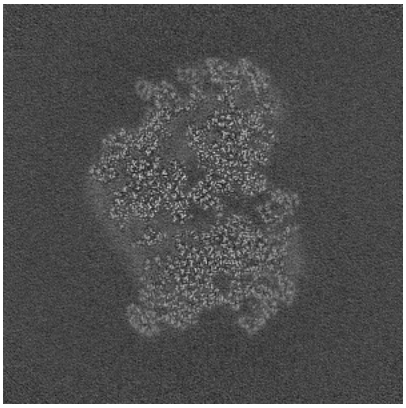
6.3.1 Primary map

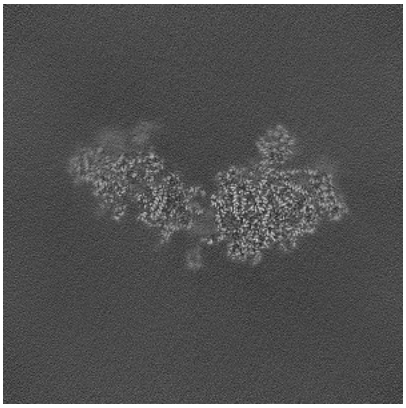

X Index: 243

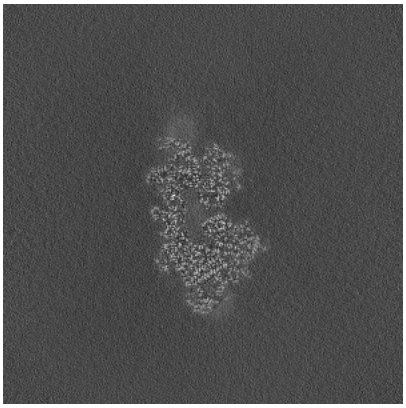

Y Index: 272


Z Index: 287

6.3.2 Raw map


X Index: 243

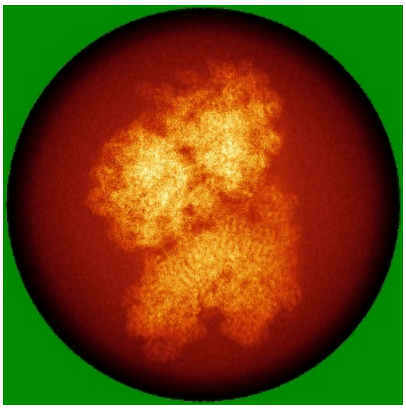

Y Index: 271

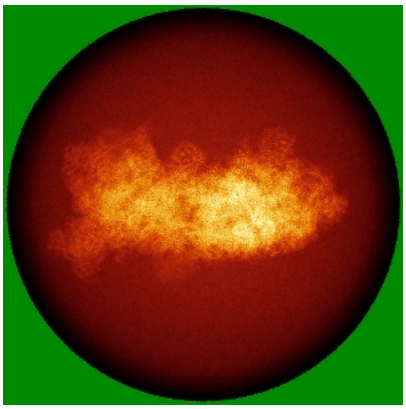

Z Index: 284

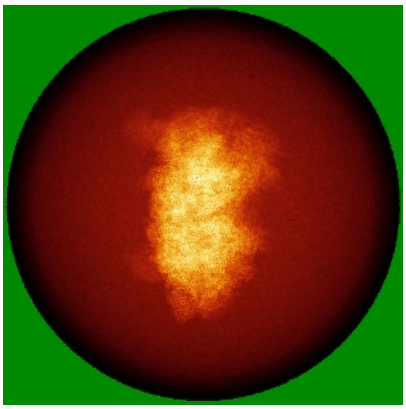
The images above show the largest variance slices of the map in three orthogonal directions.

