Full wwPDB EM Validation Report

Jun 10, 2024 – 09:31 PM EDT

PDB ID	:	8UGH
EMDB ID	:	EMD-42225
Title	:	In-situ structure of typeA supercomplex with lipids in respiratory chain (composite)
Authors	:	Zheng, W.; Zhang, K.; Zhu, J.
Deposited on	:	2023-10-05
Resolution	:	2.10 Å(reported)

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

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

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

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

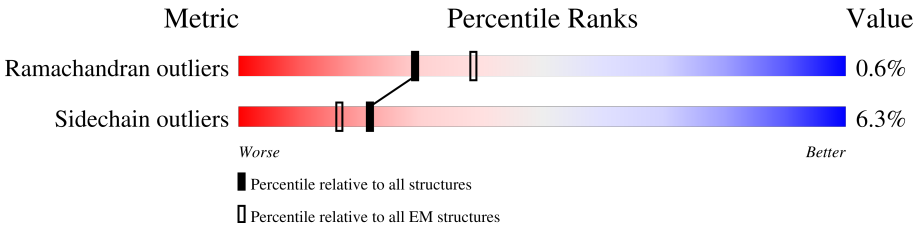
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	91% 8% ·
2	1B	258	55% 5% 40%
3	1C	264	77% · 21%
4	1D	466	88% · 8%
5	1E	249	83% · 14%
6	1F	464	88% 5% 7%
7	1G	727	89% 7% ·
8	1H	318	95% 5%
9	1I	239	71% · 26%

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Mol	Chain	Length	Quality of chain
10	1J	175	90% 9%
11	1K	98	91% 9%
12	1L	606	91% 9%
13	1M	459	95% 5%
14	1N	347	95% 5%
15	1O	357	81% 9% 10%
16	1P	377	85% 5% 9%
17	1Q	175	66% 7% 26%
18	1R	123	72% 6% 22%
19	1S	99	79% 9% 12%
20	1T	156	48% 6% 46%
20	1U	156	52% 45%
21	1V	116	95%
22	1W	128	88% 10%
23	1X	172	92% 7%
24	1Y	141	92% 6%
25	1Z	144	95%
26	1a	70	97%
27	1b	84	89% 10%
28	1c	76	58% 7% 36%
29	1d	122	91% 7%
30	1e	106	89% 5% 7%
31	1f	135	36% 6% 58%
32	1g	154	58% 7% 35%
33	1h	189	69% 27%

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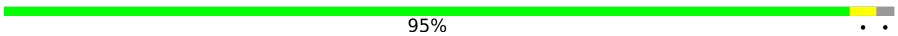
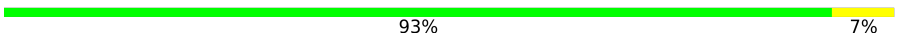
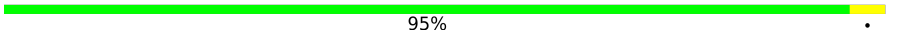
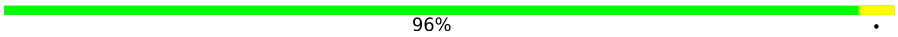
Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	

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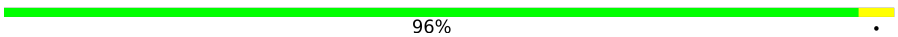
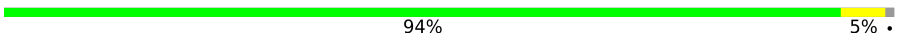
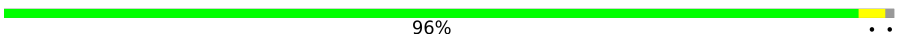
Mol	Chain	Length	Quality of chain
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	64	
53	3W	64	
54	3X	56	
54	3Y	56	
55	4A	514	
56	4B	229	
57	4C	261	
58	4D	169	
59	4E	152	
60	4F	129	
61	4G	97	
62	4H	86	
63	4I	75	
64	4J	80	
65	4K	80	
66	4L	63	
67	4M	70	
68	4N	82	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 124052 atoms, of which 0 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	115	916	616	134	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	155	1242	791	226	211	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	209	1740	1125	297	316	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	429	3452	2207	593	628	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	1g	100	835	535	138	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			464	305	82	77		
53	3W	56	Total	C	N	O	0	0
			464	305	82	77		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

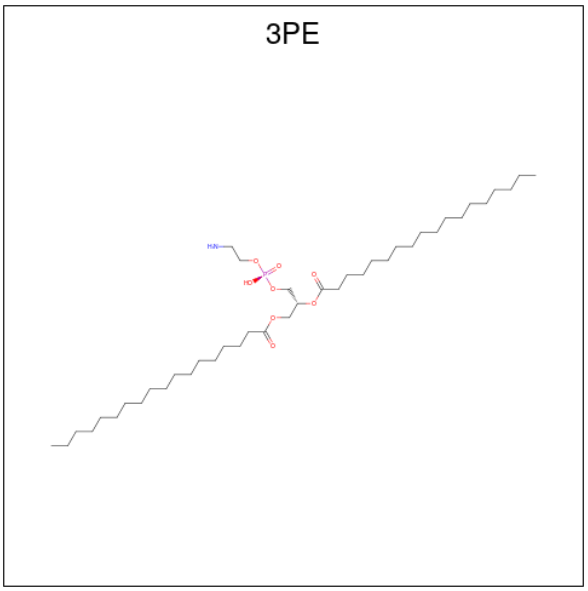
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1A	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	1B	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1B	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1J	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1L	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1L	1	Total	C	N	O	P	0
			38	28	1	8	1	
69	1L	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	1L	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1M	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1b	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1d	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1d	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1e	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1f	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1f	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	1f	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1f	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1g	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1g	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1k	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1l	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1l	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1l	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1m	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	1m	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1m	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1m	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1m	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1o	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3A	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	3C	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3C	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	3C	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	3D	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	3D	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	3E	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3E	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	3G	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	

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Mol	Chain	Residues	Atoms	AltConf
69	3G	1	Total C N O P 33 23 1 8 1	0
69	3G	1	Total C N O P 33 23 1 8 1	0
69	3G	1	Total C N O P 33 23 1 8 1	0
69	3G	1	Total C N O P 33 23 1 8 1	0
69	3G	1	Total C N O P 33 23 1 8 1	0
69	3G	1	Total C N O P 33 23 1 8 1	0
69	3G	1	Total C N O P 51 41 1 8 1	0
69	3G	1	Total C N O P 43 33 1 8 1	0
69	3G	1	Total C N O P 48 38 1 8 1	0
69	3J	1	Total C N O P 47 37 1 8 1	0
69	3J	1	Total C N O P 38 28 1 8 1	0
69	3J	1	Total C N O P 51 41 1 8 1	0
69	3J	1	Total C N O P 51 41 1 8 1	0
69	3J	1	Total C N O P 51 41 1 8 1	0
69	3N	1	Total C N O P 51 41 1 8 1	0
69	3N	1	Total C N O P 51 41 1 8 1	0
69	3P	1	Total C N O P 51 41 1 8 1	0
69	3P	1	Total C N O P 38 28 1 8 1	0
69	3P	1	Total C N O P 32 22 1 8 1	0
69	3P	1	Total C N O P 51 41 1 8 1	0
69	3P	1	Total C N O P 51 41 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 48	C 38	N 1	O 8	P 1	0
69	3P	1	Total 45	C 35	N 1	O 8	P 1	0
69	3P	1	Total 48	C 38	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3Q	1	Total 41	C 31	N 1	O 8	P 1	0
69	3Q	1	Total 46	C 36	N 1	O 8	P 1	0
69	3Q	1	Total 46	C 36	N 1	O 8	P 1	0
69	3R	1	Total 51	C 41	N 1	O 8	P 1	0
69	3R	1	Total 51	C 41	N 1	O 8	P 1	0
69	3R	1	Total 51	C 41	N 1	O 8	P 1	0
69	3S	1	Total 51	C 41	N 1	O 8	P 1	0
69	3T	1	Total 51	C 41	N 1	O 8	P 1	0
69	3W	1	Total 51	C 41	N 1	O 8	P 1	0
69	3W	1	Total 42	C 32	N 1	O 8	P 1	0

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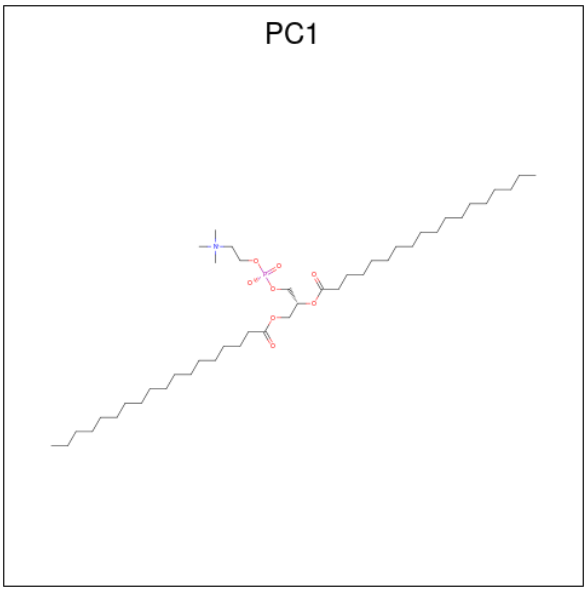
Mol	Chain	Residues	Atoms					AltConf
69	3W	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	4G	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	4G	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	

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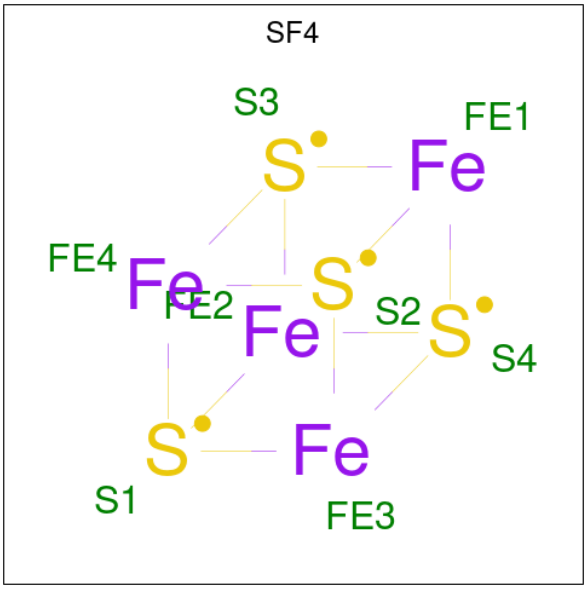
Mol	Chain	Residues	Atoms					AltConf
70	1h	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	3J	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3P	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3R	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3T	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3X	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 71 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

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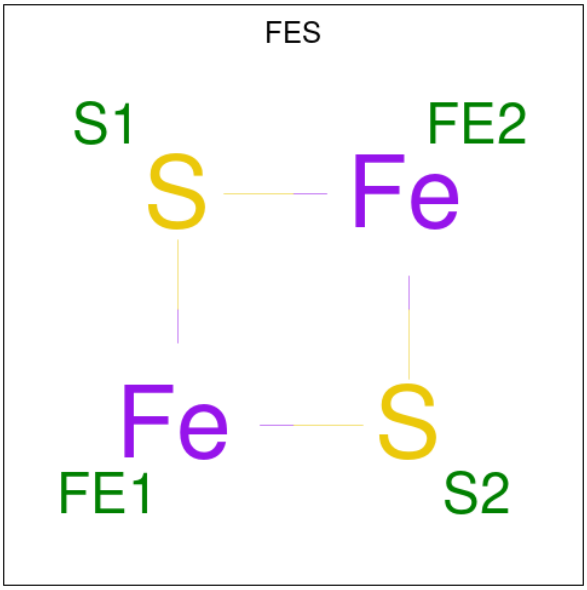
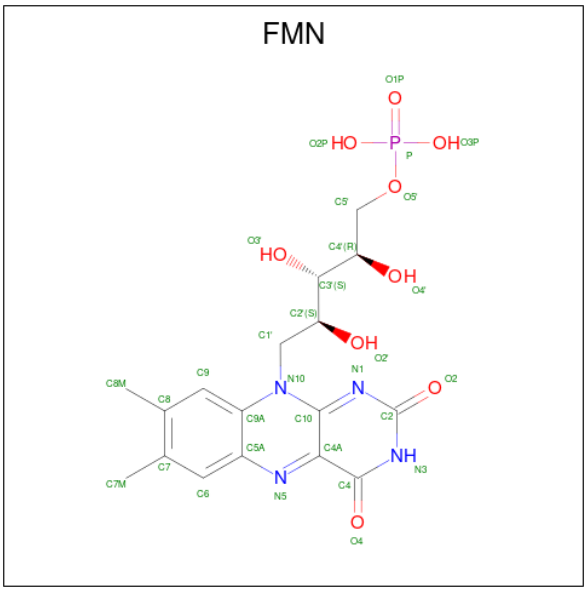
Mol	Chain	Residues	Atoms	AltConf
71	1I	1	Total Fe S 8 4 4	0

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
72	1E	1	Total Fe S 4 2 2	0
72	1G	1	Total Fe S 4 2 2	0
72	3E	1	Total Fe S 4 2 2	0
72	3R	1	Total Fe S 4 2 2	0

- Molecule 73 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

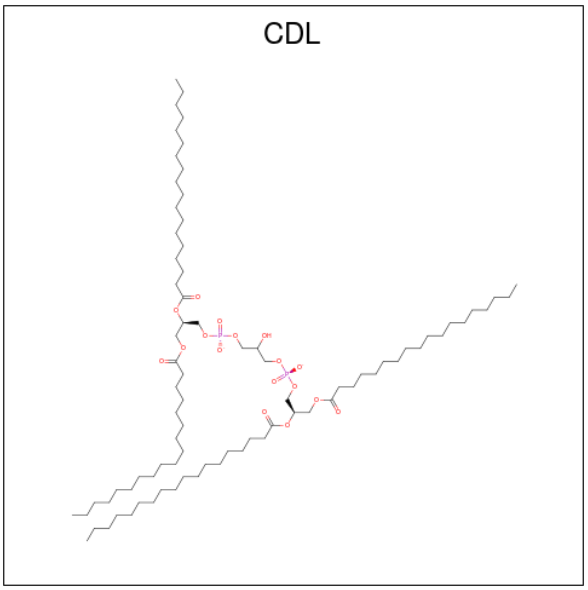


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (three-letter code: K) (formula: K).

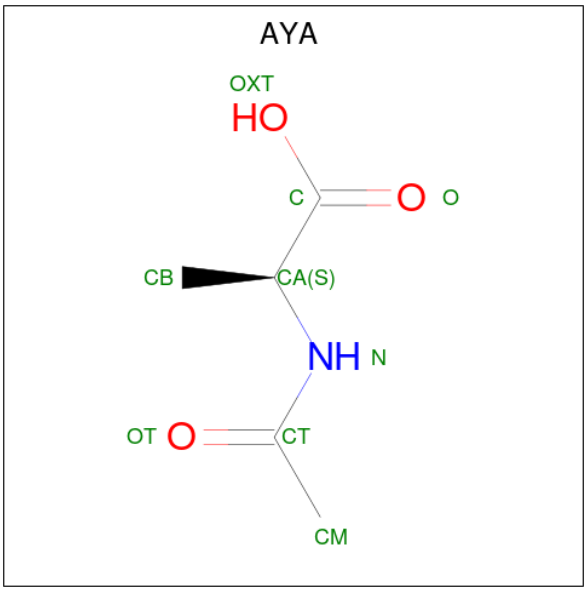
Mol	Chain	Residues	Atoms		AltConf
74	1G	1	Total	K	0
			1	1	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



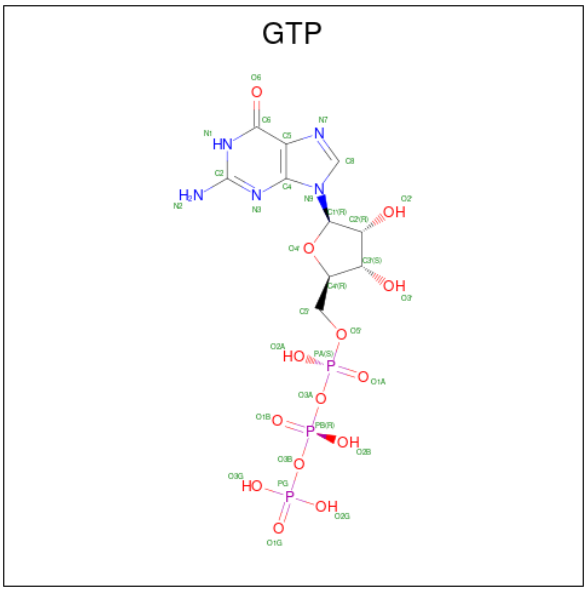
Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			87	68	17	2	
75	1N	1	Total	C	O	P	0
			77	58	17	2	
75	1Y	1	Total	C	O	P	0
			100	81	17	2	
75	1d	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			93	74	17	2	
75	1g	1	Total	C	O	P	0
			100	81	17	2	
75	1i	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	1q	1	Total	C	O	P	0
			100	81	17	2	
75	3A	1	Total	C	O	P	0
			98	79	17	2	
75	3D	1	Total	C	O	P	0
			56	37	17	2	
75	3F	1	Total	C	O	P	0
			100	81	17	2	
75	3N	1	Total	C	O	P	0
			100	81	17	2	
75	3P	1	Total	C	O	P	0
			100	81	17	2	
75	3T	1	Total	C	O	P	0
			57	38	17	2	
75	3X	1	Total	C	O	P	0
			100	81	17	2	
75	3Y	1	Total	C	O	P	0
			100	81	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is N-ACETYLALANINE (three-letter code: AYA) (formula: $C_5H_9NO_3$).



Mol	Chain	Residues	Atoms				AltConf
76	1I	1	Total	C	N	O	0
			8	5	1	2	

- Molecule 77 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

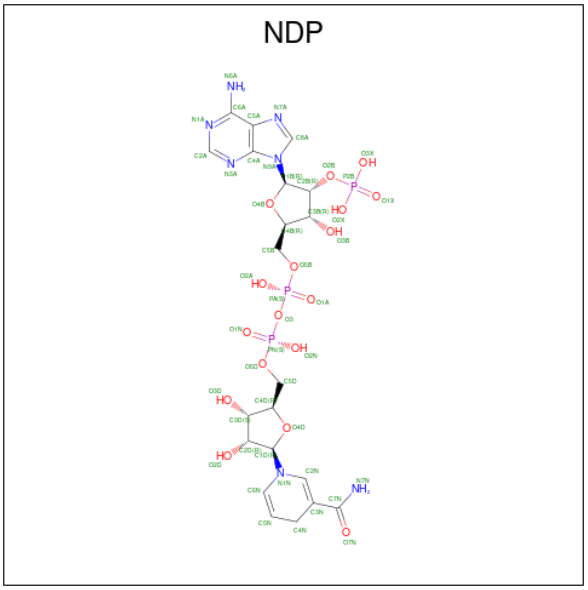


Mol	Chain	Residues	Atoms					AltConf
77	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
78	1O	1	Total Mg 1 1	0
78	4A	1	Total Mg 1 1	0

- Molecule 79 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

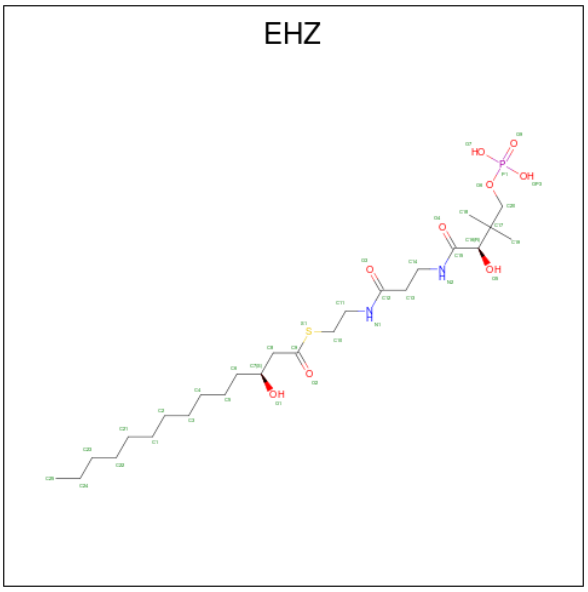


Mol	Chain	Residues	Atoms	AltConf
79	1P	1	Total C N O P 48 21 7 17 3	0

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

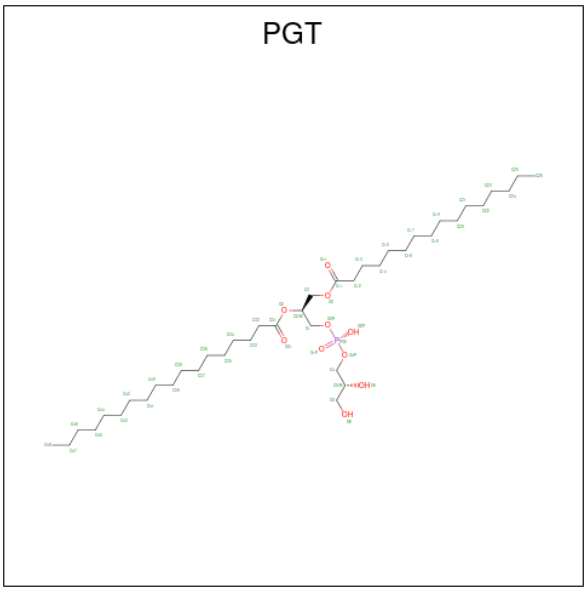
Mol	Chain	Residues	Atoms	AltConf
80	1R	1	Total Zn 1 1	0
80	4F	1	Total Zn 1 1	0

- Molecule 81 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



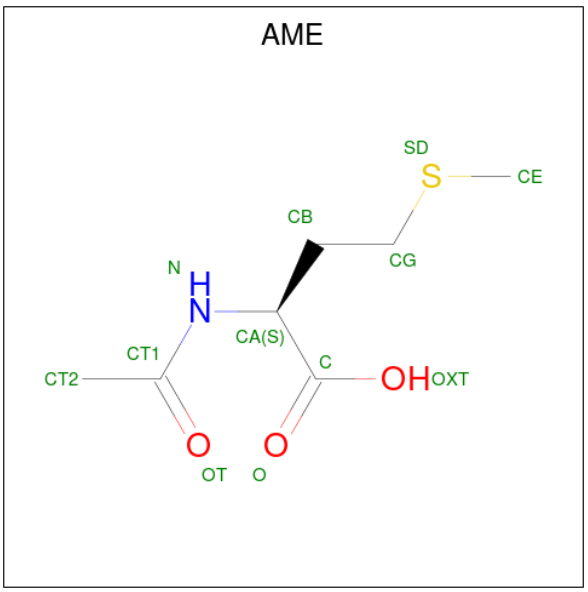
Mol	Chain	Residues	Atoms						AltConf
81	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 82 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



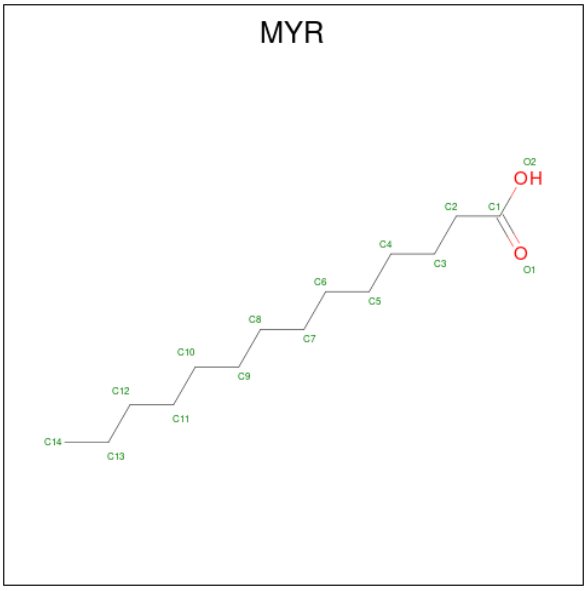
Mol	Chain	Residues	Atoms				AltConf
82	1Y	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 83 is N-ACETYLMETHIONINE (three-letter code: AME) (formula: $C_7H_{13}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
83	1h	1	11	7	1	2	1	0

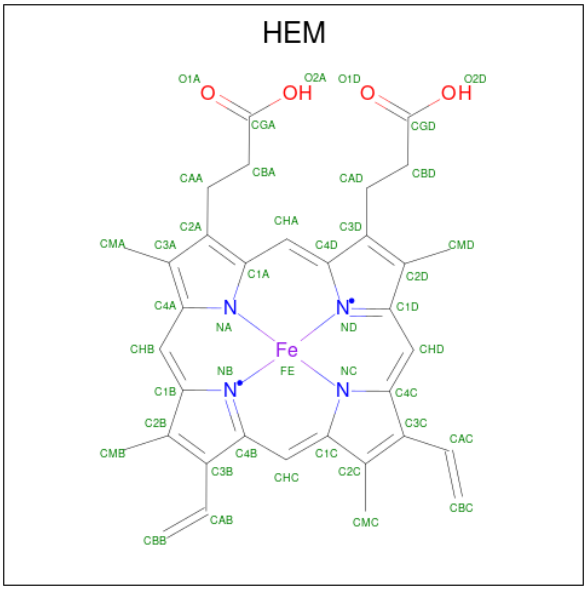
- Molecule 84 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
84	1l	1	15	14	1	0

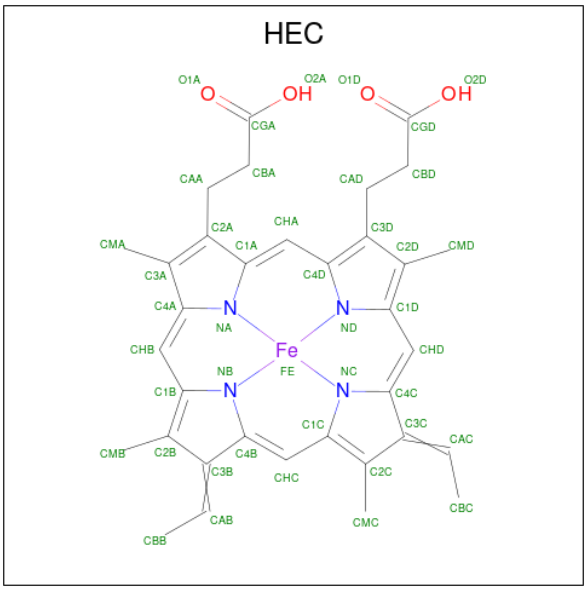
- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



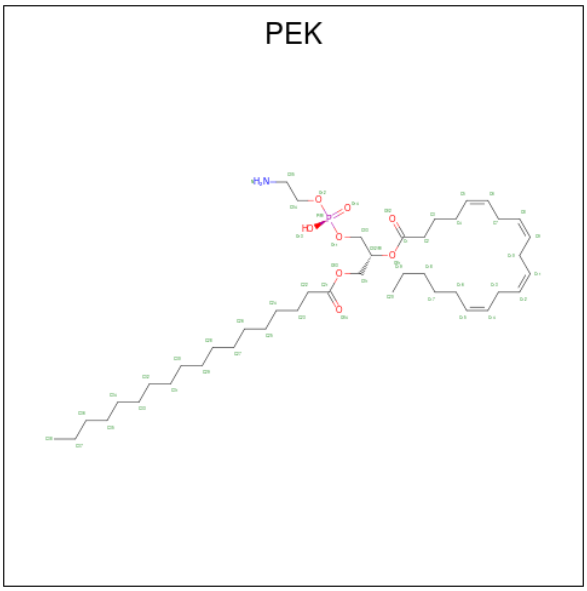
Mol	Chain	Residues	Atoms					AltConf
85	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
85	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
85	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
85	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 86 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



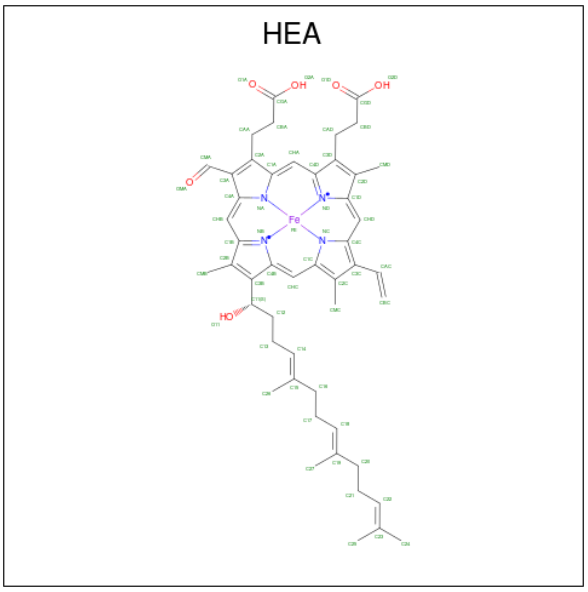
Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
86	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 87 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
87	3X	1	Total	C	N	O	P	0
			53	43	1	8	1	
87	4G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 88 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
88	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
88	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

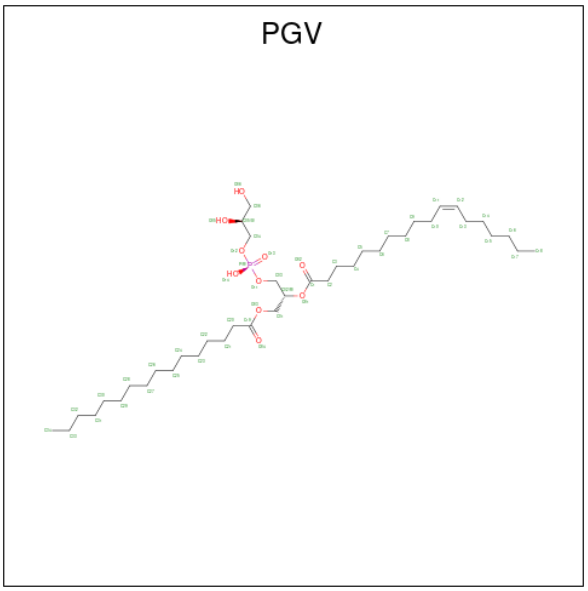
- Molecule 89 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
89	4A	1	Total	Cu	0
			1	1	

- Molecule 90 is SODIUM ION (three-letter code: NA) (formula: Na).

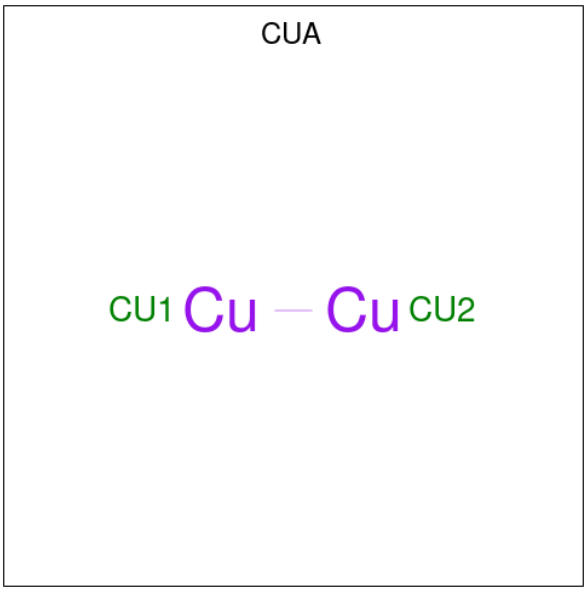
Mol	Chain	Residues	Atoms		AltConf
90	4A	1	Total	Na	0
			1	1	

- Molecule 91 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



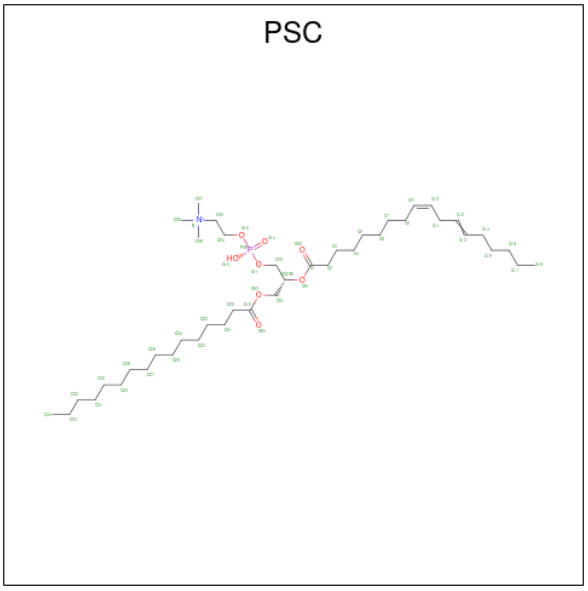
Mol	Chain	Residues	Atoms				AltConf
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4G	1	Total	C	O	P	0
			51	40	10	1	
91	4J	1	Total	C	O	P	0
			42	31	10	1	
91	4K	1	Total	C	O	P	0
			43	32	10	1	
91	4N	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 92 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



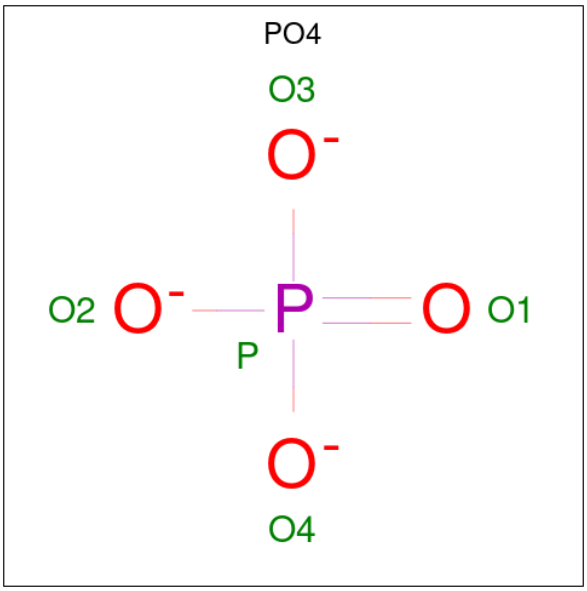
Mol	Chain	Residues	Atoms		AltConf
92	4B	1	Total	Cu	0
			2	2	

- Molecule 93 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
93	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 94 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



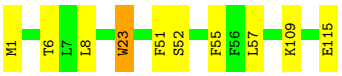
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
94	4H	1	5	4	1	0

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.

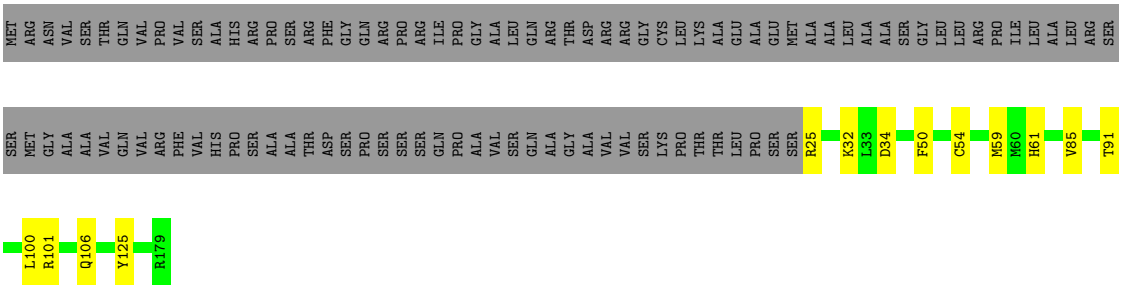
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain 1A:



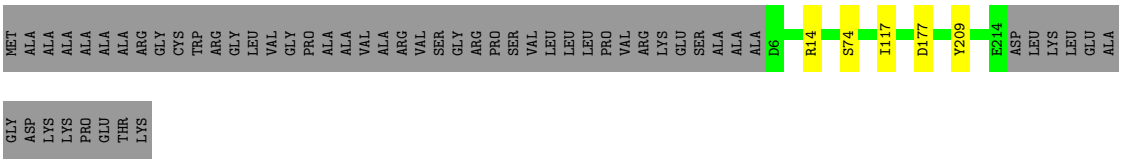
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 1B:



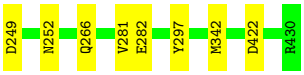
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain 1C:



• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D:



• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

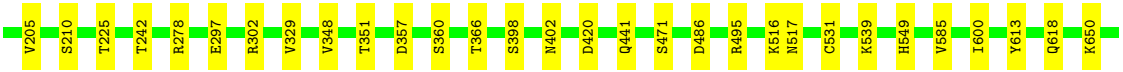
Chain 1E:

• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F:

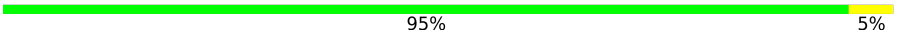
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G:



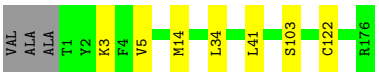
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:



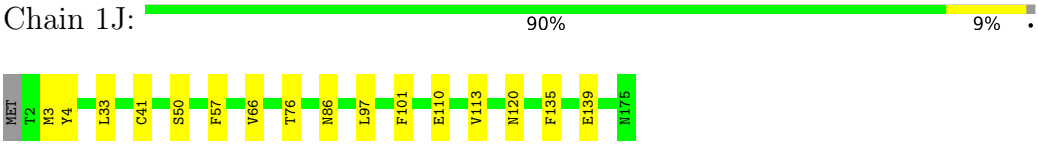
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I:



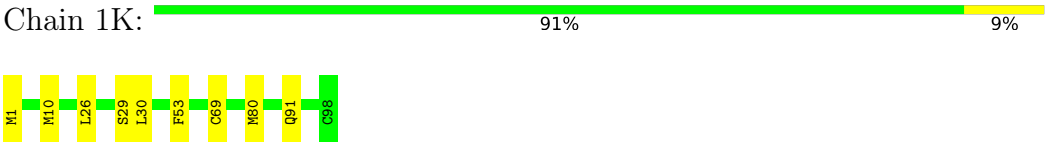
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:



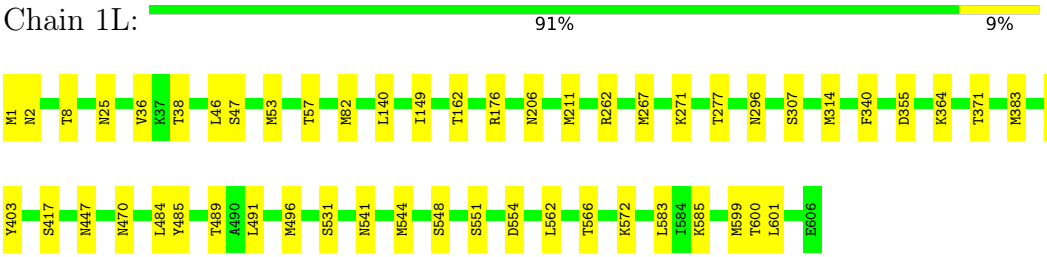
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:



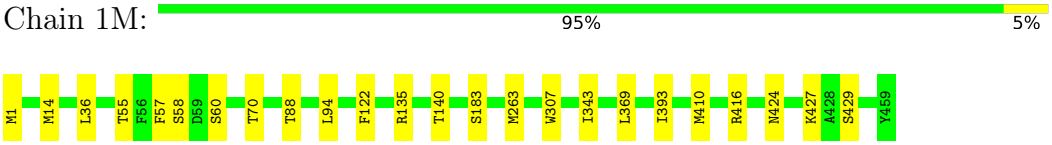
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L:



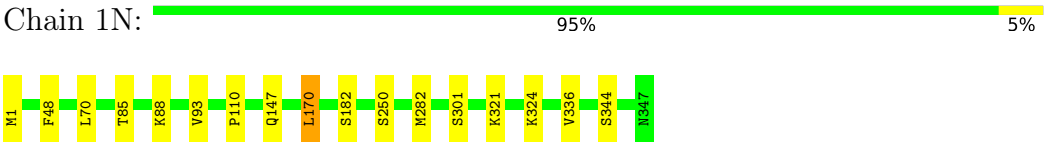
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:



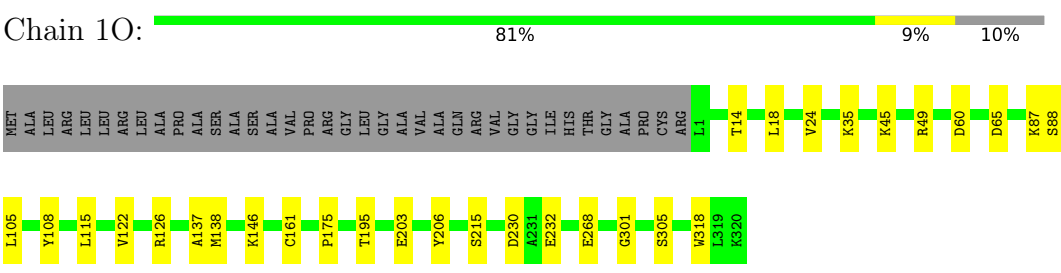
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:



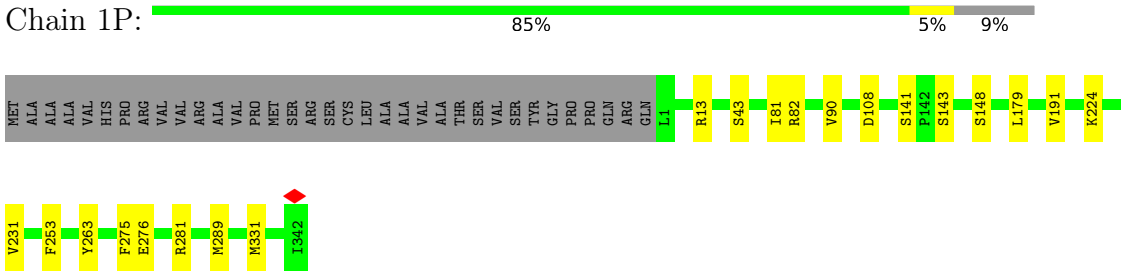
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:



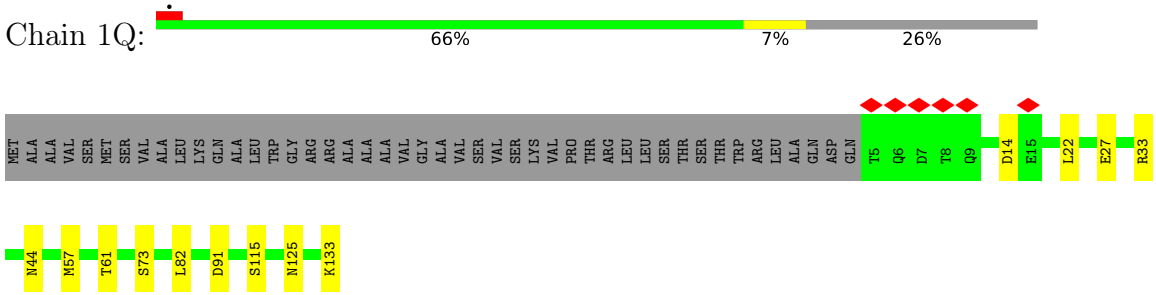
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:



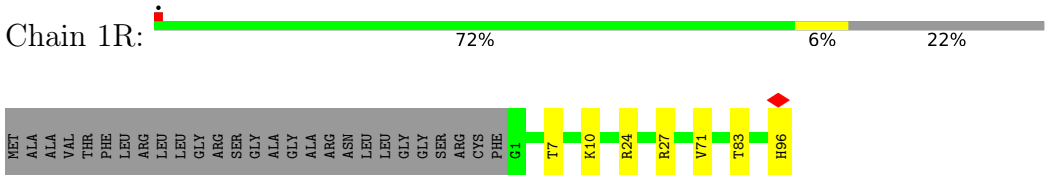
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:



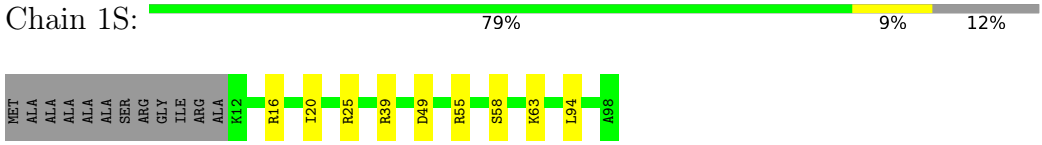
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



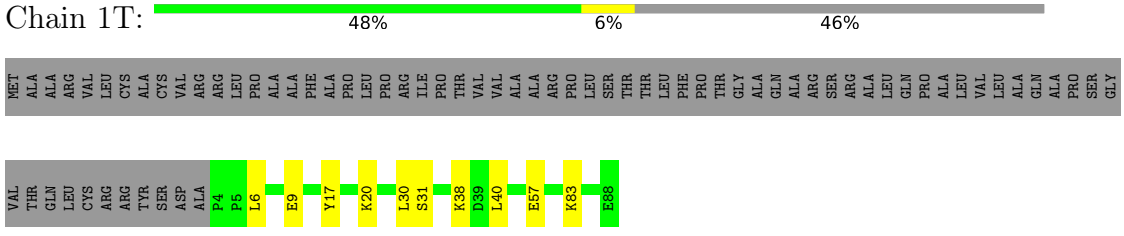
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S:



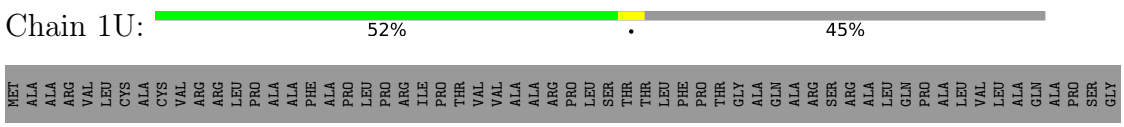
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

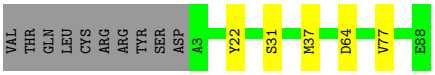
Chain 1T:



• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

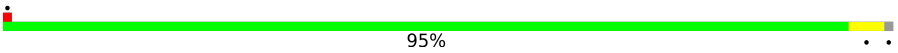
Chain 1U:

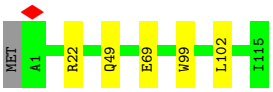




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

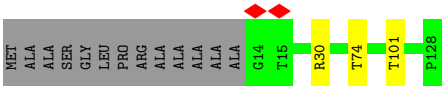
Chain 1V:





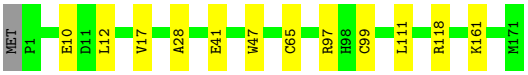
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain 1W:



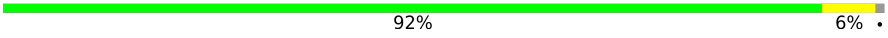
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X:



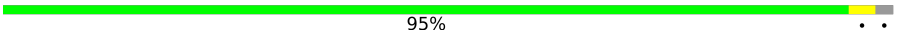
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

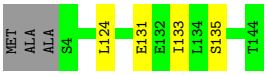
Chain 1Y:



• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

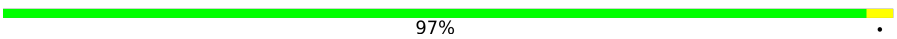
Chain 1Z:





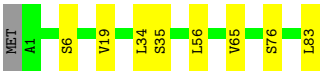
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a:



• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b:

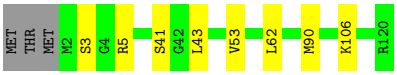


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c:

• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d:

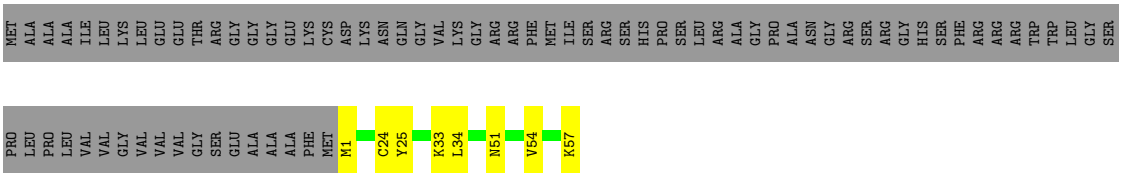


• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:

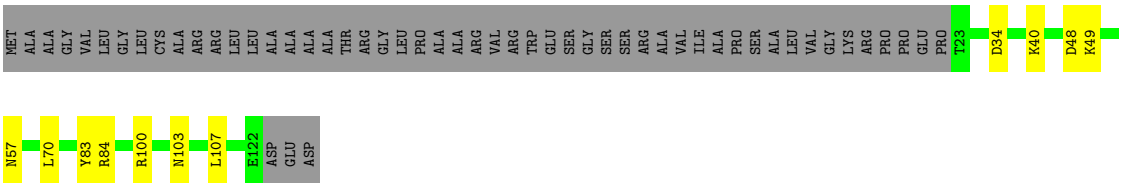
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f:



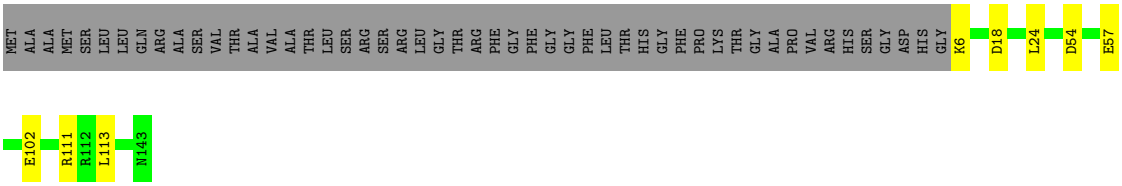
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:

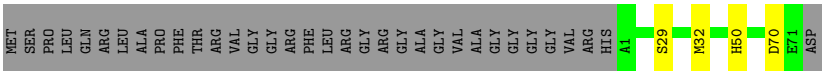


• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:

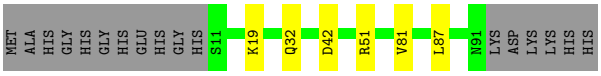
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:

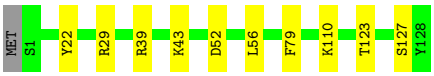


• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l:

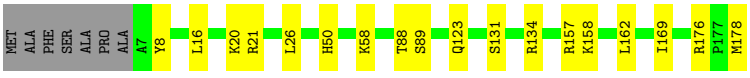
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m:



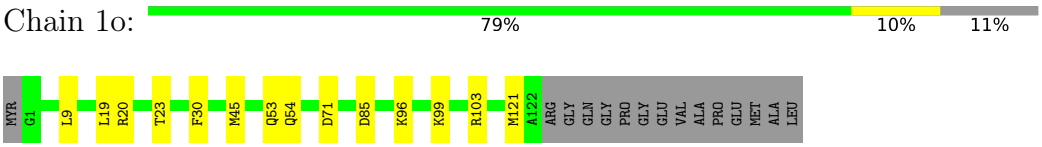
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n:



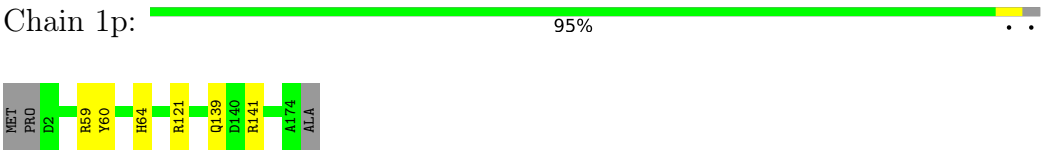
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:



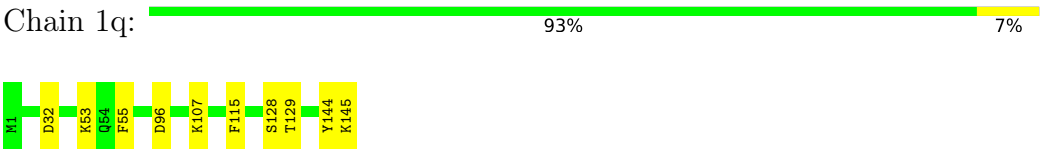
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p:



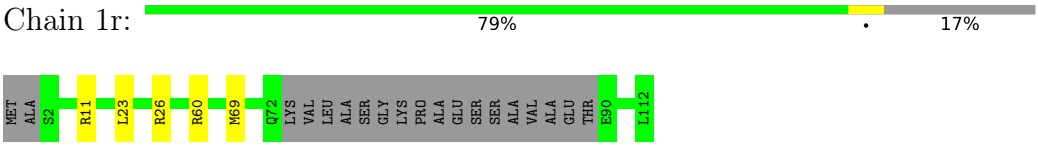
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:



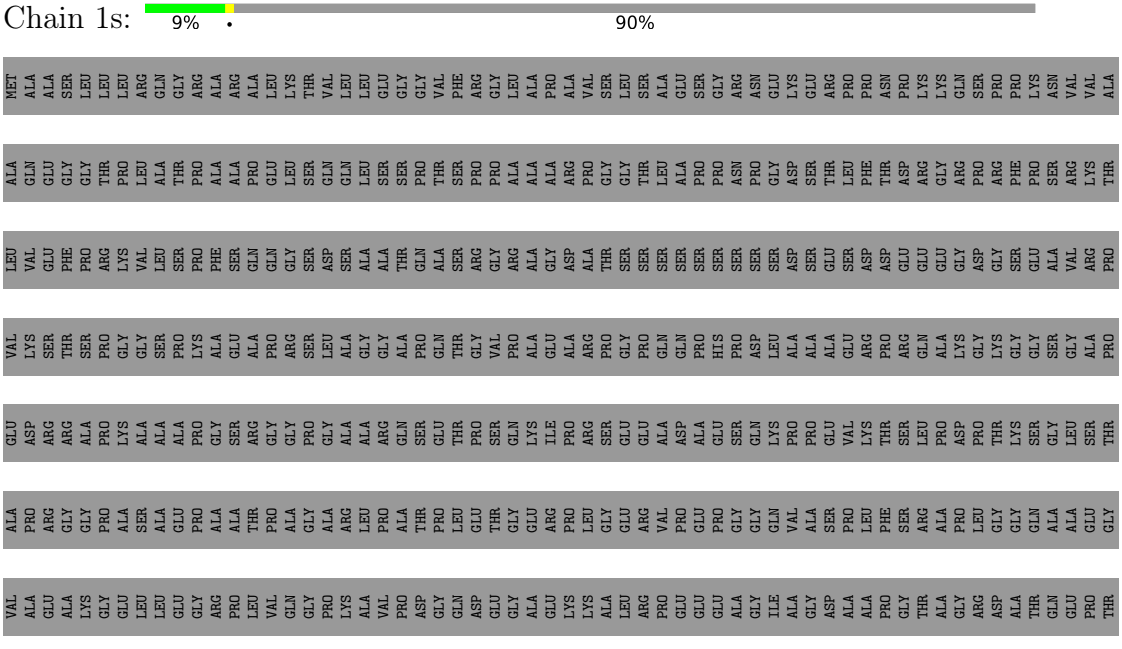
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

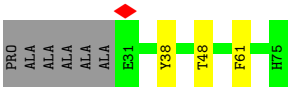
Chain 1r:



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

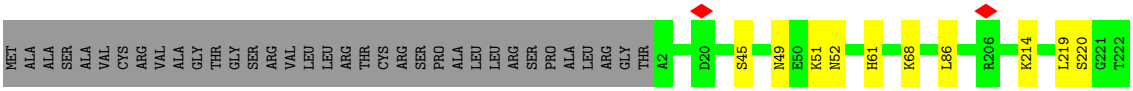
Chain 1s:

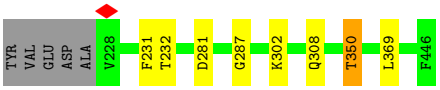




• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 3A:



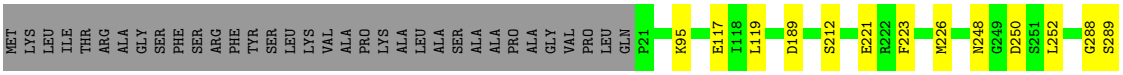


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 3N:

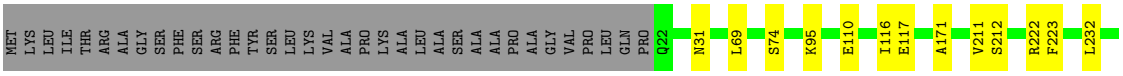
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B:



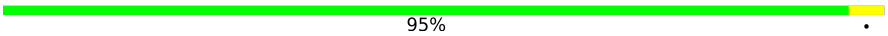
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

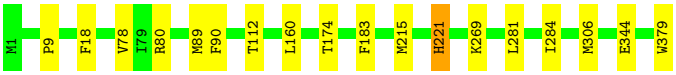
Chain 3O:



• Molecule 47: Cytochrome b

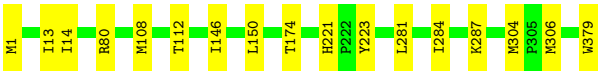
Chain 3C:





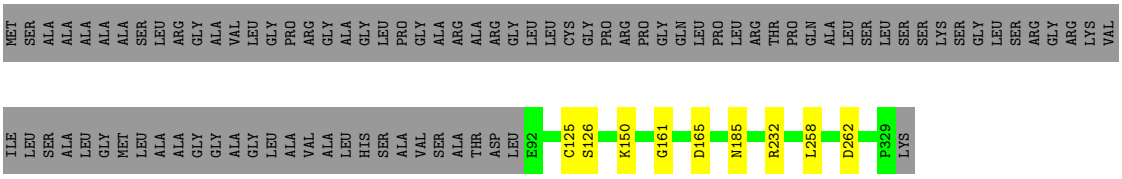
• Molecule 47: Cytochrome b

Chain 3P:



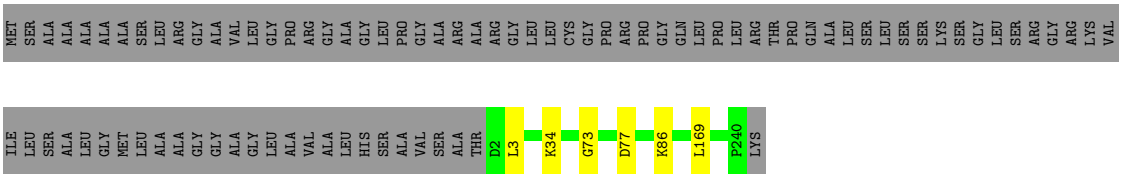
• Molecule 48: Cytochrome c1

Chain 3D:



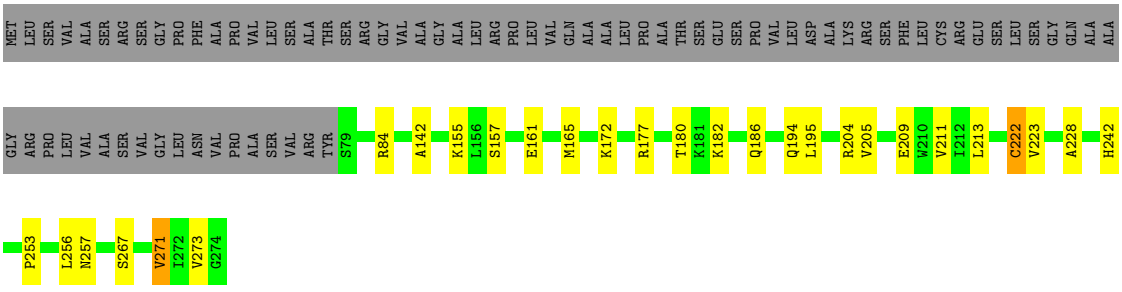
• Molecule 48: Cytochrome c1

Chain 3Q:



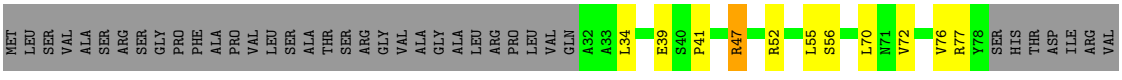
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

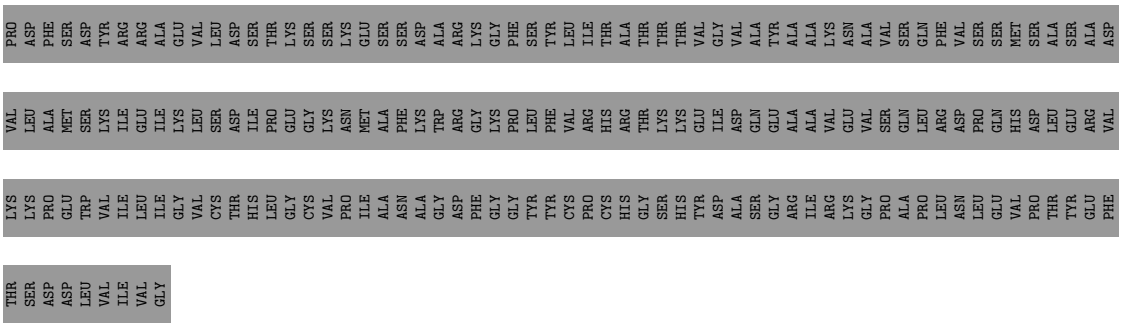
Chain 3E:



• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

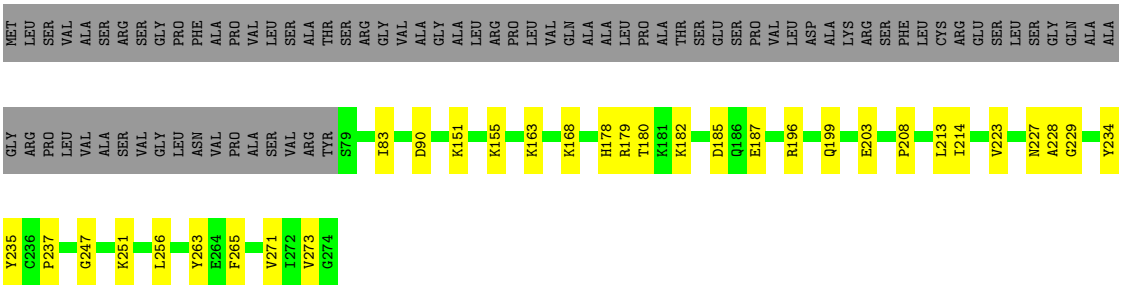
Chain 3I:





• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3R:

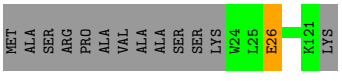


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3V:

• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3F:

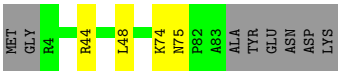


• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3S:

• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3G:

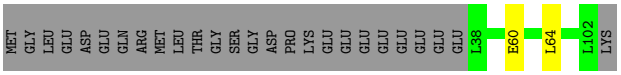


• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T:

• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H:



• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

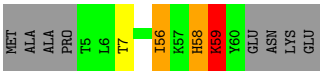
Chain 3U:

• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J:

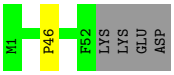
• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W:



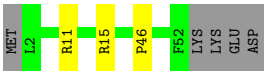
• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X:



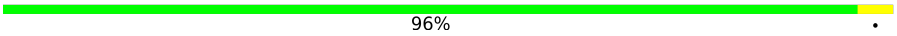
• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y:



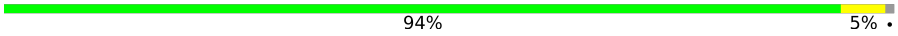
• Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A:



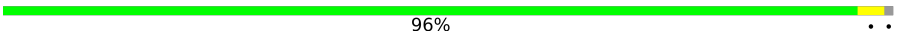
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B:



• Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C:



• Molecule 58: Cytochrome c oxidase subunit 4

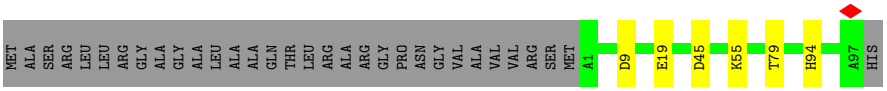
Chain 4D:

• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

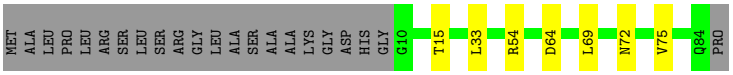
Chain 4E:

• Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 4F:

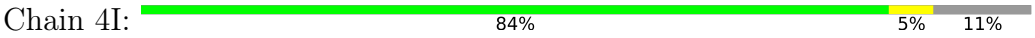


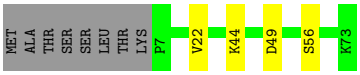
• Molecule 61: Cytochrome c oxidase subunit 6A2



• Molecule 62: Cytochrome c oxidase subunit 6B1

• Molecule 63: Cytochrome c oxidase subunit 6C



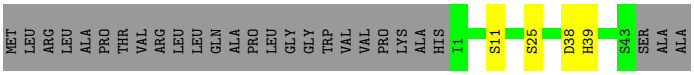


• Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

• Molecule 65: Cytochrome c oxidase subunit 7B

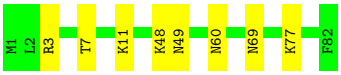
• Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial

• Molecule 67: Cytochrome c oxidase subunit 8



• Molecule 68: Cytochrome c oxidase subunit NDUFA4

Chain 4N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.404	Depositor
Minimum map value	-0.225	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, PGV, CDL, PC1, HEA, SF4, MG, PEK, K, 3PE, ZN, NDP, PGT, NA, FMN, CUA, FES, HEC, EHZ, AME, PSC, GTP, MYR, HEM, CU, PO4, AYA, SAC

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	1A	0.34	0/930	0.55	0/1271
2	1B	0.46	0/1273	0.63	0/1722
3	1C	0.25	0/1791	0.49	0/2439
4	1D	0.30	0/3545	0.50	0/4806
5	1E	0.33	0/1698	0.54	0/2311
6	1F	0.34	0/3401	0.55	0/4595
7	1G	0.34	0/5451	0.57	0/7387
8	1H	0.39	0/2566	0.60	4/3509 (0.1%)
9	1I	0.55	0/1443	0.69	0/1952
10	1J	0.45	0/1364	0.67	0/1850
11	1K	0.42	0/751	0.61	0/1018
12	1L	0.32	0/4939	0.47	1/6718 (0.0%)
13	1M	0.38	0/3713	0.50	0/5063
14	1N	0.37	0/2765	0.54	1/3758 (0.0%)
15	1O	0.46	2/2650 (0.1%)	0.63	4/3588 (0.1%)
16	1P	0.28	0/2828	0.51	0/3834
17	1Q	0.27	0/1070	0.51	0/1446
18	1R	0.26	0/755	0.56	0/1018
19	1S	0.24	0/711	0.51	0/956
20	1T	0.26	0/701	0.52	0/946
20	1U	0.25	0/706	0.46	0/954
21	1V	0.24	0/946	0.45	0/1281
22	1W	0.25	0/995	0.52	0/1340
23	1X	0.26	0/1436	0.48	0/1938
24	1Y	0.63	0/1037	0.70	0/1404
25	1Z	0.36	0/1199	0.55	0/1617
26	1a	0.38	0/577	0.53	0/777
27	1b	0.25	0/664	0.46	0/912
28	1c	0.25	0/430	0.47	0/581
29	1d	0.34	0/1016	0.52	0/1374
30	1e	0.24	0/836	0.49	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	1f	0.39	0/499	0.65	2/673 (0.3%)
32	1g	0.27	0/858	0.51	0/1165
33	1h	0.26	0/1184	0.49	0/1603
34	1i	0.26	0/1131	0.54	1/1541 (0.1%)
35	1j	0.24	0/627	0.46	0/858
36	1k	0.26	0/668	0.50	1/903 (0.1%)
37	1l	0.25	0/1365	0.48	0/1867
38	1m	0.30	0/1092	0.57	0/1481
39	1n	0.26	0/1549	0.53	0/2098
40	1o	0.24	0/1069	0.54	0/1430
41	1p	0.25	0/1481	0.53	0/1997
42	1q	0.41	0/1253	0.53	0/1704
43	1r	0.36	0/777	0.57	0/1051
44	1s	0.29	0/394	0.56	0/533
45	3A	0.46	0/3481	0.59	1/4722 (0.0%)
45	3N	0.47	0/3496	0.61	0/4723
46	3B	0.46	0/3190	0.57	0/4317
46	3O	0.45	0/3175	0.58	0/4292
47	3C	0.44	0/3123	0.57	0/4269
47	3P	0.43	0/3122	0.57	1/4269 (0.0%)
48	3D	0.47	0/1946	0.58	0/2641
48	3Q	0.44	0/1962	0.57	0/2663
49	3E	0.36	0/1551	0.56	0/2098
49	3I	0.59	0/342	0.74	0/465
49	3R	0.40	0/1551	0.56	0/2098
49	3V	0.44	0/225	0.59	0/303
50	3F	0.49	0/888	0.61	1/1193 (0.1%)
50	3S	0.44	0/888	0.53	0/1193
51	3G	0.51	0/648	0.58	0/874
51	3T	0.45	0/649	0.53	0/878
52	3H	0.49	0/538	0.61	0/721
52	3U	0.56	0/539	0.69	0/724
53	3J	1.19	2/476 (0.4%)	3.74	9/641 (1.4%)
53	3W	1.21	3/475 (0.6%)	3.72	8/638 (1.3%)
54	3X	0.42	0/445	0.57	0/608
54	3Y	0.43	0/437	0.54	0/598
55	4A	0.31	0/4156	0.47	0/5679
56	4B	0.29	0/1865	0.51	0/2544
57	4C	0.32	0/2179	0.45	0/2981
58	4D	0.29	0/1197	0.45	0/1617
59	4E	0.29	0/871	0.51	0/1182
60	4F	0.28	0/749	0.54	0/1016
61	4G	0.27	0/644	0.49	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
62	4H	0.33	0/708	0.59	1/956 (0.1%)
63	4I	0.30	0/563	0.50	0/748
64	4J	0.27	0/466	0.44	0/631
65	4K	0.26	0/396	0.47	0/543
66	4L	0.28	0/394	0.47	0/528
67	4M	0.29	0/349	0.45	0/477
68	4N	0.31	0/680	0.49	0/921
All	All	0.39	7/116498 (0.0%)	0.64	35/158019 (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
6	1F	0	1
10	1J	0	1
12	1L	0	1
15	1O	0	1
26	1a	0	1
45	3N	0	2
49	3I	0	2
53	3J	0	3
53	3W	0	3
All	All	0	15

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	3J	59	LYS	C-N	19.61	1.79	1.34
53	3W	56	ILE	C-N	-17.33	0.94	1.34
53	3W	58	HIS	C-N	-13.55	1.02	1.34
53	3J	56	ILE	C-N	-11.47	1.07	1.34
15	1O	175	PRO	CG-CD	-11.18	1.13	1.50
53	3W	59	LYS	C-N	10.71	1.58	1.34
15	1O	175	PRO	N-CD	5.91	1.56	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	3J	58	HIS	O-C-N	-62.41	22.84	122.70
53	3W	56	ILE	CA-C-N	-46.78	14.29	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	3W	59	LYS	C-N-CA	-42.18	16.25	121.70
53	3J	57	LYS	O-C-N	-41.91	55.65	122.70
53	3W	56	ILE	C-N-CA	-35.75	32.31	121.70
53	3W	58	HIS	CA-C-N	-34.62	41.04	117.20
53	3J	56	ILE	CA-C-N	-33.35	43.82	117.20
53	3W	59	LYS	CA-C-N	-32.31	46.11	117.20
53	3J	56	ILE	C-N-CA	-30.05	46.59	121.70
53	3W	58	HIS	C-N-CA	-24.54	60.35	121.70
53	3J	57	LYS	CA-C-N	-19.32	74.69	117.20
53	3J	56	ILE	O-C-N	18.55	152.38	122.70
53	3W	58	HIS	O-C-N	-18.47	93.15	122.70
53	3W	59	LYS	O-C-N	13.87	144.89	122.70
53	3J	57	LYS	C-N-CA	-13.77	87.27	121.70
15	1O	175	PRO	N-CD-CG	-11.95	85.27	103.20
15	1O	175	PRO	CA-N-CD	-11.61	95.24	111.50
8	1H	252	PRO	CA-N-CD	-8.02	100.27	111.50
53	3J	59	LYS	O-C-N	7.32	134.41	122.70
34	1i	117	PRO	CA-N-CD	-7.19	101.44	111.50
53	3J	59	LYS	CA-C-N	-6.78	102.29	117.20
15	1O	175	PRO	CA-CB-CG	-6.72	91.23	104.00
8	1H	252	PRO	N-CD-CG	-6.70	93.15	103.20
62	4H	49	ASP	CB-CG-OD1	6.59	124.23	118.30
8	1H	252	PRO	CA-CB-CG	-5.65	93.27	104.00
31	1f	34	LEU	N-CA-C	-5.61	95.84	111.00
50	3F	26	GLU	N-CA-C	-5.56	96.00	111.00
36	1k	42	ASP	CB-CG-OD1	5.53	123.28	118.30
47	3P	223	TYR	N-CA-C	5.45	125.72	111.00
12	1L	585	LYS	N-CA-CB	-5.35	100.97	110.60
45	3A	232	THR	N-CA-C	-5.14	97.13	111.00
14	1N	170	LEU	CA-CB-CG	5.13	127.11	115.30
15	1O	105	LEU	N-CA-C	-5.12	97.18	111.00
8	1H	101	GLY	N-CA-C	5.04	125.70	113.10
31	1f	24	CYS	O-C-N	-5.03	114.66	122.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
10	1J	86	ASN	Mainchain
12	1L	583	LEU	Mainchain
15	1O	301	GLY	Mainchain

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Mol	Chain	Res	Type	Group
26	1a	37	ARG	Mainchain
49	3I	47	ARG	Sidechain
49	3I	52	ARG	Sidechain
53	3J	56	ILE	Mainchain
53	3J	57	LYS	Mainchain
53	3J	58	HIS	Mainchain
45	3N	206	ARG	Mainchain
53	3W	56	ILE	Mainchain
53	3W	58	HIS	Mainchain
53	3W	59	LYS	Mainchain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	1A	113/115 (98%)	101 (89%)	9 (8%)	3 (3%)	5 1
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100 100
3	1C	207/264 (78%)	198 (96%)	9 (4%)	0	100 100
4	1D	427/466 (92%)	411 (96%)	16 (4%)	0	100 100
5	1E	212/249 (85%)	198 (93%)	12 (6%)	2 (1%)	17 12
6	1F	430/464 (93%)	404 (94%)	22 (5%)	4 (1%)	17 12
7	1G	697/727 (96%)	667 (96%)	27 (4%)	3 (0%)	34 32
8	1H	316/318 (99%)	297 (94%)	17 (5%)	2 (1%)	25 21
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100 100
10	1J	172/175 (98%)	160 (93%)	11 (6%)	1 (1%)	25 21
11	1K	96/98 (98%)	95 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	1L	604/606 (100%)	567 (94%)	33 (6%)	4 (1%)	22	18
13	1M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	1N	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	41	41
15	1O	318/357 (89%)	296 (93%)	17 (5%)	5 (2%)	9	5
16	1P	340/377 (90%)	328 (96%)	11 (3%)	1 (0%)	41	41
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	81 (98%)	2 (2%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	21
24	1Y	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
25	1Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	53 (96%)	2 (4%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
33	1h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	1i	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	164 (96%)	6 (4%)	0	100	100
40	1o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	1q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	84 (93%)	6 (7%)	0	100	100
44	1s	43/471 (9%)	40 (93%)	3 (7%)	0	100	100
45	3A	436/480 (91%)	418 (96%)	13 (3%)	5 (1%)	14	9
45	3N	444/480 (92%)	426 (96%)	12 (3%)	6 (1%)	11	6
46	3B	414/453 (91%)	387 (94%)	21 (5%)	6 (1%)	11	6
46	3O	413/453 (91%)	393 (95%)	19 (5%)	1 (0%)	47	49
47	3C	377/379 (100%)	368 (98%)	8 (2%)	1 (0%)	41	41
47	3P	377/379 (100%)	367 (97%)	9 (2%)	1 (0%)	41	41
48	3D	235/326 (72%)	228 (97%)	6 (3%)	1 (0%)	34	32
48	3Q	237/326 (73%)	224 (94%)	12 (5%)	1 (0%)	34	32
49	3E	194/274 (71%)	166 (86%)	18 (9%)	10 (5%)	2	0
49	3I	45/274 (16%)	31 (69%)	12 (27%)	2 (4%)	2	0
49	3R	194/274 (71%)	163 (84%)	22 (11%)	9 (5%)	2	0
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	70/82 (85%)	69 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	61/91 (67%)	60 (98%)	1 (2%)	0	100	100
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/64 (84%)	50 (93%)	2 (4%)	2 (4%)	3	1
53	3W	52/64 (81%)	50 (96%)	1 (2%)	1 (2%)	8	3
54	3X	50/56 (89%)	46 (92%)	3 (6%)	1 (2%)	7	3
54	3Y	49/56 (88%)	45 (92%)	3 (6%)	1 (2%)	7	3
55	4A	512/514 (100%)	488 (95%)	21 (4%)	3 (1%)	25	21
56	4B	225/229 (98%)	211 (94%)	14 (6%)	0	100	100
57	4C	257/261 (98%)	245 (95%)	12 (5%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
60	4F	95/129 (74%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	72 (90%)	8 (10%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
66	4L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
All	All	14067/16999 (83%)	13359 (95%)	630 (4%)	78 (1%)	29	21

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	115	ASP
8	1H	92	PRO
10	1J	66	VAL
12	1L	562	LEU
15	1O	138	MET
16	1P	276	GLU
23	1X	28	ALA
45	3A	369	LEU
46	3B	226	MET
46	3B	250	ASP
46	3B	309	VAL
49	3E	157	SER
49	3E	228	ALA
49	3E	271	VAL
53	3J	57	LYS
45	3N	71	PRO
45	3N	172	GLU
45	3N	224	VAL
49	3R	182	LYS
49	3R	228	ALA
53	3W	59	LYS
54	3X	46	PRO
54	3Y	46	PRO
1	1A	23	TRP
6	1F	205	LEU
8	1H	208	VAL

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Mol	Chain	Res	Type
12	1L	601	LEU
15	1O	35	LYS
15	1O	137	ALA
45	3A	220	SER
45	3A	287	GLY
46	3B	288	GLY
48	3D	161	GLY
49	3E	253	PRO
49	3E	256	LEU
49	3E	273	VAL
53	3J	54	LYS
45	3N	72	GLY
45	3N	214	LYS
48	3Q	73	GLY
49	3R	151	LYS
49	3R	229	GLY
49	3R	247	GLY
49	3R	273	VAL
55	4A	290	HIS
1	1A	52	SER
1	1A	109	LYS
6	1F	249	ARG
6	1F	297	VAL
12	1L	600	THR
15	1O	126	ARG
45	3A	350	THR
46	3B	289	SER
49	3E	142	ALA
49	3E	222	CYS
5	1E	110	LEU
5	1E	157	ASN
49	3E	223	VAL
49	3I	41	PRO
49	3I	56	SER
45	3N	287	GLY
46	3O	171	ALA
7	1G	654	GLN
15	1O	305	SER
45	3A	231	PHE
49	3E	267	SER
47	3P	221	HIS
6	1F	207	PRO

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Mol	Chain	Res	Type
46	3B	248	ASN
49	3R	223	VAL
55	4A	128	VAL
7	1G	111	GLY
47	3C	221	HIS
55	4A	3	VAL
12	1L	2	ASN
14	1N	110	PRO
49	3R	208	PRO
49	3R	237	PRO

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	1A	99/99 (100%)	92 (93%)	7 (7%)	14 11
2	1B	131/212 (62%)	118 (90%)	13 (10%)	8 5
3	1C	190/227 (84%)	185 (97%)	5 (3%)	46 50
4	1D	371/396 (94%)	352 (95%)	19 (5%)	24 22
5	1E	183/207 (88%)	176 (96%)	7 (4%)	33 34
6	1F	346/368 (94%)	326 (94%)	20 (6%)	20 17
7	1G	588/610 (96%)	540 (92%)	48 (8%)	11 8
8	1H	274/274 (100%)	262 (96%)	12 (4%)	28 28
9	1I	151/201 (75%)	144 (95%)	7 (5%)	27 26
10	1J	140/141 (99%)	126 (90%)	14 (10%)	7 5
11	1K	84/84 (100%)	76 (90%)	8 (10%)	8 5
12	1L	539/539 (100%)	492 (91%)	47 (9%)	10 7
13	1M	408/408 (100%)	385 (94%)	23 (6%)	21 18
14	1N	310/310 (100%)	295 (95%)	15 (5%)	25 24
15	1O	283/307 (92%)	260 (92%)	23 (8%)	11 8
16	1P	296/323 (92%)	277 (94%)	19 (6%)	17 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	1Q	117/152 (77%)	104 (89%)	13 (11%)	6 3
18	1R	79/97 (81%)	72 (91%)	7 (9%)	9 6
19	1S	77/82 (94%)	68 (88%)	9 (12%)	5 3
20	1T	79/133 (59%)	69 (87%)	10 (13%)	4 2
20	1U	79/133 (59%)	74 (94%)	5 (6%)	18 15
21	1V	100/101 (99%)	95 (95%)	5 (5%)	24 23
22	1W	107/112 (96%)	104 (97%)	3 (3%)	43 47
23	1X	153/154 (99%)	142 (93%)	11 (7%)	14 11
24	1Y	101/102 (99%)	92 (91%)	9 (9%)	9 6
25	1Z	123/124 (99%)	119 (97%)	4 (3%)	38 40
26	1a	58/58 (100%)	57 (98%)	1 (2%)	60 67
27	1b	69/70 (99%)	61 (88%)	8 (12%)	5 3
28	1c	45/66 (68%)	40 (89%)	5 (11%)	6 3
29	1d	106/109 (97%)	98 (92%)	8 (8%)	13 10
30	1e	87/94 (93%)	82 (94%)	5 (6%)	20 18
31	1f	54/113 (48%)	48 (89%)	6 (11%)	6 3
32	1g	92/129 (71%)	81 (88%)	11 (12%)	5 2
33	1h	121/158 (77%)	113 (93%)	8 (7%)	16 14
34	1i	119/120 (99%)	111 (93%)	8 (7%)	16 13
35	1j	62/84 (74%)	58 (94%)	4 (6%)	17 14
36	1k	63/76 (83%)	58 (92%)	5 (8%)	12 9
37	1l	141/161 (88%)	130 (92%)	11 (8%)	12 9
38	1m	113/114 (99%)	103 (91%)	10 (9%)	10 6
39	1n	156/160 (98%)	138 (88%)	18 (12%)	5 3
40	1o	110/119 (92%)	96 (87%)	14 (13%)	4 2
41	1p	154/156 (99%)	148 (96%)	6 (4%)	32 33
42	1q	131/131 (100%)	121 (92%)	10 (8%)	13 10
43	1r	85/98 (87%)	80 (94%)	5 (6%)	19 17
44	1s	44/351 (12%)	41 (93%)	3 (7%)	16 13
45	3A	367/397 (92%)	354 (96%)	13 (4%)	36 38
45	3N	372/397 (94%)	353 (95%)	19 (5%)	24 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	3B	328/355 (92%)	314 (96%)	14 (4%)	29 29
46	3O	327/355 (92%)	314 (96%)	13 (4%)	31 32
47	3C	332/332 (100%)	314 (95%)	18 (5%)	22 20
47	3P	332/332 (100%)	317 (96%)	15 (4%)	27 27
48	3D	202/259 (78%)	194 (96%)	8 (4%)	31 32
48	3Q	204/259 (79%)	199 (98%)	5 (2%)	47 52
49	3E	166/225 (74%)	146 (88%)	20 (12%)	5 2
49	3I	36/225 (16%)	28 (78%)	8 (22%)	1 0
49	3R	166/225 (74%)	143 (86%)	23 (14%)	3 1
49	3V	24/225 (11%)	23 (96%)	1 (4%)	30 30
50	3F	90/99 (91%)	89 (99%)	1 (1%)	73 79
50	3S	90/99 (91%)	89 (99%)	1 (1%)	73 79
51	3G	67/73 (92%)	63 (94%)	4 (6%)	19 16
51	3T	67/73 (92%)	63 (94%)	4 (6%)	19 16
52	3H	62/85 (73%)	60 (97%)	2 (3%)	39 41
52	3U	62/85 (73%)	56 (90%)	6 (10%)	8 5
53	3J	46/52 (88%)	46 (100%)	0	100 100
53	3W	46/52 (88%)	45 (98%)	1 (2%)	52 57
54	3X	42/46 (91%)	42 (100%)	0	100 100
54	3Y	41/46 (89%)	39 (95%)	2 (5%)	25 23
55	4A	424/424 (100%)	408 (96%)	16 (4%)	33 34
56	4B	210/211 (100%)	199 (95%)	11 (5%)	23 21
57	4C	223/225 (99%)	214 (96%)	9 (4%)	31 32
58	4D	124/149 (83%)	115 (93%)	9 (7%)	14 11
59	4E	92/124 (74%)	91 (99%)	1 (1%)	73 79
60	4F	80/101 (79%)	74 (92%)	6 (8%)	13 10
61	4G	65/80 (81%)	58 (89%)	7 (11%)	6 3
62	4H	73/76 (96%)	69 (94%)	4 (6%)	21 19
63	4I	54/61 (88%)	50 (93%)	4 (7%)	13 10
64	4J	49/68 (72%)	47 (96%)	2 (4%)	30 31
65	4K	38/66 (58%)	37 (97%)	1 (3%)	46 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
66	4L	39/55 (71%)	37 (95%)	2 (5%)	24 22
67	4M	37/57 (65%)	33 (89%)	4 (11%)	6 3
68	4N	70/70 (100%)	62 (89%)	8 (11%)	5 3
All	All	12265/14326 (86%)	11494 (94%)	771 (6%)	21 15

All (771) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	6	THR
1	1A	8	LEU
1	1A	23	TRP
1	1A	51	PHE
1	1A	55	PHE
1	1A	57	LEU
1	1A	115	GLU
2	1B	25	ARG
2	1B	32	LYS
2	1B	34	ASP
2	1B	50	PHE
2	1B	54	CYS
2	1B	59	MET
2	1B	61	HIS
2	1B	85	VAL
2	1B	91	THR
2	1B	100	LEU
2	1B	101	ARG
2	1B	106	GLN
2	1B	125	TYR
3	1C	14	ARG
3	1C	74	SER
3	1C	117	ILE
3	1C	177	ASP
3	1C	209	TYR
4	1D	29	LYS
4	1D	40	LYS
4	1D	61	VAL
4	1D	72	MET
4	1D	79	HIS
4	1D	108	TYR
4	1D	109	VAL
4	1D	140	LEU

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Mol	Chain	Res	Type
4	1D	164	MET
4	1D	209	ASP
4	1D	219	SER
4	1D	249	ASP
4	1D	252	ASN
4	1D	266	GLN
4	1D	281	VAL
4	1D	282	GLU
4	1D	297	TYR
4	1D	342	MET
4	1D	422	ASP
5	1E	75	VAL
5	1E	110	LEU
5	1E	114	ASP
5	1E	190	ARG
5	1E	192	SER
5	1E	199	LEU
5	1E	217	LEU
6	1F	10	THR
6	1F	32	ARG
6	1F	44	LYS
6	1F	91	LYS
6	1F	94	VAL
6	1F	104	THR
6	1F	114	ASP
6	1F	151	VAL
6	1F	164	LYS
6	1F	171	TYR
6	1F	175	VAL
6	1F	188	GLU
6	1F	231	SER
6	1F	250	ASN
6	1F	277	LYS
6	1F	287	VAL
6	1F	312	CYS
6	1F	385	ARG
6	1F	404	ILE
6	1F	437	HIS
7	1G	39	ARG
7	1G	65	VAL
7	1G	77	TRP
7	1G	98	LEU

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Mol	Chain	Res	Type
7	1G	116	LEU
7	1G	137	VAL
7	1G	146	VAL
7	1G	151	THR
7	1G	153	CYS
7	1G	156	CYS
7	1G	172	LEU
7	1G	180	ASP
7	1G	190	MET
7	1G	199	ILE
7	1G	205	VAL
7	1G	210	SER
7	1G	225	THR
7	1G	242	THR
7	1G	278	ARG
7	1G	297	GLU
7	1G	302	ARG
7	1G	329	VAL
7	1G	348	VAL
7	1G	351	THR
7	1G	357	ASP
7	1G	360	SER
7	1G	366	THR
7	1G	398	SER
7	1G	402	ASN
7	1G	420	ASP
7	1G	441	GLN
7	1G	471	SER
7	1G	486	ASP
7	1G	495	ARG
7	1G	516	LYS
7	1G	517	ASN
7	1G	531	CYS
7	1G	539	LYS
7	1G	549	HIS
7	1G	585	VAL
7	1G	600	ILE
7	1G	613	TYR
7	1G	618	GLN
7	1G	650	LYS
7	1G	669	LYS
7	1G	675	ASP

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Mol	Chain	Res	Type
7	1G	682	GLN
7	1G	689	LYS
8	1H	70	MET
8	1H	87	VAL
8	1H	105	MET
8	1H	119	SER
8	1H	126	LYS
8	1H	156	MET
8	1H	178	SER
8	1H	220	PHE
8	1H	234	MET
8	1H	237	PHE
8	1H	271	LEU
8	1H	274	ARG
9	1I	3	LYS
9	1I	5	VAL
9	1I	14	MET
9	1I	34	LEU
9	1I	41	LEU
9	1I	103	SER
9	1I	122	CYS
10	1J	3	MET
10	1J	4	TYR
10	1J	33	LEU
10	1J	41	CYS
10	1J	50	SER
10	1J	57	PHE
10	1J	76	THR
10	1J	97	LEU
10	1J	101	PHE
10	1J	110	GLU
10	1J	113	VAL
10	1J	120	ASN
10	1J	135	PHE
10	1J	139	GLU
11	1K	10	MET
11	1K	26	LEU
11	1K	29	SER
11	1K	30	LEU
11	1K	53	PHE
11	1K	69	CYS
11	1K	80	MET

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Mol	Chain	Res	Type
11	1K	91	GLN
12	1L	8	THR
12	1L	25	ASN
12	1L	36	VAL
12	1L	38	THR
12	1L	46	LEU
12	1L	47	SER
12	1L	53	MET
12	1L	57	THR
12	1L	82	MET
12	1L	140	LEU
12	1L	149	ILE
12	1L	162	THR
12	1L	176	ARG
12	1L	206	ASN
12	1L	211	MET
12	1L	262	ARG
12	1L	267	MET
12	1L	271	LYS
12	1L	277	THR
12	1L	296	ASN
12	1L	307	SER
12	1L	314	MET
12	1L	340	PHE
12	1L	355	ASP
12	1L	364	LYS
12	1L	371	THR
12	1L	383	MET
12	1L	387	THR
12	1L	393	ASP
12	1L	403	TYR
12	1L	417	SER
12	1L	447	ASN
12	1L	470	ASN
12	1L	484	LEU
12	1L	485	TYR
12	1L	489	THR
12	1L	491	LEU
12	1L	496	MET
12	1L	531	SER
12	1L	541	ASN
12	1L	544	MET

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Mol	Chain	Res	Type
12	1L	548	SER
12	1L	551	SER
12	1L	554	ASP
12	1L	566	THR
12	1L	572	LYS
12	1L	599	MET
13	1M	14	MET
13	1M	36	LEU
13	1M	55	THR
13	1M	57	PHE
13	1M	58	SER
13	1M	60	SER
13	1M	70	THR
13	1M	88	THR
13	1M	94	LEU
13	1M	122	PHE
13	1M	135	ARG
13	1M	140	THR
13	1M	183	SER
13	1M	263	MET
13	1M	307	TRP
13	1M	343	ILE
13	1M	369	LEU
13	1M	393	ILE
13	1M	410	MET
13	1M	416	ARG
13	1M	424	ASN
13	1M	427	LYS
13	1M	429	SER
14	1N	48	PHE
14	1N	70	LEU
14	1N	85	THR
14	1N	88	LYS
14	1N	93	VAL
14	1N	147	GLN
14	1N	170	LEU
14	1N	182	SER
14	1N	250	SER
14	1N	282	MET
14	1N	301	SER
14	1N	321	LYS
14	1N	324	LYS

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Mol	Chain	Res	Type
14	1N	336	VAL
14	1N	344	SER
15	1O	14	THR
15	1O	18	LEU
15	1O	24	VAL
15	1O	45	LYS
15	1O	49	ARG
15	1O	60	ASP
15	1O	65	ASP
15	1O	87	LYS
15	1O	88	SER
15	1O	96	LEU
15	1O	108	TYR
15	1O	115	LEU
15	1O	122	VAL
15	1O	146	LYS
15	1O	161	CYS
15	1O	195	THR
15	1O	203	GLU
15	1O	206	TYR
15	1O	215	SER
15	1O	230	ASP
15	1O	232	GLU
15	1O	268	GLU
15	1O	318	TRP
16	1P	13	ARG
16	1P	43	SER
16	1P	81	ILE
16	1P	82	ARG
16	1P	90	VAL
16	1P	108	ASP
16	1P	141	SER
16	1P	143	SER
16	1P	148	SER
16	1P	179	LEU
16	1P	191	VAL
16	1P	224	LYS
16	1P	231	VAL
16	1P	253	PHE
16	1P	263	TYR
16	1P	275	PHE
16	1P	281	ARG

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Mol	Chain	Res	Type
16	1P	289	MET
16	1P	331	MET
17	1Q	14	ASP
17	1Q	22	LEU
17	1Q	27	GLU
17	1Q	33	ARG
17	1Q	44	ASN
17	1Q	57	MET
17	1Q	61	THR
17	1Q	73	SER
17	1Q	82	LEU
17	1Q	91	ASP
17	1Q	115	SER
17	1Q	125	ASN
17	1Q	133	LYS
18	1R	7	THR
18	1R	10	LYS
18	1R	24	ARG
18	1R	27	ARG
18	1R	71	VAL
18	1R	83	THR
18	1R	96	HIS
19	1S	16	ARG
19	1S	20	ILE
19	1S	25	ARG
19	1S	39	ARG
19	1S	49	ASP
19	1S	55	ARG
19	1S	58	SER
19	1S	63	LYS
19	1S	94	LEU
20	1T	6	LEU
20	1T	9	GLU
20	1T	17	TYR
20	1T	20	LYS
20	1T	30	LEU
20	1T	31	SER
20	1T	38	LYS
20	1T	40	LEU
20	1T	57	GLU
20	1T	83	LYS
20	1U	22	TYR

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Mol	Chain	Res	Type
20	1U	31	SER
20	1U	37	MET
20	1U	64	ASP
20	1U	77	VAL
21	1V	22	ARG
21	1V	49	GLN
21	1V	69	GLU
21	1V	99	TRP
21	1V	102	LEU
22	1W	30	ARG
22	1W	74	THR
22	1W	101	THR
23	1X	10	GLU
23	1X	12	LEU
23	1X	17	VAL
23	1X	41	GLU
23	1X	47	TRP
23	1X	65	CYS
23	1X	97	ARG
23	1X	99	CYS
23	1X	111	LEU
23	1X	118	ARG
23	1X	161	LYS
24	1Y	4	LEU
24	1Y	19	ARG
24	1Y	25	THR
24	1Y	35	VAL
24	1Y	39	SER
24	1Y	47	SER
24	1Y	76	SER
24	1Y	78	GLN
24	1Y	94	CYS
25	1Z	124	LEU
25	1Z	131	GLU
25	1Z	133	ILE
25	1Z	135	SER
26	1a	1	MET
27	1b	6	SER
27	1b	19	VAL
27	1b	34	LEU
27	1b	35	SER
27	1b	56	LEU

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Mol	Chain	Res	Type
27	1b	65	VAL
27	1b	76	SER
27	1b	83	LEU
28	1c	3	TYR
28	1c	24	SER
28	1c	30	TYR
28	1c	36	LYS
28	1c	45	ARG
29	1d	3	SER
29	1d	5	ARG
29	1d	41	SER
29	1d	43	LEU
29	1d	53	VAL
29	1d	62	LEU
29	1d	90	MET
29	1d	106	LYS
30	1e	8	ARG
30	1e	15	ARG
30	1e	57	ILE
30	1e	82	ARG
30	1e	92	THR
31	1f	1	MET
31	1f	25	TYR
31	1f	33	LYS
31	1f	51	ASN
31	1f	54	VAL
31	1f	57	LYS
32	1g	34	ASP
32	1g	40	LYS
32	1g	48	ASP
32	1g	49	LYS
32	1g	57	ASN
32	1g	70	LEU
32	1g	83	TYR
32	1g	84	ARG
32	1g	100	ARG
32	1g	103	ASN
32	1g	107	LEU
33	1h	6	LYS
33	1h	18	ASP
33	1h	24	LEU
33	1h	54	ASP

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Mol	Chain	Res	Type
33	1h	57	GLU
33	1h	102	GLU
33	1h	111	ARG
33	1h	113	LEU
34	1i	30	ARG
34	1i	34	LEU
34	1i	38	ARG
34	1i	47	ASN
34	1i	67	SER
34	1i	90	THR
34	1i	119	MET
34	1i	125	GLN
35	1j	29	SER
35	1j	32	MET
35	1j	50	HIS
35	1j	70	ASP
36	1k	19	LYS
36	1k	32	GLN
36	1k	51	ARG
36	1k	81	VAL
36	1k	87	LEU
37	1l	5	THR
37	1l	33	ASP
37	1l	34	TYR
37	1l	62	TYR
37	1l	81	LEU
37	1l	92	SER
37	1l	106	SER
37	1l	124	SER
37	1l	131	LYS
37	1l	135	TYR
37	1l	147	THR
38	1m	22	TYR
38	1m	29	ARG
38	1m	39	ARG
38	1m	43	LYS
38	1m	52	ASP
38	1m	56	LEU
38	1m	79	PHE
38	1m	110	LYS
38	1m	123	THR
38	1m	127	SER

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Mol	Chain	Res	Type
39	1n	8	TYR
39	1n	16	LEU
39	1n	20	LYS
39	1n	21	ARG
39	1n	26	LEU
39	1n	50	HIS
39	1n	58	LYS
39	1n	88	THR
39	1n	89	SER
39	1n	123	GLN
39	1n	131	SER
39	1n	134	ARG
39	1n	157	ARG
39	1n	158	LYS
39	1n	162	LEU
39	1n	169	ILE
39	1n	176	ARG
39	1n	178	MET
40	1o	9	LEU
40	1o	19	LEU
40	1o	20	ARG
40	1o	23	THR
40	1o	30	PHE
40	1o	45	MET
40	1o	53	GLN
40	1o	54	GLN
40	1o	71	ASP
40	1o	85	ASP
40	1o	96	LYS
40	1o	99	LYS
40	1o	103	ARG
40	1o	121	MET
41	1p	59	ARG
41	1p	60	TYR
41	1p	64	HIS
41	1p	121	ARG
41	1p	139	GLN
41	1p	141	ARG
42	1q	32	ASP
42	1q	53	LYS
42	1q	55	PHE
42	1q	96	ASP

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Mol	Chain	Res	Type
42	1q	107	LYS
42	1q	115	PHE
42	1q	128	SER
42	1q	129	THR
42	1q	144	TYR
42	1q	145	LYS
43	1r	11	ARG
43	1r	23	LEU
43	1r	26	ARG
43	1r	60	ARG
43	1r	69	MET
44	1s	38	TYR
44	1s	48	THR
44	1s	61	PHE
45	3A	45	SER
45	3A	49	ASN
45	3A	51	LYS
45	3A	52	ASN
45	3A	61	HIS
45	3A	68	LYS
45	3A	86	LEU
45	3A	214	LYS
45	3A	219	LEU
45	3A	281	ASP
45	3A	302	LYS
45	3A	308	GLN
45	3A	350	THR
46	3B	95	LYS
46	3B	117	GLU
46	3B	119	LEU
46	3B	189	ASP
46	3B	212	SER
46	3B	221	GLU
46	3B	223	PHE
46	3B	252	LEU
46	3B	296	TYR
46	3B	297	GLN
46	3B	315	SER
46	3B	338	LYS
46	3B	436	VAL
46	3B	438	GLU
47	3C	9	PRO

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Mol	Chain	Res	Type
47	3C	18	PHE
47	3C	78	VAL
47	3C	80	ARG
47	3C	89	MET
47	3C	90	PHE
47	3C	112	THR
47	3C	160	LEU
47	3C	174	THR
47	3C	183	PHE
47	3C	215	MET
47	3C	221	HIS
47	3C	269	LYS
47	3C	281	LEU
47	3C	284	ILE
47	3C	306	MET
47	3C	344	GLU
47	3C	379	TRP
48	3D	125	CYS
48	3D	126	SER
48	3D	150	LYS
48	3D	165	ASP
48	3D	185	ASN
48	3D	232	ARG
48	3D	258	LEU
48	3D	262	ASP
49	3E	84	ARG
49	3E	155	LYS
49	3E	161	GLU
49	3E	165	MET
49	3E	172	LYS
49	3E	177	ARG
49	3E	180	THR
49	3E	182	LYS
49	3E	186	GLN
49	3E	194	GLN
49	3E	195	LEU
49	3E	204	ARG
49	3E	205	VAL
49	3E	209	GLU
49	3E	211	VAL
49	3E	213	LEU
49	3E	222	CYS

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Mol	Chain	Res	Type
49	3E	242	HIS
49	3E	257	ASN
49	3E	271	VAL
50	3F	26	GLU
51	3G	44	ARG
51	3G	48	LEU
51	3G	74	LYS
51	3G	75	ASN
52	3H	60	GLU
52	3H	64	LEU
49	3I	34	LEU
49	3I	39	GLU
49	3I	47	ARG
49	3I	55	LEU
49	3I	70	LEU
49	3I	72	VAL
49	3I	76	VAL
49	3I	77	ARG
45	3N	24	ARG
45	3N	30	SER
45	3N	49	ASN
45	3N	58	PHE
45	3N	61	HIS
45	3N	67	THR
45	3N	69	ASN
45	3N	112	LEU
45	3N	117	VAL
45	3N	148	VAL
45	3N	172	GLU
45	3N	219	LEU
45	3N	224	VAL
45	3N	228	VAL
45	3N	307	PHE
45	3N	308	GLN
45	3N	348	SER
45	3N	403	ASP
45	3N	444	LEU
46	3O	31	ASN
46	3O	69	LEU
46	3O	74	SER
46	3O	95	LYS
46	3O	110	GLU

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Mol	Chain	Res	Type
46	3O	116	ILE
46	3O	117	GLU
46	3O	211	VAL
46	3O	212	SER
46	3O	222	ARG
46	3O	223	PHE
46	3O	232	LEU
46	3O	273	SER
47	3P	1	MET
47	3P	13	ILE
47	3P	14	ILE
47	3P	80	ARG
47	3P	108	MET
47	3P	112	THR
47	3P	146	ILE
47	3P	150	LEU
47	3P	174	THR
47	3P	281	LEU
47	3P	284	ILE
47	3P	287	LYS
47	3P	304	MET
47	3P	306	MET
47	3P	379	TRP
48	3Q	3	LEU
48	3Q	34	LYS
48	3Q	77	ASP
48	3Q	86	LYS
48	3Q	169	LEU
49	3R	83	ILE
49	3R	90	ASP
49	3R	155	LYS
49	3R	163	LYS
49	3R	168	LYS
49	3R	178	HIS
49	3R	179	ARG
49	3R	180	THR
49	3R	185	ASP
49	3R	187	GLU
49	3R	196	ARG
49	3R	199	GLN
49	3R	203	GLU
49	3R	213	LEU