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

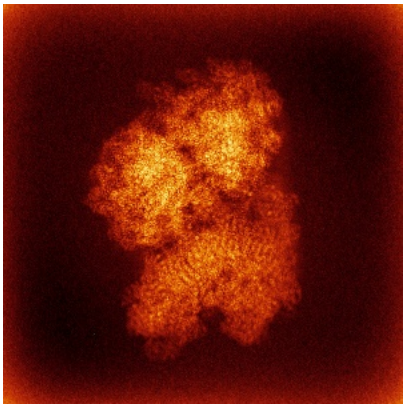
6.4.1 Primary map

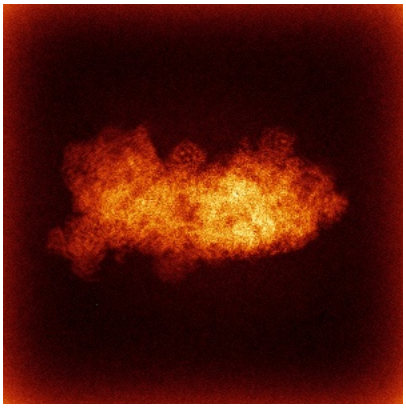

X

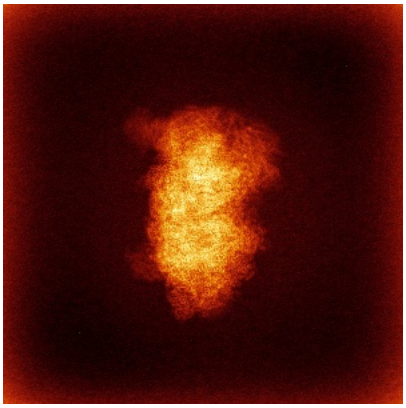

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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

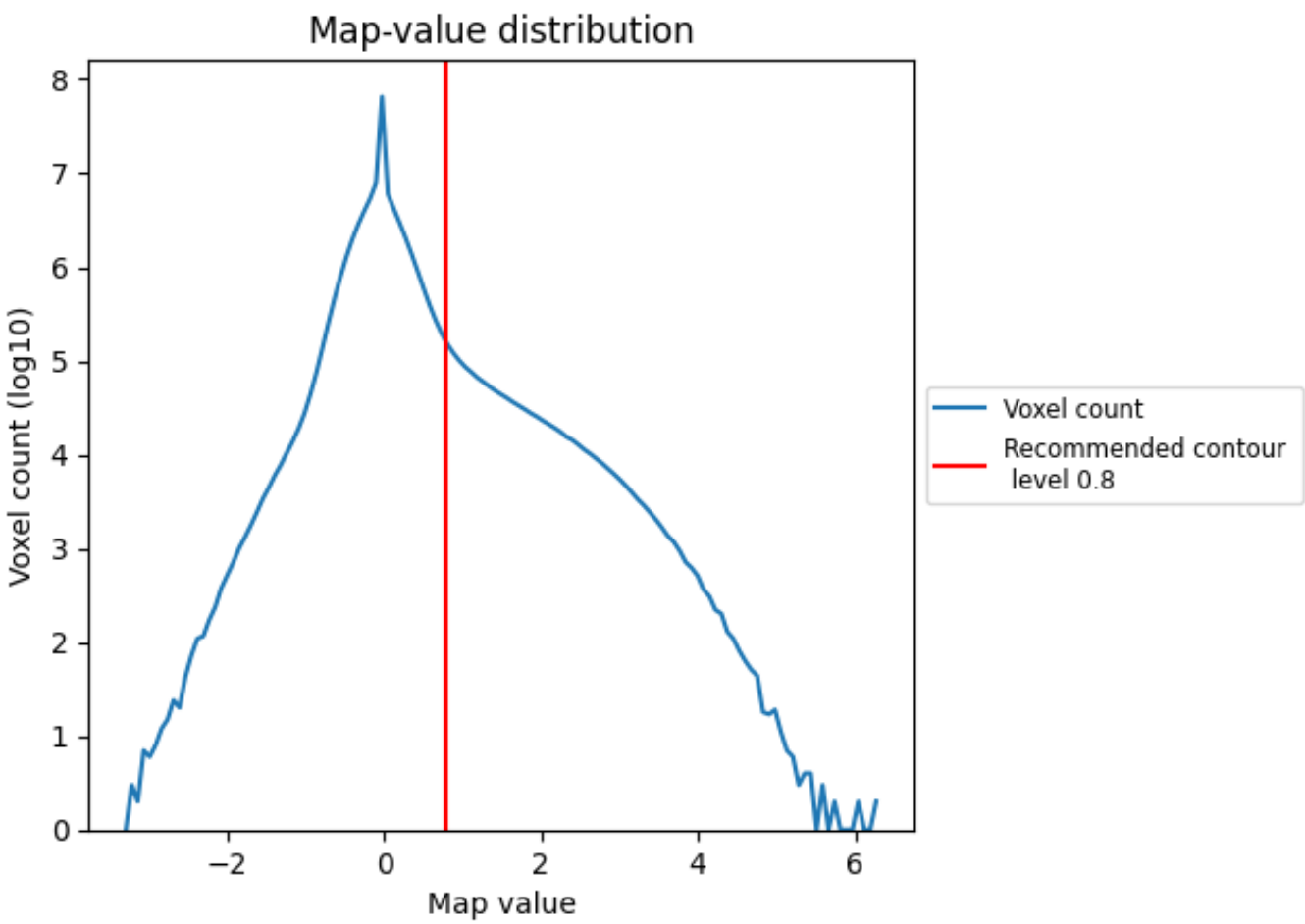
6.6 Mask visualisation (i)

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

7 Map analysis (i)

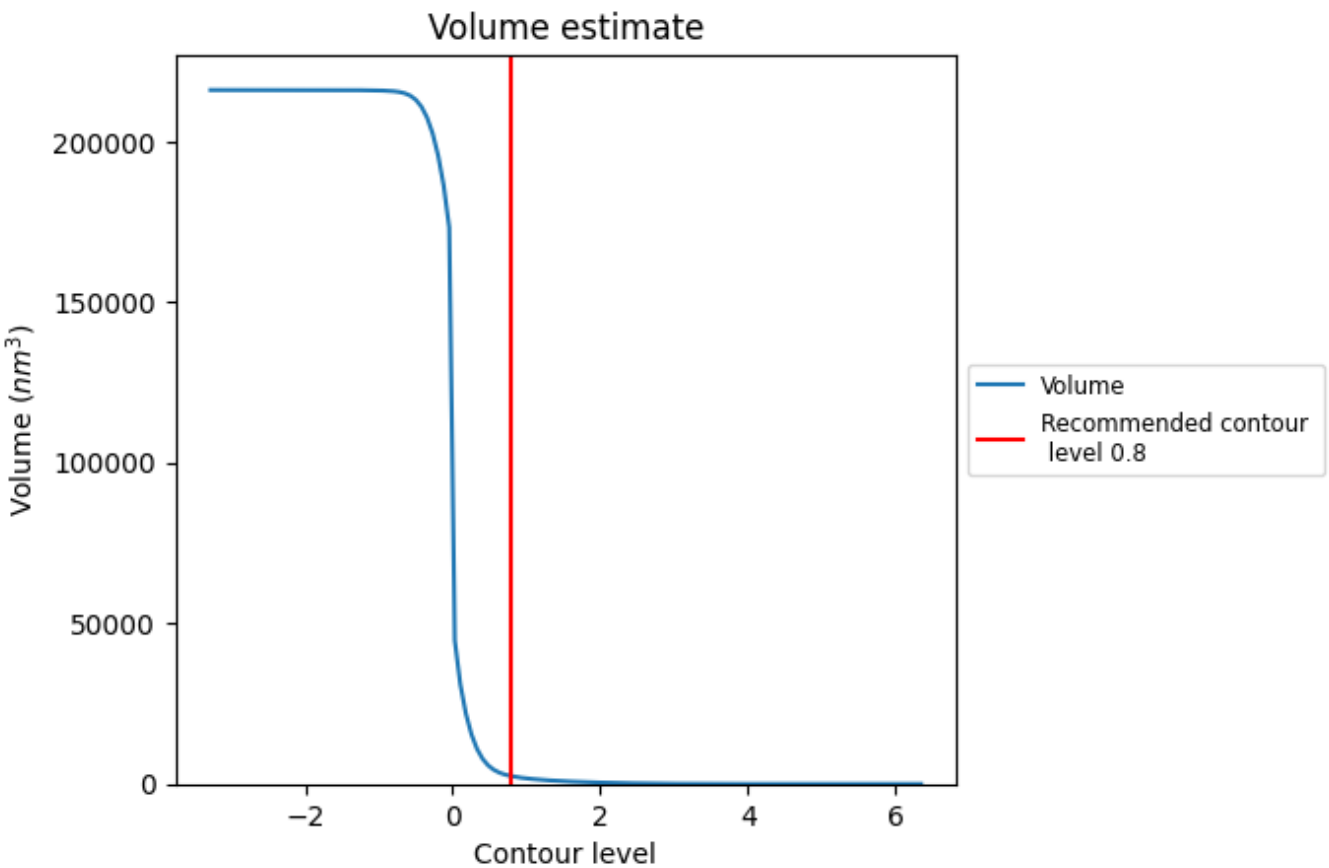
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