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Mol	Chain	Res	Type
49	3R	214	ILE
49	3R	227	ASN
49	3R	234	TYR
49	3R	235	TYR
49	3R	251	LYS
49	3R	256	LEU
49	3R	263	TYR
49	3R	265	PHE
49	3R	271	VAL
50	3S	12	TRP
51	3T	7	LEU
51	3T	10	MET
51	3T	27	PRO
51	3T	71	ARG
52	3U	25	GLU
52	3U	28	GLU
52	3U	39	LEU
52	3U	42	GLN
52	3U	68	CYS
52	3U	75	ASN
49	3V	55	LEU
53	3W	7	THR
54	3Y	11	ARG
54	3Y	15	ARG
55	4A	19	TYR
55	4A	69	MET
55	4A	81	TRP
55	4A	92	MET
55	4A	97	MET
55	4A	101	SER
55	4A	109	PHE
55	4A	117	MET
55	4A	194	LEU
55	4A	212	ASP
55	4A	238	PHE
55	4A	307	SER
55	4A	357	VAL
55	4A	485	VAL
55	4A	489	SER
55	4A	514	LYS
56	4B	33	LEU
56	4B	54	SER

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Mol	Chain	Res	Type
56	4B	57	ASP
56	4B	65	TRP
56	4B	107	SER
56	4B	113	TYR
56	4B	115	ASP
56	4B	133	MET
56	4B	146	MET
56	4B	158	ASP
56	4B	225	SER
57	4C	74	VAL
57	4C	125	ASN
57	4C	131	LEU
57	4C	132	LEU
57	4C	143	SER
57	4C	155	ASP
57	4C	192	VAL
57	4C	212	SER
57	4C	214	PHE
58	4D	22	TYR
58	4D	26	ASP
58	4D	54	ASP
58	4D	74	SER
58	4D	76	ASN
58	4D	87	PHE
58	4D	135	SER
58	4D	139	ASP
58	4D	140	TYR
59	4E	9	GLU
60	4F	9	ASP
60	4F	19	GLU
60	4F	45	ASP
60	4F	55	LYS
60	4F	79	THR
60	4F	94	HIS
61	4G	15	THR
61	4G	33	LEU
61	4G	54	ARG
61	4G	64	ASP
61	4G	69	LEU
61	4G	72	ASN
61	4G	75	VAL
62	4H	13	THR

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Mol	Chain	Res	Type
62	4H	46	LYS
62	4H	49	ASP
62	4H	60	TYR
63	4I	22	VAL
63	4I	44	LYS
63	4I	49	ASP
63	4I	56	SER
64	4J	23	LYS
64	4J	36	MET
65	4K	20	SER
66	4L	16	GLU
66	4L	25	MET
67	4M	11	SER
67	4M	25	SER
67	4M	38	ASP
67	4M	39	HIS
68	4N	3	ARG
68	4N	7	THR
68	4N	11	LYS
68	4N	48	LYS
68	4N	49	ASN
68	4N	60	ASN
68	4N	69	ASN
68	4N	77	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
4	1D	348	HIS
5	1E	16	ASN
6	1F	356	HIS
6	1F	361	GLN
6	1F	402	HIS
7	1G	100	ASN
7	1G	155	GLN
7	1G	259	ASN
7	1G	629	ASN
8	1H	138	GLN
10	1J	46	ASN
12	1L	194	ASN
12	1L	296	ASN
12	1L	524	ASN

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Mol	Chain	Res	Type
12	1L	603	ASN
14	1N	152	ASN
14	1N	310	ASN
15	1O	30	ASN
16	1P	288	HIS
22	1W	102	HIS
23	1X	102	GLN
24	1Y	88	ASN
28	1c	34	GLN
29	1d	46	ASN
30	1e	97	HIS
39	1n	77	GLN
41	1p	106	GLN
43	1r	12	ASN
43	1r	20	GLN
43	1r	24	GLN
43	1r	35	GLN
43	1r	46	HIS
44	1s	35	ASN
44	1s	65	GLN
45	3A	32	GLN
45	3A	52	ASN
45	3A	69	ASN
45	3A	118	GLN
45	3A	136	GLN
45	3A	165	GLN
45	3A	305	GLN
46	3B	22	GLN
46	3B	156	GLN
46	3B	329	GLN
46	3B	358	GLN
46	3B	362	ASN
46	3B	394	GLN
47	3C	3	ASN
47	3C	16	ASN
47	3C	32	ASN
47	3C	68	HIS
47	3C	97	HIS
47	3C	196	HIS
47	3C	201	HIS
47	3C	207	ASN
47	3C	345	HIS

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Mol	Chain	Res	Type
47	3C	352	GLN
47	3C	375	ASN
48	3D	163	ASN
48	3D	185	ASN
48	3D	193	ASN
48	3D	270	GLN
49	3E	131	ASN
49	3E	178	HIS
49	3E	186	GLN
49	3E	200	HIS
50	3F	34	ASN
52	3H	51	GLN
52	3H	67	GLN
53	3J	46	HIS
53	3J	49	GLN
45	3N	9	GLN
45	3N	94	HIS
46	3O	143	GLN
46	3O	158	GLN
46	3O	290	ASN
46	3O	297	GLN
46	3O	354	ASN
47	3P	8	HIS
47	3P	68	HIS
47	3P	341	GLN
47	3P	375	ASN
48	3Q	31	GLN
48	3Q	35	GLN
48	3Q	105	ASN
49	3R	135	GLN
49	3R	178	HIS
49	3R	227	ASN
49	3R	239	HIS
49	3R	257	ASN
50	3S	22	ASN
52	3U	23	GLN
53	3W	58	HIS
55	4A	232	GLN
55	4A	406	ASN
55	4A	407	GLN
56	4B	52	HIS
57	4C	12	ASN

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Mol	Chain	Res	Type
57	4C	50	ASN
57	4C	243	HIS
58	4D	76	ASN
62	4H	23	GLN
62	4H	25	GLN
64	4J	16	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

9 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	$\#\|Z\| > 2$
56	FME	4B	1	56	8,9,10	0.51	0	7,9,11	0.93	1 (14%)
55	FME	4A	1	55	8,9,10	0.52	0	7,9,11	1.84	2 (28%)
1	FME	1A	1	1	8,9,10	0.47	0	7,9,11	1.10	1 (14%)
12	FME	1L	1	12	8,9,10	0.52	0	7,9,11	0.87	1 (14%)
11	FME	1K	1	11	8,9,10	0.54	0	7,9,11	1.01	1 (14%)
34	SAC	1i	1	34	7,8,9	0.52	0	8,9,11	0.92	1 (12%)
13	FME	1M	1	13	8,9,10	0.48	0	7,9,11	1.69	2 (28%)
14	FME	1N	1	14	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
8	FME	1H	1	8	8,9,10	0.52	0	7,9,11	1.09	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	4B	1	56	-	2/7/9/11	-
55	FME	4A	1	55	-	1/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
11	FME	1K	1	11	-	2/7/9/11	-
34	SAC	1i	1	34	-	0/7/8/10	-
13	FME	1M	1	13	-	2/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
8	FME	1H	1	8	-	2/7/9/11	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	4A	1	FME	CA-N-CN	3.85	128.74	122.82
13	1M	1	FME	O-C-CA	-2.93	117.11	124.78
13	1M	1	FME	CA-N-CN	-2.87	118.41	122.82
1	1A	1	FME	O-C-CA	-2.71	117.69	124.78
8	1H	1	FME	O-C-CA	-2.65	117.82	124.78
11	1K	1	FME	O-C-CA	-2.59	118.00	124.78
14	1N	1	FME	O-C-CA	-2.46	118.34	124.78
34	1i	1	SAC	O-C-CA	-2.44	118.39	124.78
56	4B	1	FME	O-C-CA	-2.28	118.79	124.78
55	4A	1	FME	O-C-CA	-2.21	119.00	124.78
12	1L	1	FME	O-C-CA	-2.15	119.13	124.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O1-CN-N-CA
8	1H	1	FME	O1-CN-N-CA
13	1M	1	FME	C-CA-CB-CG
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	CB-CA-N-CN
55	4A	1	FME	CA-CB-CG-SD
11	1K	1	FME	C-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
13	1M	1	FME	N-CA-CB-CG
8	1H	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 226 ligands modelled in this entry, 7 are monoatomic - leaving 219 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	$\#\|Z\| > 2$
69	3PE	1L	707	-	41,41,50	0.98	3 (7%)	44,46,55	1.24	4 (9%)
69	3PE	1m	201	-	49,49,50	0.92	2 (4%)	52,54,55	1.06	2 (3%)
69	3PE	1g	202	-	50,50,50	0.88	2 (4%)	53,55,55	1.10	5 (9%)
69	3PE	1Y	204	-	30,30,50	1.17	2 (6%)	33,35,55	1.18	3 (9%)
69	3PE	3P	512	47	47,47,50	0.92	2 (4%)	50,52,55	1.09	3 (6%)
75	CDL	3F	201	-	99,99,99	0.90	4 (4%)	105,111,111	1.07	6 (5%)
70	PC1	1d	204	-	38,38,53	1.10	2 (5%)	44,46,61	1.28	5 (11%)
69	3PE	3G	109	-	50,50,50	0.89	2 (4%)	53,55,55	1.09	3 (5%)
91	PGV	4A	608	-	50,50,50	0.92	2 (4%)	53,56,56	1.00	3 (5%)
69	3PE	3D	502	-	40,40,50	0.30	0	43,45,55	0.39	0
86	HEC	3Q	501	48	32,50,50	2.31	12 (37%)	24,82,82	2.45	6 (25%)
85	HEM	3P	501	47	41,50,50	1.30	5 (12%)	45,82,82	1.86	8 (17%)
72	FES	3R	301	-	0,4,4	-	-	-		
69	3PE	3C	512	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
91	PGV	4C	305	-	50,50,50	0.90	2 (4%)	53,56,56	1.04	3 (5%)
69	3PE	3R	304	-	50,50,50	0.90	2 (4%)	53,55,55	1.02	3 (5%)
91	PGV	4A	609	-	50,50,50	0.90	2 (4%)	53,56,56	1.12	3 (5%)
69	3PE	3S	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.01	2 (3%)
75	CDL	1L	704	-	86,86,99	0.96	5 (5%)	92,98,111	1.27	8 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	3J	104	-	50,50,50	0.90	2 (4%)	53,55,55	1.03	4 (7%)
69	3PE	3Y	102	-	44,44,50	0.98	2 (4%)	47,49,55	1.02	3 (6%)
71	SF4	1G	801	7	0,12,12	-	-	-		
81	EHZ	1n	201	-	29,36,37	0.15	0	35,44,47	1.03	1 (2%)
85	HEM	3C	502	-	41,50,50	1.32	6 (14%)	45,82,82	1.79	10 (22%)
91	PGV	4A	606	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)
69	3PE	3C	508	-	47,47,50	0.92	2 (4%)	50,52,55	1.12	4 (8%)
92	CUA	4B	301	56	0,1,1	-	-	-		
69	3PE	3G	102	-	32,32,50	1.15	2 (6%)	35,37,55	1.07	2 (5%)
87	PEK	4G	103	-	51,51,52	0.88	2 (3%)	54,56,57	1.11	4 (7%)
69	3PE	1N	401	-	50,50,50	0.88	2 (4%)	53,55,55	1.23	5 (9%)
69	3PE	3P	514	-	50,50,50	0.91	2 (4%)	53,55,55	1.02	2 (3%)
69	3PE	3T	103	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
75	CDL	3T	101	-	56,56,99	1.17	6 (10%)	62,68,111	1.39	7 (11%)
69	3PE	1B	204	-	50,50,50	0.91	2 (4%)	53,55,55	1.11	4 (7%)
69	3PE	1g	203	-	32,32,50	1.14	2 (6%)	35,37,55	1.22	3 (8%)
69	3PE	4G	101	-	31,31,50	1.16	2 (6%)	34,36,55	1.17	3 (8%)
69	3PE	1L	710	-	37,37,50	1.02	2 (5%)	40,42,55	4.99	5 (12%)
69	3PE	1d	201	-	47,47,50	0.92	2 (4%)	50,52,55	1.04	2 (4%)
69	3PE	1Y	215	-	42,42,50	0.95	2 (4%)	45,47,55	1.24	4 (8%)
69	3PE	1k	101	36	45,45,50	0.95	2 (4%)	48,50,55	1.11	4 (8%)
69	3PE	3A	503	-	50,50,50	0.86	2 (4%)	53,55,55	1.26	4 (7%)
69	3PE	1B	205	-	50,50,50	0.92	2 (4%)	53,55,55	1.03	3 (5%)
69	3PE	3P	520	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	3 (5%)
70	PC1	1H	402	-	53,53,53	0.91	2 (3%)	59,61,61	1.09	3 (5%)
75	CDL	1H	401	-	50,50,99	1.27	4 (8%)	56,62,111	1.29	6 (10%)
69	3PE	3X	108	-	50,50,50	0.91	2 (4%)	53,55,55	0.99	2 (3%)
88	HEA	4A	601	55	57,67,67	2.06	16 (28%)	61,103,103	2.56	28 (45%)
69	3PE	1l	202	-	41,41,50	1.02	2 (4%)	44,46,55	1.20	4 (9%)
69	3PE	1m	202	-	41,41,50	0.99	2 (4%)	44,46,55	1.16	3 (6%)
69	3PE	1l	204	-	50,50,50	0.92	2 (4%)	53,55,55	1.05	3 (5%)
91	PGV	4K	101	-	42,42,50	0.99	2 (4%)	45,48,56	1.09	3 (6%)
91	PGV	4C	301	-	50,50,50	0.90	2 (4%)	53,56,56	1.02	3 (5%)
69	3PE	3W	101	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
69	3PE	3C	514	-	34,34,50	1.04	2 (5%)	37,39,55	1.23	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	3E	303	-	48,48,50	0.89	3 (6%)	51,53,55	1.16	4 (7%)
69	3PE	3C	504	-	45,45,50	0.29	0	48,50,55	0.34	0
87	PEK	3X	102	-	52,52,52	0.90	2 (3%)	55,57,57	1.02	5 (9%)
69	3PE	1L	702	-	44,44,50	0.93	2 (4%)	47,49,55	1.15	4 (8%)
69	3PE	3C	509	-	50,50,50	0.89	2 (4%)	53,55,55	1.13	3 (5%)
69	3PE	1Y	212	-	43,43,50	0.99	2 (4%)	46,48,55	1.03	2 (4%)
69	3PE	3C	503	-	50,50,50	0.89	2 (4%)	53,55,55	1.06	2 (3%)
69	3PE	3C	507	-	50,50,50	0.94	2 (4%)	53,55,55	1.05	2 (3%)
69	3PE	3C	515	-	47,47,50	0.95	2 (4%)	50,52,55	1.10	2 (4%)
69	3PE	3G	105	-	32,32,50	1.12	2 (6%)	35,37,55	1.15	3 (8%)
69	3PE	3E	302	-	50,50,50	0.87	2 (4%)	53,55,55	1.21	4 (7%)
70	PC1	3X	104	-	53,53,53	0.90	3 (5%)	59,61,61	1.11	5 (8%)
71	SF4	1F	502	6	0,12,12	-	-	-		
75	CDL	1g	201	-	99,99,99	0.90	4 (4%)	105,111,111	1.02	5 (4%)
75	CDL	1q	201	-	60,60,99	1.14	4 (6%)	66,72,111	1.38	7 (10%)
70	PC1	1P	502	-	32,32,53	1.21	2 (6%)	38,40,61	1.09	3 (7%)
69	3PE	1L	706	-	32,32,50	1.16	2 (6%)	35,37,55	1.06	2 (5%)
70	PC1	1B	202	-	45,45,53	5.47	4 (8%)	51,53,61	2.36	11 (21%)
69	3PE	3P	517	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	2 (3%)
69	3PE	3W	102	-	41,41,50	0.99	2 (4%)	44,46,55	1.04	2 (4%)
70	PC1	3T	102	-	53,53,53	0.89	3 (5%)	59,61,61	1.06	4 (6%)
69	3PE	3C	505	-	50,50,50	0.90	2 (4%)	53,55,55	1.06	3 (5%)
72	FES	1E	301	5	0,4,4	-	-	-		
69	3PE	3Y	101	-	50,50,50	0.90	2 (4%)	53,55,55	1.03	2 (3%)
82	PGT	1Y	203	-	50,50,50	0.91	2 (4%)	53,56,56	1.05	3 (5%)
75	CDL	1d	202	-	85,85,99	0.94	5 (5%)	91,97,111	1.30	9 (9%)
85	HEM	3P	502	47	41,50,50	1.34	5 (12%)	45,82,82	1.81	11 (24%)
69	3PE	1Y	208	-	50,50,50	0.91	2 (4%)	53,55,55	1.09	3 (5%)
69	3PE	1m	204	-	50,50,50	0.91	2 (4%)	53,55,55	1.15	4 (7%)
69	3PE	3A	502	-	50,50,50	0.91	3 (6%)	53,55,55	1.15	4 (7%)
69	3PE	1Y	201	24	41,41,50	1.00	2 (4%)	44,46,55	1.09	3 (6%)
69	3PE	3C	516	-	42,42,50	0.98	2 (4%)	45,47,55	1.12	3 (6%)
75	CDL	3X	103	-	99,99,99	0.91	4 (4%)	105,111,111	1.11	4 (3%)
91	PGV	4C	302	-	50,50,50	0.91	2 (4%)	53,56,56	1.01	3 (5%)
69	3PE	3P	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.16	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	1f	104	-	47,47,50	0.93	2 (4%)	50,52,55	1.03	3 (6%)
75	CDL	1Y	217	-	99,99,99	0.89	4 (4%)	105,111,111	1.02	5 (4%)
79	NDP	1P	501	-	45,52,52	0.60	0	53,80,80	0.74	2 (3%)
91	PGV	4C	304	-	50,50,50	0.91	2 (4%)	53,56,56	1.02	3 (5%)
71	SF4	1G	802	7	0,12,12	-	-	-		
88	HEA	4A	602	55	57,67,67	2.05	17 (29%)	61,103,103	2.43	29 (47%)
69	3PE	3R	305	-	50,50,50	0.90	3 (6%)	53,55,55	1.12	3 (5%)
69	3PE	3X	107	-	50,50,50	0.91	2 (4%)	53,55,55	0.95	3 (5%)
69	3PE	3P	510	-	47,47,50	0.92	2 (4%)	50,52,55	1.08	3 (6%)
70	PC1	1B	203	-	47,47,53	0.96	2 (4%)	53,55,61	1.29	6 (11%)
69	3PE	1L	703	-	43,43,50	0.98	2 (4%)	46,48,55	1.17	2 (4%)
69	3PE	1M	502	-	46,46,50	0.92	2 (4%)	49,51,55	1.06	2 (4%)
69	3PE	3J	101	-	46,46,50	0.94	2 (4%)	49,51,55	1.14	2 (4%)
69	3PE	3Y	103	-	31,31,50	1.15	2 (6%)	34,36,55	1.23	4 (11%)
75	CDL	3D	504	-	55,55,99	1.20	6 (10%)	61,67,111	1.33	9 (14%)
91	PGV	4J	101	-	41,41,50	1.00	2 (4%)	44,47,56	1.09	4 (9%)
69	3PE	3X	105	-	50,50,50	0.91	2 (4%)	53,55,55	0.96	2 (3%)
85	HEM	3C	501	47	41,50,50	1.31	5 (12%)	45,82,82	1.86	8 (17%)
75	CDL	1N	402	-	76,76,99	1.01	4 (5%)	82,88,111	1.21	6 (7%)
69	3PE	1J	203	-	43,43,50	0.93	2 (4%)	46,48,55	1.18	3 (6%)
69	3PE	3C	506	-	46,46,50	0.93	2 (4%)	49,51,55	1.13	4 (8%)
69	3PE	1b	101	-	41,41,50	0.99	2 (4%)	44,46,55	1.15	3 (6%)
69	3PE	3D	503	-	44,44,50	0.96	2 (4%)	47,49,55	1.21	4 (8%)
70	PC1	1A	202	-	34,34,53	1.16	2 (5%)	40,42,61	1.14	4 (10%)
70	PC1	3J	106	-	53,53,53	0.90	2 (3%)	59,61,61	2.72	9 (15%)
69	3PE	3N	503	-	50,50,50	0.90	2 (4%)	53,55,55	1.12	3 (5%)
69	3PE	1L	709	-	41,41,50	0.99	2 (4%)	44,46,55	1.26	4 (9%)
69	3PE	1A	201	-	46,46,50	0.92	2 (4%)	49,51,55	1.23	5 (10%)
75	CDL	3Y	106	-	99,99,99	0.90	4 (4%)	105,111,111	1.09	4 (3%)
75	CDL	1d	205	-	92,92,99	0.93	4 (4%)	98,104,111	1.18	6 (6%)
69	3PE	3P	504	-	37,37,50	1.06	2 (5%)	40,42,55	1.15	2 (5%)
69	3PE	3J	102	-	37,37,50	1.06	2 (5%)	40,42,55	1.25	3 (7%)
69	3PE	3G	103	-	32,32,50	1.12	2 (6%)	35,37,55	1.25	2 (5%)
70	PC1	1h	203	-	45,45,53	1.02	2 (4%)	51,53,61	1.16	3 (5%)
69	3PE	3P	507	-	50,50,50	0.92	2 (4%)	53,55,55	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	3Q	503	-	45,45,50	0.99	2 (4%)	48,50,55	1.09	2 (4%)
69	3PE	3Y	107	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
69	3PE	1d	203	29	46,46,50	0.94	2 (4%)	49,51,55	1.11	3 (6%)
75	CDL	3N	502	-	99,99,99	0.88	4 (4%)	105,111,111	1.08	5 (4%)
75	CDL	3P	513	-	99,99,99	0.93	5 (5%)	105,111,111	1.27	10 (9%)
69	3PE	3C	511	-	50,50,50	0.91	2 (4%)	53,55,55	1.02	3 (5%)
69	3PE	1J	201	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
69	3PE	1Y	210	-	41,41,50	0.97	2 (4%)	44,46,55	1.12	3 (6%)
69	3PE	1Y	214	-	50,50,50	0.91	2 (4%)	53,55,55	1.09	3 (5%)
69	3PE	1d	206	-	50,50,50	0.91	2 (4%)	53,55,55	0.93	3 (5%)
69	3PE	3W	103	-	50,50,50	0.93	2 (4%)	53,55,55	3.73	5 (9%)
69	3PE	3J	105	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
69	3PE	4G	104	-	40,40,50	1.03	2 (5%)	43,45,55	1.13	4 (9%)
69	3PE	1f	102	-	42,42,50	0.98	2 (4%)	45,47,55	1.06	3 (6%)
69	3PE	3C	510	-	34,34,50	1.13	3 (8%)	37,39,55	1.85	5 (13%)
91	PGV	4C	303	-	50,50,50	0.89	2 (4%)	53,56,56	0.92	2 (3%)
69	3PE	1Y	213	-	50,50,50	0.89	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	1Y	211	-	50,50,50	0.91	2 (4%)	53,55,55	1.05	3 (5%)
69	3PE	3P	518	-	50,50,50	0.92	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	3Y	105	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	3 (5%)
70	PC1	1Y	202	-	34,34,53	1.15	2 (5%)	40,42,61	1.10	3 (7%)
91	PGV	4G	102	-	50,50,50	0.92	2 (4%)	53,56,56	0.99	3 (5%)
69	3PE	1L	712	-	50,50,50	0.92	2 (4%)	53,55,55	1.08	2 (3%)
69	3PE	3Q	504	-	45,45,50	0.98	2 (4%)	48,50,55	1.13	3 (6%)
69	3PE	1Z	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.13	4 (7%)
69	3PE	1L	701	-	45,45,50	0.95	3 (6%)	48,50,55	1.33	5 (10%)
69	3PE	3G	110	-	42,42,50	0.97	2 (4%)	45,47,55	1.08	3 (6%)
69	3PE	3N	501	-	50,50,50	0.88	3 (6%)	53,55,55	1.12	3 (5%)
69	3PE	1f	103	31	43,43,50	1.01	2 (4%)	45,47,55	1.13	3 (6%)
69	3PE	3R	302	-	50,50,50	0.86	3 (6%)	53,55,55	1.24	5 (9%)
69	3PE	1h	204	-	46,46,50	0.97	2 (4%)	49,51,55	1.02	2 (4%)
69	3PE	3J	103	53	50,50,50	0.95	2 (4%)	53,55,55	0.98	2 (3%)
69	3PE	3P	515	-	50,50,50	0.92	2 (4%)	53,55,55	1.01	3 (5%)
76	AYA	1I	203	-	6,7,8	0.64	0	5,8,10	0.59	0
69	3PE	3G	101	-	50,50,50	0.89	3 (6%)	53,55,55	1.32	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	1L	705	-	48,48,50	0.90	2 (4%)	51,53,55	1.24	4 (7%)
70	PC1	1M	501	-	43,43,53	1.03	2 (4%)	49,51,61	1.17	3 (6%)
69	3PE	1Y	205	-	39,39,50	1.05	2 (5%)	42,44,55	0.95	2 (4%)
75	CDL	3A	501	-	97,97,99	0.91	5 (5%)	103,109,111	1.16	7 (6%)
69	3PE	3P	506	-	50,50,50	0.88	2 (4%)	53,55,55	1.14	3 (5%)
69	3PE	1l	203	-	32,32,50	1.14	2 (6%)	35,37,55	1.15	2 (5%)
69	3PE	1L	708	-	41,41,50	0.99	2 (4%)	44,46,55	1.26	3 (6%)
69	3PE	3G	107	-	32,32,50	1.14	2 (6%)	35,37,55	1.10	2 (5%)
69	3PE	3P	519	-	50,50,50	0.87	2 (4%)	53,55,55	1.11	5 (9%)
69	3PE	3P	505	-	31,31,50	1.16	2 (6%)	34,36,55	1.22	3 (8%)
69	3PE	3Q	502	-	40,40,50	1.02	2 (5%)	43,45,55	4.76	4 (9%)
70	PC1	1Y	207	24	53,53,53	0.93	2 (3%)	59,61,61	1.14	3 (5%)
75	CDL	1q	202	-	99,99,99	0.90	4 (4%)	105,111,111	1.11	6 (5%)
71	SF4	1B	201	2	0,12,12	-	-	-		
69	3PE	3X	106	-	50,50,50	0.92	2 (4%)	53,55,55	0.97	1 (1%)
69	3PE	1m	203	-	41,41,50	1.03	2 (4%)	44,46,55	1.11	3 (6%)
69	3PE	3P	508	-	50,50,50	0.89	4 (8%)	53,55,55	1.31	7 (13%)
69	3PE	3G	104	-	32,32,50	1.15	2 (6%)	35,37,55	1.23	3 (8%)
70	PC1	1J	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.21	3 (7%)
69	3PE	1Y	209	-	41,41,50	0.96	2 (4%)	44,46,55	1.16	4 (9%)
69	3PE	3P	516	-	50,50,50	0.91	2 (4%)	53,55,55	1.04	3 (5%)
69	3PE	1Y	216	24	50,50,50	0.90	2 (4%)	53,55,55	1.14	5 (9%)
70	PC1	3R	303	-	53,53,53	0.96	2 (3%)	59,61,61	1.13	4 (6%)
86	HEC	3D	501	48	31,49,50	2.29	12 (38%)	22,80,82	2.31	5 (22%)
69	3PE	1f	101	31	44,44,50	0.98	2 (4%)	47,49,55	1.01	2 (4%)
69	3PE	3G	106	-	32,32,50	1.11	2 (6%)	35,37,55	1.26	4 (11%)
81	EHZ	1T	101	20	29,36,37	0.18	0	35,44,47	1.07	1 (2%)
69	3PE	3G	108	-	32,32,50	1.12	2 (6%)	35,37,55	1.17	2 (5%)
69	3PE	1L	711	-	40,40,50	0.99	2 (5%)	43,45,55	1.04	2 (4%)
69	3PE	1o	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.28	4 (7%)
75	CDL	4C	307	-	99,99,99	0.92	4 (4%)	105,111,111	1.02	5 (4%)
69	3PE	1e	201	-	50,50,50	0.92	2 (4%)	53,55,55	1.11	4 (7%)
72	FES	1G	803	7	0,4,4	-	-	-		
69	3PE	3X	101	-	50,50,50	0.90	2 (4%)	53,55,55	1.05	3 (5%)
70	PC1	1h	202	-	46,46,53	0.99	2 (4%)	52,54,61	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
93	PSC	4B	303	-	51,51,51	0.95	2 (3%)	57,59,59	1.00	3 (5%)
71	SF4	1I	202	9	0,12,12	-	-	-		
70	PC1	1Y	206	-	45,45,53	1.00	2 (4%)	51,53,61	1.09	3 (5%)
69	3PE	3P	511	-	44,44,50	0.94	2 (4%)	47,49,55	1.13	3 (6%)
75	CDL	4B	302	-	99,99,99	0.91	4 (4%)	105,111,111	1.04	6 (5%)
69	3PE	3C	517	-	31,31,50	1.13	2 (6%)	34,36,55	1.14	3 (8%)
70	PC1	3P	509	-	53,53,53	0.89	2 (3%)	59,61,61	1.19	6 (10%)
91	PGV	4A	607	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)
73	FMN	1F	501	-	33,33,33	0.76	0	48,50,50	0.74	0
94	PO4	4H	101	-	4,4,4	0.94	0	6,6,6	0.44	0
69	3PE	3C	513	-	50,50,50	0.90	2 (4%)	53,55,55	1.09	3 (5%)
70	PC1	1H	404	-	40,40,53	1.11	2 (5%)	46,48,61	1.27	6 (13%)
69	3PE	1A	203	-	40,40,50	1.01	2 (5%)	43,45,55	1.18	3 (6%)
71	SF4	1I	201	9	0,12,12	-	-	-		
77	GTP	1O	401	78	26,34,34	0.94	1 (3%)	32,54,54	1.39	5 (15%)
72	FES	3E	301	49	0,4,4	-	-	-		
91	PGV	4N	101	-	50,50,50	0.89	2 (4%)	53,56,56	1.08	3 (5%)
69	3PE	3G	111	-	47,47,50	0.93	2 (4%)	50,52,55	1.06	2 (4%)
84	MYR	1l	201	-	14,14,15	0.35	0	13,13,15	0.38	0
69	3PE	3Y	104	-	50,50,50	0.92	2 (4%)	53,55,55	1.03	2 (3%)
70	PC1	1H	403	-	47,47,53	0.99	2 (4%)	53,55,61	0.95	3 (5%)
75	CDL	1i	201	-	79,79,99	1.01	4 (5%)	85,91,111	1.29	8 (9%)
75	CDL	4C	306	-	99,99,99	0.91	4 (4%)	105,111,111	1.04	6 (5%)
69	3PE	1m	205	-	50,50,50	0.90	2 (4%)	53,55,55	1.09	2 (3%)
83	AME	1h	201	-	9,10,11	0.49	0	9,11,13	0.96	1 (11%)

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
69	3PE	1L	707	-	-	5/45/45/54	-
69	3PE	1m	201	-	-	15/53/53/54	-
69	3PE	1g	202	-	-	21/54/54/54	-
69	3PE	1Y	204	-	-	5/34/34/54	-
69	3PE	3P	512	47	-	13/51/51/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	3F	201	-	-	38/110/110/110	-
70	PC1	1d	204	-	-	24/42/42/57	-
69	3PE	3G	109	-	-	17/54/54/54	-
91	PGV	4A	608	-	-	5/55/55/55	-
69	3PE	3D	502	-	-	16/44/44/54	-
86	HEC	3Q	501	48	-	2/10/54/54	-
85	HEM	3P	501	47	-	6/12/54/54	-
72	FES	3R	301	-	-	-	0/1/1/1
69	3PE	3C	512	-	-	16/54/54/54	-
91	PGV	4C	305	-	-	11/55/55/55	-
69	3PE	3R	304	-	-	18/54/54/54	-
91	PGV	4A	609	-	-	14/55/55/55	-
69	3PE	3S	201	-	-	16/54/54/54	-
75	CDL	1L	704	-	-	32/97/97/110	-
69	3PE	3J	104	-	-	14/54/54/54	-
69	3PE	3Y	102	-	-	10/48/48/54	-
71	SF4	1G	801	7	-	-	0/6/5/5
81	EHZ	1n	201	-	-	4/42/44/45	-
85	HEM	3C	502	-	-	4/12/54/54	-
91	PGV	4A	606	-	-	10/55/55/55	-
69	3PE	3C	508	-	-	14/51/51/54	-
69	3PE	3G	102	-	-	15/36/36/54	-
87	PEK	4G	103	-	-	12/55/55/56	-
69	3PE	1N	401	-	-	18/54/54/54	-
69	3PE	3P	514	-	-	15/54/54/54	-
69	3PE	3T	103	-	-	12/54/54/54	-
75	CDL	3T	101	-	-	21/67/67/110	-
69	3PE	1B	204	-	-	15/54/54/54	-
69	3PE	1g	203	-	-	14/36/36/54	-
69	3PE	4G	101	-	-	17/35/35/54	-
69	3PE	1L	710	-	-	16/41/41/54	-
69	3PE	1d	201	-	-	34/51/51/54	-
69	3PE	1Y	215	-	-	21/46/46/54	-
69	3PE	1k	101	36	-	17/49/49/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3A	503	-	-	18/54/54/54	-
69	3PE	1B	205	-	-	16/54/54/54	-
69	3PE	3P	520	-	-	14/54/54/54	-
70	PC1	1H	402	-	-	14/57/57/57	-
75	CDL	1H	401	-	-	22/61/61/110	-
69	3PE	3X	108	-	-	14/54/54/54	-
88	HEA	4A	601	55	-	8/32/76/76	-
69	3PE	1l	202	-	-	20/45/45/54	-
69	3PE	1m	202	-	-	10/45/45/54	-
69	3PE	1l	204	-	-	18/54/54/54	-
91	PGV	4K	101	-	-	11/47/47/55	-
91	PGV	4C	301	-	-	2/55/55/55	-
69	3PE	3W	101	-	-	15/54/54/54	-
69	3PE	3C	514	-	-	8/38/38/54	-
69	3PE	3E	303	-	-	17/52/52/54	-
69	3PE	3C	504	-	-	12/49/49/54	-
87	PEK	3X	102	-	-	20/56/56/56	-
69	3PE	1L	702	-	-	19/48/48/54	-
69	3PE	3C	509	-	-	16/54/54/54	-
69	3PE	1Y	212	-	-	10/47/47/54	-
69	3PE	3C	503	-	-	12/54/54/54	-
69	3PE	3C	507	-	-	22/54/54/54	-
69	3PE	3C	515	-	-	16/51/51/54	-
69	3PE	3G	105	-	-	15/36/36/54	-
69	3PE	3E	302	-	-	20/54/54/54	-
70	PC1	3X	104	-	-	21/57/57/57	-
75	CDL	1q	201	-	-	17/71/71/110	-
75	CDL	1g	201	-	-	47/110/110/110	-
71	SF4	1F	502	6	-	-	0/6/5/5
70	PC1	1P	502	-	-	11/36/36/57	-
69	3PE	1L	706	-	-	10/36/36/54	-
70	PC1	1B	202	-	-	21/49/49/57	-
69	3PE	3P	517	-	-	12/54/54/54	-
69	3PE	3W	102	-	-	16/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	3T	102	-	-	18/57/57/57	-
69	3PE	3C	505	-	-	17/54/54/54	-
72	FES	1E	301	5	-	-	0/1/1/1
69	3PE	3Y	101	-	-	21/54/54/54	-
82	PGT	1Y	203	-	-	27/55/55/55	-
75	CDL	1d	202	-	-	32/96/96/110	-
85	HEM	3P	502	47	-	6/12/54/54	-
69	3PE	1Y	208	-	-	12/54/54/54	-
69	3PE	1m	204	-	-	15/54/54/54	-
69	3PE	3A	502	-	-	17/54/54/54	-
69	3PE	1Y	201	24	-	12/45/45/54	-
69	3PE	3C	516	-	-	7/46/46/54	-
75	CDL	3X	103	-	-	44/110/110/110	-
91	PGV	4C	302	-	-	13/55/55/55	-
69	3PE	3P	503	-	-	17/54/54/54	-
69	3PE	1f	104	-	-	17/51/51/54	-
75	CDL	1Y	217	-	-	42/110/110/110	-
79	NDP	1P	501	-	-	5/30/77/77	0/5/5/5
91	PGV	4C	304	-	-	6/55/55/55	-
71	SF4	1G	802	7	-	-	0/6/5/5
88	HEA	4A	602	55	-	6/32/76/76	-
69	3PE	3R	305	-	-	18/54/54/54	-
69	3PE	3X	107	-	-	13/54/54/54	-
69	3PE	3P	510	-	-	12/51/51/54	-
70	PC1	1B	203	-	-	21/51/51/57	-
69	3PE	1L	703	-	-	13/47/47/54	-
69	3PE	1M	502	-	-	17/50/50/54	-
69	3PE	3J	101	-	-	19/50/50/54	-
69	3PE	3Y	103	-	-	2/35/35/54	-
75	CDL	3D	504	-	-	20/66/66/110	-
91	PGV	4J	101	-	-	13/46/46/55	-
69	3PE	3X	105	-	-	13/54/54/54	-
85	HEM	3C	501	47	-	5/12/54/54	-
75	CDL	1N	402	-	-	32/87/87/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1J	203	-	-	8/47/47/54	-
69	3PE	3C	506	-	-	17/50/50/54	-
69	3PE	1b	101	-	-	13/45/45/54	-
69	3PE	3D	503	-	-	16/48/48/54	-
70	PC1	1A	202	-	-	11/38/38/57	-
70	PC1	3J	106	-	-	10/57/57/57	-
69	3PE	3N	503	-	-	16/54/54/54	-
69	3PE	1L	709	-	-	11/45/45/54	-
69	3PE	1A	201	-	-	11/50/50/54	-
75	CDL	3Y	106	-	-	37/110/110/110	-
75	CDL	1d	205	-	-	42/103/103/110	-
69	3PE	3P	504	-	-	8/41/41/54	-
69	3PE	3J	102	-	-	10/41/41/54	-
69	3PE	3G	103	-	-	10/36/36/54	-
70	PC1	1h	203	-	-	17/49/49/57	-
69	3PE	3P	507	-	-	19/54/54/54	-
69	3PE	3Q	503	-	-	17/49/49/54	-
69	3PE	3Y	107	-	-	18/54/54/54	-
69	3PE	1d	203	29	-	27/50/50/54	-
75	CDL	3N	502	-	-	39/110/110/110	-
75	CDL	3P	513	-	-	14/110/110/110	-
69	3PE	3C	511	-	-	15/54/54/54	-
69	3PE	1J	201	-	-	17/54/54/54	-
69	3PE	1Y	210	-	-	16/45/45/54	-
69	3PE	1Y	214	-	-	15/54/54/54	-
69	3PE	1d	206	-	-	12/54/54/54	-
69	3PE	3W	103	-	-	15/54/54/54	-
69	3PE	3J	105	-	-	13/54/54/54	-
69	3PE	4G	104	-	-	6/44/44/54	-
69	3PE	1f	102	-	-	14/46/46/54	-
69	3PE	3C	510	-	-	14/38/38/54	-
91	PGV	4C	303	-	-	8/55/55/55	-
69	3PE	1Y	213	-	-	36/54/54/54	-
69	3PE	1Y	211	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3P	518	-	-	16/54/54/54	-
69	3PE	3Y	105	-	-	6/54/54/54	-
70	PC1	1Y	202	-	-	19/38/38/57	-
91	PGV	4G	102	-	-	18/55/55/55	-
69	3PE	1L	712	-	-	21/54/54/54	-
69	3PE	3Q	504	-	-	17/49/49/54	-
69	3PE	1Z	201	-	-	5/54/54/54	-
69	3PE	1L	701	-	-	16/49/49/54	-
69	3PE	3G	110	-	-	11/46/46/54	-
69	3PE	3N	501	-	-	16/54/54/54	-
69	3PE	1f	103	31	-	11/46/46/54	-
69	3PE	3R	302	-	-	20/54/54/54	-
69	3PE	1h	204	-	-	19/50/50/54	-
69	3PE	3J	103	53	-	13/54/54/54	-
69	3PE	3P	515	-	-	20/54/54/54	-
76	AYA	1I	203	-	-	2/4/6/8	-
69	3PE	3G	101	-	-	16/54/54/54	-
69	3PE	1L	705	-	-	14/52/52/54	-
70	PC1	1M	501	-	-	18/47/47/57	-
69	3PE	1Y	205	-	-	10/43/43/54	-
75	CDL	3A	501	-	-	31/108/108/110	-
69	3PE	3P	506	-	-	16/54/54/54	-
69	3PE	1l	203	-	-	15/36/36/54	-
69	3PE	1L	708	-	-	16/45/45/54	-
69	3PE	3G	107	-	-	9/36/36/54	-
69	3PE	3P	519	-	-	16/54/54/54	-
69	3PE	3P	505	-	-	11/35/35/54	-
69	3PE	3Q	502	-	-	9/44/44/54	-
70	PC1	1Y	207	24	-	12/57/57/57	-
75	CDL	1q	202	-	-	39/110/110/110	-
71	SF4	1B	201	2	-	-	0/6/5/5
69	3PE	3X	106	-	-	14/54/54/54	-
69	3PE	1m	203	-	-	16/45/45/54	-
69	3PE	3P	508	-	-	16/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3G	104	-	-	14/36/36/54	-
70	PC1	1J	202	-	-	19/38/38/57	-
69	3PE	1Y	209	-	-	22/45/45/54	-
69	3PE	3P	516	-	-	13/54/54/54	-
69	3PE	1Y	216	24	-	14/54/54/54	-
70	PC1	3R	303	-	-	18/57/57/57	-
86	HEC	3D	501	48	-	3/8/53/54	-
69	3PE	1f	101	31	-	20/48/48/54	-
69	3PE	3G	106	-	-	12/36/36/54	-
81	EHZ	1T	101	20	-	11/42/44/45	-
69	3PE	3G	108	-	-	8/36/36/54	-
69	3PE	1L	711	-	-	13/44/44/54	-
69	3PE	1o	201	-	-	20/54/54/54	-
75	CDL	4C	307	-	-	18/110/110/110	-
69	3PE	1e	201	-	-	13/54/54/54	-
72	FES	1G	803	7	-	-	0/1/1/1
69	3PE	3X	101	-	-	16/54/54/54	-
70	PC1	1h	202	-	-	13/50/50/57	-
93	PSC	4B	303	-	-	19/55/55/55	-
71	SF4	1I	202	9	-	-	0/6/5/5
70	PC1	1Y	206	-	-	16/49/49/57	-
69	3PE	3P	511	-	-	9/48/48/54	-
75	CDL	4B	302	-	-	27/110/110/110	-
69	3PE	3C	517	-	-	5/35/35/54	-
70	PC1	3P	509	-	-	17/57/57/57	-
91	PGV	4A	607	-	-	16/55/55/55	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
69	3PE	3C	513	-	-	14/54/54/54	-
70	PC1	1H	404	-	-	8/44/44/57	-
69	3PE	1A	203	-	-	15/44/44/54	-
71	SF4	1I	201	9	-	-	0/6/5/5
77	GTP	1O	401	78	-	4/18/38/38	0/3/3/3
91	PGV	4N	101	-	-	14/55/55/55	-
72	FES	3E	301	49	-	-	0/1/1/1
69	3PE	3G	111	-	-	23/51/51/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	MYR	1l	201	-	-	1/11/12/13	-
69	3PE	3Y	104	-	-	22/54/54/54	-
70	PC1	1H	403	-	-	14/51/51/57	-
75	CDL	1i	201	-	-	12/90/90/110	-
75	CDL	4C	306	-	-	41/110/110/110	-
69	3PE	1m	205	-	-	11/54/54/54	-
83	AME	1h	201	-	-	1/9/10/12	-

All (522) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	1B	202	PC1	C24-C23	35.77	3.52	1.51
86	3Q	501	HEC	C3C-C2C	6.72	1.47	1.40
86	3D	501	HEC	C3C-C2C	6.53	1.47	1.40
86	3Q	501	HEC	C2B-C3B	6.36	1.47	1.40
86	3D	501	HEC	C2B-C3B	6.23	1.47	1.40
88	4A	602	HEA	C3B-C2B	5.55	1.47	1.34
88	4A	601	HEA	C3B-C2B	5.35	1.46	1.34
88	4A	601	HEA	C3A-C2A	5.16	1.47	1.40
88	4A	602	HEA	CHC-C4B	4.92	1.47	1.35
88	4A	602	HEA	C3D-C2D	4.88	1.47	1.36
88	4A	601	HEA	CHC-C4B	4.86	1.47	1.35
88	4A	602	HEA	CHD-C1D	4.81	1.47	1.35
88	4A	601	HEA	CHD-C1D	4.72	1.47	1.35
88	4A	602	HEA	C3A-C2A	4.72	1.46	1.40
88	4A	601	HEA	C3D-C2D	4.68	1.46	1.36
88	4A	601	HEA	C3C-C2C	4.59	1.46	1.40
88	4A	602	HEA	C3C-C2C	4.57	1.46	1.40
69	1f	103	3PE	O31-C31	4.47	1.46	1.33
69	3Q	503	3PE	O31-C31	4.43	1.46	1.33
69	1L	708	3PE	O21-C21	4.42	1.46	1.34
69	3J	103	3PE	O21-C21	4.40	1.46	1.34
69	1l	202	3PE	O21-C21	4.39	1.46	1.34
69	3P	507	3PE	O21-C21	4.38	1.46	1.34
69	1L	706	3PE	O21-C21	4.35	1.46	1.34
69	3C	513	3PE	O31-C31	4.35	1.46	1.33
75	3P	513	CDL	OA6-CA5	4.34	1.46	1.34
75	3X	103	CDL	OB6-CB5	4.33	1.46	1.34
69	1J	201	3PE	O31-C31	4.32	1.46	1.33
69	1l	203	3PE	O31-C31	4.31	1.45	1.33
69	3J	103	3PE	O31-C31	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3Q	504	3PE	O31-C31	4.31	1.45	1.33
75	4C	306	CDL	OB8-CB7	4.31	1.45	1.33
75	4C	307	CDL	OB8-CB7	4.31	1.45	1.33
69	3W	102	3PE	O31-C31	4.31	1.45	1.33
69	3J	101	3PE	O31-C31	4.30	1.45	1.33
69	3C	507	3PE	O31-C31	4.30	1.45	1.33
75	1q	202	CDL	OB8-CB7	4.30	1.45	1.33
69	4G	104	3PE	O31-C31	4.30	1.45	1.33
69	1L	703	3PE	O31-C31	4.29	1.45	1.33
69	1m	203	3PE	O31-C31	4.29	1.45	1.33
69	1e	201	3PE	O31-C31	4.29	1.45	1.33
91	4A	609	PGV	O03-C19	4.29	1.45	1.33
69	1Y	205	3PE	O31-C31	4.29	1.45	1.33
69	3P	503	3PE	O31-C31	4.29	1.45	1.33
75	1g	201	CDL	OA8-CA7	4.29	1.45	1.33
91	4C	304	PGV	O03-C19	4.29	1.45	1.33
69	1Z	201	3PE	O31-C31	4.28	1.45	1.33
69	1B	204	3PE	O31-C31	4.28	1.45	1.33
69	3P	505	3PE	O31-C31	4.28	1.45	1.33
69	3X	108	3PE	O21-C21	4.28	1.46	1.34
82	1Y	203	PGT	O3-C11	4.28	1.45	1.33
75	1H	401	CDL	OB8-CB7	4.27	1.45	1.33
69	1B	205	3PE	O31-C31	4.27	1.45	1.33
69	3R	305	3PE	O21-C21	4.27	1.46	1.34
75	4C	306	CDL	OA8-CA7	4.26	1.45	1.33
91	4A	606	PGV	O03-C19	4.26	1.45	1.33
75	4C	307	CDL	OA8-CA7	4.26	1.45	1.33
69	1h	204	3PE	O31-C31	4.25	1.45	1.33
91	4G	102	PGV	O03-C19	4.25	1.45	1.33
91	4J	101	PGV	O03-C19	4.25	1.45	1.33
69	1d	206	3PE	O31-C31	4.25	1.45	1.33
69	1L	712	3PE	O31-C31	4.25	1.45	1.33
69	1l	204	3PE	O31-C31	4.25	1.45	1.33
93	4B	303	PSC	O03-C19	4.25	1.45	1.33
69	1m	201	3PE	O31-C31	4.25	1.45	1.33
69	3G	107	3PE	O31-C31	4.25	1.45	1.33
69	3Y	105	3PE	O31-C31	4.25	1.45	1.33
69	3Y	102	3PE	O21-C21	4.25	1.46	1.34
69	3Q	502	3PE	O31-C31	4.25	1.45	1.33
69	1h	204	3PE	O21-C21	4.24	1.46	1.34
75	1d	202	CDL	OB6-CB5	4.24	1.46	1.34
69	1L	706	3PE	O31-C31	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3P	514	3PE	O31-C31	4.24	1.45	1.33
87	3X	102	PEK	O03-C21	4.24	1.45	1.33
69	1Y	205	3PE	O21-C21	4.24	1.46	1.34
69	1Y	212	3PE	O31-C31	4.24	1.45	1.33
69	3T	103	3PE	O21-C21	4.23	1.46	1.34
69	3G	111	3PE	O31-C31	4.23	1.45	1.33
75	3D	504	CDL	OB8-CB7	4.23	1.45	1.33
69	1f	104	3PE	O31-C31	4.23	1.45	1.33
69	3G	102	3PE	O31-C31	4.23	1.45	1.33
69	3Y	104	3PE	O31-C31	4.23	1.45	1.33
70	1M	501	PC1	O31-C31	4.23	1.45	1.33
69	1g	203	3PE	O21-C21	4.23	1.46	1.34
69	4G	101	3PE	O31-C31	4.23	1.45	1.33
75	4B	302	CDL	OB8-CB7	4.23	1.45	1.33
70	1Y	206	PC1	O31-C31	4.23	1.45	1.33
69	3Y	103	3PE	O31-C31	4.23	1.45	1.33
69	3G	102	3PE	O21-C21	4.23	1.46	1.34
91	4C	302	PGV	O03-C19	4.22	1.45	1.33
69	3P	517	3PE	O21-C21	4.22	1.46	1.34
75	3X	103	CDL	OA8-CA7	4.22	1.45	1.33
69	1m	204	3PE	O31-C31	4.22	1.45	1.33
75	1d	205	CDL	OA8-CA7	4.21	1.45	1.33
91	4A	608	PGV	O03-C19	4.21	1.45	1.33
69	1A	203	3PE	O31-C31	4.21	1.45	1.33
69	1f	101	3PE	O21-C21	4.21	1.46	1.34
69	3P	504	3PE	O21-C21	4.21	1.46	1.34
69	3C	515	3PE	O31-C31	4.21	1.45	1.33
69	1g	202	3PE	O31-C31	4.21	1.45	1.33
69	1Y	204	3PE	O31-C31	4.20	1.45	1.33
69	1g	203	3PE	O31-C31	4.20	1.45	1.33
69	3P	503	3PE	O21-C21	4.20	1.46	1.34
70	1Y	202	PC1	O31-C31	4.20	1.45	1.33
69	3X	105	3PE	O31-C31	4.20	1.45	1.33
69	3P	518	3PE	O31-C31	4.20	1.45	1.33
75	1L	704	CDL	OA8-CA7	4.19	1.45	1.33
91	4C	305	PGV	O03-C19	4.19	1.45	1.33
69	1L	712	3PE	O21-C21	4.19	1.46	1.34
69	3G	104	3PE	O31-C31	4.19	1.45	1.33
75	1H	401	CDL	OA6-CA5	4.19	1.46	1.34
69	3W	103	3PE	O21-C21	4.19	1.46	1.34
75	1q	201	CDL	OB8-CB7	4.19	1.45	1.33
87	3X	102	PEK	O01-C1	4.19	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3P	515	3PE	O21-C21	4.19	1.46	1.34
69	3W	101	3PE	O21-C21	4.18	1.46	1.34
69	1Y	214	3PE	O31-C31	4.18	1.45	1.33
69	3G	104	3PE	O21-C21	4.18	1.46	1.34
70	1d	204	PC1	O21-C21	4.18	1.46	1.34
69	1f	102	3PE	O31-C31	4.18	1.45	1.33
70	1Y	207	PC1	O31-C31	4.18	1.45	1.33
69	3C	511	3PE	O31-C31	4.18	1.45	1.33
70	1H	403	PC1	O31-C31	4.18	1.45	1.33
69	3J	105	3PE	O31-C31	4.18	1.45	1.33
69	3J	102	3PE	O21-C21	4.17	1.46	1.34
69	3X	106	3PE	O31-C31	4.17	1.45	1.33
69	3W	103	3PE	O31-C31	4.17	1.45	1.33
91	4C	301	PGV	O03-C19	4.17	1.45	1.33
69	1A	201	3PE	O31-C31	4.17	1.45	1.33
75	4B	302	CDL	OA8-CA7	4.17	1.45	1.33
69	1o	201	3PE	O31-C31	4.17	1.45	1.33
69	3G	106	3PE	O31-C31	4.17	1.45	1.33
69	3C	515	3PE	O21-C21	4.17	1.46	1.34
69	3C	507	3PE	O21-C21	4.17	1.46	1.34
69	3P	510	3PE	O31-C31	4.17	1.45	1.33
69	3X	107	3PE	O31-C31	4.16	1.45	1.33
69	3X	105	3PE	O21-C21	4.16	1.46	1.34
69	3W	101	3PE	O31-C31	4.16	1.45	1.33
75	1H	401	CDL	OA8-CA7	4.16	1.45	1.33
69	3G	105	3PE	O31-C31	4.16	1.45	1.33
75	3Y	106	CDL	OB6-CB5	4.16	1.46	1.34
91	4K	101	PGV	O03-C19	4.16	1.45	1.33
69	4G	101	3PE	O21-C21	4.16	1.46	1.34
69	3Q	504	3PE	O21-C21	4.16	1.46	1.34
70	1P	502	PC1	O31-C31	4.16	1.45	1.33
69	3P	516	3PE	O31-C31	4.16	1.45	1.33
70	1A	202	PC1	O31-C31	4.16	1.45	1.33
69	3X	106	3PE	O21-C21	4.16	1.46	1.34
69	3P	520	3PE	O31-C31	4.15	1.45	1.33
69	3Q	503	3PE	O21-C21	4.15	1.46	1.34
69	1k	101	3PE	O31-C31	4.15	1.45	1.33
69	3P	520	3PE	O21-C21	4.15	1.46	1.34
69	3P	518	3PE	O21-C21	4.15	1.46	1.34
69	3C	512	3PE	O31-C31	4.14	1.45	1.33
69	3Y	107	3PE	O31-C31	4.14	1.45	1.33
69	1m	203	3PE	O21-C21	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	1l	204	3PE	O21-C21	4.14	1.46	1.34
69	1m	205	3PE	O21-C21	4.14	1.46	1.34
69	1Y	216	3PE	O31-C31	4.14	1.45	1.33
69	1Y	211	3PE	O31-C31	4.14	1.45	1.33
69	3Y	101	3PE	O31-C31	4.14	1.45	1.33
75	1N	402	CDL	OB8-CB7	4.13	1.45	1.33
69	3G	107	3PE	O21-C21	4.13	1.46	1.34
69	3Y	104	3PE	O21-C21	4.13	1.46	1.34
69	3X	101	3PE	O31-C31	4.13	1.45	1.33
69	3P	506	3PE	O31-C31	4.13	1.45	1.33
69	1L	710	3PE	O31-C31	4.13	1.45	1.33
69	3T	103	3PE	O31-C31	4.13	1.45	1.33
69	3J	104	3PE	O31-C31	4.13	1.45	1.33
69	3N	503	3PE	O31-C31	4.13	1.45	1.33
69	1d	203	3PE	O31-C31	4.12	1.45	1.33
69	1b	101	3PE	O31-C31	4.12	1.45	1.33
69	3G	108	3PE	O31-C31	4.12	1.45	1.33
70	3T	102	PC1	O31-C31	4.12	1.45	1.33
75	3F	201	CDL	OA8-CA7	4.12	1.45	1.33
91	4A	607	PGV	O03-C19	4.12	1.45	1.33
69	1Y	201	3PE	O21-C21	4.11	1.45	1.34
69	3C	516	3PE	O31-C31	4.11	1.45	1.33
69	3C	508	3PE	O21-C21	4.11	1.45	1.34
75	3F	201	CDL	OB6-CB5	4.11	1.45	1.34
69	1Y	215	3PE	O31-C31	4.11	1.45	1.33
69	3P	512	3PE	O31-C31	4.11	1.45	1.33
91	4C	302	PGV	O01-C1	4.11	1.45	1.34
69	3J	105	3PE	O21-C21	4.11	1.45	1.34
75	3F	201	CDL	OA6-CA5	4.11	1.45	1.34
75	1q	202	CDL	OA8-CA7	4.11	1.45	1.33
69	3Y	102	3PE	O31-C31	4.11	1.45	1.33
91	4A	608	PGV	O01-C1	4.10	1.45	1.34
69	1B	205	3PE	O21-C21	4.10	1.45	1.34
75	1i	201	CDL	OB6-CB5	4.10	1.45	1.34
75	3Y	106	CDL	OA8-CA7	4.10	1.45	1.33
69	3G	103	3PE	O31-C31	4.10	1.45	1.33
69	3G	103	3PE	O21-C21	4.10	1.45	1.34
69	1Y	210	3PE	O31-C31	4.09	1.45	1.33
91	4C	303	PGV	O01-C1	4.09	1.45	1.34
69	3C	510	3PE	O31-C31	4.09	1.45	1.33
69	1f	103	3PE	O21-C21	4.09	1.45	1.34
69	3G	109	3PE	O31-C31	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	1L	709	3PE	O31-C31	4.09	1.45	1.33
69	3C	503	3PE	O21-C21	4.09	1.45	1.34
91	4N	101	PGV	O03-C19	4.09	1.45	1.33
69	1d	201	3PE	O31-C31	4.09	1.45	1.33
69	3P	504	3PE	O31-C31	4.09	1.45	1.33
69	1Y	208	3PE	O31-C31	4.09	1.45	1.33
69	3C	517	3PE	O31-C31	4.09	1.45	1.33
70	1B	202	PC1	O31-C31	4.08	1.45	1.33
70	3R	303	PC1	O31-C31	4.08	1.45	1.33
69	1m	202	3PE	O21-C21	4.08	1.45	1.34
91	4A	607	PGV	O01-C1	4.08	1.45	1.34
69	1k	101	3PE	O21-C21	4.08	1.45	1.34
91	4G	102	PGV	O01-C1	4.08	1.45	1.34
69	3P	515	3PE	O31-C31	4.08	1.45	1.33
69	3R	304	3PE	O31-C31	4.07	1.45	1.33
75	4C	307	CDL	OA6-CA5	4.07	1.45	1.34
70	1A	202	PC1	O21-C21	4.07	1.45	1.34
75	1L	704	CDL	OB6-CB5	4.07	1.45	1.34
69	1Y	208	3PE	O21-C21	4.07	1.45	1.34
69	3P	514	3PE	O21-C21	4.07	1.45	1.34
69	1Y	212	3PE	O21-C21	4.07	1.45	1.34
69	3C	505	3PE	O21-C21	4.07	1.45	1.34
69	3G	108	3PE	O21-C21	4.07	1.45	1.34
69	3X	108	3PE	O31-C31	4.06	1.45	1.33
69	1M	502	3PE	O31-C31	4.06	1.45	1.33
69	3C	512	3PE	O21-C21	4.06	1.45	1.34
69	1Y	204	3PE	O21-C21	4.06	1.45	1.34
69	1Y	201	3PE	O31-C31	4.06	1.45	1.33
70	1P	502	PC1	O21-C21	4.06	1.45	1.34
69	3C	509	3PE	O31-C31	4.06	1.45	1.33
75	1Y	217	CDL	OB8-CB7	4.06	1.45	1.33
69	3P	505	3PE	O21-C21	4.06	1.45	1.34
69	1L	702	3PE	O31-C31	4.06	1.45	1.33
91	4K	101	PGV	O01-C1	4.06	1.45	1.34
69	1Y	209	3PE	O31-C31	4.06	1.45	1.33
69	3Y	107	3PE	O21-C21	4.06	1.45	1.34
69	3J	102	3PE	O31-C31	4.05	1.45	1.33
69	3Y	103	3PE	O21-C21	4.05	1.45	1.34
69	1Y	213	3PE	O31-C31	4.05	1.45	1.33
69	3J	104	3PE	O21-C21	4.05	1.45	1.34
69	1Y	216	3PE	O21-C21	4.05	1.45	1.34
70	1Y	202	PC1	O21-C21	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	1H	404	PC1	O21-C21	4.05	1.45	1.34
69	3C	511	3PE	O21-C21	4.05	1.45	1.34
75	4B	302	CDL	OA6-CA5	4.05	1.45	1.34
69	1f	101	3PE	O31-C31	4.05	1.45	1.33
70	3J	106	PC1	O31-C31	4.04	1.45	1.33
91	4C	303	PGV	O03-C19	4.04	1.45	1.33
82	1Y	203	PGT	O2-C31	4.04	1.45	1.34
75	1d	205	CDL	OB6-CB5	4.04	1.45	1.34
75	3Y	106	CDL	OA6-CA5	4.04	1.45	1.34
70	1H	403	PC1	O21-C21	4.04	1.45	1.34
69	3X	107	3PE	O21-C21	4.04	1.45	1.34
70	3P	509	PC1	O31-C31	4.04	1.45	1.33
69	1d	203	3PE	O21-C21	4.04	1.45	1.34
69	3C	516	3PE	O21-C21	4.03	1.45	1.34
69	3R	304	3PE	O21-C21	4.03	1.45	1.34
69	1J	201	3PE	O21-C21	4.03	1.45	1.34
69	3C	506	3PE	O31-C31	4.03	1.45	1.33
69	1m	205	3PE	O31-C31	4.03	1.45	1.33
75	3X	103	CDL	OA6-CA5	4.03	1.45	1.34
91	4C	301	PGV	O01-C1	4.02	1.45	1.34
69	3P	519	3PE	O21-C21	4.02	1.45	1.34
91	4N	101	PGV	O01-C1	4.02	1.45	1.34
75	3F	201	CDL	OB8-CB7	4.02	1.45	1.33
70	1J	202	PC1	O31-C31	4.02	1.45	1.33
69	3S	201	3PE	O21-C21	4.01	1.45	1.34
75	1Y	217	CDL	OA6-CA5	4.01	1.45	1.34
93	4B	303	PSC	O01-C1	4.01	1.45	1.34
75	3T	101	CDL	OB8-CB7	4.01	1.45	1.33
91	4C	304	PGV	O01-C1	4.01	1.45	1.34
69	1b	101	3PE	O21-C21	4.01	1.45	1.34
69	3Y	101	3PE	O21-C21	4.01	1.45	1.34
69	3Y	105	3PE	O21-C21	4.01	1.45	1.34
69	3P	511	3PE	O21-C21	4.00	1.45	1.34
69	1Y	214	3PE	O21-C21	4.00	1.45	1.34
69	3N	501	3PE	O31-C31	4.00	1.45	1.33
69	1m	201	3PE	O21-C21	4.00	1.45	1.34
69	3P	511	3PE	O31-C31	4.00	1.45	1.33
69	1Y	211	3PE	O21-C21	4.00	1.45	1.34
70	1Y	207	PC1	O21-C21	4.00	1.45	1.34
69	1l	202	3PE	O31-C31	4.00	1.45	1.33
69	1L	705	3PE	O31-C31	4.00	1.45	1.33
75	4B	302	CDL	OB6-CB5	3.99	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4G	103	PEK	O03-C21	3.99	1.45	1.33
91	4C	305	PGV	O01-C1	3.99	1.45	1.34
75	1q	202	CDL	OB6-CB5	3.99	1.45	1.34
69	3S	201	3PE	O31-C31	3.99	1.45	1.33
70	1h	202	PC1	O21-C21	3.98	1.45	1.34
69	3J	101	3PE	O21-C21	3.98	1.45	1.34
69	3G	110	3PE	O31-C31	3.98	1.45	1.33
87	4G	103	PEK	O01-C1	3.98	1.45	1.34
69	3P	516	3PE	O21-C21	3.98	1.45	1.34
69	3G	111	3PE	O21-C21	3.98	1.45	1.34
75	1g	201	CDL	OB6-CB5	3.98	1.45	1.34
69	4G	104	3PE	O21-C21	3.98	1.45	1.34
69	3C	505	3PE	O31-C31	3.98	1.45	1.33
75	1i	201	CDL	OA8-CA7	3.97	1.45	1.33
69	1d	206	3PE	O21-C21	3.97	1.45	1.34
69	1A	203	3PE	O21-C21	3.97	1.45	1.34
69	3G	110	3PE	O21-C21	3.97	1.45	1.34
70	1J	202	PC1	O21-C21	3.97	1.45	1.34
69	3X	101	3PE	O21-C21	3.97	1.45	1.34
75	1g	201	CDL	OA6-CA5	3.97	1.45	1.34
91	4J	101	PGV	O01-C1	3.97	1.45	1.34
75	1g	201	CDL	OB8-CB7	3.97	1.44	1.33
69	3P	517	3PE	O31-C31	3.97	1.44	1.33
69	3Q	502	3PE	O21-C21	3.96	1.45	1.34
75	4C	307	CDL	OB6-CB5	3.96	1.45	1.34
75	3P	513	CDL	OB8-CB7	3.96	1.44	1.33
91	4A	606	PGV	O01-C1	3.96	1.45	1.34
69	3C	514	3PE	O31-C31	3.96	1.44	1.33
75	4C	306	CDL	OB6-CB5	3.96	1.45	1.34
70	1Y	206	PC1	O21-C21	3.96	1.45	1.34
75	1i	201	CDL	OA6-CA5	3.96	1.45	1.34
69	1f	102	3PE	O21-C21	3.95	1.45	1.34
75	3Y	106	CDL	OB8-CB7	3.95	1.44	1.33
69	3C	508	3PE	O31-C31	3.95	1.44	1.33
69	3C	517	3PE	O21-C21	3.95	1.45	1.34
69	1M	502	3PE	O21-C21	3.95	1.45	1.34
69	1e	201	3PE	O21-C21	3.95	1.45	1.34
75	4C	306	CDL	OA6-CA5	3.94	1.45	1.34
70	1H	402	PC1	O21-C21	3.94	1.45	1.34
70	1h	202	PC1	O31-C31	3.94	1.44	1.33
70	1H	404	PC1	O31-C31	3.94	1.44	1.33
75	3A	501	CDL	OB6-CB5	3.94	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	1m	204	3PE	O21-C21	3.94	1.45	1.34
69	1N	401	3PE	O21-C21	3.93	1.45	1.34
70	3R	303	PC1	O21-C21	3.93	1.45	1.34
69	1L	709	3PE	O21-C21	3.92	1.45	1.34
69	1m	202	3PE	O31-C31	3.92	1.44	1.33
70	1h	203	PC1	O21-C21	3.92	1.45	1.34
69	3D	503	3PE	O21-C21	3.92	1.45	1.34
70	3J	106	PC1	O21-C21	3.92	1.45	1.34
75	1H	401	CDL	OB6-CB5	3.92	1.45	1.34
75	3N	502	CDL	OA8-CA7	3.91	1.44	1.33
75	1N	402	CDL	OA6-CA5	3.91	1.45	1.34
69	3C	506	3PE	O21-C21	3.91	1.45	1.34
69	3C	503	3PE	O31-C31	3.91	1.44	1.33
69	3G	105	3PE	O21-C21	3.91	1.45	1.34
70	1h	203	PC1	O31-C31	3.91	1.44	1.33
69	1L	711	3PE	O31-C31	3.90	1.44	1.33
69	3A	502	3PE	O31-C31	3.90	1.44	1.33
69	1J	203	3PE	O31-C31	3.90	1.44	1.33
75	1N	402	CDL	OA8-CA7	3.90	1.44	1.33
70	1B	202	PC1	O21-C21	3.90	1.45	1.34
75	1Y	217	CDL	OA8-CA7	3.90	1.44	1.33
75	1N	402	CDL	OB6-CB5	3.90	1.45	1.34
69	3E	302	3PE	O21-C21	3.90	1.45	1.34
69	1f	104	3PE	O21-C21	3.89	1.45	1.34
69	1B	204	3PE	O21-C21	3.89	1.45	1.34
75	3T	101	CDL	OA6-CA5	3.88	1.45	1.34
69	1l	203	3PE	O21-C21	3.88	1.45	1.34
70	1B	203	PC1	O21-C21	3.88	1.45	1.34
69	1L	711	3PE	O21-C21	3.88	1.45	1.34
69	3P	512	3PE	O21-C21	3.88	1.45	1.34
69	3W	102	3PE	O21-C21	3.87	1.45	1.34
69	3D	503	3PE	O31-C31	3.87	1.44	1.33
69	1L	708	3PE	O31-C31	3.87	1.44	1.33
69	3A	503	3PE	O31-C31	3.87	1.44	1.33
69	3G	109	3PE	O21-C21	3.86	1.45	1.34
75	3D	504	CDL	OA6-CA5	3.86	1.45	1.34
69	3G	101	3PE	O31-C31	3.86	1.44	1.33
75	3P	513	CDL	OA8-CA7	3.86	1.44	1.33
75	1Y	217	CDL	OB6-CB5	3.86	1.45	1.34
69	3G	106	3PE	O21-C21	3.86	1.45	1.34
69	1L	703	3PE	O21-C21	3.85	1.45	1.34
75	1d	205	CDL	OB8-CB7	3.85	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	1L	705	3PE	O21-C21	3.85	1.45	1.34
69	1d	201	3PE	O21-C21	3.85	1.45	1.34
69	3A	502	3PE	O21-C21	3.85	1.45	1.34
69	1Y	213	3PE	O21-C21	3.85	1.45	1.34
75	1d	202	CDL	OA8-CA7	3.84	1.44	1.33
69	3C	509	3PE	O21-C21	3.84	1.45	1.34
91	4A	609	PGV	O01-C1	3.84	1.45	1.34
69	3C	513	3PE	O21-C21	3.83	1.45	1.34
69	3E	302	3PE	O31-C31	3.83	1.44	1.33
75	3X	103	CDL	OB8-CB7	3.83	1.44	1.33
75	3A	501	CDL	OB8-CB7	3.83	1.44	1.33
69	1o	201	3PE	O21-C21	3.82	1.45	1.34
70	1H	402	PC1	O31-C31	3.82	1.44	1.33
69	3P	506	3PE	O21-C21	3.82	1.45	1.34
75	3A	501	CDL	OA8-CA7	3.82	1.44	1.33
75	1d	205	CDL	OA6-CA5	3.82	1.45	1.34
69	3N	503	3PE	O21-C21	3.81	1.45	1.34
69	1L	710	3PE	O21-C21	3.81	1.45	1.34
70	1d	204	PC1	O31-C31	3.81	1.44	1.33
69	3P	519	3PE	O31-C31	3.81	1.44	1.33
69	1L	701	3PE	O21-C21	3.80	1.45	1.34
69	3P	510	3PE	O21-C21	3.80	1.45	1.34
75	1q	201	CDL	OB6-CB5	3.79	1.45	1.34
75	3D	504	CDL	OA8-CA7	3.78	1.44	1.33
69	1Y	210	3PE	O21-C21	3.78	1.45	1.34
75	1q	201	CDL	OA8-CA7	3.77	1.44	1.33
69	1L	702	3PE	O21-C21	3.75	1.44	1.34
69	1N	401	3PE	O31-C31	3.75	1.44	1.33
75	1q	202	CDL	OA6-CA5	3.75	1.44	1.34
75	3N	502	CDL	OB8-CB7	3.75	1.44	1.33
69	3R	302	3PE	O21-C21	3.74	1.44	1.34
69	3G	101	3PE	O21-C21	3.74	1.44	1.34
69	1A	201	3PE	O21-C21	3.72	1.44	1.34
69	1L	707	3PE	O31-C31	3.72	1.44	1.33
70	1M	501	PC1	O21-C21	3.72	1.44	1.34
69	1Z	201	3PE	O21-C21	3.70	1.44	1.34
69	3E	303	3PE	O31-C31	3.70	1.44	1.33
70	1B	203	PC1	O31-C31	3.70	1.44	1.33
69	1J	203	3PE	O21-C21	3.69	1.44	1.34
69	1Y	209	3PE	O21-C21	3.69	1.44	1.34
75	1q	201	CDL	OA6-CA5	3.69	1.44	1.34
75	1L	704	CDL	OB8-CB7	3.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3P	507	3PE	O31-C31	3.67	1.44	1.33
69	3P	508	3PE	O31-C31	3.67	1.44	1.33
75	1i	201	CDL	OB8-CB7	3.65	1.44	1.33
69	3C	514	3PE	O21-C21	3.64	1.44	1.34
75	1L	704	CDL	OA6-CA5	3.64	1.44	1.34
75	3A	501	CDL	OA6-CA5	3.63	1.44	1.34
69	1L	707	3PE	O21-C21	3.63	1.44	1.34
69	1g	202	3PE	O21-C21	3.63	1.44	1.34
69	1Y	215	3PE	O21-C21	3.63	1.44	1.34
70	3P	509	PC1	O21-C21	3.62	1.44	1.34
70	3X	104	PC1	O21-C21	3.61	1.44	1.34
75	3T	101	CDL	OA8-CA7	3.59	1.43	1.33
75	1d	202	CDL	OA6-CA5	3.59	1.44	1.34
69	3A	503	3PE	O21-C21	3.59	1.44	1.34
69	3R	305	3PE	O31-C31	3.57	1.43	1.33
69	1L	701	3PE	O31-C31	3.57	1.43	1.33
70	3T	102	PC1	O21-C21	3.55	1.44	1.34
75	3N	502	CDL	OB6-CB5	3.55	1.44	1.34
69	3N	501	3PE	O21-C21	3.55	1.44	1.34
69	3E	303	3PE	O21-C21	3.54	1.44	1.34
75	3N	502	CDL	OA6-CA5	3.53	1.44	1.34
75	3P	513	CDL	OB6-CB5	3.51	1.44	1.34
85	3P	502	HEM	C1B-NB	-3.48	1.34	1.40
69	3R	302	3PE	O31-C31	3.47	1.43	1.33
85	3C	502	HEM	C1B-NB	-3.47	1.34	1.40
75	3T	101	CDL	OB6-CB5	3.47	1.44	1.34
75	3D	504	CDL	OB6-CB5	3.46	1.44	1.34
70	3X	104	PC1	O31-C31	3.44	1.43	1.33
85	3C	501	HEM	C1B-NB	-3.43	1.34	1.40
75	1d	202	CDL	OB8-CB7	3.42	1.43	1.33
85	3P	501	HEM	C1B-NB	-3.39	1.34	1.40
85	3P	502	HEM	C4D-ND	-3.39	1.34	1.40
69	3P	508	3PE	O21-C21	3.30	1.43	1.34
85	3C	502	HEM	C4D-ND	-3.30	1.34	1.40
86	3Q	501	HEC	C2A-C3A	3.28	1.47	1.37
86	3D	501	HEC	C3D-C2D	3.26	1.47	1.37
85	3P	501	HEM	C4D-ND	-3.25	1.34	1.40
86	3D	501	HEC	C2A-C3A	3.24	1.47	1.37
69	3C	510	3PE	O21-C21	3.24	1.43	1.34
86	3Q	501	HEC	C3D-C2D	3.23	1.47	1.37
69	3C	510	3PE	O21-C2	-3.20	1.38	1.46
85	3C	501	HEM	C4D-ND	-3.12	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	4A	601	HEA	FE-ND	3.08	2.12	1.96
88	4A	602	HEA	FE-ND	3.06	2.12	1.96
88	4A	601	HEA	FE-NB	3.06	2.12	1.96
88	4A	601	HEA	C4B-C3B	3.05	1.49	1.44
88	4A	602	HEA	FE-NB	3.04	2.11	1.96
85	3C	501	HEM	FE-NB	2.99	2.11	1.96
85	3P	501	HEM	FE-NB	2.98	2.11	1.96
86	3D	501	HEC	C4B-C3B	2.97	1.48	1.43
85	3C	502	HEM	FE-NB	2.86	2.11	1.96
85	3P	502	HEM	FE-NB	2.84	2.10	1.96
86	3Q	501	HEC	C3C-C4C	2.84	1.48	1.43
86	3D	501	HEC	C3C-C4C	2.83	1.48	1.43
88	4A	602	HEA	C1D-ND	-2.81	1.35	1.40
86	3Q	501	HEC	C4B-C3B	2.80	1.48	1.43
88	4A	601	HEA	C1D-ND	-2.74	1.35	1.40
86	3Q	501	HEC	C3A-C4A	2.72	1.48	1.42
88	4A	602	HEA	C4B-C3B	2.70	1.49	1.44
88	4A	601	HEA	C2A-C1A	2.69	1.48	1.42
88	4A	602	HEA	C4B-NB	-2.66	1.35	1.40
88	4A	601	HEA	C4B-NB	-2.57	1.35	1.40
86	3D	501	HEC	C2A-C1A	2.55	1.48	1.42
86	3D	501	HEC	C3A-C4A	2.52	1.48	1.42
86	3Q	501	HEC	C1D-CHD	2.48	1.47	1.41
86	3D	501	HEC	C1D-CHD	2.48	1.47	1.41
69	1L	701	3PE	O21-C2	-2.47	1.40	1.46
86	3Q	501	HEC	C1C-CHC	2.45	1.47	1.41
86	3D	501	HEC	C4D-CHA	2.45	1.47	1.41
88	4A	602	HEA	C2A-C1A	2.45	1.48	1.42
86	3Q	501	HEC	C2A-C1A	2.45	1.48	1.42
77	1O	401	GTP	C6-N1	-2.44	1.34	1.37
86	3D	501	HEC	C1C-CHC	2.40	1.47	1.41
86	3Q	501	HEC	C1B-CHB	2.38	1.47	1.41
88	4A	601	HEA	C4D-C3D	2.37	1.49	1.45
86	3Q	501	HEC	C4D-CHA	2.34	1.47	1.41
70	1B	202	PC1	C25-C24	-2.33	1.38	1.51
88	4A	602	HEA	C4C-CHD	2.30	1.47	1.41
88	4A	602	HEA	C1D-C2D	2.29	1.49	1.44
88	4A	601	HEA	C1C-CHC	2.24	1.47	1.41
70	3X	104	PC1	O21-C2	-2.24	1.41	1.46
88	4A	602	HEA	C1C-CHC	2.23	1.47	1.41
69	1L	707	3PE	O21-C2	-2.23	1.41	1.46
75	3P	513	CDL	OB6-CB4	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	3D	504	CDL	OB6-CB4	-2.21	1.41	1.46
69	3E	303	3PE	O21-C2	-2.20	1.41	1.46
88	4A	601	HEA	C4C-CHD	2.20	1.47	1.41
69	3N	501	3PE	O21-C2	-2.20	1.41	1.46
86	3D	501	HEC	C1B-CHB	2.18	1.47	1.41
85	3C	502	HEM	C1D-ND	-2.14	1.34	1.38
85	3P	502	HEM	C1D-ND	-2.13	1.34	1.38
85	3C	501	HEM	CHB-C1B	2.13	1.40	1.35
75	1d	202	CDL	OA6-CA4	-2.11	1.41	1.46
69	3P	508	3PE	O21-C2	-2.11	1.41	1.46
69	3R	305	3PE	O21-C2	-2.10	1.41	1.46
85	3C	501	HEM	C4B-NB	-2.09	1.34	1.38
69	3A	502	3PE	O21-C2	-2.09	1.41	1.46
75	3T	101	CDL	OA6-CA4	-2.09	1.41	1.46
69	3P	508	3PE	O31-C3	-2.08	1.40	1.45
85	3P	501	HEM	CHB-C1B	2.08	1.40	1.35
85	3C	502	HEM	C4B-NB	-2.07	1.34	1.38
88	4A	602	HEA	C1B-C2B	2.06	1.48	1.44
88	4A	602	HEA	CHB-C1B	2.06	1.47	1.41
88	4A	601	HEA	C1D-C2D	2.05	1.48	1.44
75	3T	101	CDL	OB6-CB4	-2.03	1.41	1.46
75	3A	501	CDL	OB6-CB4	-2.03	1.41	1.46
69	3R	302	3PE	O21-C2	-2.02	1.41	1.46
69	3G	101	3PE	O21-C2	-2.02	1.41	1.46
75	3D	504	CDL	OA6-CA4	-2.01	1.41	1.46
85	3P	501	HEM	C1D-ND	-2.01	1.34	1.38
70	3T	102	PC1	O21-C2	-2.01	1.41	1.46
75	1L	704	CDL	OA6-CA4	-2.01	1.41	1.46
85	3P	502	HEM	C4B-NB	-2.01	1.34	1.38
85	3C	502	HEM	CHB-C1B	2.00	1.40	1.35