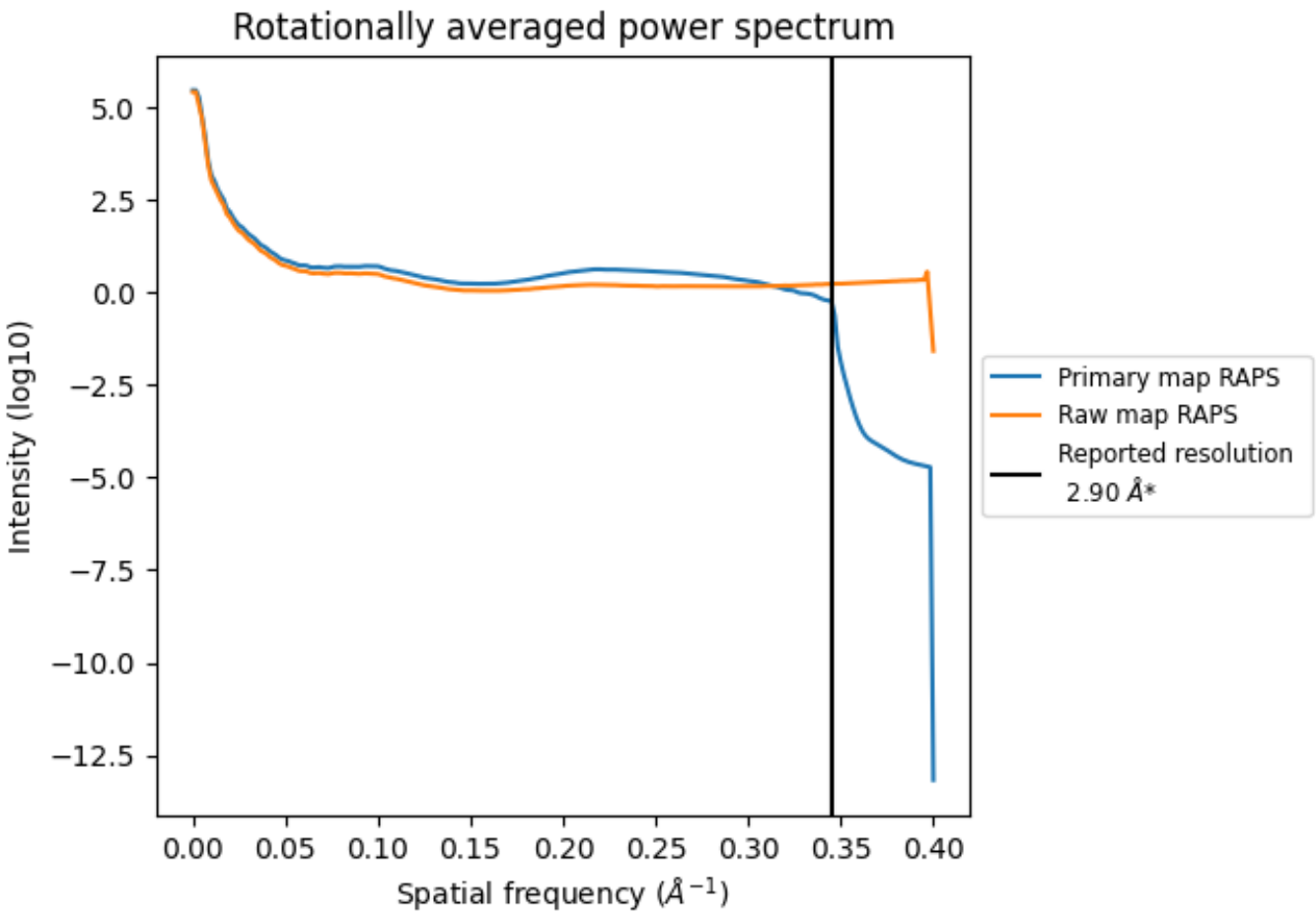
7.2 Volume estimate (i)



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

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

7.3 Rotationally averaged power spectrum (i)

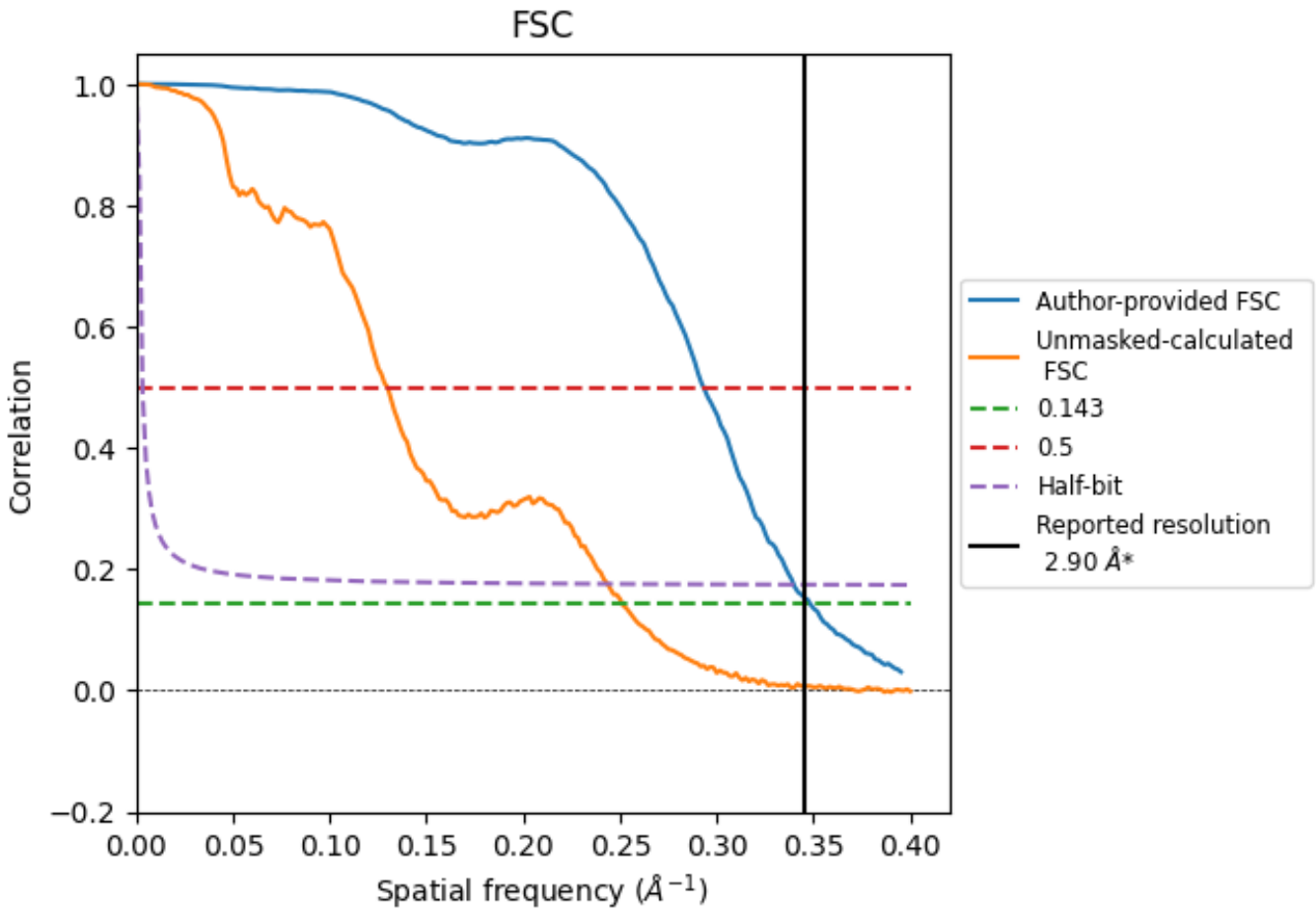


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

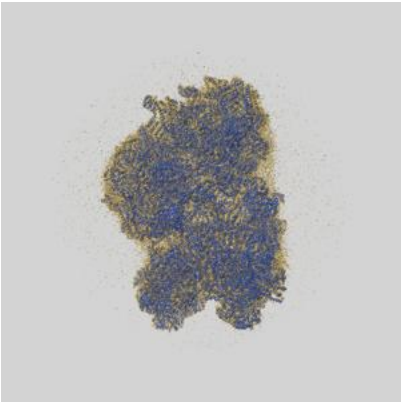
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.41	2.94
Unmasked-calculated*	3.98	7.70	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.9 by more than 10 %