All (805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1L	710	3PE	O21-C21-C22	22.38	159.74	111.50
69	3Q	502	3PE	O21-C21-C22	21.69	158.26	111.50
69	3W	103	3PE	O31-C31-O32	-18.85	76.02	123.59
69	3Q	502	3PE	O21-C21-O22	-18.74	78.41	123.70
69	1L	710	3PE	O21-C21-O22	-18.30	79.47	123.70
69	3W	103	3PE	O31-C31-C32	15.02	159.05	111.91
70	3J	106	PC1	C15-N-C14	-12.11	77.84	108.97
70	3J	106	PC1	C15-N-C13	-11.90	78.38	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	3Q	502	3PE	O22-C21-C22	-11.25	79.85	123.73
69	1L	710	3PE	O22-C21-C22	-11.13	80.30	123.73
69	3W	103	3PE	O32-C31-C32	-10.42	83.06	123.73
70	1B	202	PC1	C2B-C2A-C29	-8.86	46.16	113.42
70	3J	106	PC1	C15-N-C12	-8.04	77.01	109.92
88	4A	602	HEA	C3D-C4D-ND	6.71	116.86	110.36
69	3C	510	3PE	C2-O21-C21	-6.70	101.29	117.79
86	3Q	501	HEC	C1D-C2D-C3D	-6.46	102.50	107.00
86	3D	501	HEC	C1D-C2D-C3D	-6.41	102.54	107.00
88	4A	601	HEA	C3D-C4D-ND	6.39	116.55	110.36
88	4A	601	HEA	C2B-C1B-NB	5.83	116.86	109.88
81	1T	101	EHZ	C10-S1-C9	5.78	119.88	101.87
70	1B	202	PC1	C25-C24-C23	5.73	143.51	114.42
81	1n	201	EHZ	C10-S1-C9	5.72	119.68	101.87
85	3P	501	HEM	CHC-C4B-NB	5.58	130.49	124.43
70	1B	202	PC1	C28-C27-C26	-5.52	86.39	114.42
69	3A	503	3PE	C2-O21-C21	-5.48	104.29	117.79
88	4A	602	HEA	C2D-C1D-ND	5.48	116.33	109.84
85	3C	501	HEM	CHC-C4B-NB	5.47	130.37	124.43
75	1L	704	CDL	OB6-CB5-C51	5.45	123.26	111.50
70	1B	202	PC1	C26-C25-C24	-5.41	86.98	114.42
69	1o	201	3PE	O21-C21-C22	5.37	123.08	111.50
75	1i	201	CDL	OB6-CB5-C51	5.37	123.07	111.50
88	4A	601	HEA	C2D-C1D-ND	5.34	116.17	109.84
88	4A	602	HEA	C3B-C4B-NB	5.34	116.16	109.84
88	4A	602	HEA	C2B-C1B-NB	5.29	116.22	109.88
88	4A	601	HEA	C3B-C4B-NB	5.23	116.03	109.84
75	1d	202	CDL	OB6-CB5-C51	5.13	122.55	111.50
75	3P	513	CDL	OB6-CB5-C51	5.12	122.53	111.50
70	1B	202	PC1	O21-C21-C22	5.07	122.44	111.50
70	1B	203	PC1	O21-C21-C22	5.01	122.30	111.50
69	3G	104	3PE	O21-C21-C22	4.91	122.08	111.50
69	3P	503	3PE	O21-C21-C22	4.89	122.05	111.50
70	3R	303	PC1	O21-C21-C22	4.84	121.93	111.50
85	3P	502	HEM	CHC-C4B-NB	4.81	129.66	124.43
86	3Q	501	HEC	CMC-C2C-C3C	4.81	131.47	125.82
70	1B	202	PC1	C27-C26-C25	-4.79	90.10	114.42
86	3D	501	HEC	CMC-C2C-C3C	4.79	131.45	125.82
70	1d	204	PC1	O21-C21-C22	4.75	121.75	111.50
75	3Y	106	CDL	OB6-CB5-C51	4.73	121.70	111.50
88	4A	601	HEA	CBA-CAA-C2A	-4.71	104.66	112.60
85	3C	502	HEM	CHC-C4B-NB	4.69	129.53	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	1d	205	CDL	OA6-CA5-C11	4.68	121.59	111.50
70	1h	203	PC1	O21-C21-C22	4.68	121.59	111.50
75	1q	202	CDL	OA6-CA5-C11	4.67	121.56	111.50
69	3R	305	3PE	O21-C21-C22	4.65	121.53	111.50
69	1L	708	3PE	O21-C21-C22	4.65	121.52	111.50
69	3G	101	3PE	O21-C21-C22	4.64	121.51	111.50
69	3J	102	3PE	O21-C21-C22	4.64	121.50	111.50
69	1m	204	3PE	O21-C21-C22	4.63	121.47	111.50
75	1q	201	CDL	OB6-CB5-C51	4.61	121.44	111.50
69	1d	203	3PE	O21-C21-C22	4.60	121.42	111.50
75	3D	504	CDL	OA6-CA5-C11	4.59	121.40	111.50
69	1B	204	3PE	O21-C21-C22	4.58	121.38	111.50
69	3J	105	3PE	O21-C21-C22	4.56	121.33	111.50
75	1i	201	CDL	OA6-CA5-C11	4.56	121.32	111.50
70	3P	509	PC1	O21-C21-C22	4.55	121.30	111.50
69	1g	203	3PE	O21-C21-C22	4.54	121.29	111.50
69	3C	508	3PE	O21-C21-C22	4.53	121.26	111.50
85	3P	501	HEM	CHD-C1D-ND	4.53	129.35	124.43
69	3C	509	3PE	O21-C21-C22	4.50	121.20	111.50
70	1M	501	PC1	O21-C21-C22	4.49	121.19	111.50
69	1N	401	3PE	O21-C21-C22	4.49	121.17	111.50
75	1q	201	CDL	OA6-CA5-C11	4.47	121.13	111.50
69	3G	103	3PE	O21-C21-C22	4.47	121.13	111.50
86	3D	501	HEC	CMB-C2B-C3B	4.43	131.03	125.82
69	1e	201	3PE	O21-C21-C22	4.42	121.02	111.50
75	3P	513	CDL	OA6-CA5-C11	4.41	121.02	111.50
69	1A	203	3PE	O21-C21-C22	4.40	120.98	111.50
69	1L	703	3PE	O21-C21-C22	4.39	120.97	111.50
88	4A	602	HEA	C1D-C2D-C3D	-4.39	102.34	106.96
75	3A	501	CDL	OA6-CA5-C11	4.39	120.96	111.50
75	3T	101	CDL	OA6-CA5-C11	4.39	120.96	111.50
69	4G	101	3PE	O21-C21-C22	4.38	120.95	111.50
85	3C	501	HEM	CHD-C1D-ND	4.38	129.19	124.43
70	3J	106	PC1	O21-C21-C22	4.36	120.90	111.50
69	3C	515	3PE	O21-C21-C22	4.36	120.89	111.50
69	1L	712	3PE	O21-C21-C22	4.35	120.88	111.50
75	3F	201	CDL	OA6-CA5-C11	4.34	120.85	111.50
69	1k	101	3PE	O21-C21-C22	4.34	120.84	111.50
75	3P	513	CDL	CB4-OB6-CB5	-4.33	107.12	117.79
69	3P	511	3PE	O21-C21-C22	4.33	120.83	111.50
75	3X	103	CDL	OA6-CA5-C11	4.33	120.82	111.50
69	1L	707	3PE	O21-C21-C22	4.30	120.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	3P	508	3PE	O21-C21-C22	4.30	120.78	111.50
85	3P	502	HEM	C1B-NB-C4B	4.30	109.51	105.07
69	3W	103	3PE	O21-C21-C22	4.29	120.75	111.50
69	1l	202	3PE	O21-C21-C22	4.28	120.73	111.50
69	1Y	216	3PE	O21-C21-C22	4.27	120.71	111.50
69	3Y	107	3PE	O21-C21-C22	4.27	120.70	111.50
69	1L	701	3PE	O21-C21-C22	4.27	120.70	111.50
69	1A	201	3PE	O21-C21-C22	4.27	120.70	111.50
85	3C	502	HEM	C1B-NB-C4B	4.26	109.48	105.07
69	3E	303	3PE	O21-C21-C22	4.26	120.69	111.50
69	1L	709	3PE	O21-C21-C22	4.26	120.68	111.50
75	1N	402	CDL	OB6-CB5-C51	4.25	120.65	111.50
69	3P	515	3PE	O21-C21-C22	4.24	120.64	111.50
69	3C	512	3PE	O21-C21-C22	4.24	120.64	111.50
75	4B	302	CDL	OB6-CB5-C51	4.24	120.64	111.50
69	3Q	503	3PE	O21-C21-C22	4.24	120.63	111.50
86	3Q	501	HEC	CMB-C2B-C3B	4.23	130.79	125.82
70	1H	402	PC1	O21-C21-C22	4.22	120.60	111.50
69	3R	302	3PE	O21-C21-C22	4.22	120.59	111.50
86	3Q	501	HEC	CBD-CAD-C3D	-4.22	105.42	112.62
75	3F	201	CDL	OB6-CB5-C51	4.22	120.59	111.50
85	3C	501	HEM	C1B-NB-C4B	4.21	109.42	105.07
70	1Y	207	PC1	O21-C21-C22	4.20	120.56	111.50
69	3C	516	3PE	O21-C21-C22	4.20	120.55	111.50
70	1J	202	PC1	O21-C21-C22	4.20	120.55	111.50
75	3A	501	CDL	OB6-CB5-C51	4.20	120.54	111.50
91	4N	101	PGV	O01-C1-C2	4.19	120.54	111.50
87	4G	103	PEK	O01-C1-C2	4.18	120.52	111.50
69	1m	202	3PE	O21-C21-C22	4.16	120.48	111.50
69	3J	101	3PE	O21-C21-C22	4.16	120.47	111.50
69	3E	302	3PE	O21-C21-C22	4.15	120.45	111.50
69	3P	504	3PE	O21-C21-C22	4.15	120.45	111.50
69	3C	510	3PE	O21-C21-C22	4.15	120.44	111.50
91	4C	304	PGV	O01-C1-C2	4.15	120.44	111.50
69	3C	505	3PE	O21-C21-C22	4.14	120.43	111.50
69	3D	503	3PE	O21-C21-C22	4.14	120.42	111.50
75	1d	205	CDL	CA4-OA6-CA5	-4.12	107.64	117.79
85	3C	502	HEM	CHD-C1D-ND	4.12	128.91	124.43
69	1B	205	3PE	O21-C21-C22	4.12	120.38	111.50
69	3C	514	3PE	O21-C21-C22	4.12	120.37	111.50
75	3N	502	CDL	OA6-CA5-C11	4.12	120.37	111.50
69	3C	506	3PE	O21-C21-C22	4.11	120.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	1A	202	PC1	O21-C21-C22	4.11	120.37	111.50
75	4C	307	CDL	OB6-CB5-C51	4.11	120.36	111.50
70	1H	404	PC1	O21-C21-C22	4.10	120.34	111.50
75	3X	103	CDL	OB6-CB5-C51	4.10	120.33	111.50
69	3C	507	3PE	O21-C21-C22	4.09	120.33	111.50
85	3P	502	HEM	CHD-C1D-ND	4.07	128.85	124.43
69	3Q	504	3PE	O21-C21-C22	4.07	120.27	111.50
91	4K	101	PGV	O01-C1-C2	4.07	120.26	111.50
69	1Y	215	3PE	O21-C21-C22	4.06	120.25	111.50
70	1h	202	PC1	O21-C21-C22	4.05	120.23	111.50
85	3P	501	HEM	C1B-NB-C4B	4.05	109.25	105.07
69	3A	502	3PE	O21-C21-C22	4.04	120.20	111.50
75	1Y	217	CDL	OB6-CB5-C51	4.04	120.20	111.50
69	1m	205	3PE	O21-C21-C22	4.03	120.19	111.50
69	3Y	103	3PE	O21-C21-C22	4.02	120.17	111.50
69	1Y	208	3PE	O21-C21-C22	4.02	120.16	111.50
69	1f	103	3PE	O21-C21-C22	4.02	120.16	111.50
69	1m	203	3PE	O21-C21-C22	4.01	120.15	111.50
69	3G	108	3PE	O21-C21-C22	4.00	120.13	111.50
88	4A	601	HEA	C13-C12-C11	-4.00	108.34	114.35
75	1d	202	CDL	OA6-CA5-C11	4.00	120.12	111.50
69	1b	101	3PE	O21-C21-C22	4.00	120.12	111.50
82	1Y	203	PGT	O2-C31-C32	4.00	120.12	111.50
91	4A	606	PGV	O01-C1-C2	4.00	120.11	111.50
69	3P	516	3PE	O21-C21-C22	4.00	120.11	111.50
69	3P	512	3PE	O21-C21-C22	3.99	120.11	111.50
88	4A	601	HEA	C3C-C4C-NC	3.99	114.37	109.21
69	3C	513	3PE	O21-C21-C22	3.97	120.07	111.50
69	1J	201	3PE	O21-C21-C22	3.97	120.06	111.50
69	1f	101	3PE	O21-C21-C22	3.97	120.06	111.50
75	1g	201	CDL	OB6-CB5-C51	3.97	120.05	111.50
69	1h	204	3PE	O21-C21-C22	3.97	120.05	111.50
88	4A	601	HEA	CHA-C4D-ND	-3.96	120.12	124.43
69	3C	511	3PE	O21-C21-C22	3.96	120.03	111.50
69	1Z	201	3PE	O21-C21-C22	3.95	120.02	111.50
75	1N	402	CDL	OA6-CA5-C11	3.95	120.02	111.50
91	4J	101	PGV	O01-C1-C2	3.95	120.01	111.50
70	1Y	202	PC1	O21-C21-C22	3.94	120.00	111.50
75	4B	302	CDL	OA6-CA5-C11	3.94	120.00	111.50
75	1d	205	CDL	OB6-CB5-C51	3.94	120.00	111.50
91	4C	301	PGV	O01-C1-C2	3.93	119.98	111.50
69	1L	705	3PE	O21-C21-C22	3.91	119.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	3Q	501	HEC	CAA-CBA-CGA	-3.91	102.79	113.76
75	1q	202	CDL	OB6-CB5-C51	3.91	119.93	111.50
69	3P	518	3PE	O21-C21-C22	3.90	119.91	111.50
91	4C	302	PGV	O01-C1-C2	3.90	119.91	111.50
69	1l	204	3PE	O21-C21-C22	3.90	119.90	111.50
69	3N	501	3PE	O21-C21-C22	3.90	119.90	111.50
75	1H	401	CDL	OA6-CA5-C11	3.89	119.87	111.50
91	4A	607	PGV	O01-C1-C2	3.88	119.86	111.50
69	1L	706	3PE	O21-C21-C22	3.87	119.85	111.50
69	3C	503	3PE	O21-C21-C22	3.87	119.83	111.50
69	1Y	212	3PE	O21-C21-C22	3.86	119.82	111.50
91	4A	609	PGV	O01-C1-C2	3.85	119.81	111.50
85	3P	502	HEM	CHA-C4D-ND	3.85	129.14	124.38
69	1Y	213	3PE	O21-C21-C22	3.84	119.79	111.50
69	3J	104	3PE	O21-C21-C22	3.82	119.74	111.50
91	4A	608	PGV	O01-C1-C2	3.82	119.74	111.50
69	1f	104	3PE	O21-C21-C22	3.82	119.74	111.50
69	3P	520	3PE	O21-C21-C22	3.82	119.73	111.50
69	1L	702	3PE	O21-C21-C22	3.82	119.73	111.50
75	4C	306	CDL	OA6-CA5-C11	3.82	119.73	111.50
75	3T	101	CDL	OB6-CB5-C51	3.81	119.72	111.50
88	4A	602	HEA	C3C-C4C-NC	3.81	114.14	109.21
69	3P	505	3PE	O21-C21-C22	3.80	119.70	111.50
69	3S	201	3PE	O21-C21-C22	3.79	119.68	111.50
88	4A	601	HEA	C1D-C2D-C3D	-3.79	102.97	106.96
69	3X	106	3PE	O21-C21-C22	3.79	119.67	111.50
93	4B	303	PSC	O01-C1-C2	3.79	119.67	111.50
69	3G	101	3PE	O31-C31-C32	3.79	123.81	111.91
69	3G	107	3PE	O21-C21-C22	3.78	119.65	111.50
69	3N	503	3PE	O21-C21-C22	3.78	119.65	111.50
69	3P	514	3PE	O21-C21-C22	3.78	119.65	111.50
69	3X	101	3PE	O21-C21-C22	3.78	119.65	111.50
69	3Y	104	3PE	O21-C21-C22	3.77	119.63	111.50
69	1Y	204	3PE	O21-C21-C22	3.77	119.62	111.50
69	1Y	210	3PE	O21-C21-C22	3.76	119.60	111.50
69	3G	110	3PE	O21-C21-C22	3.75	119.59	111.50
69	3R	304	3PE	O21-C21-C22	3.75	119.59	111.50
69	3W	102	3PE	O21-C21-C22	3.74	119.56	111.50
69	3G	105	3PE	O21-C21-C22	3.73	119.54	111.50
69	1J	203	3PE	O21-C21-C22	3.73	119.53	111.50
69	3G	102	3PE	O21-C21-C22	3.72	119.52	111.50
69	1Y	214	3PE	O21-C21-C22	3.72	119.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	4G	104	3PE	O21-C21-C22	3.72	119.51	111.50
91	4C	305	PGV	O01-C1-C2	3.72	119.51	111.50
75	1L	704	CDL	OA6-CA5-C11	3.71	119.50	111.50
69	3P	519	3PE	O21-C21-C22	3.71	119.49	111.50
69	3W	101	3PE	O21-C21-C22	3.70	119.47	111.50
69	3Y	101	3PE	O21-C21-C22	3.70	119.47	111.50
70	1Y	206	PC1	O21-C21-C22	3.69	119.46	111.50
88	4A	601	HEA	C13-C14-C15	-3.68	118.79	127.66
69	1Y	201	3PE	O21-C21-C22	3.68	119.43	111.50
70	3T	102	PC1	O21-C21-C22	3.67	119.41	111.50
69	3Y	102	3PE	O21-C21-C22	3.67	119.41	111.50
69	1d	201	3PE	O21-C21-C22	3.67	119.40	111.50
85	3C	502	HEM	CHA-C4D-ND	3.66	128.91	124.38
69	1L	701	3PE	O31-C31-C32	3.65	123.35	111.91
69	3E	302	3PE	C2-O21-C21	-3.63	108.85	117.79
69	3G	111	3PE	O21-C21-C22	3.63	119.33	111.50
85	3C	502	HEM	CHB-C1B-NB	3.62	128.85	124.38
69	3T	103	3PE	O21-C21-C22	3.62	119.29	111.50
69	3G	109	3PE	O21-C21-C22	3.61	119.29	111.50
69	3P	510	3PE	O21-C21-C22	3.61	119.29	111.50
69	3J	103	3PE	O21-C21-C22	3.61	119.27	111.50
69	1Y	211	3PE	C2-O21-C21	-3.60	108.94	117.79
69	1Y	209	3PE	O21-C21-C22	3.59	119.25	111.50
91	4A	609	PGV	C02-O01-C1	-3.59	108.96	117.79
69	3G	101	3PE	C2-O21-C21	-3.57	108.99	117.79
88	4A	601	HEA	CAD-C3D-C4D	3.57	130.90	124.66
69	3G	106	3PE	O21-C21-C22	3.57	119.20	111.50
69	3C	517	3PE	O21-C21-C22	3.57	119.19	111.50
85	3P	502	HEM	CHB-C1B-NB	3.57	128.79	124.38
75	3N	502	CDL	OB6-CB5-C51	3.56	119.18	111.50
69	3Y	105	3PE	O21-C21-C22	3.55	119.16	111.50
75	1H	401	CDL	OB6-CB5-C51	3.54	119.14	111.50
69	1g	202	3PE	O21-C21-C22	3.54	119.13	111.50
70	3X	104	PC1	O21-C21-C22	3.53	119.10	111.50
77	1O	401	GTP	PB-O3B-PG	-3.52	120.73	132.83
69	3X	108	3PE	O21-C21-C22	3.52	119.08	111.50
75	4C	306	CDL	OB6-CB5-C51	3.52	119.08	111.50
69	3C	510	3PE	O31-C31-C32	3.51	122.94	111.91
69	1l	203	3PE	O21-C21-C22	3.51	119.06	111.50
69	3N	503	3PE	C2-O21-C21	-3.51	109.16	117.79
69	3C	510	3PE	O21-C21-O22	-3.49	115.27	123.70
69	1o	201	3PE	C2-O21-C21	-3.48	109.23	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	1B	202	PC1	C2-O21-C21	-3.47	109.25	117.79
70	1P	502	PC1	O21-C21-C22	3.47	118.97	111.50
69	3A	503	3PE	O21-C21-C22	3.46	118.96	111.50
75	3Y	106	CDL	OA6-CA5-C11	3.46	118.96	111.50
91	4G	102	PGV	O01-C1-C2	3.45	118.94	111.50
69	3P	517	3PE	O21-C21-C22	3.45	118.93	111.50
75	1q	202	CDL	CA4-OA6-CA5	-3.44	109.31	117.79
69	1Y	211	3PE	O21-C21-C22	3.44	118.92	111.50
88	4A	601	HEA	C1B-C2B-C3B	-3.44	102.69	106.80
69	3R	302	3PE	C2-O21-C21	-3.42	109.36	117.79
69	1M	502	3PE	O21-C21-C22	3.40	118.83	111.50
88	4A	602	HEA	C1B-C2B-C3B	-3.40	102.74	106.80
69	3P	506	3PE	C2-O21-C21	-3.39	109.43	117.79
75	3D	504	CDL	OB6-CB5-C51	3.38	118.79	111.50
88	4A	601	HEA	C4D-C3D-C2D	-3.35	102.01	106.90
69	1L	709	3PE	O31-C31-C32	3.35	122.43	111.91
69	3A	502	3PE	C2-O21-C21	-3.34	109.57	117.79
70	3T	102	PC1	C2-O21-C21	-3.34	109.57	117.79
69	1l	202	3PE	O31-C31-C32	3.32	122.34	111.91
69	3X	105	3PE	O21-C21-C22	3.32	118.66	111.50
70	1B	203	PC1	C2-O21-C21	-3.32	109.62	117.79
70	1H	403	PC1	O21-C21-C22	3.32	118.65	111.50
69	3P	508	3PE	O31-C31-C32	3.31	122.29	111.91
69	3G	106	3PE	C2-O21-C21	-3.30	109.68	117.79
69	3P	507	3PE	O21-C21-C22	3.29	118.59	111.50
75	1H	401	CDL	CB4-OB6-CB5	-3.29	109.69	117.79
69	3C	513	3PE	O31-C31-C32	3.28	122.20	111.91
87	3X	102	PEK	O01-C1-C2	3.28	118.56	111.50
70	3P	509	PC1	C2-O21-C21	-3.27	109.73	117.79
69	1f	102	3PE	O21-C21-C22	3.27	118.54	111.50
85	3C	501	HEM	CHA-C4D-ND	3.25	128.40	124.38
86	3D	501	HEC	CAA-CBA-CGA	-3.25	104.64	113.76
85	3C	501	HEM	CHB-C1B-NB	3.24	128.38	124.38
75	1L	704	CDL	OA8-CA7-C31	3.23	122.05	111.91
75	3T	101	CDL	CA4-OA6-CA5	-3.22	109.88	117.79
69	1L	711	3PE	O21-C21-C22	3.20	118.41	111.50
69	3P	506	3PE	O21-C21-C22	3.20	118.40	111.50
85	3P	501	HEM	CHA-C4D-ND	3.20	128.34	124.38
88	4A	601	HEA	C26-C15-C16	3.20	120.65	115.27
69	1m	201	3PE	O21-C21-C22	3.20	118.40	111.50
69	3P	507	3PE	O31-C31-C32	3.19	121.91	111.91
69	1L	707	3PE	O31-C31-C32	3.19	121.90	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	1d	202	CDL	OA8-CA7-C31	3.18	121.90	111.91
69	3J	102	3PE	C2-O21-C21	-3.18	109.95	117.79
77	1O	401	GTP	PA-O3A-PB	-3.17	121.95	132.83
75	1L	704	CDL	OB8-CB7-C71	3.15	121.78	111.91
88	4A	602	HEA	C4D-C3D-C2D	-3.13	102.33	106.90
88	4A	602	HEA	CMC-C2C-C3C	3.13	130.53	124.68
69	1Y	205	3PE	O21-C21-C22	3.11	118.21	111.50
69	1L	702	3PE	O31-C31-C32	3.11	121.67	111.91
75	1g	201	CDL	OB8-CB7-C71	3.11	121.66	111.91
75	1g	201	CDL	OA6-CA5-C11	3.10	118.19	111.50
69	3P	518	3PE	C2-O21-C21	-3.09	110.17	117.79
75	3T	101	CDL	OB8-CB7-C71	3.09	121.61	111.91
75	3A	501	CDL	CB4-OB6-CB5	-3.09	110.19	117.79
69	3D	503	3PE	O31-C31-C32	3.09	121.59	111.91
75	1i	201	CDL	OA8-CA7-C31	3.07	121.55	111.91
88	4A	601	HEA	C4B-C3B-C2B	-3.06	102.17	107.41
70	1H	402	PC1	O31-C31-C32	3.06	121.53	111.91
70	1Y	207	PC1	C2-O21-C21	-3.06	110.25	117.79
69	1b	101	3PE	C2-O21-C21	-3.06	110.25	117.79
88	4A	602	HEA	C13-C12-C11	-3.06	109.75	114.35
75	4C	307	CDL	CB4-OB6-CB5	-3.05	110.28	117.79
69	3C	508	3PE	O31-C31-C32	3.05	121.48	111.91
91	4C	303	PGV	O01-C1-C2	3.05	118.07	111.50
75	3X	103	CDL	OB8-CB7-C71	3.05	121.47	111.91
69	3D	503	3PE	C2-O21-C21	-3.04	110.31	117.79
70	1H	404	PC1	C11-C12-N	-3.04	105.63	115.78
88	4A	601	HEA	CMC-C2C-C3C	3.04	130.36	124.68
75	1q	201	CDL	OA8-CA7-C31	3.04	121.44	111.91
69	4G	104	3PE	O31-C31-C32	3.04	121.44	111.91
69	3T	103	3PE	O31-C31-C32	3.03	121.41	111.91
75	1Y	217	CDL	OA6-CA5-C11	3.03	118.02	111.50
70	3R	303	PC1	O31-C31-C32	3.03	121.40	111.91
69	3C	510	3PE	O21-C2-C1	-3.02	97.46	108.40
88	4A	602	HEA	C4B-C3B-C2B	-3.02	102.26	107.41
69	1L	710	3PE	O31-C31-C32	3.01	121.35	111.91
75	3D	504	CDL	OA8-CA7-C31	3.01	121.34	111.91
69	3X	107	3PE	O31-C31-C32	3.00	121.33	111.91
69	1m	204	3PE	C2-O21-C21	-3.00	110.41	117.79
88	4A	602	HEA	CBA-CAA-C2A	-2.99	107.56	112.60
69	3C	507	3PE	O31-C31-C32	2.99	121.28	111.91
87	3X	102	PEK	O03-C21-C22	2.98	121.26	111.91
69	3X	107	3PE	O21-C21-C22	2.98	117.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1f	103	3PE	O31-C31-C32	2.98	121.25	111.91
85	3P	501	HEM	CHB-C1B-NB	2.98	128.06	124.38
69	1Y	213	3PE	C2-O21-C21	-2.97	110.47	117.79
75	1N	402	CDL	OB8-CB7-C71	2.97	121.23	111.91
69	1l	203	3PE	O31-C31-C32	2.97	121.23	111.91
75	3T	101	CDL	CB4-OB6-CB5	-2.97	110.48	117.79
85	3P	501	HEM	CBA-CAA-C2A	-2.96	107.57	112.62
69	1L	708	3PE	O31-C31-C32	2.96	121.19	111.91
69	3P	506	3PE	O31-C31-C32	2.96	121.19	111.91
85	3P	501	HEM	CHD-C1D-C2D	-2.94	120.38	124.98
69	3Y	103	3PE	C2-O21-C21	-2.94	110.55	117.79
69	1Y	215	3PE	C2-O21-C21	-2.93	110.57	117.79
69	3C	506	3PE	C2-O21-C21	-2.93	110.57	117.79
69	1A	201	3PE	C2-O21-C21	-2.93	110.58	117.79
75	1i	201	CDL	CA4-OA6-CA5	-2.92	110.59	117.79
69	1A	203	3PE	C2-O21-C21	-2.92	110.61	117.79
75	4C	307	CDL	OA6-CA5-C11	2.92	117.79	111.50
70	1A	202	PC1	O31-C31-C32	2.91	121.04	111.91
69	1f	104	3PE	C2-O21-C21	-2.91	110.62	117.79
69	1g	202	3PE	O31-C31-C32	2.91	121.03	111.91
70	1h	203	PC1	O31-C31-C32	2.90	121.01	111.91
88	4A	602	HEA	C13-C14-C15	-2.90	120.69	127.66
91	4A	606	PGV	O03-C19-C20	2.89	120.98	111.91
75	1q	201	CDL	OB8-CB7-C71	2.89	120.98	111.91
69	3G	106	3PE	O31-C31-C32	2.89	120.97	111.91
75	4C	306	CDL	CA4-OA6-CA5	-2.89	110.68	117.79
75	3Y	106	CDL	OB8-CB7-C71	2.88	120.96	111.91
69	3Q	504	3PE	C2-O21-C21	-2.88	110.69	117.79
70	1Y	207	PC1	O31-C31-C32	2.88	120.95	111.91
69	3R	302	3PE	O31-C31-C32	2.88	120.94	111.91
69	3P	505	3PE	O31-C31-C32	2.88	120.94	111.91
69	1L	705	3PE	O31-C31-C32	2.88	120.94	111.91
91	4J	101	PGV	C02-O01-C1	-2.88	110.71	117.79
70	1H	404	PC1	O31-C31-C32	2.87	120.93	111.91
69	1L	701	3PE	O31-C31-O32	-2.87	116.34	123.59
75	3N	502	CDL	OA8-CA7-C31	2.87	120.90	111.91
75	1d	202	CDL	OB8-CB7-C71	2.86	120.89	111.91
70	1J	202	PC1	C2-O21-C21	-2.86	110.75	117.79
69	1m	205	3PE	O31-C31-C32	2.86	120.89	111.91
69	3C	515	3PE	O31-C31-C32	2.86	120.88	111.91
69	3G	110	3PE	O31-C31-C32	2.86	120.88	111.91
70	1P	502	PC1	O31-C31-C32	2.85	120.85	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1l	204	3PE	O31-C31-C32	2.85	120.85	111.91
69	3P	508	3PE	C3-C2-C1	-2.85	105.05	111.79
88	4A	602	HEA	C1D-ND-C4D	-2.85	102.13	105.07
69	3G	102	3PE	O31-C31-C32	2.84	120.83	111.91
75	1L	704	CDL	CA4-OA6-CA5	-2.84	110.79	117.79
69	3Q	504	3PE	O31-C31-C32	2.84	120.83	111.91
69	3C	516	3PE	O31-C31-C32	2.83	120.80	111.91
69	3G	101	3PE	O31-C31-O32	-2.83	116.44	123.59
69	3E	303	3PE	O31-C31-C32	2.83	120.79	111.91
75	1d	202	CDL	OB8-CB7-OB9	-2.83	116.45	123.59
69	1A	201	3PE	O31-C31-C32	2.83	120.78	111.91
91	4A	608	PGV	O03-C19-C20	2.82	120.77	111.91
75	3D	504	CDL	CB4-OB6-CB5	-2.82	110.84	117.79
69	3Y	104	3PE	O31-C31-C32	2.82	120.76	111.91
69	1k	101	3PE	O31-C31-C32	2.82	120.75	111.91
69	3P	510	3PE	O31-C31-C32	2.82	120.75	111.91
69	3G	105	3PE	C2-O21-C21	-2.82	110.85	117.79
69	1L	705	3PE	C23-C22-C21	-2.82	103.37	113.62
69	3Y	105	3PE	O31-C31-C32	2.82	120.74	111.91
75	3P	513	CDL	CA4-OA6-CA5	-2.81	110.86	117.79
70	3X	104	PC1	O31-C31-C32	2.81	120.73	111.91
69	3E	302	3PE	O31-C31-C32	2.81	120.73	111.91
75	1q	202	CDL	OB8-CB7-C71	2.81	120.72	111.91
70	3J	106	PC1	O31-C31-C32	2.81	120.72	111.91
87	4G	103	PEK	O03-C21-C22	2.80	120.70	111.91
93	4B	303	PSC	C02-O01-C1	-2.80	110.89	117.79
75	1q	201	CDL	CB4-OB6-CB5	-2.80	110.90	117.79
69	1Z	201	3PE	O31-C31-C32	2.80	120.69	111.91
69	3G	109	3PE	O31-C31-C32	2.80	120.69	111.91
69	1Y	204	3PE	C2-O21-C21	-2.80	110.91	117.79
69	3W	102	3PE	O31-C31-C32	2.79	120.68	111.91
69	3C	514	3PE	C2-O21-C21	-2.79	110.93	117.79
91	4A	609	PGV	O03-C19-C20	2.78	120.65	111.91
75	1i	201	CDL	OB8-CB7-C71	2.78	120.64	111.91
75	4C	306	CDL	OA8-CA7-C31	2.78	120.64	111.91
69	1J	203	3PE	O31-C31-C32	2.78	120.62	111.91
70	3R	303	PC1	C2-O21-C21	-2.77	110.97	117.79
91	4C	305	PGV	O03-C19-C20	2.77	120.59	111.91
69	3N	503	3PE	O31-C31-C32	2.77	120.59	111.91
88	4A	602	HEA	C26-C15-C16	2.76	119.92	115.27
70	3X	104	PC1	C2-O21-C21	-2.76	110.98	117.79
69	3P	517	3PE	O31-C31-C32	2.76	120.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	4A	602	HEA	C27-C19-C20	2.76	119.92	115.27
69	1f	102	3PE	C2-O21-C21	-2.76	110.99	117.79
69	1L	711	3PE	O31-C31-C32	2.76	120.57	111.91
75	4C	306	CDL	OB8-CB7-C71	2.76	120.56	111.91
75	3D	504	CDL	OB8-CB7-C71	2.75	120.55	111.91
70	3T	102	PC1	O31-C31-C32	2.75	120.53	111.91
70	3J	106	PC1	C2-O21-C21	-2.75	111.03	117.79
69	3S	201	3PE	O31-C31-C32	2.75	120.52	111.91
69	3Y	103	3PE	O31-C31-C32	2.74	120.52	111.91
88	4A	601	HEA	C4B-NB-C1B	-2.74	102.24	105.07
69	3G	108	3PE	O31-C31-C32	2.74	120.51	111.91
83	1h	201	AME	O-C-CA	-2.74	117.60	124.78
70	1B	203	PC1	C11-C12-N	-2.74	106.63	115.78
69	3P	507	3PE	O31-C31-O32	-2.73	116.71	123.59
69	1Z	201	3PE	C2-O21-C21	-2.73	111.08	117.79
69	1Y	208	3PE	C2-O21-C21	-2.72	111.08	117.79
85	3C	501	HEM	CHD-C1D-C2D	-2.72	120.73	124.98
75	1d	202	CDL	CB6-CB4-CB3	-2.72	105.36	111.79
87	4G	103	PEK	C02-O01-C1	-2.72	111.10	117.79
75	3D	504	CDL	CA4-OA6-CA5	-2.71	111.12	117.79
69	3C	511	3PE	O31-C31-C32	2.71	120.40	111.91
69	3Q	503	3PE	O31-C31-C32	2.70	120.37	111.91
69	3A	502	3PE	O31-C31-C32	2.70	120.37	111.91
70	1Y	206	PC1	C2-O21-C21	-2.69	111.16	117.79
70	1B	202	PC1	O31-C31-C32	2.69	120.36	111.91
75	1g	201	CDL	OA8-CA7-C31	2.69	120.36	111.91
75	3A	501	CDL	OA8-CA7-C31	2.69	120.35	111.91
69	1L	703	3PE	O31-C31-C32	2.69	120.34	111.91
69	4G	104	3PE	C2-O21-C21	-2.69	111.17	117.79
88	4A	601	HEA	C1D-ND-C4D	-2.69	102.30	105.07
75	1Y	217	CDL	OA8-CA7-C31	2.68	120.33	111.91
69	1Y	201	3PE	O31-C31-C32	2.68	120.33	111.91
75	1H	401	CDL	OA8-CA7-C31	2.68	120.33	111.91
69	1m	203	3PE	C2-O21-C21	-2.68	111.19	117.79
91	4G	102	PGV	O03-C19-C20	2.68	120.32	111.91
70	1d	204	PC1	C11-C12-N	-2.68	106.84	115.78
69	1Y	211	3PE	O31-C31-C32	2.68	120.31	111.91
75	1d	202	CDL	CA4-OA6-CA5	-2.68	111.20	117.79
69	1d	206	3PE	O21-C21-C22	2.68	117.27	111.50
75	4C	306	CDL	CB4-OB6-CB5	-2.67	111.21	117.79
75	3Y	106	CDL	OA8-CA7-C31	2.67	120.29	111.91
70	1d	204	PC1	O31-C31-C32	2.67	120.28	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	4C	301	PGV	O03-C19-C20	2.67	120.28	111.91
69	1Y	201	3PE	C2-O21-C21	-2.67	111.22	117.79
75	1d	205	CDL	OA8-CA7-C31	2.67	120.28	111.91
69	1o	201	3PE	O31-C31-C32	2.67	120.28	111.91
70	1Y	206	PC1	O31-C31-C32	2.67	120.28	111.91
88	4A	601	HEA	CAD-CBD-CGD	-2.67	107.86	113.60
88	4A	602	HEA	CHA-C4D-ND	-2.66	121.54	124.43
69	1e	201	3PE	C2-O21-C21	-2.66	111.25	117.79
82	1Y	203	PGT	O3-C11-C12	2.66	120.25	111.91
69	1M	502	3PE	O31-C31-C32	2.65	120.24	111.91
75	4B	302	CDL	OB8-CB7-C71	2.65	120.23	111.91
69	3A	503	3PE	O31-C31-C32	2.65	120.22	111.91
70	3J	106	PC1	C11-C12-N	-2.64	106.95	115.78
69	1Y	212	3PE	O31-C31-C32	2.64	120.20	111.91
75	3F	201	CDL	OB8-CB7-C71	2.64	120.19	111.91
69	1f	102	3PE	O31-C31-C32	2.64	120.18	111.91
69	1h	204	3PE	O31-C31-C32	2.64	120.18	111.91
69	1B	204	3PE	O31-C31-C32	2.64	120.18	111.91
70	1B	203	PC1	O31-C31-C32	2.64	120.18	111.91
88	4A	602	HEA	OMA-CMA-C3A	-2.63	119.17	124.91
69	1J	201	3PE	O31-C31-C32	2.63	120.17	111.91
69	3P	512	3PE	C2-O21-C21	-2.63	111.31	117.79
69	3G	103	3PE	O31-C31-C32	2.63	120.15	111.91
69	1L	709	3PE	C2-O21-C21	-2.63	111.33	117.79
88	4A	601	HEA	C27-C19-C20	2.62	119.69	115.27
69	1Y	214	3PE	C2-O21-C21	-2.62	111.33	117.79
70	1B	202	PC1	C24-C23-C22	2.62	122.62	113.19
69	1Y	209	3PE	O31-C31-C32	2.62	120.14	111.91
69	1g	203	3PE	O31-C31-C32	2.62	120.13	111.91
69	3C	506	3PE	O31-C31-C32	2.62	120.13	111.91
69	3P	516	3PE	O31-C31-C32	2.62	120.13	111.91
69	1d	206	3PE	O31-C31-C32	2.62	120.13	111.91
69	1l	204	3PE	C2-O21-C21	-2.62	111.34	117.79
69	1f	104	3PE	O31-C31-C32	2.62	120.12	111.91
69	1m	203	3PE	O31-C31-C32	2.61	120.11	111.91
69	3X	105	3PE	O31-C31-C32	2.61	120.10	111.91
69	1L	706	3PE	O31-C31-C32	2.61	120.10	111.91
69	3G	111	3PE	O31-C31-C32	2.61	120.10	111.91
69	3R	304	3PE	O31-C31-C32	2.61	120.09	111.91
75	3X	103	CDL	OA8-CA7-C31	2.60	120.08	111.91
69	3C	517	3PE	O31-C31-C32	2.60	120.07	111.91
70	3P	509	PC1	O31-C31-C32	2.60	120.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1f	103	3PE	C2-O21-C21	-2.59	111.40	117.79
69	1d	203	3PE	O31-C31-C32	2.59	120.05	111.91
70	1M	501	PC1	O31-C31-C32	2.59	120.05	111.91
87	3X	102	PEK	C2-C3-C4	-2.59	108.61	113.23
69	3N	501	3PE	O31-C31-C32	2.59	120.03	111.91
75	1Y	217	CDL	OB8-CB7-C71	2.59	120.03	111.91
69	1N	401	3PE	C2-O21-C21	-2.58	111.43	117.79
69	1m	204	3PE	O31-C31-C32	2.58	120.01	111.91
69	3X	101	3PE	O31-C31-C32	2.58	120.00	111.91
69	3X	108	3PE	O31-C31-C32	2.57	119.99	111.91
69	3C	512	3PE	O31-C31-C32	2.57	119.98	111.91
69	1B	205	3PE	O31-C31-C32	2.57	119.98	111.91
69	1Y	216	3PE	C3-C2-C1	-2.57	105.71	111.79
91	4A	607	PGV	O03-C19-C20	2.57	119.96	111.91
69	3P	511	3PE	C2-O21-C21	-2.56	111.49	117.79
69	3N	501	3PE	C2-O21-C21	-2.56	111.49	117.79
69	1Y	205	3PE	O31-C31-C32	2.56	119.93	111.91
69	3P	520	3PE	C2-O21-C21	-2.56	111.50	117.79
91	4C	302	PGV	O03-C19-C20	2.56	119.93	111.91
69	3G	107	3PE	O31-C31-C32	2.55	119.92	111.91
75	1H	401	CDL	OB8-CB7-C71	2.55	119.92	111.91
75	3T	101	CDL	OA8-CA7-C31	2.55	119.90	111.91
70	1d	204	PC1	C3-C2-C1	-2.55	105.77	111.79
75	3F	201	CDL	OA8-CA7-C31	2.54	119.89	111.91
75	1N	402	CDL	CB4-OB6-CB5	-2.54	111.54	117.79
85	3C	502	HEM	CHD-C1D-C2D	-2.54	121.02	124.98
69	1Y	216	3PE	O31-C31-C32	2.54	119.87	111.91
69	1d	201	3PE	O31-C31-C32	2.53	119.86	111.91
75	4B	302	CDL	OA8-CA7-C31	2.53	119.84	111.91
85	3P	502	HEM	C4D-ND-C1D	2.53	107.68	105.07
91	4N	101	PGV	C02-O01-C1	-2.53	111.57	117.79
70	1H	404	PC1	C2-O21-C21	-2.53	111.57	117.79
70	1M	501	PC1	C11-C12-N	-2.52	107.35	115.78
91	4C	304	PGV	O03-C19-C20	2.52	119.83	111.91
69	3P	505	3PE	C2-O21-C21	-2.52	111.58	117.79
70	1Y	202	PC1	O31-C31-C32	2.52	119.81	111.91
70	1h	202	PC1	O31-C31-C32	2.52	119.81	111.91
69	1Y	213	3PE	O31-C31-C32	2.51	119.79	111.91
70	1H	403	PC1	O31-C31-C32	2.51	119.78	111.91
69	1J	201	3PE	C2-O21-C21	-2.51	111.62	117.79
69	3P	508	3PE	O21-C21-O22	-2.51	117.65	123.70
75	4C	307	CDL	OA8-CA7-C31	2.50	119.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	3Y	107	3PE	O31-C31-C32	2.50	119.76	111.91
75	1d	205	CDL	OB8-CB7-C71	2.50	119.76	111.91
79	1P	501	NDP	O4D-C1D-C2D	-2.50	101.19	106.64
91	4N	101	PGV	O03-C19-C20	2.50	119.75	111.91
77	1O	401	GTP	C5-C6-N1	2.50	118.36	113.95
91	4C	305	PGV	C02-O01-C1	-2.50	111.64	117.79
69	3P	520	3PE	O31-C31-C32	2.49	119.73	111.91
69	1L	712	3PE	O31-C31-C32	2.49	119.73	111.91
69	3J	101	3PE	O31-C31-C32	2.49	119.72	111.91
69	3W	103	3PE	C2-O21-C21	-2.49	111.66	117.79
77	1O	401	GTP	C3'-C2'-C1'	2.49	104.72	100.98
69	3P	503	3PE	O31-C31-C32	2.49	119.71	111.91
75	3P	513	CDL	C32-C31-CA7	-2.48	104.59	113.62
69	1Y	204	3PE	O31-C31-C32	2.48	119.69	111.91
69	3C	503	3PE	O31-C31-C32	2.48	119.69	111.91
93	4B	303	PSC	O03-C19-C20	2.48	119.68	111.91
69	1Y	210	3PE	O31-C31-C32	2.48	119.67	111.91
69	1Y	208	3PE	O31-C31-C32	2.47	119.66	111.91
75	1q	202	CDL	OA8-CA7-C31	2.47	119.65	111.91
70	1J	202	PC1	O31-C31-C32	2.46	119.62	111.91
69	3C	514	3PE	O31-C31-C32	2.46	119.62	111.91
75	3P	513	CDL	OB8-CB7-C71	2.46	119.62	111.91
69	1Y	209	3PE	C2-O21-C21	-2.46	111.75	117.79
69	3P	508	3PE	C2-O21-C21	-2.46	111.75	117.79
69	4G	101	3PE	O31-C31-C32	2.45	119.60	111.91
69	1L	710	3PE	C2-O21-C21	-2.45	111.76	117.79
88	4A	602	HEA	CAD-CBD-CGD	-2.45	108.33	113.60
75	4B	302	CDL	CB4-OB6-CB5	-2.45	111.76	117.79
69	3P	514	3PE	O31-C31-C32	2.45	119.59	111.91
69	3P	510	3PE	C2-O21-C21	-2.45	111.77	117.79
91	4J	101	PGV	O03-C19-C20	2.44	119.58	111.91
69	1L	701	3PE	C2-O21-C21	-2.44	111.78	117.79
69	3P	512	3PE	O31-C31-C32	2.44	119.56	111.91
85	3C	502	HEM	C4D-ND-C1D	2.44	107.59	105.07
69	1L	702	3PE	C2-O21-C21	-2.43	111.80	117.79
69	1e	201	3PE	O31-C31-C32	2.43	119.54	111.91
91	4A	607	PGV	C02-O01-C1	-2.43	111.81	117.79
75	1L	704	CDL	OB8-CB7-OB9	-2.43	117.46	123.59
69	3P	518	3PE	O31-C31-C32	2.42	119.51	111.91
75	4C	307	CDL	OB8-CB7-C71	2.42	119.51	111.91
75	1N	402	CDL	OA8-CA7-C31	2.42	119.51	111.91
69	1o	201	3PE	O21-C21-O22	-2.42	117.86	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1L	707	3PE	O31-C31-O32	-2.42	117.49	123.59
69	1A	203	3PE	O31-C31-C32	2.42	119.49	111.91
91	4C	302	PGV	C02-O01-C1	-2.41	111.86	117.79
69	1N	401	3PE	O31-C31-C32	2.41	119.46	111.91
69	3P	515	3PE	O31-C31-C32	2.41	119.46	111.91
75	3P	513	CDL	OB6-CB5-OB7	-2.40	117.91	123.70
88	4A	601	HEA	C17-C18-C19	-2.40	121.89	127.66
69	3C	509	3PE	O31-C31-C32	2.39	119.42	111.91
70	1d	204	PC1	O31-C31-O32	-2.39	117.56	123.59
75	1q	201	CDL	OA8-CA7-OA9	-2.39	117.56	123.59
88	4A	602	HEA	C25-C23-C24	2.39	119.88	114.60
75	3P	513	CDL	CB6-CB4-CB3	-2.39	106.14	111.79
88	4A	601	HEA	CHB-C1B-C2B	-2.39	121.25	124.98
88	4A	602	HEA	C4B-NB-C1B	-2.38	102.61	105.07
69	3C	508	3PE	O31-C31-O32	-2.38	117.58	123.59
69	3Y	102	3PE	O31-C31-C32	2.38	119.37	111.91
69	3G	101	3PE	C33-C32-C31	-2.37	104.99	113.62
88	4A	601	HEA	CMD-C2D-C1D	2.37	128.65	125.04
69	3P	508	3PE	O31-C31-O32	-2.37	117.62	123.59
69	3P	515	3PE	O21-C21-O22	-2.37	117.98	123.70
70	3J	106	PC1	O31-C31-O32	-2.37	117.62	123.59
70	1H	404	PC1	P-O13-C11	-2.37	109.94	121.59
69	1m	201	3PE	O31-C31-C32	2.36	119.33	111.91
69	1m	202	3PE	O31-C31-C32	2.36	119.32	111.91
69	3E	303	3PE	C2-O21-C21	-2.36	111.97	117.79
88	4A	602	HEA	CMB-C2B-C1B	2.36	128.63	125.04
69	3R	305	3PE	O31-C31-O32	-2.36	117.64	123.59
70	3J	106	PC1	C14-N-C13	2.36	115.04	108.97
75	1i	201	CDL	OA8-CA7-OA9	-2.36	117.65	123.59
88	4A	601	HEA	C25-C23-C24	2.35	119.80	114.60
69	3G	101	3PE	O21-C21-O22	-2.35	118.02	123.70
69	3P	504	3PE	O31-C31-C32	2.35	119.29	111.91
69	3Y	101	3PE	O31-C31-C32	2.35	119.29	111.91
69	1b	101	3PE	O31-C31-C32	2.35	119.28	111.91
69	3G	105	3PE	O31-C31-C32	2.35	119.28	111.91
91	4G	102	PGV	C02-O01-C1	-2.34	112.02	117.79
69	1L	708	3PE	O31-C31-O32	-2.34	117.67	123.59
75	1i	201	CDL	CB6-CB4-CB3	-2.34	106.25	111.79
88	4A	601	HEA	CHB-C1B-NB	-2.34	121.89	124.43
69	3P	516	3PE	C2-O21-C21	-2.34	112.03	117.79
70	1A	202	PC1	C2-O21-C21	-2.34	112.03	117.79
69	3Q	502	3PE	O31-C31-C32	2.33	119.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1k	101	3PE	O31-C31-O32	-2.33	117.70	123.59
69	1N	401	3PE	C3-C2-C1	-2.33	106.28	111.79
70	3R	303	PC1	O21-C21-O22	-2.33	118.08	123.70
77	1O	401	GTP	C8-N7-C5	2.33	107.42	102.99
69	1g	202	3PE	C2-O21-C21	-2.33	112.06	117.79
69	3G	104	3PE	O31-C31-C32	2.32	119.20	111.91
69	3R	302	3PE	O31-C31-O32	-2.32	117.73	123.59
87	3X	102	PEK	C3-C2-C1	-2.32	105.18	113.62
69	3D	503	3PE	O31-C31-O32	-2.32	117.73	123.59
69	3G	109	3PE	C2-O21-C21	-2.32	112.08	117.79
69	3J	105	3PE	O31-C31-C32	2.32	119.18	111.91
91	4C	303	PGV	O03-C19-C20	2.32	119.18	111.91
91	4K	101	PGV	O03-C19-C20	2.32	119.18	111.91
85	3P	502	HEM	CHA-C4D-C3D	-2.32	120.98	125.33
79	1P	501	NDP	C5A-C6A-N6A	2.32	123.87	120.35
69	3X	101	3PE	C2-O21-C21	-2.31	112.10	117.79
91	4C	304	PGV	C02-O01-C1	-2.31	112.11	117.79
69	3C	505	3PE	C2-O21-C21	-2.30	112.12	117.79
69	3C	512	3PE	C2-O21-C21	-2.30	112.13	117.79
88	4A	601	HEA	CMB-C2B-C1B	2.30	128.54	125.04
85	3P	502	HEM	CHD-C1D-C2D	-2.30	121.39	124.98
75	1g	201	CDL	OB8-CB7-OB9	-2.29	117.80	123.59
70	3P	509	PC1	C11-C12-N	-2.29	108.13	115.78
91	4K	101	PGV	C02-O01-C1	-2.29	112.15	117.79
70	1B	203	PC1	O21-C21-O22	-2.29	118.18	123.70
70	1Y	202	PC1	C2-O21-C21	-2.28	112.18	117.79
70	3X	104	PC1	O31-C31-O32	-2.28	117.84	123.59
75	1i	201	CDL	OB8-CB7-OB9	-2.28	117.84	123.59
69	1Y	215	3PE	O31-C31-C32	2.28	119.06	111.91
70	1B	202	PC1	O21-C21-O22	-2.28	118.20	123.70
70	3P	509	PC1	O21-C21-O22	-2.28	118.20	123.70
75	3A	501	CDL	OB8-CB7-C71	2.28	119.05	111.91
88	4A	601	HEA	CHD-C1D-C2D	-2.27	120.45	126.72
69	1L	705	3PE	C2-O21-C21	-2.27	112.21	117.79
91	4C	301	PGV	C02-O01-C1	-2.26	112.22	117.79
69	3E	303	3PE	O21-C21-O22	-2.26	118.23	123.70
69	1J	203	3PE	C2-O21-C21	-2.26	112.23	117.79
75	3N	502	CDL	CB4-OB6-CB5	-2.26	112.23	117.79
69	3G	110	3PE	C2-O21-C21	-2.26	112.24	117.79
69	3J	103	3PE	O31-C31-C32	2.25	118.98	111.91
75	3N	502	CDL	OB8-CB7-C71	2.25	118.96	111.91
85	3C	502	HEM	O2A-CGA-CBA	2.25	121.25	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	1L	704	CDL	OB6-CB5-OB7	-2.25	118.27	123.70
69	1N	401	3PE	O21-C21-O22	-2.25	118.28	123.70
69	1Y	209	3PE	C23-C22-C21	-2.24	105.46	113.62
69	3C	514	3PE	O21-C21-O22	-2.24	118.28	123.70
88	4A	602	HEA	CHB-C1B-NB	-2.24	122.00	124.43
69	1Y	216	3PE	C2-O21-C21	-2.24	112.28	117.79
87	4G	103	PEK	O03-C21-O04	-2.24	117.94	123.59
69	3C	509	3PE	C2-O21-C21	-2.24	112.29	117.79
69	1l	202	3PE	C3-C2-C1	-2.23	106.50	111.79
69	3P	503	3PE	C2-O21-C21	-2.23	112.29	117.79
69	3T	103	3PE	O31-C31-O32	-2.23	117.96	123.59
69	3P	511	3PE	O31-C31-C32	2.22	118.89	111.91
69	3W	101	3PE	O31-C31-C32	2.22	118.88	111.91
69	1d	206	3PE	C23-C22-C21	-2.22	105.56	113.62
75	1q	202	CDL	OA6-CA5-OA7	-2.21	118.35	123.70
75	1d	205	CDL	OA6-CA5-OA7	-2.21	118.35	123.70
88	4A	602	HEA	CHA-C4D-C3D	-2.21	121.59	124.84
69	1e	201	3PE	O21-C21-O22	-2.21	118.37	123.70
69	4G	101	3PE	O21-C21-O22	-2.21	118.37	123.70
69	1Y	214	3PE	O31-C31-C32	2.21	118.83	111.91
70	1H	403	PC1	C2-O21-C21	-2.21	112.36	117.79
75	1q	201	CDL	OA6-CA5-OA7	-2.20	118.38	123.70
69	3C	505	3PE	O31-C31-C32	2.20	118.81	111.91
75	3F	201	CDL	CB4-OB6-CB5	-2.20	112.38	117.79
85	3C	501	HEM	CBA-CAA-C2A	-2.19	108.88	112.62
75	3D	504	CDL	OA8-CA7-OA9	-2.19	118.06	123.59
88	4A	602	HEA	C17-C18-C19	-2.19	122.40	127.66
69	3J	104	3PE	C33-C32-C31	-2.18	105.67	113.62
69	3P	519	3PE	O31-C31-C32	2.18	118.76	111.91
88	4A	602	HEA	CMD-C2D-C1D	2.18	128.36	125.04
69	1L	701	3PE	C23-C22-C21	-2.18	105.70	113.62
69	3Y	105	3PE	C2-O21-C21	-2.18	112.43	117.79
69	1l	202	3PE	O31-C31-O32	-2.18	118.10	123.59
69	1A	201	3PE	O21-C21-O22	-2.17	118.46	123.70
69	1B	204	3PE	O21-C21-O22	-2.17	118.47	123.70
75	3T	101	CDL	CA6-CA4-CA3	-2.17	106.67	111.79
69	4G	104	3PE	O31-C31-O32	-2.16	118.13	123.59
69	3A	503	3PE	O31-C31-O32	-2.16	118.14	123.59
70	1H	402	PC1	O31-C31-O32	-2.16	118.14	123.59
86	3D	501	HEC	CMA-C3A-C2A	2.16	129.01	124.94
70	1B	203	PC1	O31-C31-O32	-2.15	118.16	123.59
88	4A	601	HEA	CHC-C4B-NB	-2.15	121.73	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1f	101	3PE	O31-C31-C32	2.15	118.65	111.91
69	3E	302	3PE	O31-C31-O32	-2.15	118.17	123.59
69	1L	702	3PE	O31-C31-O32	-2.14	118.20	123.59
69	3Y	102	3PE	C3-C2-C1	-2.14	106.74	111.79
85	3P	502	HEM	O2D-CGD-CBD	2.13	120.89	114.03
75	1H	401	CDL	CA4-OA6-CA5	-2.13	112.54	117.79
85	3C	502	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
69	3J	104	3PE	O31-C31-C32	2.13	118.59	111.91
69	1L	707	3PE	C3-C2-C1	-2.12	106.76	111.79
75	3A	501	CDL	OA6-CA5-OA7	-2.12	118.58	123.70
69	3Y	107	3PE	C2-O21-C21	-2.11	112.59	117.79
69	3P	519	3PE	C34-C33-C32	-2.11	105.60	113.19
69	3C	517	3PE	C2-O21-C21	-2.11	112.60	117.79
69	1m	204	3PE	O21-C21-O22	-2.11	118.61	123.70
75	1d	202	CDL	OA8-CA7-OA9	-2.11	118.28	123.59
70	1P	502	PC1	C2-O21-C21	-2.10	112.62	117.79
75	1L	704	CDL	OA8-CA7-OA9	-2.09	118.31	123.59
88	4A	602	HEA	CHD-C1D-C2D	-2.09	120.93	126.72
91	4A	608	PGV	C02-O01-C1	-2.09	112.64	117.79
69	1B	204	3PE	C2-O21-C21	-2.09	112.65	117.79
69	1Z	201	3PE	O21-C21-O22	-2.09	118.66	123.70
75	3F	201	CDL	OB6-CB5-OB7	-2.09	118.66	123.70
75	1Y	217	CDL	OA8-CA7-OA9	-2.09	118.32	123.59
69	1k	101	3PE	O21-C21-O22	-2.08	118.67	123.70
69	1d	203	3PE	O21-C21-O22	-2.08	118.67	123.70
82	1Y	203	PGT	C2-O2-C31	-2.08	112.67	117.79
69	3C	511	3PE	C2-O21-C21	-2.08	112.67	117.79
75	3P	513	CDL	OA8-CA7-C31	2.08	118.43	111.91
75	3A	501	CDL	CB6-CB4-CB3	-2.08	106.87	111.79
85	3C	501	HEM	C4D-ND-C1D	2.08	107.22	105.07
69	1g	203	3PE	C23-C22-C21	-2.08	106.07	113.62
69	3R	305	3PE	O31-C31-C32	2.08	118.42	111.91
69	3P	503	3PE	O21-C21-O22	-2.07	118.69	123.70
69	3P	519	3PE	C3-C2-C1	-2.07	106.88	111.79
69	1Y	210	3PE	C2-O21-C21	-2.07	112.69	117.79
75	4B	302	CDL	CA4-OA6-CA5	-2.07	112.69	117.79
70	1H	404	PC1	O31-C31-O32	-2.07	118.36	123.59
69	3X	107	3PE	O31-C31-O32	-2.07	118.36	123.59
69	3Y	103	3PE	O21-C21-O22	-2.07	118.70	123.70
75	1d	202	CDL	C12-C11-CA5	-2.07	106.10	113.62
69	3A	502	3PE	O31-C31-O32	-2.07	118.38	123.59
69	3R	302	3PE	O21-C21-O22	-2.06	118.71	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	1Y	215	3PE	O21-C21-O22	-2.06	118.71	123.70
70	1A	202	PC1	O31-C31-O32	-2.06	118.39	123.59
75	3D	504	CDL	OB6-CB5-OB7	-2.06	118.72	123.70
70	3P	509	PC1	O31-C31-O32	-2.06	118.39	123.59
70	1h	202	PC1	C11-C12-N	-2.06	108.91	115.78
69	3C	513	3PE	O31-C31-O32	-2.06	118.40	123.59
88	4A	602	HEA	CHB-C1B-C2B	-2.05	121.77	124.98
88	4A	602	HEA	C21-C22-C23	-2.05	120.73	127.75
85	3P	502	HEM	O2A-CGA-CBA	2.05	120.61	114.03
75	3D	504	CDL	OA6-CA5-OA7	-2.05	118.75	123.70
86	3Q	501	HEC	CMA-C3A-C2A	2.05	128.80	124.94
69	1m	202	3PE	C2-O21-C21	-2.05	112.76	117.79
69	3G	106	3PE	O21-C21-O22	-2.04	118.76	123.70
75	3P	513	CDL	CA6-CA4-CA3	-2.04	106.95	111.79
69	1g	202	3PE	O21-C21-O22	-2.04	118.77	123.70
70	3X	104	PC1	C23-C22-C21	-2.04	106.20	113.62
69	3J	105	3PE	O21-C21-O22	-2.04	118.77	123.70
75	1N	402	CDL	C32-C31-CA7	-2.04	106.21	113.62
69	1A	201	3PE	O31-C31-O32	-2.03	118.46	123.59
69	3C	506	3PE	O21-C21-O22	-2.03	118.80	123.70
69	1g	202	3PE	O31-C31-O32	-2.03	118.47	123.59
69	1L	709	3PE	O21-C21-O22	-2.03	118.80	123.70
85	3P	501	HEM	CHA-C4D-C3D	-2.02	121.53	125.33
69	3J	102	3PE	O21-C21-O22	-2.02	118.82	123.70
70	3T	102	PC1	O21-C21-O22	-2.02	118.83	123.70
69	3P	508	3PE	O13-C11-C12	-2.02	101.55	109.10
70	1h	203	PC1	C3-C2-C1	-2.02	107.02	111.79
69	3C	508	3PE	O21-C21-O22	-2.02	118.83	123.70
69	3G	104	3PE	O21-C21-O22	-2.01	118.83	123.70
70	1B	202	PC1	C3-C2-C1	-2.01	107.03	111.79
85	3C	502	HEM	CHB-C1B-C2B	-2.01	121.16	126.72
69	1Y	216	3PE	O31-C31-O32	-2.01	118.51	123.59
69	3R	304	3PE	C2-O21-C21	-2.01	112.84	117.79
69	1B	205	3PE	O21-C21-O22	-2.01	118.84	123.70
87	3X	102	PEK	O03-C21-O04	-2.01	118.52	123.59
91	4J	101	PGV	O01-C1-O02	-2.01	118.85	123.70
69	3J	104	3PE	C2-O21-C21	-2.00	112.86	117.79
69	3P	519	3PE	C36-C35-C34	-2.00	104.25	114.42
85	3P	502	HEM	CHB-C1B-C2B	-2.00	121.18	126.72
91	4A	606	PGV	O01-C1-O02	-2.00	118.86	123.70
69	3C	516	3PE	O21-C21-O22	-2.00	118.86	123.70

There are no chirality outliers.

All (3221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O12
69	1A	201	3PE	C11-O13-P-O14
69	1A	203	3PE	C11-O13-P-O11
69	1A	203	3PE	C11-O13-P-O12
69	1A	203	3PE	C11-O13-P-O14
69	1B	204	3PE	C1-O11-P-O14
69	1B	205	3PE	C1-O11-P-O14
69	1B	205	3PE	C11-O13-P-O12
69	1B	205	3PE	C11-O13-P-O14
69	1B	205	3PE	C1-C2-O21-C21
69	1B	205	3PE	O22-C21-O21-C2
69	1B	205	3PE	C22-C21-O21-C2
69	1J	201	3PE	C1-O11-P-O13
69	1J	201	3PE	C1-O11-P-O14
69	1L	701	3PE	C11-O13-P-O12
69	1L	701	3PE	C11-O13-P-O14
69	1L	702	3PE	O22-C21-O21-C2
69	1L	702	3PE	C22-C21-O21-C2
69	1L	703	3PE	C11-O13-P-O11
69	1L	703	3PE	C12-C11-O13-P
69	1L	705	3PE	C1-O11-P-O13
69	1L	705	3PE	C1-O11-P-O14
69	1L	706	3PE	C1-O11-P-O14
69	1L	707	3PE	O13-C11-C12-N
69	1L	708	3PE	C1-O11-P-O14
69	1L	708	3PE	O22-C21-O21-C2
69	1L	709	3PE	C1-O11-P-O12
69	1L	709	3PE	O22-C21-O21-C2
69	1L	709	3PE	C22-C21-O21-C2
69	1L	710	3PE	O22-C21-O21-C2
69	1L	711	3PE	O11-C1-C2-O21
69	1L	712	3PE	C11-O13-P-O11
69	1L	712	3PE	C11-O13-P-O12
69	1L	712	3PE	C11-O13-P-O14
69	1M	502	3PE	C11-O13-P-O14
69	1M	502	3PE	O11-C1-C2-O21
69	1M	502	3PE	C32-C31-O31-C3
69	1Y	201	3PE	C11-O13-P-O12
69	1Y	201	3PE	C22-C21-O21-C2
69	1Y	204	3PE	C22-C21-O21-C2
69	1Y	205	3PE	C11-O13-P-O14
69	1Y	208	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	1Y	208	3PE	C11-O13-P-O14
69	1Y	208	3PE	C12-C11-O13-P
69	1Y	209	3PE	C1-O11-P-O12
69	1Y	209	3PE	C1-O11-P-O13
69	1Y	209	3PE	C11-O13-P-O11
69	1Y	209	3PE	C11-O13-P-O12
69	1Y	209	3PE	C11-O13-P-O14
69	1Y	209	3PE	C22-C21-O21-C2
69	1Y	210	3PE	C12-C11-O13-P
69	1Y	211	3PE	C11-O13-P-O12
69	1Y	211	3PE	O22-C21-O21-C2
69	1Y	211	3PE	C22-C21-O21-C2
69	1Y	212	3PE	C1-O11-P-O14
69	1Y	212	3PE	C11-O13-P-O12
69	1Y	212	3PE	C11-O13-P-O14
69	1Y	213	3PE	C1-O11-P-O14
69	1Y	213	3PE	O13-C11-C12-N
69	1Y	213	3PE	C32-C31-O31-C3
69	1Y	213	3PE	O22-C21-O21-C2
69	1Y	215	3PE	C1-O11-P-O14
69	1Y	215	3PE	O32-C31-O31-C3
69	1Y	215	3PE	C32-C31-O31-C3
69	1Y	215	3PE	O22-C21-O21-C2
69	1Y	216	3PE	C1-O11-P-O12
69	1Y	216	3PE	C1-O11-P-O14
69	1Y	216	3PE	C22-C21-O21-C2
69	1b	101	3PE	C22-C21-O21-C2
69	1d	201	3PE	C11-O13-P-O11
69	1d	201	3PE	O32-C31-O31-C3
69	1d	201	3PE	C32-C31-O31-C3
69	1d	203	3PE	C1-O11-P-O12
69	1d	203	3PE	C1-O11-P-O13
69	1d	203	3PE	C1-O11-P-O14
69	1d	203	3PE	O13-C11-C12-N
69	1d	203	3PE	O22-C21-O21-C2
69	1d	203	3PE	C22-C21-O21-C2
69	1d	206	3PE	C11-O13-P-O11
69	1e	201	3PE	C1-O11-P-O14
69	1e	201	3PE	C11-O13-P-O14
69	1f	101	3PE	C1-O11-P-O12
69	1f	101	3PE	C11-O13-P-O14
69	1f	102	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	1f	102	3PE	O13-C11-C12-N
69	1f	102	3PE	C22-C21-O21-C2
69	1f	103	3PE	C11-O13-P-O12
69	1f	103	3PE	O22-C21-O21-C2
69	1f	103	3PE	C22-C21-O21-C2
69	1f	104	3PE	C11-O13-P-O12
69	1f	104	3PE	C11-O13-P-O14
69	1g	202	3PE	C11-O13-P-O12
69	1g	202	3PE	C12-C11-O13-P
69	1g	202	3PE	C22-C21-O21-C2
69	1g	203	3PE	C1-O11-P-O12
69	1h	204	3PE	C1-O11-P-O12
69	1h	204	3PE	C1-O11-P-O13
69	1h	204	3PE	C1-O11-P-O14
69	1h	204	3PE	C11-O13-P-O12
69	1h	204	3PE	C11-O13-P-O14
69	1h	204	3PE	O22-C21-O21-C2
69	1k	101	3PE	O21-C2-C3-O31
69	1k	101	3PE	O22-C21-O21-C2
69	1l	202	3PE	C11-O13-P-O12
69	1l	203	3PE	C11-O13-P-O14
69	1l	203	3PE	C22-C21-O21-C2
69	1l	204	3PE	C11-O13-P-O11
69	1l	204	3PE	C11-O13-P-O12
69	1l	204	3PE	C11-O13-P-O14
69	1l	204	3PE	O22-C21-O21-C2
69	1m	202	3PE	C22-C21-O21-C2
69	1m	203	3PE	C1-O11-P-O12
69	1m	203	3PE	C1-O11-P-O14
69	1m	203	3PE	O22-C21-O21-C2
69	1m	203	3PE	C22-C21-O21-C2
69	1m	205	3PE	C11-O13-P-O12
69	1m	205	3PE	C22-C21-O21-C2
69	1o	201	3PE	C1-O11-P-O12
69	1o	201	3PE	C1-O11-P-O13
69	1o	201	3PE	C1-O11-P-O14
69	1o	201	3PE	C11-O13-P-O11
69	1o	201	3PE	C11-O13-P-O12
69	1o	201	3PE	C11-O13-P-O14
69	3A	502	3PE	C1-O11-P-O12
69	3A	502	3PE	C11-O13-P-O11
69	3A	502	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	3A	502	3PE	O22-C21-O21-C2
69	3A	502	3PE	C22-C21-O21-C2
69	3A	503	3PE	C1-O11-P-O13
69	3A	503	3PE	C1-O11-P-O14
69	3A	503	3PE	C11-O13-P-O12
69	3A	503	3PE	C12-C11-O13-P
69	3A	503	3PE	O22-C21-O21-C2
69	3A	503	3PE	C22-C21-O21-C2
69	3C	506	3PE	C1-O11-P-O14
69	3C	507	3PE	C1-O11-P-O12
69	3C	507	3PE	C1-O11-P-O14
69	3C	507	3PE	C11-O13-P-O11
69	3C	507	3PE	C11-O13-P-O12
69	3C	507	3PE	C11-O13-P-O14
69	3C	507	3PE	C22-C21-O21-C2
69	3C	508	3PE	O22-C21-O21-C2
69	3C	509	3PE	C1-O11-P-O12
69	3C	509	3PE	C1-O11-P-O13
69	3C	509	3PE	C11-O13-P-O14
69	3C	510	3PE	C1-O11-P-O14
69	3C	510	3PE	C11-O13-P-O14
69	3C	510	3PE	O21-C2-C3-O31
69	3C	511	3PE	O22-C21-O21-C2
69	3C	511	3PE	C22-C21-O21-C2
69	3C	512	3PE	O13-C11-C12-N
69	3C	512	3PE	O22-C21-O21-C2
69	3C	513	3PE	C1-O11-P-O12
69	3C	513	3PE	C1-O11-P-O13
69	3C	513	3PE	C22-C21-O21-C2
69	3C	515	3PE	C1-O11-P-O12
69	3C	515	3PE	C1-O11-P-O14
69	3C	515	3PE	C11-O13-P-O14
69	3C	515	3PE	C22-C21-O21-C2
69	3C	516	3PE	C11-O13-P-O14
69	3C	516	3PE	C1-C2-O21-C21
69	3C	516	3PE	O22-C21-O21-C2
69	3C	516	3PE	C22-C21-O21-C2
69	3D	502	3PE	C2-C1-O11-P
69	3D	502	3PE	C22-C21-O21-C2
69	3D	503	3PE	C11-O13-P-O12
69	3D	503	3PE	O13-C11-C12-N
69	3D	503	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	3E	302	3PE	C1-O11-P-O12
69	3E	302	3PE	C1-O11-P-O13
69	3E	302	3PE	C11-O13-P-O11
69	3E	302	3PE	C11-O13-P-O12
69	3E	302	3PE	C11-O13-P-O14
69	3E	303	3PE	C1-O11-P-O14
69	3G	101	3PE	C11-O13-P-O14
69	3G	102	3PE	C11-O13-P-O12
69	3G	103	3PE	C11-O13-P-O11
69	3G	103	3PE	C11-O13-P-O12
69	3G	103	3PE	C11-O13-P-O14
69	3G	103	3PE	C22-C21-O21-C2
69	3G	104	3PE	C1-O11-P-O14
69	3G	104	3PE	C11-O13-P-O11
69	3G	104	3PE	C11-O13-P-O12
69	3G	104	3PE	C11-O13-P-O14
69	3G	104	3PE	O22-C21-O21-C2
69	3G	104	3PE	C22-C21-O21-C2
69	3G	105	3PE	C1-O11-P-O12
69	3G	105	3PE	C1-O11-P-O13
69	3G	105	3PE	C1-O11-P-O14
69	3G	105	3PE	C11-O13-P-O12
69	3G	105	3PE	C11-O13-P-O14
69	3G	105	3PE	C22-C21-O21-C2
69	3G	106	3PE	C1-O11-P-O14
69	3G	106	3PE	C2-C3-O31-C31
69	3G	106	3PE	O22-C21-O21-C2
69	3G	106	3PE	C22-C21-O21-C2
69	3G	108	3PE	C1-O11-P-O14
69	3G	108	3PE	O11-C1-C2-O21
69	3G	108	3PE	C22-C21-O21-C2
69	3G	109	3PE	C1-O11-P-O13
69	3G	109	3PE	C11-O13-P-O14
69	3G	109	3PE	C2-C1-O11-P
69	3G	110	3PE	C1-O11-P-O14
69	3G	110	3PE	C22-C21-O21-C2
69	3G	111	3PE	C1-O11-P-O13
69	3G	111	3PE	C11-O13-P-O12
69	3G	111	3PE	C11-O13-P-O14
69	3G	111	3PE	C22-C21-O21-C2
69	3J	101	3PE	C1-O11-P-O12
69	3J	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
69	3J	101	3PE	C2-C3-O31-C31
69	3J	101	3PE	O22-C21-O21-C2
69	3J	102	3PE	C11-O13-P-O12
69	3J	103	3PE	C1-O11-P-O14
69	3J	103	3PE	C11-O13-P-O11
69	3J	104	3PE	C1-O11-P-O14
69	3J	104	3PE	C22-C21-O21-C2
69	3J	105	3PE	C11-O13-P-O14
69	3J	105	3PE	C22-C21-O21-C2
69	3N	501	3PE	C1-O11-P-O14
69	3N	501	3PE	C11-O13-P-O14
69	3N	501	3PE	O13-C11-C12-N
69	3N	501	3PE	C22-C21-O21-C2
69	3N	503	3PE	C1-O11-P-O13
69	3N	503	3PE	C1-O11-P-O14
69	3N	503	3PE	C11-O13-P-O11
69	3N	503	3PE	C11-O13-P-O12
69	3N	503	3PE	O22-C21-O21-C2
69	3N	503	3PE	C22-C21-O21-C2
69	3P	503	3PE	C1-O11-P-O14
69	3P	503	3PE	C22-C21-O21-C2
69	3P	504	3PE	C22-C21-O21-C2
69	3P	505	3PE	O22-C21-O21-C2
69	3P	505	3PE	C22-C21-O21-C2
69	3P	506	3PE	C1-O11-P-O12
69	3P	506	3PE	C12-C11-O13-P
69	3P	506	3PE	O22-C21-O21-C2
69	3P	507	3PE	C1-O11-P-O14
69	3P	507	3PE	C11-O13-P-O12
69	3P	508	3PE	O13-C11-C12-N
69	3P	510	3PE	C1-O11-P-O14
69	3P	512	3PE	C11-O13-P-O12
69	3P	512	3PE	C11-O13-P-O14
69	3P	514	3PE	C11-O13-P-O11
69	3P	514	3PE	C11-O13-P-O12
69	3P	514	3PE	C11-O13-P-O14
69	3P	514	3PE	C22-C21-O21-C2
69	3P	515	3PE	C1-O11-P-O14
69	3P	515	3PE	C11-O13-P-O11
69	3P	515	3PE	C11-O13-P-O12
69	3P	515	3PE	C11-O13-P-O14
69	3P	515	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
69	3P	515	3PE	C3-C2-O21-C21
69	3P	515	3PE	O22-C21-O21-C2
69	3P	515	3PE	C22-C21-O21-C2
69	3P	516	3PE	C1-O11-P-O13
69	3P	516	3PE	C11-O13-P-O14
69	3P	517	3PE	C1-O11-P-O14
69	3P	517	3PE	C2-C1-O11-P
69	3P	518	3PE	C1-O11-P-O12
69	3P	518	3PE	C1-O11-P-O14
69	3P	518	3PE	C11-O13-P-O12
69	3P	518	3PE	O22-C21-O21-C2
69	3P	518	3PE	C22-C21-O21-C2
69	3P	519	3PE	C11-O13-P-O12
69	3P	519	3PE	C11-O13-P-O14
69	3P	520	3PE	C1-O11-P-O14
69	3P	520	3PE	O22-C21-O21-C2
69	3Q	502	3PE	O22-C21-O21-C2
69	3Q	503	3PE	C2-C3-O31-C31
69	3Q	503	3PE	C22-C21-O21-C2
69	3Q	504	3PE	C22-C21-O21-C2
69	3R	302	3PE	C1-O11-P-O12
69	3R	302	3PE	C11-O13-P-O11
69	3R	302	3PE	C11-O13-P-O12
69	3R	302	3PE	C11-O13-P-O14
69	3R	304	3PE	C11-O13-P-O12
69	3R	304	3PE	C11-O13-P-O14
69	3R	305	3PE	C11-O13-P-O14
69	3R	305	3PE	C12-C11-O13-P
69	3R	305	3PE	O32-C31-O31-C3
69	3R	305	3PE	C32-C31-O31-C3
69	3R	305	3PE	O22-C21-O21-C2
69	3S	201	3PE	C1-O11-P-O13
69	3S	201	3PE	C11-O13-P-O12
69	3S	201	3PE	C22-C21-O21-C2
69	3W	101	3PE	C1-O11-P-O12
69	3W	101	3PE	C1-O11-P-O13
69	3W	101	3PE	C1-O11-P-O14
69	3W	101	3PE	O13-C11-C12-N
69	3W	101	3PE	C22-C21-O21-C2
69	3W	102	3PE	C1-O11-P-O12
69	3W	102	3PE	C1-O11-P-O14
69	3W	102	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
69	3W	102	3PE	O32-C31-O31-C3
69	3W	102	3PE	C32-C31-O31-C3
69	3W	103	3PE	C22-C21-O21-C2
69	3X	101	3PE	C1-O11-P-O14
69	3X	105	3PE	C1-O11-P-O12
69	3X	105	3PE	C1-O11-P-O14
69	3X	106	3PE	C1-O11-P-O14
69	3X	106	3PE	O32-C31-O31-C3
69	3X	106	3PE	C32-C31-O31-C3
69	3X	106	3PE	C22-C21-O21-C2
69	3X	107	3PE	C11-O13-P-O12
69	3X	107	3PE	C11-O13-P-O14
69	3Y	101	3PE	C1-O11-P-O12
69	3Y	101	3PE	C1-O11-P-O13
69	3Y	101	3PE	C1-O11-P-O14
69	3Y	101	3PE	C11-O13-P-O12
69	3Y	101	3PE	C11-O13-P-O14
69	3Y	102	3PE	C1-O11-P-O12
69	3Y	102	3PE	O32-C31-O31-C3
69	3Y	104	3PE	C1-O11-P-O14
69	3Y	107	3PE	C1-O11-P-O14
69	3Y	107	3PE	C11-O13-P-O14
69	3Y	107	3PE	C22-C21-O21-C2
69	4G	101	3PE	C1-O11-P-O14
69	4G	101	3PE	C2-C3-O31-C31
69	4G	101	3PE	C22-C21-O21-C2
70	1A	202	PC1	C1-O11-P-O12
70	1A	202	PC1	O22-C21-O21-C2
70	1B	202	PC1	C11-O13-P-O12
70	1B	202	PC1	C1-O11-P-O14
70	1B	203	PC1	C11-O13-P-O14
70	1B	203	PC1	C1-O11-P-O12
70	1B	203	PC1	C1-O11-P-O14
70	1H	402	PC1	C11-O13-P-O14
70	1J	202	PC1	C11-O13-P-O14
70	1J	202	PC1	C1-O11-P-O14
70	1M	501	PC1	C11-O13-P-O14
70	1M	501	PC1	C1-O11-P-O12
70	1M	501	PC1	C1-O11-P-O14
70	1P	502	PC1	C1-O11-P-O12
70	1P	502	PC1	C1-O11-P-O14
70	1P	502	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
70	1P	502	PC1	O13-C11-C12-N
70	1Y	202	PC1	C11-O13-P-O12
70	1Y	202	PC1	C11-O13-P-O14
70	1Y	202	PC1	C1-O11-P-O12
70	1Y	202	PC1	C1-O11-P-O14
70	1Y	202	PC1	C1-O11-P-O13
70	1Y	202	PC1	C22-C21-O21-C2
70	1Y	206	PC1	C1-O11-P-O12
70	1Y	207	PC1	C11-O13-P-O12
70	1Y	207	PC1	C11-O13-P-O14
70	1Y	207	PC1	C11-O13-P-O11
70	1Y	207	PC1	O32-C31-O31-C3
70	1Y	207	PC1	C32-C31-O31-C3
70	1d	204	PC1	C11-O13-P-O12
70	1d	204	PC1	C1-O11-P-O14
70	1d	204	PC1	C12-C11-O13-P
70	1d	204	PC1	O13-C11-C12-N
70	1d	204	PC1	C2-C1-O11-P
70	1d	204	PC1	C22-C21-O21-C2
70	1d	204	PC1	O32-C31-O31-C3
70	1d	204	PC1	C32-C31-O31-C3
70	1h	203	PC1	C1-O11-P-O12
70	1h	203	PC1	C1-O11-P-O14
70	1h	203	PC1	C1-O11-P-O13
70	3J	106	PC1	C1-O11-P-O14
70	3P	509	PC1	O13-C11-C12-N
70	3R	303	PC1	C11-O13-P-O12
70	3R	303	PC1	C11-O13-P-O11
70	3T	102	PC1	C22-C21-O21-C2
70	3X	104	PC1	C11-O13-P-O12
75	1H	401	CDL	CA2-OA2-PA1-OA3
75	1H	401	CDL	CA2-OA2-PA1-OA5
75	1H	401	CDL	CA3-OA5-PA1-OA4
75	1H	401	CDL	CB2-OB2-PB2-OB3
75	1H	401	CDL	CB3-OB5-PB2-OB2
75	1H	401	CDL	CB3-OB5-PB2-OB3
75	1H	401	CDL	CB3-OB5-PB2-OB4
75	1H	401	CDL	OB7-CB5-OB6-CB4
75	1H	401	CDL	C51-CB5-OB6-CB4
75	1L	704	CDL	CB3-OB5-PB2-OB3
75	1L	704	CDL	OB7-CB5-OB6-CB4
75	1N	402	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
75	1N	402	CDL	CA2-OA2-PA1-OA5
75	1N	402	CDL	CA3-OA5-PA1-OA4
75	1N	402	CDL	CB2-OB2-PB2-OB4
75	1Y	217	CDL	C1-CA2-OA2-PA1
75	1Y	217	CDL	CA2-OA2-PA1-OA5
75	1Y	217	CDL	CA3-OA5-PA1-OA3
75	1Y	217	CDL	C1-CB2-OB2-PB2
75	1Y	217	CDL	CB3-OB5-PB2-OB3
75	1d	202	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CB2-OB2-PB2-OB3
75	1d	202	CDL	OB7-CB5-OB6-CB4
75	1d	202	CDL	C51-CB5-OB6-CB4
75	1d	205	CDL	CA3-OA5-PA1-OA3
75	1d	205	CDL	CB3-OB5-PB2-OB3
75	1g	201	CDL	CA2-OA2-PA1-OA3
75	1g	201	CDL	CA2-OA2-PA1-OA4
75	1g	201	CDL	CA3-OA5-PA1-OA3
75	1g	201	CDL	CB2-OB2-PB2-OB4
75	1g	201	CDL	C51-CB5-OB6-CB4
75	1i	201	CDL	CA2-OA2-PA1-OA4
75	1i	201	CDL	OB7-CB5-OB6-CB4
75	1q	201	CDL	CA2-OA2-PA1-OA4
75	1q	201	CDL	CA3-OA5-PA1-OA3
75	1q	201	CDL	C11-CA5-OA6-CA4
75	1q	202	CDL	CB2-OB2-PB2-OB3
75	1q	202	CDL	CB3-OB5-PB2-OB2
75	1q	202	CDL	CB3-OB5-PB2-OB3
75	1q	202	CDL	CB3-OB5-PB2-OB4
75	1q	202	CDL	OB6-CB4-CB6-OB8
75	3A	501	CDL	CA2-OA2-PA1-OA3
75	3A	501	CDL	CA2-OA2-PA1-OA5
75	3A	501	CDL	CB2-OB2-PB2-OB3
75	3A	501	CDL	CB3-OB5-PB2-OB3
75	3A	501	CDL	OB7-CB5-OB6-CB4
75	3D	504	CDL	CA2-OA2-PA1-OA4
75	3D	504	CDL	C11-CA5-OA6-CA4
75	3D	504	CDL	CB2-OB2-PB2-OB3
75	3F	201	CDL	CA2-OA2-PA1-OA4
75	3F	201	CDL	CA3-OA5-PA1-OA3
75	3F	201	CDL	CA3-OA5-PA1-OA4
75	3F	201	CDL	CB3-OB5-PB2-OB2
75	3F	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
75	3F	201	CDL	CB3-OB5-PB2-OB4
75	3F	201	CDL	OB7-CB5-OB6-CB4
75	3F	201	CDL	C51-CB5-OB6-CB4
75	3N	502	CDL	CA3-OA5-PA1-OA4
75	3N	502	CDL	C11-CA5-OA6-CA4
75	3N	502	CDL	CB2-OB2-PB2-OB3
75	3N	502	CDL	CB2-OB2-PB2-OB4
75	3N	502	CDL	C51-CB5-OB6-CB4
75	3P	513	CDL	CA2-OA2-PA1-OA4
75	3T	101	CDL	CA2-OA2-PA1-OA3
75	3T	101	CDL	CA2-OA2-PA1-OA4
75	3T	101	CDL	CA2-OA2-PA1-OA5
75	3T	101	CDL	CB3-OB5-PB2-OB3
75	3T	101	CDL	CB3-OB5-PB2-OB4
75	3T	101	CDL	OB6-CB4-CB6-OB8
75	3X	103	CDL	CA3-OA5-PA1-OA3
75	3X	103	CDL	C11-CA5-OA6-CA4
75	3X	103	CDL	CB2-OB2-PB2-OB3
75	3X	103	CDL	CB2-OB2-PB2-OB4
75	3X	103	CDL	CB2-OB2-PB2-OB5
75	3X	103	CDL	CB3-OB5-PB2-OB3
75	3X	103	CDL	CB3-OB5-PB2-OB4
75	3X	103	CDL	CB4-CB3-OB5-PB2
75	3X	103	CDL	C51-CB5-OB6-CB4
75	3Y	106	CDL	O1-C1-CA2-OA2
75	3Y	106	CDL	CA2-OA2-PA1-OA4
75	3Y	106	CDL	CA3-OA5-PA1-OA3
75	3Y	106	CDL	CA3-OA5-PA1-OA4
75	3Y	106	CDL	CB2-OB2-PB2-OB3
75	3Y	106	CDL	CB3-OB5-PB2-OB4
75	3Y	106	CDL	OB7-CB5-OB6-CB4
75	3Y	106	CDL	C51-CB5-OB6-CB4
75	4B	302	CDL	CB3-OB5-PB2-OB3
75	4B	302	CDL	CB3-OB5-PB2-OB4
75	4C	306	CDL	CA3-OA5-PA1-OA3
75	4C	306	CDL	CA3-OA5-PA1-OA4
75	4C	306	CDL	C11-CA5-OA6-CA4
75	4C	306	CDL	CB2-OB2-PB2-OB3
75	4C	306	CDL	CB3-OB5-PB2-OB3
75	4C	306	CDL	CB3-OB5-PB2-OB4
75	4C	306	CDL	OB7-CB5-OB6-CB4
75	4C	307	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
75	4C	307	CDL	CA3-OA5-PA1-OA4
81	1T	101	EHZ	N2-C15-C16-O5
81	1n	201	EHZ	C7-C8-C9-O2
82	1Y	203	PGT	C32-C31-O2-C2
82	1Y	203	PGT	O31-C31-O2-C2
82	1Y	203	PGT	C1-O3P-P-O2P
82	1Y	203	PGT	C4-O4P-P-O2P
82	1Y	203	PGT	O11-C11-O3-C3
82	1Y	203	PGT	C12-C11-O3-C3
85	3C	501	HEM	C2B-C3B-CAB-CBB
85	3C	502	HEM	C2B-C3B-CAB-CBB
85	3P	502	HEM	C2B-C3B-CAB-CBB
87	3X	102	PEK	C03-O11-P-O14
87	3X	102	PEK	C04-O12-P-O14
87	3X	102	PEK	C11-C10-C9-C8
87	4G	103	PEK	C04-O12-P-O14
88	4A	601	HEA	C3B-C11-C12-C13
91	4A	606	PGV	C01-C02-O01-C1
91	4A	606	PGV	C2-C1-O01-C02
91	4A	607	PGV	C03-O11-P-O13
91	4A	607	PGV	C04-O12-P-O13
91	4A	608	PGV	C03-O11-P-O14
91	4C	302	PGV	C03-O11-P-O14
91	4C	304	PGV	O02-C1-O01-C02
91	4C	305	PGV	C04-O12-P-O11
91	4C	305	PGV	C04-O12-P-O13
91	4C	305	PGV	C04-O12-P-O14
91	4G	102	PGV	C03-O11-P-O13
91	4G	102	PGV	C03-O11-P-O14
91	4G	102	PGV	C04-O12-P-O13
91	4G	102	PGV	C04-O12-P-O14
91	4J	101	PGV	C03-O11-P-O13
91	4K	101	PGV	C03-O11-P-O13
91	4N	101	PGV	C03-O11-P-O13
91	4N	101	PGV	C04-O12-P-O11
91	4N	101	PGV	C04-O12-P-O13
91	4N	101	PGV	C04-O12-P-O14
93	4B	303	PSC	C03-O11-P-O13
93	4B	303	PSC	C03-O11-P-O14
93	4B	303	PSC	C04-O12-P-O14
93	4B	303	PSC	O12-C04-C05-N
93	4B	303	PSC	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
93	4B	303	PSC	C2-C1-O01-C02
69	1B	205	3PE	O32-C31-O31-C3
69	1M	502	3PE	O32-C31-O31-C3
69	1Y	213	3PE	O32-C31-O31-C3
69	1l	203	3PE	O32-C31-O31-C3
69	3C	513	3PE	O32-C31-O31-C3
69	3P	511	3PE	O32-C31-O31-C3
69	3Y	107	3PE	O32-C31-O31-C3
70	1J	202	PC1	O32-C31-O31-C3
75	3N	502	CDL	OB9-CB7-OB8-CB6
75	4B	302	CDL	OB9-CB7-OB8-CB6
69	3P	507	3PE	C2-C3-O31-C31
70	1Y	202	PC1	C2-C3-O31-C31
75	1H	401	CDL	CB4-CB6-OB8-CB7
69	1l	203	3PE	C32-C31-O31-C3
69	3C	513	3PE	C32-C31-O31-C3
69	3P	511	3PE	C32-C31-O31-C3
70	1J	202	PC1	C32-C31-O31-C3
75	3N	502	CDL	C71-CB7-OB8-CB6
75	4B	302	CDL	C71-CB7-OB8-CB6
69	1L	701	3PE	O32-C31-O31-C3
69	1Y	201	3PE	O32-C31-O31-C3
69	1b	101	3PE	O32-C31-O31-C3
69	1l	204	3PE	O32-C31-O31-C3
69	1m	204	3PE	O32-C31-O31-C3
69	3C	503	3PE	O32-C31-O31-C3
69	3C	506	3PE	O32-C31-O31-C3
69	3D	502	3PE	O32-C31-O31-C3
69	3G	106	3PE	O32-C31-O31-C3
69	3N	501	3PE	O32-C31-O31-C3
69	3W	103	3PE	O32-C31-O31-C3
69	3X	101	3PE	O32-C31-O31-C3
69	4G	104	3PE	O32-C31-O31-C3
75	1d	205	CDL	OA9-CA7-OA8-CA6
75	3T	101	CDL	OB9-CB7-OB8-CB6
75	4B	302	CDL	OA9-CA7-OA8-CA6
75	4C	306	CDL	OB9-CB7-OB8-CB6
69	1Y	201	3PE	O22-C21-O21-C2
69	1Y	204	3PE	O22-C21-O21-C2
69	1Y	216	3PE	O22-C21-O21-C2
69	1b	101	3PE	O22-C21-O21-C2
69	1d	201	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	1f	102	3PE	O22-C21-O21-C2
69	1g	202	3PE	O22-C21-O21-C2
69	1l	203	3PE	O22-C21-O21-C2
69	1m	205	3PE	O22-C21-O21-C2
69	3C	507	3PE	O22-C21-O21-C2
69	3C	513	3PE	O22-C21-O21-C2
69	3C	515	3PE	O22-C21-O21-C2
69	3D	502	3PE	O22-C21-O21-C2
69	3D	503	3PE	O22-C21-O21-C2
69	3G	103	3PE	O22-C21-O21-C2
69	3G	105	3PE	O22-C21-O21-C2
69	3G	108	3PE	O22-C21-O21-C2
69	3G	110	3PE	O22-C21-O21-C2
69	3G	111	3PE	O22-C21-O21-C2
69	3J	104	3PE	O22-C21-O21-C2
69	3J	105	3PE	O22-C21-O21-C2
69	3P	504	3PE	O22-C21-O21-C2
69	3P	514	3PE	O22-C21-O21-C2
69	3Q	503	3PE	O22-C21-O21-C2
69	3Q	504	3PE	O22-C21-O21-C2
69	3S	201	3PE	O22-C21-O21-C2
69	3W	101	3PE	O22-C21-O21-C2
69	3W	103	3PE	O22-C21-O21-C2
69	3X	106	3PE	O22-C21-O21-C2
69	3Y	107	3PE	O22-C21-O21-C2
69	4G	101	3PE	O22-C21-O21-C2
70	1Y	202	PC1	O22-C21-O21-C2
70	3T	102	PC1	O22-C21-O21-C2
75	1H	401	CDL	OA7-CA5-OA6-CA4
75	1g	201	CDL	OB7-CB5-OB6-CB4
75	1q	201	CDL	OA7-CA5-OA6-CA4
75	3D	504	CDL	OA7-CA5-OA6-CA4
75	3N	502	CDL	OA7-CA5-OA6-CA4
75	3N	502	CDL	OB7-CB5-OB6-CB4
75	3X	103	CDL	OA7-CA5-OA6-CA4
75	3X	103	CDL	OB7-CB5-OB6-CB4
75	3Y	106	CDL	OA7-CA5-OA6-CA4
75	4C	306	CDL	OA7-CA5-OA6-CA4
91	4A	606	PGV	O02-C1-O01-C02
91	4A	606	PGV	O04-C19-O03-C01
69	1h	204	3PE	C2-C3-O31-C31
69	1B	205	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	1L	701	3PE	C32-C31-O31-C3
69	1Y	201	3PE	C32-C31-O31-C3
69	1k	101	3PE	C32-C31-O31-C3
69	1l	204	3PE	C32-C31-O31-C3
69	1m	204	3PE	C32-C31-O31-C3
69	3C	506	3PE	C32-C31-O31-C3
69	3D	502	3PE	C32-C31-O31-C3
69	3G	106	3PE	C32-C31-O31-C3
69	3N	501	3PE	C32-C31-O31-C3
69	3R	304	3PE	C32-C31-O31-C3
69	3X	101	3PE	C32-C31-O31-C3
69	3Y	102	3PE	C32-C31-O31-C3
69	3Y	107	3PE	C32-C31-O31-C3
69	4G	104	3PE	C32-C31-O31-C3
75	1Y	217	CDL	C71-CB7-OB8-CB6
75	3T	101	CDL	C31-CA7-OA8-CA6
75	3T	101	CDL	C71-CB7-OB8-CB6
75	4B	302	CDL	C31-CA7-OA8-CA6
75	4C	306	CDL	C71-CB7-OB8-CB6
69	1L	708	3PE	C22-C21-O21-C2
69	1Y	213	3PE	C22-C21-O21-C2
69	1Y	215	3PE	C22-C21-O21-C2
69	1h	204	3PE	C22-C21-O21-C2
69	1k	101	3PE	C22-C21-O21-C2
69	1l	204	3PE	C22-C21-O21-C2
69	3C	508	3PE	C22-C21-O21-C2
69	3C	512	3PE	C22-C21-O21-C2
69	3J	101	3PE	C22-C21-O21-C2
69	3P	506	3PE	C22-C21-O21-C2
69	3P	520	3PE	C22-C21-O21-C2
69	3R	305	3PE	C22-C21-O21-C2
70	1A	202	PC1	C22-C21-O21-C2
75	1H	401	CDL	C11-CA5-OA6-CA4
75	1L	704	CDL	C51-CB5-OB6-CB4
75	1i	201	CDL	C51-CB5-OB6-CB4
75	3A	501	CDL	C51-CB5-OB6-CB4
75	3Y	106	CDL	C11-CA5-OA6-CA4
75	4C	306	CDL	C51-CB5-OB6-CB4
91	4C	304	PGV	C2-C1-O01-C02
69	3C	507	3PE	O32-C31-O31-C3
70	1M	501	PC1	O32-C31-O31-C3
81	1T	101	EHZ	C13-C12-N1-C11

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Mol	Chain	Res	Type	Atoms
69	1o	201	3PE	O32-C31-O31-C3
69	3C	514	3PE	O32-C31-O31-C3
75	3T	101	CDL	OA9-CA7-OA8-CA6
69	1Y	209	3PE	C32-C31-O31-C3
69	1Y	212	3PE	C32-C31-O31-C3
69	1Y	214	3PE	C32-C31-O31-C3
69	1b	101	3PE	C32-C31-O31-C3
69	1d	203	3PE	C32-C31-O31-C3
69	1m	202	3PE	C32-C31-O31-C3
69	1m	203	3PE	C32-C31-O31-C3
69	1o	201	3PE	C32-C31-O31-C3
69	3C	503	3PE	C32-C31-O31-C3
69	3C	511	3PE	C32-C31-O31-C3
69	3G	105	3PE	C32-C31-O31-C3
69	3J	101	3PE	C32-C31-O31-C3
69	3P	504	3PE	C32-C31-O31-C3
69	3P	508	3PE	C32-C31-O31-C3
69	4G	101	3PE	C32-C31-O31-C3
70	1P	502	PC1	C32-C31-O31-C3
75	1L	704	CDL	C71-CB7-OB8-CB6
75	1N	402	CDL	C31-CA7-OA8-CA6
75	1N	402	CDL	C71-CB7-OB8-CB6
75	1d	205	CDL	C31-CA7-OA8-CA6
91	4A	606	PGV	C20-C19-O03-C01
93	4B	303	PSC	C20-C19-O03-C01
69	1Y	209	3PE	O22-C21-O21-C2
69	1m	202	3PE	O22-C21-O21-C2
69	3N	501	3PE	O22-C21-O21-C2
69	3P	503	3PE	O22-C21-O21-C2
70	1d	204	PC1	O22-C21-O21-C2
75	3F	201	CDL	OA7-CA5-OA6-CA4
69	1Y	209	3PE	O32-C31-O31-C3
69	1k	101	3PE	O32-C31-O31-C3
69	3G	105	3PE	O32-C31-O31-C3
69	3J	101	3PE	O32-C31-O31-C3
70	1h	203	PC1	O32-C31-O31-C3
75	1L	704	CDL	OB9-CB7-OB8-CB6
75	1N	402	CDL	OA9-CA7-OA8-CA6
75	1Y	217	CDL	OB9-CB7-OB8-CB6
70	1h	202	PC1	C11-C12-N-C14
75	3T	101	CDL	CA4-CA6-OA8-CA7
75	1L	704	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
75	1g	201	CDL	O1-C1-CA2-OA2
75	3A	501	CDL	O1-C1-CA2-OA2
69	3C	507	3PE	C32-C31-O31-C3
69	3C	514	3PE	C32-C31-O31-C3
69	3C	517	3PE	C32-C31-O31-C3
69	3G	104	3PE	C32-C31-O31-C3
69	3P	506	3PE	C32-C31-O31-C3
69	3P	520	3PE	C32-C31-O31-C3
69	3S	201	3PE	C32-C31-O31-C3
75	3A	501	CDL	C31-CA7-OA8-CA6
75	3X	103	CDL	C71-CB7-OB8-CB6
69	1Y	212	3PE	O32-C31-O31-C3
69	1m	205	3PE	O32-C31-O31-C3
69	3C	511	3PE	O32-C31-O31-C3
69	3R	304	3PE	O32-C31-O31-C3
70	1Y	202	PC1	O32-C31-O31-C3
69	1Y	210	3PE	C22-C21-O21-C2
69	1Y	212	3PE	C22-C21-O21-C2
69	1d	201	3PE	C22-C21-O21-C2
69	1f	104	3PE	C22-C21-O21-C2
69	3C	506	3PE	C22-C21-O21-C2
69	3C	514	3PE	C22-C21-O21-C2
69	3G	107	3PE	C22-C21-O21-C2
69	3G	109	3PE	C22-C21-O21-C2
69	3W	102	3PE	C22-C21-O21-C2
69	3Y	101	3PE	C22-C21-O21-C2
69	3Y	103	3PE	C22-C21-O21-C2
70	1h	202	PC1	C22-C21-O21-C2
70	1h	203	PC1	C22-C21-O21-C2
75	1Y	217	CDL	C11-CA5-OA6-CA4
75	3F	201	CDL	C11-CA5-OA6-CA4
75	4C	307	CDL	C51-CB5-OB6-CB4
69	1d	201	3PE	C32-C33-C34-C35
69	1l	202	3PE	C33-C34-C35-C36
69	1d	201	3PE	C34-C35-C36-C37
69	1d	203	3PE	C2D-C2E-C2F-C2G
69	3C	509	3PE	C23-C24-C25-C26
70	3P	509	PC1	C28-C29-C2A-C2B
69	1d	201	3PE	C38-C39-C3A-C3B
77	1O	401	GTP	O4'-C4'-C5'-O5'
69	1m	205	3PE	C32-C31-O31-C3
69	3W	103	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
70	1M	501	PC1	C32-C31-O31-C3
70	1Y	202	PC1	C32-C31-O31-C3
70	1h	203	PC1	C32-C31-O31-C3
70	1h	202	PC1	O22-C21-O21-C2
75	1Y	217	CDL	C11-C12-C13-C14
75	1g	201	CDL	CB4-CB3-OB5-PB2
75	3X	103	CDL	C1-CB2-OB2-PB2
69	1d	203	3PE	O32-C31-O31-C3
69	1m	202	3PE	O32-C31-O31-C3
69	3P	508	3PE	O32-C31-O31-C3
69	3S	201	3PE	O32-C31-O31-C3
69	4G	101	3PE	O32-C31-O31-C3
75	3A	501	CDL	OA9-CA7-OA8-CA6
93	4B	303	PSC	O04-C19-O03-C01
69	3A	503	3PE	C35-C36-C37-C38
69	1Y	214	3PE	O32-C31-O31-C3
69	1m	203	3PE	O32-C31-O31-C3
69	3G	104	3PE	O32-C31-O31-C3
69	3P	504	3PE	O32-C31-O31-C3
70	1P	502	PC1	O32-C31-O31-C3
75	1N	402	CDL	OB9-CB7-OB8-CB6
69	1f	101	3PE	C32-C31-O31-C3
69	3J	105	3PE	C32-C31-O31-C3
75	1H	401	CDL	C31-CA7-OA8-CA6
75	3N	502	CDL	C31-CA7-OA8-CA6
81	1T	101	EHZ	O3-C12-N1-C11
69	3C	517	3PE	O32-C31-O31-C3
69	3P	506	3PE	O32-C31-O31-C3
69	3P	520	3PE	O32-C31-O31-C3
75	3X	103	CDL	OB9-CB7-OB8-CB6
69	1d	201	3PE	C36-C37-C38-C39
75	3Y	106	CDL	CB2-C1-CA2-OA2
69	1Y	212	3PE	O22-C21-O21-C2
69	3G	107	3PE	O22-C21-O21-C2
69	3G	109	3PE	O22-C21-O21-C2
69	3W	102	3PE	O22-C21-O21-C2
69	3Y	101	3PE	O22-C21-O21-C2
70	1h	203	PC1	O22-C21-O21-C2
69	1f	101	3PE	O32-C31-O31-C3
69	3J	105	3PE	O32-C31-O31-C3
75	1H	401	CDL	OA9-CA7-OA8-CA6
75	3N	502	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
75	3X	103	CDL	OA9-CA7-OA8-CA6
70	1Y	206	PC1	C11-C12-N-C13
70	1Y	206	PC1	C11-C12-N-C15
70	1h	202	PC1	C11-C12-N-C13
69	1L	711	3PE	C32-C31-O31-C3
69	1L	712	3PE	C32-C31-O31-C3
69	1N	401	3PE	C32-C31-O31-C3
69	1l	202	3PE	C32-C31-O31-C3
69	3C	509	3PE	C32-C31-O31-C3
69	3C	512	3PE	C32-C31-O31-C3
69	3D	503	3PE	C32-C31-O31-C3
69	3E	302	3PE	C32-C31-O31-C3
69	3G	109	3PE	C32-C31-O31-C3
69	3P	507	3PE	C32-C31-O31-C3
69	3P	514	3PE	C32-C31-O31-C3
69	3Q	502	3PE	C32-C31-O31-C3
69	3Q	503	3PE	C32-C31-O31-C3
69	3Q	504	3PE	C32-C31-O31-C3
69	3X	107	3PE	C32-C31-O31-C3
69	3Y	101	3PE	C32-C31-O31-C3
70	1A	202	PC1	C32-C31-O31-C3
75	1g	201	CDL	C31-CA7-OA8-CA6
75	1i	201	CDL	C31-CA7-OA8-CA6
75	1q	202	CDL	C71-CB7-OB8-CB6
75	3D	504	CDL	C71-CB7-OB8-CB6
75	3F	201	CDL	C71-CB7-OB8-CB6
75	3X	103	CDL	C31-CA7-OA8-CA6
75	3Y	106	CDL	C71-CB7-OB8-CB6
91	4A	607	PGV	C20-C19-O03-C01
91	4K	101	PGV	C20-C19-O03-C01
69	1L	712	3PE	C2A-C2B-C2C-C2D
70	3T	102	PC1	C23-C24-C25-C26
79	1P	501	NDP	O4D-C1D-N1N-C6N
69	1Y	215	3PE	C36-C37-C38-C39
75	1L	704	CDL	O1-C1-CA2-OA2
69	1o	201	3PE	C31-C32-C33-C34
69	1J	201	3PE	O21-C2-C3-O31
69	3J	103	3PE	O21-C2-C3-O31
69	1L	710	3PE	C32-C31-O31-C3
91	4C	302	PGV	C20-C19-O03-C01
69	1m	201	3PE	C28-C29-C2A-C2B
69	3Y	107	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
70	1J	202	PC1	C24-C25-C26-C27
69	1L	712	3PE	O32-C31-O31-C3
69	3C	512	3PE	O32-C31-O31-C3
75	1i	201	CDL	OA9-CA7-OA8-CA6
69	1Y	215	3PE	C25-C26-C27-C28
69	1Y	210	3PE	O22-C21-O21-C2
69	3C	506	3PE	O22-C21-O21-C2
75	1Y	217	CDL	OA7-CA5-OA6-CA4
69	1L	710	3PE	C22-C21-O21-C2
69	3C	505	3PE	C22-C21-O21-C2
69	1d	206	3PE	C24-C25-C26-C27
75	1i	201	CDL	C13-C14-C15-C16
69	1N	401	3PE	O32-C31-O31-C3
69	1l	202	3PE	O32-C31-O31-C3
69	3C	509	3PE	O32-C31-O31-C3
69	3E	302	3PE	O32-C31-O31-C3
69	3G	109	3PE	O32-C31-O31-C3
69	3Q	503	3PE	O32-C31-O31-C3
69	3X	107	3PE	O32-C31-O31-C3
75	1g	201	CDL	OA9-CA7-OA8-CA6
75	1q	202	CDL	OB9-CB7-OB8-CB6
91	4A	607	PGV	O04-C19-O03-C01
69	1l	204	3PE	C26-C27-C28-C29
69	3C	506	3PE	C27-C28-C29-C2A
69	3G	109	3PE	C22-C23-C24-C25
69	1Y	210	3PE	C23-C24-C25-C26
69	3C	505	3PE	C32-C31-O31-C3
87	3X	102	PEK	C31-C32-C33-C34
69	1d	201	3PE	C21-C22-C23-C24
69	3W	103	3PE	C31-C32-C33-C34
70	1J	202	PC1	C21-C22-C23-C24
75	1d	205	CDL	CA5-C11-C12-C13
69	1d	201	3PE	C27-C28-C29-C2A
75	1q	201	CDL	C17-C18-C19-C20
91	4A	607	PGV	C24-C25-C26-C27
69	1L	701	3PE	C31-C32-C33-C34
69	1Y	213	3PE	C31-C32-C33-C34
69	1o	201	3PE	C21-C22-C23-C24
69	3D	502	3PE	C31-C32-C33-C34
69	3P	508	3PE	C21-C22-C23-C24
70	1B	202	PC1	C21-C22-C23-C24
70	3P	509	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
70	3X	104	PC1	C31-C32-C33-C34
75	1L	704	CDL	CA7-C31-C32-C33
75	1i	201	CDL	CA7-C31-C32-C33
75	3P	513	CDL	CB5-C51-C52-C53
69	1B	204	3PE	C29-C2A-C2B-C2C
69	3P	503	3PE	C39-C3A-C3B-C3C
69	3G	110	3PE	C32-C31-O31-C3
69	3J	104	3PE	C32-C31-O31-C3
69	3P	517	3PE	C32-C31-O31-C3
69	3C	513	3PE	C2-C3-O31-C31
75	1g	201	CDL	CA4-CA6-OA8-CA7
69	1Y	216	3PE	C24-C25-C26-C27
69	1m	205	3PE	C32-C33-C34-C35
69	1f	104	3PE	O22-C21-O21-C2
69	3C	514	3PE	O22-C21-O21-C2
69	3P	507	3PE	C34-C35-C36-C37
75	1Y	217	CDL	C17-C18-C19-C20
69	3Y	101	3PE	O32-C31-O31-C3
70	1Y	202	PC1	C11-C12-N-C15
69	1b	101	3PE	C31-C32-C33-C34
69	1e	201	3PE	C21-C22-C23-C24
70	1J	202	PC1	C31-C32-C33-C34
69	1L	711	3PE	C22-C21-O21-C2
69	3P	519	3PE	C22-C21-O21-C2
91	4A	609	PGV	C2-C1-O01-C02
75	1d	202	CDL	C11-C12-C13-C14
69	3C	505	3PE	O32-C31-O31-C3
69	3P	507	3PE	O32-C31-O31-C3
69	3Q	502	3PE	O32-C31-O31-C3
70	1A	202	PC1	O32-C31-O31-C3
75	3F	201	CDL	OB9-CB7-OB8-CB6
69	3G	111	3PE	C23-C24-C25-C26
70	1H	404	PC1	C3C-C3D-C3E-C3F
69	3C	508	3PE	C36-C37-C38-C39
75	3D	504	CDL	OB9-CB7-OB8-CB6
91	4K	101	PGV	O04-C19-O03-C01
88	4A	601	HEA	C19-C20-C21-C22
75	4C	306	CDL	C51-C52-C53-C54
69	3G	111	3PE	C31-C32-C33-C34
69	3A	502	3PE	C22-C23-C24-C25
69	3P	517	3PE	C27-C28-C29-C2A
75	1g	201	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
69	3P	519	3PE	O22-C21-O21-C2
69	3Y	103	3PE	O22-C21-O21-C2
75	4C	307	CDL	OB7-CB5-OB6-CB4
69	3J	102	3PE	C32-C31-O31-C3
91	4C	303	PGV	C20-C19-O03-C01
69	1A	203	3PE	C36-C37-C38-C39
69	1L	711	3PE	O32-C31-O31-C3
69	3D	503	3PE	O32-C31-O31-C3
69	3P	514	3PE	O32-C31-O31-C3
69	3Q	504	3PE	O32-C31-O31-C3
75	3Y	106	CDL	OB9-CB7-OB8-CB6
91	4C	302	PGV	O04-C19-O03-C01
69	1L	710	3PE	C21-C22-C23-C24
69	1Y	213	3PE	C21-C22-C23-C24
69	1Y	210	3PE	C35-C36-C37-C38
69	1L	710	3PE	O32-C31-O31-C3
69	3G	110	3PE	O32-C31-O31-C3
70	1B	202	PC1	C22-C21-O21-C2
69	1A	201	3PE	C11-O13-P-O11
69	1B	204	3PE	C1-O11-P-O13
69	1B	205	3PE	C11-O13-P-O11
69	1J	201	3PE	C11-O13-P-O11
69	1L	701	3PE	C11-O13-P-O11
69	1L	703	3PE	C1-O11-P-O13
69	1L	706	3PE	C11-O13-P-O11
69	1L	708	3PE	C1-O11-P-O13
69	1L	709	3PE	C1-O11-P-O13
69	1L	709	3PE	C11-O13-P-O11
69	1L	712	3PE	C1-O11-P-O13
69	1M	502	3PE	C1-O11-P-O13
69	1M	502	3PE	C11-O13-P-O11
69	1Y	201	3PE	C11-O13-P-O11
69	1Y	205	3PE	C1-O11-P-O13
69	1Y	210	3PE	C1-O11-P-O13
69	1Y	212	3PE	C11-O13-P-O11
69	1Y	213	3PE	C1-O11-P-O13
69	1Y	215	3PE	C1-O11-P-O13
69	1Y	215	3PE	C11-O13-P-O11
69	1Y	216	3PE	C1-O11-P-O13
69	1f	101	3PE	C1-O11-P-O13
69	1f	101	3PE	C11-O13-P-O11
69	1f	103	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	1f	104	3PE	C1-O11-P-O13
69	1f	104	3PE	C11-O13-P-O11
69	1g	203	3PE	C1-O11-P-O13
69	1h	204	3PE	C11-O13-P-O11
69	1k	101	3PE	C1-O11-P-O13
69	1l	202	3PE	C11-O13-P-O11
69	1l	203	3PE	C11-O13-P-O11
69	1m	201	3PE	C1-O11-P-O13
69	1m	203	3PE	C1-O11-P-O13
69	1m	205	3PE	C11-O13-P-O11
69	3A	503	3PE	C11-O13-P-O11
69	3C	505	3PE	C1-O11-P-O13
69	3C	507	3PE	C1-O11-P-O13
69	3C	510	3PE	C1-O11-P-O13
69	3C	511	3PE	C1-O11-P-O13
69	3C	512	3PE	C1-O11-P-O13
69	3C	514	3PE	C1-O11-P-O13
69	3C	515	3PE	C1-O11-P-O13
69	3C	516	3PE	C11-O13-P-O11
69	3D	502	3PE	C1-O11-P-O13
69	3D	503	3PE	C11-O13-P-O11
69	3E	303	3PE	C11-O13-P-O11
69	3G	102	3PE	C1-O11-P-O13
69	3G	103	3PE	C1-O11-P-O13
69	3G	104	3PE	C1-O11-P-O13
69	3G	105	3PE	C11-O13-P-O11
69	3G	106	3PE	C1-O11-P-O13
69	3G	108	3PE	C1-O11-P-O13
69	3G	111	3PE	C11-O13-P-O11
69	3J	101	3PE	C1-O11-P-O13
69	3J	101	3PE	C11-O13-P-O11
69	3J	102	3PE	C1-O11-P-O13
69	3J	102	3PE	C11-O13-P-O11
69	3J	103	3PE	C1-O11-P-O13
69	3J	104	3PE	C1-O11-P-O13
69	3P	503	3PE	C1-O11-P-O13
69	3P	504	3PE	C11-O13-P-O11
69	3P	506	3PE	C1-O11-P-O13
69	3P	507	3PE	C11-O13-P-O11
69	3P	508	3PE	C11-O13-P-O11
69	3P	510	3PE	C1-O11-P-O13
69	3P	512	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	3P	515	3PE	C1-O11-P-O13
69	3P	518	3PE	C1-O11-P-O13
69	3P	518	3PE	C11-O13-P-O11
69	3P	519	3PE	C1-O11-P-O13
69	3P	519	3PE	C11-O13-P-O11
69	3Q	504	3PE	C1-O11-P-O13
69	3R	304	3PE	C1-O11-P-O13
69	3R	304	3PE	C11-O13-P-O11
69	3S	201	3PE	C11-O13-P-O11
69	3T	103	3PE	C1-O11-P-O13
69	3T	103	3PE	C11-O13-P-O11
69	3W	102	3PE	C1-O11-P-O13
69	3W	102	3PE	C11-O13-P-O11
69	3X	101	3PE	C1-O11-P-O13
69	3X	105	3PE	C1-O11-P-O13
69	3X	106	3PE	C1-O11-P-O13
69	3X	107	3PE	C11-O13-P-O11
69	3X	108	3PE	C11-O13-P-O11
69	3Y	101	3PE	C11-O13-P-O11
69	3Y	102	3PE	C1-O11-P-O13
69	3Y	104	3PE	C11-O13-P-O11
69	4G	101	3PE	C11-O13-P-O11
70	1A	202	PC1	C1-O11-P-O13
70	1B	202	PC1	C11-O13-P-O11
70	1B	202	PC1	C1-O11-P-O13
70	1B	203	PC1	C11-O13-P-O11
70	1B	203	PC1	C1-O11-P-O13
70	1M	501	PC1	C11-O13-P-O11
70	1M	501	PC1	C1-O11-P-O13
70	1Y	202	PC1	C11-O13-P-O11
70	1Y	206	PC1	C1-O11-P-O13
70	1d	204	PC1	C11-O13-P-O11
70	1d	204	PC1	C1-O11-P-O13
70	1h	203	PC1	C11-O13-P-O11
70	3J	106	PC1	C1-O11-P-O13
70	3P	509	PC1	C11-O13-P-O11
70	3T	102	PC1	C11-O13-P-O11
70	3T	102	PC1	C1-O11-P-O13
75	1L	704	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CA3-OA5-PA1-OA2
75	1d	202	CDL	CB2-OB2-PB2-OB5
75	1d	205	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
75	1d	205	CDL	CA3-OA5-PA1-OA2
75	1g	201	CDL	CA2-OA2-PA1-OA5
75	1g	201	CDL	CB2-OB2-PB2-OB5
75	1i	201	CDL	CA2-OA2-PA1-OA5
75	3A	501	CDL	CB2-OB2-PB2-OB5
75	3D	504	CDL	CA2-OA2-PA1-OA5
75	3D	504	CDL	CB2-OB2-PB2-OB5
75	3F	201	CDL	CA2-OA2-PA1-OA5
75	3F	201	CDL	CA3-OA5-PA1-OA2
75	3F	201	CDL	CB2-OB2-PB2-OB5
75	3N	502	CDL	CB2-OB2-PB2-OB5
75	3N	502	CDL	CB3-OB5-PB2-OB2
75	3T	101	CDL	CB3-OB5-PB2-OB2
75	3X	103	CDL	CA3-OA5-PA1-OA2
75	3X	103	CDL	CB3-OB5-PB2-OB2
75	3Y	106	CDL	CA2-OA2-PA1-OA5
75	3Y	106	CDL	CA3-OA5-PA1-OA2
75	3Y	106	CDL	CB3-OB5-PB2-OB2
75	4B	302	CDL	CB2-OB2-PB2-OB5
75	4B	302	CDL	CB3-OB5-PB2-OB2
75	4C	306	CDL	CA3-OA5-PA1-OA2
75	4C	306	CDL	CB3-OB5-PB2-OB2
75	4C	307	CDL	CA3-OA5-PA1-OA2
75	4C	307	CDL	CB2-OB2-PB2-OB5
75	4C	307	CDL	CB3-OB5-PB2-OB2
87	4G	103	PEK	C04-O12-P-O11
91	4A	606	PGV	C03-O11-P-O12
91	4A	607	PGV	C04-O12-P-O11
91	4A	608	PGV	C03-O11-P-O12
91	4A	609	PGV	C04-O12-P-O11
91	4C	302	PGV	C03-O11-P-O12
91	4C	303	PGV	C04-O12-P-O11
91	4C	305	PGV	C03-O11-P-O12
91	4G	102	PGV	C03-O11-P-O12
91	4G	102	PGV	C04-O12-P-O11
91	4J	101	PGV	C03-O11-P-O12
91	4K	101	PGV	C03-O11-P-O12
93	4B	303	PSC	C03-O11-P-O12
69	3X	107	3PE	C21-C22-C23-C24
69	1d	206	3PE	C32-C31-O31-C3
69	1g	203	3PE	C32-C31-O31-C3
69	3G	102	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
75	1g	201	CDL	C71-CB7-OB8-CB6
75	3A	501	CDL	C71-CB7-OB8-CB6
69	1h	204	3PE	C35-C36-C37-C38
75	1L	704	CDL	CA2-C1-CB2-OB2
75	1g	201	CDL	CA2-C1-CB2-OB2
75	3A	501	CDL	CB2-C1-CA2-OA2
69	1L	711	3PE	O22-C21-O21-C2
69	3C	505	3PE	O22-C21-O21-C2
91	4A	609	PGV	O02-C1-O01-C02
69	1L	710	3PE	C25-C26-C27-C28
75	1i	201	CDL	C17-C18-C19-C20
75	3N	502	CDL	C36-C37-C38-C39
75	3N	502	CDL	C59-C60-C61-C62
75	1Y	217	CDL	C21-C22-C23-C24
70	1d	204	PC1	C11-C12-N-C13
70	1d	204	PC1	C11-C12-N-C14
70	3T	102	PC1	C11-C12-N-C13
70	3T	102	PC1	C11-C12-N-C15
93	4B	303	PSC	C04-C05-N-C06
93	4B	303	PSC	C04-C05-N-C08
69	1J	201	3PE	C32-C31-O31-C3
69	1L	705	3PE	C32-C31-O31-C3
69	1L	706	3PE	C32-C31-O31-C3
91	4N	101	PGV	C20-C19-O03-C01
69	1m	201	3PE	C35-C36-C37-C38
69	3P	519	3PE	C3E-C3F-C3G-C3H
69	1L	708	3PE	C23-C24-C25-C26
69	1L	712	3PE	C33-C34-C35-C36
69	1o	201	3PE	C25-C26-C27-C28
69	1m	203	3PE	C26-C27-C28-C29
69	3G	105	3PE	C25-C26-C27-C28
69	3T	103	3PE	C36-C37-C38-C39
69	1L	712	3PE	C22-C21-O21-C2
69	1Y	208	3PE	C22-C21-O21-C2
69	3P	512	3PE	C22-C21-O21-C2
69	3Y	102	3PE	C22-C21-O21-C2
70	1P	502	PC1	C22-C21-O21-C2
70	1Y	206	PC1	C22-C21-O21-C2
70	3X	104	PC1	C22-C21-O21-C2
69	1L	708	3PE	C28-C29-C2A-C2B
69	1Y	213	3PE	C32-C33-C34-C35
69	1Y	213	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
69	1d	201	3PE	C2A-C2B-C2C-C2D
69	1d	201	3PE	C2C-C2D-C2E-C2F
69	3C	508	3PE	C35-C36-C37-C38
69	3C	508	3PE	C39-C3A-C3B-C3C
69	3R	302	3PE	C22-C23-C24-C25
70	1B	203	PC1	C29-C2A-C2B-C2C
70	1M	501	PC1	C28-C29-C2A-C2B
75	1d	202	CDL	C31-C32-C33-C34
75	1d	205	CDL	C14-C15-C16-C17
75	1g	201	CDL	C57-C58-C59-C60
69	1Y	204	3PE	C32-C31-O31-C3
69	1Y	213	3PE	C3C-C3D-C3E-C3F
69	1d	201	3PE	C24-C25-C26-C27
69	1d	203	3PE	C33-C34-C35-C36
69	3G	111	3PE	C24-C25-C26-C27
69	3P	506	3PE	C34-C35-C36-C37
75	3P	513	CDL	C36-C37-C38-C39
87	3X	102	PEK	C25-C26-C27-C28
91	4C	304	PGV	C5-C6-C7-C8
69	1g	202	3PE	C1-C2-O21-C21
69	3J	105	3PE	C1-C2-O21-C21
69	3W	102	3PE	C3-C2-O21-C21
69	3X	105	3PE	C1-C2-O21-C21
69	3X	108	3PE	C1-C2-O21-C21
69	4G	101	3PE	C3-C2-O21-C21
75	1Y	217	CDL	CA3-CA4-OA6-CA5
75	3N	502	CDL	CA3-CA4-OA6-CA5
75	3X	103	CDL	CA3-CA4-OA6-CA5
69	1L	712	3PE	O22-C21-O21-C2
69	1Y	208	3PE	O22-C21-O21-C2
69	3X	105	3PE	O22-C21-O21-C2
69	3Y	102	3PE	O22-C21-O21-C2
70	1B	202	PC1	O22-C21-O21-C2
70	1P	502	PC1	O22-C21-O21-C2
70	1Y	206	PC1	O22-C21-O21-C2
70	3X	104	PC1	O22-C21-O21-C2
69	3G	101	3PE	C21-C22-C23-C24
69	3R	302	3PE	C38-C39-C3A-C3B
69	3S	201	3PE	C35-C36-C37-C38
69	3X	106	3PE	C2B-C2C-C2D-C2E
70	1B	203	PC1	C24-C25-C26-C27
70	1J	202	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
69	1Y	204	3PE	C2-C1-O11-P
69	1g	203	3PE	C2-C1-O11-P
69	3G	102	3PE	C2-C1-O11-P
91	4J	101	PGV	C02-C03-O11-P
75	4B	302	CDL	C62-C63-C64-C65
75	1Y	217	CDL	O1-C1-CA2-OA2
69	1d	201	3PE	C33-C34-C35-C36
75	1g	201	CDL	C37-C38-C39-C40
75	3X	103	CDL	C14-C15-C16-C17
69	1N	401	3PE	C22-C23-C24-C25
69	1Y	205	3PE	C2A-C2B-C2C-C2D
69	1Y	209	3PE	C32-C33-C34-C35
69	1Y	211	3PE	C2A-C2B-C2C-C2D
69	1Y	213	3PE	C2B-C2C-C2D-C2E
69	1d	201	3PE	C28-C29-C2A-C2B
69	1d	203	3PE	C2C-C2D-C2E-C2F
69	1l	202	3PE	C35-C36-C37-C38
69	3J	104	3PE	O32-C31-O31-C3
75	3A	501	CDL	C61-C62-C63-C64
75	4C	306	CDL	C75-C76-C77-C78
70	1B	202	PC1	C22-C23-C24-C25
70	3R	303	PC1	C36-C37-C38-C39
69	3J	102	3PE	O32-C31-O31-C3
69	3P	517	3PE	O32-C31-O31-C3
69	1d	203	3PE	C23-C24-C25-C26
69	1o	201	3PE	C3C-C3D-C3E-C3F
69	3W	102	3PE	C3A-C3B-C3C-C3D
69	3P	512	3PE	O22-C21-O21-C2
75	4B	302	CDL	OA7-CA5-OA6-CA4
69	1L	705	3PE	C22-C21-O21-C2
69	3C	510	3PE	C22-C21-O21-C2
69	3X	105	3PE	C22-C21-O21-C2
75	4B	302	CDL	C11-CA5-OA6-CA4
91	4C	302	PGV	C2-C1-O01-C02
69	3G	109	3PE	C33-C34-C35-C36
70	1h	203	PC1	C34-C35-C36-C37
75	1Y	217	CDL	C39-C40-C41-C42
91	4J	101	PGV	C20-C21-C22-C23
69	3W	102	3PE	C31-C32-C33-C34
70	1d	204	PC1	C31-C32-C33-C34
93	4B	303	PSC	C1-C2-C3-C4
69	1L	702	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
69	1Y	201	3PE	C36-C37-C38-C39
69	1k	101	3PE	C32-C33-C34-C35
69	1k	101	3PE	C29-C2A-C2B-C2C
69	3G	101	3PE	C3A-C3B-C3C-C3D
70	1B	202	PC1	C24-C25-C26-C27
75	1Y	217	CDL	C74-C75-C76-C77
75	1g	201	CDL	C36-C37-C38-C39
87	3X	102	PEK	C23-C24-C25-C26
70	1Y	206	PC1	C11-C12-N-C14
70	1d	204	PC1	C11-C12-N-C15
70	3T	102	PC1	C11-C12-N-C14
70	3X	104	PC1	C11-C12-N-C14
93	4B	303	PSC	C04-C05-N-C07
69	1e	201	3PE	C22-C23-C24-C25
69	1m	202	3PE	C23-C24-C25-C26
69	3P	514	3PE	C37-C38-C39-C3A
69	3X	108	3PE	C32-C33-C34-C35
69	4G	104	3PE	C22-C23-C24-C25
70	1d	204	PC1	C37-C38-C39-C3A
70	3J	106	PC1	C23-C24-C25-C26
70	3T	102	PC1	C37-C38-C39-C3A
75	1g	201	CDL	C63-C64-C65-C66
69	1d	201	3PE	O13-C11-C12-N
69	3E	303	3PE	O13-C11-C12-N
69	3P	515	3PE	O13-C11-C12-N
69	3P	520	3PE	O13-C11-C12-N
69	1Y	213	3PE	C22-C23-C24-C25
69	1m	202	3PE	C22-C23-C24-C25
69	3X	106	3PE	C27-C28-C29-C2A
69	3X	107	3PE	C34-C35-C36-C37
75	1N	402	CDL	C31-C32-C33-C34
75	1N	402	CDL	C34-C35-C36-C37
75	4B	302	CDL	C51-C52-C53-C54
75	4B	302	CDL	C58-C59-C60-C61
69	1J	201	3PE	O32-C31-O31-C3
75	1g	201	CDL	OB9-CB7-OB8-CB6
69	3C	509	3PE	C28-C29-C2A-C2B
70	3X	104	PC1	C26-C27-C28-C29
70	3X	104	PC1	C35-C36-C37-C38
69	1Y	216	3PE	C32-C31-O31-C3
69	3G	101	3PE	C32-C31-O31-C3
75	1d	202	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
69	3C	507	3PE	C3A-C3B-C3C-C3D
69	3W	101	3PE	C23-C24-C25-C26
88	4A	602	HEA	C2A-CAA-CBA-CGA
75	3P	513	CDL	CA4-CA6-OA8-CA7
69	1o	201	3PE	C2B-C2C-C2D-C2E
69	3S	201	3PE	C2E-C2F-C2G-C2H
70	1H	403	PC1	C28-C29-C2A-C2B
75	4C	306	CDL	C17-C18-C19-C20
91	4A	609	PGV	C21-C22-C23-C24
69	1g	203	3PE	O32-C31-O31-C3
69	3G	102	3PE	O32-C31-O31-C3
75	3A	501	CDL	OB9-CB7-OB8-CB6
91	4C	303	PGV	O04-C19-O03-C01
91	4N	101	PGV	O04-C19-O03-C01
69	1d	201	3PE	C29-C2A-C2B-C2C
75	1Y	217	CDL	C81-C82-C83-C84
75	1g	201	CDL	C53-C54-C55-C56
75	3N	502	CDL	C17-C18-C19-C20
75	3X	103	CDL	C75-C76-C77-C78
75	3Y	106	CDL	C73-C74-C75-C76
69	1f	101	3PE	C1-C2-C3-O31
91	4C	302	PGV	O02-C1-O01-C02
69	1L	709	3PE	C22-C23-C24-C25
69	1N	401	3PE	C23-C24-C25-C26
75	4B	302	CDL	C59-C60-C61-C62
69	1Y	208	3PE	C34-C35-C36-C37
69	1d	201	3PE	C25-C26-C27-C28
69	3P	508	3PE	C29-C2A-C2B-C2C
70	3R	303	PC1	C2A-C2B-C2C-C2D
69	1d	206	3PE	O32-C31-O31-C3
69	1B	204	3PE	C32-C31-O31-C3
69	3P	503	3PE	C32-C31-O31-C3
69	1L	703	3PE	C22-C21-O21-C2
70	3P	509	PC1	C22-C21-O21-C2
70	3R	303	PC1	C22-C21-O21-C2
69	1L	702	3PE	C2-C3-O31-C31
69	3X	105	3PE	C36-C37-C38-C39
69	1d	206	3PE	C22-C23-C24-C25
69	3G	101	3PE	C25-C26-C27-C28
70	1h	203	PC1	C32-C33-C34-C35
70	3X	104	PC1	C2B-C2C-C2D-C2E
69	1L	706	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	1d	203	3PE	C36-C37-C38-C39
75	4B	302	CDL	C14-C15-C16-C17
77	1O	401	GTP	C3'-C4'-C5'-O5'
69	3P	520	3PE	C22-C23-C24-C25
75	4B	302	CDL	C74-C75-C76-C77
69	1L	702	3PE	C25-C26-C27-C28
69	1Y	213	3PE	C2A-C2B-C2C-C2D
69	1l	203	3PE	C23-C24-C25-C26
69	3X	101	3PE	C2A-C2B-C2C-C2D
69	3Y	102	3PE	C23-C24-C25-C26
69	1L	705	3PE	O32-C31-O31-C3
69	1Y	204	3PE	O32-C31-O31-C3
75	1Y	217	CDL	CB2-C1-CA2-OA2
70	1H	402	PC1	C32-C33-C34-C35
75	1L	704	CDL	C13-C14-C15-C16
69	1L	703	3PE	O22-C21-O21-C2
69	3C	510	3PE	O22-C21-O21-C2
70	3P	509	PC1	O22-C21-O21-C2
70	3R	303	PC1	O22-C21-O21-C2
87	3X	102	PEK	O02-C1-O01-C02
75	1Y	217	CDL	C83-C84-C85-C86
69	1d	206	3PE	C37-C38-C39-C3A
75	1d	205	CDL	C23-C24-C25-C26
70	1Y	202	PC1	C11-C12-N-C14
70	1h	202	PC1	C11-C12-N-C15
70	3J	106	PC1	C11-C12-N-C15
70	3P	509	PC1	C11-C12-N-C15
87	4G	103	PEK	C21-C22-C23-C24
69	1A	201	3PE	C32-C33-C34-C35
69	1L	710	3PE	C23-C24-C25-C26
69	3C	512	3PE	C25-C26-C27-C28
69	3P	508	3PE	C34-C35-C36-C37
75	3F	201	CDL	C71-C72-C73-C74
69	3X	108	3PE	C32-C31-O31-C3
75	1q	202	CDL	C31-CA7-OA8-CA6
75	3Y	106	CDL	C31-CA7-OA8-CA6
75	4C	306	CDL	C31-CA7-OA8-CA6
69	1Y	214	3PE	C22-C21-O21-C2
70	1H	402	PC1	C22-C21-O21-C2
69	1f	104	3PE	C24-C25-C26-C27
69	1h	204	3PE	C3B-C3C-C3D-C3E
69	3G	104	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
69	3Q	503	3PE	C22-C23-C24-C25
69	3T	103	3PE	C28-C29-C2A-C2B
69	3Y	101	3PE	C3A-C3B-C3C-C3D
75	4C	306	CDL	C61-C62-C63-C64
69	1Y	211	3PE	C21-C22-C23-C24
69	1m	201	3PE	C21-C22-C23-C24
69	3J	103	3PE	C21-C22-C23-C24
69	1J	201	3PE	C3A-C3B-C3C-C3D
69	1N	401	3PE	C36-C37-C38-C39
69	1d	203	3PE	C27-C28-C29-C2A
70	3T	102	PC1	C33-C34-C35-C36
69	1Y	213	3PE	C26-C27-C28-C29
69	1Y	215	3PE	C22-C23-C24-C25
69	3A	502	3PE	C32-C33-C34-C35
69	1B	204	3PE	O32-C31-O31-C3
69	1Y	216	3PE	O32-C31-O31-C3
69	3G	101	3PE	O32-C31-O31-C3
69	3P	503	3PE	O32-C31-O31-C3
75	1q	202	CDL	OA9-CA7-OA8-CA6
75	4C	306	CDL	C38-C39-C40-C41
87	3X	102	PEK	C35-C36-C37-C38
69	1L	705	3PE	O22-C21-O21-C2
70	1B	203	PC1	O22-C21-O21-C2
69	1B	205	3PE	C31-C32-C33-C34
69	3C	514	3PE	C21-C22-C23-C24
70	1A	202	PC1	C21-C22-C23-C24
69	1f	103	3PE	C32-C31-O31-C3
69	3N	503	3PE	C32-C31-O31-C3
87	3X	102	PEK	C22-C21-O03-C01
69	3E	302	3PE	C2A-C2B-C2C-C2D
69	3J	104	3PE	C2C-C2D-C2E-C2F
69	3C	505	3PE	C3C-C3D-C3E-C3F
70	3X	104	PC1	C2D-C2E-C2F-C2G
91	4A	609	PGV	C4-C5-C6-C7
91	4K	101	PGV	C3-C4-C5-C6
69	1Y	214	3PE	C28-C29-C2A-C2B
69	1l	202	3PE	C32-C33-C34-C35
69	3C	504	3PE	C34-C35-C36-C37
70	1J	202	PC1	C34-C35-C36-C37
69	1L	702	3PE	C21-C22-C23-C24
69	3C	504	3PE	C21-C22-C23-C24
69	3P	507	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
91	4A	606	PGV	C19-C20-C21-C22
69	1m	204	3PE	C27-C28-C29-C2A
91	4G	102	PGV	C2-C3-C4-C5
85	3P	501	HEM	C2B-C3B-CAB-CBB
69	1Y	213	3PE	C33-C34-C35-C36
69	1g	202	3PE	C22-C23-C24-C25
91	4A	609	PGV	C20-C19-O03-C01
69	1L	712	3PE	C38-C39-C3A-C3B
69	1f	104	3PE	C36-C37-C38-C39
69	1g	202	3PE	C27-C28-C29-C2A
69	1m	204	3PE	C33-C34-C35-C36
69	3J	102	3PE	C22-C23-C24-C25
69	3S	201	3PE	C32-C33-C34-C35
70	3J	106	PC1	C27-C28-C29-C2A
75	4C	306	CDL	C12-C13-C14-C15
69	3C	513	3PE	C31-C32-C33-C34
69	3E	302	3PE	C31-C32-C33-C34
75	1q	202	CDL	CA5-C11-C12-C13
69	1A	201	3PE	C22-C21-O21-C2
69	1A	203	3PE	C22-C21-O21-C2
69	1B	204	3PE	C22-C21-O21-C2
69	1f	101	3PE	C22-C21-O21-C2
69	3C	504	3PE	C22-C21-O21-C2
69	3G	102	3PE	C22-C21-O21-C2
69	3P	507	3PE	C22-C21-O21-C2
69	3R	302	3PE	C22-C21-O21-C2
69	3X	108	3PE	C22-C21-O21-C2
69	3Y	104	3PE	C22-C21-O21-C2
70	1B	203	PC1	C22-C21-O21-C2
70	1J	202	PC1	C22-C21-O21-C2
75	1N	402	CDL	C51-CB5-OB6-CB4
75	1d	202	CDL	C11-CA5-OA6-CA4
75	3P	513	CDL	C51-CB5-OB6-CB4
87	3X	102	PEK	C2-C1-O01-C02
91	4A	607	PGV	C2-C1-O01-C02
91	4N	101	PGV	C2-C1-O01-C02
69	3C	509	3PE	O11-C1-C2-O21
69	3C	510	3PE	O11-C1-C2-O21
69	3R	302	3PE	O11-C1-C2-O21
91	4G	102	PGV	O01-C02-C03-O11
85	3C	501	HEM	C4B-C3B-CAB-CBB
85	3C	502	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
85	3P	502	HEM	C4B-C3B-CAB-CBB
69	1L	706	3PE	C22-C23-C24-C25
69	3C	503	3PE	C2C-C2D-C2E-C2F
70	1Y	206	PC1	C27-C28-C29-C2A
69	1A	201	3PE	O22-C21-O21-C2
69	1B	204	3PE	O22-C21-O21-C2
69	1Y	214	3PE	O22-C21-O21-C2
69	1f	101	3PE	O22-C21-O21-C2
69	3G	102	3PE	O22-C21-O21-C2
69	3X	108	3PE	O22-C21-O21-C2
69	3Y	104	3PE	O22-C21-O21-C2
70	1J	202	PC1	O22-C21-O21-C2
91	4N	101	PGV	O02-C1-O01-C02
75	1d	205	CDL	CB5-C51-C52-C53
69	1Y	214	3PE	C35-C36-C37-C38
75	3N	502	CDL	OA6-CA4-CA6-OA8
69	1L	702	3PE	C32-C33-C34-C35
69	1k	101	3PE	C35-C36-C37-C38
70	1Y	202	PC1	C11-C12-N-C13
69	1f	101	3PE	C39-C3A-C3B-C3C
69	3G	111	3PE	C32-C33-C34-C35
70	3R	303	PC1	C25-C26-C27-C28
75	1d	205	CDL	C71-C72-C73-C74
75	3A	501	CDL	C31-C32-C33-C34
69	3P	516	3PE	C31-C32-C33-C34
75	1q	201	CDL	CB5-C51-C52-C53
69	3S	201	3PE	C34-C35-C36-C37
69	1h	204	3PE	C37-C38-C39-C3A
69	3Y	107	3PE	C23-C24-C25-C26
70	1Y	206	PC1	C35-C36-C37-C38
75	1N	402	CDL	C55-C56-C57-C58
69	3E	303	3PE	C38-C39-C3A-C3B
69	3N	503	3PE	C28-C29-C2A-C2B
75	4B	302	CDL	C31-C32-C33-C34
69	1Y	211	3PE	C32-C33-C34-C35
69	3P	506	3PE	C32-C33-C34-C35
69	3X	108	3PE	O32-C31-O31-C3
75	1d	202	CDL	OB9-CB7-OB8-CB6
75	4C	306	CDL	OA9-CA7-OA8-CA6
69	1A	203	3PE	O22-C21-O21-C2
69	3C	504	3PE	O22-C21-O21-C2
69	3P	507	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
70	1H	402	PC1	O22-C21-O21-C2
75	1N	402	CDL	OB7-CB5-OB6-CB4
91	4A	607	PGV	O02-C1-O01-C02
69	1L	701	3PE	C22-C21-O21-C2
69	1m	204	3PE	C22-C21-O21-C2
70	1H	403	PC1	C22-C21-O21-C2
69	1Y	213	3PE	C37-C38-C39-C3A
69	1Y	214	3PE	C34-C35-C36-C37
69	1d	201	3PE	C37-C38-C39-C3A
69	3G	111	3PE	C38-C39-C3A-C3B
91	4C	303	PGV	C11-C12-C13-C14
69	1B	205	3PE	C1-O11-P-O13
69	1L	706	3PE	C1-O11-P-O13
69	1Y	205	3PE	C11-O13-P-O11
69	1Y	212	3PE	C1-O11-P-O13
69	1Y	213	3PE	C11-O13-P-O11
69	1b	101	3PE	C11-O13-P-O11
69	1e	201	3PE	C11-O13-P-O11
69	1m	203	3PE	C11-O13-P-O11
69	1m	204	3PE	C1-O11-P-O13
69	3C	503	3PE	C11-O13-P-O11
69	3C	515	3PE	C11-O13-P-O11
69	3E	303	3PE	C1-O11-P-O13
69	3G	109	3PE	C11-O13-P-O11
69	3P	517	3PE	C1-O11-P-O13
69	3P	520	3PE	C1-O11-P-O13
69	3X	107	3PE	C1-O11-P-O13
69	3Y	107	3PE	C1-O11-P-O13
69	3Y	107	3PE	C11-O13-P-O11
70	1Y	206	PC1	C11-O13-P-O11
75	1H	401	CDL	CB2-OB2-PB2-OB5
75	1L	704	CDL	CB3-OB5-PB2-OB2
75	1N	402	CDL	CB2-OB2-PB2-OB5
75	1g	201	CDL	CA3-OA5-PA1-OA2
75	3D	504	CDL	CA3-OA5-PA1-OA2
75	3N	502	CDL	CA3-OA5-PA1-OA2
75	3P	513	CDL	CA2-OA2-PA1-OA5
75	4C	306	CDL	CB2-OB2-PB2-OB5
87	3X	102	PEK	C04-O12-P-O11
91	4A	609	PGV	C03-O11-P-O12
69	1N	401	3PE	C2B-C2C-C2D-C2E
75	1q	202	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
69	3C	507	3PE	C21-C22-C23-C24
75	3Y	106	CDL	CB4-CB3-OB5-PB2
69	3C	516	3PE	C38-C39-C3A-C3B
69	3Y	101	3PE	C38-C39-C3A-C3B
69	1L	711	3PE	O11-C1-C2-C3
69	1M	502	3PE	O11-C1-C2-C3
69	3G	108	3PE	O11-C1-C2-C3
69	3P	510	3PE	O11-C1-C2-C3
75	1L	704	CDL	OA5-CA3-CA4-CA6
91	4G	102	PGV	C01-C02-C03-O11
69	1L	703	3PE	C24-C25-C26-C27
69	3W	103	3PE	C2C-C2D-C2E-C2F
70	1J	202	PC1	C36-C37-C38-C39
75	3T	101	CDL	C54-C55-C56-C57
75	4C	307	CDL	C20-C21-C22-C23
88	4A	601	HEA	O11-C11-C12-C13
69	1L	701	3PE	C38-C39-C3A-C3B
69	1e	201	3PE	C29-C2A-C2B-C2C
69	3E	303	3PE	C26-C27-C28-C29
69	3Y	101	3PE	C37-C38-C39-C3A
69	1l	204	3PE	C2-C3-O31-C31
69	3P	514	3PE	C2-C3-O31-C31
69	1N	401	3PE	C2A-C2B-C2C-C2D
69	3C	509	3PE	C38-C39-C3A-C3B
69	3D	503	3PE	C3C-C3D-C3E-C3F
69	3J	101	3PE	C24-C25-C26-C27
75	1Y	217	CDL	C35-C36-C37-C38
75	1q	202	CDL	C73-C74-C75-C76
69	1l	204	3PE	C32-C33-C34-C35
69	3P	512	3PE	C34-C35-C36-C37
75	1L	704	CDL	C12-C13-C14-C15
69	3P	505	3PE	C32-C31-O31-C3
75	1g	201	CDL	CB2-C1-CA2-OA2
69	1L	701	3PE	O22-C21-O21-C2
69	3Q	504	3PE	C26-C27-C28-C29
70	1H	402	PC1	C3C-C3D-C3E-C3F
75	1d	205	CDL	C11-C12-C13-C14
69	1g	202	3PE	C25-C26-C27-C28
69	3Q	503	3PE	C23-C24-C25-C26
69	3W	101	3PE	C27-C28-C29-C2A
69	3X	101	3PE	C32-C33-C34-C35
70	1B	202	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
69	1f	103	3PE	O32-C31-O31-C3
69	3N	503	3PE	O32-C31-O31-C3
75	3Y	106	CDL	OA9-CA7-OA8-CA6
69	1l	203	3PE	C22-C23-C24-C25
69	1J	201	3PE	C1-C2-C3-O31
69	1L	705	3PE	C1-C2-C3-O31
69	1Y	201	3PE	C39-C3A-C3B-C3C
69	1Y	209	3PE	C28-C29-C2A-C2B
69	1Y	214	3PE	C1-C2-C3-O31
69	1d	203	3PE	C1-C2-C3-O31
69	3G	111	3PE	C1-C2-C3-O31
69	3J	103	3PE	C1-C2-C3-O31
69	3Y	104	3PE	C1-C2-C3-O31
70	1H	404	PC1	C1-C2-C3-O31
75	1d	205	CDL	CB3-CB4-CB6-OB8
75	3D	504	CDL	CB3-CB4-CB6-OB8
75	3N	502	CDL	CA3-CA4-CA6-OA8
75	3Y	106	CDL	CB3-CB4-CB6-OB8
69	1Y	213	3PE	C35-C36-C37-C38
69	1Z	201	3PE	C38-C39-C3A-C3B
69	1f	102	3PE	C25-C26-C27-C28
69	1Y	215	3PE	C34-C35-C36-C37
69	1d	201	3PE	C2E-C2F-C2G-C2H
70	1B	202	PC1	C25-C26-C27-C28
69	3P	505	3PE	C31-C32-C33-C34
69	1k	101	3PE	C23-C24-C25-C26
69	3P	508	3PE	C2F-C2G-C2H-C2I
69	3R	304	3PE	C39-C3A-C3B-C3C
81	1T	101	EHZ	O4-C15-C16-O5
91	4A	609	PGV	O04-C19-O03-C01
69	1L	701	3PE	C21-C22-C23-C24
69	1Y	210	3PE	C31-C32-C33-C34
69	3J	101	3PE	C21-C22-C23-C24
69	1J	201	3PE	C35-C36-C37-C38
69	1m	204	3PE	C3A-C3B-C3C-C3D
69	3P	506	3PE	C38-C39-C3A-C3B
75	1d	205	CDL	C51-CB5-OB6-CB4
75	1q	202	CDL	C51-CB5-OB6-CB4
69	3C	505	3PE	C28-C29-C2A-C2B
70	1h	203	PC1	C3B-C3C-C3D-C3E
87	4G	103	PEK	C22-C23-C24-C25
69	3S	201	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
75	3F	201	CDL	CB5-C51-C52-C53
69	1A	203	3PE	C32-C31-O31-C3
69	1L	702	3PE	C32-C31-O31-C3
69	1d	201	3PE	C3C-C3D-C3E-C3F
69	1d	206	3PE	C2D-C2E-C2F-C2G
70	1Y	207	PC1	C24-C25-C26-C27
75	1Y	217	CDL	C79-C80-C81-C82
69	1Y	216	3PE	C1-C2-O21-C21
69	3G	107	3PE	C3-C2-O21-C21
69	3J	101	3PE	C1-C2-O21-C21
69	3S	201	3PE	C1-C2-O21-C21
69	3X	106	3PE	C3-C2-O21-C21
70	1M	501	PC1	C3-C2-O21-C21
87	3X	102	PEK	C03-C02-O01-C1
75	1d	202	CDL	OA7-CA5-OA6-CA4
75	3F	201	CDL	C35-C36-C37-C38
69	1d	203	3PE	C2B-C2C-C2D-C2E
69	3C	508	3PE	C3C-C3D-C3E-C3F
69	3X	101	3PE	C3F-C3G-C3H-C3I
69	3C	509	3PE	C2-C1-O11-P
69	3P	504	3PE	C2-C1-O11-P
91	4A	607	PGV	C05-C04-O12-P
69	1A	201	3PE	C33-C34-C35-C36
70	1Y	206	PC1	C26-C27-C28-C29
70	3J	106	PC1	C2A-C2B-C2C-C2D
91	4K	101	PGV	C27-C28-C29-C30
69	3C	504	3PE	C32-C31-O31-C3
69	3P	516	3PE	C32-C31-O31-C3
87	3X	102	PEK	O04-C21-O03-C01
69	1Y	210	3PE	O11-C1-C2-O21
69	3G	109	3PE	O11-C1-C2-O21
75	1g	201	CDL	OA5-CA3-CA4-OA6
70	3X	104	PC1	C11-C12-N-C15
69	3J	104	3PE	C21-C22-C23-C24
69	1L	706	3PE	C23-C24-C25-C26
69	1Y	209	3PE	C38-C39-C3A-C3B
69	3P	510	3PE	C2D-C2E-C2F-C2G
70	1B	202	PC1	C28-C29-C2A-C2B
70	1J	202	PC1	C22-C23-C24-C25
75	3N	502	CDL	C39-C40-C41-C42
69	1A	203	3PE	C2A-C2B-C2C-C2D
69	1Y	213	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
69	1d	203	3PE	C37-C38-C39-C3A
69	1d	203	3PE	C3B-C3C-C3D-C3E
75	3X	103	CDL	O1-C1-CB2-OB2
69	1d	206	3PE	C2C-C2D-C2E-C2F
69	3C	515	3PE	C36-C37-C38-C39
75	1q	202	CDL	CB7-C71-C72-C73
69	3P	518	3PE	C27-C28-C29-C2A
69	3Q	503	3PE	C36-C37-C38-C39
69	3Y	104	3PE	C23-C24-C25-C26
69	1Y	210	3PE	O21-C2-C3-O31
69	3Q	502	3PE	O21-C2-C3-O31
69	3W	103	3PE	O21-C2-C3-O31
75	1N	402	CDL	OA6-CA4-CA6-OA8
69	3C	512	3PE	C36-C37-C38-C39
75	3T	101	CDL	C74-C75-C76-C77
69	1o	201	3PE	C33-C34-C35-C36
69	3C	515	3PE	C34-C35-C36-C37
69	3P	519	3PE	C36-C37-C38-C39
69	3R	302	3PE	C27-C28-C29-C2A
69	1L	705	3PE	C31-C32-C33-C34
69	1Y	213	3PE	C29-C2A-C2B-C2C
69	3C	509	3PE	C25-C26-C27-C28
70	3R	303	PC1	C24-C25-C26-C27
69	1A	201	3PE	C32-C31-O31-C3
70	1H	402	PC1	C32-C31-O31-C3
75	1q	201	CDL	C71-CB7-OB8-CB6
75	3X	103	CDL	C73-C74-C75-C76
75	3Y	106	CDL	C15-C16-C17-C18
69	1f	102	3PE	C35-C36-C37-C38
69	3G	102	3PE	C36-C37-C38-C39
69	1Y	213	3PE	C3B-C3C-C3D-C3E
70	3X	104	PC1	C27-C28-C29-C2A
69	3R	302	3PE	O22-C21-O21-C2
69	3G	101	3PE	C22-C21-O21-C2
75	3D	504	CDL	C51-CB5-OB6-CB4
69	3P	515	3PE	C26-C27-C28-C29
75	1d	205	CDL	C82-C83-C84-C85
69	1A	203	3PE	O32-C31-O31-C3
69	3P	505	3PE	O32-C31-O31-C3
69	1f	102	3PE	C32-C31-O31-C3
69	1f	104	3PE	C32-C31-O31-C3
69	3P	512	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	3P	515	3PE	C32-C31-O31-C3
70	1Y	206	PC1	C32-C31-O31-C3
69	1L	711	3PE	C23-C24-C25-C26
69	1d	203	3PE	C3A-C3B-C3C-C3D
75	4C	307	CDL	C18-C19-C20-C21
69	3G	104	3PE	C21-C22-C23-C24
69	3P	520	3PE	C21-C22-C23-C24
69	1Y	205	3PE	C26-C27-C28-C29
69	1m	203	3PE	C24-C25-C26-C27
75	1d	202	CDL	C40-C41-C42-C43
87	3X	102	PEK	C24-C25-C26-C27
69	1B	204	3PE	C34-C35-C36-C37
69	1J	201	3PE	C39-C3A-C3B-C3C
69	1Y	208	3PE	C35-C36-C37-C38
69	1d	201	3PE	C35-C36-C37-C38
75	1q	201	CDL	C51-C52-C53-C54
70	3P	509	PC1	C11-C12-N-C14
69	1Y	216	3PE	O11-C1-C2-C3
69	1g	203	3PE	O11-C1-C2-C3
69	1o	201	3PE	O11-C1-C2-C3
69	3C	509	3PE	O11-C1-C2-C3
69	3C	510	3PE	O11-C1-C2-C3
69	3D	502	3PE	O11-C1-C2-C3
69	3G	109	3PE	O11-C1-C2-C3
69	3R	302	3PE	O11-C1-C2-C3
75	1g	201	CDL	OB5-CB3-CB4-CB6
75	3X	103	CDL	OB5-CB3-CB4-CB6
75	3Y	106	CDL	OB5-CB3-CB4-CB6
69	3C	512	3PE	C2D-C2E-C2F-C2G
69	3Q	504	3PE	C34-C35-C36-C37
70	3T	102	PC1	C24-C25-C26-C27
75	1q	202	CDL	C39-C40-C41-C42
93	4B	303	PSC	C23-C24-C25-C26
69	1A	203	3PE	C21-C22-C23-C24
75	4C	306	CDL	CA5-C11-C12-C13
69	1f	101	3PE	O13-C11-C12-N
69	1l	202	3PE	O13-C11-C12-N
69	3P	519	3PE	O13-C11-C12-N
69	3R	302	3PE	O13-C11-C12-N
69	1L	711	3PE	C2B-C2C-C2D-C2E
69	1b	101	3PE	C32-C33-C34-C35
75	1N	402	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
69	1N	401	3PE	C3B-C3C-C3D-C3E
69	1d	201	3PE	C31-C32-C33-C34
69	3J	102	3PE	C21-C22-C23-C24
69	3P	517	3PE	C22-C23-C24-C25
70	1H	403	PC1	O22-C21-O21-C2
75	1d	205	CDL	OB7-CB5-OB6-CB4
69	1Y	201	3PE	C33-C34-C35-C36
69	3P	510	3PE	C27-C28-C29-C2A
75	3P	513	CDL	C35-C36-C37-C38
82	1Y	203	PGT	C13-C14-C15-C16
69	3C	505	3PE	C2B-C2C-C2D-C2E
69	3N	503	3PE	C26-C27-C28-C29
70	3X	104	PC1	C3B-C3C-C3D-C3E
70	3P	509	PC1	C32-C31-O31-C3
69	1L	702	3PE	C31-C32-C33-C34
75	3A	501	CDL	C59-C60-C61-C62
69	1M	502	3PE	C2-C1-O11-P
69	1Y	214	3PE	C2-C1-O11-P
69	1Y	215	3PE	C2-C1-O11-P
75	1g	201	CDL	C1-CB2-OB2-PB2
75	3Y	106	CDL	C1-CA2-OA2-PA1
75	3Y	106	CDL	CA4-CA3-OA5-PA1
75	4C	306	CDL	CB4-CB3-OB5-PB2
91	4C	304	PGV	C02-C03-O11-P
69	1d	203	3PE	C35-C36-C37-C38
69	1g	202	3PE	C2A-C2B-C2C-C2D
86	3D	501	HEC	C3D-CAD-CBD-CGD
69	1N	401	3PE	C3A-C3B-C3C-C3D
69	1Y	213	3PE	C38-C39-C3A-C3B
69	3C	511	3PE	C22-C23-C24-C25
75	1Y	217	CDL	C42-C43-C44-C45
75	1q	202	CDL	C17-C18-C19-C20
75	3T	101	CDL	C31-C32-C33-C34
69	3C	503	3PE	C36-C37-C38-C39
69	3G	106	3PE	C24-C25-C26-C27
70	1Y	206	PC1	C36-C37-C38-C39
69	3G	111	3PE	C32-C31-O31-C3
69	3P	518	3PE	C32-C31-O31-C3
69	3Y	105	3PE	C32-C31-O31-C3
91	4J	101	PGV	C20-C19-O03-C01
69	1L	708	3PE	C1-C2-C3-O31
69	3C	510	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
75	1L	704	CDL	CB3-CB4-CB6-OB8
75	1N	402	CDL	CB3-CB4-CB6-OB8
75	3T	101	CDL	CB3-CB4-CB6-OB8
69	3C	507	3PE	C2C-C2D-C2E-C2F
69	1f	104	3PE	C26-C27-C28-C29
69	1m	201	3PE	C3B-C3C-C3D-C3E
69	3A	503	3PE	C29-C2A-C2B-C2C
69	3Y	102	3PE	C33-C34-C35-C36
82	1Y	203	PGT	C45-C46-C47-C48
69	1M	502	3PE	C22-C23-C24-C25
69	1m	203	3PE	C35-C36-C37-C38
69	3P	508	3PE	C3B-C3C-C3D-C3E
69	3R	305	3PE	C22-C23-C24-C25
75	3N	502	CDL	C80-C81-C82-C83
81	1n	201	EHZ	N2-C15-C16-C17
82	1Y	203	PGT	C31-C32-C33-C34
69	3P	515	3PE	C2C-C2D-C2E-C2F
69	1L	711	3PE	C26-C27-C28-C29
69	3W	102	3PE	C3B-C3C-C3D-C3E
70	3P	509	PC1	C35-C36-C37-C38
69	1l	203	3PE	C26-C27-C28-C29
69	3J	101	3PE	C35-C36-C37-C38
70	1M	501	PC1	C29-C2A-C2B-C2C
69	1e	201	3PE	C1-O11-P-O13
69	3P	507	3PE	C1-O11-P-O13
69	3P	516	3PE	C11-O13-P-O11
75	1N	402	CDL	CA3-OA5-PA1-OA2
75	1d	205	CDL	CB3-OB5-PB2-OB2
87	4G	103	PEK	C9-C10-C11-C12
87	4G	103	PEK	C12-C13-C14-C15
91	4K	101	PGV	C04-O12-P-O11
93	4B	303	PSC	C9-C10-C11-C12
69	3P	507	3PE	C21-C22-C23-C24
69	1L	702	3PE	O32-C31-O31-C3
69	3P	516	3PE	O32-C31-O31-C3
70	3P	509	PC1	C38-C39-C3A-C3B
69	3P	520	3PE	C34-C35-C36-C37
69	3R	305	3PE	C3B-C3C-C3D-C3E
69	1Y	216	3PE	O11-C1-C2-O21
69	1o	201	3PE	O11-C1-C2-O21
69	3D	502	3PE	O11-C1-C2-O21
70	1M	501	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
75	1Y	217	CDL	OB5-CB3-CB4-OB6
75	3P	513	CDL	OB7-CB5-OB6-CB4
69	1B	205	3PE	C37-C38-C39-C3A
69	3E	303	3PE	C39-C3A-C3B-C3C
75	1d	205	CDL	C60-C61-C62-C63
75	3X	103	CDL	C77-C78-C79-C80
69	1d	206	3PE	C31-C32-C33-C34
69	3G	103	3PE	C21-C22-C23-C24
69	1Y	213	3PE	C3E-C3F-C3G-C3H
69	3C	505	3PE	C39-C3A-C3B-C3C
69	3D	503	3PE	C24-C25-C26-C27
70	1h	203	PC1	C24-C25-C26-C27
69	1L	708	3PE	C22-C23-C24-C25
69	1A	201	3PE	O32-C31-O31-C3
69	1L	702	3PE	C23-C24-C25-C26
69	1Y	210	3PE	C32-C33-C34-C35
69	3J	101	3PE	C28-C29-C2A-C2B
69	1Y	214	3PE	O21-C2-C3-O31
69	1g	202	3PE	O21-C2-C3-O31
69	1l	202	3PE	O21-C2-C3-O31
69	3P	506	3PE	O21-C2-C3-O31
69	3R	302	3PE	O21-C2-C3-O31
69	3X	101	3PE	O21-C2-C3-O31
69	3X	108	3PE	O21-C2-C3-O31
75	1H	401	CDL	OA6-CA4-CA6-OA8
75	1N	402	CDL	OB6-CB4-CB6-OB8
75	1g	201	CDL	OA6-CA4-CA6-OA8
75	3D	504	CDL	OB6-CB4-CB6-OB8
69	1Y	216	3PE	C26-C27-C28-C29
75	3A	501	CDL	C83-C84-C85-C86
69	3Y	105	3PE	C22-C21-O21-C2
69	1g	202	3PE	C37-C38-C39-C3A
69	3R	302	3PE	C3A-C3B-C3C-C3D
82	1Y	203	PGT	C18-C19-C20-C21
69	1g	203	3PE	O22-C21-O21-C2
69	1m	204	3PE	O22-C21-O21-C2
75	1q	202	CDL	OB7-CB5-OB6-CB4
75	3D	504	CDL	OB7-CB5-OB6-CB4
69	1M	502	3PE	C2D-C2E-C2F-C2G
69	1f	101	3PE	C35-C36-C37-C38
69	3E	302	3PE	C24-C25-C26-C27
75	3A	501	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
69	3C	504	3PE	O32-C31-O31-C3
69	1N	401	3PE	C29-C2A-C2B-C2C
69	1Y	213	3PE	C3D-C3E-C3F-C3G
69	1Y	215	3PE	C24-C25-C26-C27
69	3R	304	3PE	C27-C28-C29-C2A
75	1d	202	CDL	C14-C15-C16-C17
69	1e	201	3PE	C3E-C3F-C3G-C3H
69	1A	203	3PE	C2-C1-O11-P
69	1f	104	3PE	C2-C1-O11-P
69	1l	203	3PE	C2-C1-O11-P
69	1m	201	3PE	C2-C1-O11-P
69	3A	503	3PE	C2-C1-O11-P
69	3C	504	3PE	C2-C1-O11-P
69	3C	511	3PE	C2-C1-O11-P
69	3J	103	3PE	C2-C1-O11-P
69	3N	501	3PE	C2-C1-O11-P
69	3P	515	3PE	C2-C1-O11-P
69	3P	516	3PE	C2-C1-O11-P
69	3W	101	3PE	C2-C1-O11-P
69	3W	103	3PE	C2-C1-O11-P
75	1q	202	CDL	C1-CA2-OA2-PA1
75	3F	201	CDL	CB4-CB3-OB5-PB2
75	3P	513	CDL	C1-CB2-OB2-PB2
75	3X	103	CDL	CA4-CA3-OA5-PA1
75	4C	306	CDL	CA4-CA3-OA5-PA1
82	1Y	203	PGT	C5-C4-O4P-P
91	4C	304	PGV	C05-C04-O12-P
91	4N	101	PGV	C02-C03-O11-P
69	3P	518	3PE	O32-C31-O31-C3
75	1q	201	CDL	OB9-CB7-OB8-CB6
69	1f	104	3PE	C35-C36-C37-C38
69	3X	106	3PE	C39-C3A-C3B-C3C
70	1H	402	PC1	C24-C25-C26-C27
69	1m	201	3PE	C33-C34-C35-C36
69	3X	101	3PE	C24-C25-C26-C27
75	3D	504	CDL	C52-C53-C54-C55
69	3E	303	3PE	C29-C2A-C2B-C2C
75	1d	205	CDL	C15-C16-C17-C18
69	3A	502	3PE	C24-C25-C26-C27
69	3C	510	3PE	C29-C2A-C2B-C2C
69	1L	710	3PE	C31-C32-C33-C34
85	3C	501	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
69	3G	101	3PE	O22-C21-O21-C2
69	1g	203	3PE	C22-C21-O21-C2
69	3E	303	3PE	C24-C25-C26-C27
69	1L	712	3PE	C34-C35-C36-C37
69	3P	520	3PE	C2C-C2D-C2E-C2F
70	3J	106	PC1	C26-C27-C28-C29
69	1J	203	3PE	C32-C33-C34-C35
69	3P	507	3PE	C25-C26-C27-C28
69	1L	701	3PE	O11-C1-C2-C3
69	1Y	210	3PE	O11-C1-C2-C3
69	1k	101	3PE	O11-C1-C2-C3
69	3C	503	3PE	O11-C1-C2-C3
69	3N	501	3PE	O11-C1-C2-C3
70	3X	104	PC1	O11-C1-C2-C3
75	1g	201	CDL	OA5-CA3-CA4-CA6
75	3F	201	CDL	OB5-CB3-CB4-CB6
69	1L	702	3PE	C3F-C3G-C3H-C3I
69	3C	506	3PE	C38-C39-C3A-C3B
69	3E	302	3PE	C32-C33-C34-C35
69	3Q	503	3PE	C37-C38-C39-C3A
69	1f	102	3PE	O32-C31-O31-C3
69	1L	705	3PE	C37-C38-C39-C3A
75	3N	502	CDL	C40-C41-C42-C43
69	1Y	210	3PE	C25-C26-C27-C28
70	1Y	202	PC1	C23-C24-C25-C26
69	3R	302	3PE	C35-C36-C37-C38
69	3W	102	3PE	C36-C37-C38-C39
70	1B	203	PC1	C35-C36-C37-C38
70	3R	303	PC1	C32-C33-C34-C35
69	1f	104	3PE	O32-C31-O31-C3
69	3P	512	3PE	O32-C31-O31-C3
69	1Y	213	3PE	C24-C25-C26-C27
69	1Y	214	3PE	C33-C34-C35-C36
69	3R	305	3PE	C2D-C2E-C2F-C2G
69	1B	204	3PE	C33-C34-C35-C36
75	3A	501	CDL	CB7-C71-C72-C73
69	3Y	107	3PE	C2C-C2D-C2E-C2F
69	3Y	104	3PE	C27-C28-C29-C2A
69	3C	506	3PE	C32-C33-C34-C35
69	3A	502	3PE	C25-C26-C27-C28
69	3P	505	3PE	C24-C25-C26-C27
69	3Q	502	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
69	1Y	213	3PE	C3-C2-O21-C21
69	1f	101	3PE	C3-C2-O21-C21
69	3C	510	3PE	C3-C2-O21-C21
69	3C	513	3PE	C1-C2-O21-C21
69	3G	102	3PE	C3-C2-O21-C21
69	3G	103	3PE	C1-C2-O21-C21
69	3G	111	3PE	C1-C2-O21-C21
69	3P	514	3PE	C1-C2-O21-C21
69	3W	103	3PE	C1-C2-O21-C21
75	1L	704	CDL	CB6-CB4-OB6-CB5
91	4C	303	PGV	C01-C02-O01-C1
69	1A	201	3PE	C28-C29-C2A-C2B
69	3J	104	3PE	C33-C34-C35-C36
82	1Y	203	PGT	C21-C22-C23-C24
69	3C	511	3PE	C36-C37-C38-C39
69	3C	515	3PE	C32-C31-O31-C3
70	1H	403	PC1	C32-C31-O31-C3
69	3T	103	3PE	C3B-C3C-C3D-C3E
69	3E	302	3PE	C3A-C3B-C3C-C3D
69	3G	105	3PE	C24-C25-C26-C27
75	3T	101	CDL	CA7-C31-C32-C33
69	1L	710	3PE	C2-C1-O11-P
69	1l	202	3PE	C1-C2-C3-O31
69	1l	204	3PE	C2-C1-O11-P
69	3E	302	3PE	C1-C2-C3-O31
69	3P	517	3PE	C1-C2-C3-O31
69	3Q	502	3PE	C1-C2-C3-O31
69	3R	302	3PE	C1-C2-C3-O31
69	3X	101	3PE	C1-C2-C3-O31
75	1g	201	CDL	CA3-CA4-CA6-OA8
75	1i	201	CDL	CB3-CB4-CB6-OB8
75	1q	202	CDL	CB3-CB4-CB6-OB8
75	3N	502	CDL	CB4-CB3-OB5-PB2
75	4C	307	CDL	CA4-CA3-OA5-PA1
75	4C	307	CDL	CB4-CB3-OB5-PB2
91	4K	101	PGV	C02-C03-O11-P
69	3R	304	3PE	C22-C21-O21-C2
87	4G	103	PEK	C2-C1-O01-C02
69	1L	701	3PE	O11-C1-C2-O21
69	1Y	209	3PE	O11-C1-C2-O21
69	1g	203	3PE	O11-C1-C2-O21
69	1k	101	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
69	3C	503	3PE	O11-C1-C2-O21
69	3C	507	3PE	O11-C1-C2-O21
69	3N	501	3PE	O11-C1-C2-O21
69	3P	510	3PE	O11-C1-C2-O21
70	1h	203	PC1	O11-C1-C2-O21
70	3X	104	PC1	O11-C1-C2-O21
75	1H	401	CDL	OA5-CA3-CA4-OA6
75	1L	704	CDL	OA5-CA3-CA4-OA6
75	1L	704	CDL	OB5-CB3-CB4-OB6
75	1g	201	CDL	OB5-CB3-CB4-OB6
75	1q	202	CDL	OA5-CA3-CA4-OA6
69	1m	201	3PE	C3C-C3D-C3E-C3F
69	3J	101	3PE	C23-C24-C25-C26
85	3P	501	HEM	C4B-C3B-CAB-CBB
69	1d	203	3PE	C39-C3A-C3B-C3C
69	3A	503	3PE	C3D-C3E-C3F-C3G
69	3C	506	3PE	C26-C27-C28-C29
69	3C	511	3PE	C29-C2A-C2B-C2C
69	3P	511	3PE	C22-C23-C24-C25
69	1L	711	3PE	C35-C36-C37-C38
69	1h	204	3PE	C32-C33-C34-C35
69	3Y	105	3PE	O22-C21-O21-C2
69	1m	204	3PE	C3C-C3D-C3E-C3F
69	1m	205	3PE	C3F-C3G-C3H-C3I
69	3G	111	3PE	O32-C31-O31-C3
69	3P	515	3PE	O32-C31-O31-C3
69	3Y	105	3PE	O32-C31-O31-C3
70	1H	402	PC1	O32-C31-O31-C3
70	1Y	206	PC1	O32-C31-O31-C3
70	3P	509	PC1	O32-C31-O31-C3
69	1L	712	3PE	C26-C27-C28-C29
75	3N	502	CDL	C61-C62-C63-C64
91	4C	302	PGV	C25-C26-C27-C28
69	1M	502	3PE	O21-C2-C3-O31
69	3E	302	3PE	O21-C2-C3-O31
70	1H	404	PC1	O21-C2-C3-O31
75	1L	704	CDL	OB6-CB4-CB6-OB8
75	1d	205	CDL	OB6-CB4-CB6-OB8
69	3D	502	3PE	C28-C29-C2A-C2B
69	3J	101	3PE	C38-C39-C3A-C3B
75	3P	513	CDL	C72-C73-C74-C75
91	4A	607	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
69	3C	510	3PE	C23-C24-C25-C26
75	1L	704	CDL	C37-C38-C39-C40
70	3X	104	PC1	C11-C12-N-C13
69	1b	101	3PE	C23-C24-C25-C26
69	3C	509	3PE	C2C-C2D-C2E-C2F
69	3P	506	3PE	C36-C37-C38-C39
69	3P	516	3PE	C3A-C3B-C3C-C3D
69	3R	302	3PE	C3D-C3E-C3F-C3G
91	4J	101	PGV	O04-C19-O03-C01
69	3A	503	3PE	C3E-C3F-C3G-C3H
69	3R	304	3PE	O22-C21-O21-C2
87	4G	103	PEK	O02-C1-O01-C02
91	4G	102	PGV	O02-C1-O01-C02
69	1L	702	3PE	C39-C3A-C3B-C3C
69	1L	711	3PE	C27-C28-C29-C2A
75	1Y	217	CDL	C55-C56-C57-C58
75	3A	501	CDL	C19-C20-C21-C22
75	3X	103	CDL	C82-C83-C84-C85
75	4C	306	CDL	C19-C20-C21-C22
69	3E	302	3PE	C2E-C2F-C2G-C2H
75	1L	704	CDL	C56-C57-C58-C59
69	1B	204	3PE	C2E-C2F-C2G-C2H
69	3P	508	3PE	C2A-C2B-C2C-C2D
75	1H	401	CDL	C51-C52-C53-C54
69	1L	712	3PE	C36-C37-C38-C39
69	1e	201	3PE	C2A-C2B-C2C-C2D
69	3N	501	3PE	C22-C23-C24-C25
69	3J	101	3PE	C26-C27-C28-C29
75	3P	513	CDL	C62-C63-C64-C65
83	1h	201	AME	C-CA-N-CT1
70	3P	509	PC1	C3D-C3E-C3F-C3G
69	3A	503	3PE	C26-C27-C28-C29
69	3Y	101	3PE	C2E-C2F-C2G-C2H
75	1d	205	CDL	C54-C55-C56-C57
69	1Y	211	3PE	C11-O13-P-O11
69	3C	506	3PE	C1-O11-P-O13
69	3G	101	3PE	C1-O11-P-O13
69	3G	101	3PE	C11-O13-P-O11
69	3R	305	3PE	C1-O11-P-O13
69	3Y	104	3PE	C1-O11-P-O13
70	1J	202	PC1	C1-O11-P-O13
70	3R	303	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
75	1Y	217	CDL	CA3-OA5-PA1-OA2
75	1Y	217	CDL	CB2-OB2-PB2-OB5
75	1Y	217	CDL	CB3-OB5-PB2-OB2
75	1q	201	CDL	CA2-OA2-PA1-OA5
75	1q	201	CDL	CA3-OA5-PA1-OA2
75	1q	202	CDL	CB2-OB2-PB2-OB5
82	1Y	203	PGT	C4-O4P-P-O3P
91	4N	101	PGV	C03-O11-P-O12
93	4B	303	PSC	C04-O12-P-O11
69	1L	705	3PE	C33-C34-C35-C36
69	1L	710	3PE	C32-C33-C34-C35
69	3C	508	3PE	C23-C24-C25-C26
87	4G	103	PEK	C26-C27-C28-C29
69	3A	502	3PE	C39-C3A-C3B-C3C
69	3A	502	3PE	C2C-C2D-C2E-C2F
69	1Y	201	3PE	C2-C1-O11-P
69	1Y	209	3PE	C2-C1-O11-P
69	1Y	210	3PE	C2-C1-O11-P
69	3C	503	3PE	C2-C1-O11-P
69	3G	108	3PE	C2-C1-O11-P
69	3N	503	3PE	C2-C1-O11-P
69	3P	506	3PE	C2-C1-O11-P
69	3P	507	3PE	C2-C1-O11-P
69	3R	304	3PE	C2-C1-O11-P
69	4G	101	3PE	C2-C1-O11-P
73	1F	501	FMN	C4'-C5'-O5'-P
91	4A	607	PGV	C02-C03-O11-P
91	4A	608	PGV	C02-C03-O11-P
91	4G	102	PGV	C05-C04-O12-P
70	3X	104	PC1	C2A-C2B-C2C-C2D
75	1g	201	CDL	C22-C23-C24-C25
70	1H	403	PC1	O32-C31-O31-C3
69	1B	204	3PE	C1-O11-P-O12
69	1B	205	3PE	C1-O11-P-O12
69	1J	201	3PE	C11-O13-P-O12
69	1J	201	3PE	C11-O13-P-O14
69	1L	703	3PE	C1-O11-P-O12
69	1L	703	3PE	C1-O11-P-O14
69	1L	703	3PE	C11-O13-P-O12
69	1L	706	3PE	C11-O13-P-O14
69	1L	708	3PE	C1-O11-P-O12
69	1L	709	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
69	1L	709	3PE	C11-O13-P-O14
69	1L	712	3PE	C1-O11-P-O14
69	1M	502	3PE	C1-O11-P-O14
69	1M	502	3PE	C11-O13-P-O12
69	1Y	205	3PE	C1-O11-P-O12
69	1Y	205	3PE	C11-O13-P-O12
69	1Y	209	3PE	C1-O11-P-O14
69	1Y	210	3PE	C1-O11-P-O14
69	1Y	211	3PE	C11-O13-P-O14
69	1Y	212	3PE	C1-O11-P-O12
69	1Y	213	3PE	C1-O11-P-O12
69	1Y	215	3PE	C1-O11-P-O12
69	1Y	215	3PE	C11-O13-P-O12
69	1Y	215	3PE	C11-O13-P-O14
69	1d	201	3PE	C11-O13-P-O12
69	1d	206	3PE	C11-O13-P-O12
69	1e	201	3PE	C11-O13-P-O12
69	1f	101	3PE	C1-O11-P-O14
69	1f	101	3PE	C11-O13-P-O12
69	1f	103	3PE	C11-O13-P-O14
69	1f	104	3PE	C1-O11-P-O14
69	1g	203	3PE	C1-O11-P-O14
69	1k	101	3PE	C1-O11-P-O14
69	1l	203	3PE	C11-O13-P-O12
69	1m	201	3PE	C1-O11-P-O14
69	1m	204	3PE	C1-O11-P-O12
69	1m	204	3PE	C1-O11-P-O14
69	1m	205	3PE	C11-O13-P-O14
69	3A	502	3PE	C11-O13-P-O14
69	3C	503	3PE	C11-O13-P-O12
69	3C	503	3PE	C11-O13-P-O14
69	3C	505	3PE	C1-O11-P-O14
69	3C	506	3PE	C1-O11-P-O12
69	3C	508	3PE	C11-O13-P-O14
69	3C	509	3PE	C1-O11-P-O14
69	3C	510	3PE	C1-O11-P-O12
69	3C	511	3PE	C1-O11-P-O14
69	3C	512	3PE	C1-O11-P-O12
69	3C	512	3PE	C1-O11-P-O14
69	3C	513	3PE	C1-O11-P-O14
69	3C	514	3PE	C1-O11-P-O14
69	3C	515	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	3C	516	3PE	C11-O13-P-O12
69	3D	502	3PE	C1-O11-P-O14
69	3D	503	3PE	C11-O13-P-O14
69	3E	302	3PE	C1-O11-P-O14
69	3E	303	3PE	C1-O11-P-O12
69	3E	303	3PE	C11-O13-P-O12
69	3E	303	3PE	C11-O13-P-O14
69	3G	102	3PE	C1-O11-P-O14
69	3G	103	3PE	C1-O11-P-O12
69	3G	103	3PE	C1-O11-P-O14
69	3G	104	3PE	C1-O11-P-O12
69	3G	106	3PE	C1-O11-P-O12
69	3G	108	3PE	C1-O11-P-O12
69	3G	109	3PE	C1-O11-P-O12
69	3G	111	3PE	C1-O11-P-O12
69	3J	101	3PE	C11-O13-P-O14
69	3J	102	3PE	C1-O11-P-O14
69	3J	102	3PE	C11-O13-P-O14
69	3J	103	3PE	C1-O11-P-O12
69	3J	103	3PE	C11-O13-P-O12
69	3J	104	3PE	C1-O11-P-O12
69	3N	503	3PE	C11-O13-P-O14
69	3P	503	3PE	C1-O11-P-O12
69	3P	504	3PE	C11-O13-P-O14
69	3P	508	3PE	C11-O13-P-O14
69	3P	510	3PE	C1-O11-P-O12
69	3P	515	3PE	C1-O11-P-O12
69	3P	516	3PE	C1-O11-P-O12
69	3P	519	3PE	C1-O11-P-O12
69	3P	519	3PE	C1-O11-P-O14
69	3P	520	3PE	C1-O11-P-O12
69	3Q	504	3PE	C1-O11-P-O12
69	3Q	504	3PE	C1-O11-P-O14
69	3Q	504	3PE	C11-O13-P-O12
69	3R	304	3PE	C1-O11-P-O12
69	3R	304	3PE	C1-O11-P-O14
69	3S	201	3PE	C1-O11-P-O12
69	3S	201	3PE	C11-O13-P-O14
69	3T	103	3PE	C1-O11-P-O14
69	3T	103	3PE	C11-O13-P-O14
69	3W	102	3PE	C11-O13-P-O12
69	3X	101	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
69	3X	106	3PE	C1-O11-P-O12
69	3X	108	3PE	C11-O13-P-O12
69	3X	108	3PE	C11-O13-P-O14
69	3Y	104	3PE	C11-O13-P-O12
69	3Y	104	3PE	C11-O13-P-O14
69	3Y	107	3PE	C1-O11-P-O12
69	3Y	107	3PE	C11-O13-P-O12
69	4G	101	3PE	C11-O13-P-O14
70	1B	202	PC1	C1-O11-P-O12
70	1B	202	PC1	C11-C12-N-C13
70	1B	202	PC1	C11-C12-N-C15
70	1B	203	PC1	C11-O13-P-O12
70	1M	501	PC1	C11-O13-P-O12
70	1d	204	PC1	C1-O11-P-O12
70	1h	203	PC1	C11-O13-P-O14
70	3J	106	PC1	C1-O11-P-O12
70	3P	509	PC1	C11-O13-P-O14
70	3R	303	PC1	C11-O13-P-O14
70	3T	102	PC1	C11-O13-P-O14
70	3T	102	PC1	C1-O11-P-O14
75	1L	704	CDL	CA2-OA2-PA1-OA3
75	1L	704	CDL	CB3-OB5-PB2-OB4
75	1N	402	CDL	CA2-OA2-PA1-OA3
75	1N	402	CDL	CA3-OA5-PA1-OA3
75	1N	402	CDL	CB2-OB2-PB2-OB3
75	1Y	217	CDL	CA2-OA2-PA1-OA4
75	1d	202	CDL	CA3-OA5-PA1-OA3
75	1d	202	CDL	CB2-OB2-PB2-OB4
75	1d	205	CDL	CA2-OA2-PA1-OA3
75	1d	205	CDL	CA2-OA2-PA1-OA4
75	1d	205	CDL	CA3-OA5-PA1-OA4
75	1d	205	CDL	CB3-OB5-PB2-OB4
75	1q	201	CDL	CA2-OA2-PA1-OA3
75	3A	501	CDL	CB2-OB2-PB2-OB4
75	3D	504	CDL	CA3-OA5-PA1-OA3
75	3D	504	CDL	CA3-OA5-PA1-OA4
75	3D	504	CDL	CB2-OB2-PB2-OB4
75	3F	201	CDL	CA2-OA2-PA1-OA3
75	3F	201	CDL	CB2-OB2-PB2-OB3
75	3N	502	CDL	CA3-OA5-PA1-OA3
75	3N	502	CDL	CB3-OB5-PB2-OB3
75	3P	513	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
75	3X	103	CDL	CA3-OA5-PA1-OA4
75	3Y	106	CDL	CA2-OA2-PA1-OA3
75	4B	302	CDL	CB2-OB2-PB2-OB3
75	4C	307	CDL	CB2-OB2-PB2-OB3
75	4C	307	CDL	CB3-OB5-PB2-OB4
82	1Y	203	PGT	C4-O4P-P-O1P
87	3X	102	PEK	C04-O12-P-O13
91	4A	606	PGV	C03-O11-P-O13
91	4A	607	PGV	C04-O12-P-O14
91	4A	609	PGV	C03-O11-P-O14
91	4A	609	PGV	C04-O12-P-O13
91	4C	302	PGV	C04-O12-P-O13
91	4C	303	PGV	C04-O12-P-O13
91	4C	305	PGV	C03-O11-P-O13
91	4J	101	PGV	C03-O11-P-O14
91	4K	101	PGV	C03-O11-P-O14
69	1B	204	3PE	C36-C37-C38-C39
69	1Y	214	3PE	C39-C3A-C3B-C3C
69	1m	201	3PE	C2D-C2E-C2F-C2G
69	1N	401	3PE	O11-C1-C2-C3
69	1Y	209	3PE	O11-C1-C2-C3
69	3C	505	3PE	O11-C1-C2-C3
69	3C	507	3PE	O11-C1-C2-C3
69	3G	101	3PE	O11-C1-C2-C3
69	3P	514	3PE	O11-C1-C2-C3
70	1B	203	PC1	O11-C1-C2-C3
70	1M	501	PC1	O11-C1-C2-C3
75	1H	401	CDL	OA5-CA3-CA4-CA6
75	3F	201	CDL	C59-C60-C61-C62
69	1Y	209	3PE	O13-C11-C12-N
69	1g	203	3PE	C34-C35-C36-C37
69	1l	204	3PE	C3D-C3E-C3F-C3G
69	3C	515	3PE	C28-C29-C2A-C2B
69	3G	109	3PE	C32-C33-C34-C35
69	1l	204	3PE	C27-C28-C29-C2A
70	1Y	207	PC1	C3C-C3D-C3E-C3F
69	3C	510	3PE	C25-C26-C27-C28
75	3P	513	CDL	C20-C21-C22-C23
69	1A	203	3PE	C12-C11-O13-P
69	1Y	213	3PE	C12-C11-O13-P
69	1d	206	3PE	C12-C11-O13-P
69	1o	201	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
69	3G	105	3PE	C12-C11-O13-P
69	3J	102	3PE	C12-C11-O13-P
69	3Q	502	3PE	C12-C11-O13-P
69	3Q	503	3PE	C12-C11-O13-P
69	4G	101	3PE	C12-C11-O13-P
70	1A	202	PC1	C12-C11-O13-P
70	1H	404	PC1	C12-C11-O13-P
70	1J	202	PC1	C12-C11-O13-P
69	1l	202	3PE	C31-C32-C33-C34
69	3J	104	3PE	C2B-C2C-C2D-C2E
69	3N	503	3PE	C34-C35-C36-C37
75	1d	202	CDL	C58-C59-C60-C61
69	1J	201	3PE	C2A-C2B-C2C-C2D
69	1L	705	3PE	C28-C29-C2A-C2B
69	3W	103	3PE	C27-C28-C29-C2A
69	3A	503	3PE	C31-C32-C33-C34
70	3T	102	PC1	C31-C32-C33-C34
75	1L	704	CDL	CA5-C11-C12-C13
75	1d	202	CDL	CB5-C51-C52-C53
69	1N	401	3PE	C33-C34-C35-C36
69	1Y	208	3PE	C23-C24-C25-C26
70	1B	202	PC1	C32-C31-O31-C3
75	1L	704	CDL	C31-CA7-OA8-CA6
70	1h	202	PC1	C29-C2A-C2B-C2C
75	4B	302	CDL	C13-C14-C15-C16
75	4C	306	CDL	C54-C55-C56-C57
69	1N	401	3PE	O11-C1-C2-O21
69	1d	201	3PE	O11-C1-C2-O21
69	1e	201	3PE	C31-C32-C33-C34
69	3P	503	3PE	O11-C1-C2-O21
70	1B	203	PC1	O11-C1-C2-O21
73	1F	501	FMN	N10-C1'-C2'-O2'
75	3F	201	CDL	OB5-CB3-CB4-OB6
75	3X	103	CDL	OB5-CB3-CB4-OB6
75	3Y	106	CDL	OB5-CB3-CB4-OB6
75	1N	402	CDL	C54-C55-C56-C57
69	3C	506	3PE	C36-C37-C38-C39
75	1q	202	CDL	C19-C20-C21-C22
69	3G	106	3PE	C33-C34-C35-C36
69	3P	519	3PE	C28-C29-C2A-C2B
91	4G	102	PGV	C2-C1-O01-C02
69	3E	302	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
69	3P	510	3PE	C32-C33-C34-C35
69	3Y	104	3PE	C25-C26-C27-C28
75	1d	205	CDL	C62-C63-C64-C65
69	3C	515	3PE	O32-C31-O31-C3
70	1B	202	PC1	O32-C31-O31-C3
81	1T	101	EHZ	C10-C11-N1-C12
81	1n	201	EHZ	C10-C11-N1-C12
69	3E	303	3PE	C32-C33-C34-C35
75	3N	502	CDL	C55-C56-C57-C58
75	3Y	106	CDL	C81-C82-C83-C84
91	4C	304	PGV	C4-C5-C6-C7
70	3R	303	PC1	C11-C12-N-C14
69	1L	701	3PE	C32-C33-C34-C35
69	1Y	210	3PE	C1-C2-C3-O31
69	1Z	201	3PE	C32-C33-C34-C35
69	1k	101	3PE	C1-C2-C3-O31
69	3P	505	3PE	C1-C2-C3-O31
69	3P	506	3PE	C1-C2-C3-O31
69	3W	103	3PE	C1-C2-C3-O31
69	3X	105	3PE	C3E-C3F-C3G-C3H
70	1B	203	PC1	O13-C11-C12-N
70	1H	404	PC1	O13-C11-C12-N
70	1J	202	PC1	O13-C11-C12-N
70	3T	102	PC1	O13-C11-C12-N
75	1N	402	CDL	CA3-CA4-CA6-OA8
75	1N	402	CDL	C77-C78-C79-C80
69	1L	708	3PE	O21-C2-C3-O31
69	1d	203	3PE	O21-C2-C3-O31
69	1f	101	3PE	O21-C2-C3-O31
69	3P	505	3PE	O21-C2-C3-O31
69	3Y	104	3PE	O21-C2-C3-O31
70	1B	203	PC1	O21-C2-C3-O31
75	1i	201	CDL	OB6-CB4-CB6-OB8
69	1o	201	3PE	C28-C29-C2A-C2B
69	3P	518	3PE	C2C-C2D-C2E-C2F
69	1N	401	3PE	C3E-C3F-C3G-C3H
69	1Y	213	3PE	C2E-C2F-C2G-C2H
70	1B	203	PC1	C28-C29-C2A-C2B
69	3J	103	3PE	C3E-C3F-C3G-C3H
75	1d	202	CDL	C32-C33-C34-C35
69	3P	514	3PE	C34-C35-C36-C37
69	1L	711	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
69	3Y	102	3PE	C2-C1-O11-P
75	1N	402	CDL	C1-CB2-OB2-PB2
75	1g	201	CDL	CA4-CA3-OA5-PA1
91	4C	303	PGV	C02-C03-O11-P
69	3X	107	3PE	C36-C37-C38-C39
69	1J	203	3PE	C23-C24-C25-C26
69	1Y	214	3PE	C3B-C3C-C3D-C3E
69	1g	202	3PE	C2B-C2C-C2D-C2E
75	1d	202	CDL	C23-C24-C25-C26
75	4C	307	CDL	CB4-CB6-OB8-CB7
69	1M	502	3PE	C2B-C2C-C2D-C2E
69	1Y	215	3PE	C29-C2A-C2B-C2C
75	4C	306	CDL	C22-C23-C24-C25
91	4C	305	PGV	C6-C7-C8-C9
69	3C	512	3PE	C38-C39-C3A-C3B
75	3A	501	CDL	C78-C79-C80-C81
69	3A	502	3PE	C3B-C3C-C3D-C3E
69	3C	505	3PE	C34-C35-C36-C37
69	3P	515	3PE	C22-C23-C24-C25
69	3X	101	3PE	C3E-C3F-C3G-C3H
75	1L	704	CDL	OA9-CA7-OA8-CA6
69	3Q	503	3PE	C2E-C2F-C2G-C2H
69	1L	702	3PE	C3A-C3B-C3C-C3D
69	1L	705	3PE	C2E-C2F-C2G-C2H
70	3T	102	PC1	C3C-C3D-C3E-C3F
75	4C	307	CDL	C15-C16-C17-C18
70	1P	502	PC1	C11-C12-N-C15
70	3P	509	PC1	C11-C12-N-C13
69	3Y	101	3PE	C33-C34-C35-C36
69	1A	203	3PE	C29-C2A-C2B-C2C
69	1B	204	3PE	C27-C28-C29-C2A
69	3J	105	3PE	C29-C2A-C2B-C2C
70	3R	303	PC1	C39-C3A-C3B-C3C
75	1Y	217	CDL	OB7-CB5-OB6-CB4
69	1Y	213	3PE	C25-C26-C27-C28
69	3W	103	3PE	C39-C3A-C3B-C3C
79	1P	501	NDP	O4D-C4D-C5D-O5D
69	1m	203	3PE	C2B-C2C-C2D-C2E
69	3R	305	3PE	C34-C35-C36-C37
75	3X	103	CDL	C12-C13-C14-C15
69	1l	204	3PE	C28-C29-C2A-C2B
69	3X	108	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
69	3G	110	3PE	C29-C2A-C2B-C2C
70	1d	204	PC1	C2-C3-O31-C31
69	1m	202	3PE	C2A-C2B-C2C-C2D
69	3P	512	3PE	C35-C36-C37-C38
69	1L	707	3PE	C34-C35-C36-C37
70	1h	203	PC1	C23-C24-C25-C26
69	3A	503	3PE	C3A-C3B-C3C-C3D
69	3P	519	3PE	C38-C39-C3A-C3B
69	3R	304	3PE	C3B-C3C-C3D-C3E
81	1T	101	EHZ	C21-C22-C23-C24
91	4C	305	PGV	C7-C8-C9-C10
69	1L	703	3PE	C3-C2-O21-C21
69	1L	710	3PE	C1-C2-O21-C21
69	1Y	205	3PE	C3-C2-O21-C21
69	1Y	209	3PE	C1-C2-O21-C21
69	1g	203	3PE	C1-C2-O21-C21
69	1h	204	3PE	C3-C2-O21-C21
69	1l	202	3PE	C3-C2-O21-C21
69	1l	204	3PE	C3-C2-O21-C21
69	1m	202	3PE	C1-C2-O21-C21
69	3Q	503	3PE	C1-C2-O21-C21
69	3W	101	3PE	C3-C2-O21-C21
69	3Y	101	3PE	C3-C2-O21-C21
70	1d	204	PC1	C1-C2-O21-C21
75	1d	205	CDL	CB3-CB4-OB6-CB5
75	1g	201	CDL	CA6-CA4-OA6-CA5
75	3N	502	CDL	CB6-CB4-OB6-CB5
69	1d	201	3PE	O11-C1-C2-C3
69	3P	503	3PE	O11-C1-C2-C3
69	1d	201	3PE	C3A-C3B-C3C-C3D
69	1d	203	3PE	C38-C39-C3A-C3B
69	3C	507	3PE	C32-C33-C34-C35
69	3C	507	3PE	C36-C37-C38-C39
75	1d	202	CDL	C39-C40-C41-C42
69	3G	109	3PE	C31-C32-C33-C34
69	3R	304	3PE	C31-C32-C33-C34
75	3D	504	CDL	C11-C12-C13-C14
75	3X	103	CDL	C18-C19-C20-C21
69	1Y	208	3PE	O32-C31-O31-C3
69	1Z	201	3PE	C24-C25-C26-C27
69	1g	202	3PE	C3C-C3D-C3E-C3F
69	1Y	201	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
69	3R	305	3PE	C32-C33-C34-C35
75	3Y	106	CDL	C78-C79-C80-C81
69	3Q	504	3PE	C2-C1-O11-P
70	1Y	207	PC1	C2-C1-O11-P
75	1d	202	CDL	CA4-CA3-OA5-PA1
77	1O	401	GTP	C4'-C5'-O5'-PA
82	1Y	203	PGT	C2-C1-O3P-P
91	4C	305	PGV	C05-C04-O12-P
69	3N	501	3PE	C34-C35-C36-C37
70	1H	402	PC1	C2A-C2B-C2C-C2D
75	1g	201	CDL	C56-C57-C58-C59
75	3F	201	CDL	C19-C20-C21-C22
87	4G	103	PEK	C28-C29-C30-C31
69	3C	505	3PE	O11-C1-C2-O21
69	3G	101	3PE	O11-C1-C2-O21
70	1H	403	PC1	O11-C1-C2-O21
69	3A	503	3PE	C22-C23-C24-C25
70	3R	303	PC1	C11-C12-N-C13
69	1M	502	3PE	C3A-C3B-C3C-C3D
69	3W	101	3PE	C37-C38-C39-C3A
69	3X	106	3PE	C33-C34-C35-C36
88	4A	601	HEA	C4D-C3D-CAD-CBD
69	3R	302	3PE	C33-C34-C35-C36
69	1d	201	3PE	C3B-C3C-C3D-C3E
69	3G	111	3PE	C34-C35-C36-C37
75	3X	103	CDL	C22-C23-C24-C25
69	1b	101	3PE	C29-C2A-C2B-C2C
69	3G	102	3PE	C22-C23-C24-C25
69	3P	503	3PE	C2C-C2D-C2E-C2F
91	4G	102	PGV	C26-C27-C28-C29
69	1L	705	3PE	O21-C2-C3-O31
69	1Y	209	3PE	O21-C2-C3-O31
75	3Y	106	CDL	OB6-CB4-CB6-OB8
75	1d	202	CDL	C12-C13-C14-C15
69	1L	711	3PE	C1-O11-P-O13
69	1l	203	3PE	C1-O11-P-O13
69	1m	204	3PE	C11-O13-P-O11
69	3C	504	3PE	C11-O13-P-O11
69	3C	506	3PE	C11-O13-P-O11
69	3G	107	3PE	C1-O11-P-O13
69	3J	105	3PE	C11-O13-P-O11
69	3P	517	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	3R	305	3PE	C11-O13-P-O11
69	3Y	102	3PE	C11-O13-P-O11
69	3Y	105	3PE	C11-O13-P-O11
69	4G	101	3PE	C1-O11-P-O13
70	1H	403	PC1	C1-O11-P-O13
70	1H	404	PC1	C11-O13-P-O11
70	1J	202	PC1	C11-O13-P-O11
75	1L	704	CDL	CB2-OB2-PB2-OB5
75	1g	201	CDL	CB3-OB5-PB2-OB2
75	1q	201	CDL	CB2-OB2-PB2-OB5
75	1q	202	CDL	CA2-OA2-PA1-OA5
75	1q	202	CDL	CA3-OA5-PA1-OA2
75	3N	502	CDL	CA2-OA2-PA1-OA5
75	3X	103	CDL	CA2-OA2-PA1-OA5
75	3Y	106	CDL	CB2-OB2-PB2-OB5
75	4B	302	CDL	CA2-OA2-PA1-OA5
75	4C	306	CDL	CA2-OA2-PA1-OA5
87	3X	102	PEK	C03-O11-P-O12
91	4A	607	PGV	C03-O11-P-O12
91	4A	608	PGV	C04-O12-P-O11
91	4J	101	PGV	C04-O12-P-O11
69	3C	509	3PE	C31-C32-C33-C34
69	3X	101	3PE	C31-C32-C33-C34
69	3D	502	3PE	C32-C33-C34-C35
69	3X	101	3PE	C25-C26-C27-C28
69	4G	104	3PE	C2A-C2B-C2C-C2D
69	1L	710	3PE	C38-C39-C3A-C3B
69	1M	502	3PE	C1-C2-C3-O31
75	3A	501	CDL	CA3-CA4-CA6-OA8
69	3P	515	3PE	C2D-C2E-C2F-C2G
69	3C	504	3PE	C24-C25-C26-C27
69	3D	503	3PE	C27-C28-C29-C2A
75	4C	306	CDL	C58-C59-C60-C61
69	1B	204	3PE	C3D-C3E-C3F-C3G
69	3P	519	3PE	C2A-C2B-C2C-C2D
69	3S	201	3PE	C29-C2A-C2B-C2C
69	3W	101	3PE	C39-C3A-C3B-C3C
70	1h	202	PC1	C2B-C2C-C2D-C2E
70	1B	202	PC1	C11-C12-N-C14
69	3C	511	3PE	C38-C39-C3A-C3B
69	3G	101	3PE	C2C-C2D-C2E-C2F
69	3J	101	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
69	3P	518	3PE	C2E-C2F-C2G-C2H
75	1q	202	CDL	C38-C39-C40-C41
69	1m	203	3PE	C21-C22-C23-C24
75	1g	201	CDL	C76-C77-C78-C79
69	1Y	208	3PE	C32-C31-O31-C3
69	3X	107	3PE	C28-C29-C2A-C2B
69	1Y	209	3PE	C33-C34-C35-C36
69	3J	105	3PE	C3E-C3F-C3G-C3H
69	3C	507	3PE	C29-C2A-C2B-C2C
70	1J	202	PC1	C33-C34-C35-C36
69	1m	205	3PE	C2-C1-O11-P
69	3G	104	3PE	C2-C1-O11-P
69	3G	105	3PE	C2-C1-O11-P
69	3J	104	3PE	C2-C1-O11-P
69	3R	305	3PE	C2-C1-O11-P
69	4G	104	3PE	C2-C1-O11-P
70	1A	202	PC1	C2-C1-O11-P
70	1Y	202	PC1	C2-C1-O11-P
70	1h	202	PC1	C2-C1-O11-P
75	1d	202	CDL	CB4-CB3-OB5-PB2
69	3D	502	3PE	C33-C34-C35-C36
69	3Q	504	3PE	C32-C33-C34-C35
69	3C	508	3PE	C21-C22-C23-C24
69	3G	102	3PE	C31-C32-C33-C34
91	4A	609	PGV	C9-C10-C11-C12
91	4A	609	PGV	C11-C12-C13-C14
91	4C	305	PGV	C11-C12-C13-C14
93	4B	303	PSC	C12-C13-C14-C15
69	3E	303	3PE	C37-C38-C39-C3A
75	3N	502	CDL	C31-C32-C33-C34
82	1Y	203	PGT	C36-C37-C38-C39
69	3C	513	3PE	C24-C25-C26-C27
69	3P	516	3PE	C22-C23-C24-C25
69	3C	505	3PE	C32-C33-C34-C35
70	1d	204	PC1	C3C-C3D-C3E-C3F
75	1i	201	CDL	C59-C60-C61-C62
88	4A	601	HEA	C2D-C3D-CAD-CBD
69	1J	203	3PE	C32-C31-O31-C3
75	1Y	217	CDL	C31-CA7-OA8-CA6
69	1l	202	3PE	C37-C38-C39-C3A
75	3N	502	CDL	C32-C33-C34-C35
82	1Y	203	PGT	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
69	3X	108	3PE	C3A-C3B-C3C-C3D
69	3Y	107	3PE	C34-C35-C36-C37
75	1d	205	CDL	C57-C58-C59-C60
75	4B	302	CDL	C78-C79-C80-C81
69	3C	504	3PE	C35-C36-C37-C38
69	3G	107	3PE	C25-C26-C27-C28
75	1Y	217	CDL	OA9-CA7-OA8-CA6
69	1h	204	3PE	C22-C23-C24-C25
69	3Q	503	3PE	C34-C35-C36-C37
70	1H	404	PC1	C34-C35-C36-C37
69	1b	101	3PE	C2B-C2C-C2D-C2E
70	3R	303	PC1	C23-C24-C25-C26
75	4B	302	CDL	C16-C17-C18-C19
75	4C	306	CDL	C14-C15-C16-C17
75	4C	306	CDL	OB5-CB3-CB4-CB6
69	3G	106	3PE	C32-C33-C34-C35
69	1o	201	3PE	O13-C11-C12-N
75	1Y	217	CDL	C82-C83-C84-C85
75	3F	201	CDL	C39-C40-C41-C42
81	1T	101	EHZ	C1-C21-C22-C23
69	1Y	215	3PE	O11-C1-C2-O21
69	1l	203	3PE	O11-C1-C2-O21
75	1d	205	CDL	OB5-CB3-CB4-OB6
69	1L	703	3PE	C2D-C2E-C2F-C2G
69	1Y	213	3PE	C28-C29-C2A-C2B
70	1P	502	PC1	C22-C23-C24-C25
69	1d	201	3PE	C2D-C2E-C2F-C2G
75	3P	513	CDL	C83-C84-C85-C86
75	3X	103	CDL	C78-C79-C80-C81
91	4K	101	PGV	C24-C25-C26-C27
69	1M	502	3PE	C32-C33-C34-C35
69	3P	514	3PE	C38-C39-C3A-C3B
69	3X	106	3PE	C32-C33-C34-C35
69	1Y	215	3PE	C38-C39-C3A-C3B
69	1d	203	3PE	C29-C2A-C2B-C2C
69	3Q	503	3PE	C38-C39-C3A-C3B
70	1h	202	PC1	C26-C27-C28-C29
75	1q	202	CDL	C62-C63-C64-C65
69	3Y	107	3PE	C35-C36-C37-C38
91	4J	101	PGV	O12-C04-C05-O05
69	3D	502	3PE	C2-C3-O31-C31
75	1L	704	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
75	3X	103	CDL	C15-C16-C17-C18
75	3F	201	CDL	C62-C63-C64-C65
69	1L	709	3PE	C36-C37-C38-C39
69	3C	507	3PE	O21-C2-C3-O31
69	3G	111	3PE	O21-C2-C3-O31
75	1d	205	CDL	OA6-CA4-CA6-OA8
69	3X	107	3PE	C3E-C3F-C3G-C3H
69	1f	103	3PE	C33-C34-C35-C36
69	3A	503	3PE	C28-C29-C2A-C2B
75	3N	502	CDL	C15-C16-C17-C18
69	1m	203	3PE	C2-C1-O11-P
69	3P	510	3PE	C2-C1-O11-P
75	1L	704	CDL	C82-C83-C84-C85
82	1Y	203	PGT	C17-C18-C19-C20
85	3P	501	HEM	CAA-CBA-CGA-O2A
91	4A	606	PGV	C11-C12-C13-C14
91	4A	607	PGV	C9-C10-C11-C12
69	1m	204	3PE	C2A-C2B-C2C-C2D
69	3P	510	3PE	C36-C37-C38-C39
69	1h	204	3PE	C3D-C3E-C3F-C3G
70	3X	104	PC1	C39-C3A-C3B-C3C
69	3E	302	3PE	C38-C39-C3A-C3B
69	3G	111	3PE	C25-C26-C27-C28
85	3P	502	HEM	CAA-CBA-CGA-O2A
69	3P	507	3PE	C35-C36-C37-C38
69	3P	516	3PE	C28-C29-C2A-C2B
69	1k	101	3PE	C3C-C3D-C3E-C3F
69	3G	110	3PE	C32-C33-C34-C35
75	3A	501	CDL	C40-C41-C42-C43
88	4A	601	HEA	CAD-CBD-CGD-O1D
75	3N	502	CDL	C37-C38-C39-C40
69	1m	205	3PE	C3A-C3B-C3C-C3D
69	3E	302	3PE	C34-C35-C36-C37
69	1g	202	3PE	C1-C2-C3-O31
69	3P	511	3PE	C1-C2-C3-O31
69	3R	305	3PE	C1-C2-C3-O31
70	1B	203	PC1	C1-C2-C3-O31
69	1L	712	3PE	C3A-C3B-C3C-C3D
75	3A	501	CDL	C14-C15-C16-C17
69	3C	509	3PE	C2D-C2E-C2F-C2G
69	3C	513	3PE	C2B-C2C-C2D-C2E
69	3N	503	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
70	1h	202	PC1	C24-C25-C26-C27
69	1o	201	3PE	C27-C28-C29-C2A
69	3C	505	3PE	C26-C27-C28-C29
70	1Y	207	PC1	C25-C26-C27-C28
75	3T	101	CDL	C52-C53-C54-C55
85	3C	502	HEM	CAA-CBA-CGA-O1A
69	1d	203	3PE	C22-C23-C24-C25
69	1l	204	3PE	C23-C24-C25-C26
70	3R	303	PC1	C29-C2A-C2B-C2C
91	4A	607	PGV	C20-C21-C22-C23
91	4C	301	PGV	C11-C10-C9-C8
85	3P	501	HEM	CAA-CBA-CGA-O1A
85	3P	501	HEM	CAD-CBD-CGD-O1D
85	3P	502	HEM	CAA-CBA-CGA-O1A
69	1L	706	3PE	C3-C2-O21-C21
69	1L	708	3PE	C3-C2-O21-C21
69	3J	103	3PE	C1-C2-O21-C21
69	3Q	504	3PE	C1-C2-O21-C21
75	3X	103	CDL	CB6-CB4-OB6-CB5
70	3R	303	PC1	C11-C12-N-C15
69	3A	502	3PE	C33-C34-C35-C36
69	3C	506	3PE	C33-C34-C35-C36
69	3W	102	3PE	C37-C38-C39-C3A
69	3Y	105	3PE	C33-C34-C35-C36
75	3D	504	CDL	C54-C55-C56-C57
75	1q	202	CDL	C12-C13-C14-C15
75	3Y	106	CDL	C20-C21-C22-C23
75	4C	306	CDL	C62-C63-C64-C65
69	1f	102	3PE	C11-O13-P-O11
69	3G	110	3PE	C1-O11-P-O13
69	3N	501	3PE	C1-O11-P-O13
69	3N	501	3PE	C11-O13-P-O11
82	1Y	203	PGT	C1-O3P-P-O4P
87	3X	102	PEK	C5-C6-C7-C8
69	1Y	209	3PE	C21-C22-C23-C24
85	3C	501	HEM	CAA-CBA-CGA-O2A
85	3C	502	HEM	CAA-CBA-CGA-O2A
69	1f	103	3PE	C37-C38-C39-C3A
69	3P	503	3PE	C26-C27-C28-C29
69	3P	520	3PE	C35-C36-C37-C38
69	3Y	107	3PE	C2-C1-O11-P
75	3N	502	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
69	1L	712	3PE	C39-C3A-C3B-C3C
69	1d	201	3PE	C2B-C2C-C2D-C2E
75	1g	201	CDL	C75-C76-C77-C78
75	4C	306	CDL	C11-C12-C13-C14
69	3E	303	3PE	C21-C22-C23-C24
69	3G	111	3PE	O11-C1-C2-O21
69	3N	503	3PE	O11-C1-C2-O21
69	3P	519	3PE	O11-C1-C2-O21
85	3C	501	HEM	CAA-CBA-CGA-O1A
85	3P	501	HEM	CAD-CBD-CGD-O2D
69	1L	712	3PE	C2E-C2F-C2G-C2H
69	3C	513	3PE	C28-C29-C2A-C2B
75	1Y	217	CDL	C41-C42-C43-C44
69	1Y	215	3PE	O11-C1-C2-C3
69	1l	203	3PE	O11-C1-C2-C3
69	3R	305	3PE	O11-C1-C2-C3
70	1H	403	PC1	O11-C1-C2-C3
75	1q	202	CDL	OA5-CA3-CA4-CA6
69	1L	701	3PE	C2E-C2F-C2G-C2H
69	1g	202	3PE	C33-C34-C35-C36
69	1l	202	3PE	C23-C24-C25-C26
69	3G	101	3PE	C39-C3A-C3B-C3C
69	3P	507	3PE	C2B-C2C-C2D-C2E
87	3X	102	PEK	C16-C17-C18-C19
69	1B	205	3PE	C35-C36-C37-C38
69	1d	203	3PE	C32-C33-C34-C35
69	3Y	104	3PE	C2B-C2C-C2D-C2E
75	3F	201	CDL	C72-C73-C74-C75
69	1Y	201	3PE	C32-C33-C34-C35
75	1d	205	CDL	C34-C35-C36-C37
69	3G	107	3PE	C21-C22-C23-C24
69	1A	201	3PE	C2D-C2E-C2F-C2G
69	1e	201	3PE	C39-C3A-C3B-C3C
69	1J	203	3PE	O32-C31-O31-C3
69	1l	204	3PE	C38-C39-C3A-C3B
82	1Y	203	PGT	C41-C42-C43-C44
81	1T	101	EHZ	C11-C10-S1-C9
75	1d	205	CDL	C13-C14-C15-C16
69	3C	515	3PE	C27-C28-C29-C2A
69	3P	503	3PE	C2F-C2G-C2H-C2I
69	3X	108	3PE	C38-C39-C3A-C3B
88	4A	602	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
91	4A	609	PGV	C12-C13-C14-C15
69	1m	202	3PE	C21-C22-C23-C24
69	3P	512	3PE	C22-C23-C24-C25
70	1M	501	PC1	C2A-C2B-C2C-C2D
75	1q	202	CDL	CB2-C1-CA2-OA2
88	4A	602	HEA	CAD-CBD-CGD-O2D
69	1Y	213	3PE	C3A-C3B-C3C-C3D
69	3P	515	3PE	C25-C26-C27-C28
70	1H	403	PC1	C2E-C2F-C2G-C2H
75	1g	201	CDL	C52-C53-C54-C55
88	4A	601	HEA	CAD-CBD-CGD-O2D
69	1m	201	3PE	C26-C27-C28-C29
69	1d	201	3PE	C26-C27-C28-C29
69	3X	106	3PE	C3C-C3D-C3E-C3F
75	3F	201	CDL	C77-C78-C79-C80
69	3P	511	3PE	C34-C35-C36-C37
75	1g	201	CDL	C81-C82-C83-C84
69	3W	101	3PE	C3C-C3D-C3E-C3F
75	1g	201	CDL	C42-C43-C44-C45
75	4B	302	CDL	C17-C18-C19-C20
69	1J	201	3PE	C2-C1-O11-P
69	1k	101	3PE	C33-C34-C35-C36
69	3G	102	3PE	C23-C24-C25-C26
69	3Y	101	3PE	C36-C37-C38-C39
69	1L	701	3PE	C28-C29-C2A-C2B
70	1h	203	PC1	C35-C36-C37-C38
69	1m	201	3PE	O21-C21-C22-C23
69	1B	204	3PE	C2F-C2G-C2H-C2I
69	1Y	210	3PE	C24-C25-C26-C27
69	1h	204	3PE	C27-C28-C29-C2A
69	3C	507	3PE	C1-C2-C3-O31
69	3Q	503	3PE	C29-C2A-C2B-C2C
91	4G	102	PGV	C28-C29-C30-C31
86	3Q	501	HEC	CAA-CBA-CGA-O2A
75	1Y	217	CDL	C73-C74-C75-C76
69	3G	101	3PE	C34-C35-C36-C37
69	1Y	214	3PE	C2F-C2G-C2H-C2I
91	4C	303	PGV	C15-C16-C17-C18
69	3Q	502	3PE	C22-C21-O21-C2
69	3C	511	3PE	C24-C25-C26-C27
69	3R	304	3PE	C2F-C2G-C2H-C2I
69	1A	203	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
69	3P	516	3PE	C32-C33-C34-C35
75	1N	402	CDL	C35-C36-C37-C38
91	4G	102	PGV	C30-C31-C32-C33
91	4A	608	PGV	C9-C10-C11-C12
69	1g	202	3PE	O11-C1-C2-O21
91	4A	607	PGV	C27-C28-C29-C30
69	1g	202	3PE	C2C-C2D-C2E-C2F
69	1Y	213	3PE	C2D-C2E-C2F-C2G
69	3P	505	3PE	C22-C23-C24-C25
69	4G	101	3PE	C24-C25-C26-C27
82	1Y	203	PGT	C35-C36-C37-C38
88	4A	602	HEA	CAD-CBD-CGD-O1D
70	1B	203	PC1	C32-C33-C34-C35
69	3N	503	3PE	O11-C1-C2-C3
75	1L	704	CDL	OB5-CB3-CB4-CB6
69	3C	503	3PE	C34-C35-C36-C37
69	1J	203	3PE	O13-C11-C12-N
69	1L	708	3PE	O13-C11-C12-N
69	1N	401	3PE	O13-C11-C12-N
69	3G	109	3PE	O13-C11-C12-N
69	1f	101	3PE	C23-C24-C25-C26
70	1B	202	PC1	C35-C36-C37-C38
70	1B	202	PC1	C36-C37-C38-C39
70	1H	403	PC1	C21-C22-C23-C24
69	1L	709	3PE	C34-C35-C36-C37
75	1L	704	CDL	C83-C84-C85-C86
69	3X	105	3PE	O31-C31-C32-C33
69	1g	202	3PE	C36-C37-C38-C39
69	3Q	504	3PE	C37-C38-C39-C3A
75	4C	306	CDL	C15-C16-C17-C18
75	1N	402	CDL	CB4-CB3-OB5-PB2
75	3X	103	CDL	CA2-C1-CB2-OB2
69	3X	101	3PE	C35-C36-C37-C38
69	3T	103	3PE	O32-C31-O31-C3
75	1N	402	CDL	OA7-CA5-OA6-CA4
69	1L	707	3PE	C27-C28-C29-C2A
69	1L	708	3PE	C36-C37-C38-C39
86	3D	501	HEC	CAA-CBA-CGA-O2A
69	3D	503	3PE	O31-C31-C32-C33
70	1H	402	PC1	O31-C31-C32-C33
75	1g	201	CDL	C32-C31-CA7-OA8
69	1L	701	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
69	1Y	208	3PE	C3C-C3D-C3E-C3F
75	4C	306	CDL	C23-C24-C25-C26
69	1l	202	3PE	C24-C25-C26-C27
75	1Y	217	CDL	C51-CB5-OB6-CB4
69	3C	508	3PE	C27-C28-C29-C2A
75	3X	103	CDL	C16-C17-C18-C19
75	4C	307	CDL	C36-C37-C38-C39
69	3T	103	3PE	C32-C31-O31-C3
70	3T	102	PC1	C32-C31-O31-C3
91	4C	305	PGV	C9-C10-C11-C12
69	1f	101	3PE	C3A-C3B-C3C-C3D
69	3Y	104	3PE	C3F-C3G-C3H-C3I
70	1B	203	PC1	C27-C28-C29-C2A
69	3C	511	3PE	C31-C32-C33-C34
70	1h	202	PC1	O21-C21-C22-C23
75	1d	202	CDL	C32-C31-CA7-OA8
69	1N	401	3PE	C3F-C3G-C3H-C3I
69	1f	104	3PE	C3B-C3C-C3D-C3E
69	3P	506	3PE	C24-C25-C26-C27
75	3X	103	CDL	C39-C40-C41-C42
85	3P	502	HEM	CAD-CBD-CGD-O1D
69	3C	517	3PE	C1-O11-P-O13
69	3P	511	3PE	C11-O13-P-O11
91	4A	606	PGV	C04-O12-P-O11
91	4J	101	PGV	C19-C20-C21-C22
69	3Q	503	3PE	C3A-C3B-C3C-C3D
69	1f	101	3PE	O21-C21-C22-C23
70	1M	501	PC1	O21-C21-C22-C23
75	1q	201	CDL	C52-C51-CB5-OB6
69	1e	201	3PE	C2C-C2D-C2E-C2F
69	3P	518	3PE	C2D-C2E-C2F-C2G
75	3F	201	CDL	C55-C56-C57-C58
69	1Y	215	3PE	C2C-C2D-C2E-C2F
69	1b	101	3PE	C22-C23-C24-C25
69	1f	102	3PE	C2A-C2B-C2C-C2D
69	1f	103	3PE	C25-C26-C27-C28
69	1m	203	3PE	C28-C29-C2A-C2B
69	3X	105	3PE	C3D-C3E-C3F-C3G
70	1H	403	PC1	C29-C2A-C2B-C2C
75	1Y	217	CDL	C75-C76-C77-C78
75	3X	103	CDL	C51-C52-C53-C54
75	4B	302	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
75	4C	306	CDL	C34-C35-C36-C37
69	1h	204	3PE	O21-C21-C22-C23
69	3C	508	3PE	O31-C31-C32-C33
69	3C	508	3PE	O21-C21-C22-C23
75	1N	402	CDL	C32-C31-CA7-OA8
91	4J	101	PGV	O03-C19-C20-C21
87	3X	102	PEK	C14-C15-C16-C17
87	4G	103	PEK	C14-C15-C16-C17
91	4C	301	PGV	C11-C12-C13-C14
93	4B	303	PSC	C7-C8-C9-C10
69	1A	203	3PE	C35-C36-C37-C38
69	1J	203	3PE	C24-C25-C26-C27
69	3P	510	3PE	C3A-C3B-C3C-C3D
69	1L	706	3PE	C1-C2-O21-C21
69	1L	708	3PE	C1-C2-O21-C21
69	1l	202	3PE	C1-C2-O21-C21
69	3D	502	3PE	C3-C2-O21-C21
69	3Q	504	3PE	C3-C2-O21-C21
75	3X	103	CDL	CB3-CB4-OB6-CB5
70	1Y	202	PC1	C21-C22-C23-C24
75	3F	201	CDL	C11-C12-C13-C14
75	1q	202	CDL	OA7-CA5-OA6-CA4
69	3E	302	3PE	C25-C26-C27-C28
69	1J	201	3PE	C25-C26-C27-C28
69	3J	104	3PE	C36-C37-C38-C39
69	3P	508	3PE	C2D-C2E-C2F-C2G
69	3P	517	3PE	C3B-C3C-C3D-C3E
91	4N	101	PGV	C22-C23-C24-C25
75	3N	502	CDL	C12-C11-CA5-OA6
69	3C	512	3PE	C23-C24-C25-C26
69	3P	518	3PE	C32-C33-C34-C35
69	3W	101	3PE	C35-C36-C37-C38
70	3X	104	PC1	C21-C22-C23-C24
86	3Q	501	HEC	CAA-CBA-CGA-O1A
91	4G	102	PGV	C25-C26-C27-C28
69	1J	201	3PE	O31-C31-C32-C33
69	3P	503	3PE	O21-C21-C22-C23
69	1N	401	3PE	C32-C33-C34-C35
91	4C	302	PGV	C24-C25-C26-C27
91	4C	305	PGV	C23-C24-C25-C26
88	4A	601	HEA	C15-C16-C17-C18
87	3X	102	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
69	3C	505	3PE	C2-C1-O11-P
69	3P	508	3PE	C1-C2-C3-O31
69	3T	103	3PE	C2-C1-O11-P
69	3X	108	3PE	C1-C2-C3-O31
75	1H	401	CDL	CA3-CA4-CA6-OA8
75	1d	205	CDL	CA3-CA4-CA6-OA8
75	1q	202	CDL	CB4-CB3-OB5-PB2
69	3C	512	3PE	C28-C29-C2A-C2B
69	3Y	101	3PE	C2A-C2B-C2C-C2D
69	3Y	104	3PE	C22-C23-C24-C25
75	1g	201	CDL	C61-C62-C63-C64
70	1d	204	PC1	O11-C1-C2-O21
75	1d	202	CDL	OB5-CB3-CB4-OB6
75	4C	307	CDL	OA5-CA3-CA4-OA6
69	3C	507	3PE	O31-C31-C32-C33
70	1M	501	PC1	C2D-C2E-C2F-C2G
91	4A	609	PGV	C20-C21-C22-C23
69	3P	507	3PE	C32-C33-C34-C35
69	3P	512	3PE	C3A-C3B-C3C-C3D
69	3Y	101	3PE	C35-C36-C37-C38
69	3A	502	3PE	C27-C28-C29-C2A
69	3G	107	3PE	C22-C23-C24-C25
69	3P	507	3PE	C39-C3A-C3B-C3C
69	3X	101	3PE	C33-C34-C35-C36
75	1Y	217	CDL	C24-C25-C26-C27
82	1Y	203	PGT	C43-C44-C45-C46
69	1l	203	3PE	C31-C32-C33-C34
69	1d	206	3PE	O21-C21-C22-C23
69	3J	105	3PE	O21-C21-C22-C23
82	1Y	203	PGT	O2-C31-C32-C33
69	3R	304	3PE	C3C-C3D-C3E-C3F
91	4N	101	PGV	C9-C10-C11-C12
69	1J	201	3PE	C3E-C3F-C3G-C3H
70	1Y	207	PC1	C2B-C2C-C2D-C2E
69	1L	703	3PE	O32-C31-O31-C3
88	4A	602	HEA	C26-C15-C16-C17
69	3G	111	3PE	O21-C21-C22-C23
69	3P	505	3PE	C32-C33-C34-C35
69	3T	103	3PE	C3A-C3B-C3C-C3D
70	1h	202	PC1	C25-C26-C27-C28
75	1g	201	CDL	C79-C80-C81-C82
69	1g	202	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
75	1Y	217	CDL	OB5-CB3-CB4-CB6
75	1d	205	CDL	OB5-CB3-CB4-CB6
75	3A	501	CDL	OB5-CB3-CB4-CB6
86	3D	501	HEC	CAA-CBA-CGA-O1A
69	1L	712	3PE	C28-C29-C2A-C2B
69	1N	401	3PE	C28-C29-C2A-C2B
69	1m	201	3PE	C3F-C3G-C3H-C3I
75	1d	202	CDL	C54-C55-C56-C57
69	3W	103	3PE	C22-C23-C24-C25
70	1h	203	PC1	C22-C23-C24-C25
69	1L	702	3PE	O21-C2-C3-O31
69	1g	203	3PE	O21-C2-C3-O31
69	3P	508	3PE	O21-C2-C3-O31
75	3A	501	CDL	OA6-CA4-CA6-OA8
75	3F	201	CDL	OA6-CA4-CA6-OA8
75	3T	101	CDL	OA6-CA4-CA6-OA8
69	3C	514	3PE	C31-C32-C33-C34
69	3P	503	3PE	C3D-C3E-C3F-C3G
69	3T	103	3PE	C2E-C2F-C2G-C2H
69	3A	502	3PE	C2A-C2B-C2C-C2D
69	3E	303	3PE	C2E-C2F-C2G-C2H
91	4C	302	PGV	C26-C27-C28-C29
69	3P	514	3PE	C3C-C3D-C3E-C3F
69	3W	103	3PE	C28-C29-C2A-C2B
91	4C	302	PGV	C20-C21-C22-C23
70	3T	102	PC1	O32-C31-O31-C3
69	1d	201	3PE	O31-C31-C32-C33
75	1d	205	CDL	C52-C51-CB5-OB6
75	4C	306	CDL	C72-C71-CB7-OB8
69	1b	101	3PE	C25-C26-C27-C28
76	1I	203	AYA	C-CA-N-CT
75	1q	201	CDL	C31-CA7-OA8-CA6
69	3Y	104	3PE	C31-C32-C33-C34
70	3X	104	PC1	C32-C33-C34-C35
69	1l	202	3PE	O21-C21-C22-C23
69	3J	105	3PE	C3A-C3B-C3C-C3D
69	3N	501	3PE	C3C-C3D-C3E-C3F
69	1L	707	3PE	C33-C34-C35-C36
75	1Y	217	CDL	C54-C55-C56-C57
69	3P	514	3PE	C2E-C2F-C2G-C2H
69	3R	302	3PE	C37-C38-C39-C3A
75	1d	202	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
87	4G	103	PEK	C3-C4-C5-C6
75	3F	201	CDL	C72-C71-CB7-OB8
69	3C	512	3PE	C3C-C3D-C3E-C3F
69	3Y	104	3PE	C24-C25-C26-C27
75	3T	101	CDL	C73-C74-C75-C76
69	3R	304	3PE	C33-C34-C35-C36
79	1P	501	NDP	C3D-C4D-C5D-O5D
69	3Y	101	3PE	C25-C26-C27-C28
69	3Y	104	3PE	C32-C31-O31-C3
69	1L	702	3PE	O31-C31-C32-C33
77	1O	401	GTP	PA-O3A-PB-O2B
69	3Y	104	3PE	O32-C31-O31-C3
69	3G	101	3PE	C33-C34-C35-C36
70	1Y	202	PC1	C26-C27-C28-C29
75	1N	402	CDL	C11-CA5-OA6-CA4
75	1q	202	CDL	C11-CA5-OA6-CA4
75	1N	402	CDL	C32-C31-CA7-OA9
75	1g	201	CDL	C32-C31-CA7-OA9
69	3P	506	3PE	C3B-C3C-C3D-C3E
69	3W	101	3PE	C3E-C3F-C3G-C3H
91	4G	102	PGV	O03-C19-C20-C21
69	1J	203	3PE	C27-C28-C29-C2A
69	1d	203	3PE	C25-C26-C27-C28
75	1Y	217	CDL	C51-C52-C53-C54
85	3P	502	HEM	CAD-CBD-CGD-O2D
70	1H	402	PC1	C11-C12-N-C14
69	3C	507	3PE	O32-C31-C32-C33
75	1d	202	CDL	C32-C31-CA7-OA9
69	3P	510	3PE	C2A-C2B-C2C-C2D
75	1q	202	CDL	C75-C76-C77-C78
69	3P	503	3PE	O22-C21-C22-C23
75	3X	103	CDL	OA5-CA3-CA4-OA6
69	3G	107	3PE	C32-C33-C34-C35
69	3Y	104	3PE	C3C-C3D-C3E-C3F
69	3J	103	3PE	C32-C31-O31-C3
69	1f	104	3PE	C23-C24-C25-C26
69	3P	512	3PE	C28-C29-C2A-C2B
69	3Y	107	3PE	C38-C39-C3A-C3B
70	3X	104	PC1	C36-C37-C38-C39
75	1d	205	CDL	C79-C80-C81-C82
81	1T	101	EHZ	C1-C2-C3-C4
75	1d	205	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
69	3Y	104	3PE	C21-C22-C23-C24
69	3A	503	3PE	C37-C38-C39-C3A
69	3G	110	3PE	C2C-C2D-C2E-C2F
69	1h	204	3PE	O22-C21-C22-C23
75	1q	201	CDL	C52-C51-CB5-OB7
69	1B	205	3PE	C2D-C2E-C2F-C2G
69	3D	503	3PE	C26-C27-C28-C29
70	1Y	207	PC1	C26-C27-C28-C29
91	4N	101	PGV	C11-C12-C13-C14
69	1L	705	3PE	C34-C35-C36-C37
69	3X	105	3PE	O32-C31-C32-C33
70	1h	202	PC1	O22-C21-C22-C23
69	3P	517	3PE	C3D-C3E-C3F-C3G
69	1L	702	3PE	C1-C2-C3-O31
69	3C	511	3PE	C1-C2-C3-O31
75	3F	201	CDL	CB3-CB4-CB6-OB8
69	3P	515	3PE	C3D-C3E-C3F-C3G
69	3G	102	3PE	C11-O13-P-O11
75	3A	501	CDL	CB3-OB5-PB2-OB2
69	3P	516	3PE	C3E-C3F-C3G-C3H
69	3W	103	3PE	C23-C24-C25-C26
70	1Y	206	PC1	C3B-C3C-C3D-C3E
75	1Y	217	CDL	C14-C15-C16-C17
69	1f	101	3PE	O22-C21-C22-C23
69	3C	508	3PE	O32-C31-C32-C33
69	3G	111	3PE	O22-C21-C22-C23
70	1M	501	PC1	O22-C21-C22-C23
69	1B	205	3PE	C3C-C3D-C3E-C3F
75	1d	205	CDL	C83-C84-C85-C86
75	1g	201	CDL	C34-C35-C36-C37
69	1Y	216	3PE	C35-C36-C37-C38
69	1m	202	3PE	C25-C26-C27-C28
69	3C	506	3PE	C2F-C2G-C2H-C2I
69	3P	507	3PE	C2F-C2G-C2H-C2I
69	3R	305	3PE	C36-C37-C38-C39
70	1d	204	PC1	C23-C24-C25-C26
70	3J	106	PC1	C34-C35-C36-C37
84	1l	201	MYR	C3-C4-C5-C6
69	3C	517	3PE	O22-C21-O21-C2
88	4A	602	HEA	C4D-C3D-CAD-CBD
75	1d	205	CDL	C1-CA2-OA2-PA1
91	4C	302	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
69	1L	702	3PE	O32-C31-C32-C33
69	3D	503	3PE	O32-C31-C32-C33
91	4G	102	PGV	O04-C19-C20-C21
91	4J	101	PGV	O04-C19-C20-C21
69	3Y	101	3PE	C29-C2A-C2B-C2C
69	4G	104	3PE	C24-C25-C26-C27
75	1Y	217	CDL	C32-C33-C34-C35
75	4C	306	CDL	C63-C64-C65-C66
69	1Y	208	3PE	C26-C27-C28-C29
75	1d	202	CDL	C38-C39-C40-C41
75	4B	302	CDL	C43-C44-C45-C46
69	1L	707	3PE	C1-O11-P-O14
69	1L	710	3PE	C1-O11-P-O14
69	1Y	211	3PE	C1-O11-P-O14
69	1Y	213	3PE	C11-O13-P-O14
69	1b	101	3PE	C11-O13-P-O14
69	1f	102	3PE	C11-O13-P-O14
69	1g	202	3PE	C11-O13-P-O14
69	1k	101	3PE	C1-O11-P-O12
69	1m	201	3PE	C1-O11-P-O12
69	1m	203	3PE	C11-O13-P-O14
69	1m	204	3PE	C11-O13-P-O14
69	3A	502	3PE	C1-O11-P-O14
69	3C	506	3PE	C11-O13-P-O14
69	3C	512	3PE	C11-O13-P-O14
69	3C	517	3PE	C1-O11-P-O14
69	3D	503	3PE	C1-O11-P-O14
69	3G	102	3PE	C11-O13-P-O14
69	3G	107	3PE	C1-O11-P-O14
69	3G	110	3PE	C1-O11-P-O12
69	3J	105	3PE	C11-O13-P-O12
69	3N	501	3PE	C11-O13-P-O12
69	3P	505	3PE	C1-O11-P-O14
69	3P	511	3PE	C11-O13-P-O14
69	3P	512	3PE	C1-O11-P-O14
69	3P	517	3PE	C11-O13-P-O14
69	3Q	504	3PE	C11-O13-P-O14
69	3R	302	3PE	C1-O11-P-O14
69	3X	107	3PE	C1-O11-P-O14
69	4G	101	3PE	C1-O11-P-O12
70	1A	202	PC1	C11-O13-P-O14
70	1H	402	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
70	1H	403	PC1	C1-O11-P-O14
70	1H	404	PC1	C11-O13-P-O14
70	1J	202	PC1	C11-O13-P-O12
70	1Y	206	PC1	C11-O13-P-O14
70	3X	104	PC1	C11-O13-P-O14
75	1H	401	CDL	CA3-OA5-PA1-OA3
75	1H	401	CDL	CB2-OB2-PB2-OB4
75	1L	704	CDL	CB2-OB2-PB2-OB3
75	1d	202	CDL	CA2-OA2-PA1-OA4
75	1g	201	CDL	CB3-OB5-PB2-OB3
75	1q	202	CDL	CA3-OA5-PA1-OA3
75	3A	501	CDL	CB3-OB5-PB2-OB4
75	4C	306	CDL	CA2-OA2-PA1-OA3
79	1P	501	NDP	C2N-C3N-C7N-N7N
82	1Y	203	PGT	C1-O3P-P-O1P
91	4J	101	PGV	C04-O12-P-O13
91	4K	101	PGV	C04-O12-P-O13
93	4B	303	PSC	C04-O12-P-O13
79	1P	501	NDP	O4B-C4B-C5B-O5B
69	3E	303	3PE	C33-C34-C35-C36
75	4C	307	CDL	C23-C24-C25-C26
70	1H	402	PC1	O32-C31-C32-C33
70	1d	204	PC1	O31-C31-C32-C33
69	3X	107	3PE	C32-C33-C34-C35
70	3P	509	PC1	C37-C38-C39-C3A
69	1L	712	3PE	O13-C11-C12-N
69	1m	201	3PE	O13-C11-C12-N
69	3R	305	3PE	O13-C11-C12-N
69	3C	508	3PE	O22-C21-C22-C23
82	1Y	203	PGT	O31-C31-C32-C33
69	3C	515	3PE	C35-C36-C37-C38
69	3P	519	3PE	C27-C28-C29-C2A
75	3F	201	CDL	C31-C32-C33-C34
69	1Y	205	3PE	O21-C21-C22-C23
75	3Y	106	CDL	C31-C32-C33-C34
82	1Y	203	PGT	C32-C33-C34-C35
69	3C	504	3PE	C2-C3-O31-C31
69	3G	110	3PE	C28-C29-C2A-C2B
75	4B	302	CDL	C44-C45-C46-C47
75	3N	502	CDL	C12-C11-CA5-OA7
69	3G	105	3PE	C34-C35-C36-C37
70	3R	303	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
75	3D	504	CDL	C72-C73-C74-C75
69	3C	515	3PE	O21-C21-C22-C23
70	1B	203	PC1	O21-C21-C22-C23
75	1q	202	CDL	C12-C11-CA5-OA6
75	3X	103	CDL	C72-C71-CB7-OB8
70	1H	403	PC1	C24-C25-C26-C27
69	3D	503	3PE	C21-C22-C23-C24
70	3P	509	PC1	C31-C32-C33-C34
69	1J	203	3PE	C12-C11-O13-P
69	1L	710	3PE	C3-C2-O21-C21
69	1Y	214	3PE	C12-C11-O13-P
69	1Z	201	3PE	C12-C11-O13-P
69	1f	102	3PE	C12-C11-O13-P
69	1f	103	3PE	C12-C11-O13-P
69	1g	203	3PE	C12-C11-O13-P
69	1l	202	3PE	C12-C11-O13-P
69	3C	505	3PE	C1-C2-O21-C21
69	3C	506	3PE	C12-C11-O13-P
69	3D	502	3PE	C1-C2-O21-C21
69	3G	106	3PE	C12-C11-O13-P
69	3G	111	3PE	C12-C11-O13-P
69	3P	518	3PE	C12-C11-O13-P
69	3Y	104	3PE	C12-C11-O13-P
70	1B	202	PC1	C12-C11-O13-P
70	1P	502	PC1	C12-C11-O13-P
70	1Y	202	PC1	C12-C11-O13-P
70	1Y	207	PC1	C12-C11-O13-P
81	1n	201	EHZ	O4-C15-C16-C17
69	1L	708	3PE	O32-C31-O31-C3
69	3J	105	3PE	O22-C21-C22-C23
69	1l	202	3PE	C34-C35-C36-C37
75	3Y	106	CDL	C63-C64-C65-C66
81	1T	101	EHZ	C2-C3-C4-C5
69	3G	104	3PE	O21-C21-C22-C23
75	1d	205	CDL	O1-C1-CB2-OB2
69	3P	508	3PE	C38-C39-C3A-C3B
69	3P	511	3PE	C26-C27-C28-C29
69	3P	520	3PE	C29-C2A-C2B-C2C
69	1Y	205	3PE	C24-C25-C26-C27
75	1q	202	CDL	C52-C53-C54-C55
69	1f	102	3PE	C21-C22-C23-C24
75	3Y	106	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
69	1L	703	3PE	C32-C31-O31-C3
70	1H	402	PC1	C11-C12-N-C15
91	4C	302	PGV	C9-C10-C11-C12
69	3Q	502	3PE	O21-C21-C22-C23
69	3G	109	3PE	C26-C27-C28-C29
69	3P	504	3PE	C35-C36-C37-C38
69	3P	511	3PE	C39-C3A-C3B-C3C
75	3A	501	CDL	C17-C18-C19-C20
75	3N	502	CDL	C78-C79-C80-C81
75	3T	101	CDL	C51-C52-C53-C54
69	3C	513	3PE	C3F-C3G-C3H-C3I
75	3N	502	CDL	C81-C82-C83-C84
69	1f	104	3PE	C21-C22-C23-C24
69	3P	518	3PE	C3E-C3F-C3G-C3H
69	3Q	504	3PE	C35-C36-C37-C38
70	3J	106	PC1	C28-C29-C2A-C2B
75	3A	501	CDL	C32-C33-C34-C35
91	4N	101	PGV	C13-C14-C15-C16
69	1Z	201	3PE	C23-C24-C25-C26
69	1g	202	3PE	C2D-C2E-C2F-C2G
69	1Y	209	3PE	O31-C31-C32-C33
69	4G	101	3PE	O21-C21-C22-C23
75	1q	201	CDL	OA9-CA7-OA8-CA6
69	1l	204	3PE	C2E-C2F-C2G-C2H
69	3P	508	3PE	C35-C36-C37-C38
70	1d	204	PC1	O32-C31-C32-C33
75	1d	205	CDL	C52-C51-CB5-OB7
69	3C	503	3PE	C2B-C2C-C2D-C2E
70	1M	501	PC1	C2-C1-O11-P
75	4B	302	CDL	C1-CB2-OB2-PB2
69	3Q	503	3PE	C26-C27-C28-C29
75	1d	205	CDL	C74-C75-C76-C77
69	3C	511	3PE	O11-C1-C2-O21
81	1T	101	EHZ	S1-C10-C11-N1
69	1L	710	3PE	C36-C37-C38-C39
69	1L	712	3PE	C37-C38-C39-C3A
75	3F	201	CDL	C17-C18-C19-C20
69	3J	104	3PE	O21-C21-C22-C23
75	3Y	106	CDL	C52-C51-CB5-OB6
69	1Y	216	3PE	C3B-C3C-C3D-C3E
69	3P	503	3PE	C2D-C2E-C2F-C2G
69	3Y	107	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
75	3X	103	CDL	C53-C54-C55-C56
69	4G	101	3PE	O22-C21-C22-C23
70	1B	203	PC1	O22-C21-C22-C23
75	1q	202	CDL	C12-C11-CA5-OA7
75	3F	201	CDL	C72-C71-CB7-OB9
69	1f	102	3PE	C33-C34-C35-C36
69	4G	101	3PE	C23-C24-C25-C26
69	1L	710	3PE	O21-C21-C22-C23
69	1Y	211	3PE	O31-C31-C32-C33
70	1A	202	PC1	O31-C31-C32-C33
69	1L	702	3PE	C29-C2A-C2B-C2C
75	3F	201	CDL	C80-C81-C82-C83
75	1d	202	CDL	OA9-CA7-OA8-CA6
69	1L	709	3PE	C37-C38-C39-C3A
69	1d	201	3PE	O32-C31-C32-C33
75	4C	306	CDL	C72-C71-CB7-OB9
69	3J	103	3PE	C3D-C3E-C3F-C3G
82	1Y	203	PGT	C40-C41-C42-C43
69	3X	105	3PE	C26-C27-C28-C29
75	1q	202	CDL	O1-C1-CA2-OA2
69	1m	204	3PE	O31-C31-C32-C33
69	3C	504	3PE	O31-C31-C32-C33
69	3X	105	3PE	O21-C21-C22-C23
75	1q	202	CDL	C72-C73-C74-C75
70	1H	403	PC1	C11-C12-N-C13
76	1I	203	AYA	CB-CA-N-CT
69	1L	708	3PE	C32-C31-O31-C3
69	1l	202	3PE	O22-C21-C22-C23
75	3Y	106	CDL	C60-C61-C62-C63