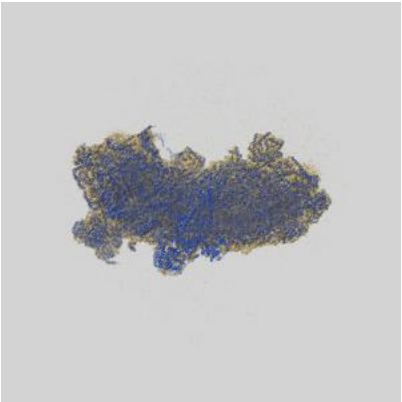
9 Map-model fit (i)

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

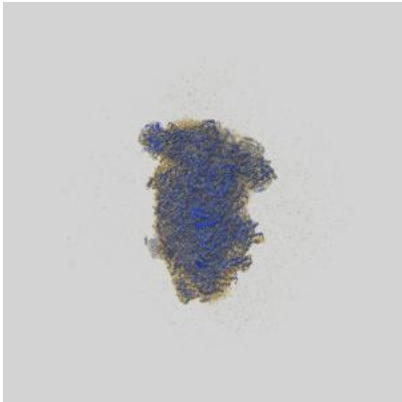
9.1 Map-model overlay (i)



X



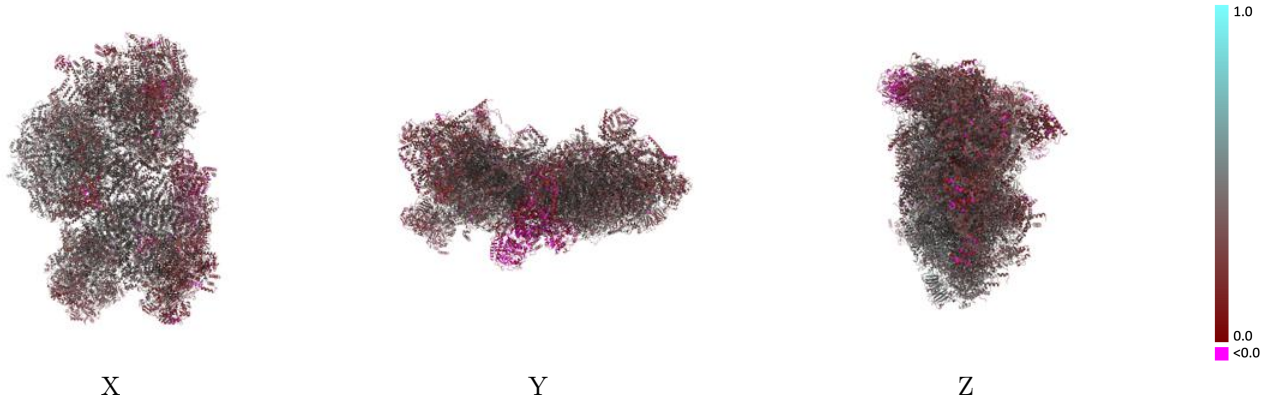
Y



Z

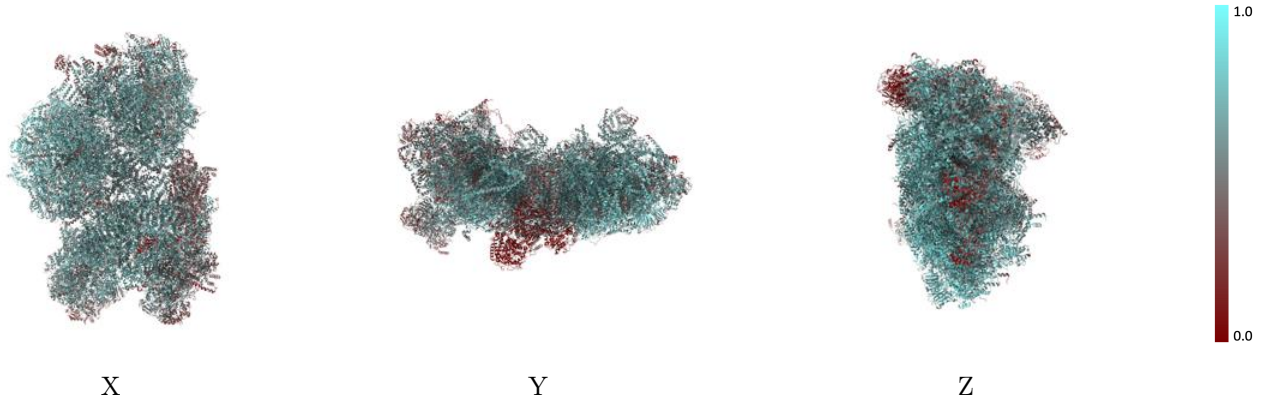
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