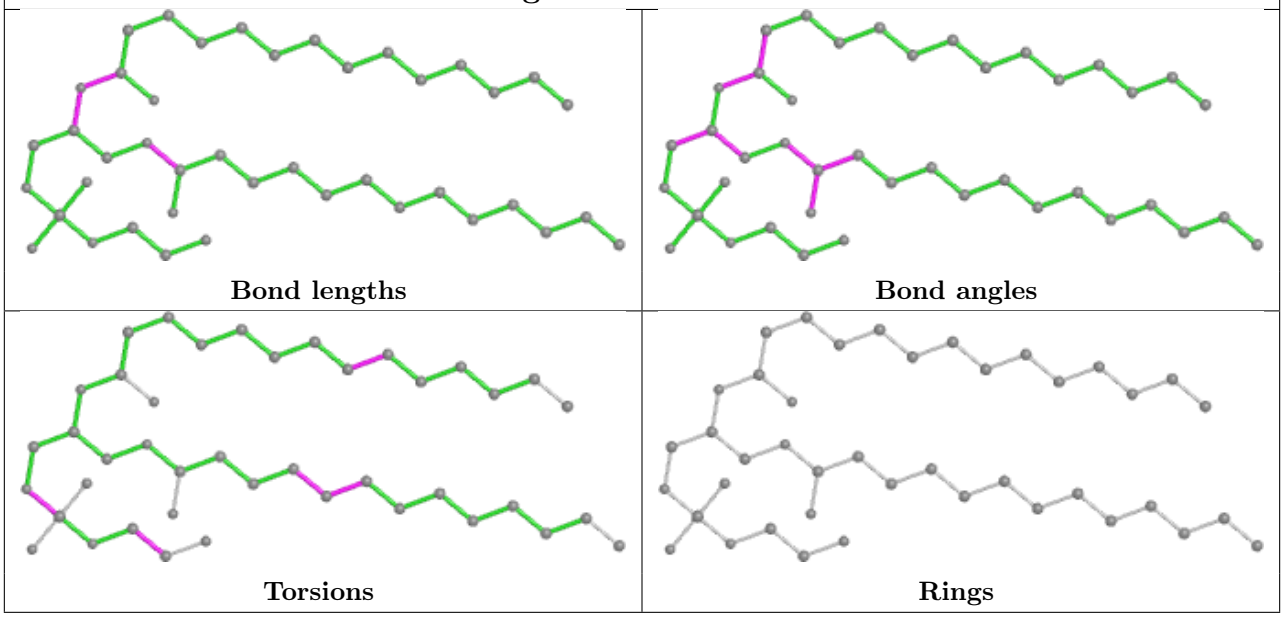
There are no ring outliers.

No monomer is involved in short contacts.

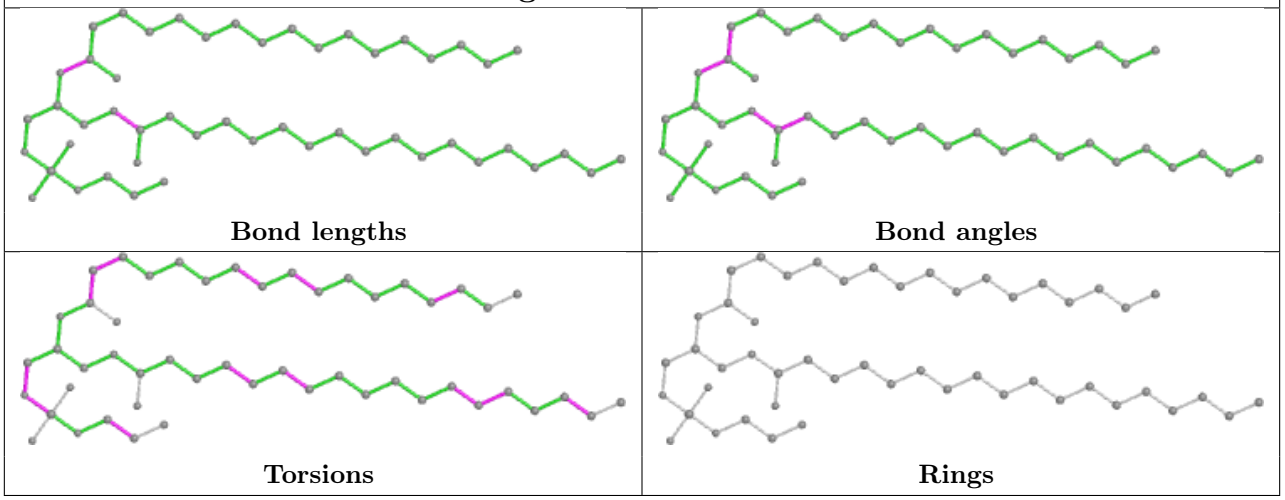
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

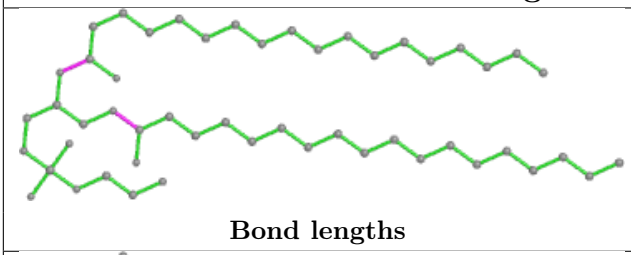
Ligand 3PE 1L 707



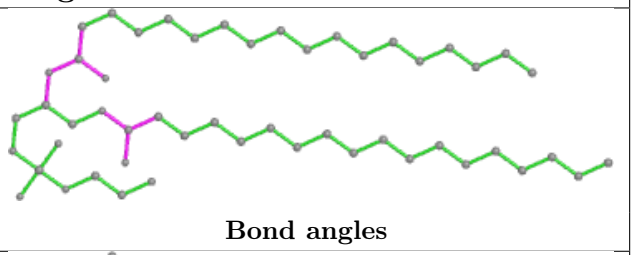
Ligand 3PE 1m 201



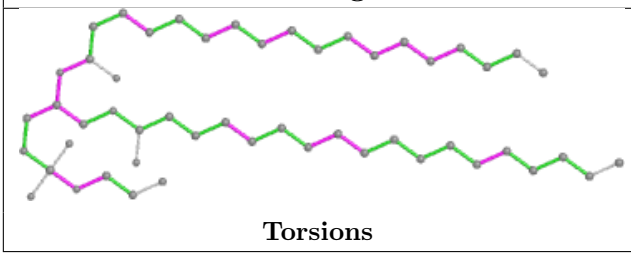
Ligand 3PE 1g 202



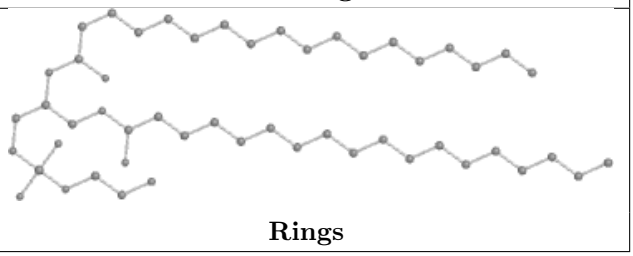
Bond lengths



Bond angles

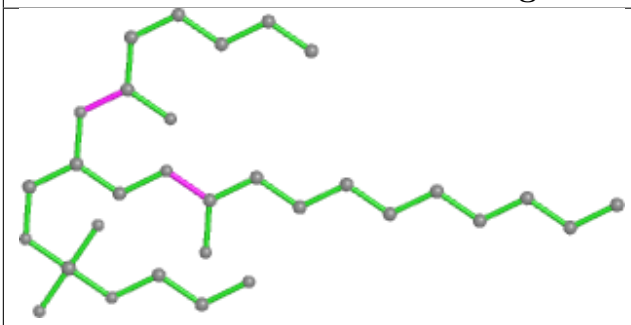


Torsions

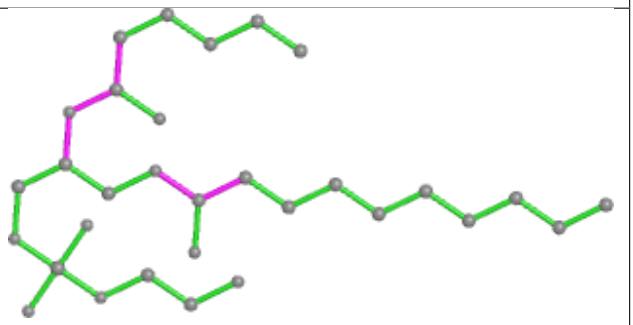


Rings

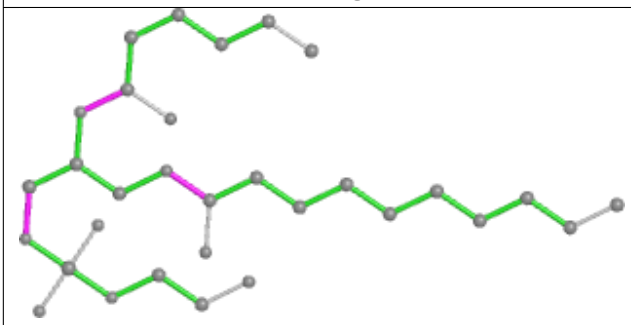
Ligand 3PE 1Y 204



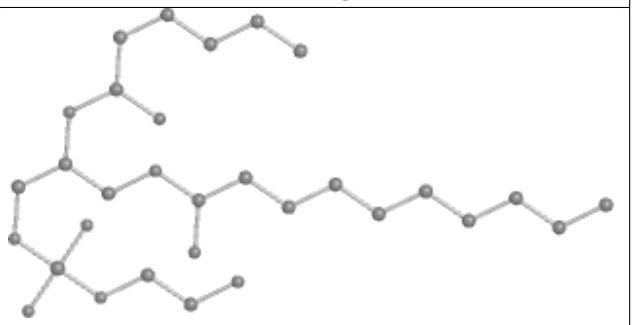
Bond lengths



Bond angles

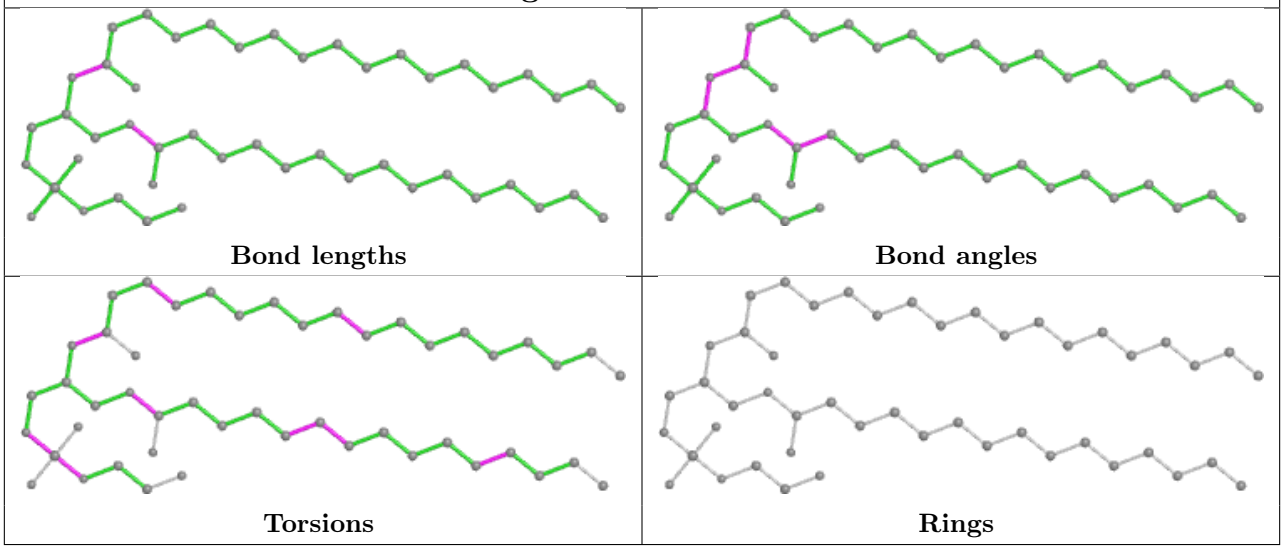


Torsions

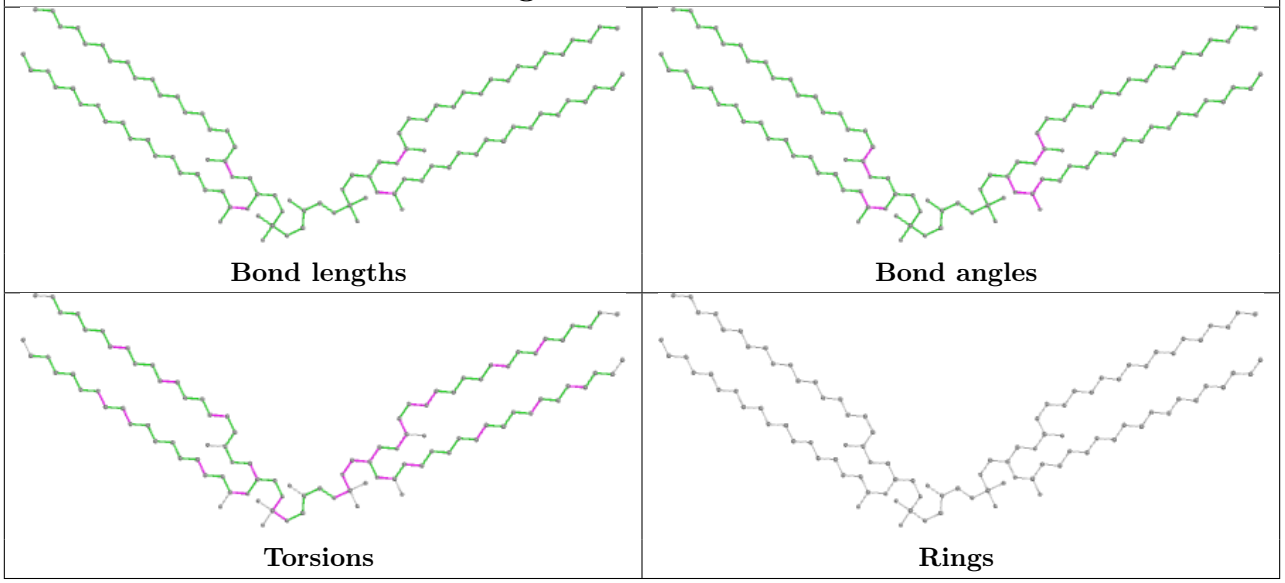


Rings

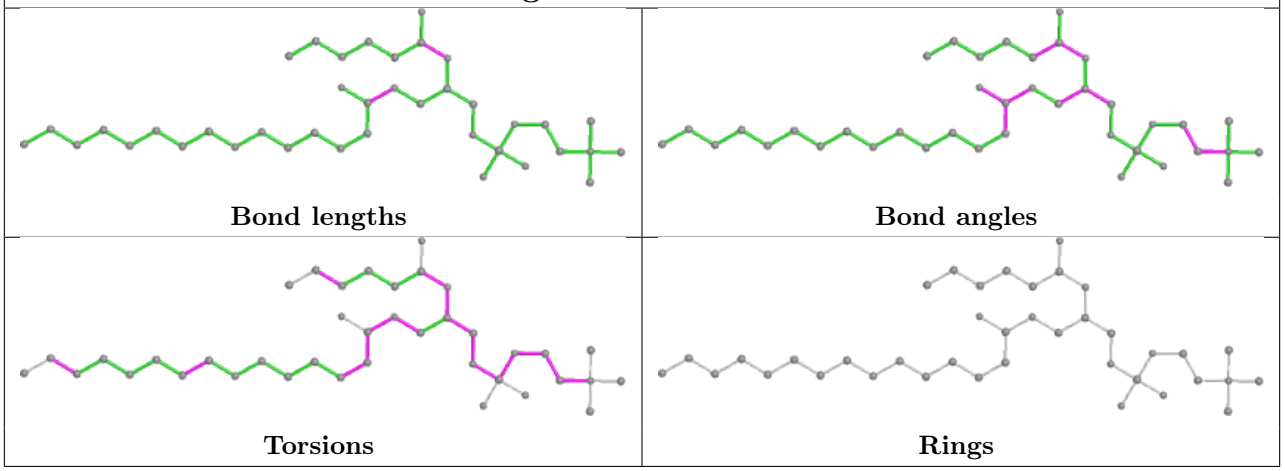
Ligand 3PE 3P 512



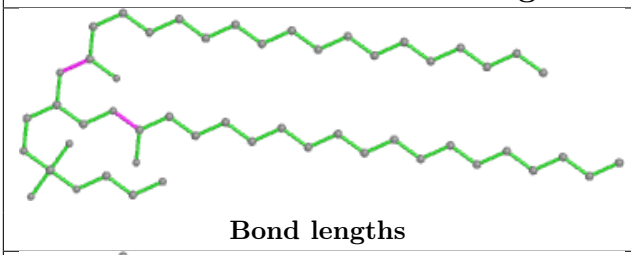
Ligand CDL 3F 201



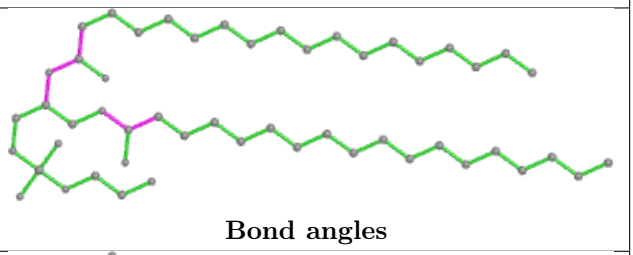
Ligand PC1 1d 204



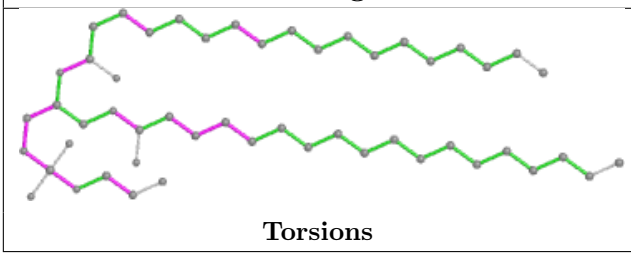
Ligand 3PE 3G 109



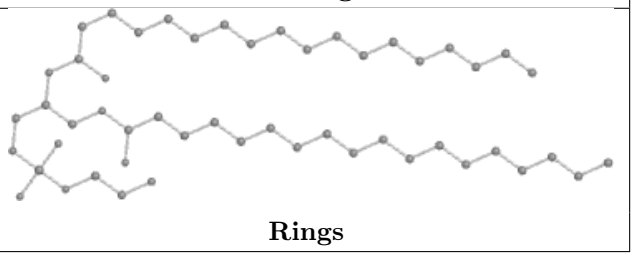
Bond lengths



Bond angles

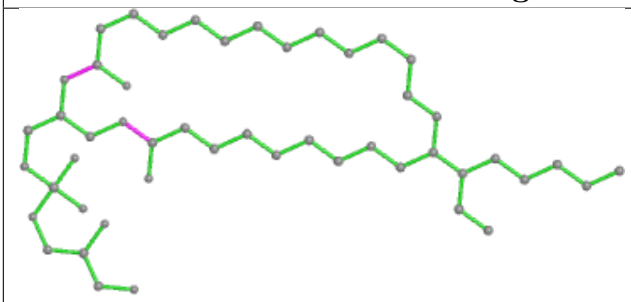


Torsions

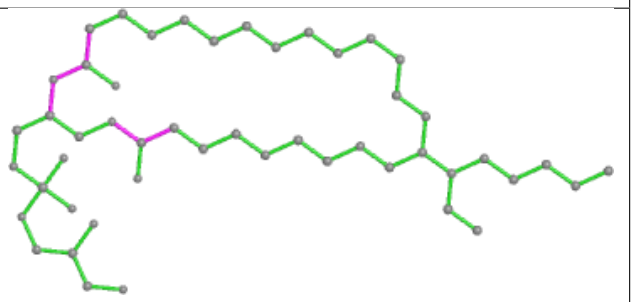


Rings

Ligand PGV 4A 608



Bond lengths



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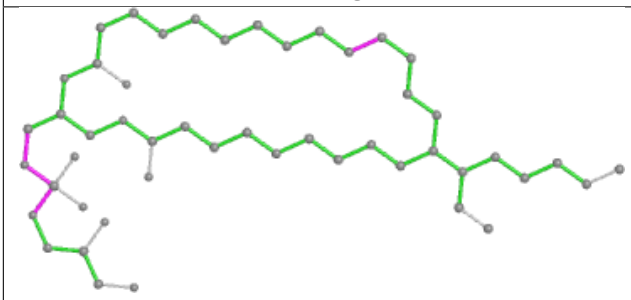

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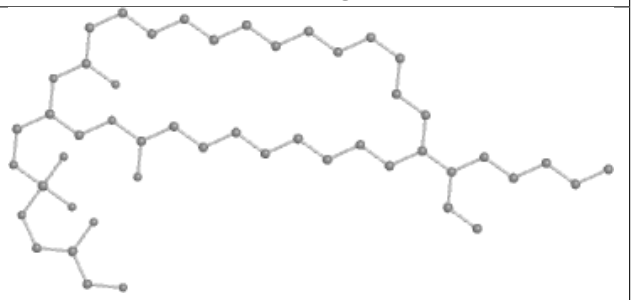

Rings

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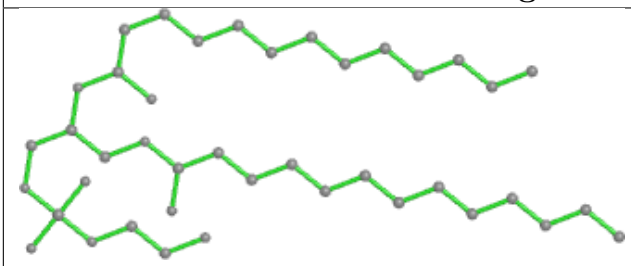

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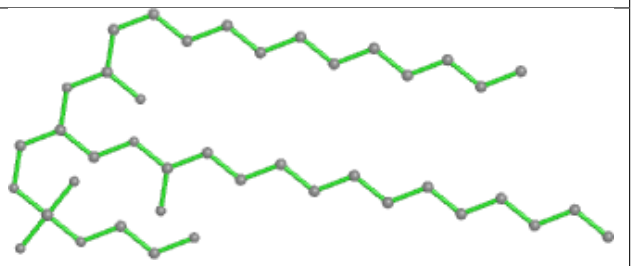

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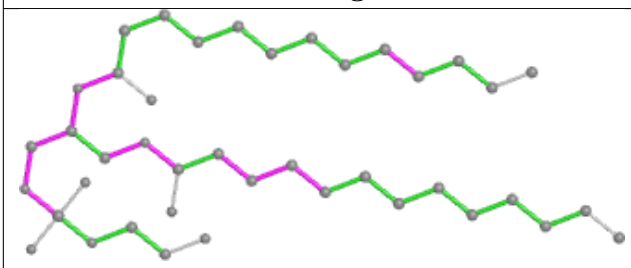

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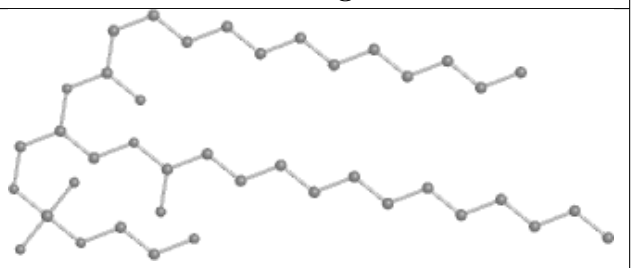
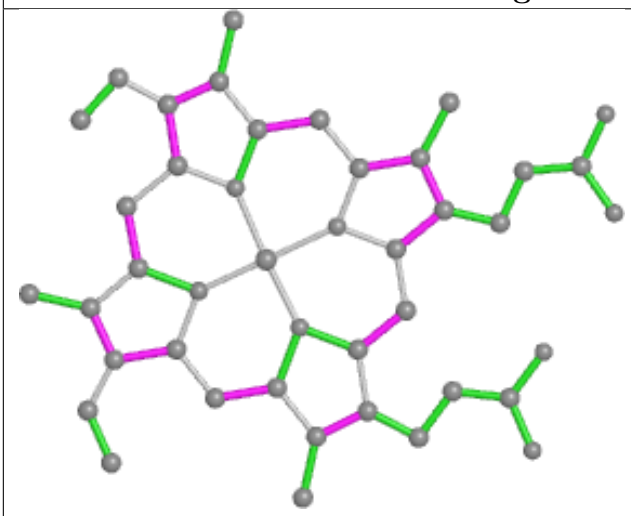
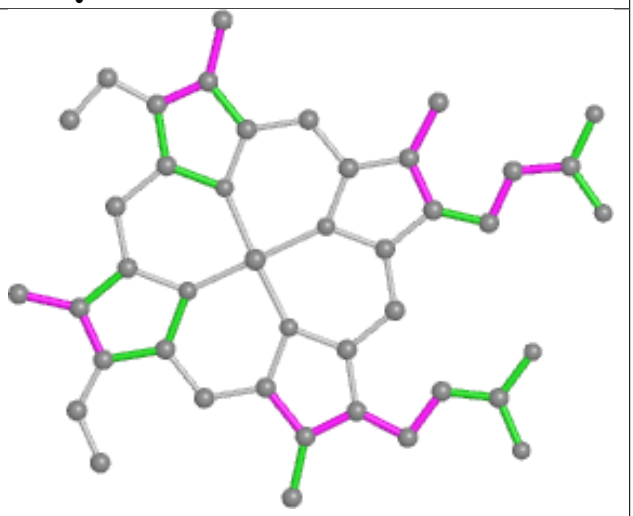


Rings

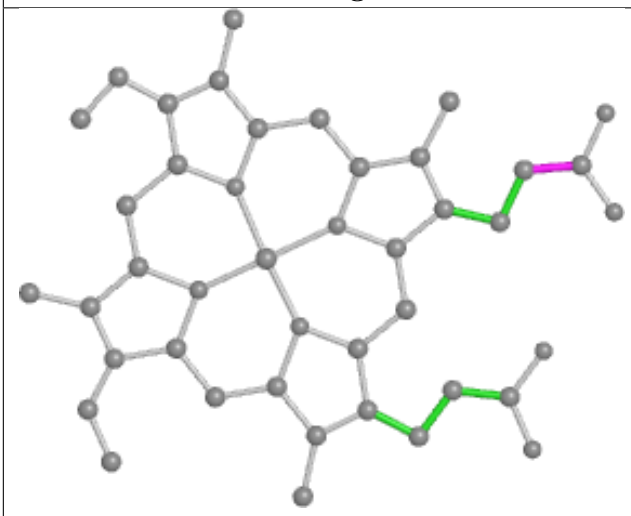
Ligand HEC 3Q 501



Bond lengths



Bond angles



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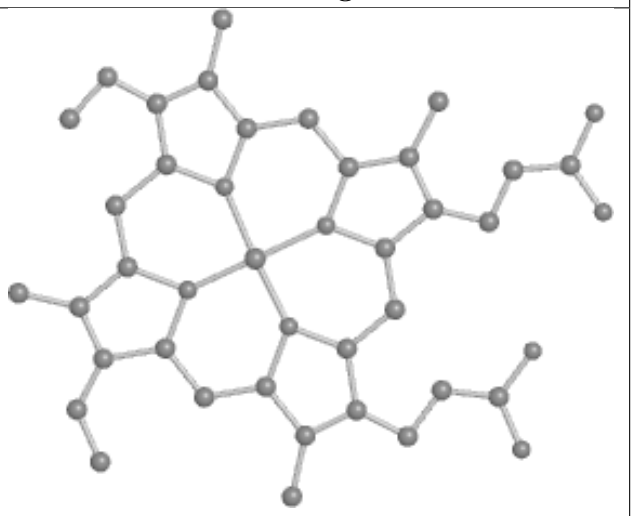
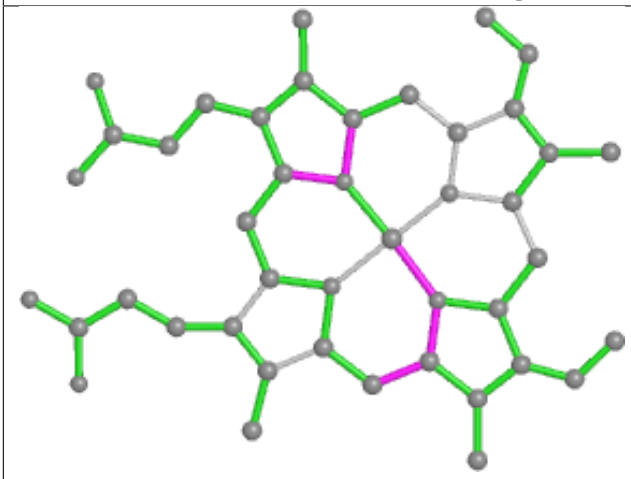
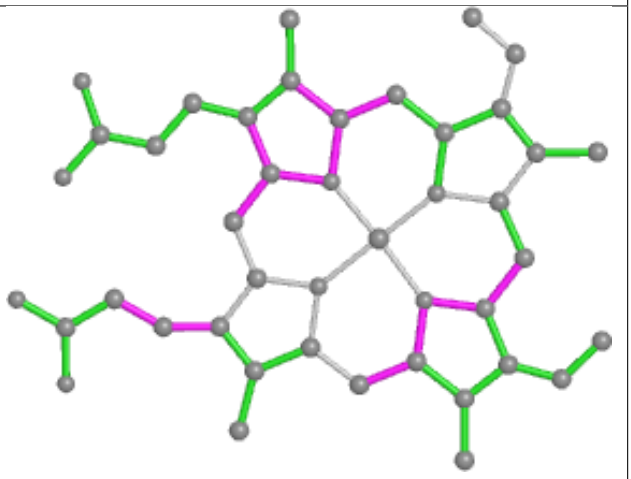


Rings

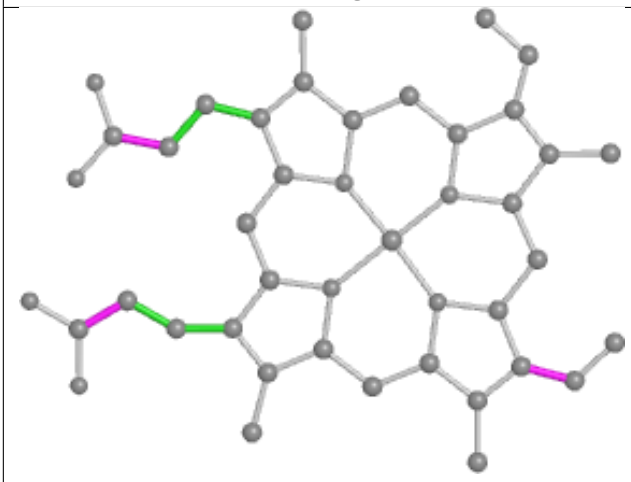
Ligand HEM 3P 501



Bond lengths



Bond angles



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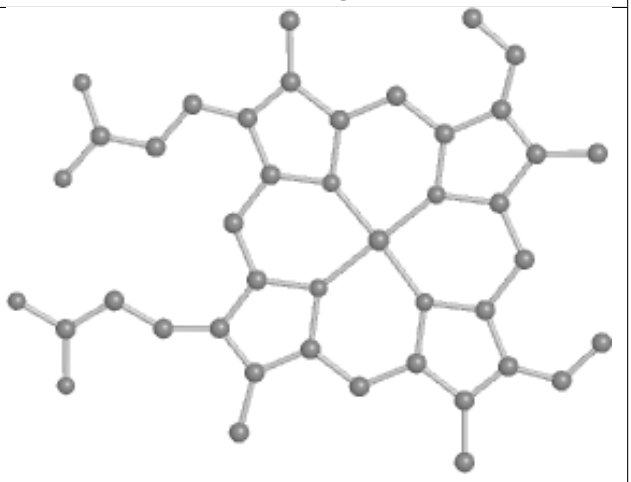
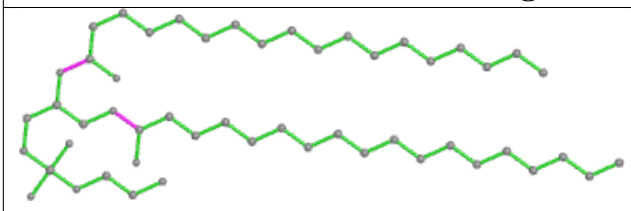
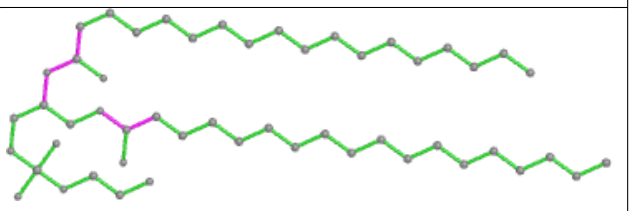


Rings

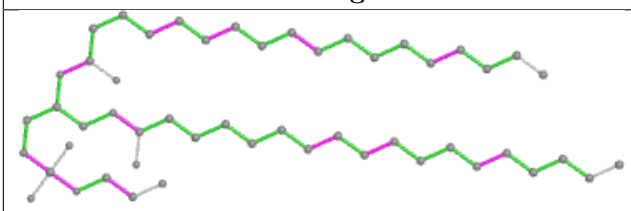
Ligand 3PE 3C 512



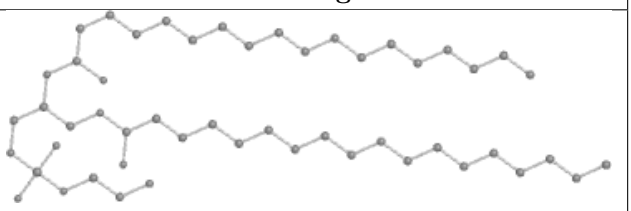
Bond lengths



Bond angles

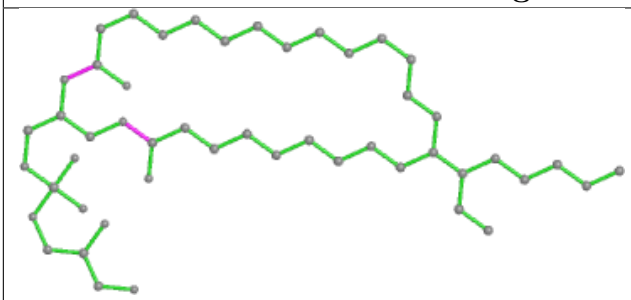


Torsions

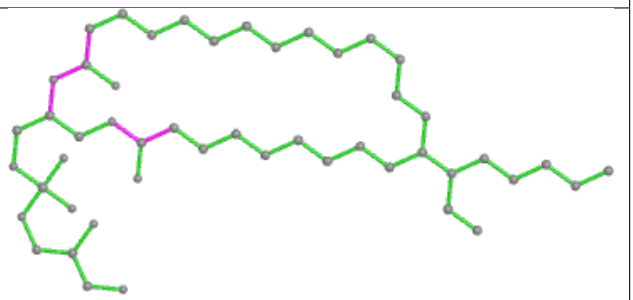


Rings

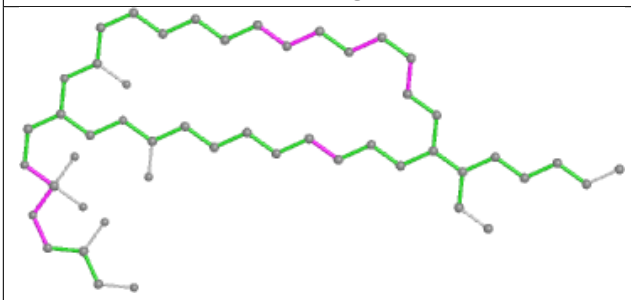
Ligand PGV 4C 305



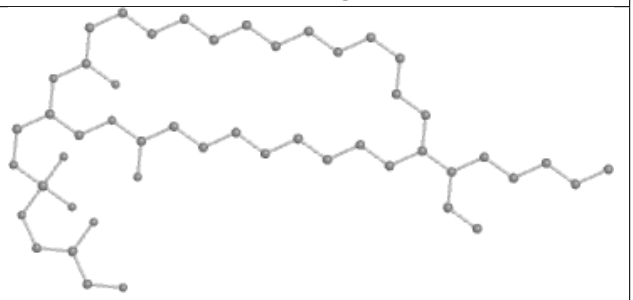
Bond lengths



Bond angles

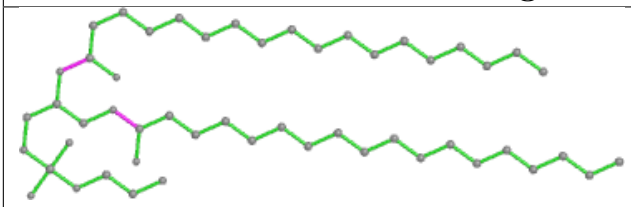


Torsions

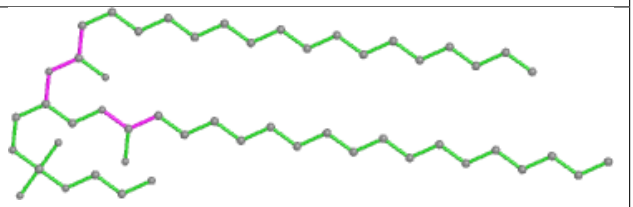


Rings

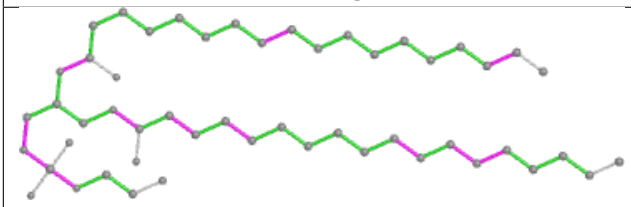
Ligand 3PE 3R 304



Bond lengths



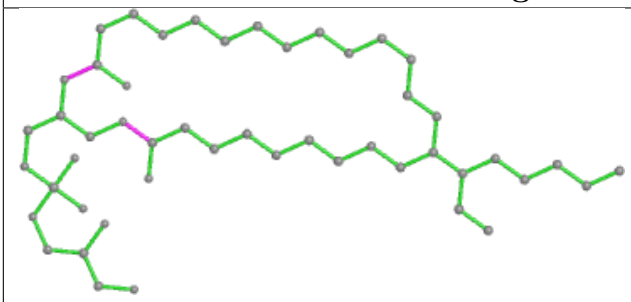
Bond angles



Torsions

Rings

Ligand PGV 4A 609



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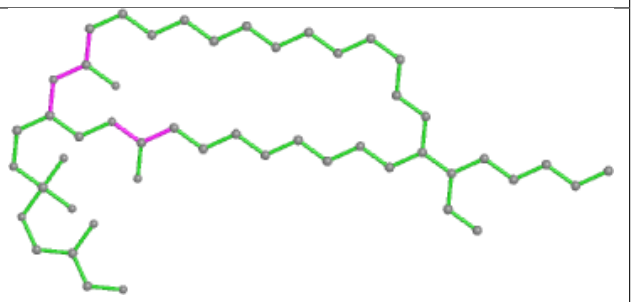
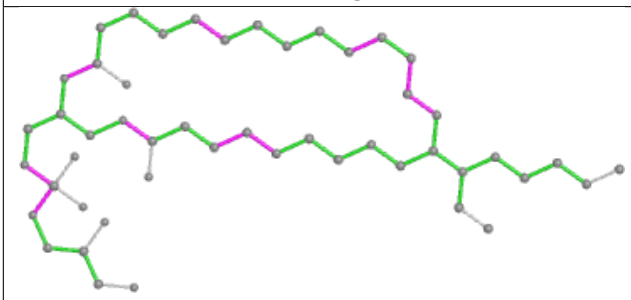
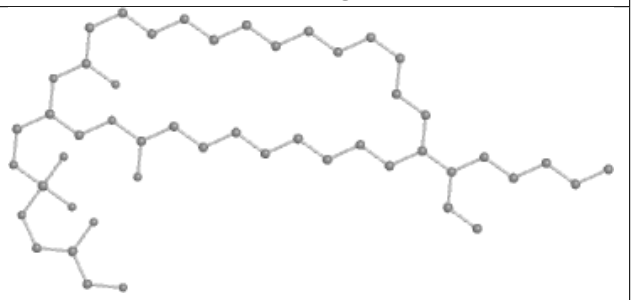


Bond angles

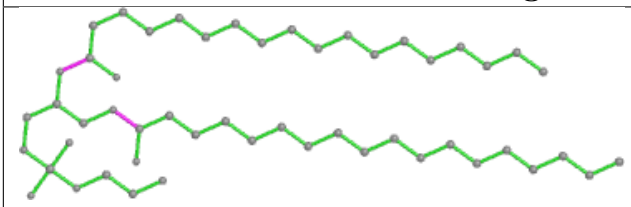


Torsions



Rings

Ligand 3PE 3S 201



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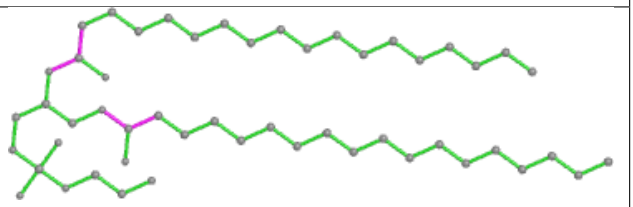
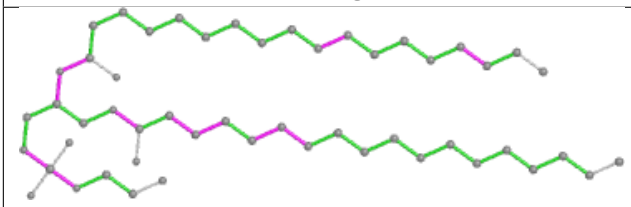


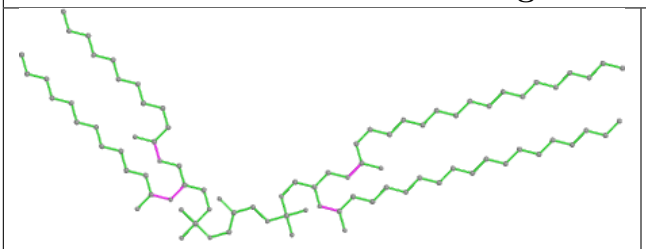
Bond angles



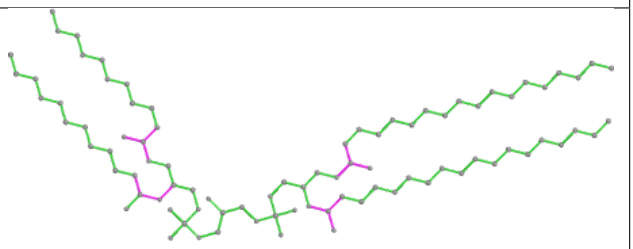
Torsions

Rings

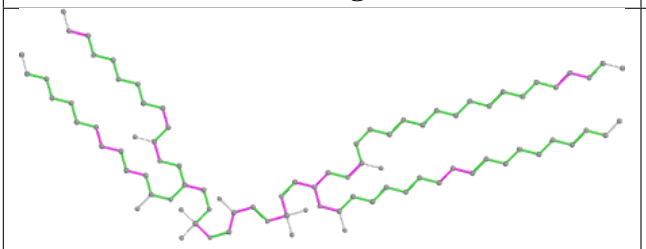
Ligand CDL 1L 704



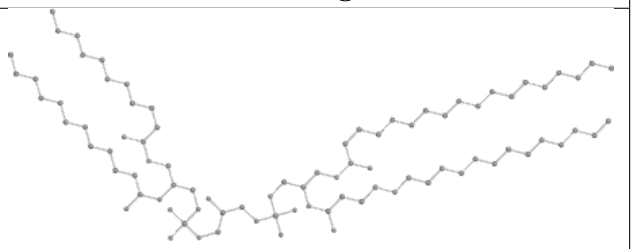
Bond lengths



Bond angles

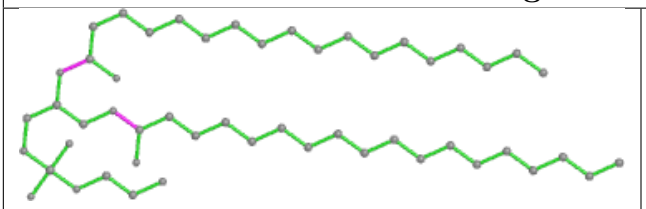


Torsions



Rings

Ligand 3PE 3J 104



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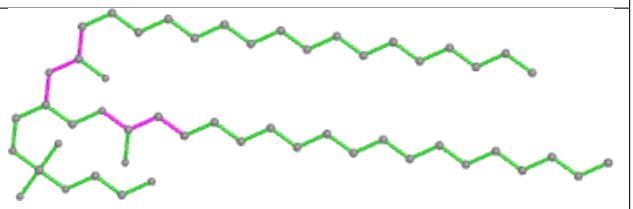
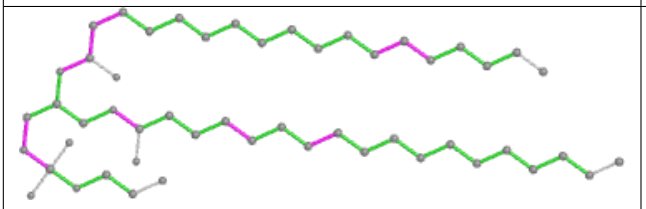


Bond angles



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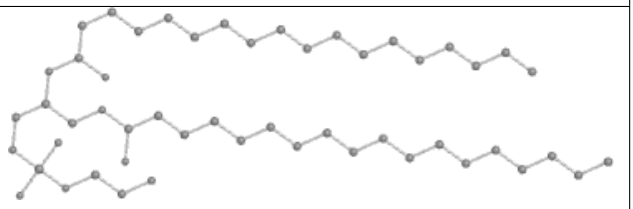
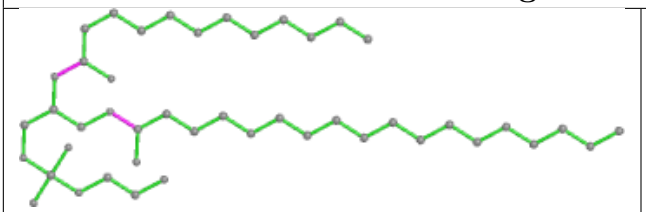


Rings

Ligand 3PE 3Y 102



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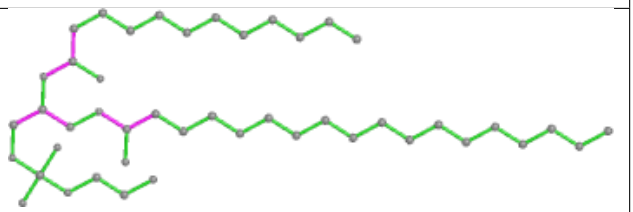
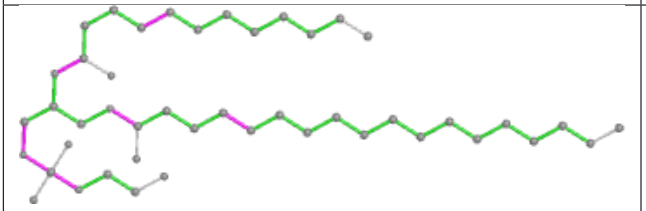
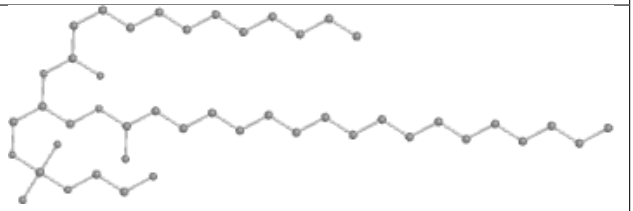


Bond angles

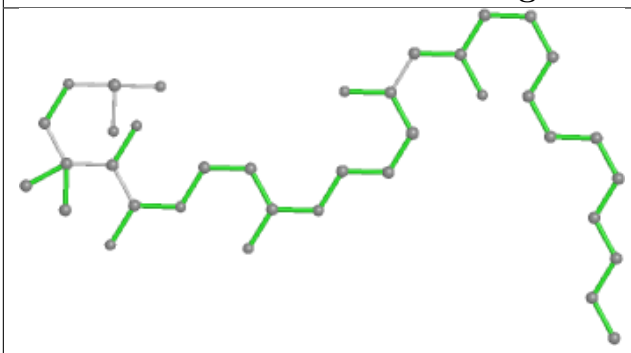


Torsions



Rings

Ligand EHZ 1n 201



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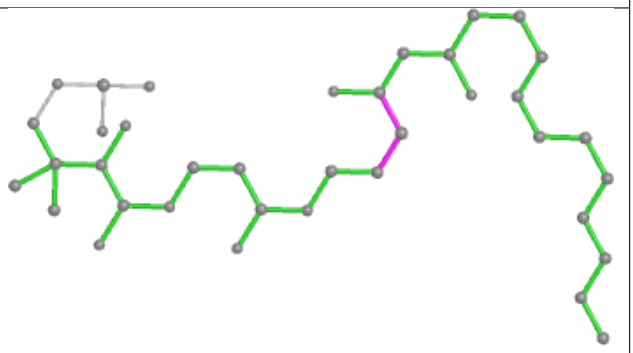
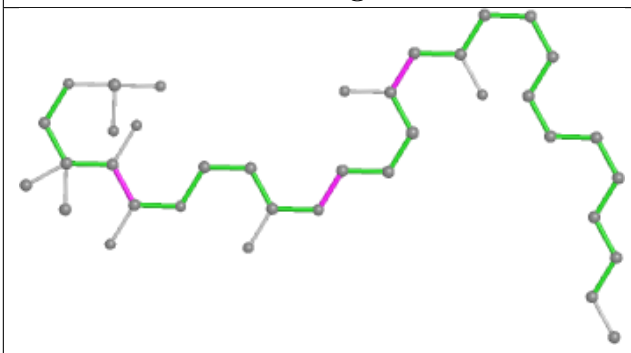


Bond angles



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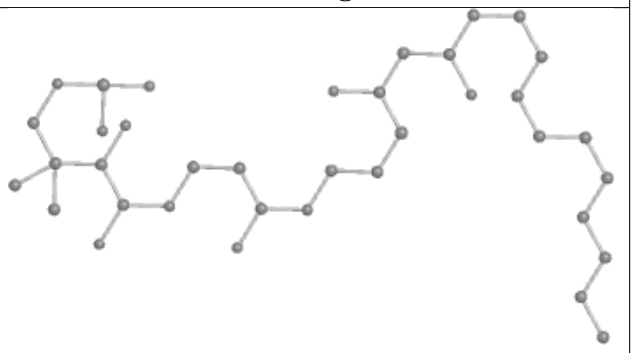
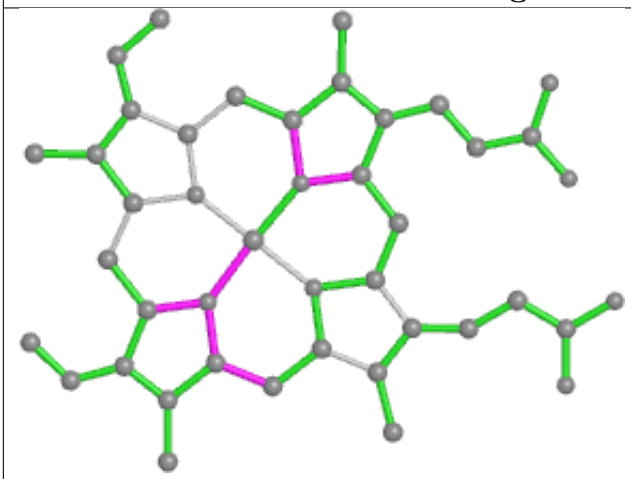
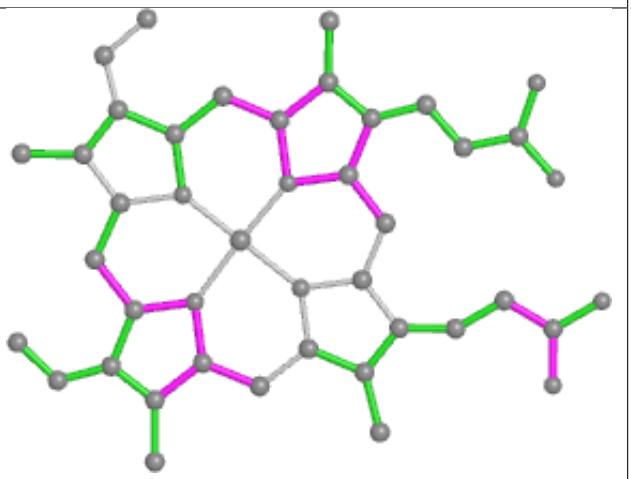


Rings

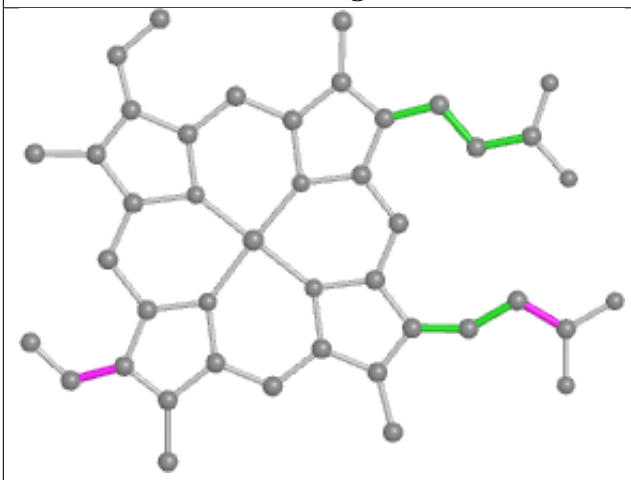
Ligand HEM 3C 502



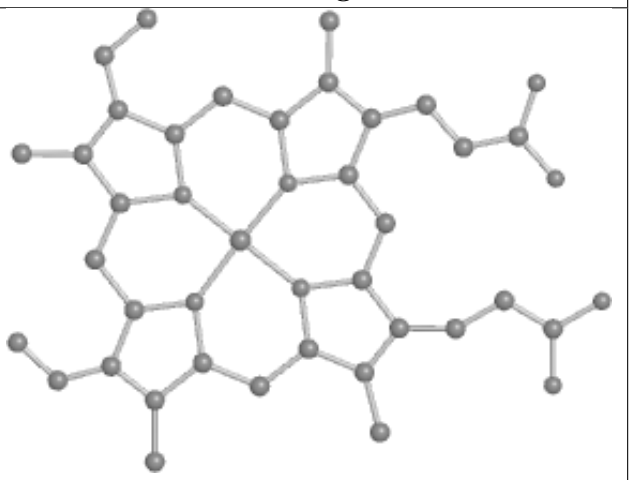
Bond lengths



Bond angles

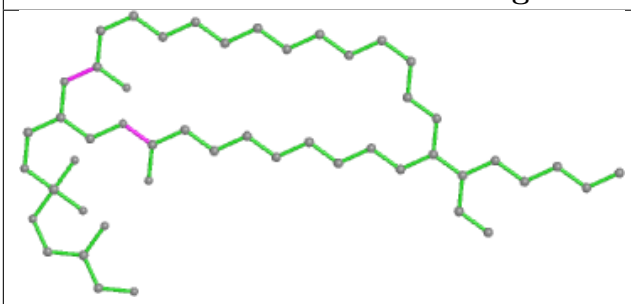


Torsions



Rings

Ligand PGV 4A 606



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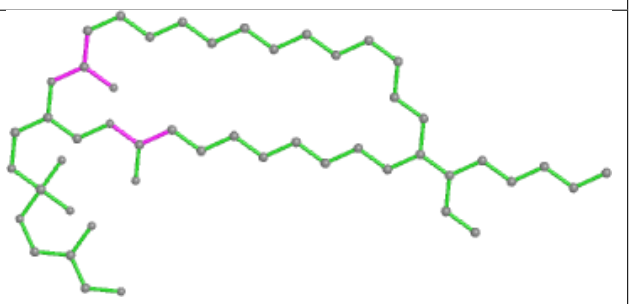
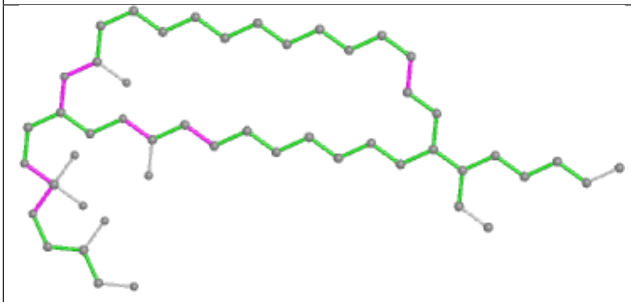
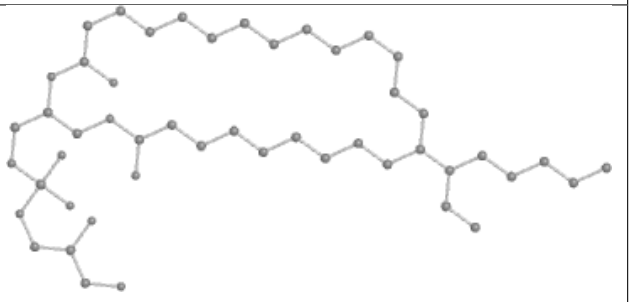


Bond angles

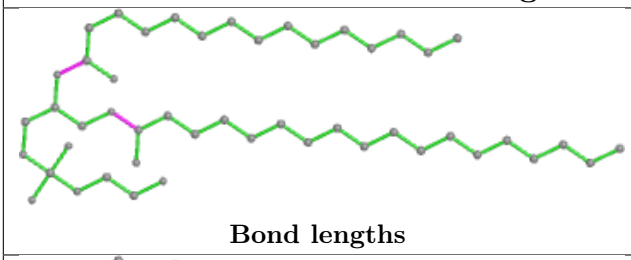


Torsions



Rings

Ligand 3PE 3C 508



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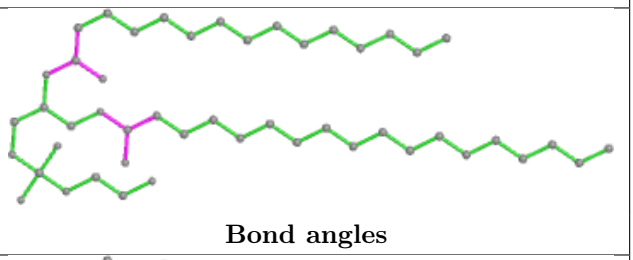
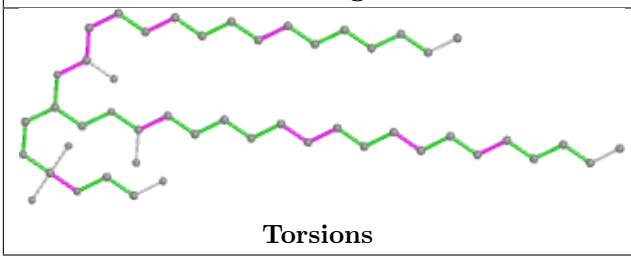


Bond angles



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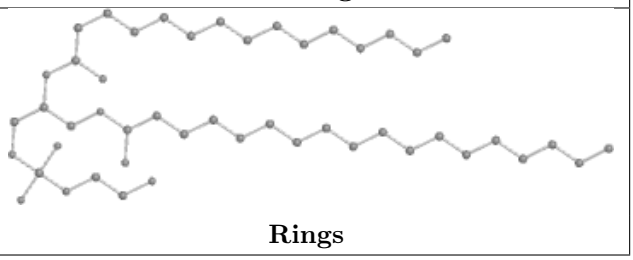
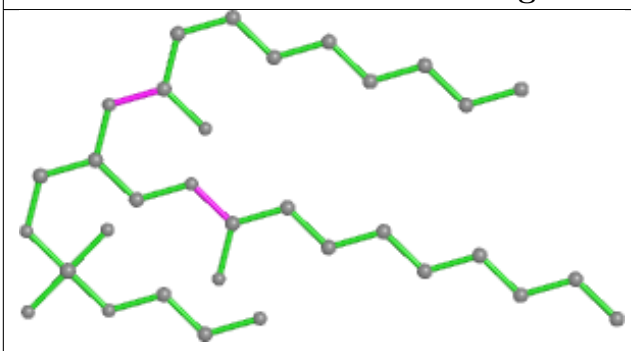
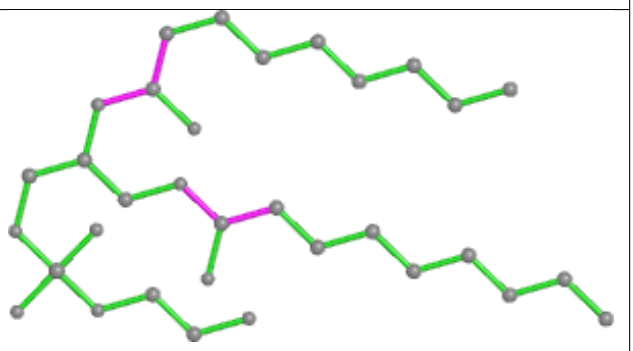


Rings

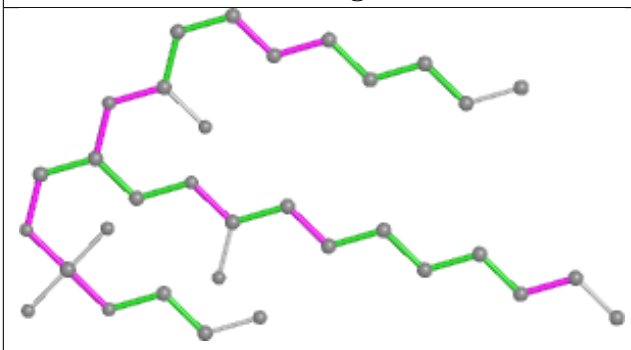
Ligand 3PE 3G 102



Bond lengths



Bond angles



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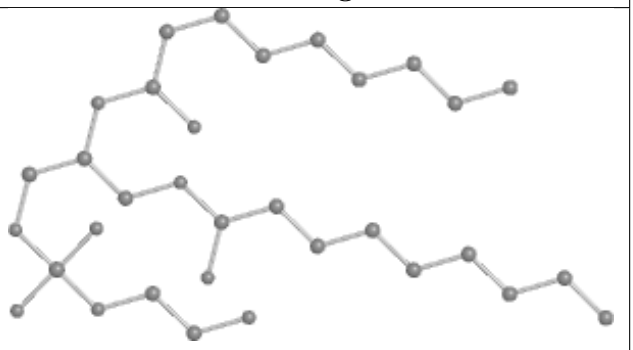
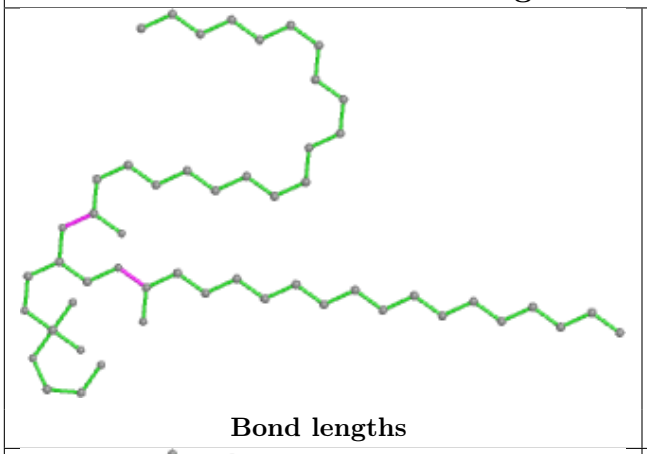
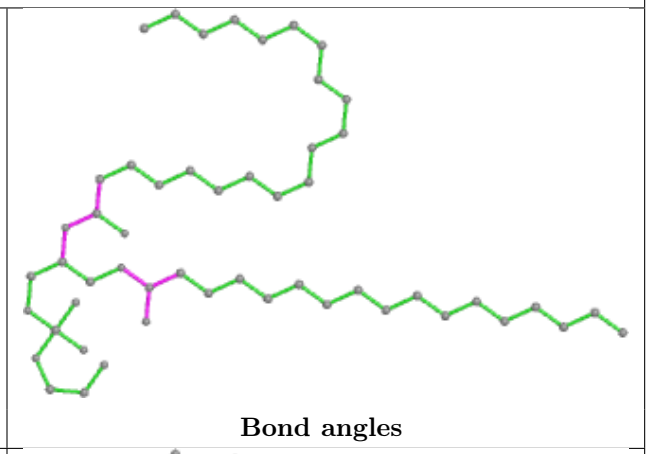


Rings

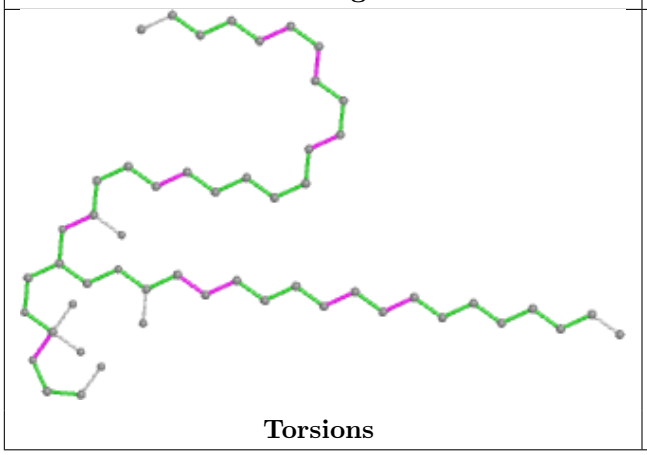
Ligand PEK 4G 103



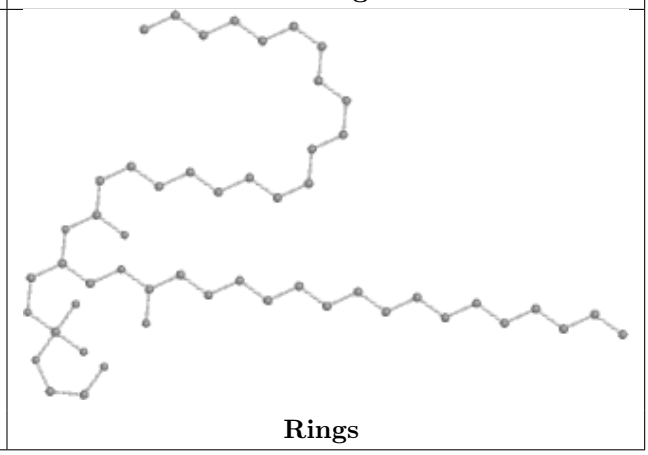
Bond lengths



Bond angles

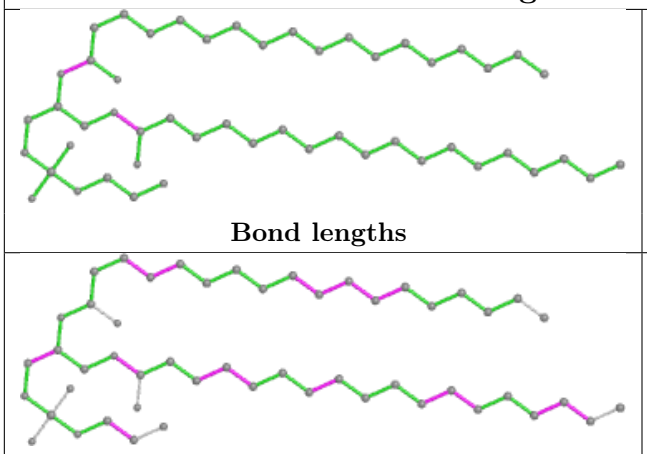


Torsions

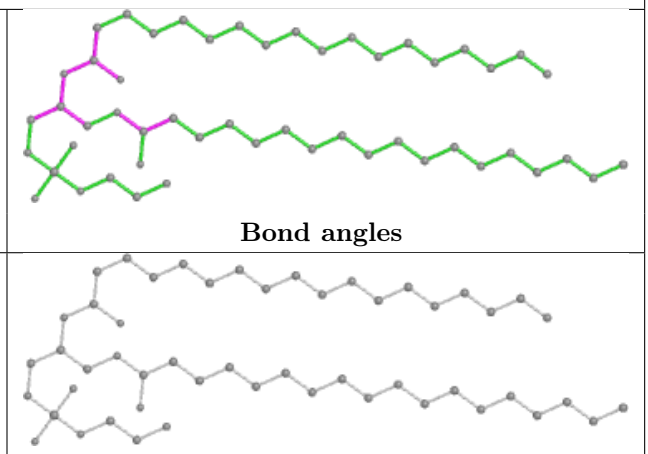


Rings

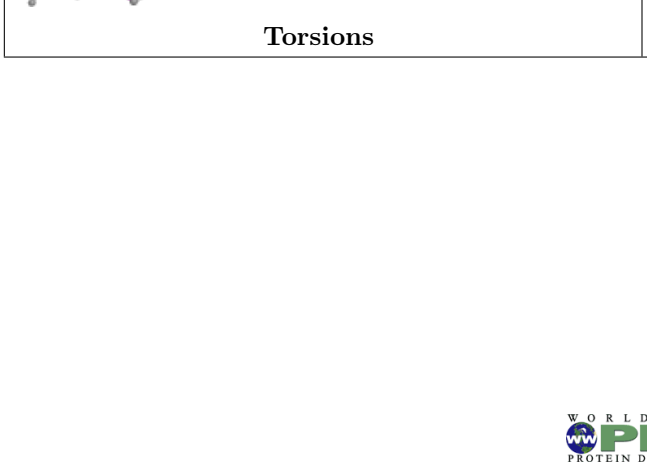
Ligand 3PE 1N 401



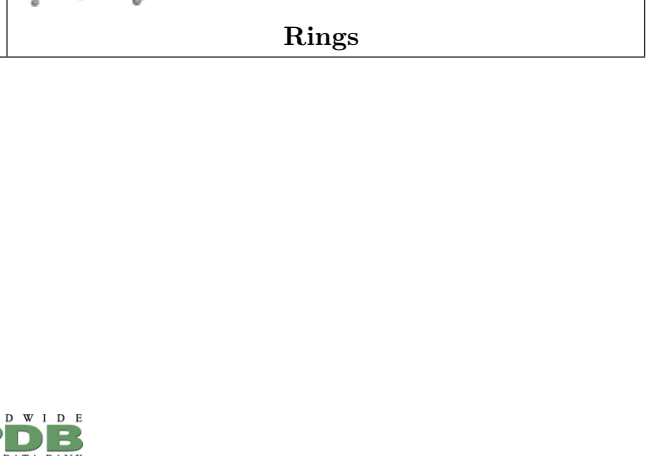
Bond lengths



Bond angles

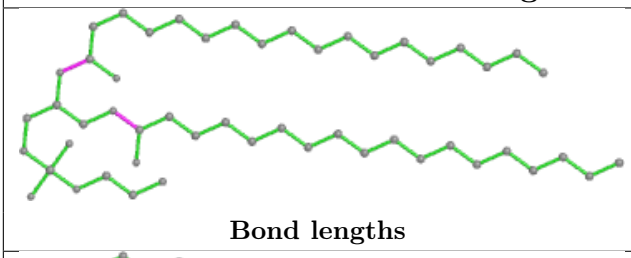


Torsions

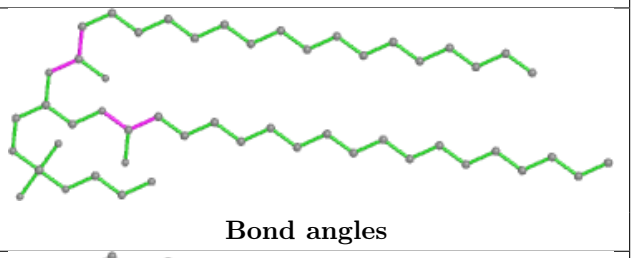


Rings

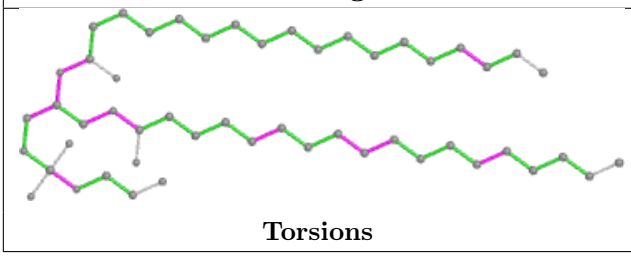
Ligand 3PE 3P 514



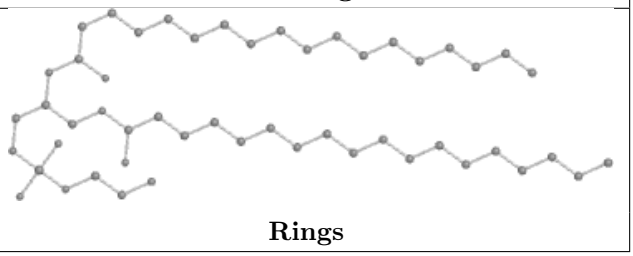
Bond lengths



Bond angles

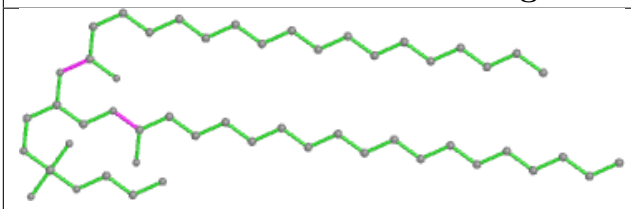


Torsions



Rings

Ligand 3PE 3T 103



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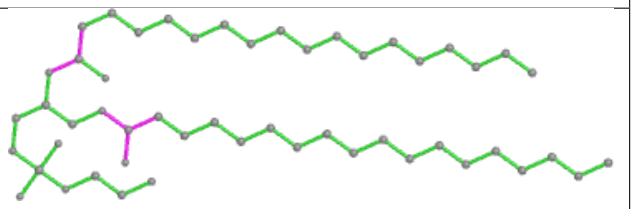
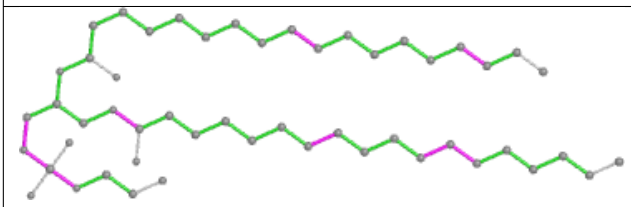


Bond angles



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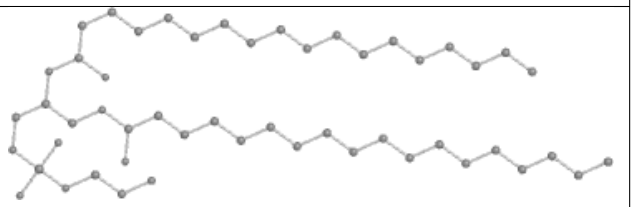
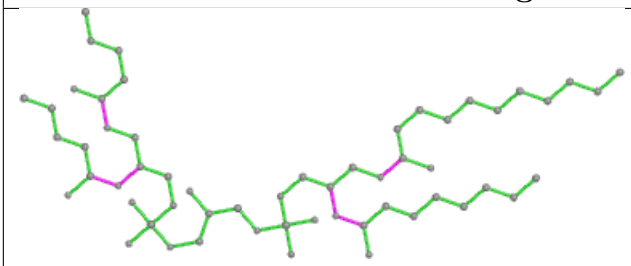
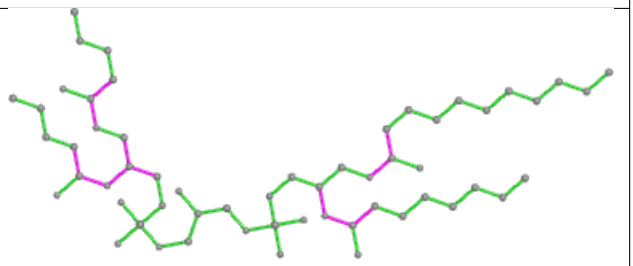


Rings

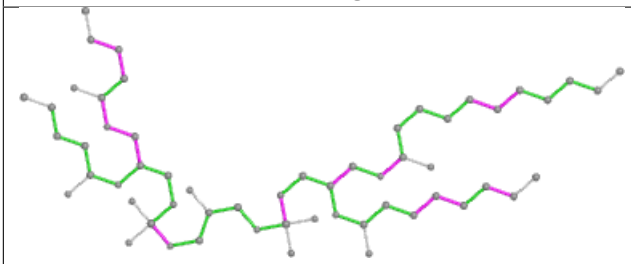
Ligand CDL 3T 101



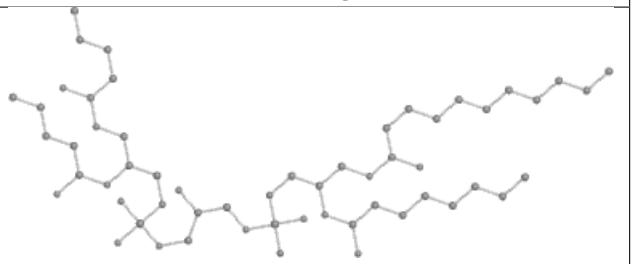
Bond lengths



Bond angles

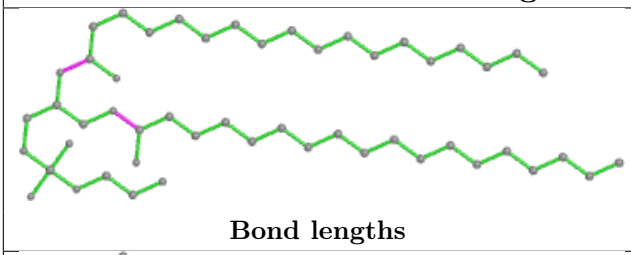


Torsions



Rings

Ligand 3PE 1B 204



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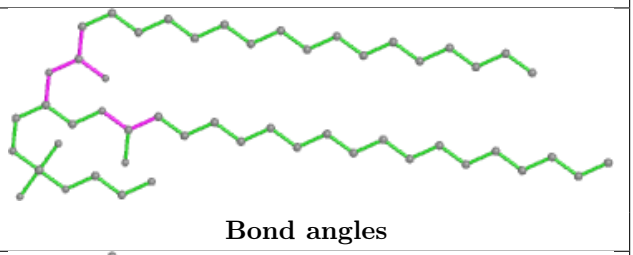
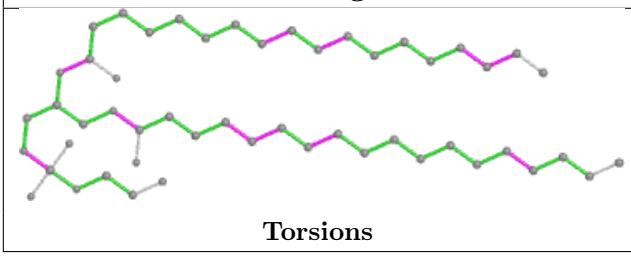


Bond angles



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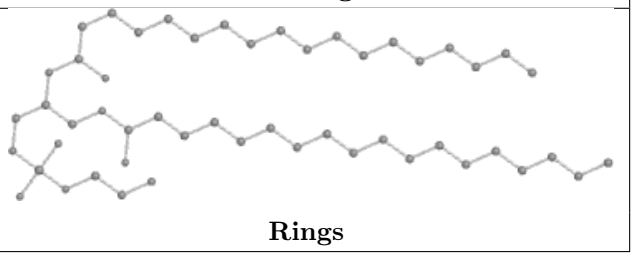
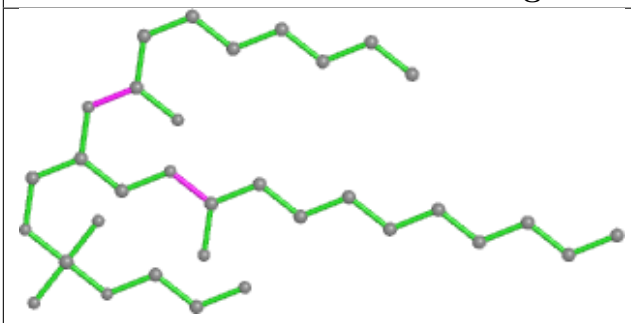
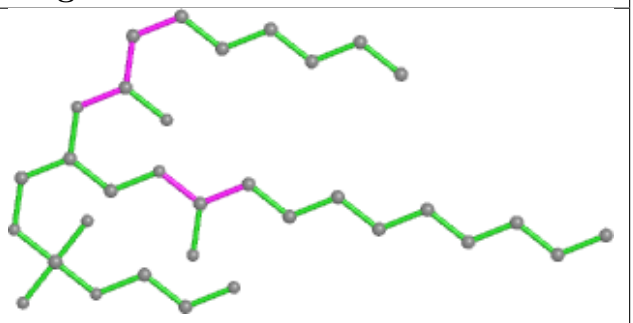


Rings

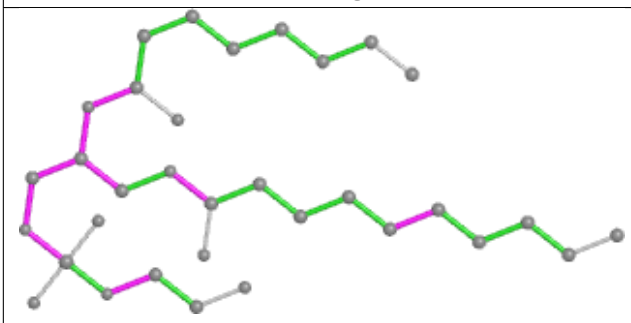
Ligand 3PE 1g 203



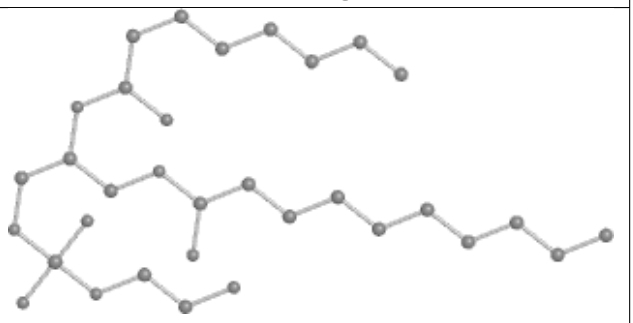
Bond lengths



Bond angles

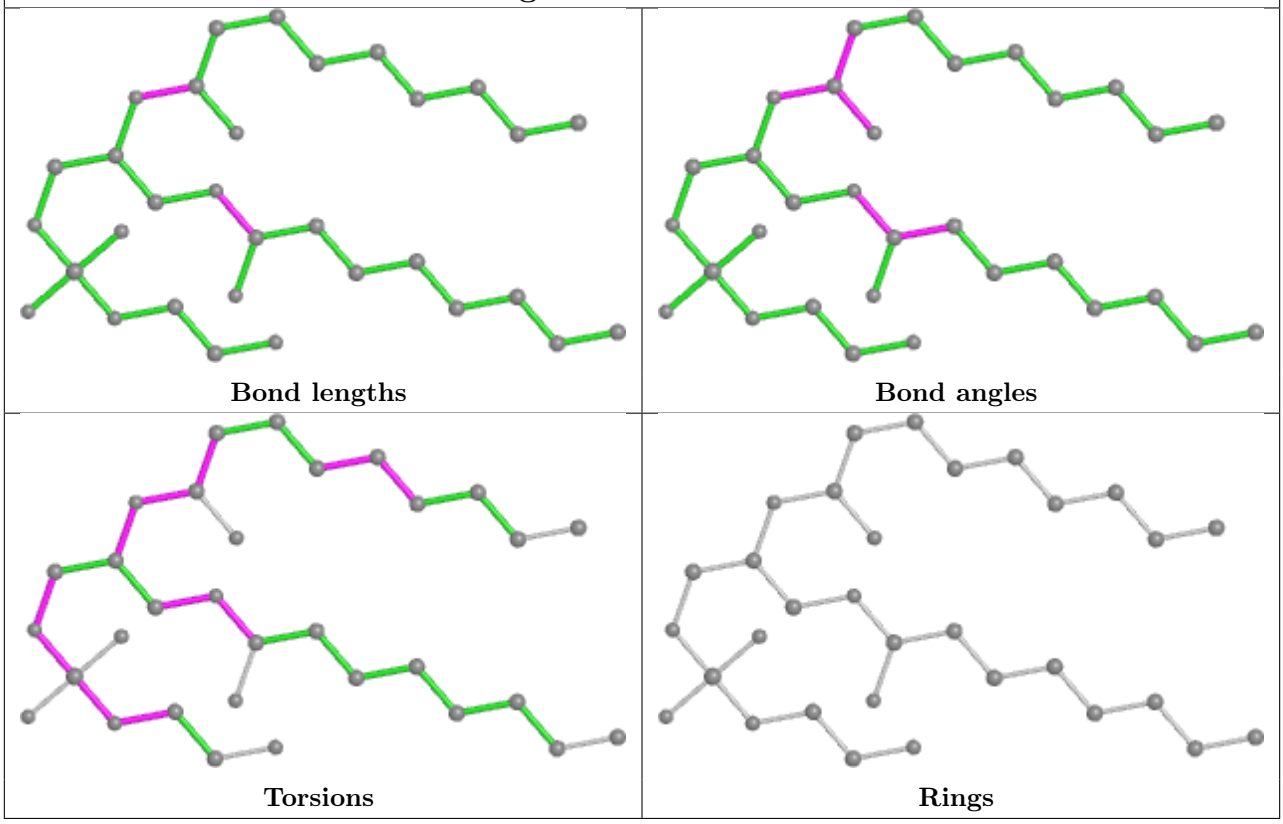


Torsions

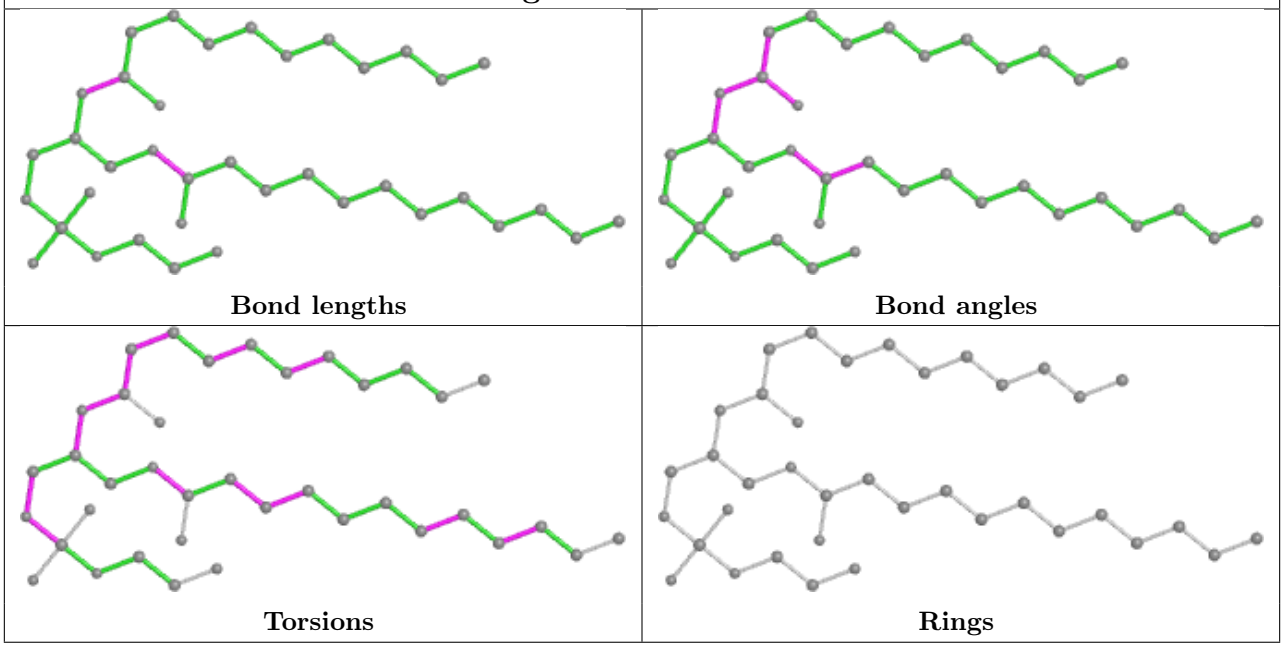


Rings

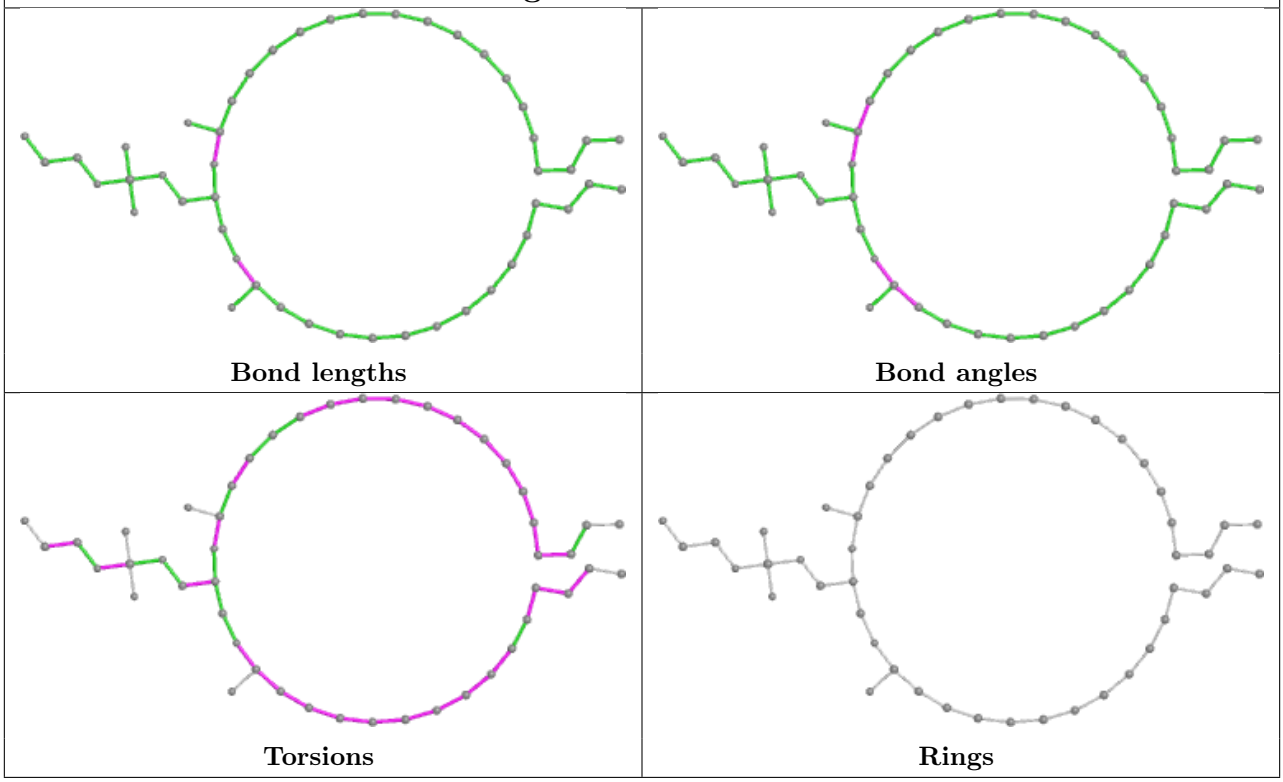
Ligand 3PE 4G 101



Ligand 3PE 1L 710



Ligand 3PE 1d 201



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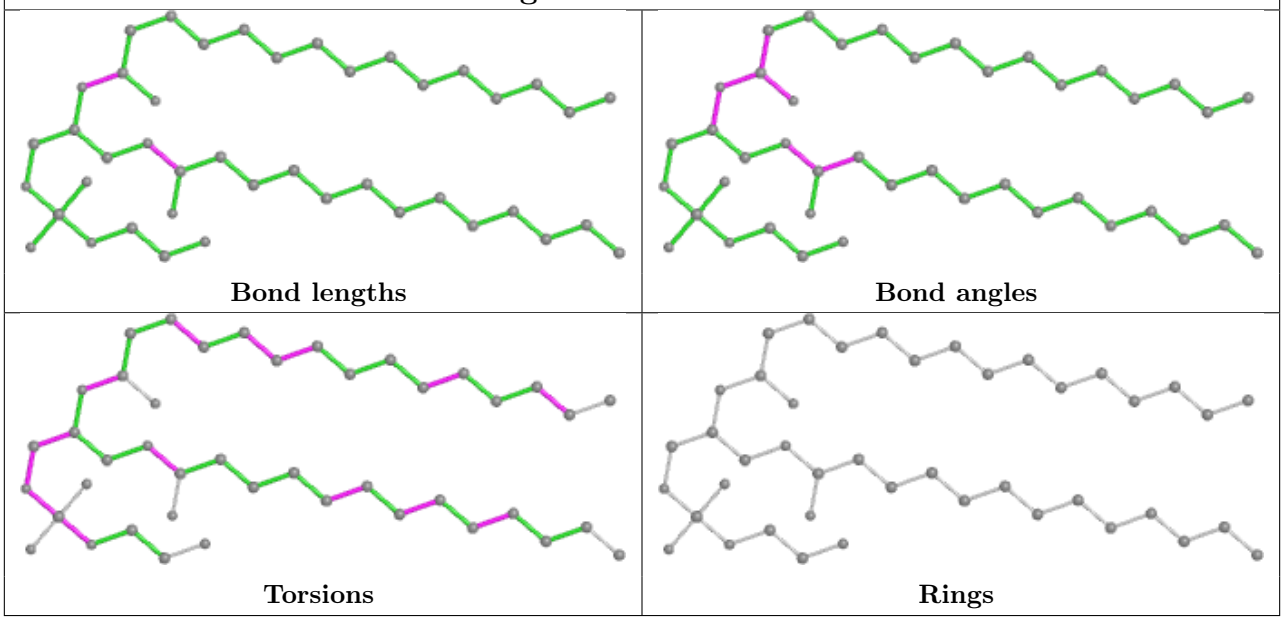

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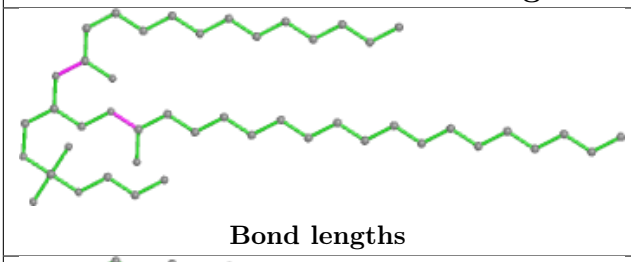
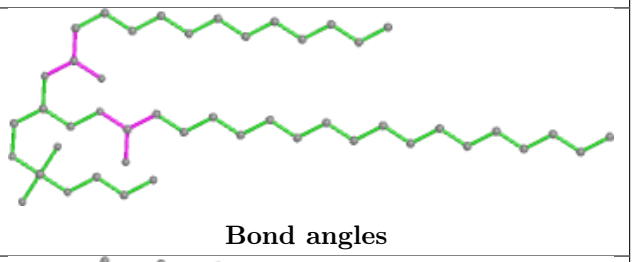
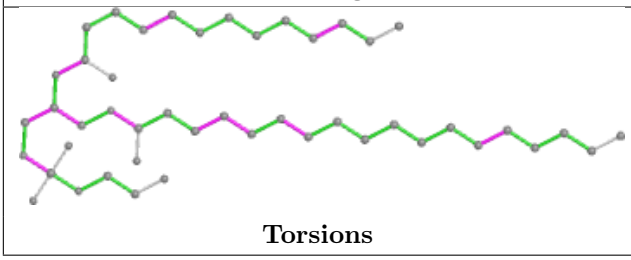


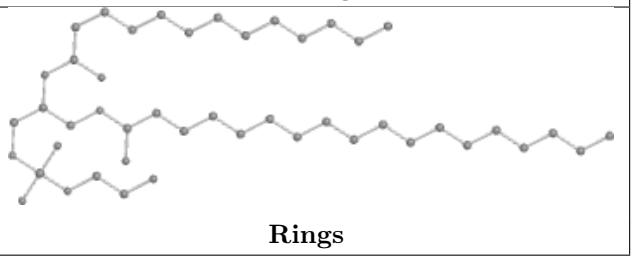
Bond lengths



Bond angles

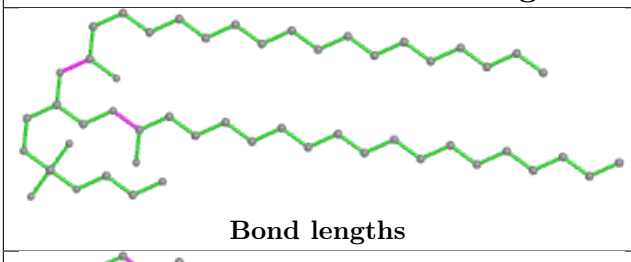


Torsions

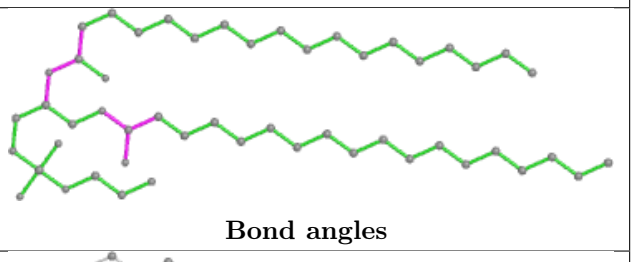


Rings

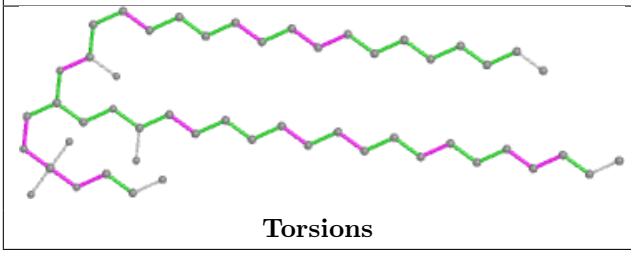
Ligand 3PE 3A 503



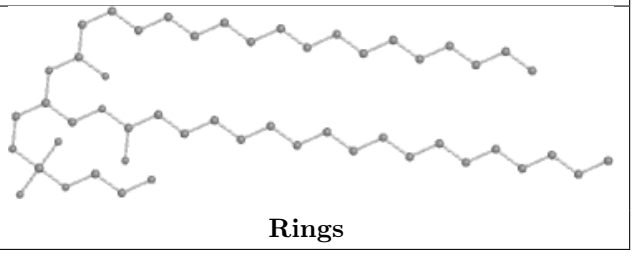
Bond lengths



Bond angles

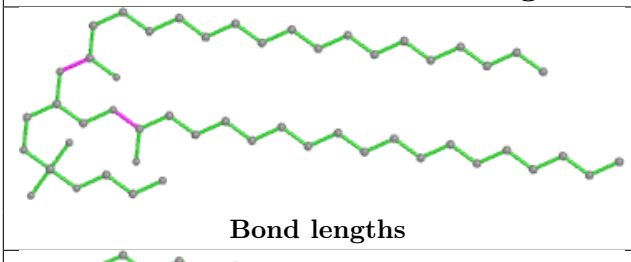


Torsions

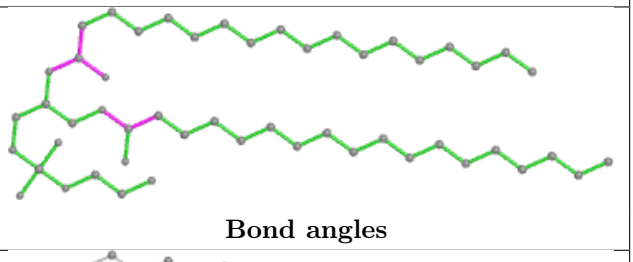


Rings

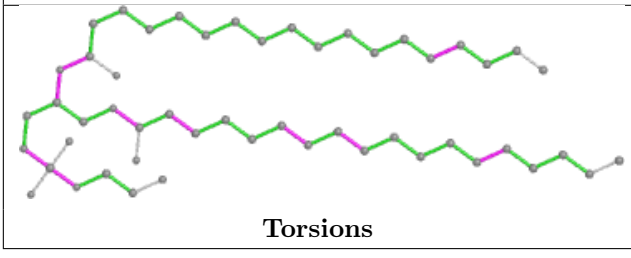
Ligand 3PE 1B 205



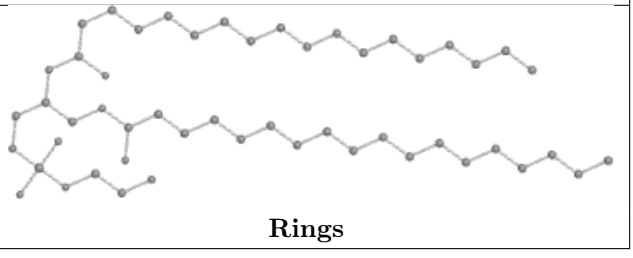
Bond lengths



Bond angles

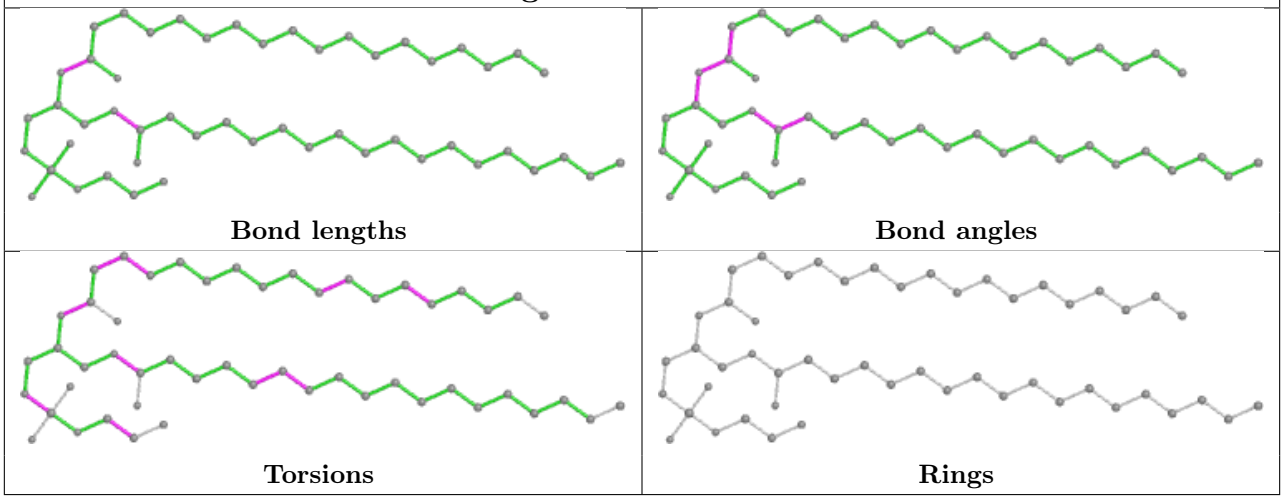


Torsions

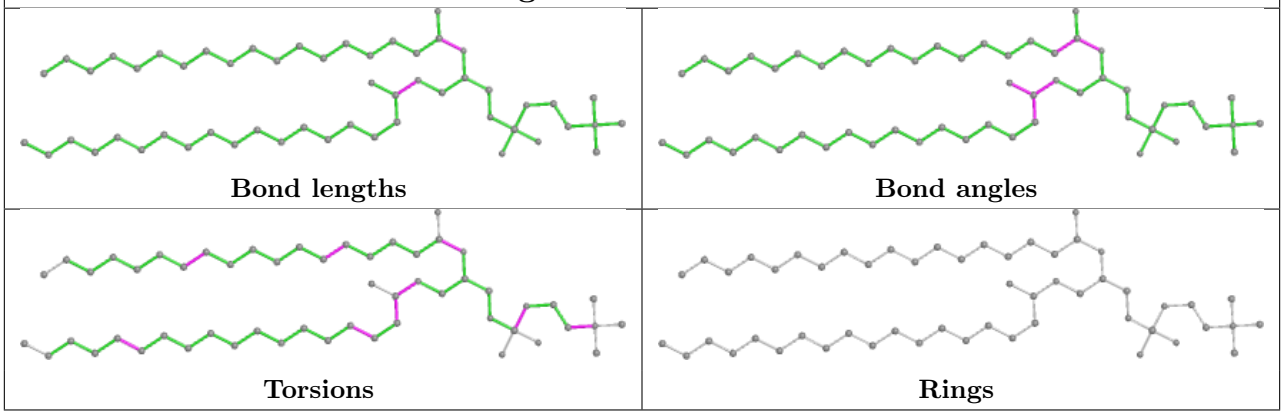


Rings

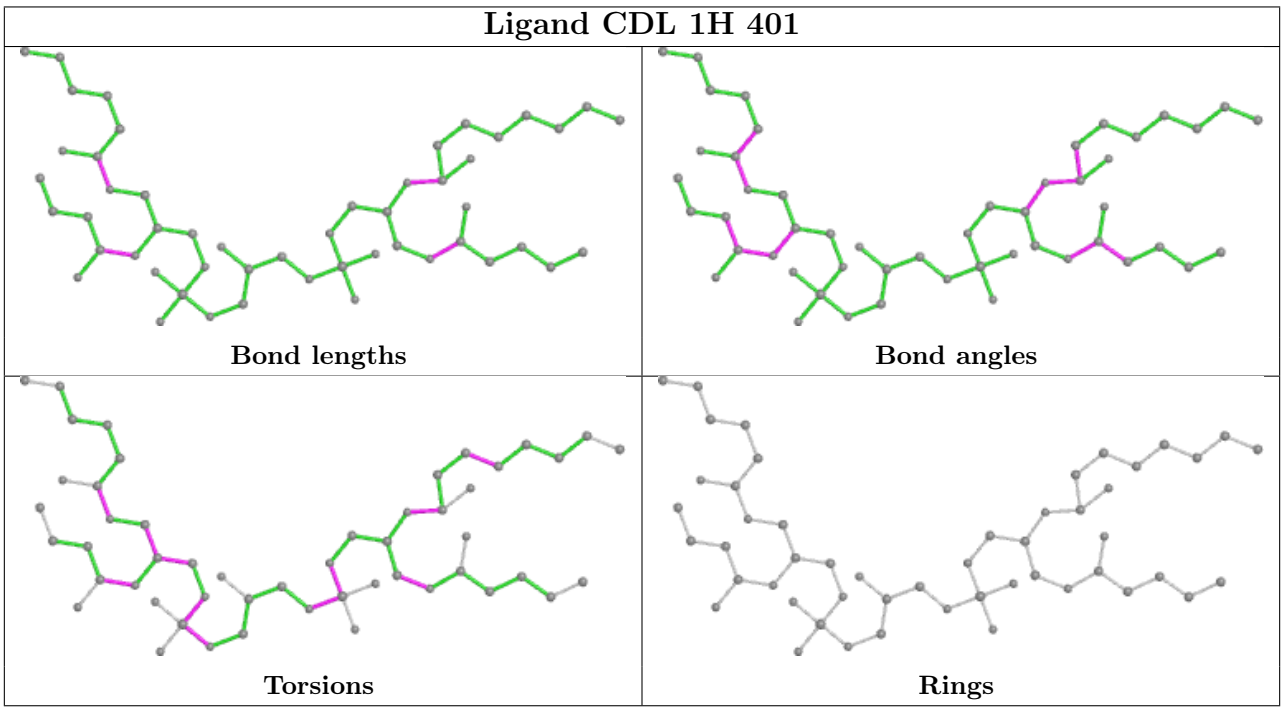
Ligand 3PE 3P 520



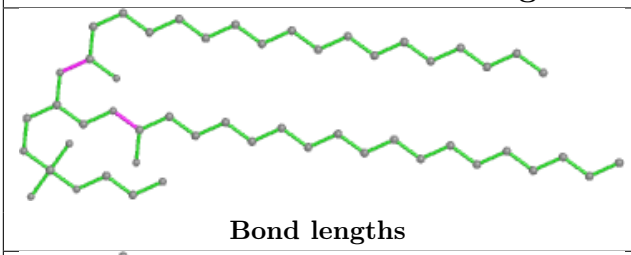
Ligand PC1 1H 402



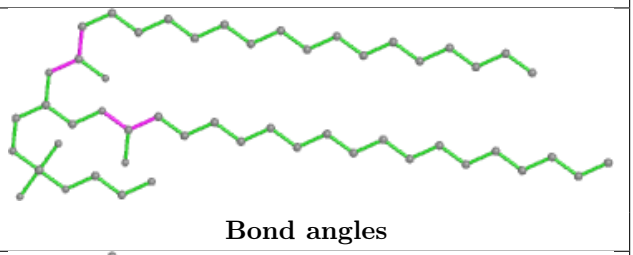
Ligand CDL 1H 401



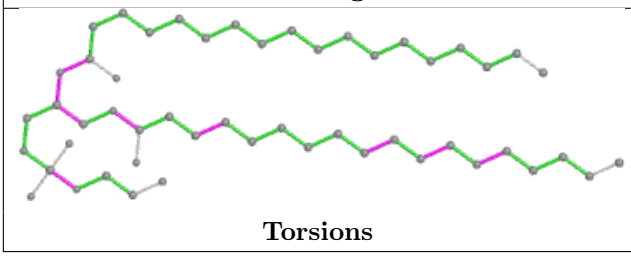
Ligand 3PE 3X 108



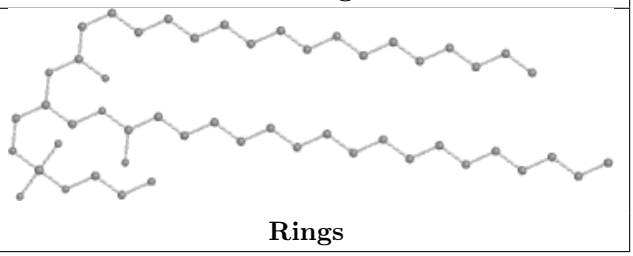
Bond lengths



Bond angles

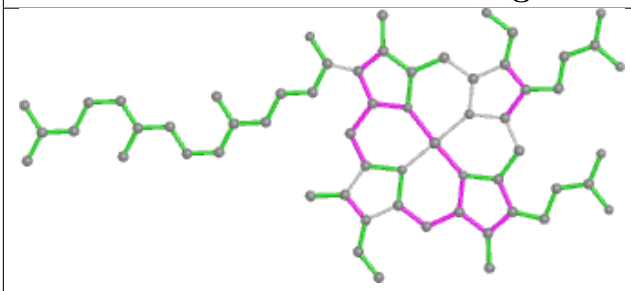


Torsions

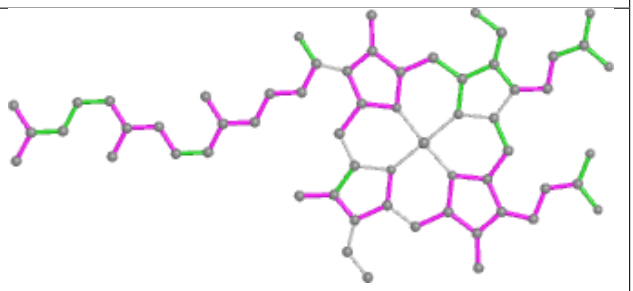


Rings

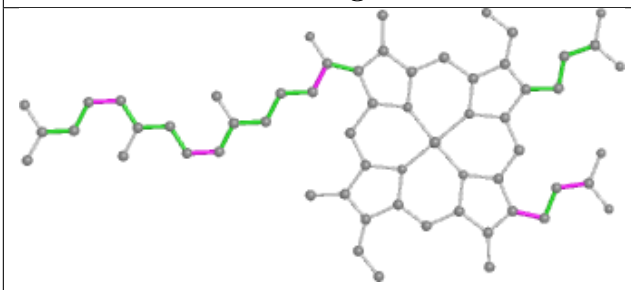
Ligand HEA 4A 601



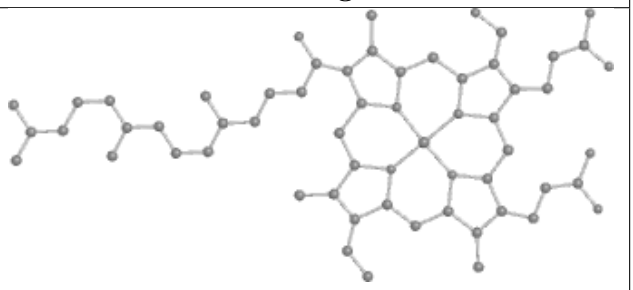
Bond lengths



Bond angles

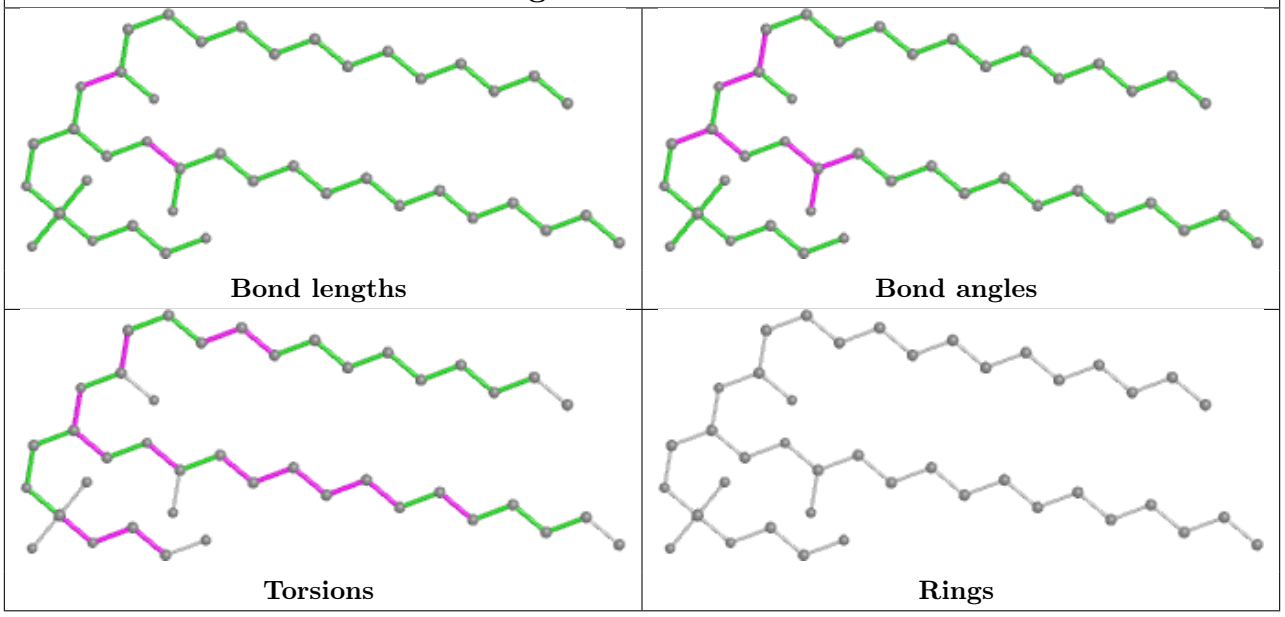


Torsions

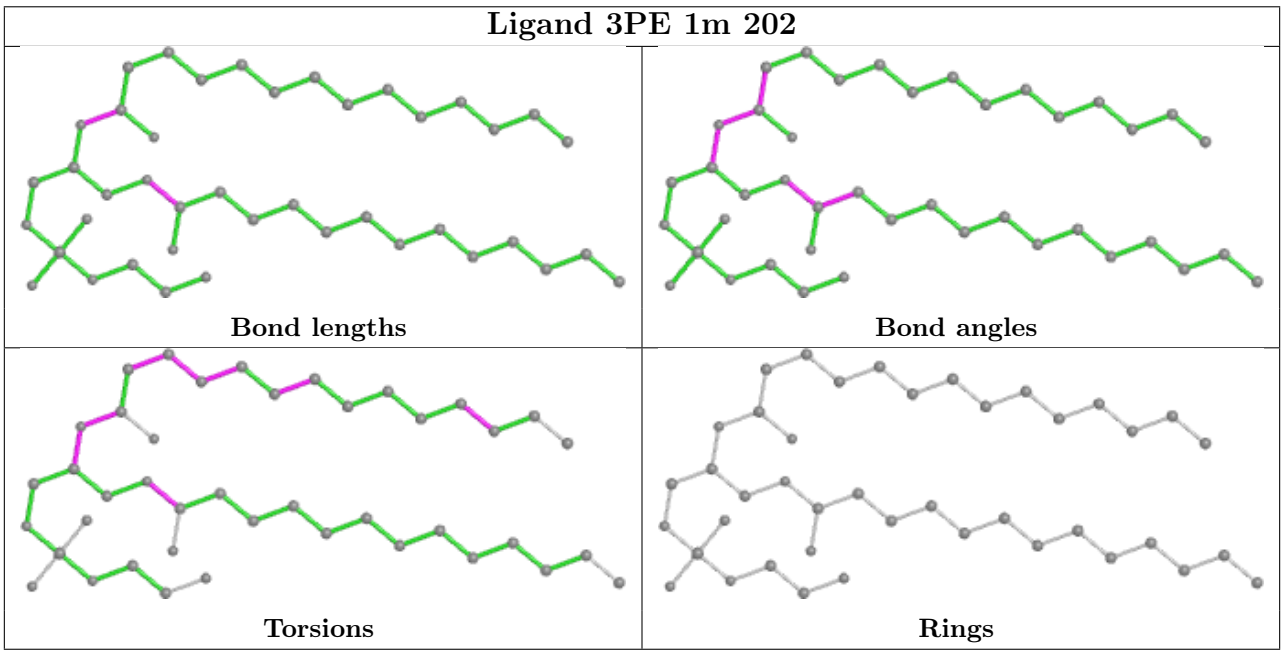


Rings

Ligand 3PE 1l 202



Ligand 3PE 1m 202



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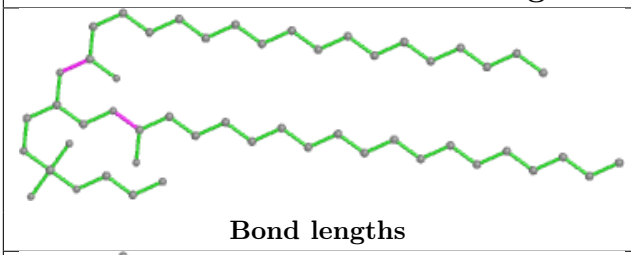
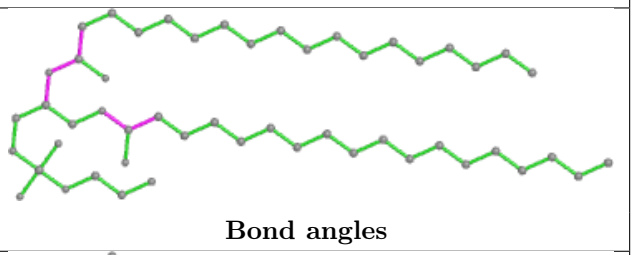
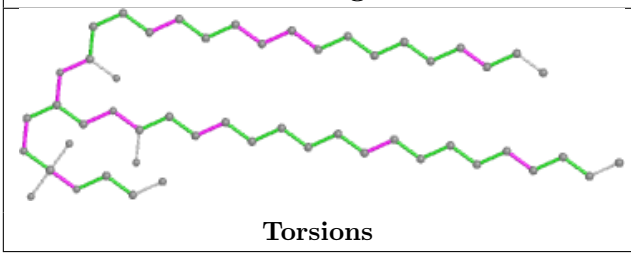


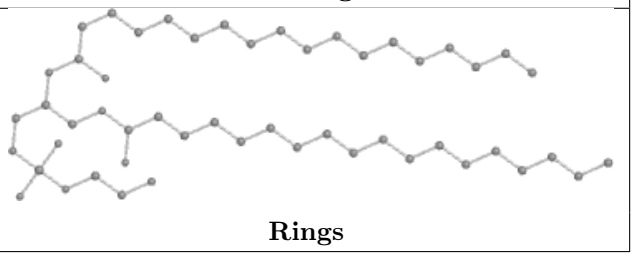
Bond lengths



Bond angles

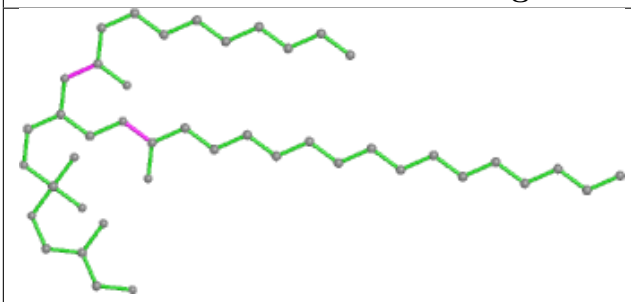


Torsions

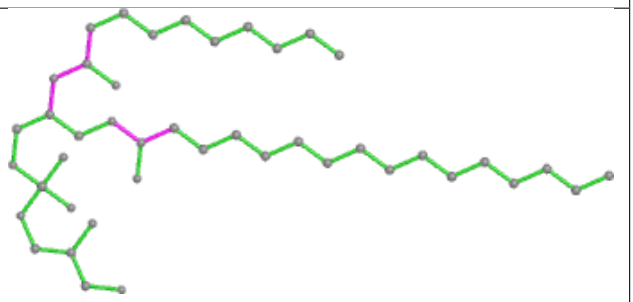


Rings

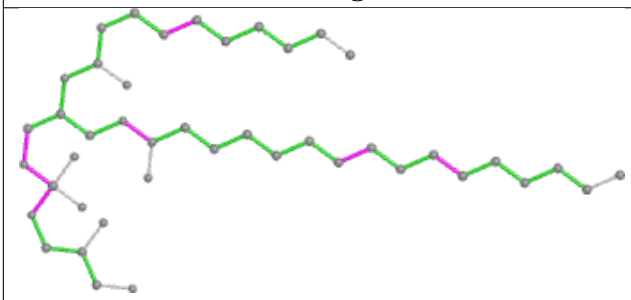
Ligand PGV 4K 101



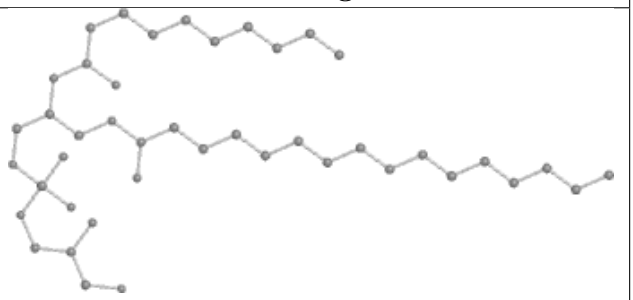
Bond lengths



Bond angles

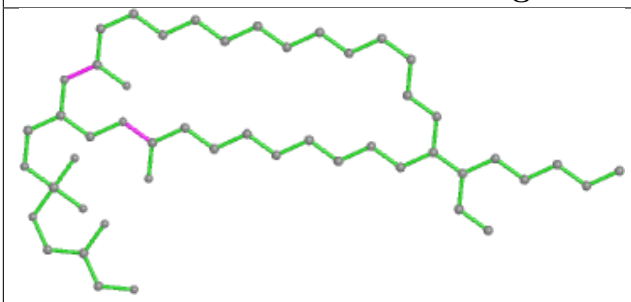


Torsions

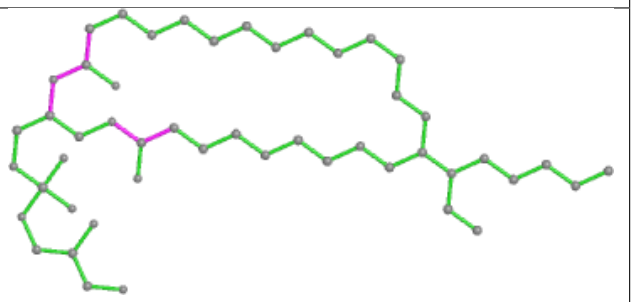


Rings

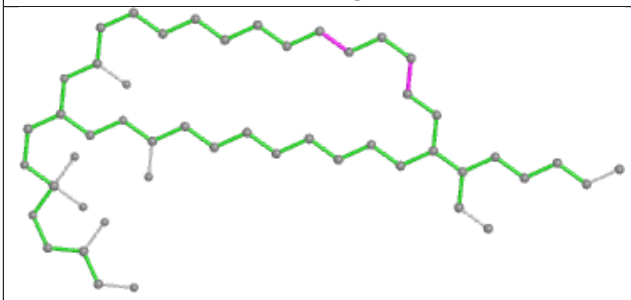
Ligand PGV 4C 301



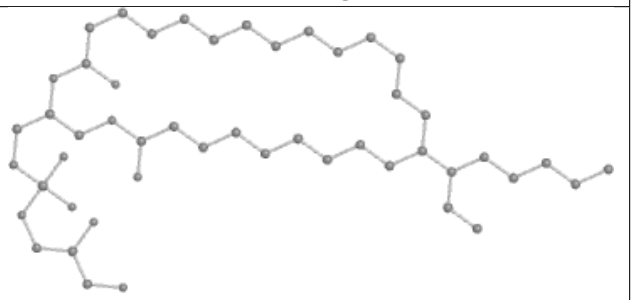
Bond lengths



Bond angles

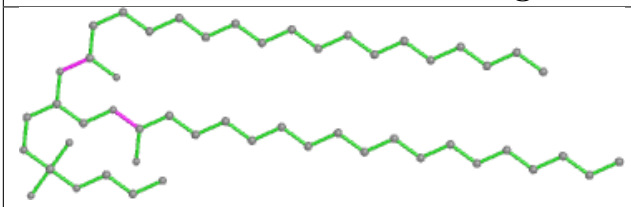


Torsions

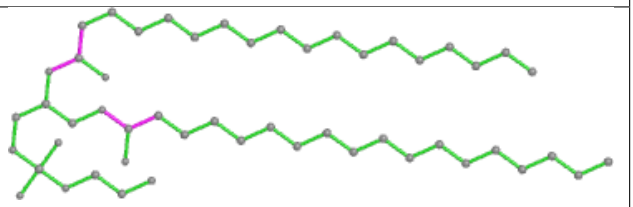


Rings

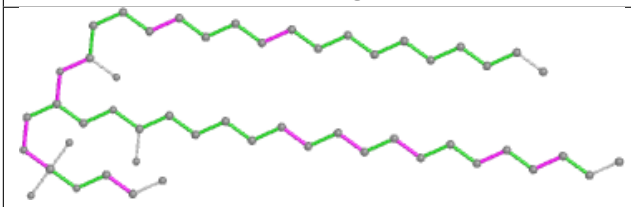
Ligand 3PE 3W 101



Bond lengths



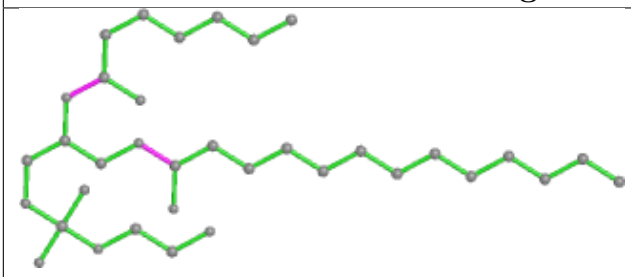
Bond angles



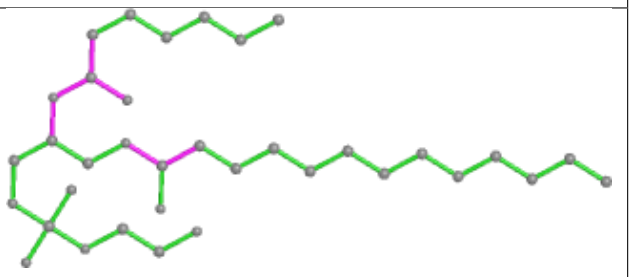
Torsions

Rings

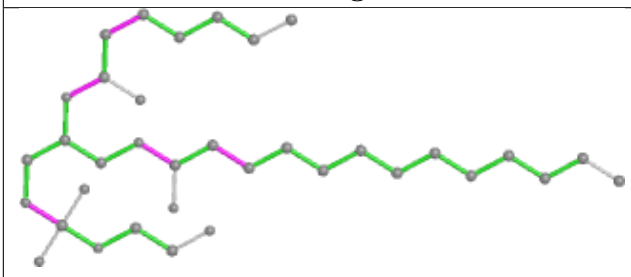
Ligand 3PE 3C 514



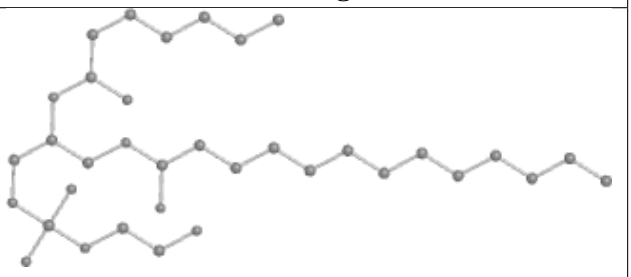
Bond lengths



Bond angles

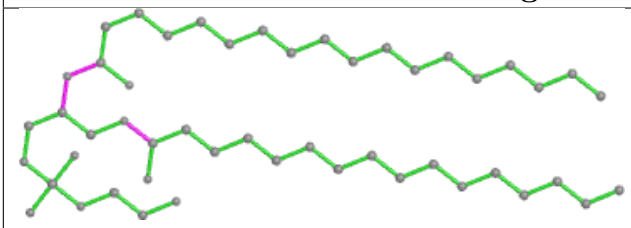


Torsions

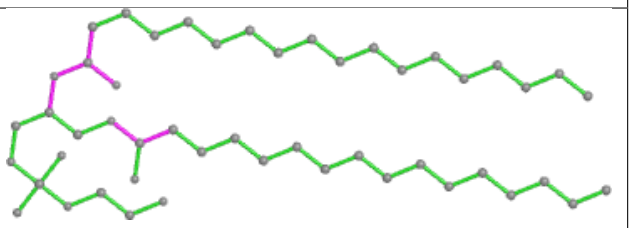


Rings

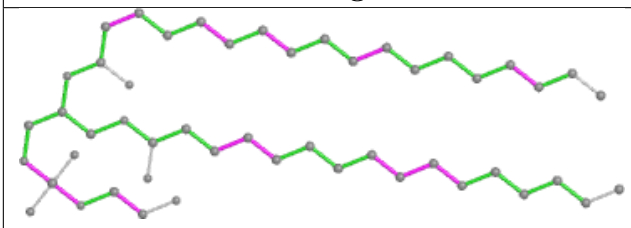
Ligand 3PE 3E 303



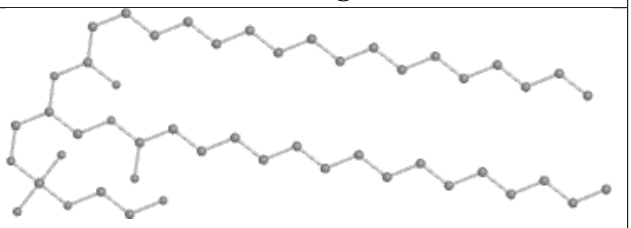
Bond lengths



Bond angles

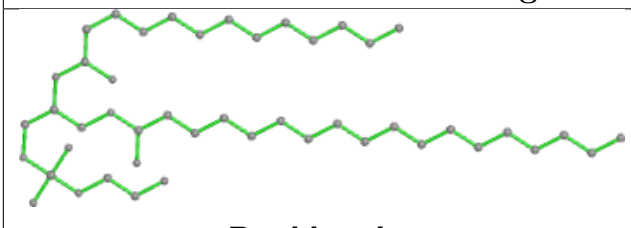


Torsions

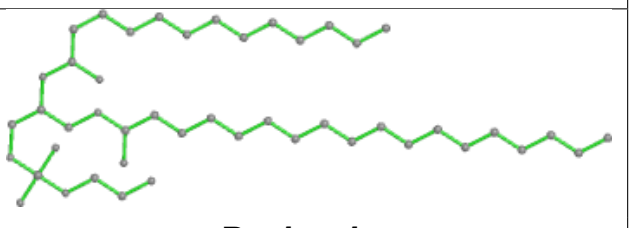


Rings

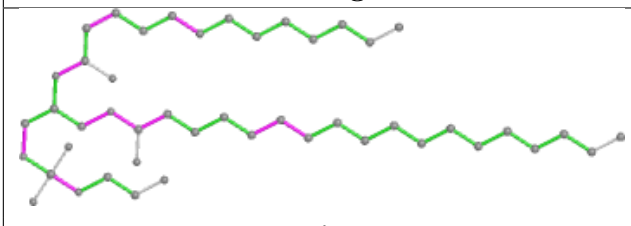
Ligand 3PE 3C 504



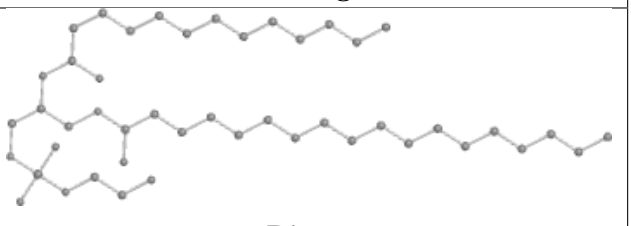
Bond lengths



Bond angles

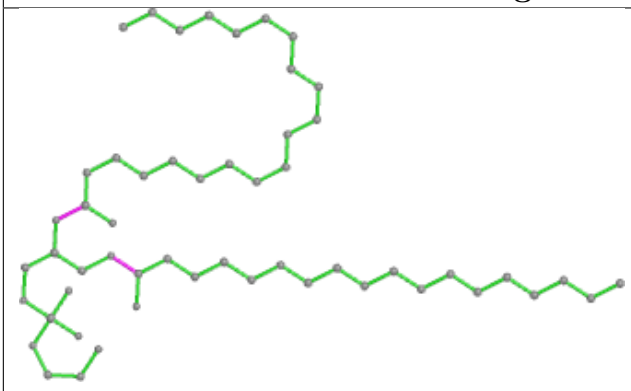


Torsions

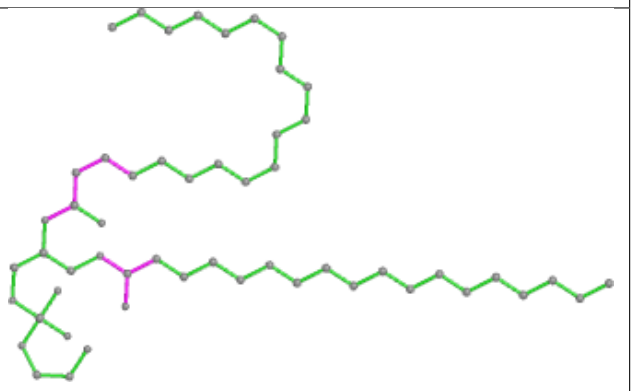


Rings

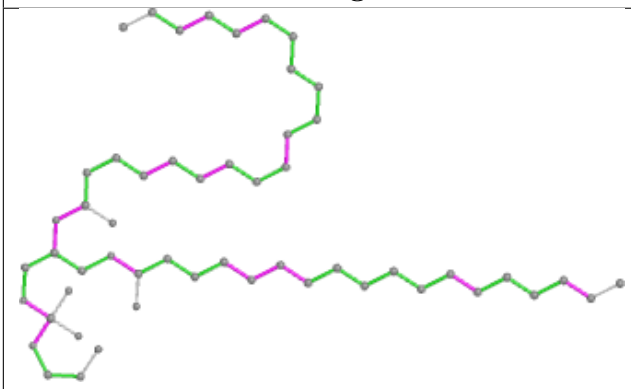
Ligand PEK 3X 102



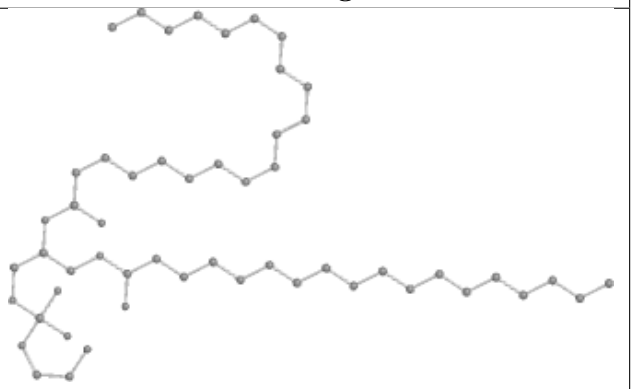
Bond lengths



Bond angles

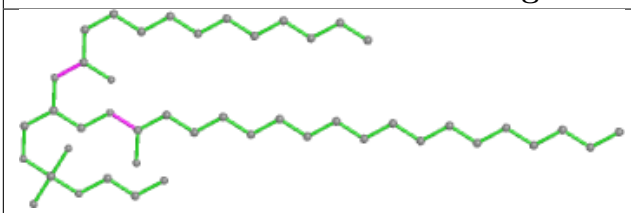


Torsions

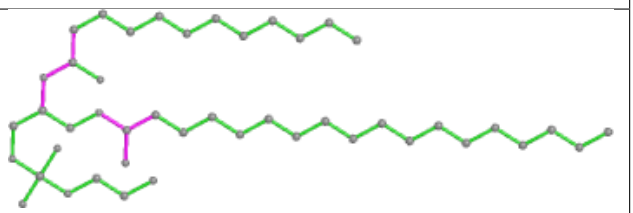


Rings

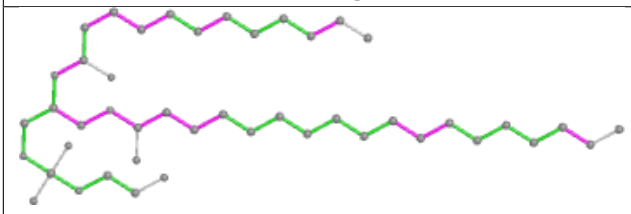
Ligand 3PE 1L 702



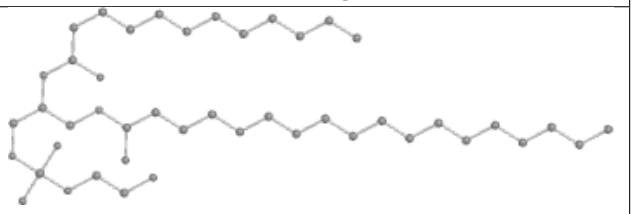
Bond lengths



Bond angles

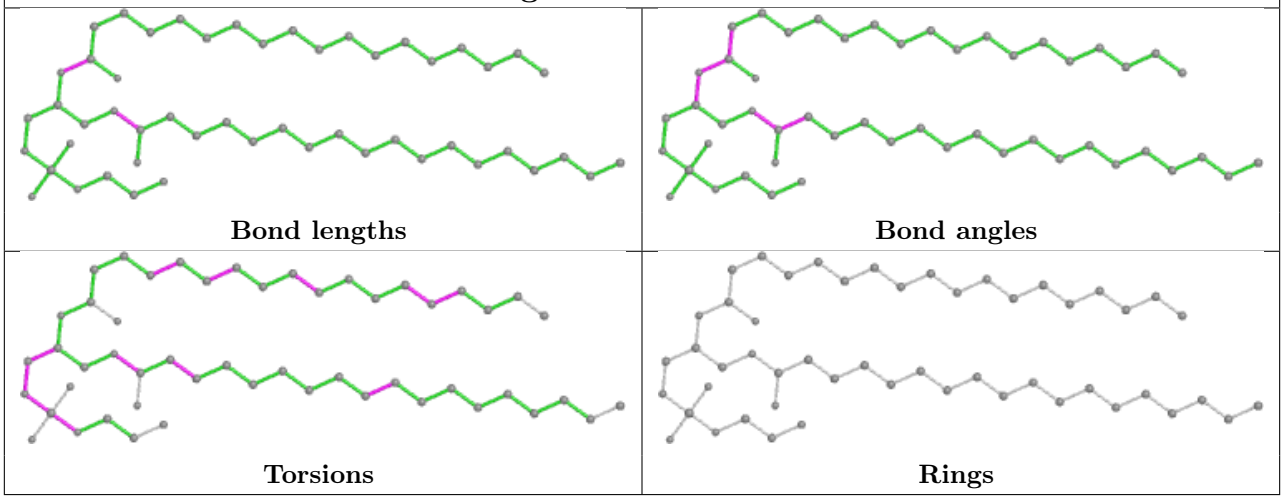


Torsions

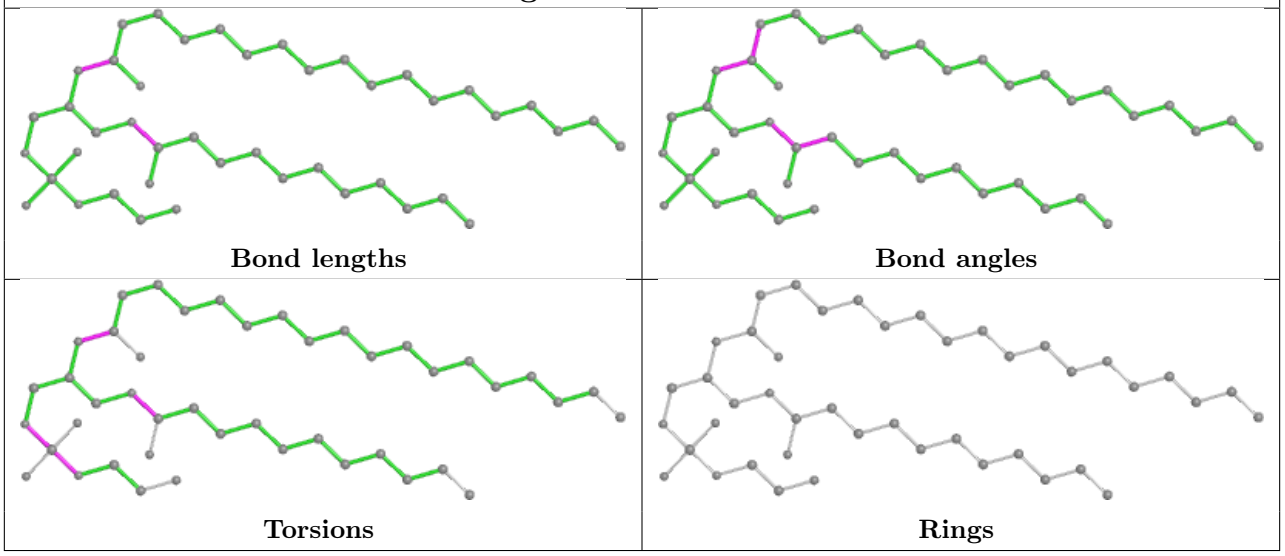


Rings

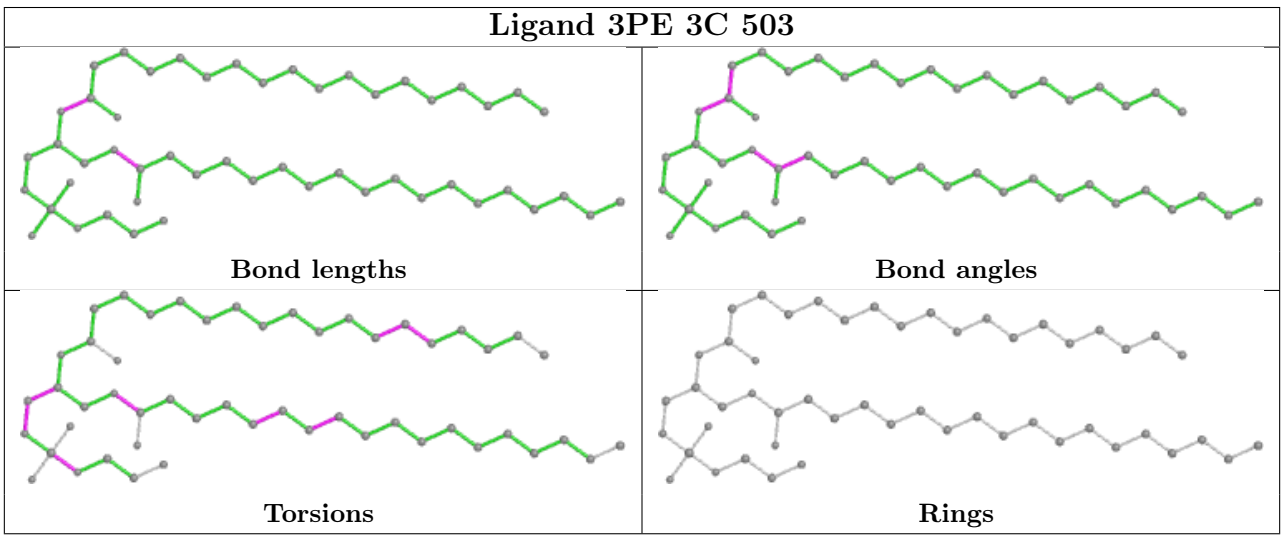
Ligand 3PE 3C 509



Ligand 3PE 1Y 212



Ligand 3PE 3C 503



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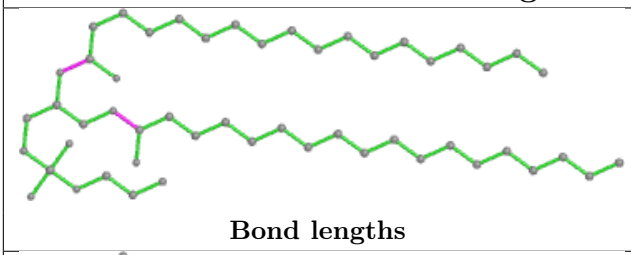
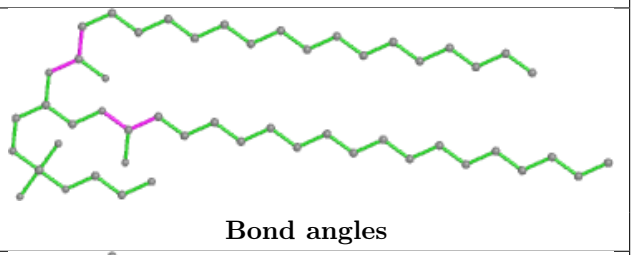
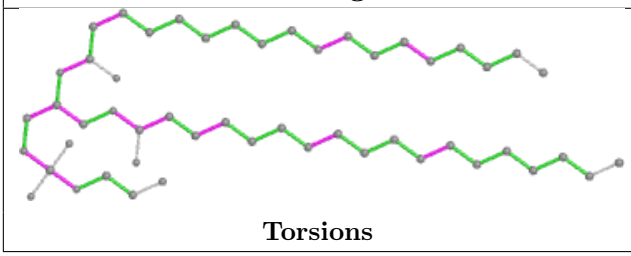


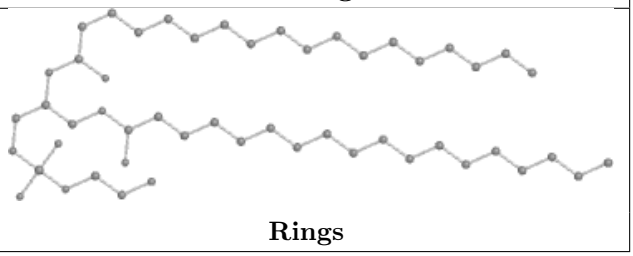
Bond lengths



Bond angles

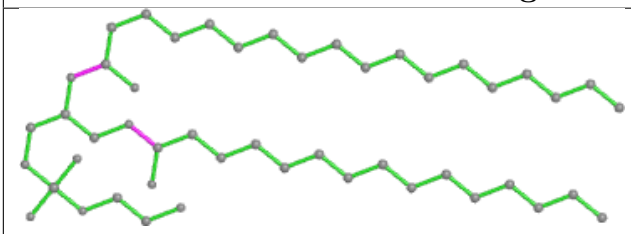


Torsions

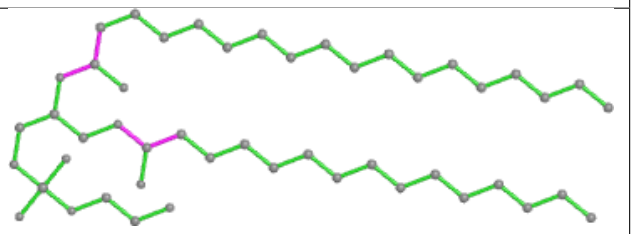


Rings

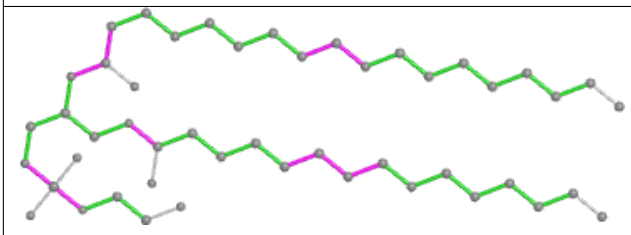
Ligand 3PE 3C 515



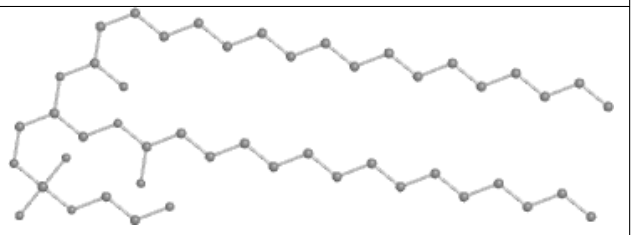
Bond lengths



Bond angles

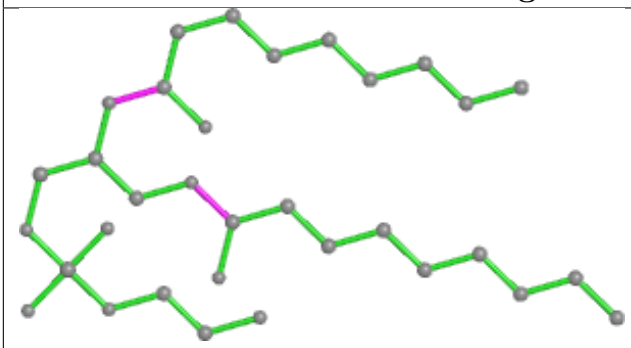


Torsions

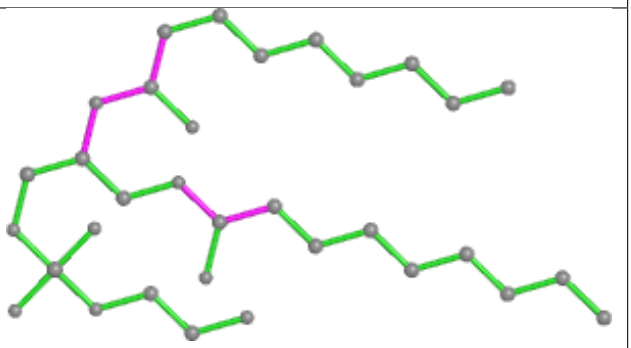


Rings

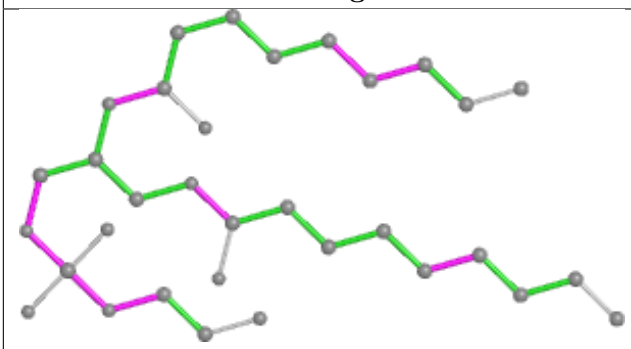
Ligand 3PE 3G 105



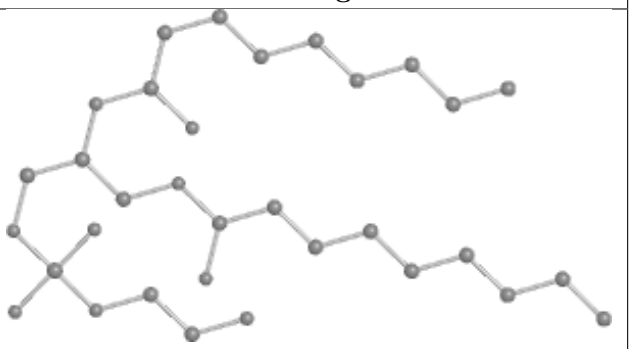
Bond lengths



Bond angles

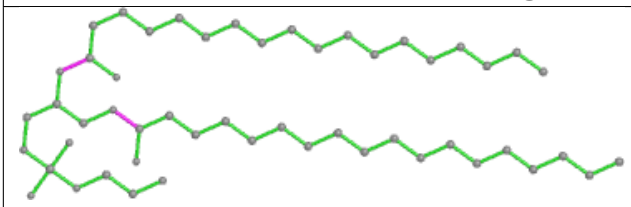


Torsions

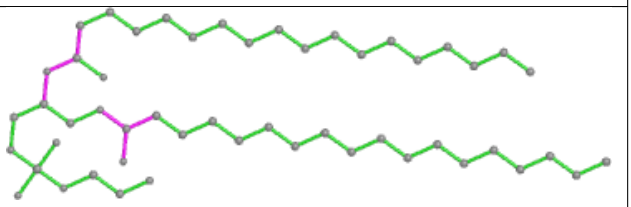


Rings

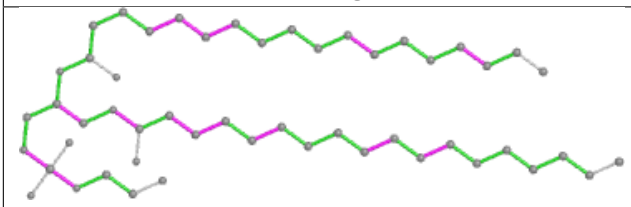
Ligand 3PE 3E 302



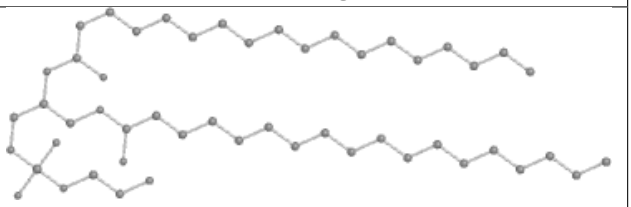
Bond lengths



Bond angles

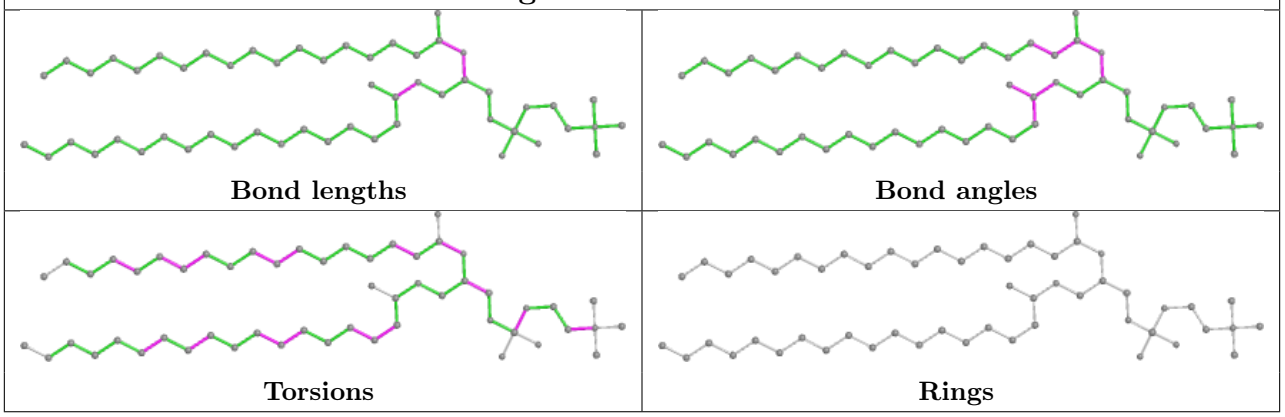


Torsions

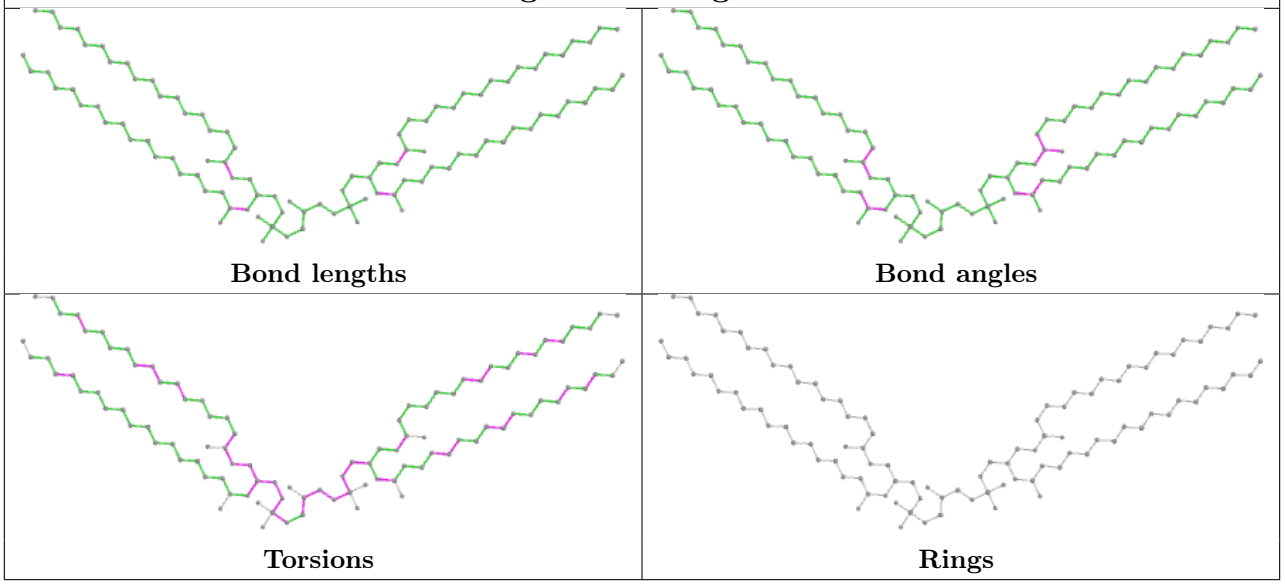


Rings

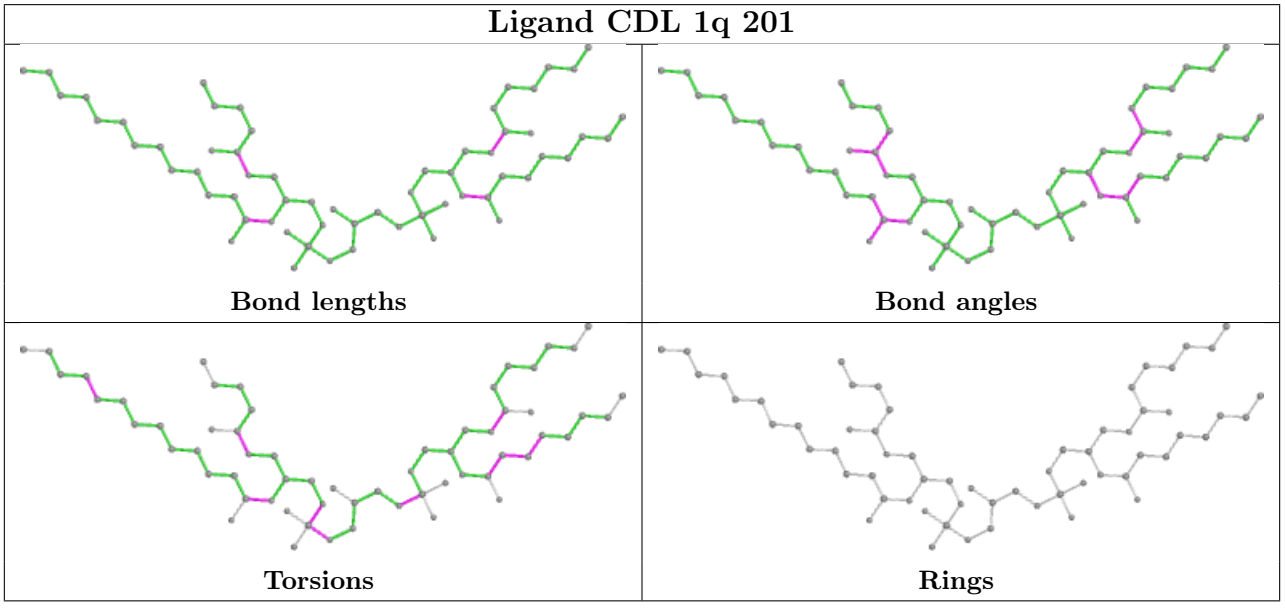
Ligand PC1 3X 104



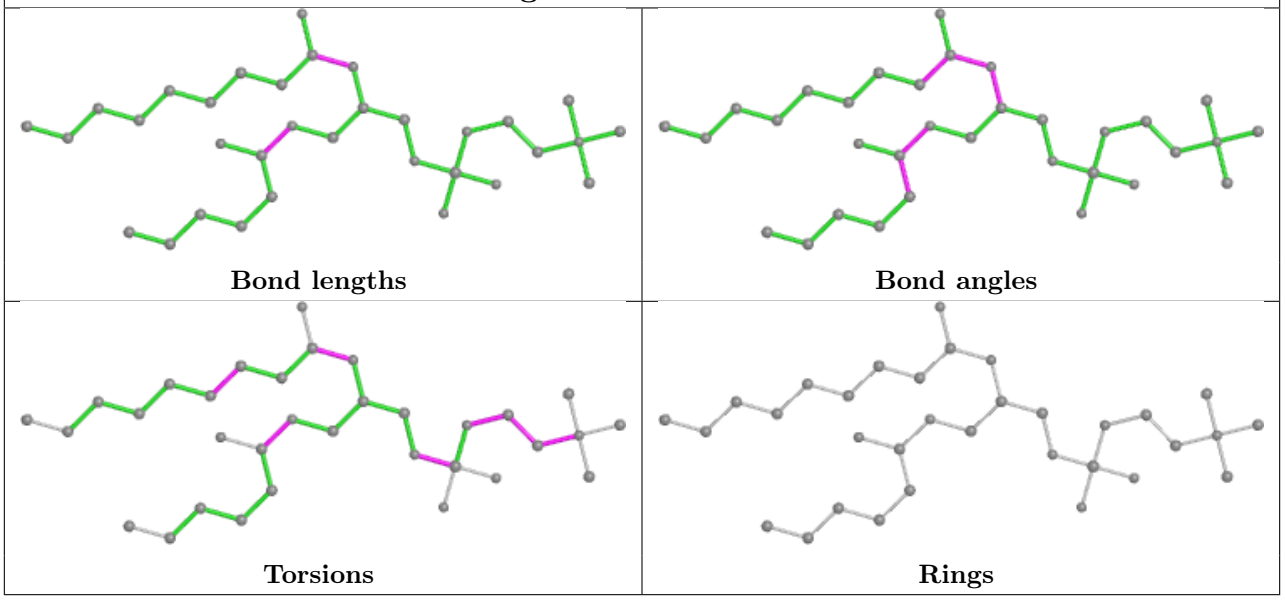
Ligand CDL 1g 201



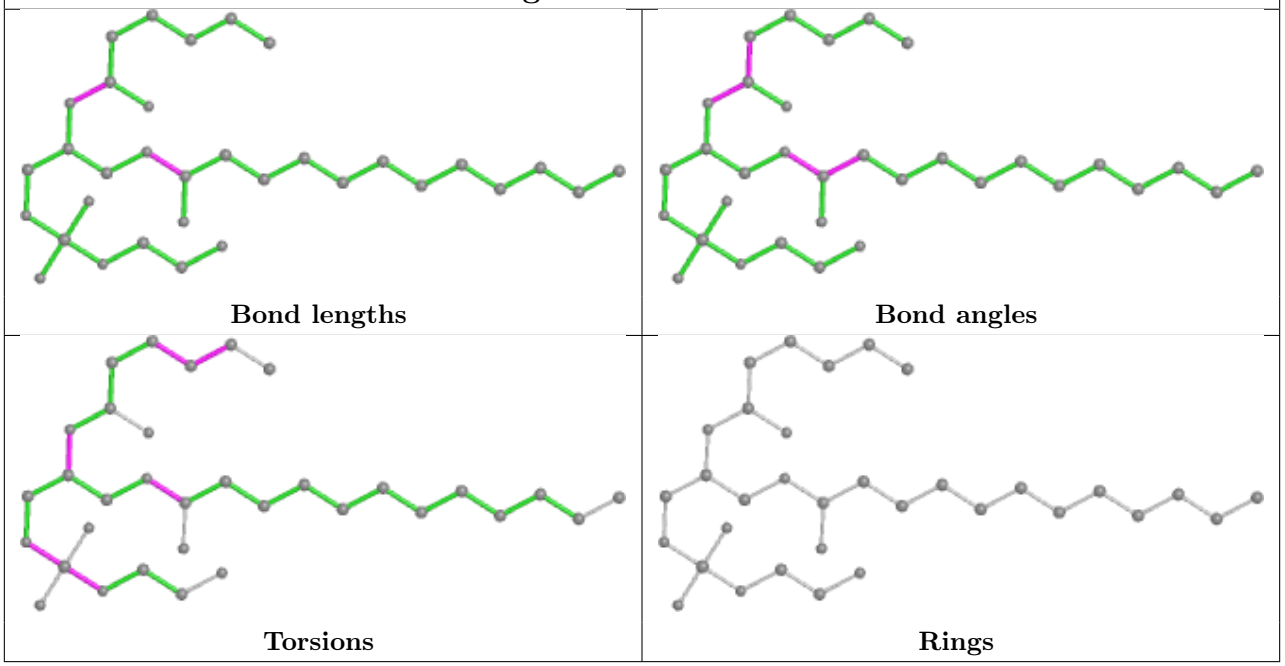
Ligand CDL 1q 201



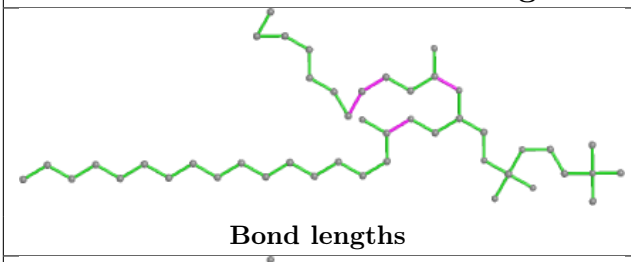
Ligand PC1 1P 502



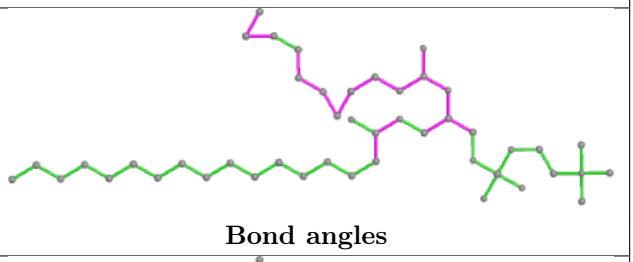
Ligand 3PE 1L 706



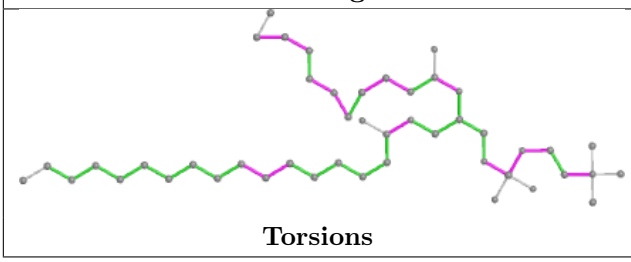
Ligand PC1 1B 202



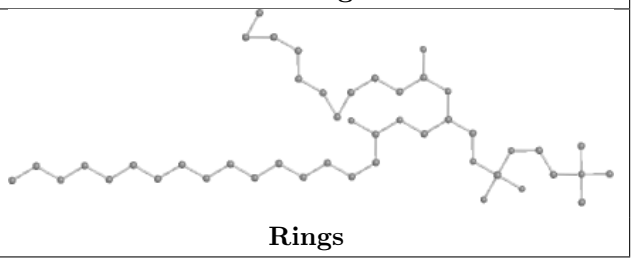
Bond lengths



Bond angles

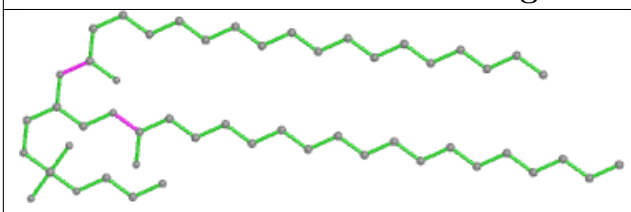


Torsions

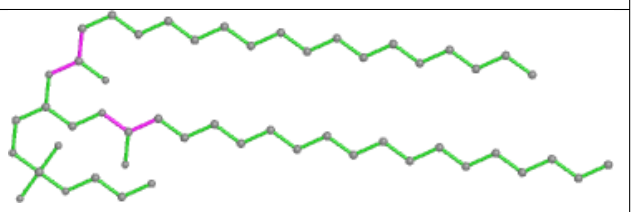


Rings

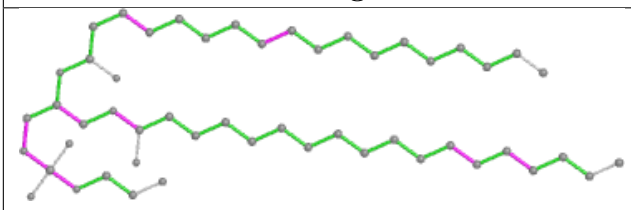
Ligand 3PE 3P 517



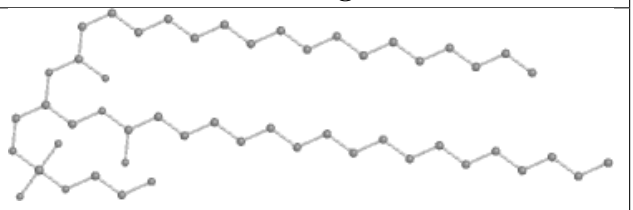
Bond lengths



Bond angles

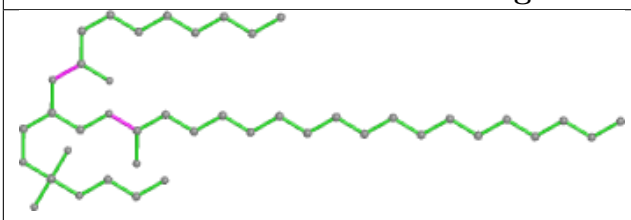


Torsions

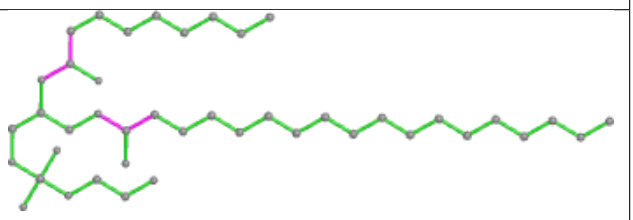


Rings

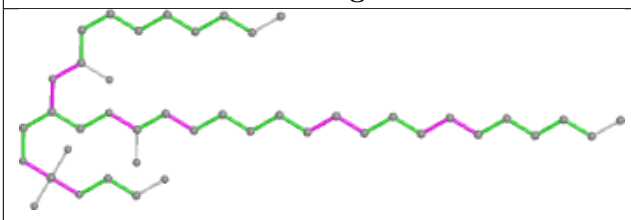
Ligand 3PE 3W 102



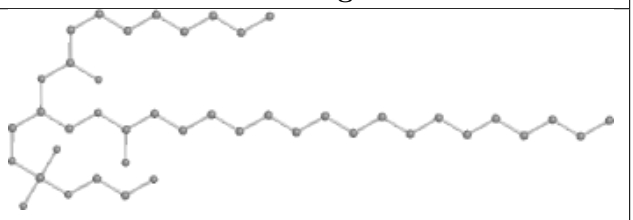
Bond lengths



Bond angles

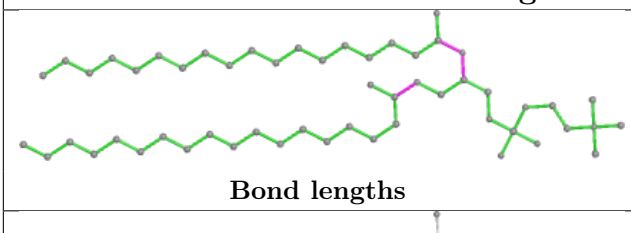


Torsions

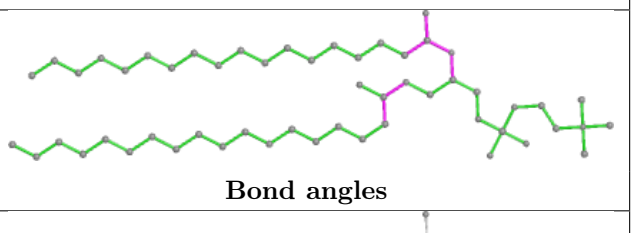


Rings

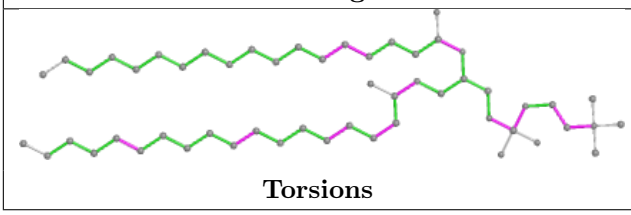
Ligand PC1 3T 102



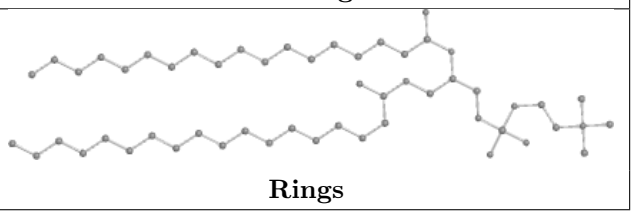
Bond lengths



Bond angles

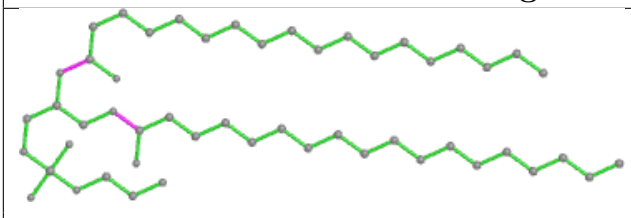


Torsions



Rings

Ligand 3PE 3C 505



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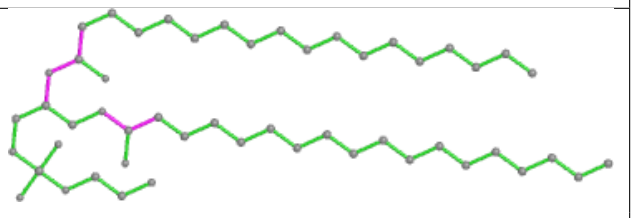
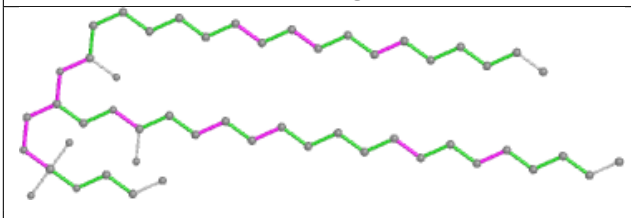
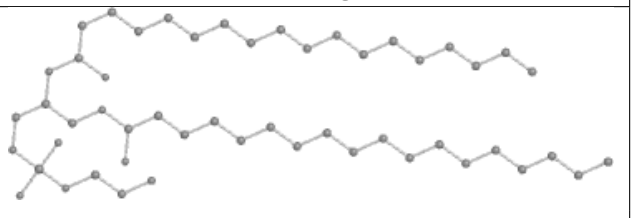


Bond angles

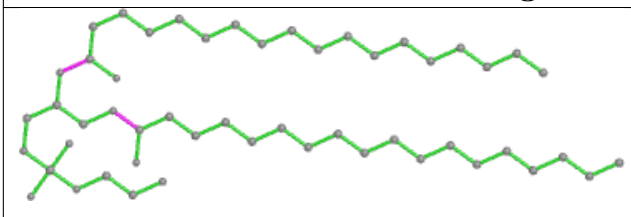


Torsions

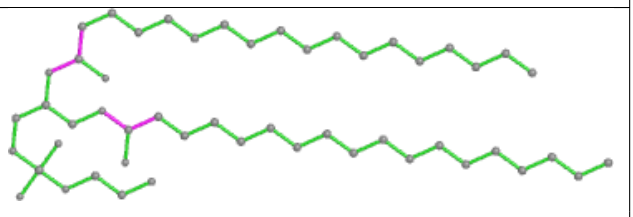


Rings

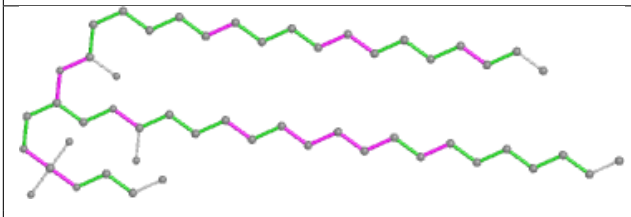
Ligand 3PE 3Y 101



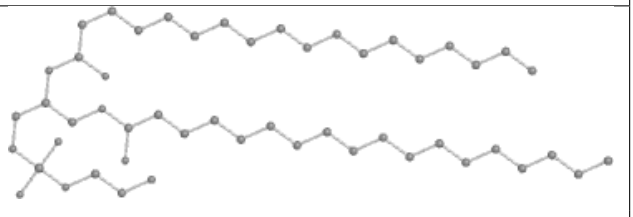
Bond lengths



Bond angles

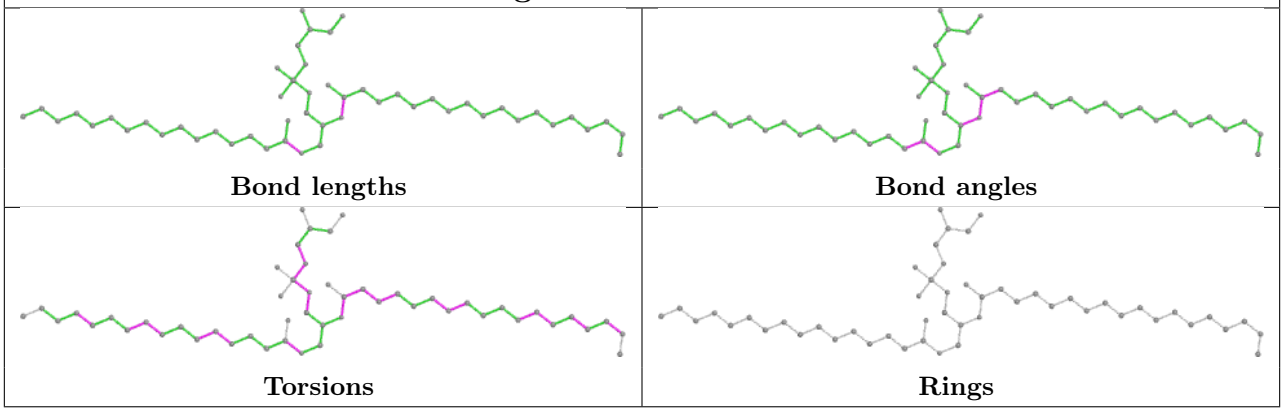


Torsions

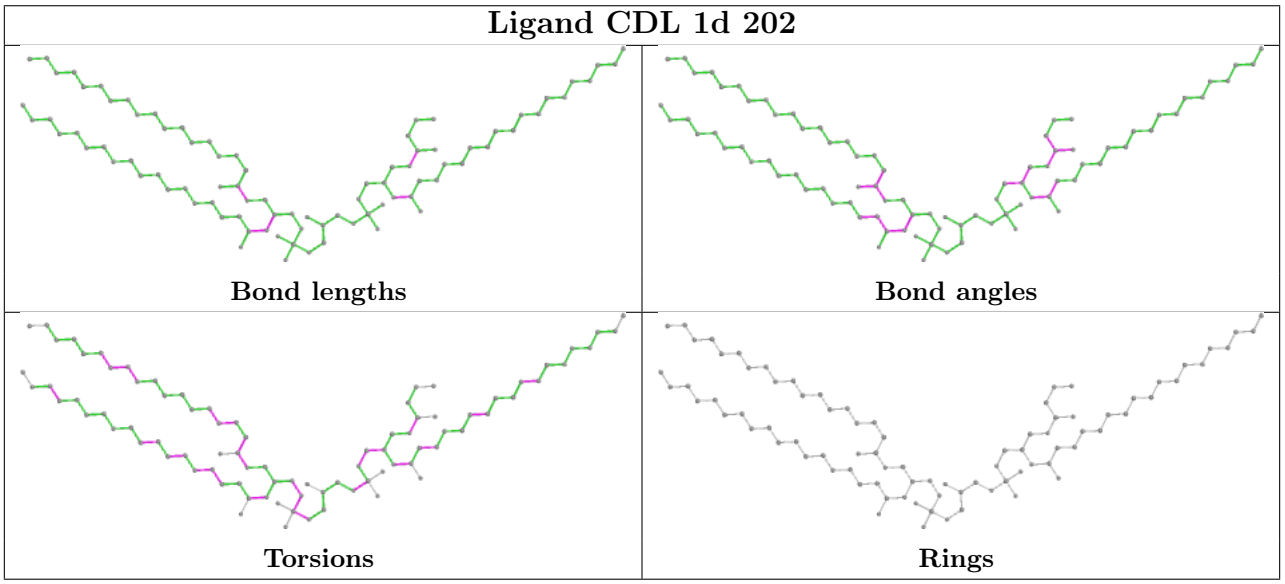


Rings

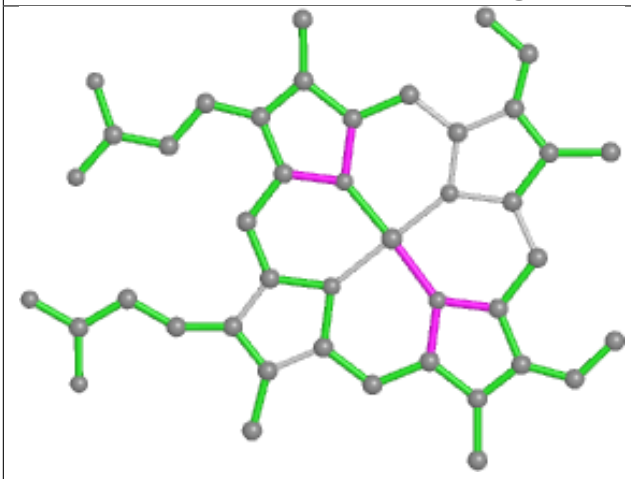
Ligand PGT 1Y 203



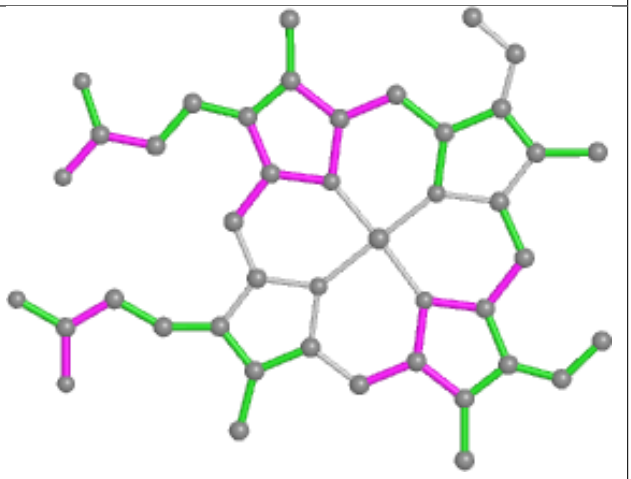
Ligand CDL 1d 202



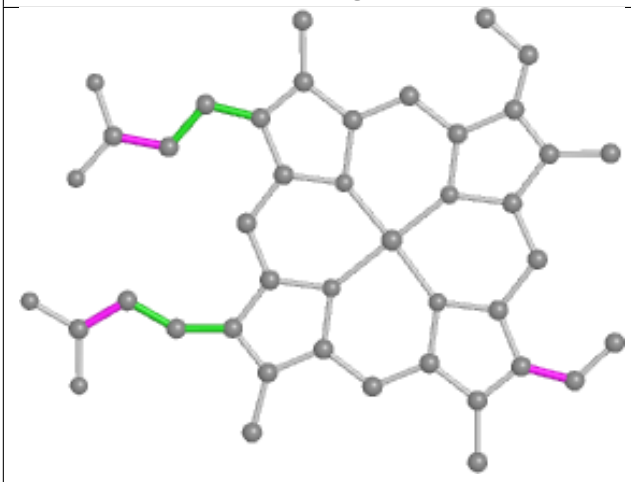
Ligand HEM 3P 502



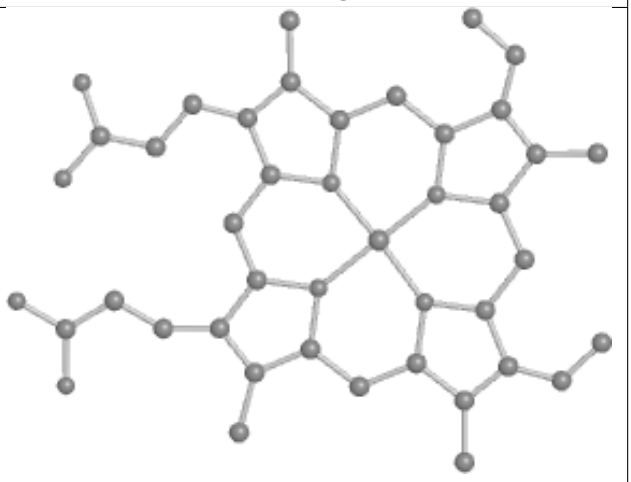
Bond lengths



Bond angles

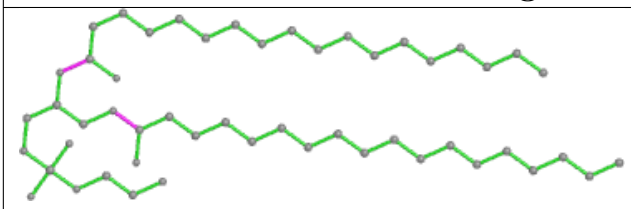


Torsions

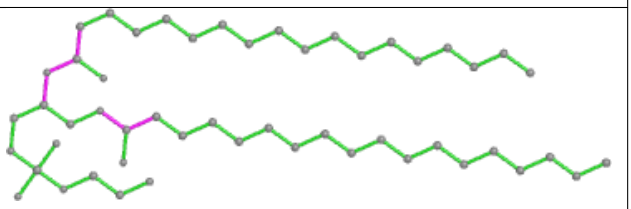


Rings

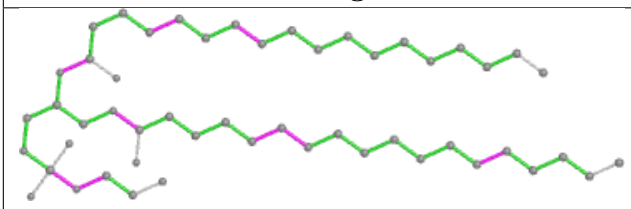
Ligand 3PE 1Y 208



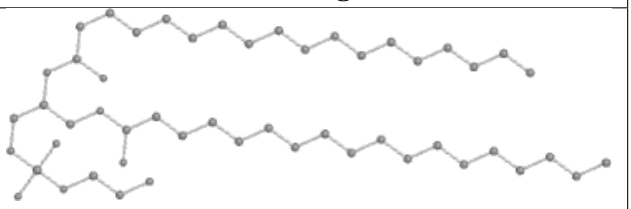
Bond lengths



Bond angles

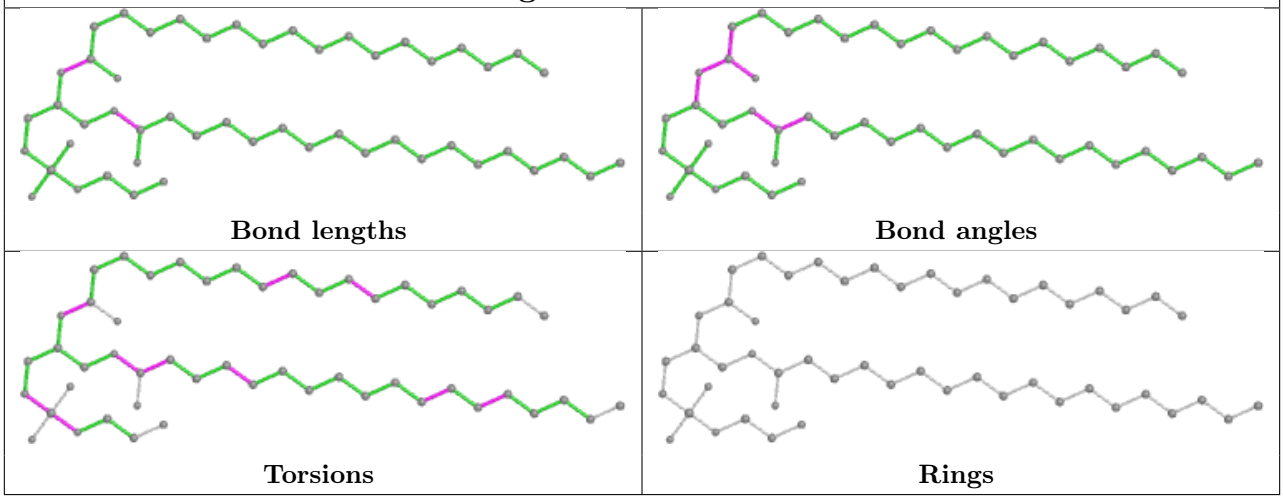


Torsions

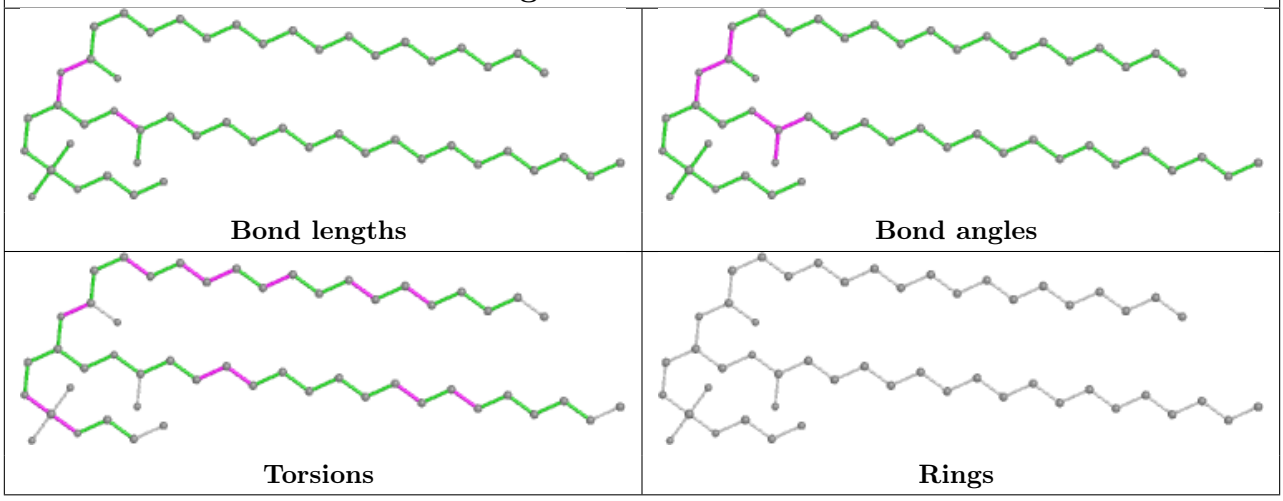


Rings

Ligand 3PE 1m 204



Ligand 3PE 3A 502



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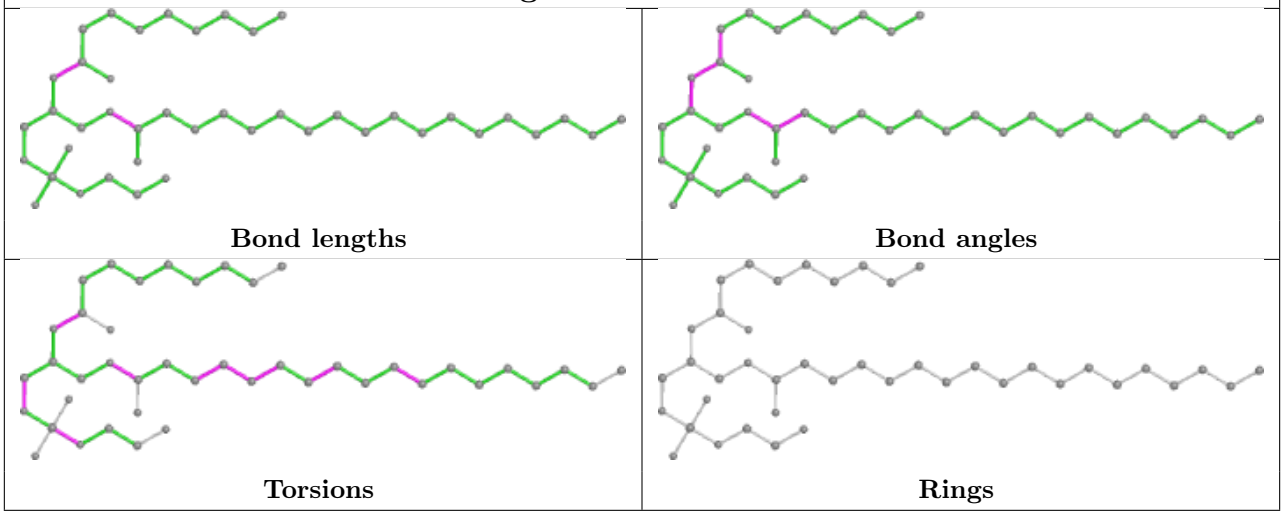
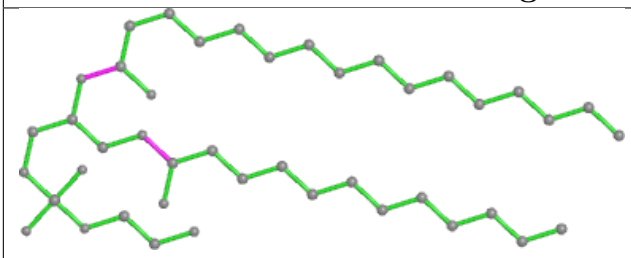
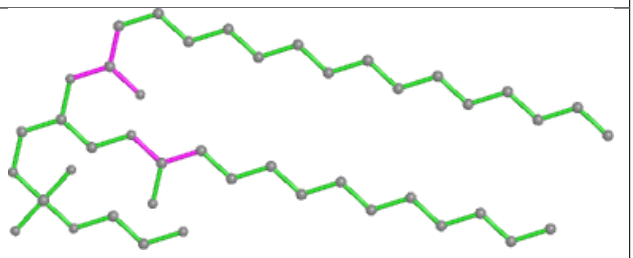