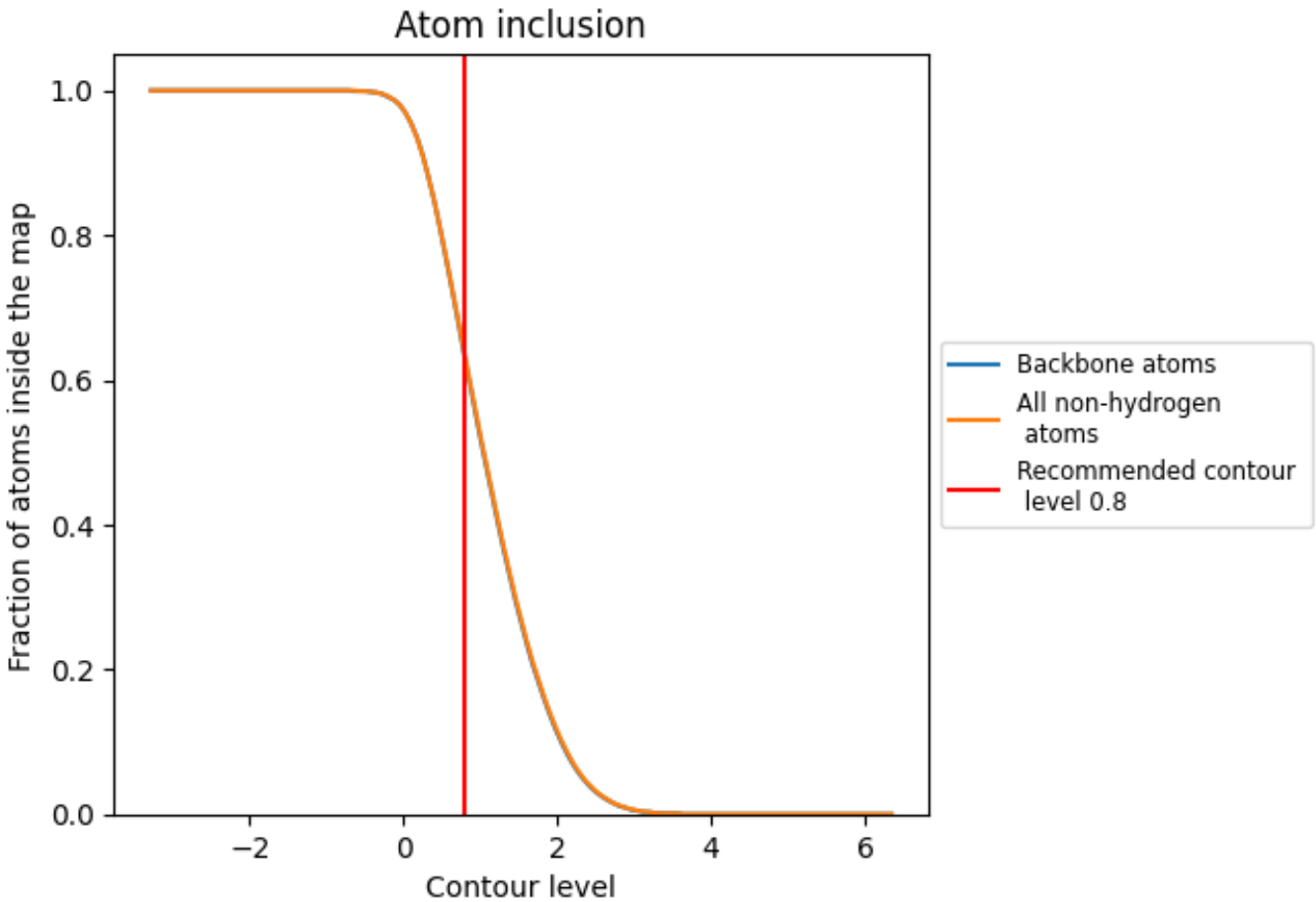
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

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

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

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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