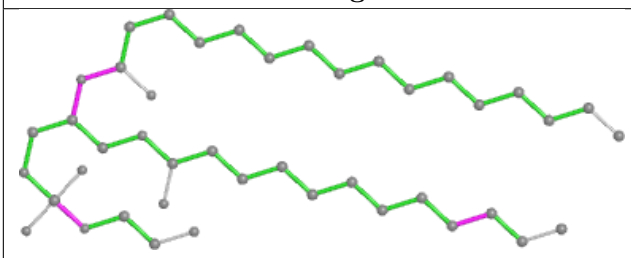
Ligand 3PE 3C 516



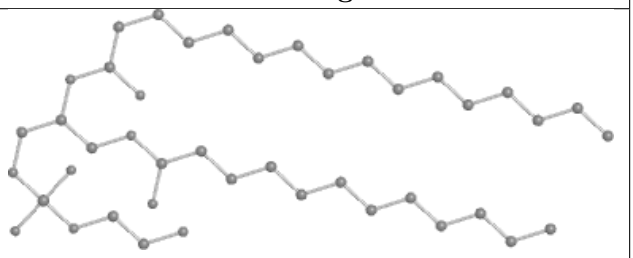
Bond lengths



Bond angles

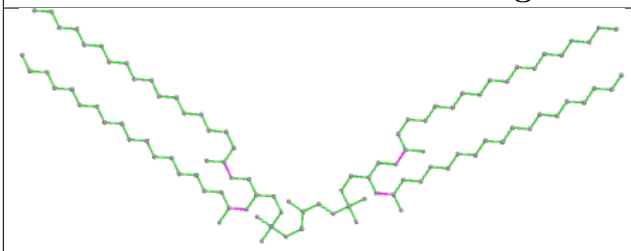


Torsions



Rings

Ligand CDL 3X 103



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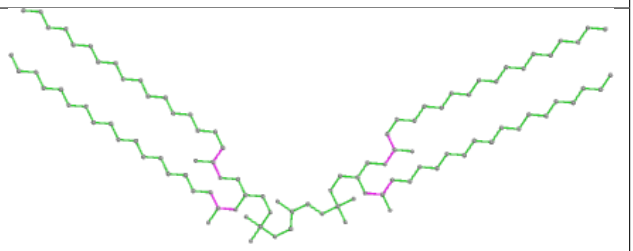
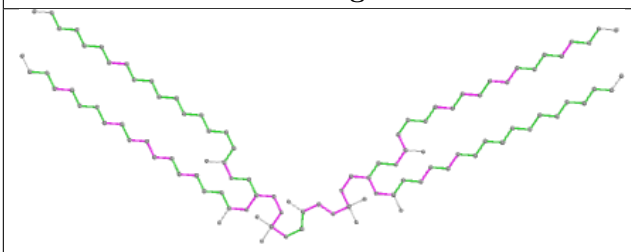
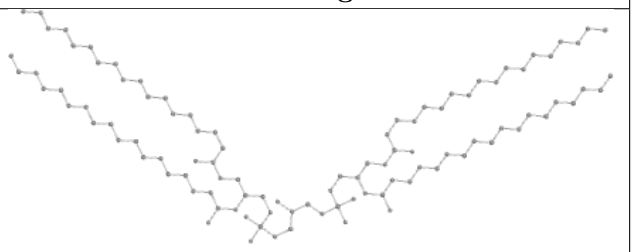


Bond angles

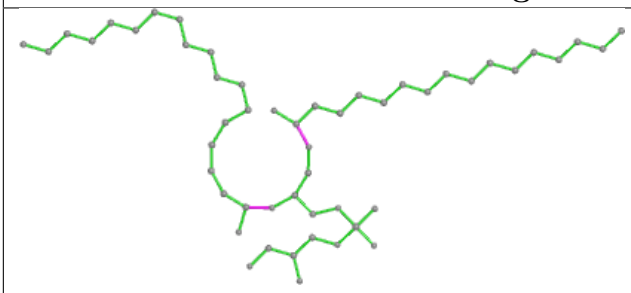


Torsions

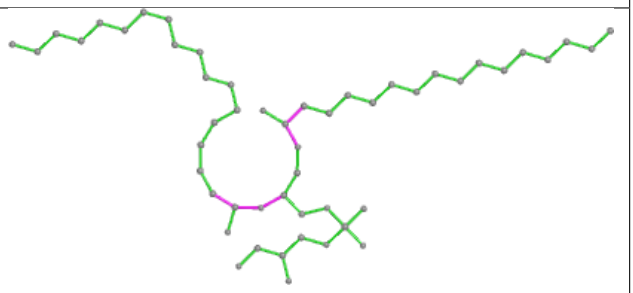


Rings

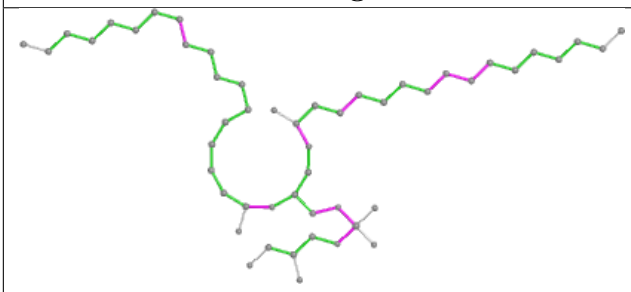
Ligand PGV 4C 302



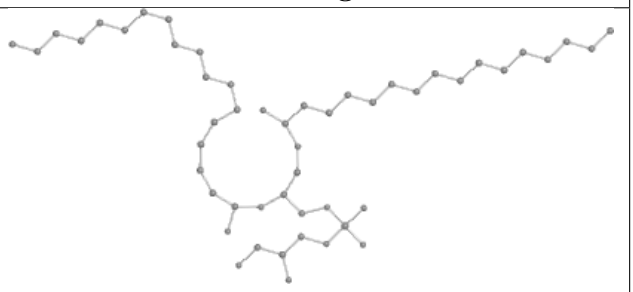
Bond lengths



Bond angles

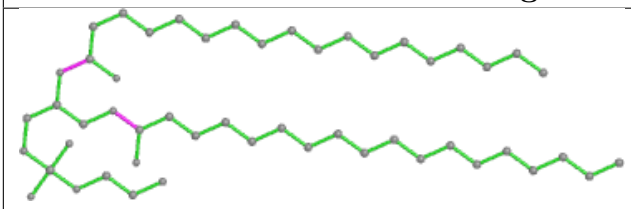


Torsions

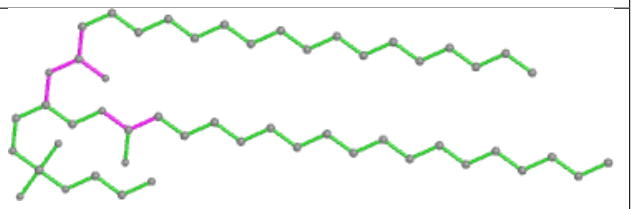


Rings

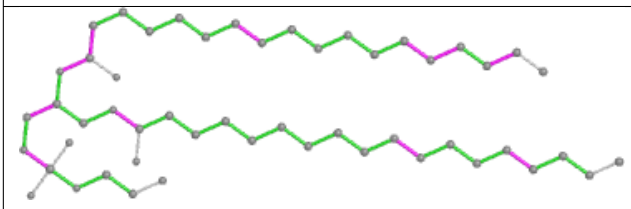
Ligand 3PE 3P 503



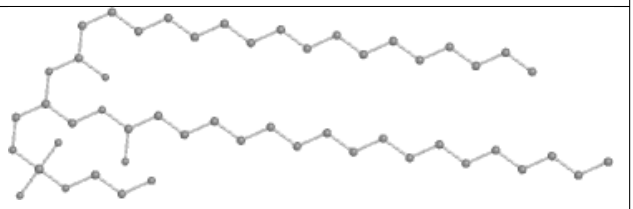
Bond lengths



Bond angles

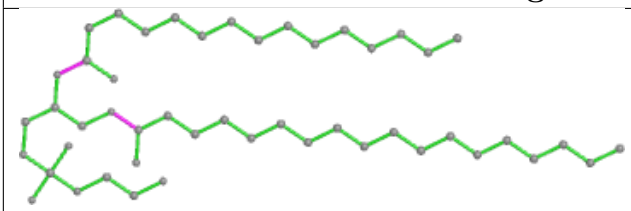


Torsions

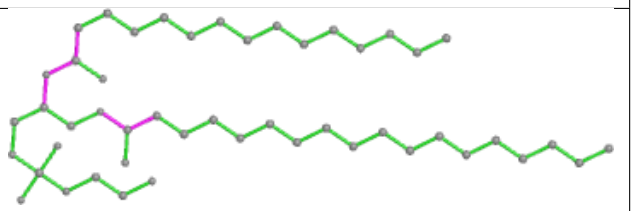


Rings

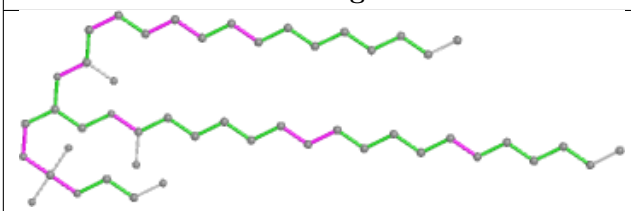
Ligand 3PE 1f 104



Bond lengths



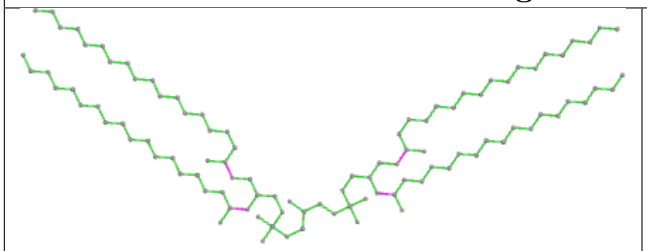
Bond angles



Torsions

Rings

Ligand CDL 1Y 217



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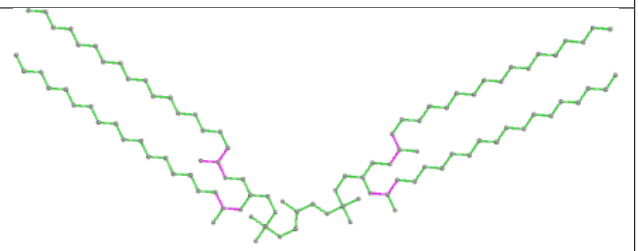
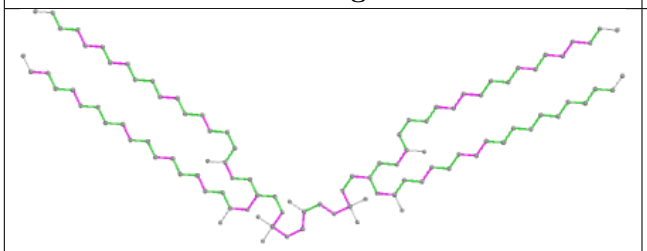
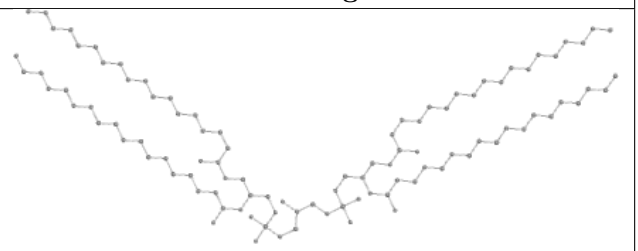


Bond angles

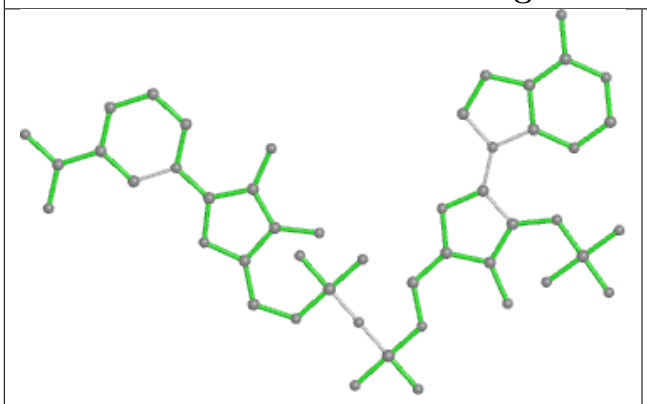


Torsions

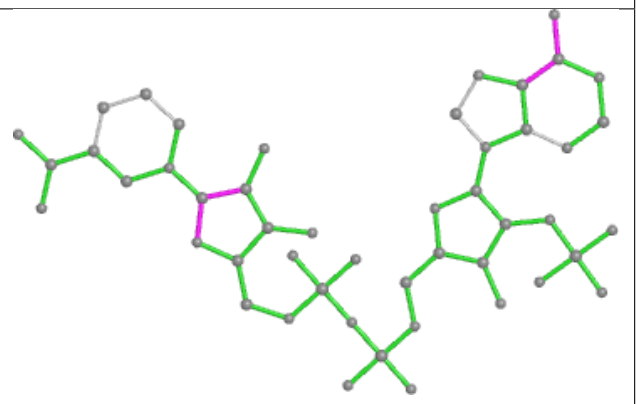


Rings

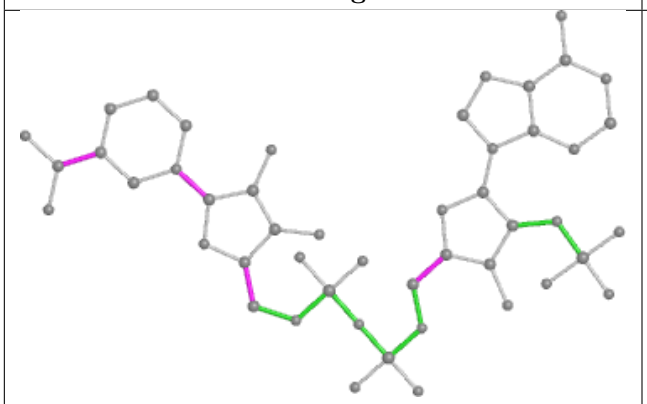
Ligand NDP 1P 501



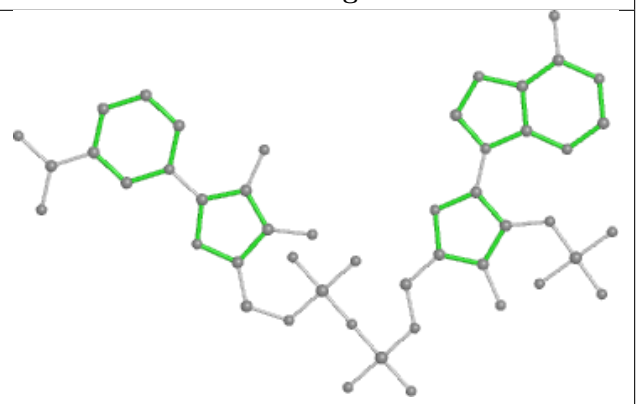
Bond lengths



Bond angles

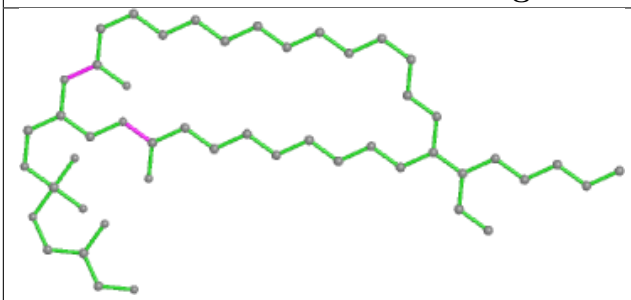


Torsions

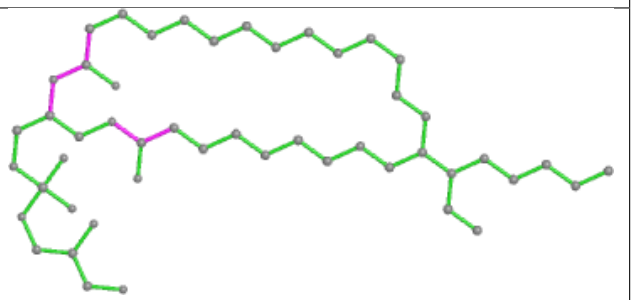


Rings

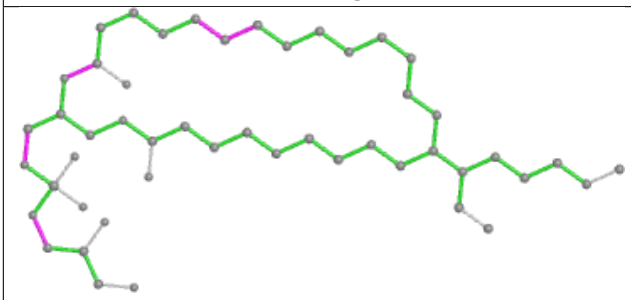
Ligand PGV 4C 304



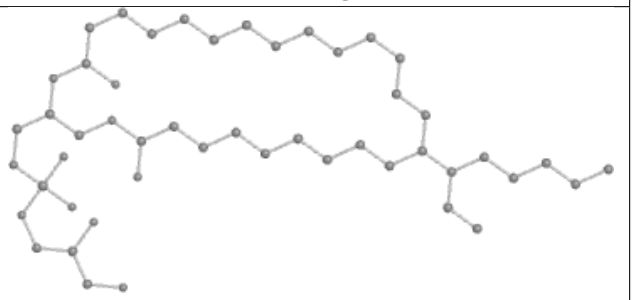
Bond lengths



Bond angles

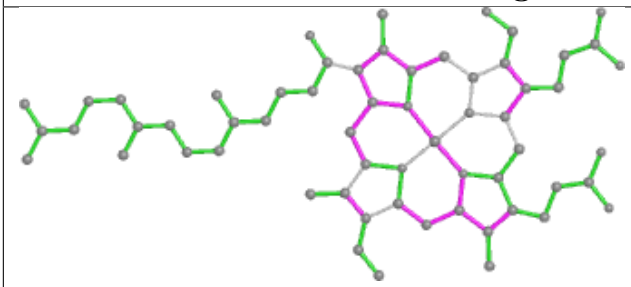


Torsions



Rings

Ligand HEA 4A 602



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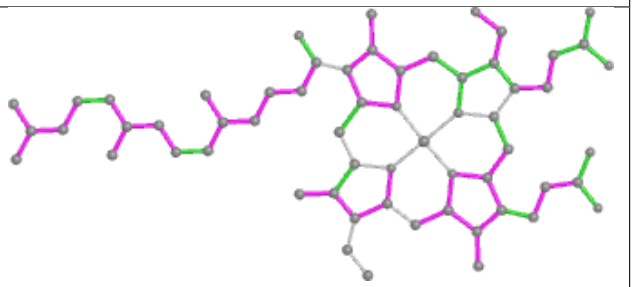

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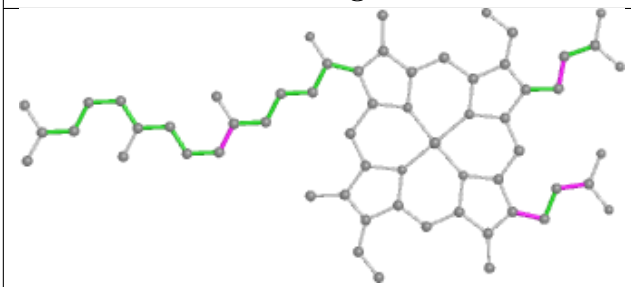

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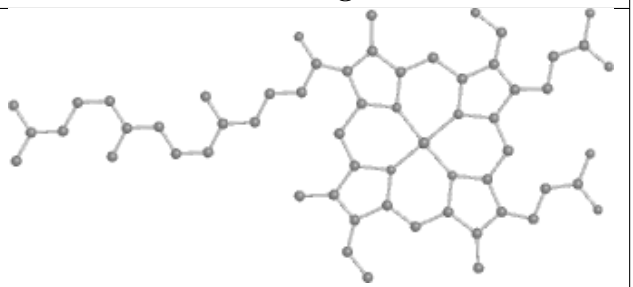
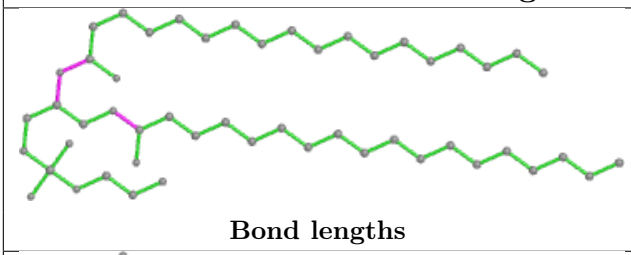


Rings

Ligand 3PE 3R 305



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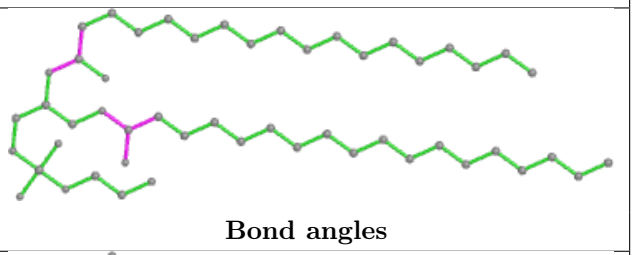
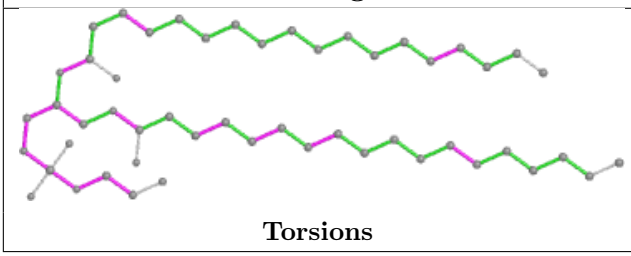


Bond angles



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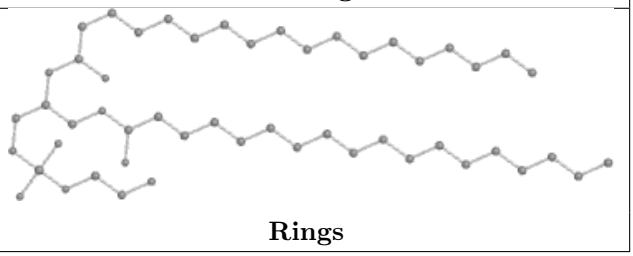
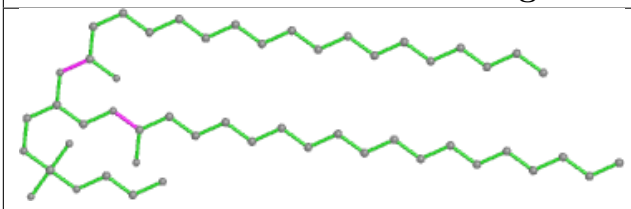


Rings

Ligand 3PE 3X 107



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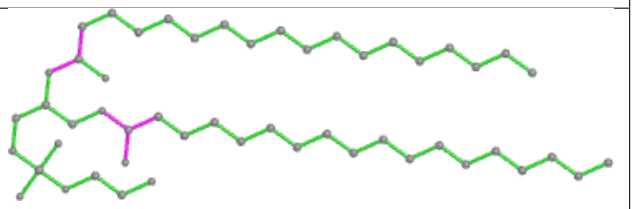
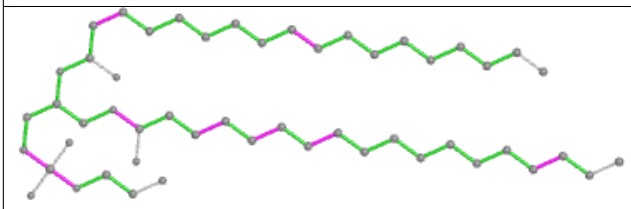


Bond angles



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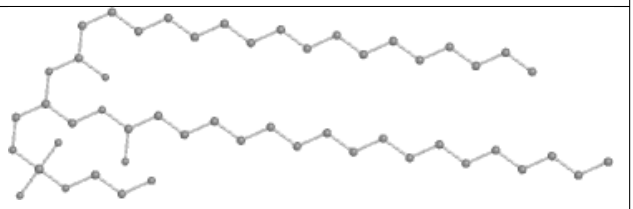
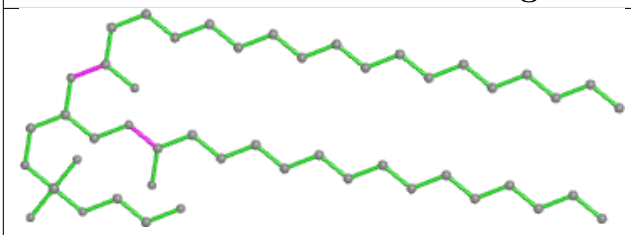
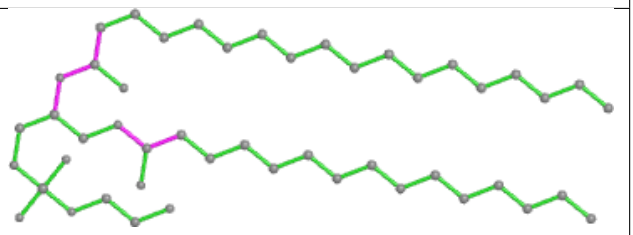


Rings

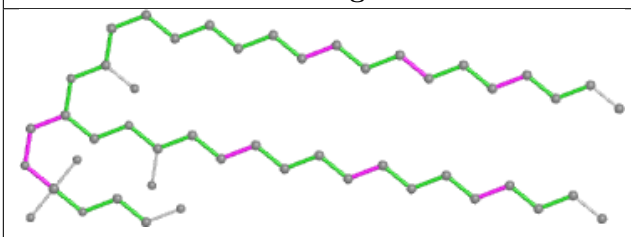
Ligand 3PE 3P 510



Bond lengths



Bond angles



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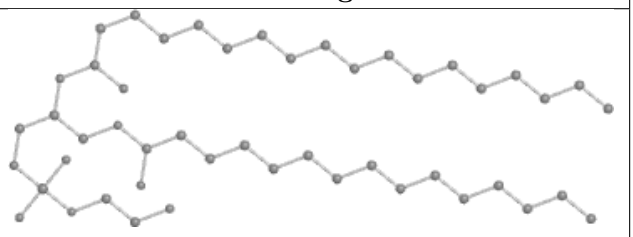
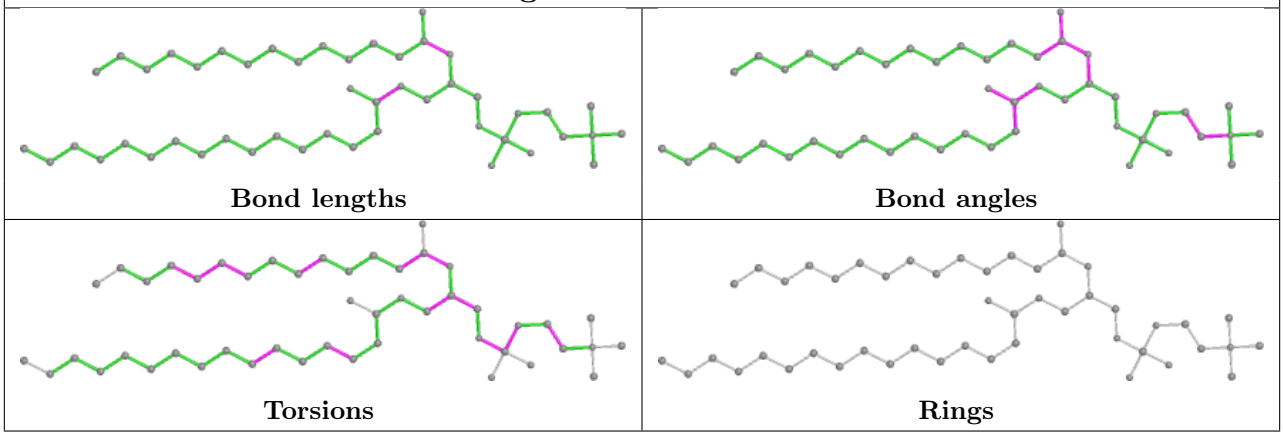
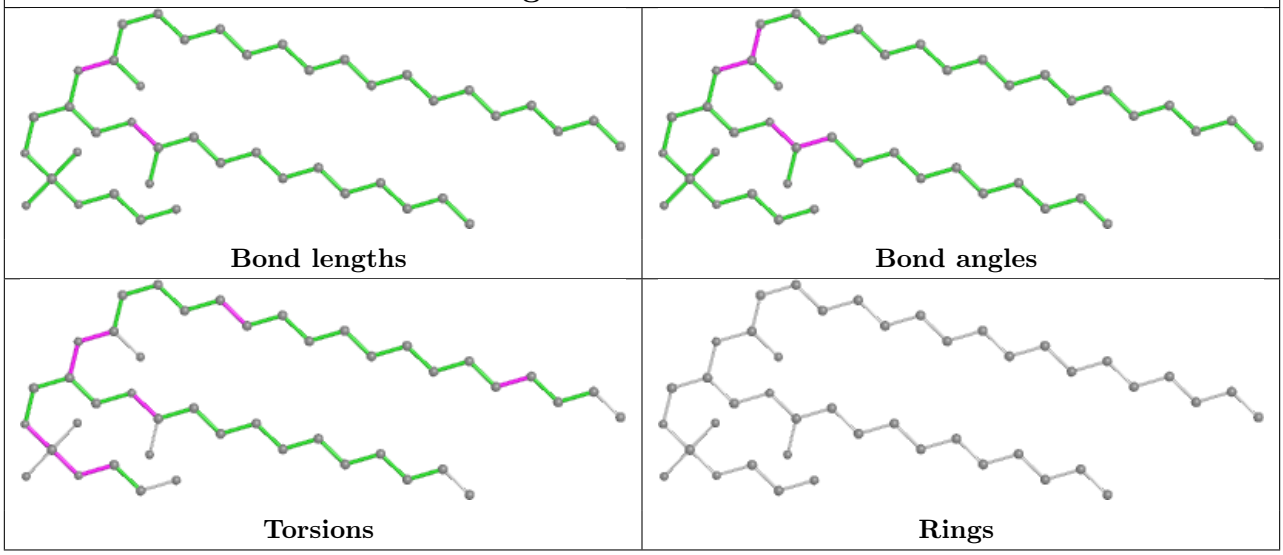


Rings

Ligand PC1 1B 203



Ligand 3PE 1L 703



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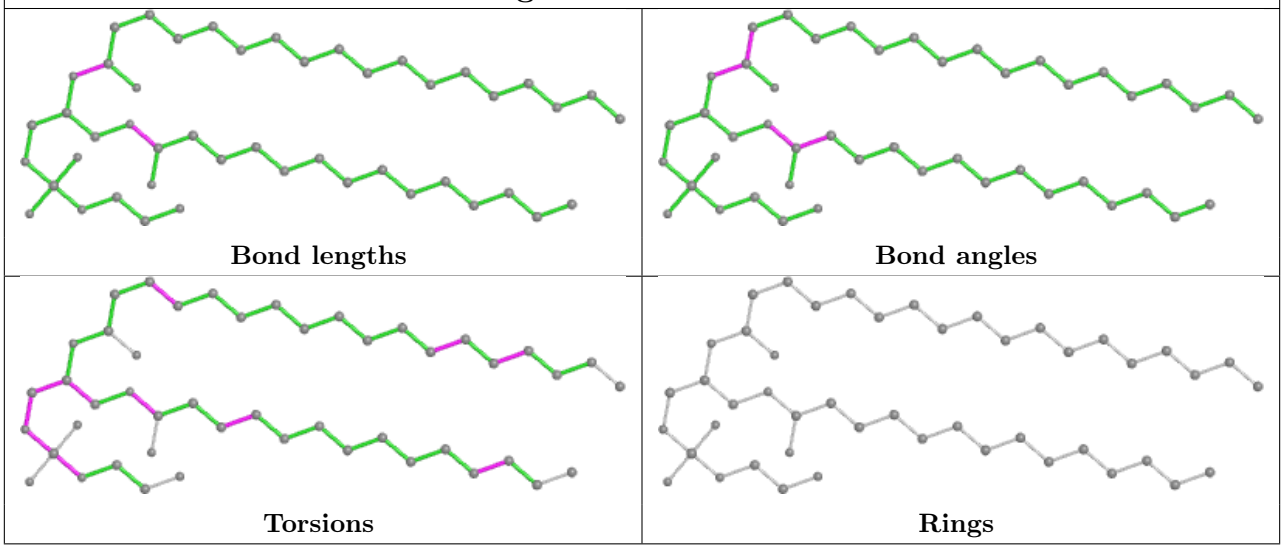
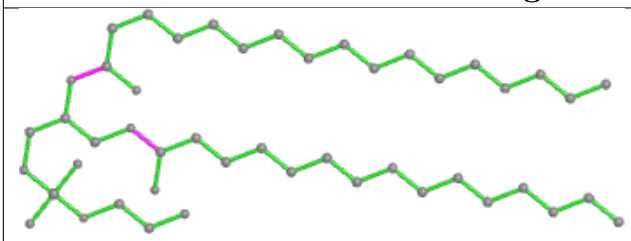
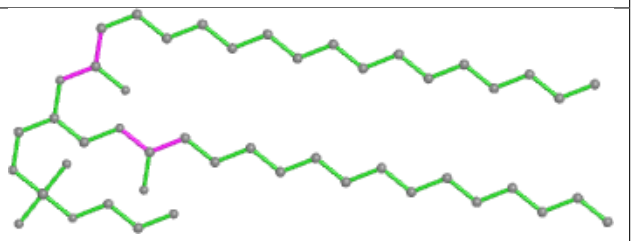


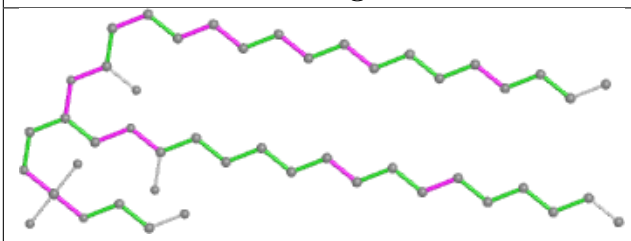
Ligand 3PE 3J 101



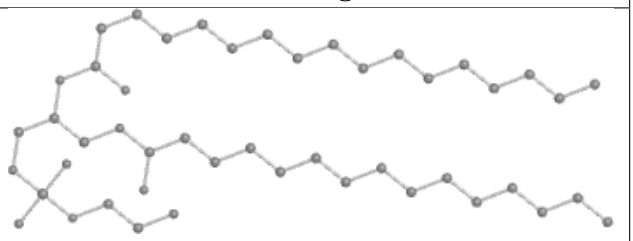
Bond lengths



Bond angles

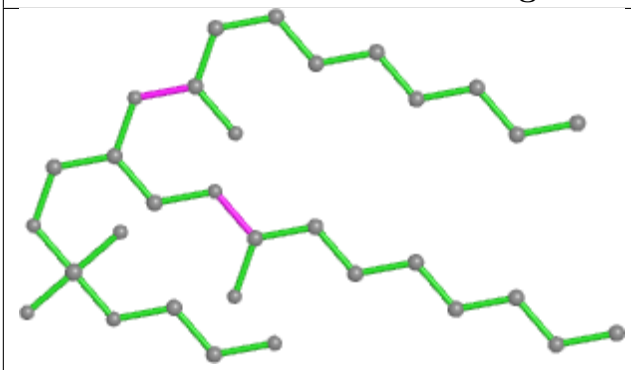


Torsions



Rings

Ligand 3PE 3Y 103



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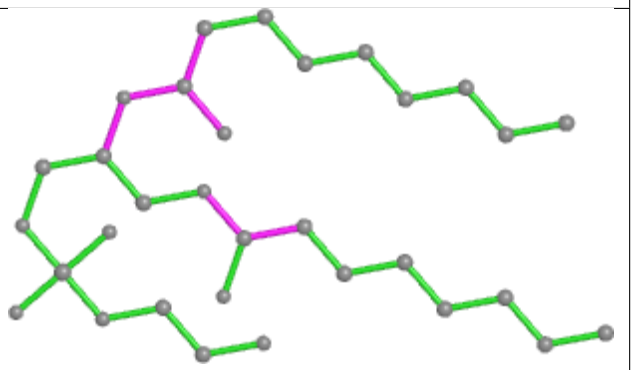
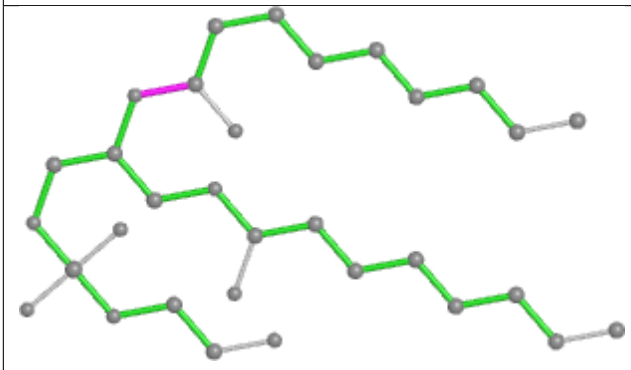


Bond angles



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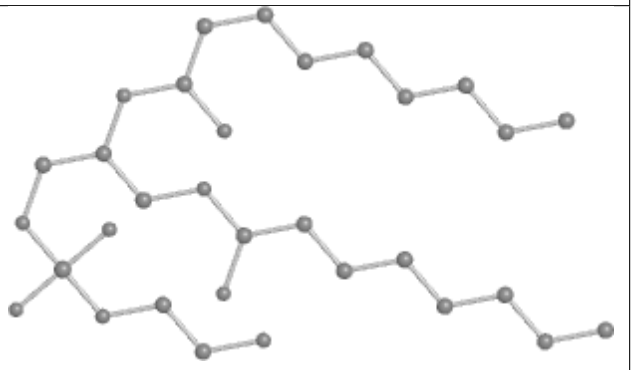
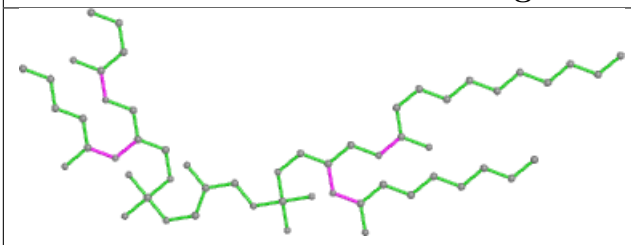


Rings

Ligand CDL 3D 504



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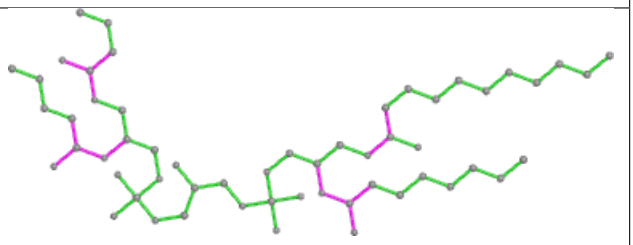
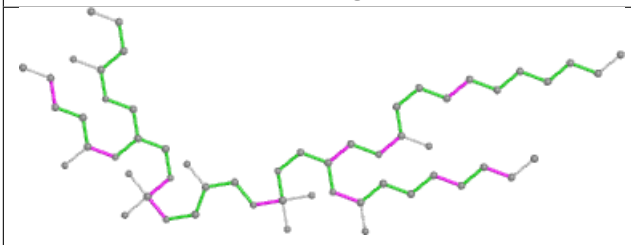
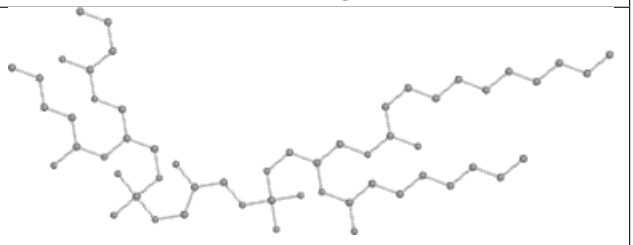


Bond angles

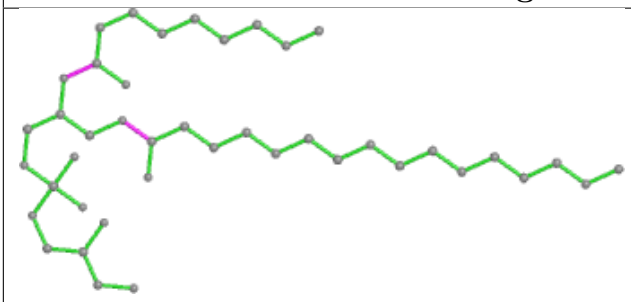


Torsions



Rings

Ligand PGV 4J 101



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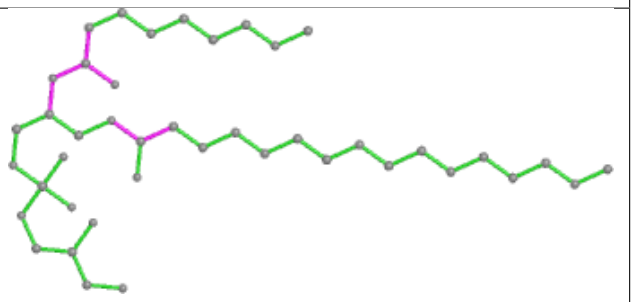
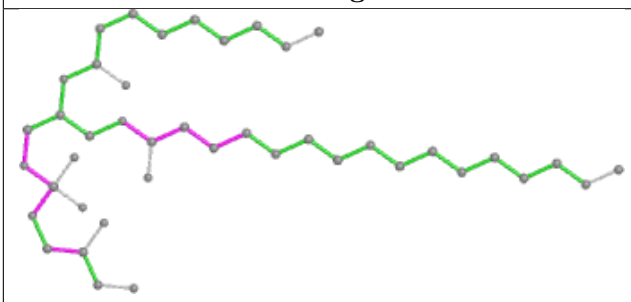


Bond angles



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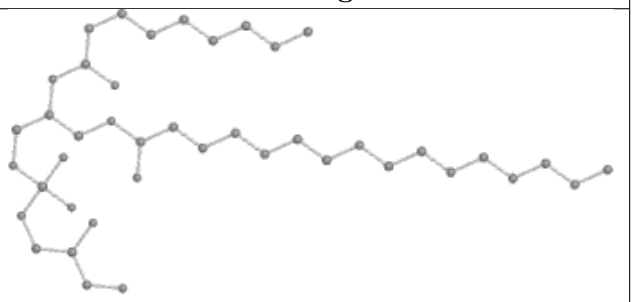
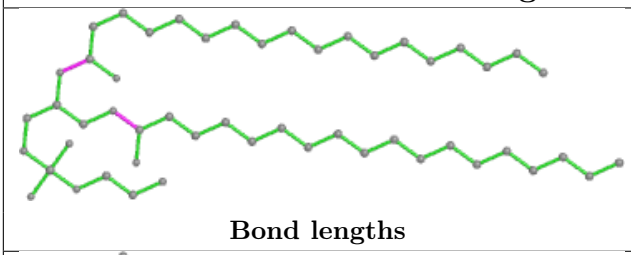


Rings

Ligand 3PE 3X 105



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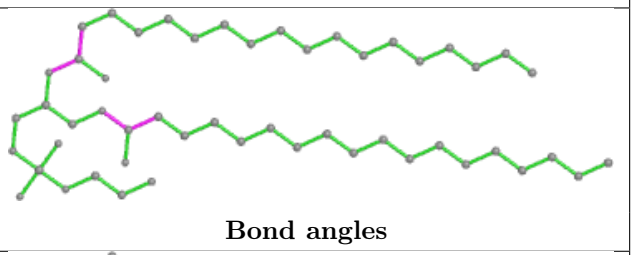
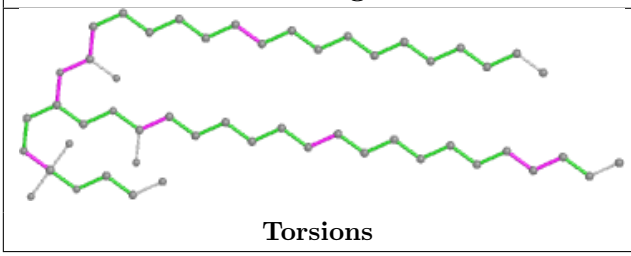


Bond angles



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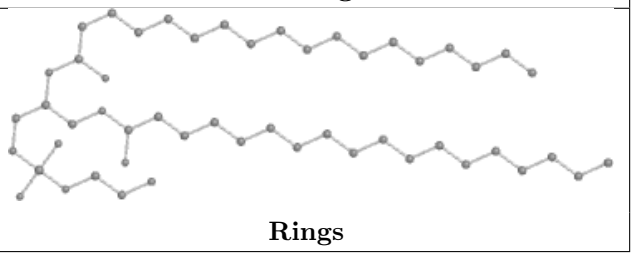
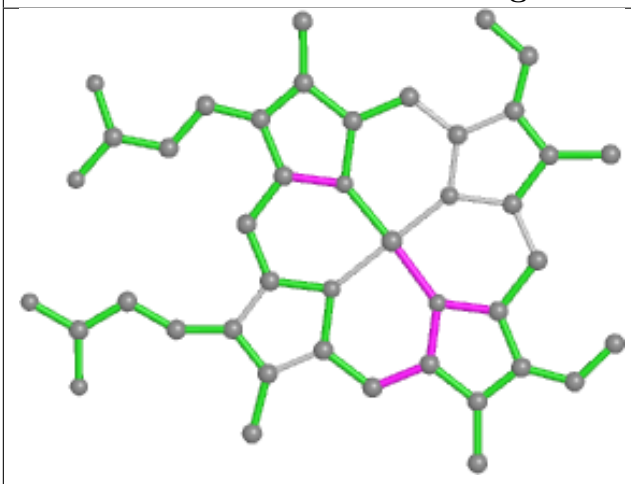


Rings

Ligand HEM 3C 501



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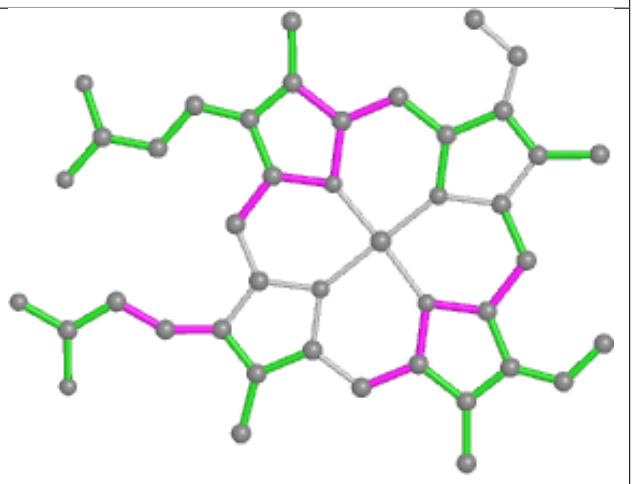
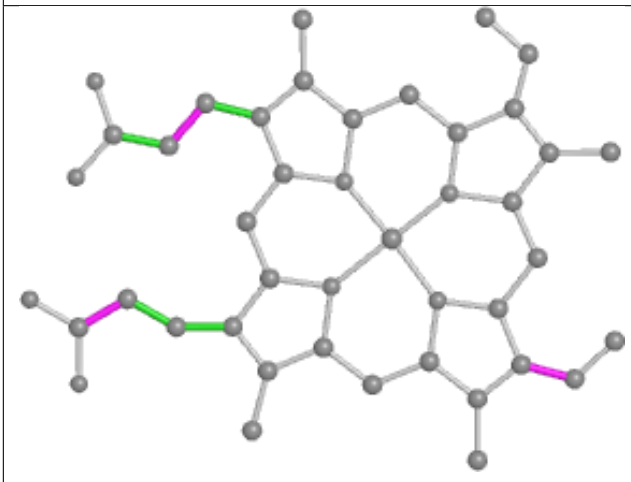


Bond angles



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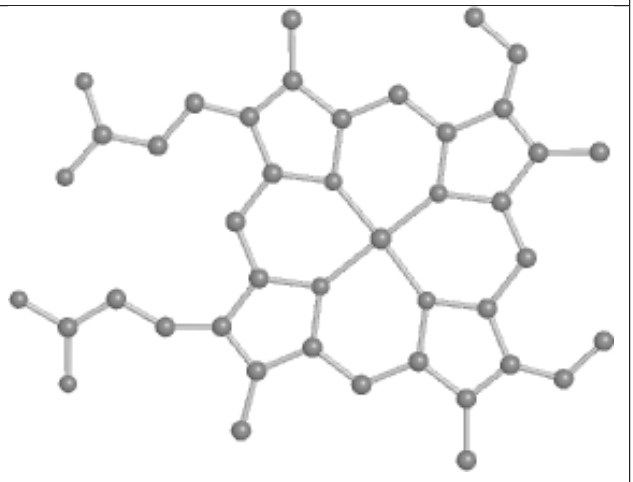
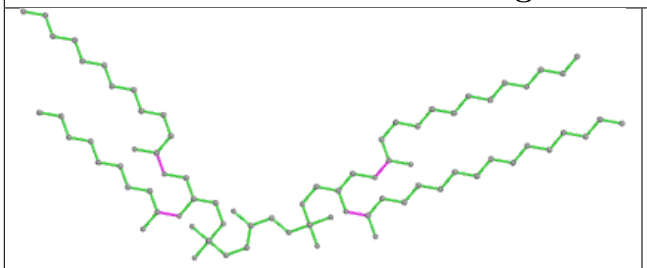


Rings

Ligand CDL 1N 402



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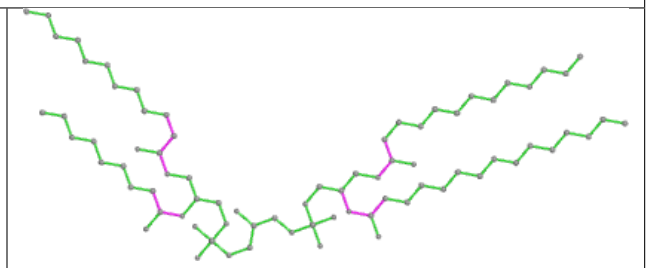
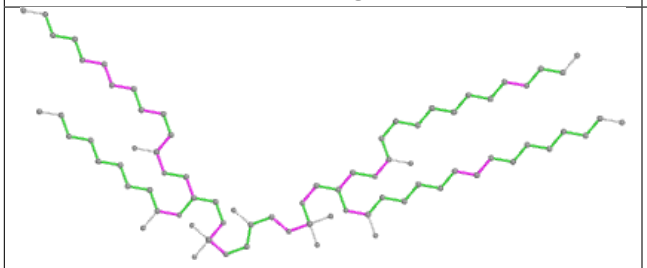


Bond angles



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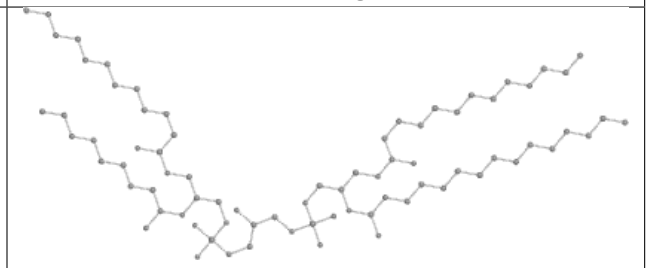
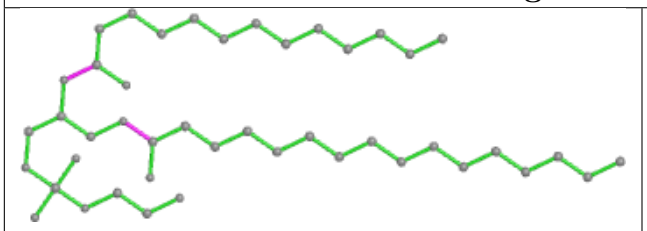
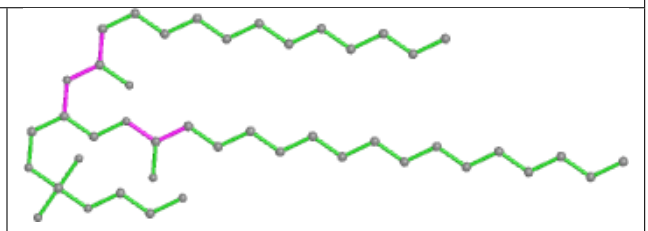


Rings

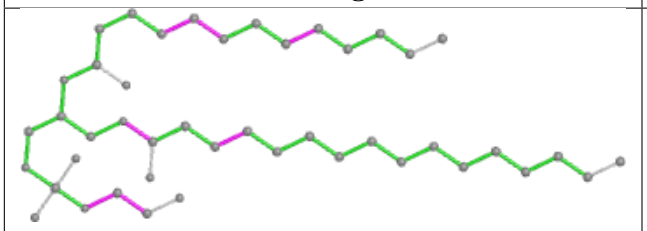
Ligand 3PE 1J 203



Bond lengths



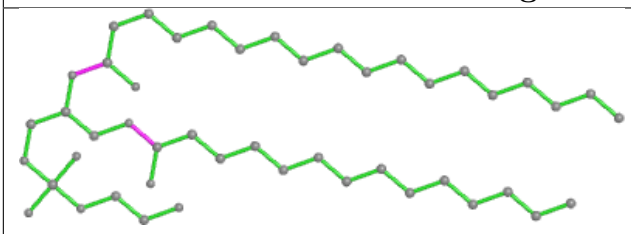
Bond angles



Torsions

Rings

Ligand 3PE 3C 506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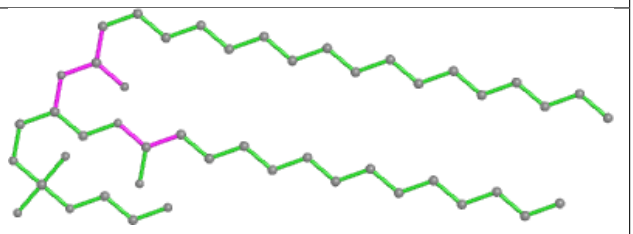
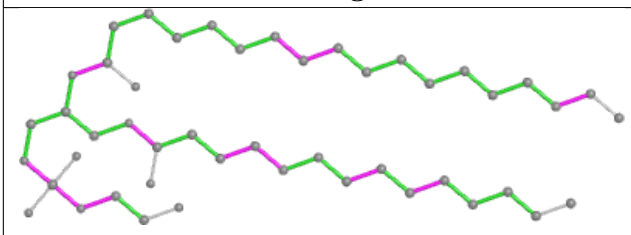
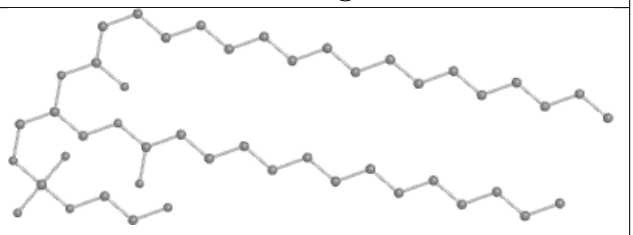
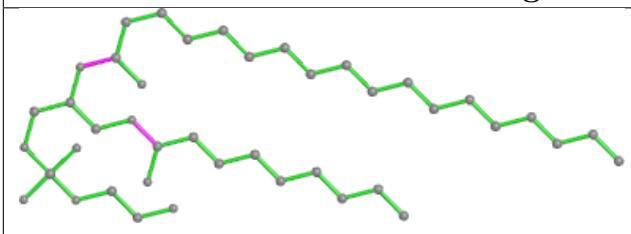
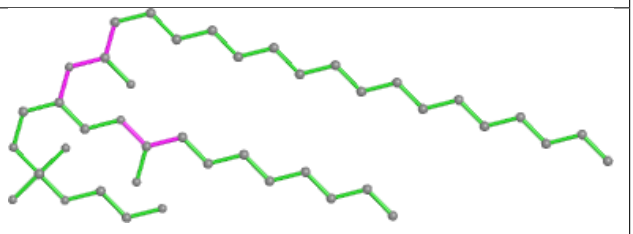

Bond angles

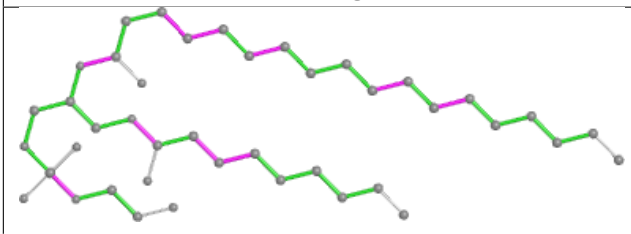

Torsions

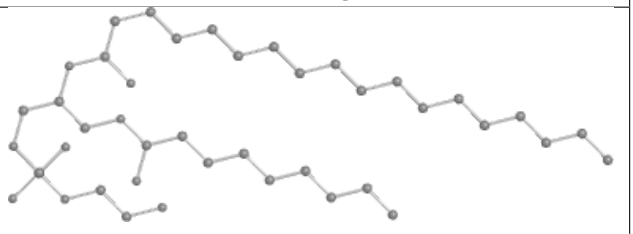

Rings

Ligand 3PE 1b 101

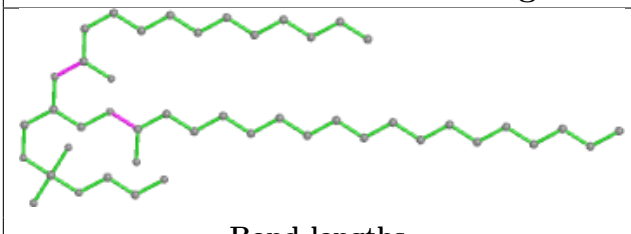

Bond lengths

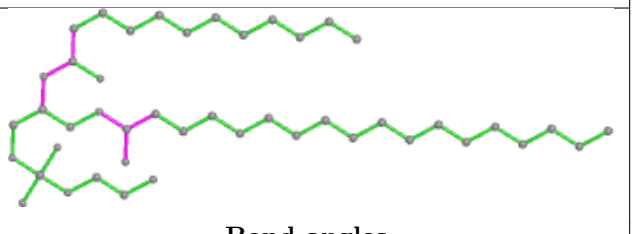

Bond angles

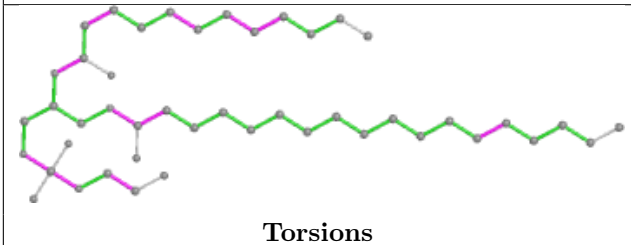

Torsions

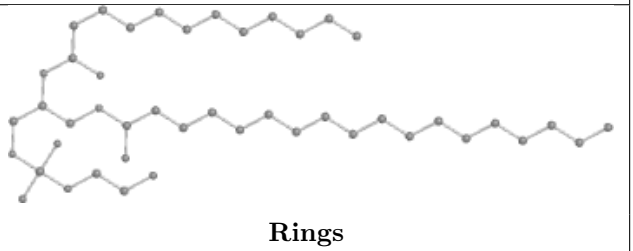

Rings

Ligand 3PE 3D 503

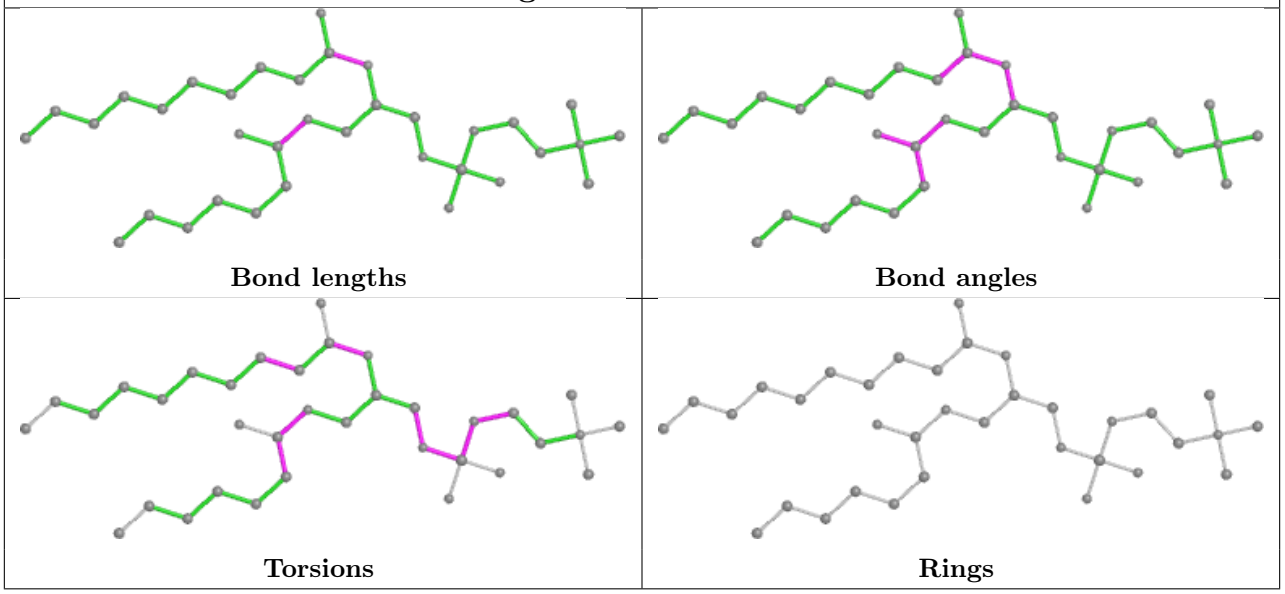

Bond lengths


Bond angles

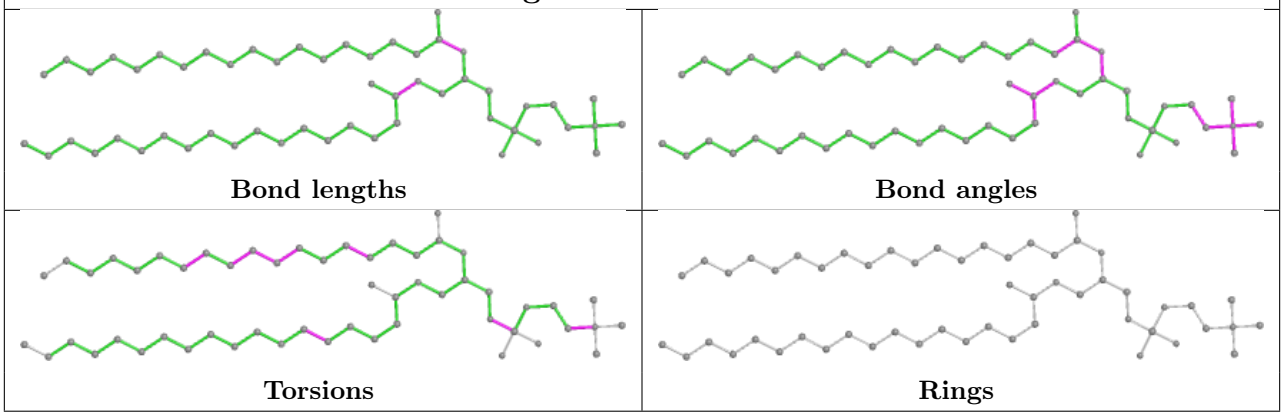

Torsions


Rings

Ligand PC1 1A 202



Ligand PC1 3J 106



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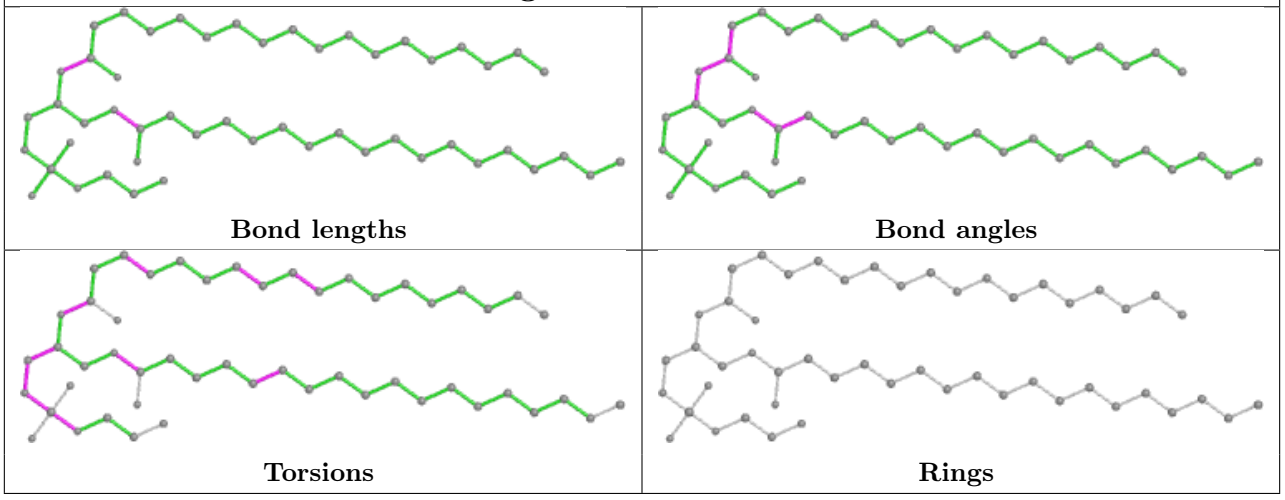
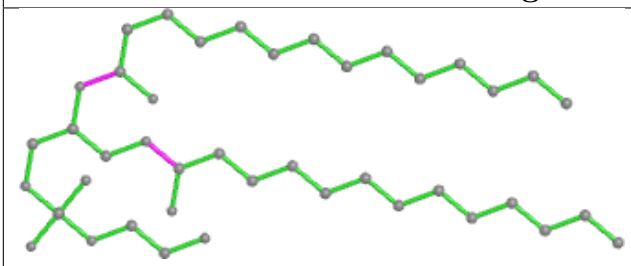
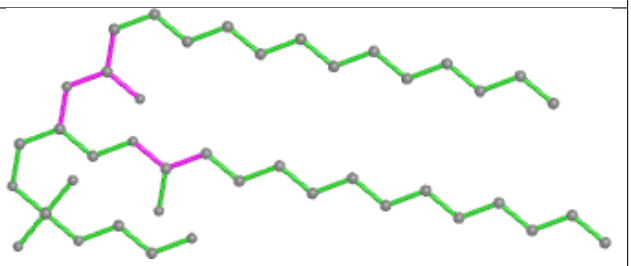


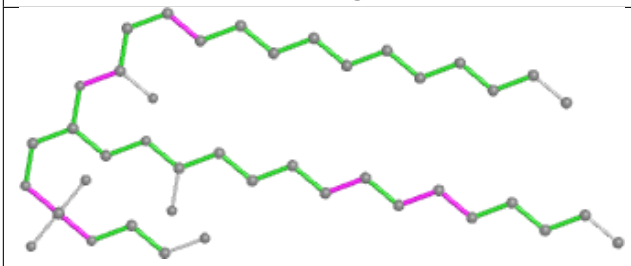
Ligand 3PE 1L 709



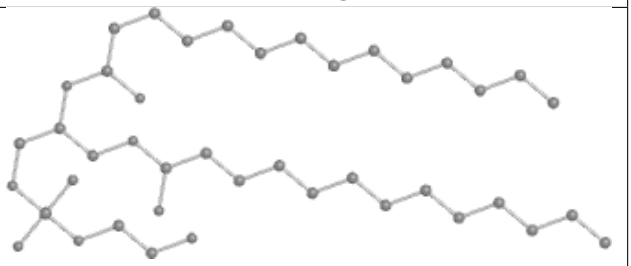
Bond lengths



Bond angles

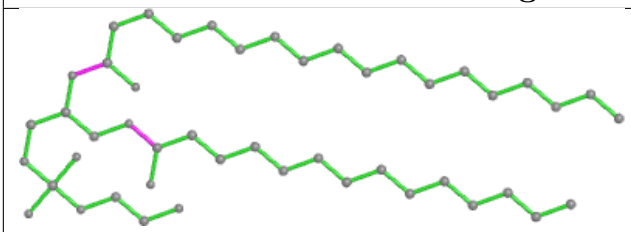


Torsions



Rings

Ligand 3PE 1A 201



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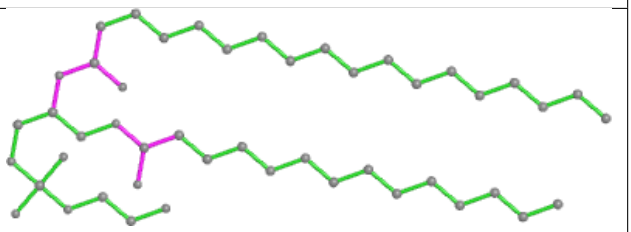
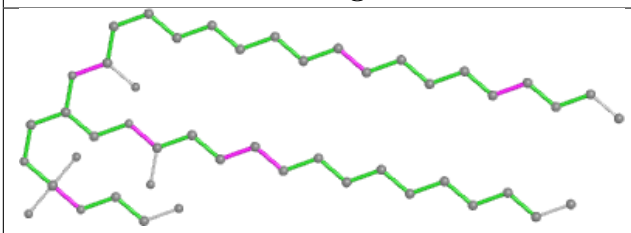


Bond angles



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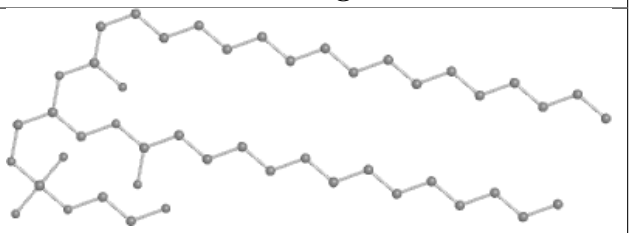
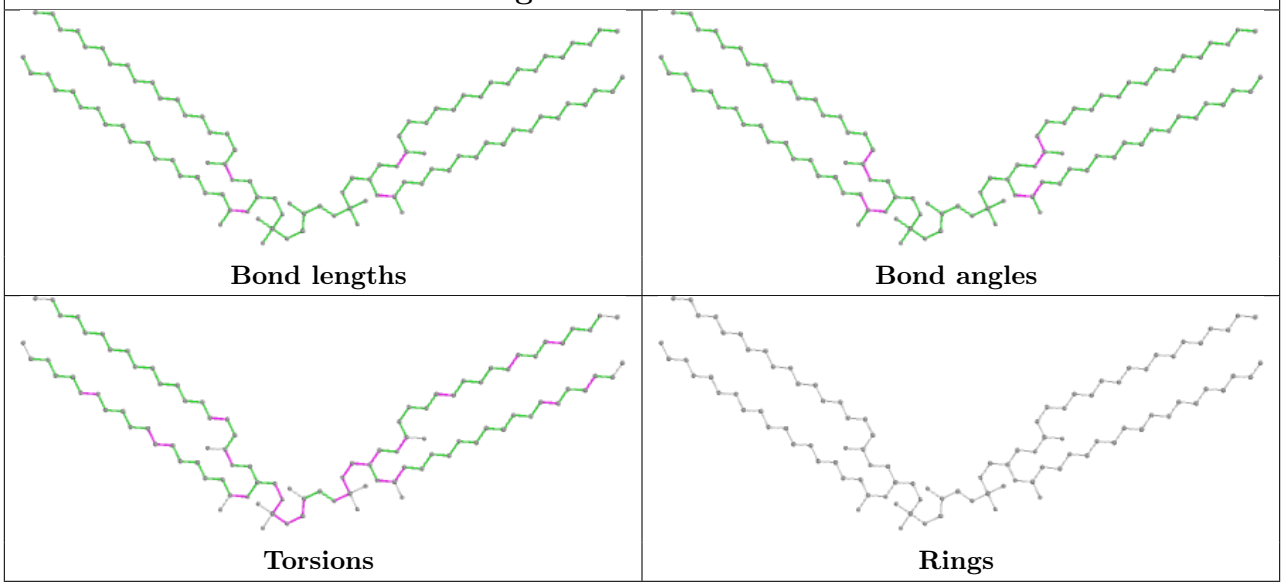
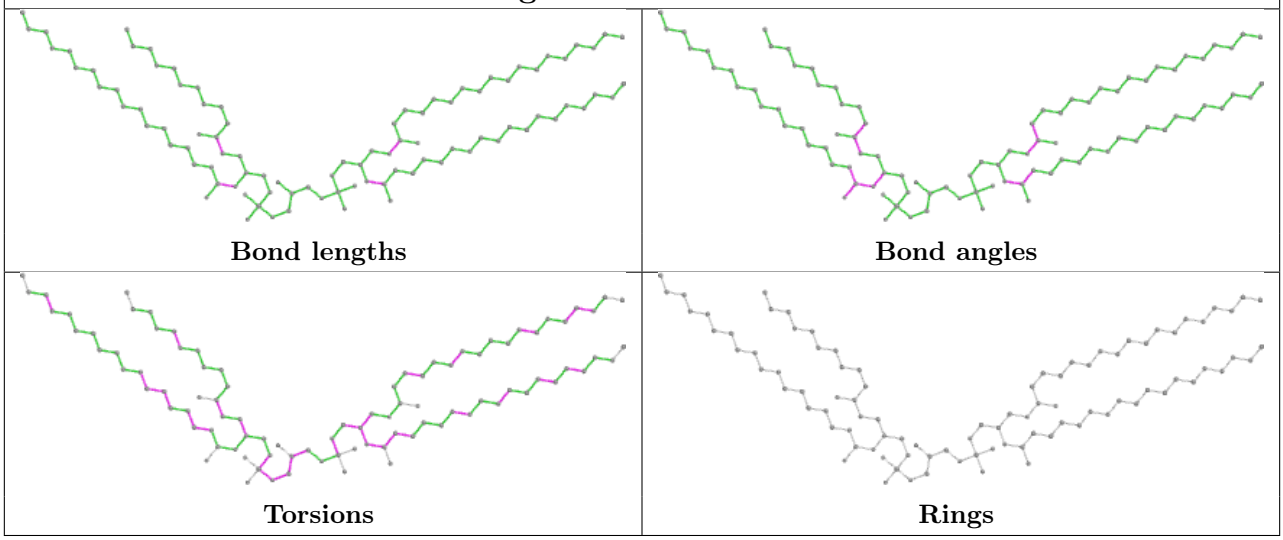


Rings

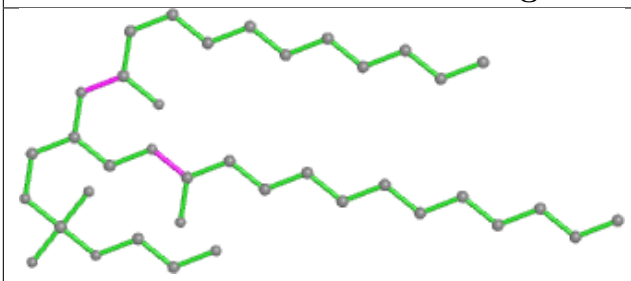
Ligand CDL 3Y 106



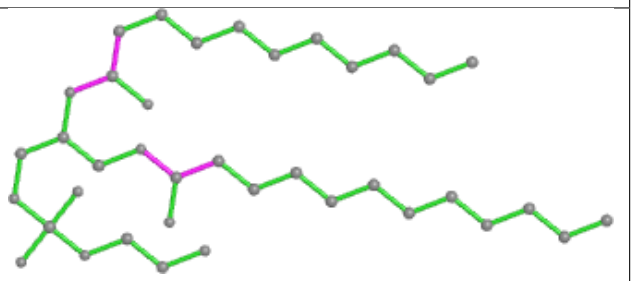
Ligand CDL 1d 205



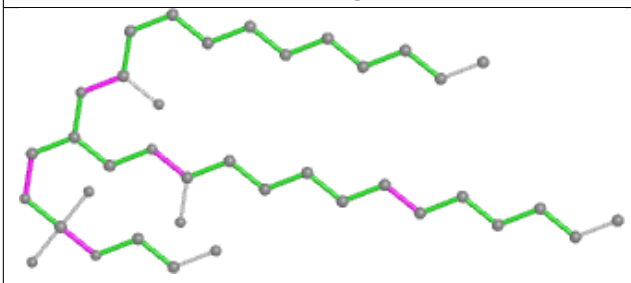
Ligand 3PE 3P 504



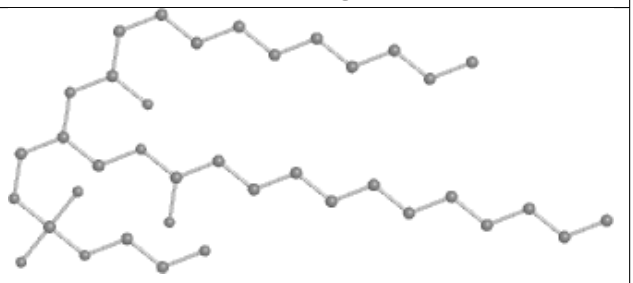
Bond lengths



Bond angles

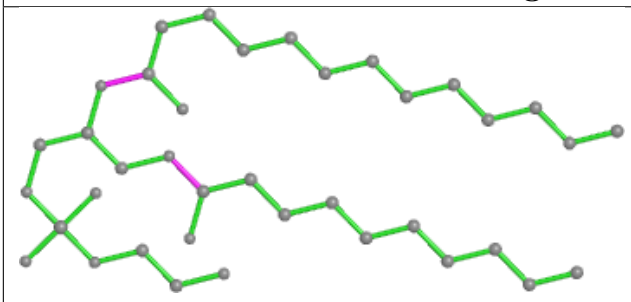


Torsions

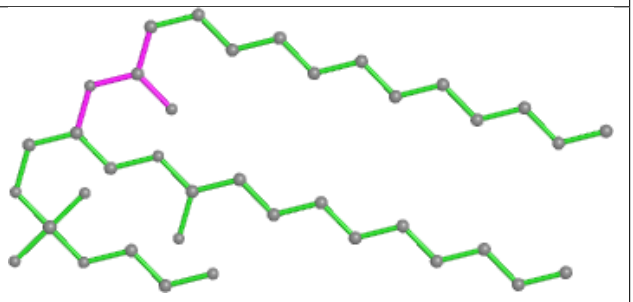


Rings

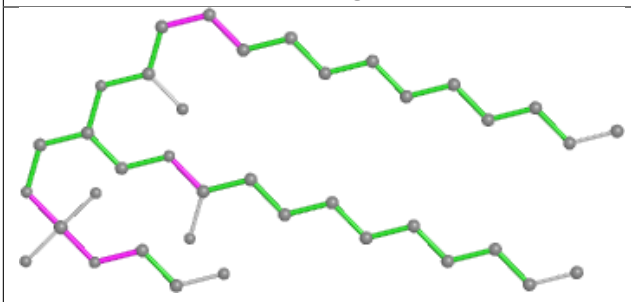
Ligand 3PE 3J 102



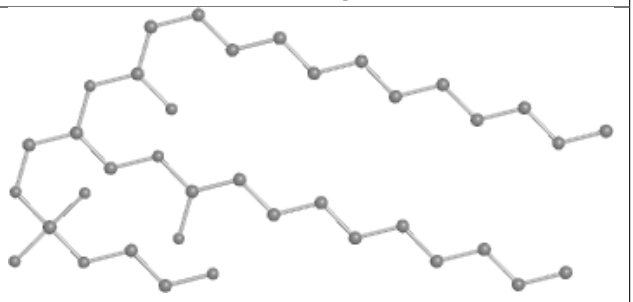
Bond lengths



Bond angles

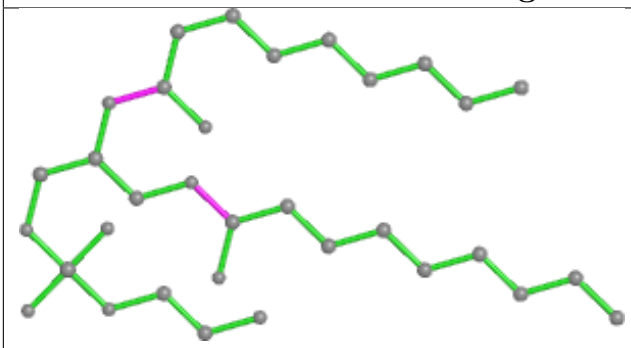


Torsions

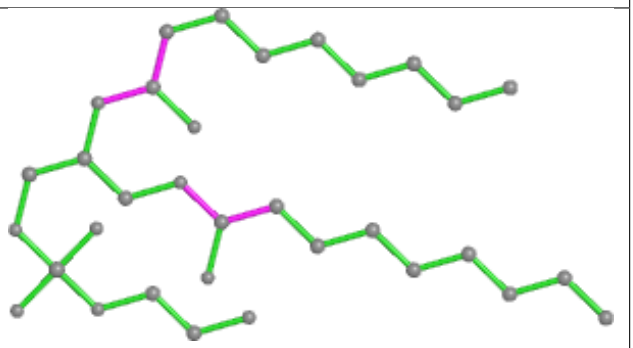


Rings

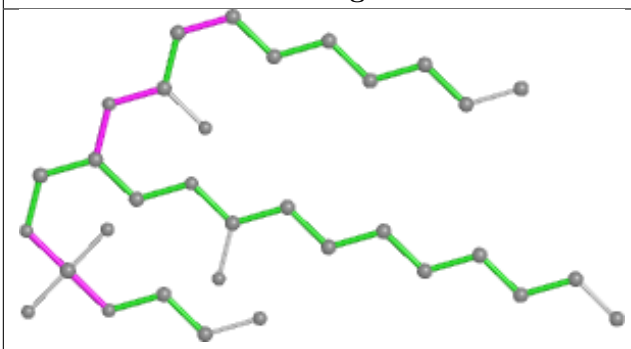
Ligand 3PE 3G 103



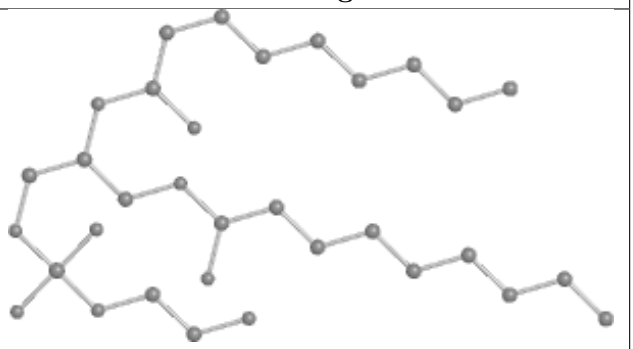
Bond lengths



Bond angles

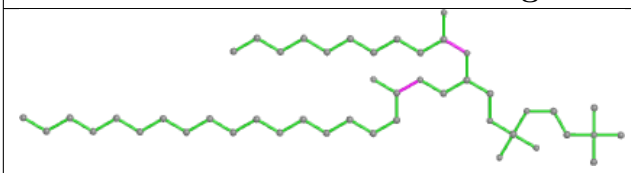


Torsions

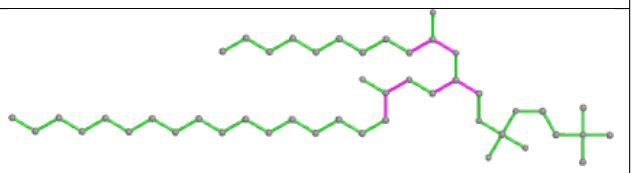


Rings

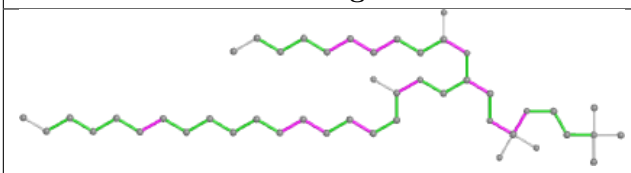
Ligand PC1 1h 203



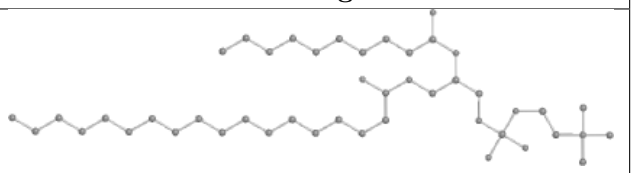
Bond lengths



Bond angles

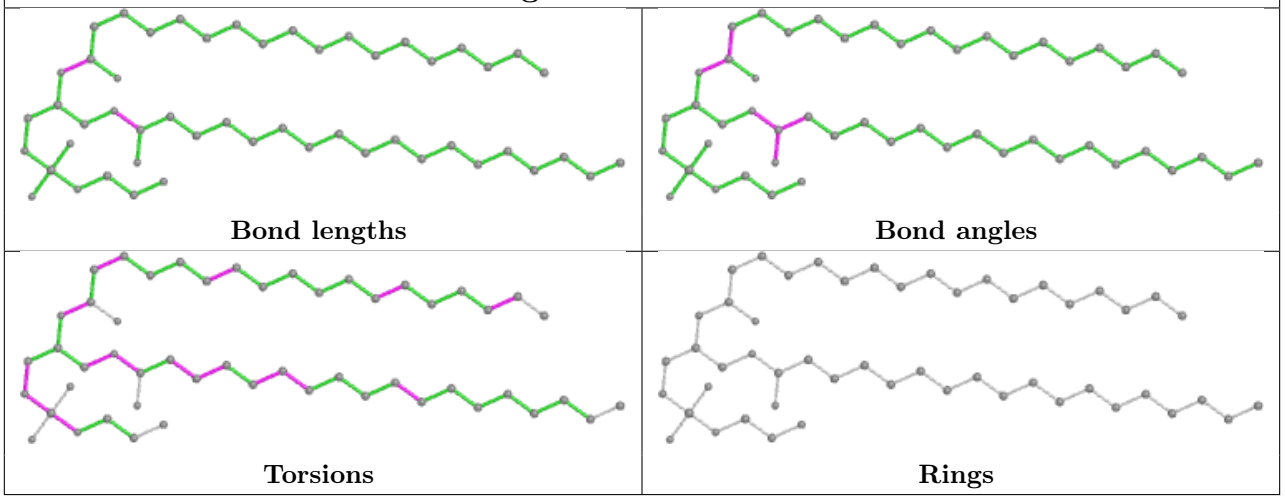


Torsions

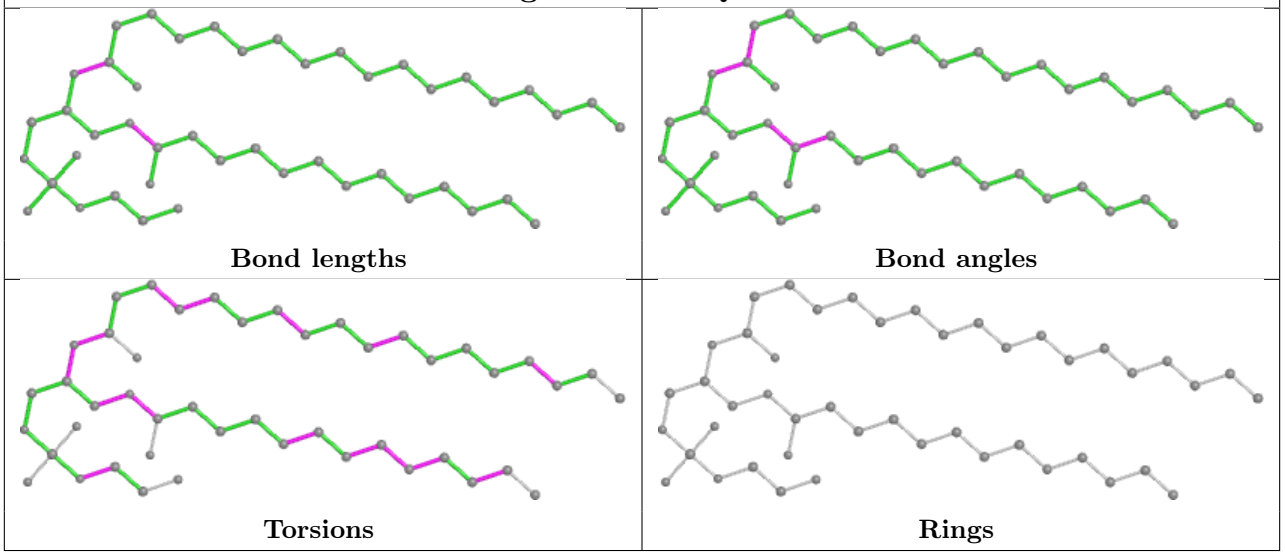


Rings

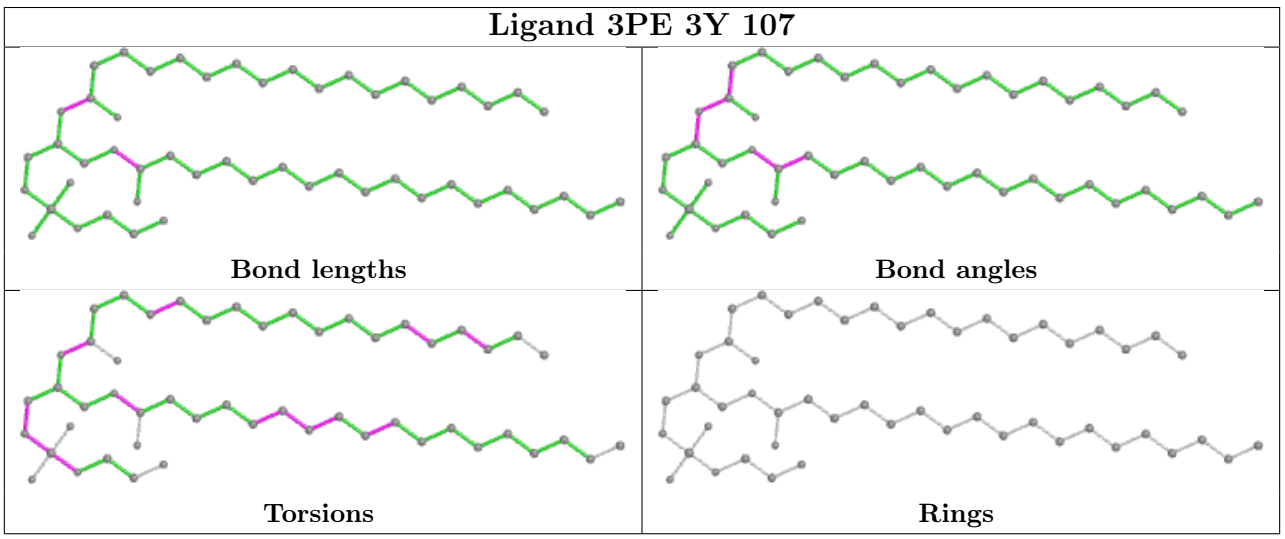
Ligand 3PE 3P 507



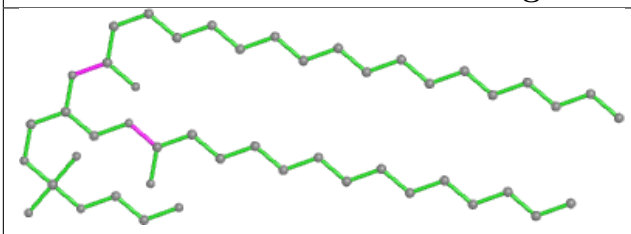
Ligand 3PE 3Q 503



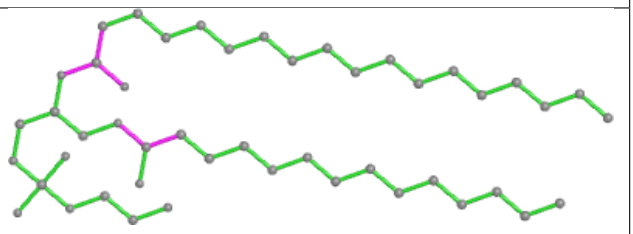
Ligand 3PE 3Y 107



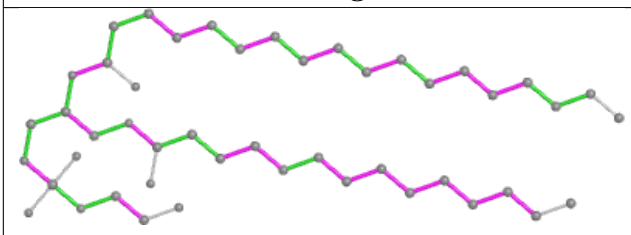
Ligand 3PE 1d 203



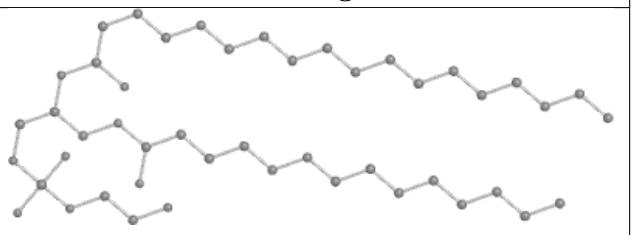
Bond lengths



Bond angles

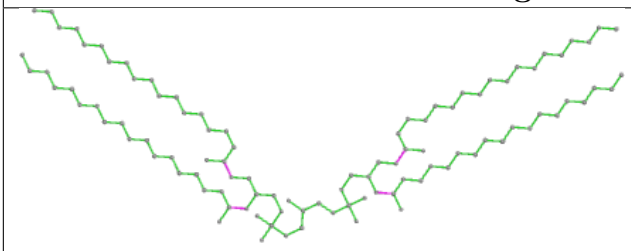


Torsions



Rings

Ligand CDL 3N 502



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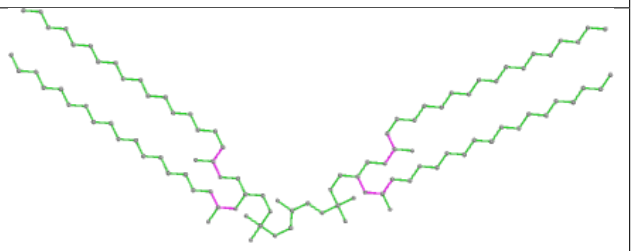
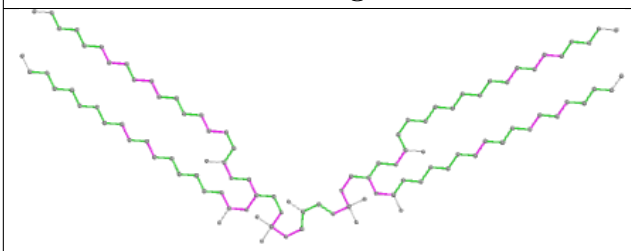
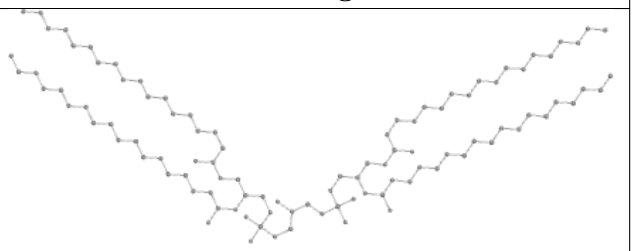


Bond angles

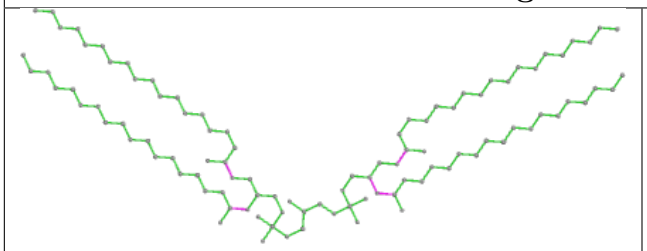


Torsions

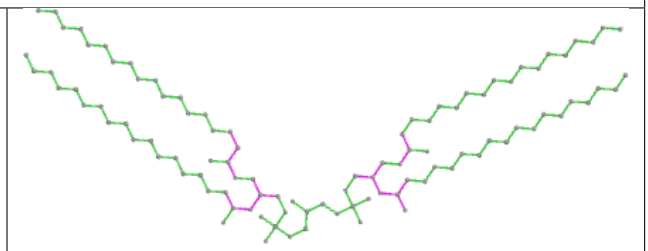


Rings

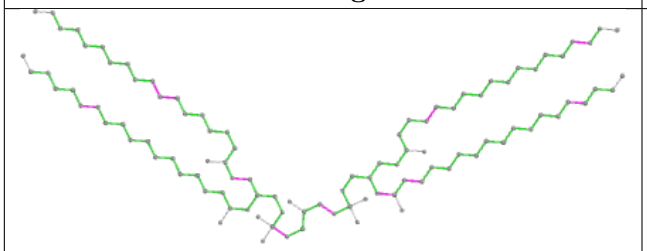
Ligand CDL 3P 513



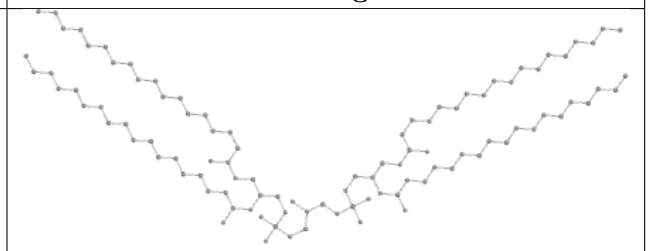
Bond lengths



Bond angles

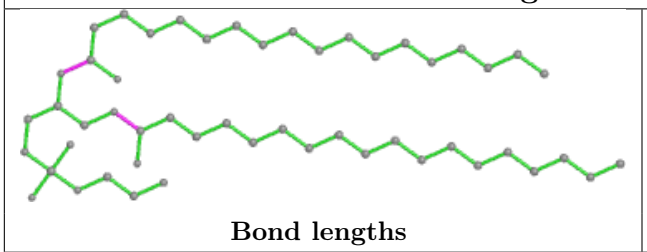


Torsions

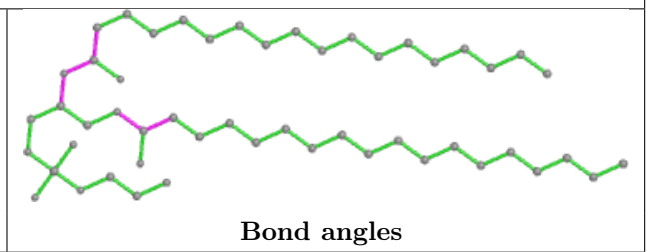


Rings

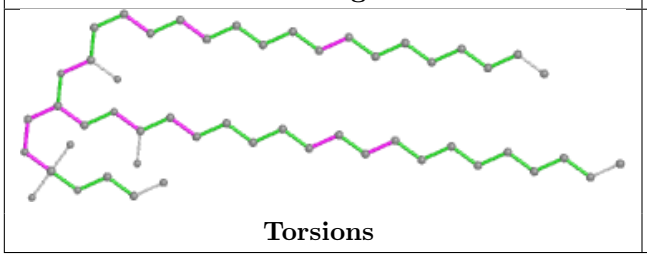
Ligand 3PE 3C 511



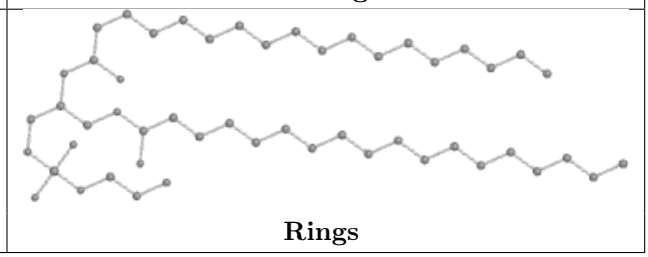
Bond lengths



Bond angles

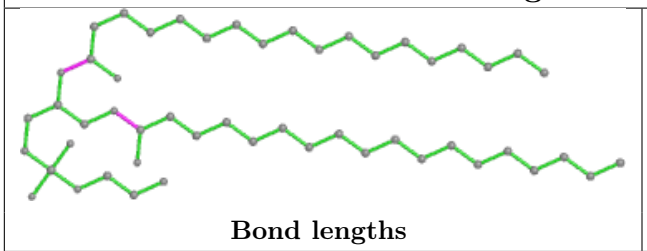


Torsions

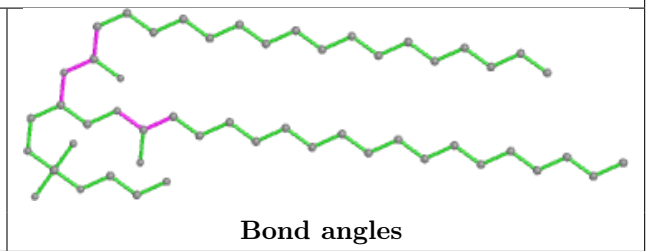


Rings

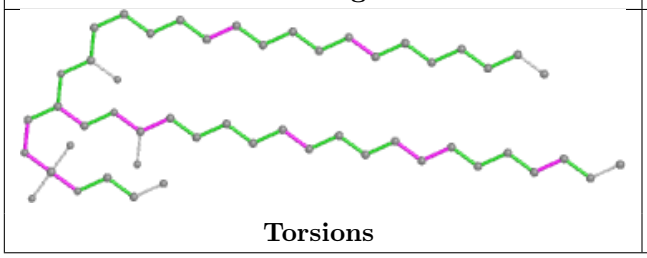
Ligand 3PE 1J 201



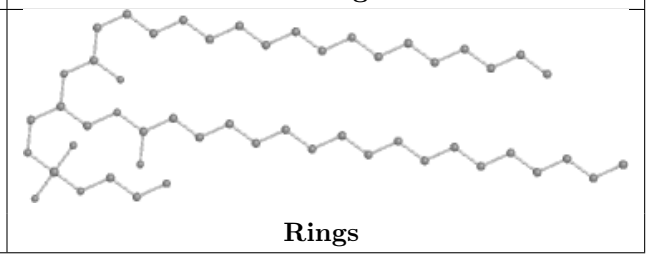
Bond lengths



Bond angles

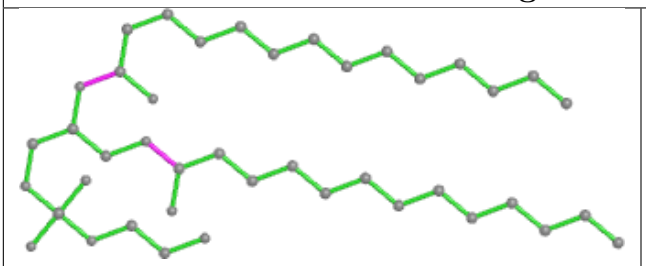


Torsions

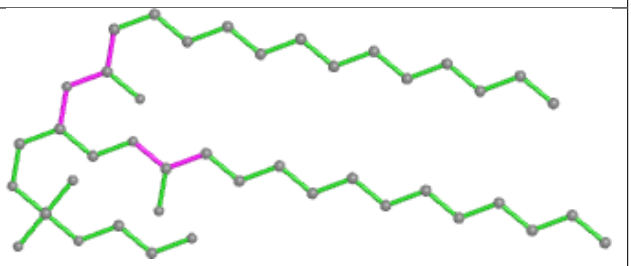


Rings

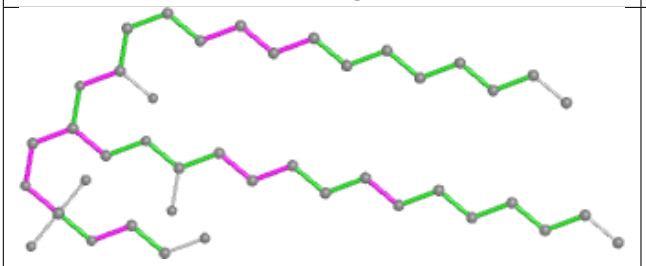
Ligand 3PE 1Y 210



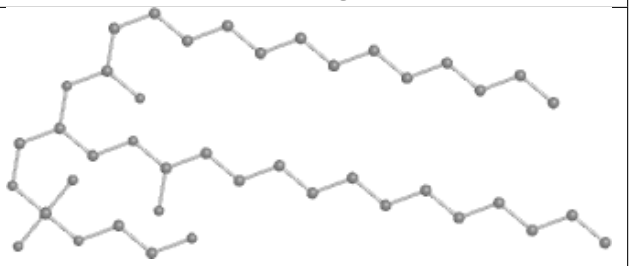
Bond lengths



Bond angles

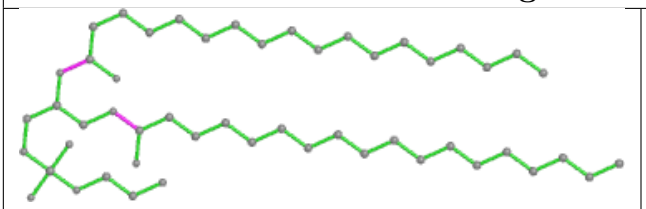


Torsions

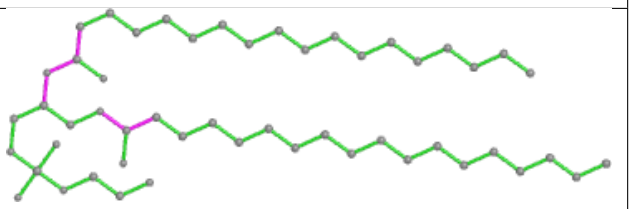


Rings

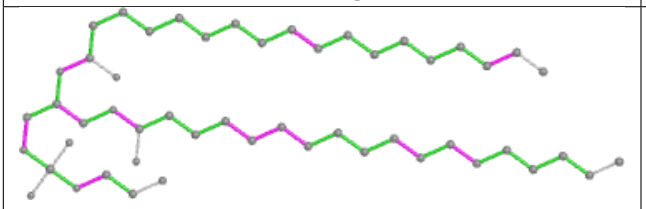
Ligand 3PE 1Y 214



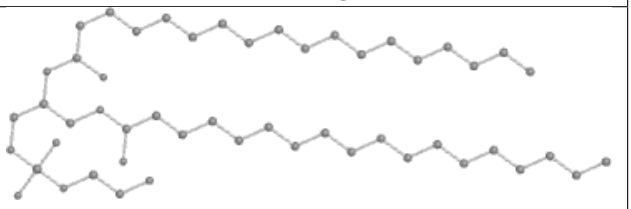
Bond lengths



Bond angles

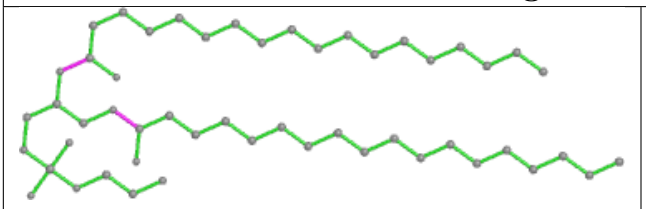


Torsions

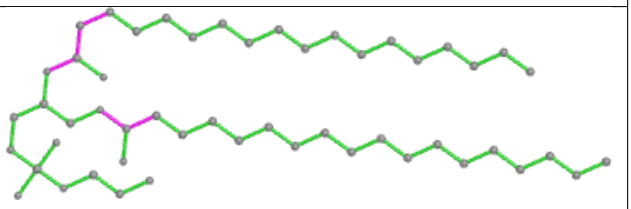


Rings

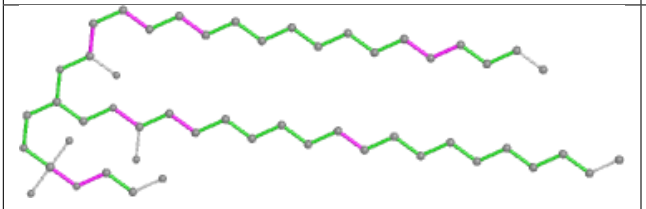
Ligand 3PE 1d 206



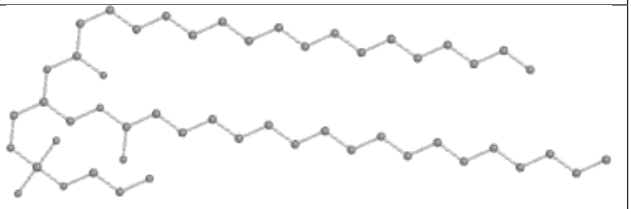
Bond lengths



Bond angles

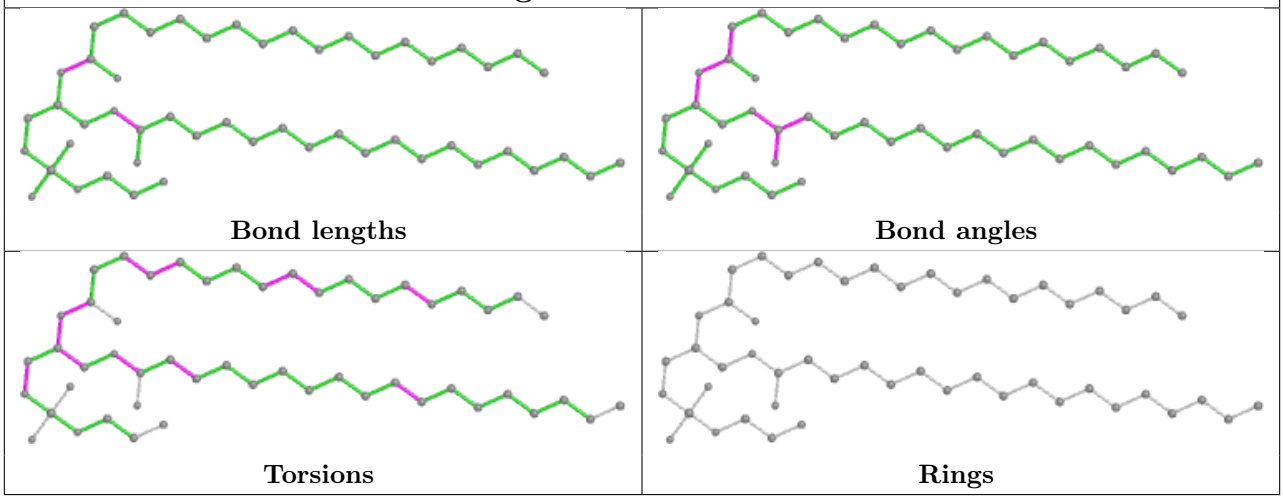


Torsions

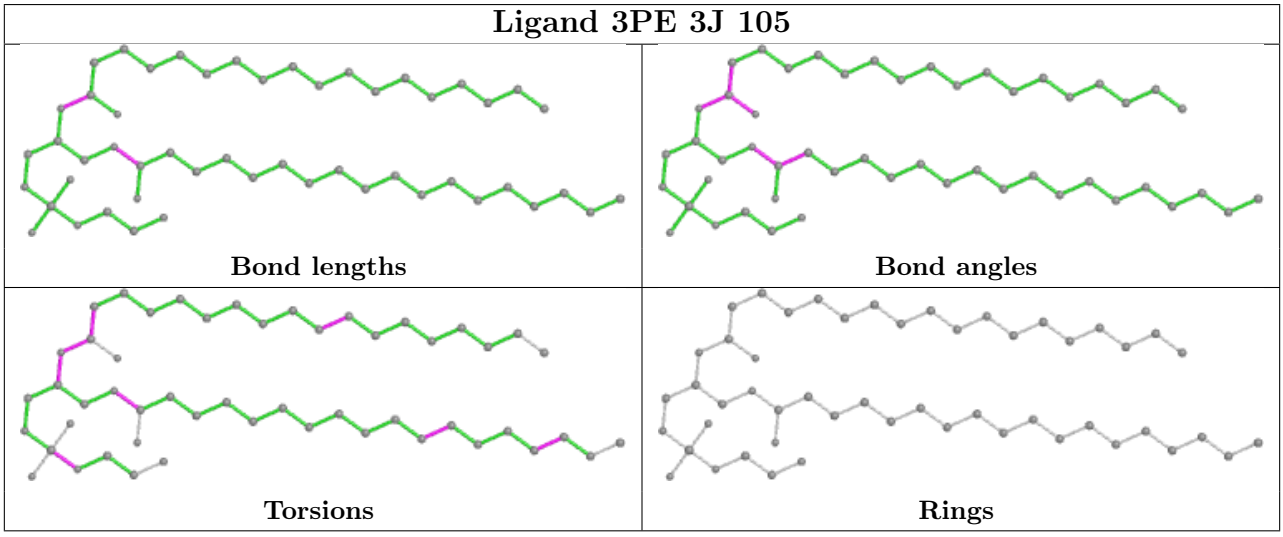


Rings

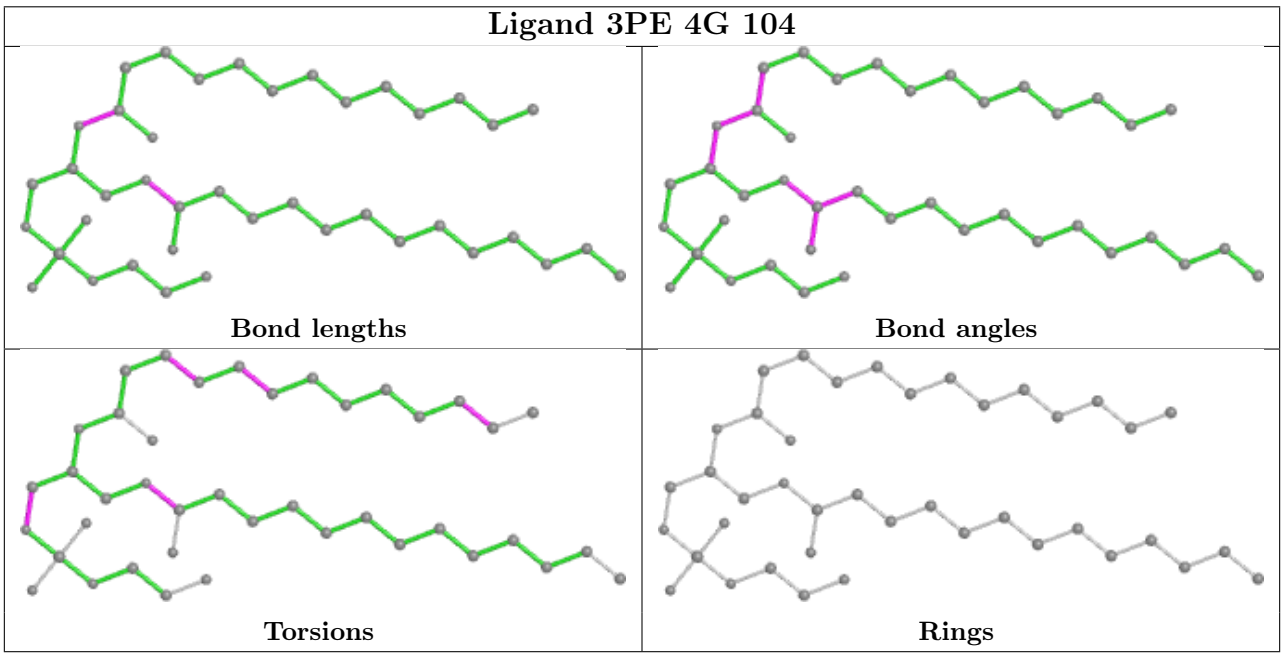
Ligand 3PE 3W 103



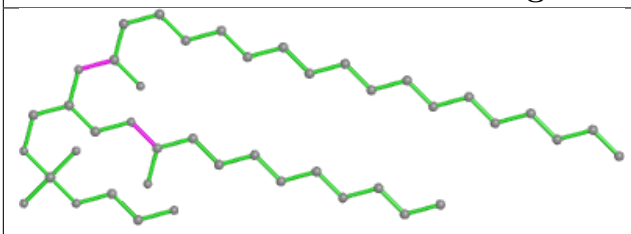
Ligand 3PE 3J 105



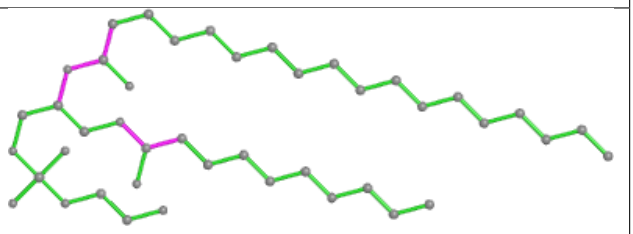
Ligand 3PE 4G 104



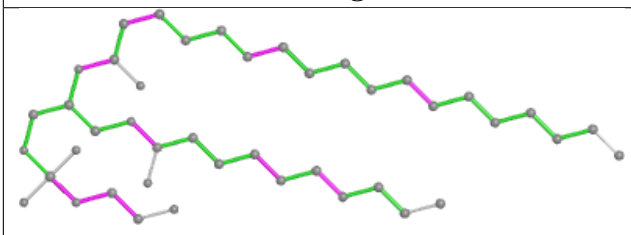
Ligand 3PE 1f 102



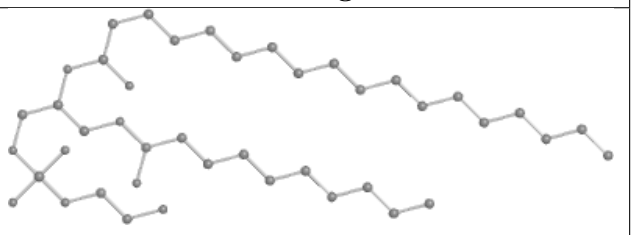
Bond lengths



Bond angles

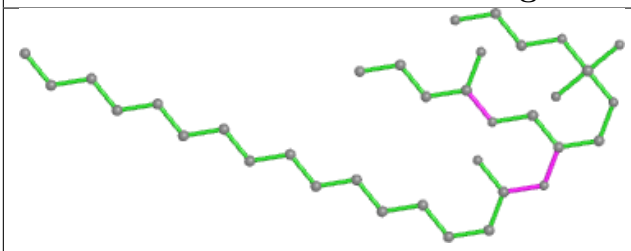


Torsions

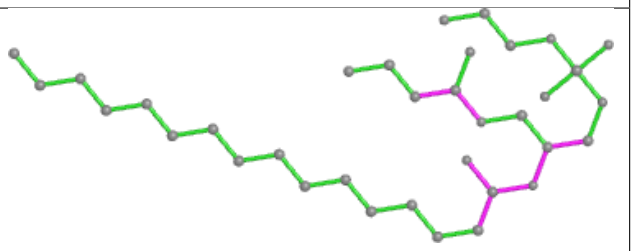


Rings

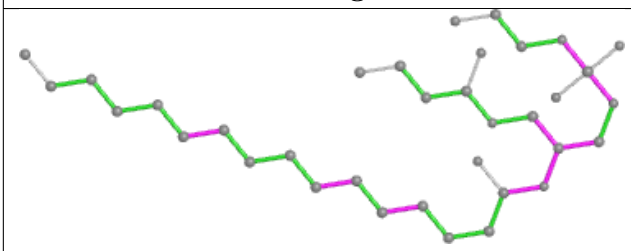
Ligand 3PE 3C 510



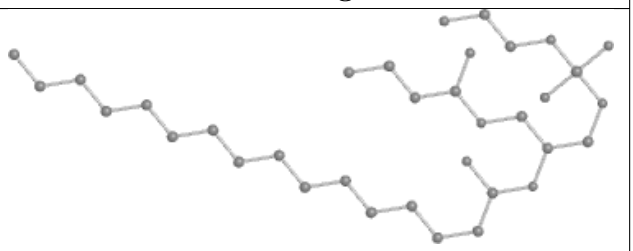
Bond lengths



Bond angles

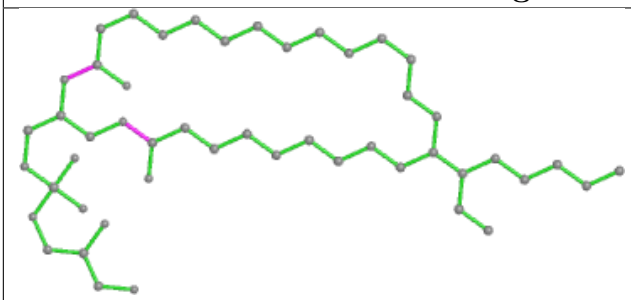


Torsions

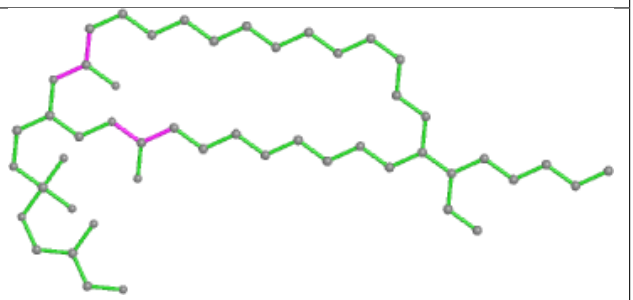


Rings

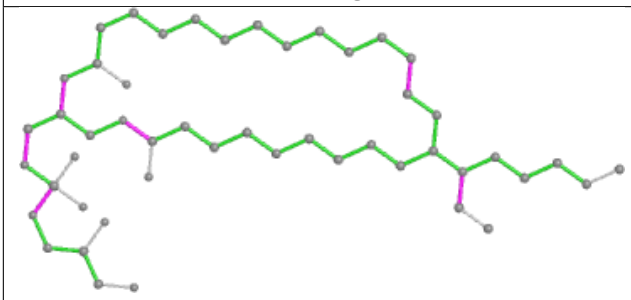
Ligand PGV 4C 303



Bond lengths



Bond angles



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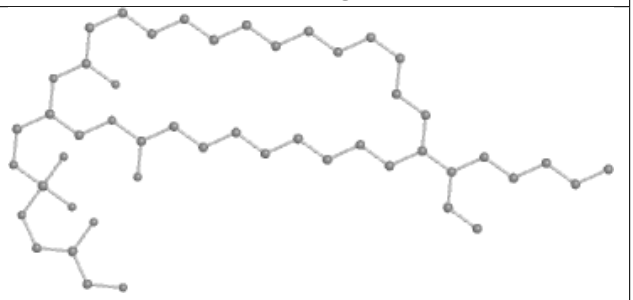
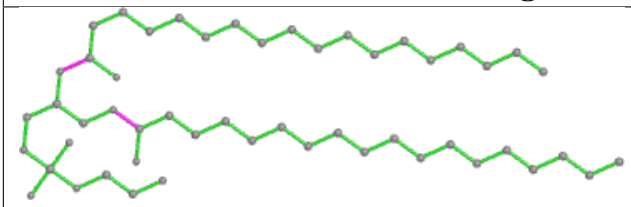
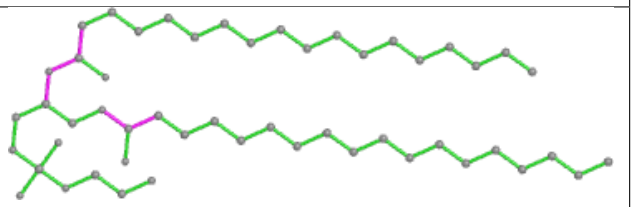


Rings

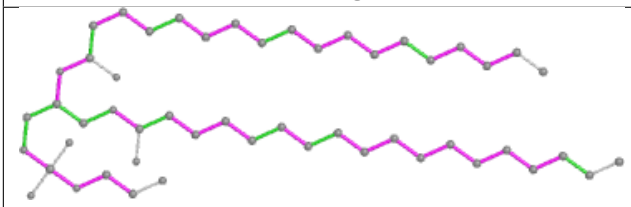
Ligand 3PE 1Y 213



Bond lengths



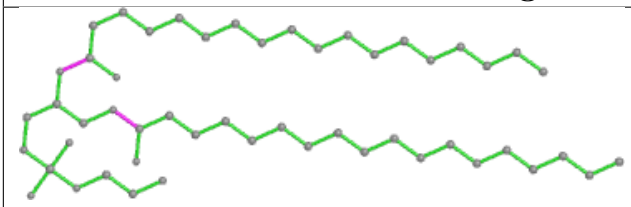
Bond angles



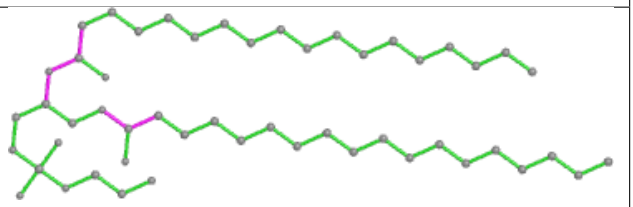
Torsions

Rings

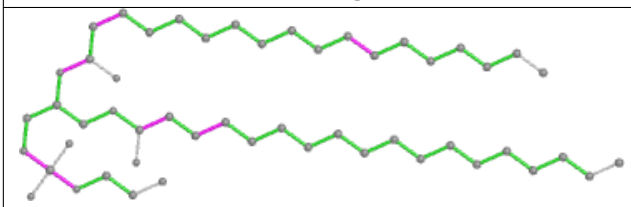
Ligand 3PE 1Y 211



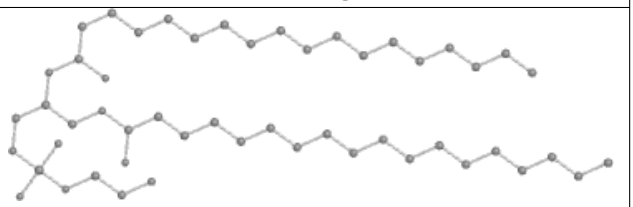
Bond lengths



Bond angles

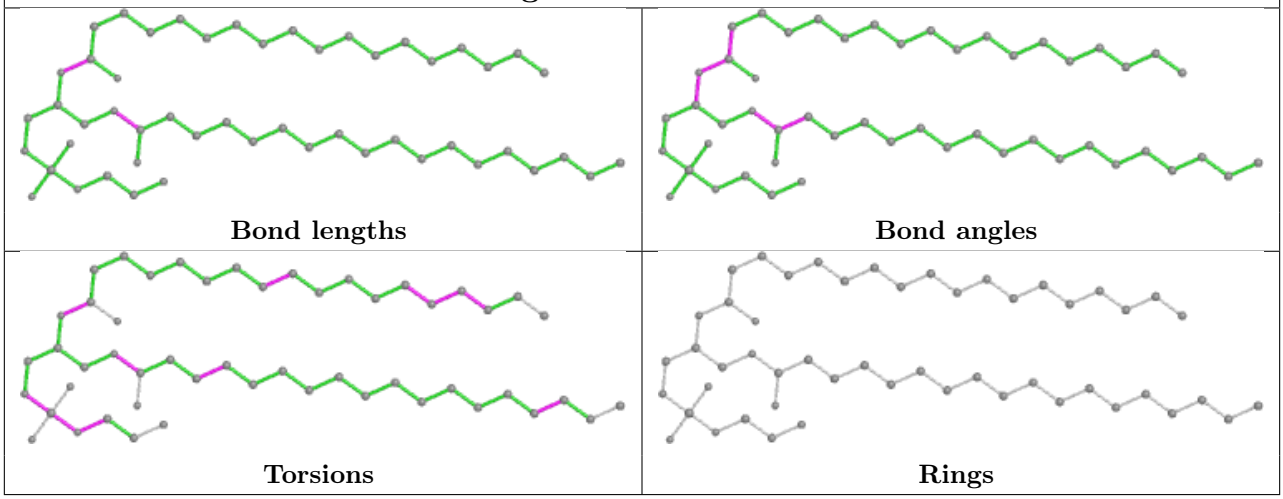


Torsions

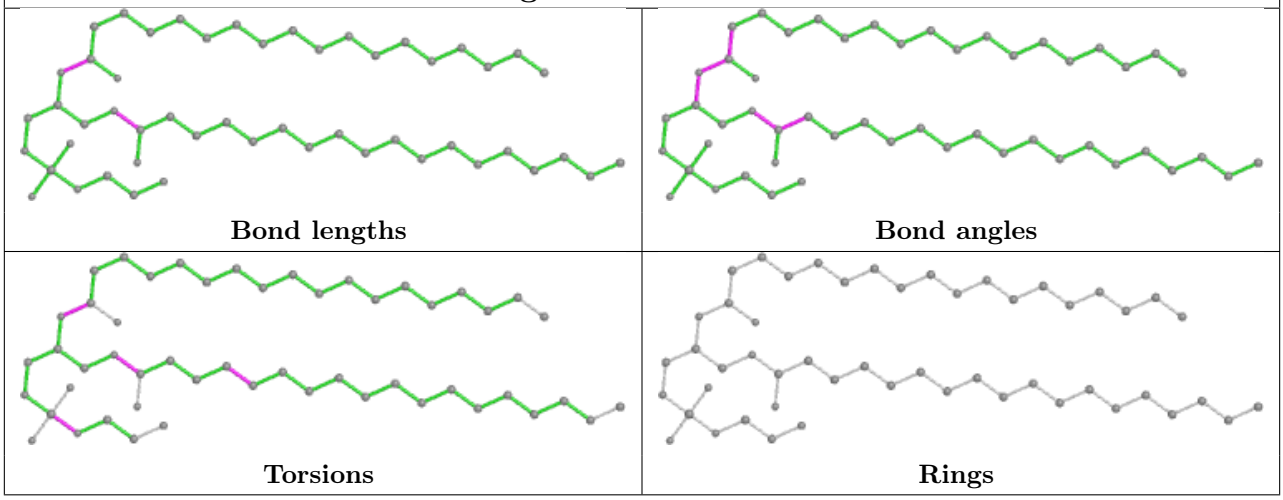


Rings

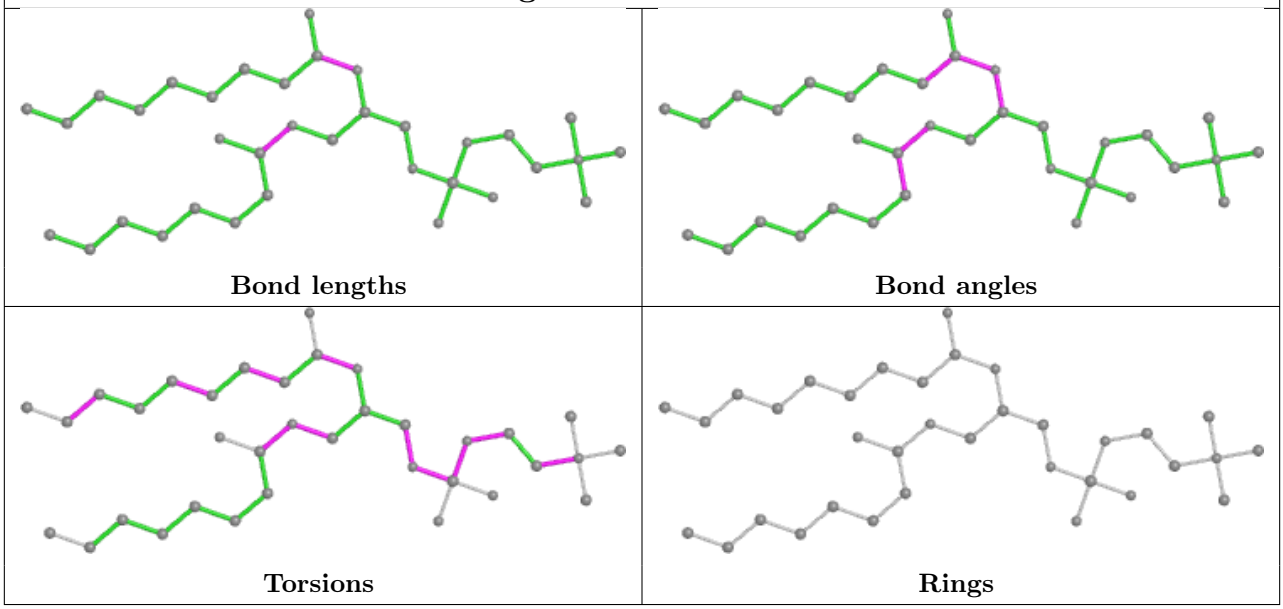
Ligand 3PE 3P 518



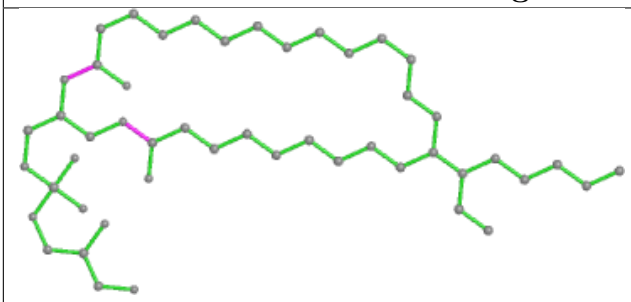
Ligand 3PE 3Y 105



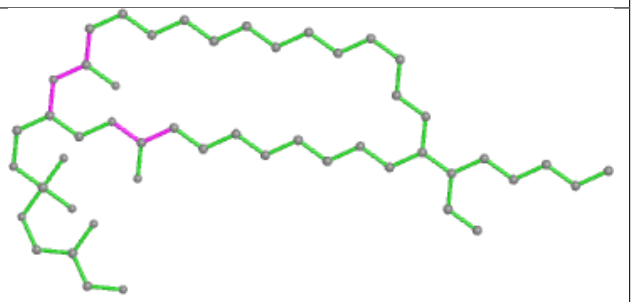
Ligand PC1 1Y 202



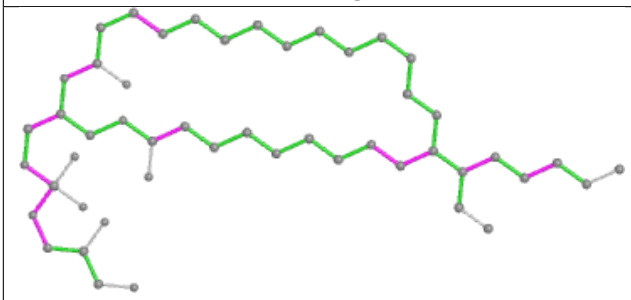
Ligand PGV 4G 102



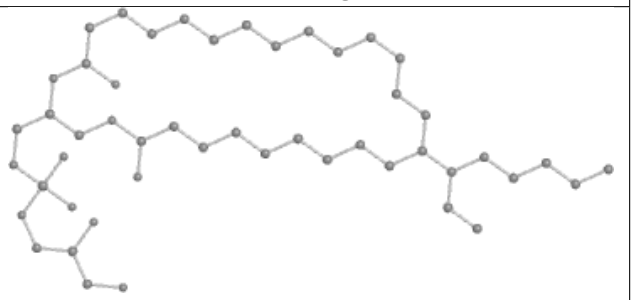
Bond lengths



Bond angles

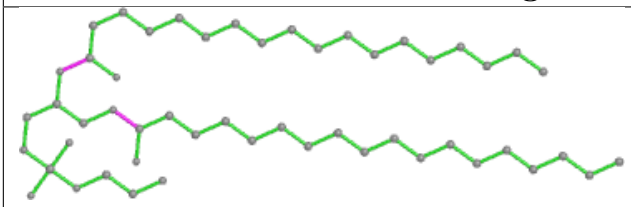


Torsions

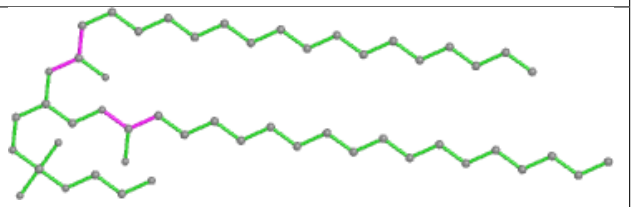


Rings

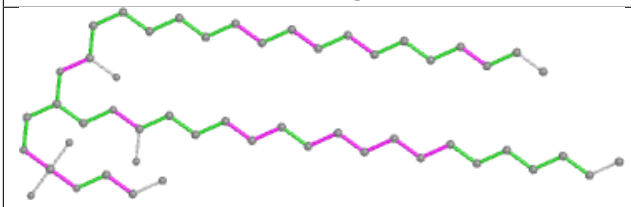
Ligand 3PE 1L 712



Bond lengths



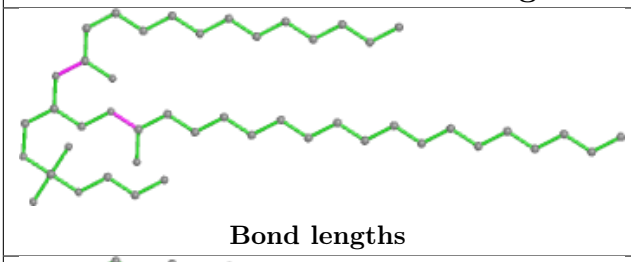
Bond angles



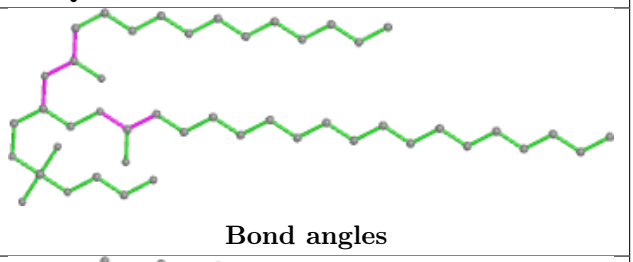
Torsions

Rings

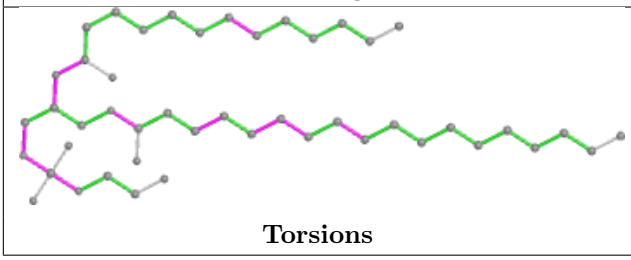
Ligand 3PE 3Q 504



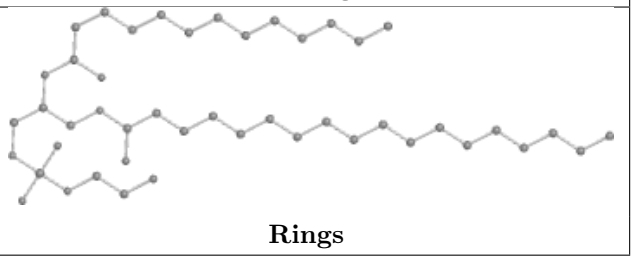
Bond lengths



Bond angles

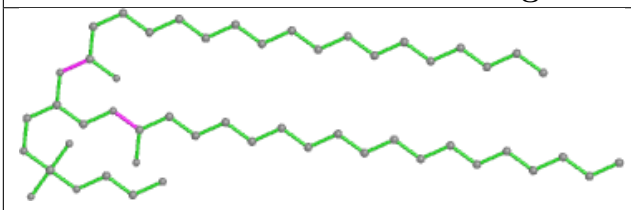


Torsions

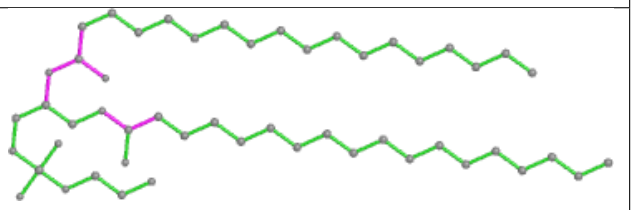


Rings

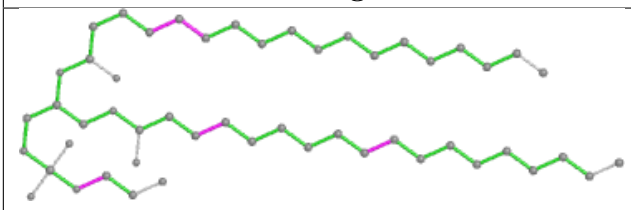
Ligand 3PE 1Z 201



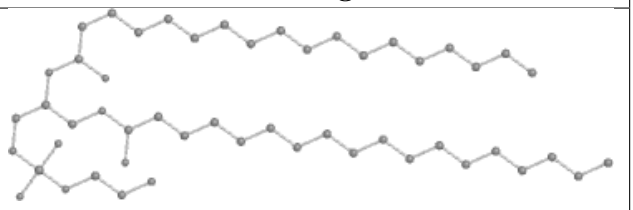
Bond lengths



Bond angles

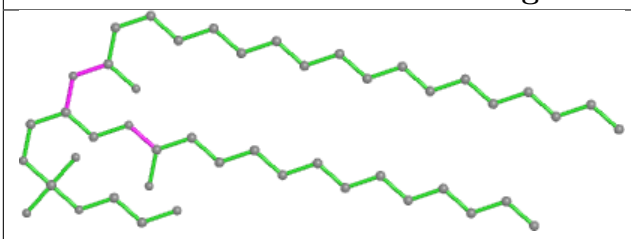


Torsions

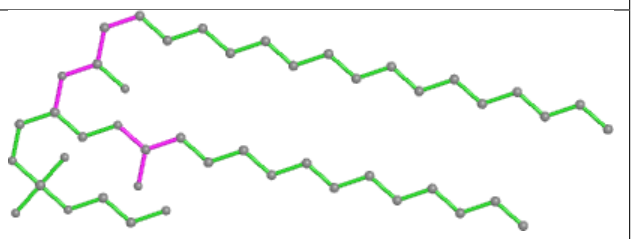


Rings

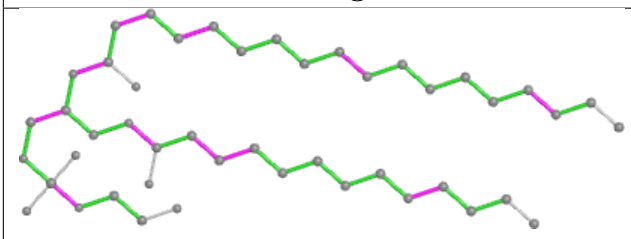
Ligand 3PE 1L 701



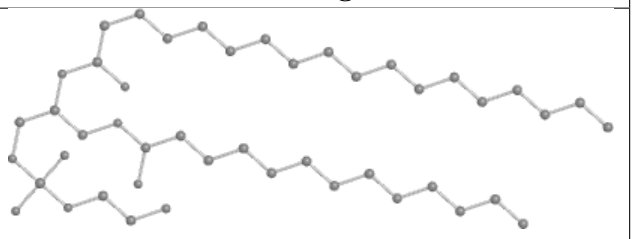
Bond lengths



Bond angles

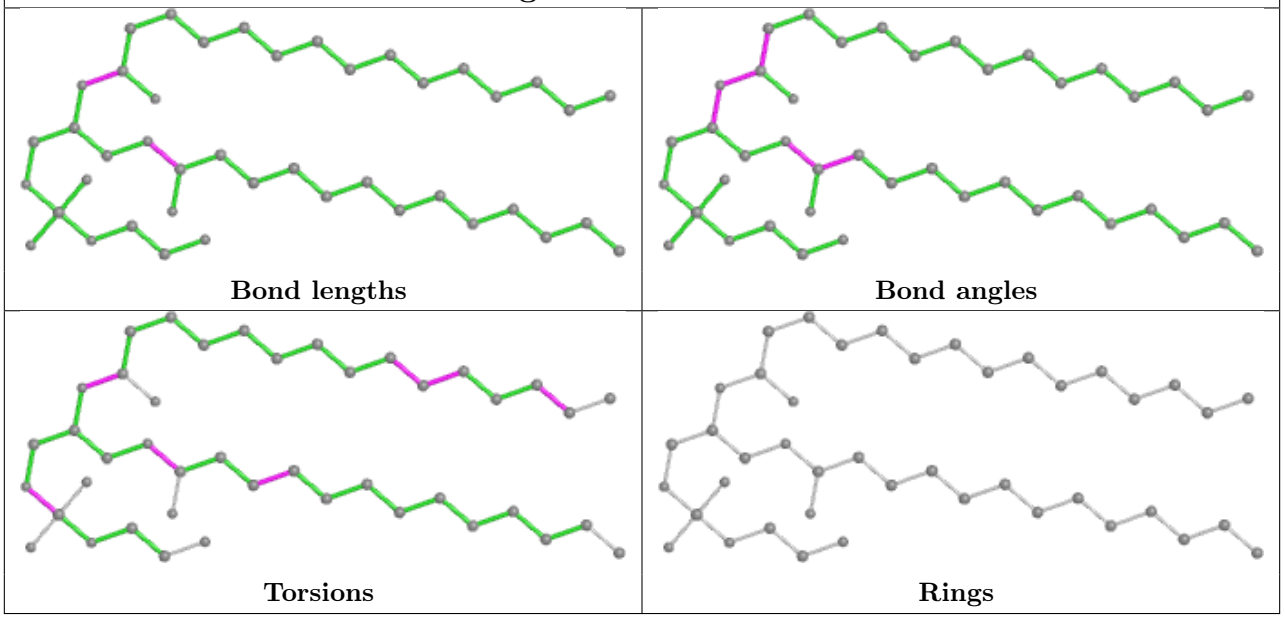


Torsions

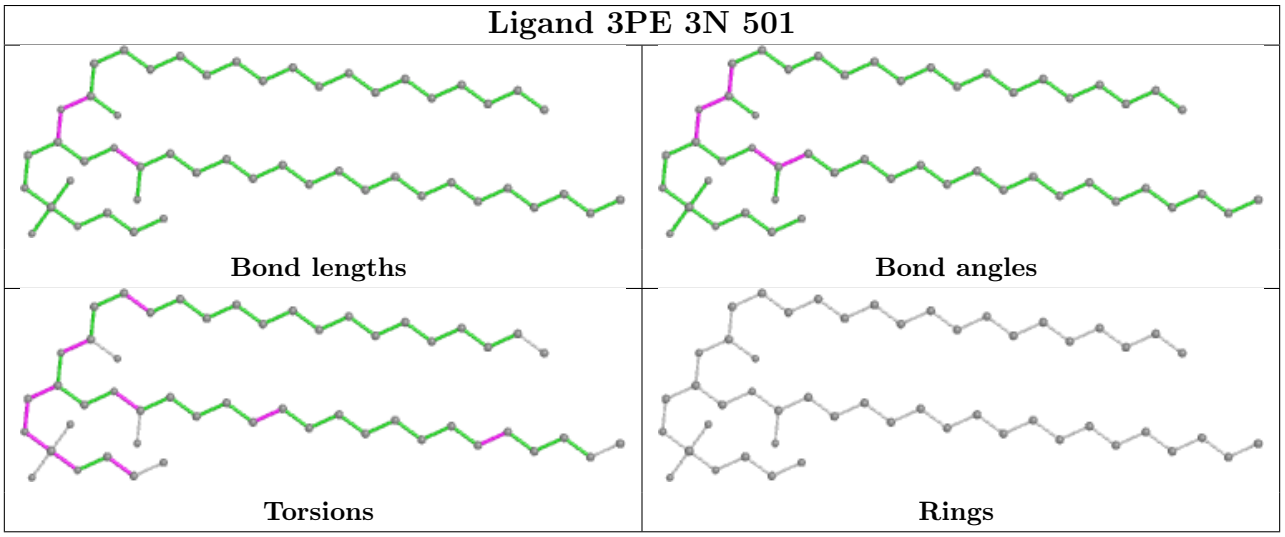


Rings

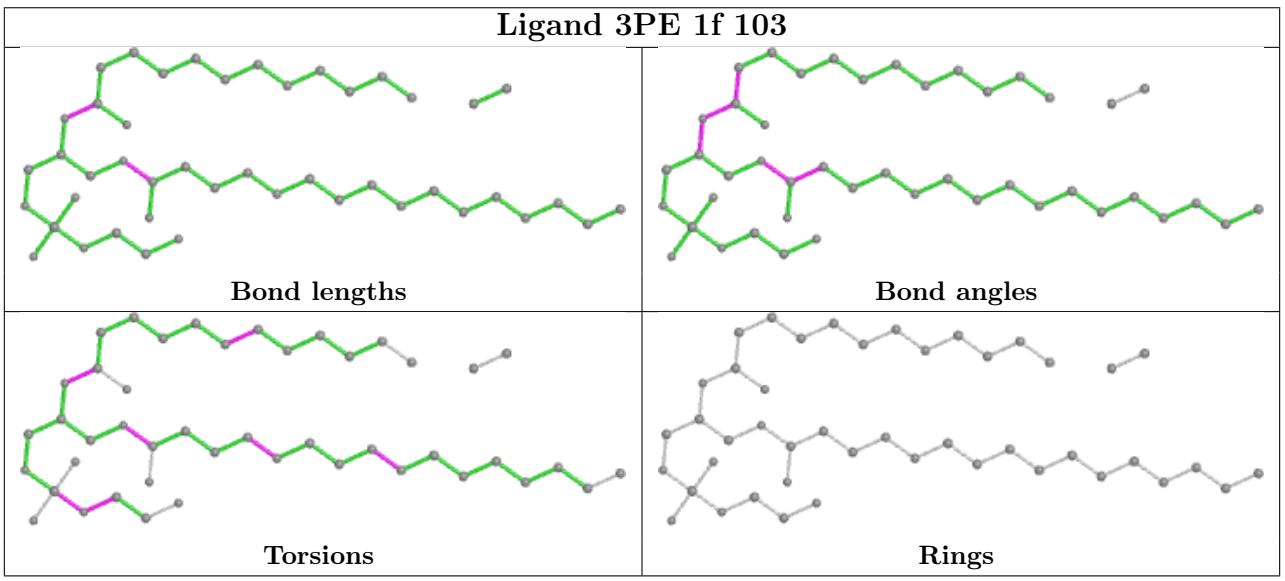
Ligand 3PE 3G 110



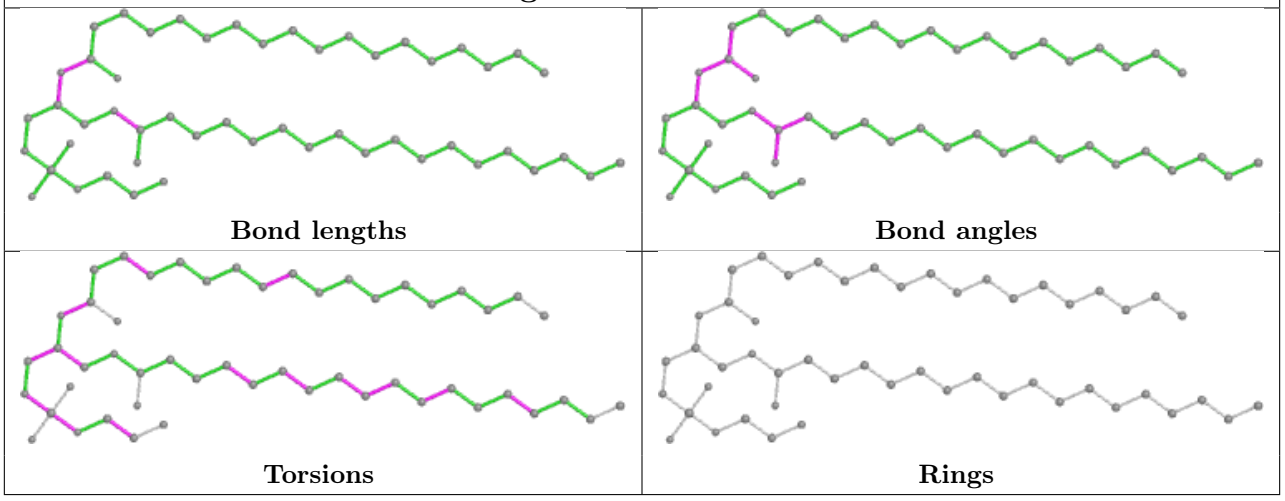
Ligand 3PE 3N 501



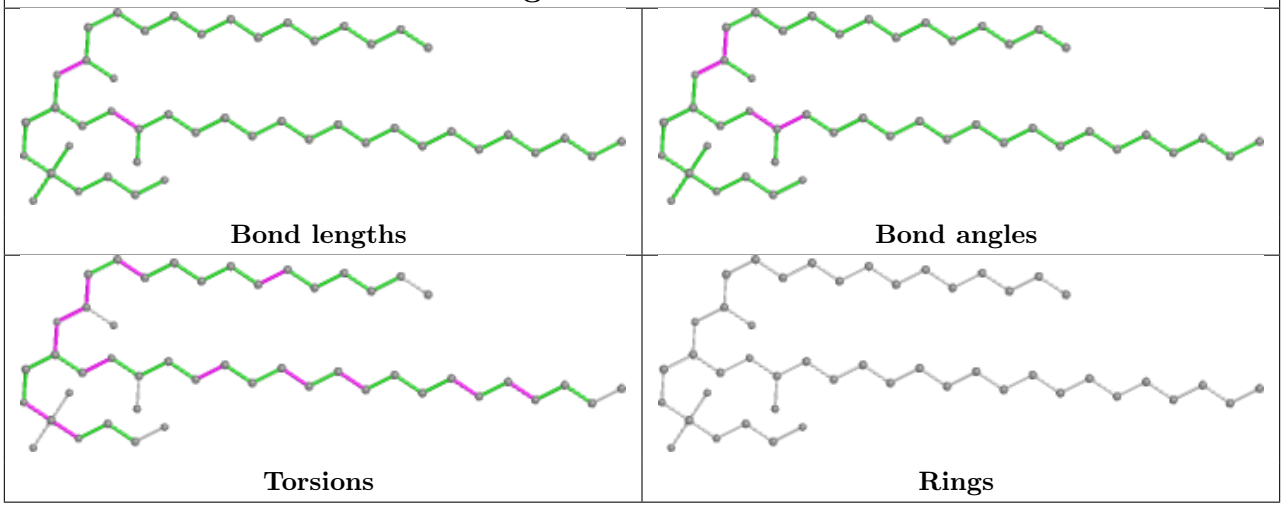
Ligand 3PE 1f 103



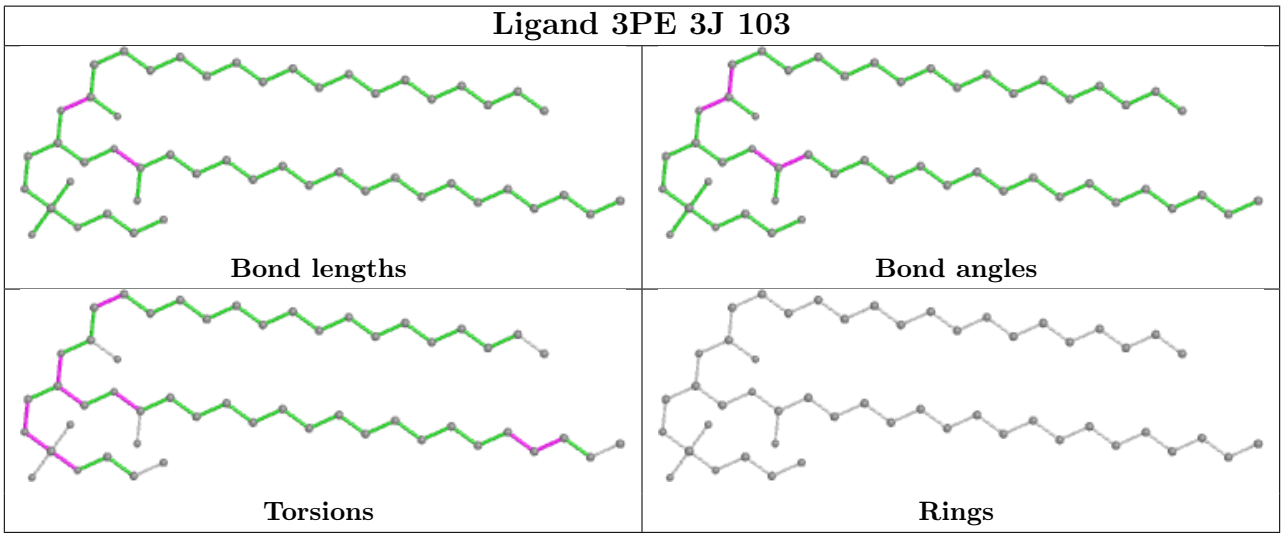
Ligand 3PE 3R 302



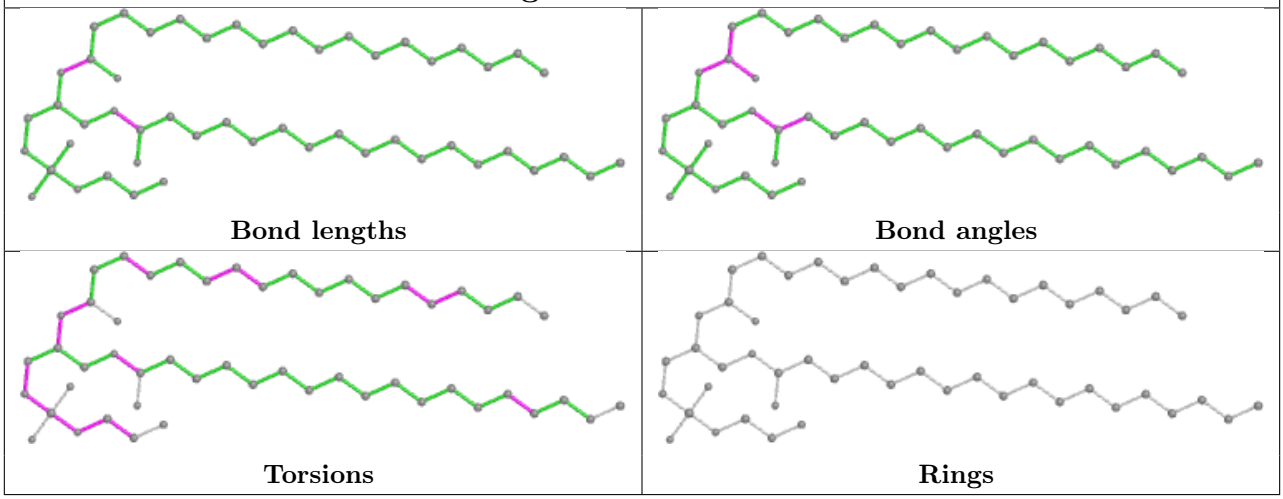
Ligand 3PE 1h 204



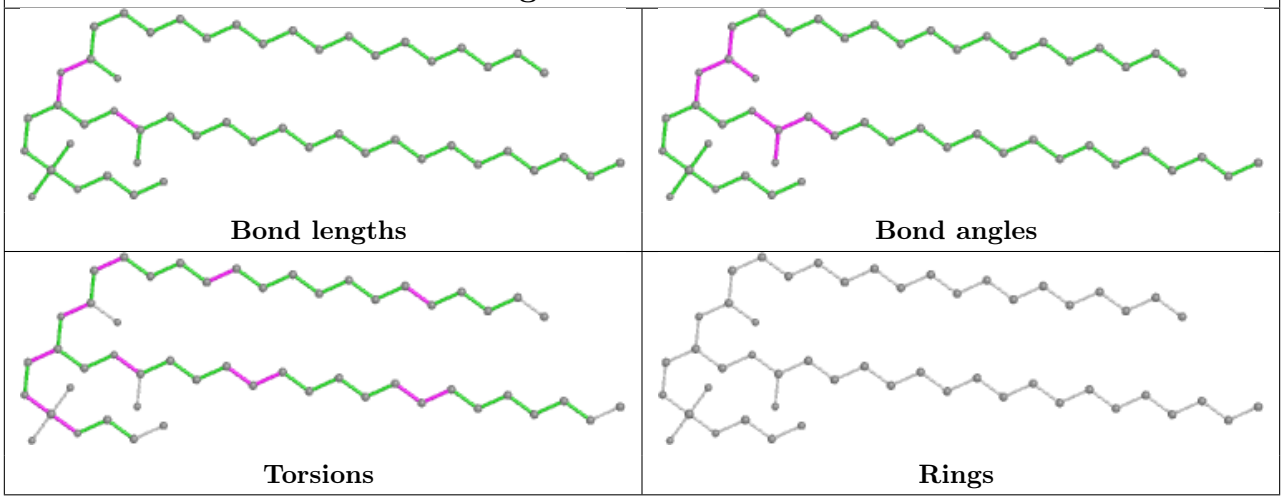
Ligand 3PE 3J 103



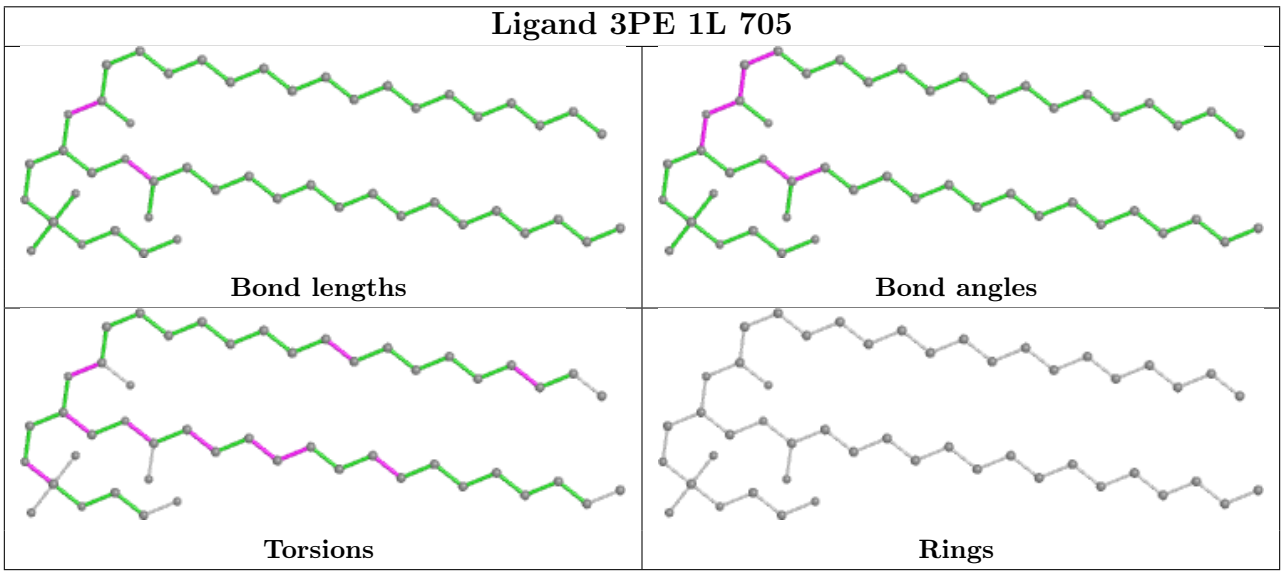
Ligand 3PE 3P 515



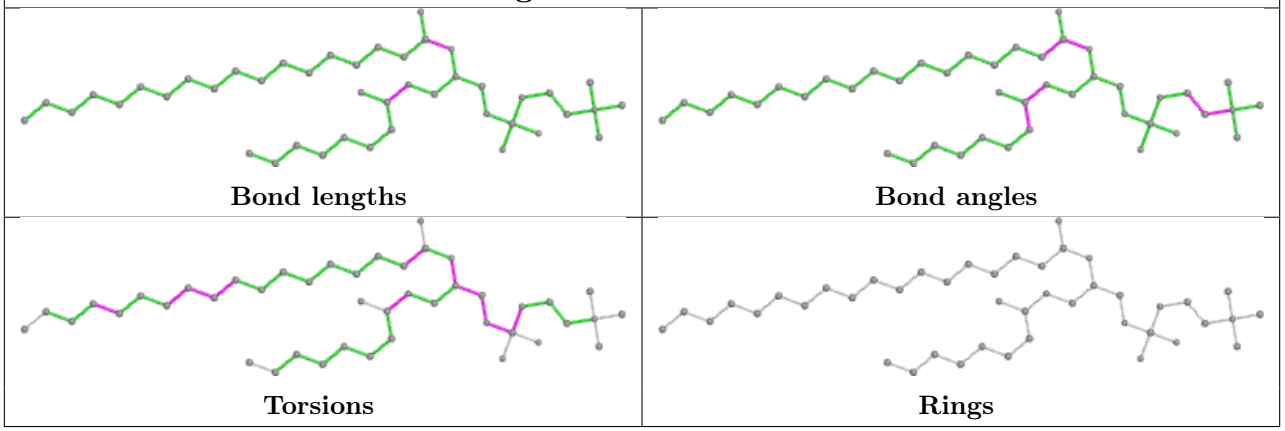
Ligand 3PE 3G 101



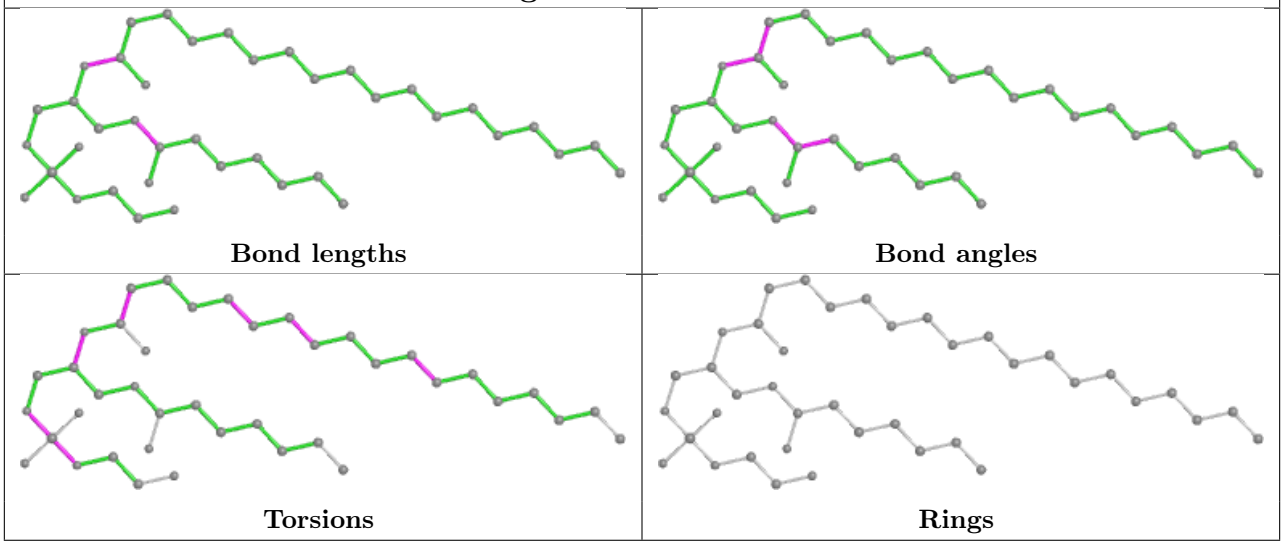
Ligand 3PE 1L 705



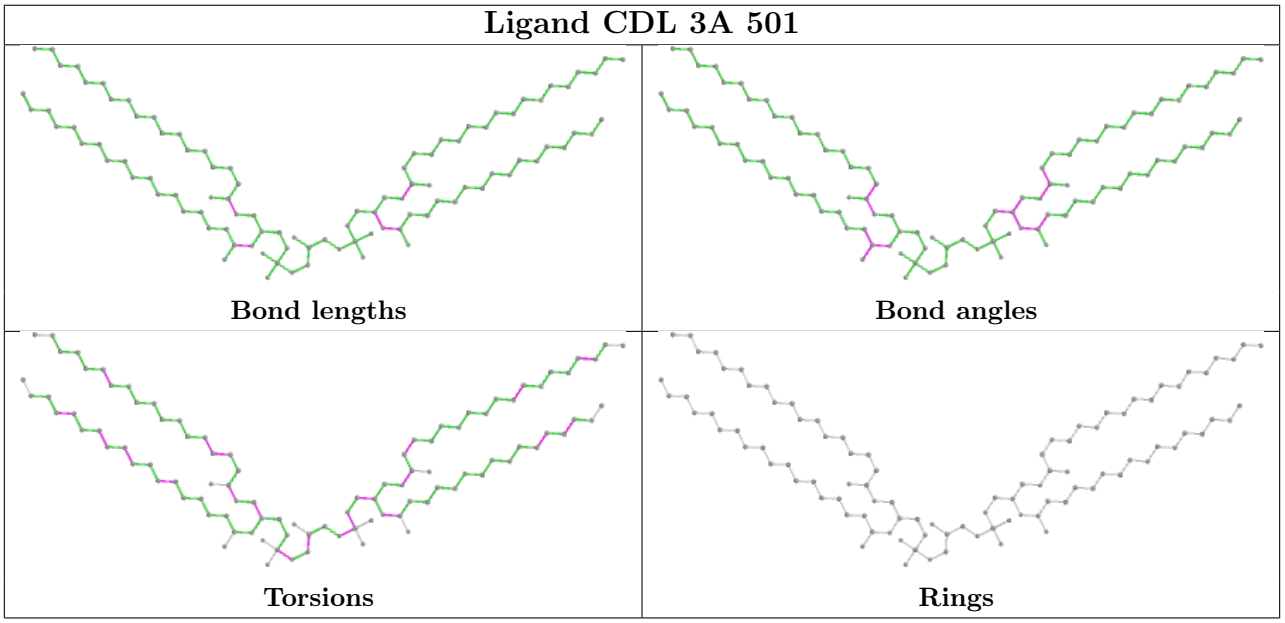
Ligand PC1 1M 501



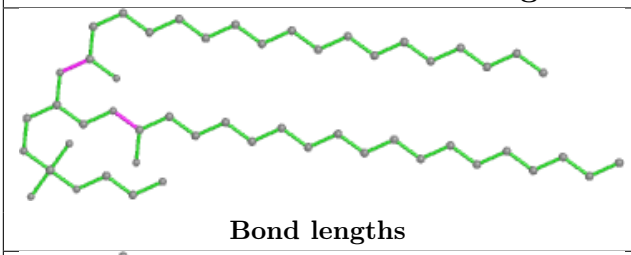
Ligand 3PE 1Y 205



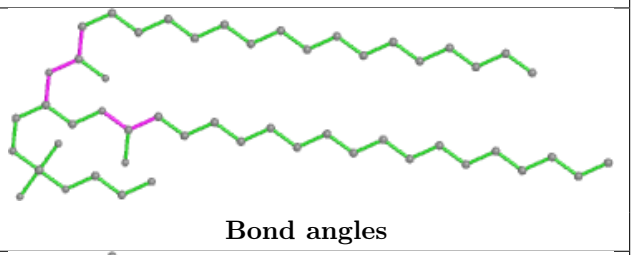
Ligand CDL 3A 501



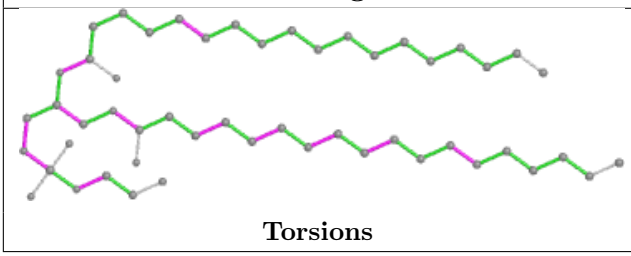
Ligand 3PE 3P 506



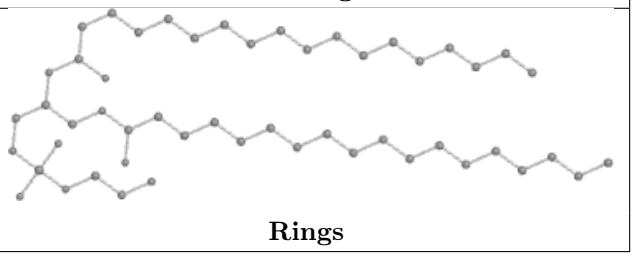
Bond lengths



Bond angles

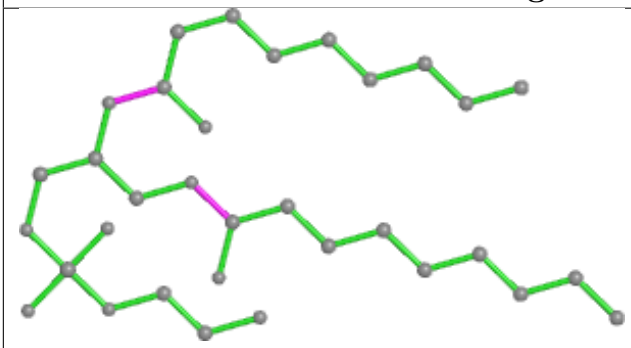


Torsions

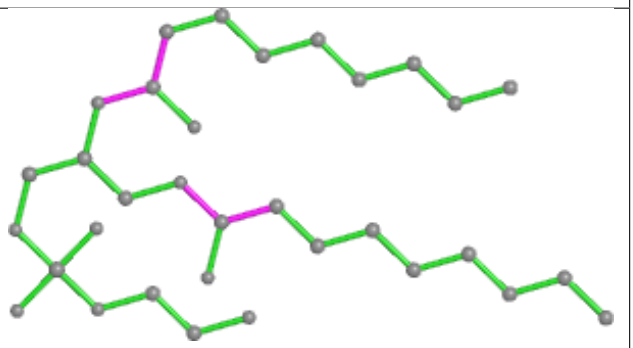


Rings

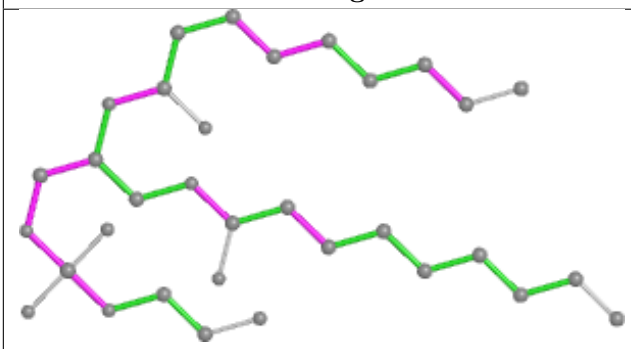
Ligand 3PE 1l 203



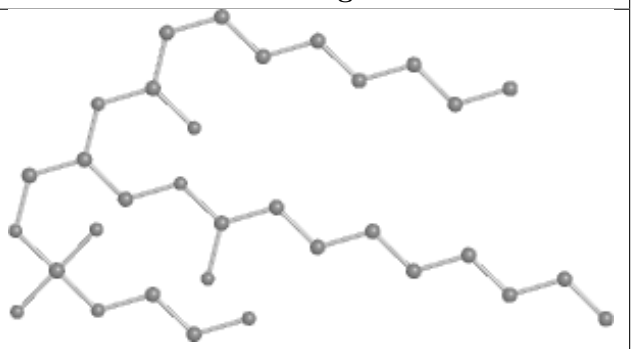
Bond lengths



Bond angles

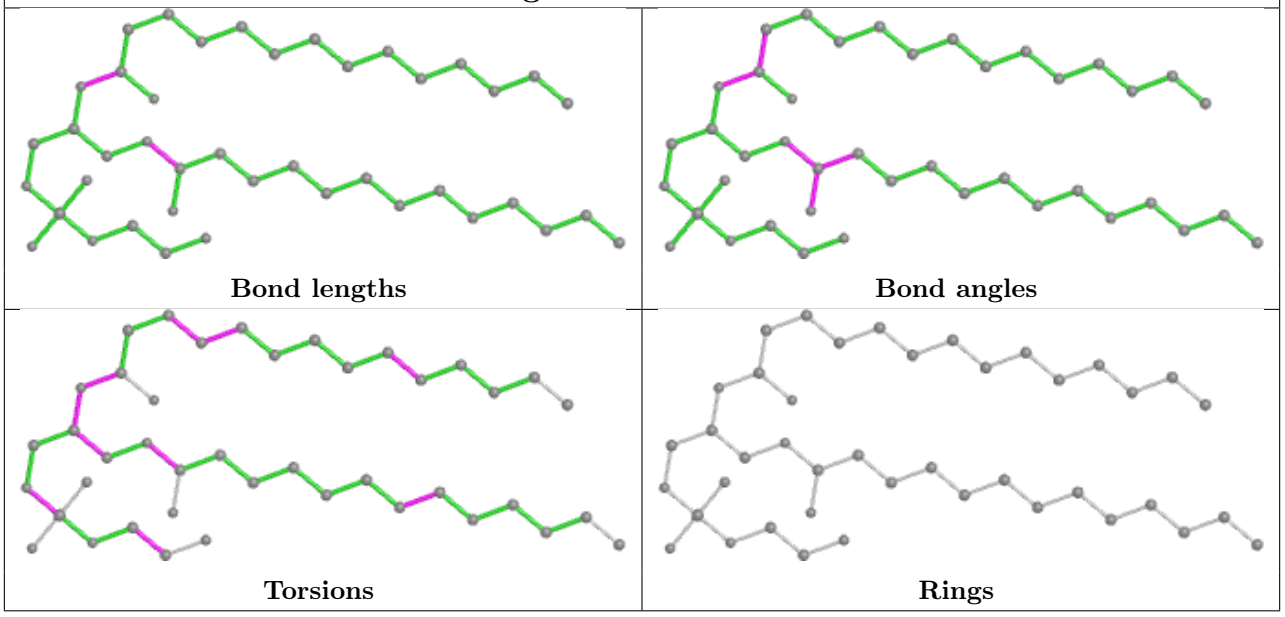


Torsions

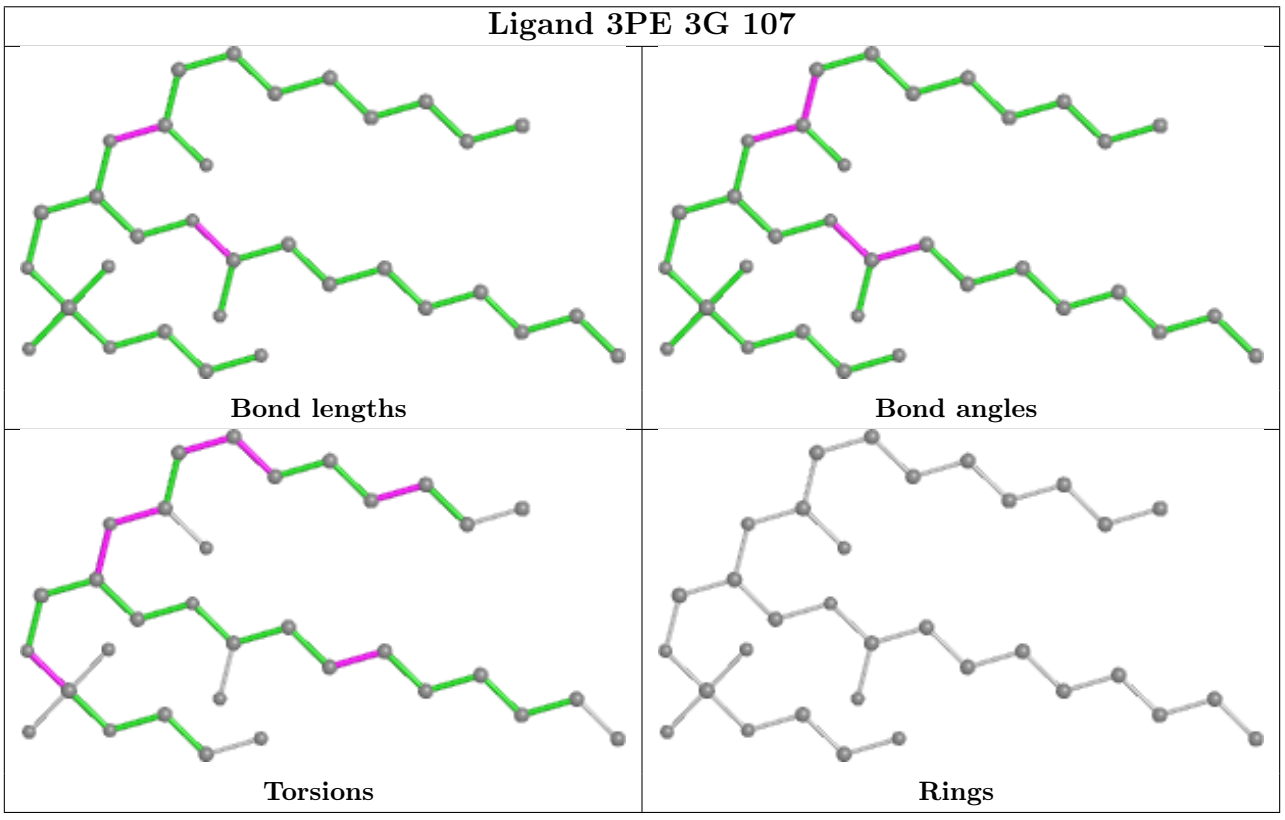


Rings

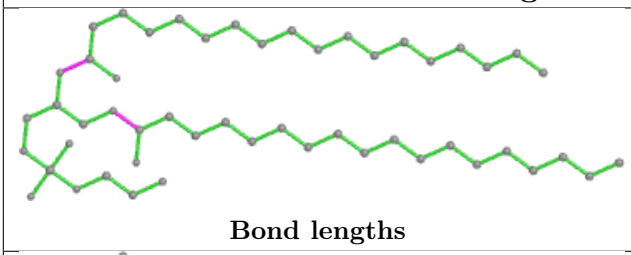
Ligand 3PE 1L 708



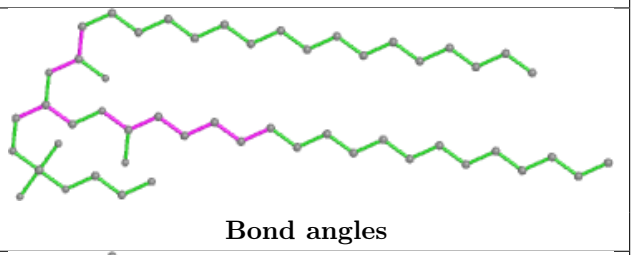
Ligand 3PE 3G 107



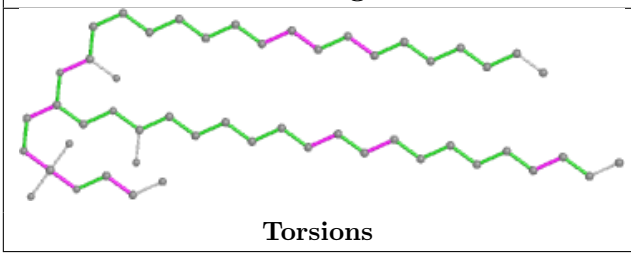
Ligand 3PE 3P 519



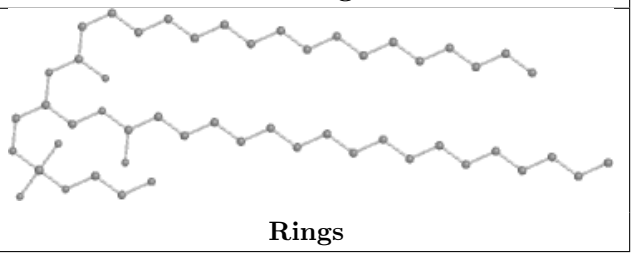
Bond lengths



Bond angles

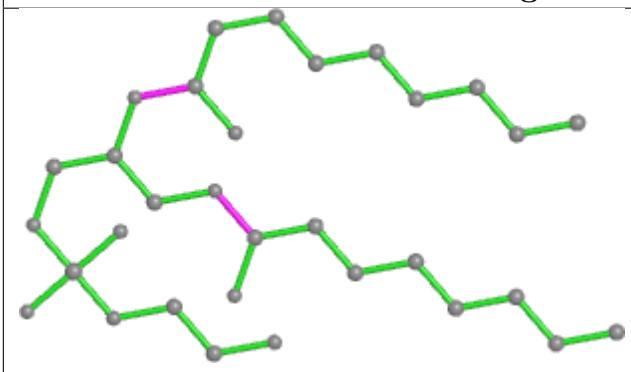


Torsions

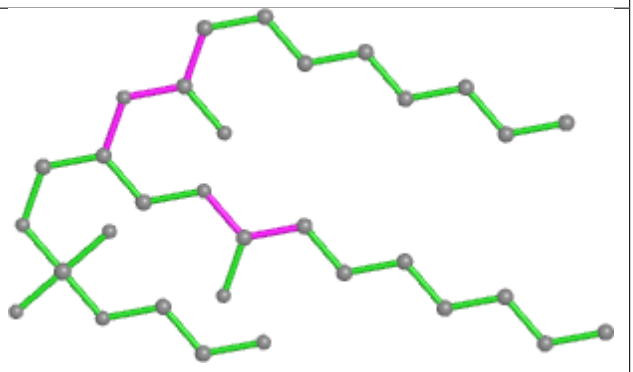


Rings

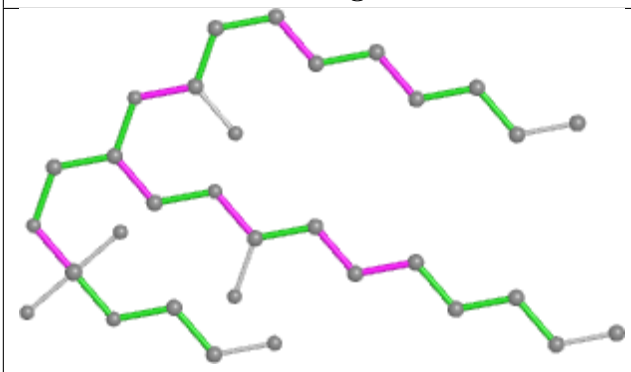
Ligand 3PE 3P 505



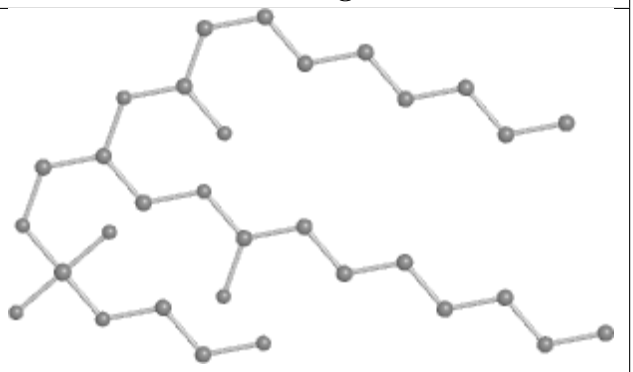
Bond lengths



Bond angles

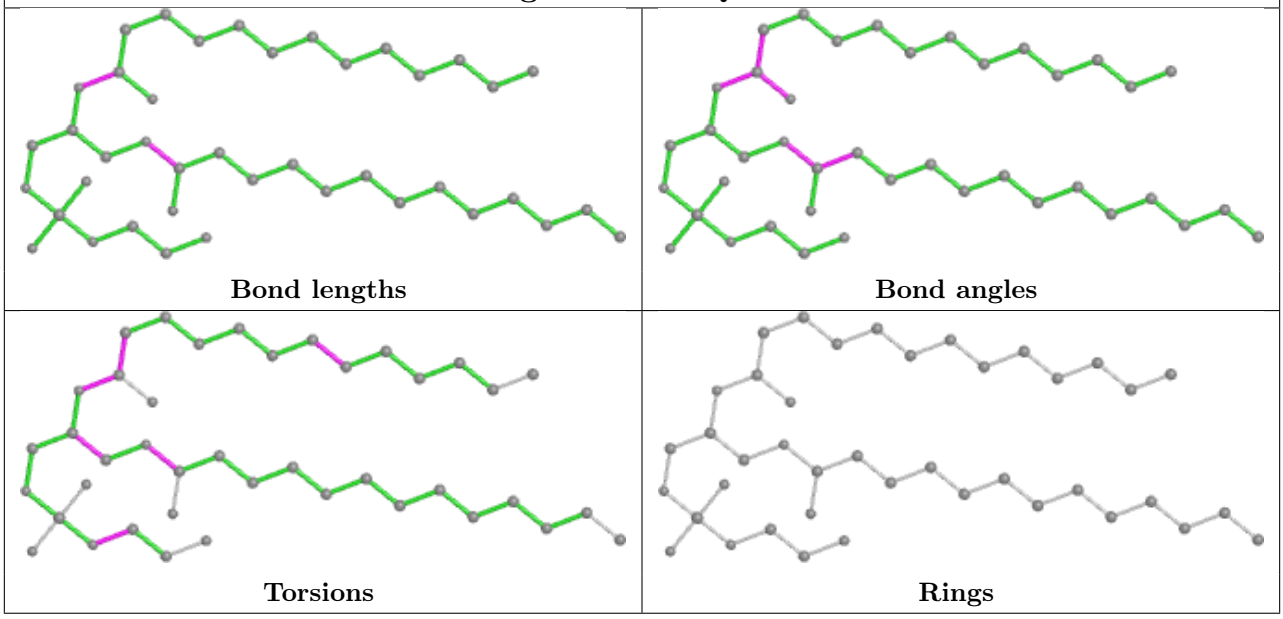


Torsions

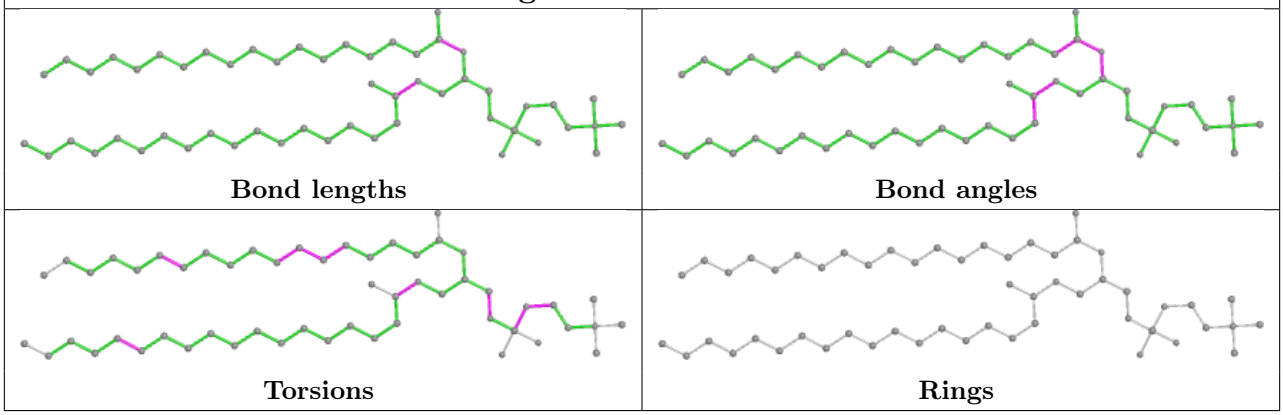


Rings

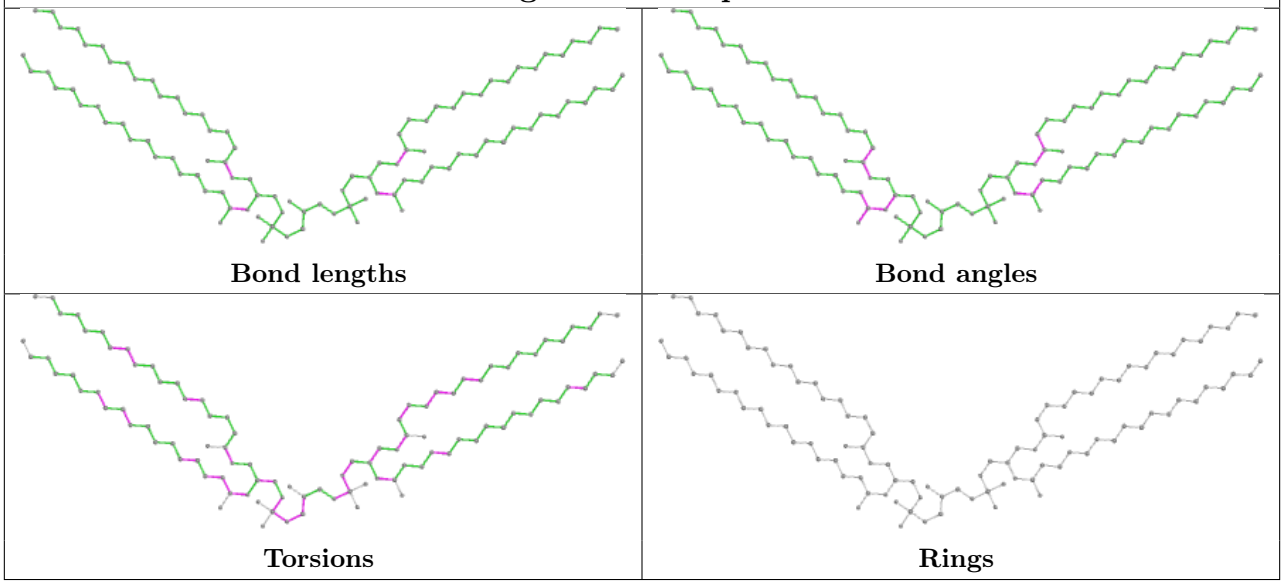
Ligand 3PE 3Q 502



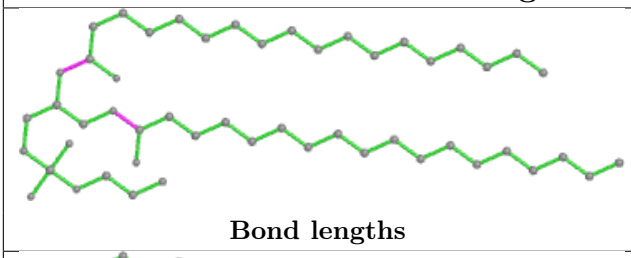
Ligand PC1 1Y 207



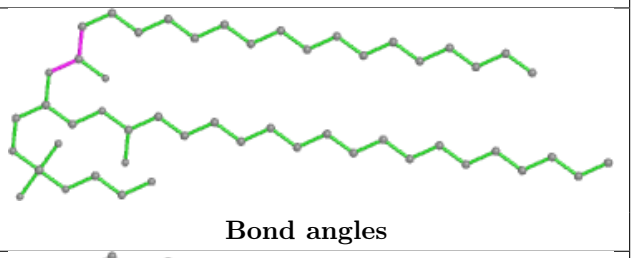
Ligand CDL 1q 202



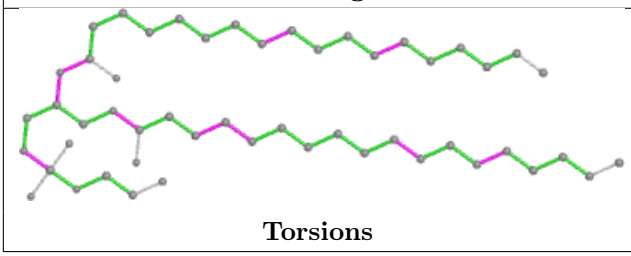
Ligand 3PE 3X 106



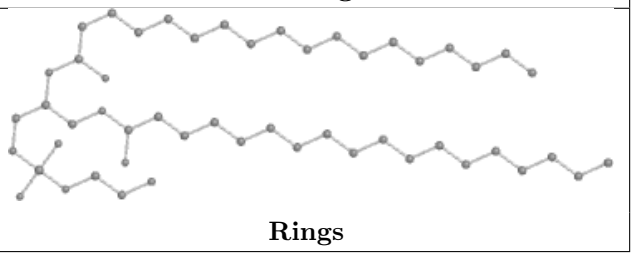
Bond lengths



Bond angles

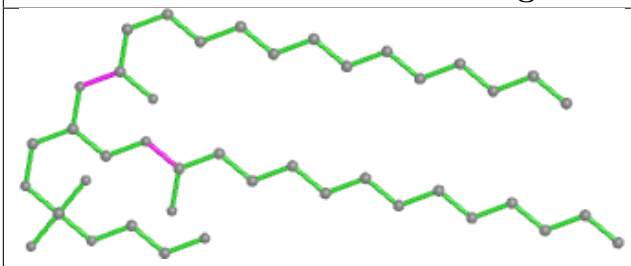


Torsions

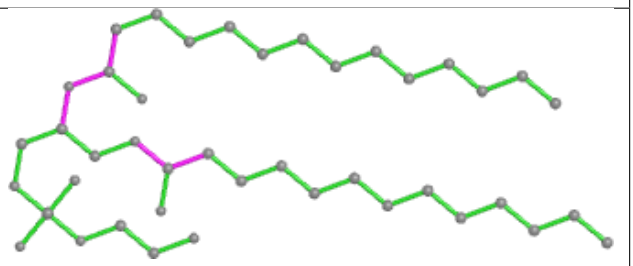


Rings

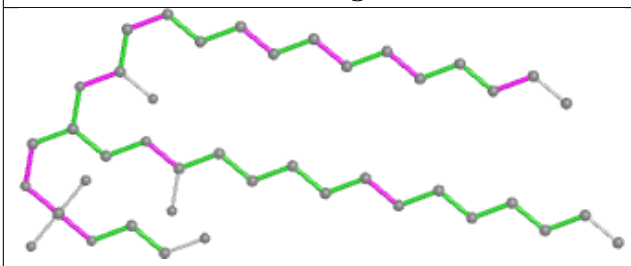
Ligand 3PE 1m 203



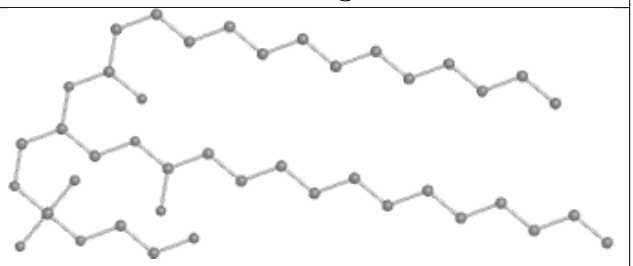
Bond lengths



Bond angles

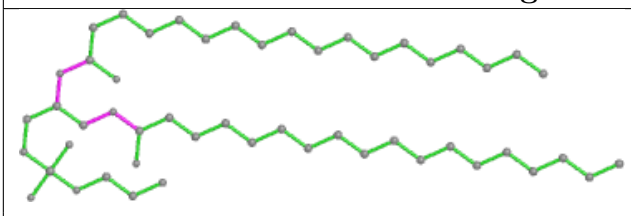


Torsions

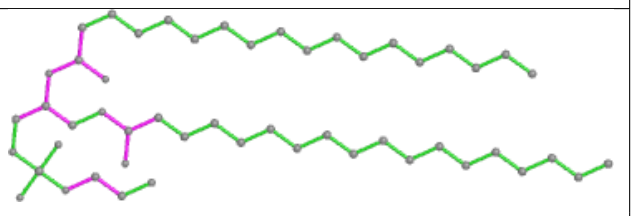


Rings

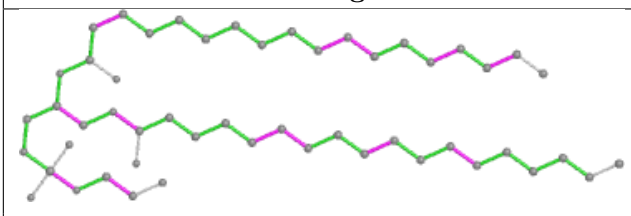
Ligand 3PE 3P 508



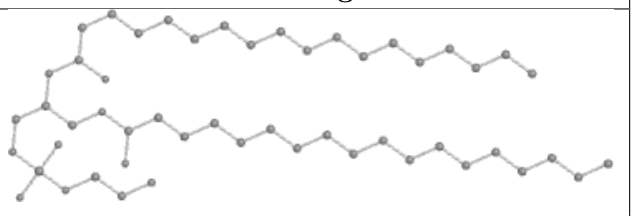
Bond lengths



Bond angles

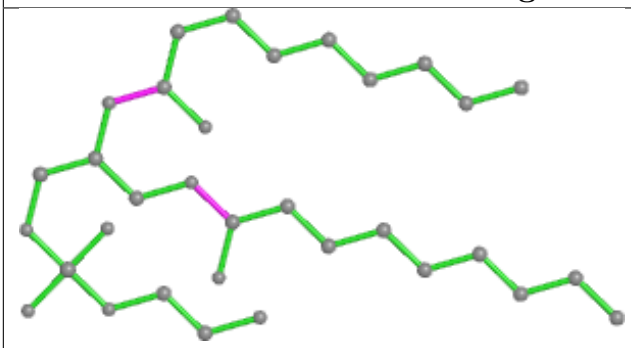


Torsions

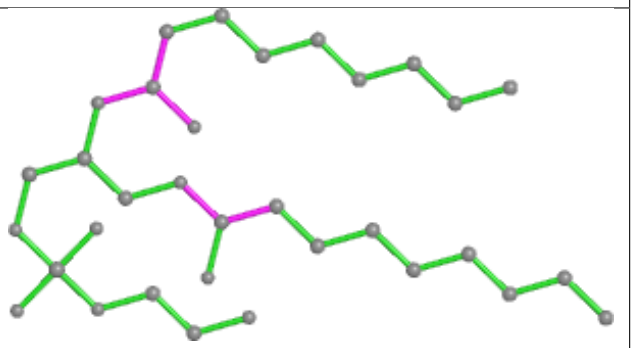


Rings

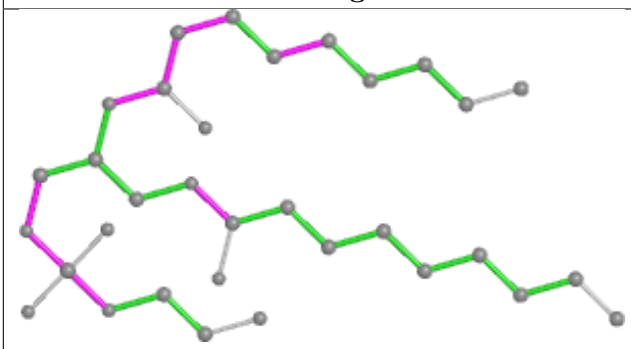
Ligand 3PE 3G 104



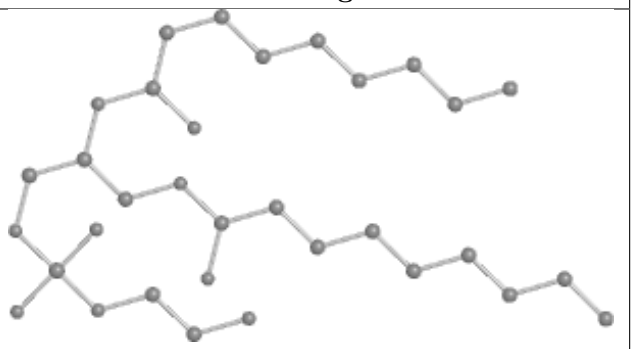
Bond lengths



Bond angles

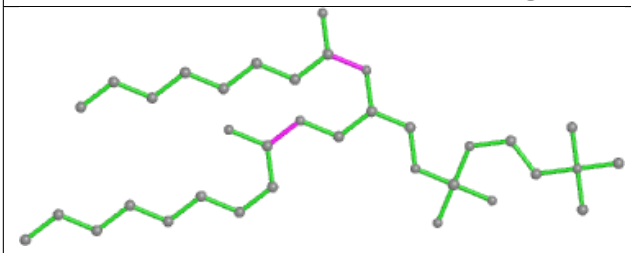


Torsions

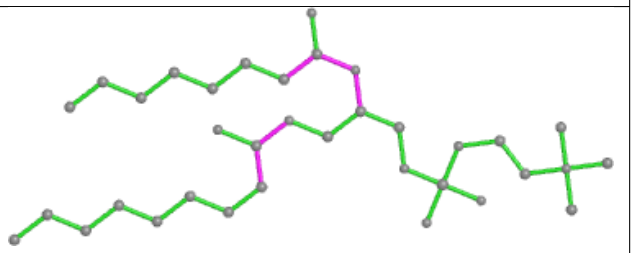


Rings

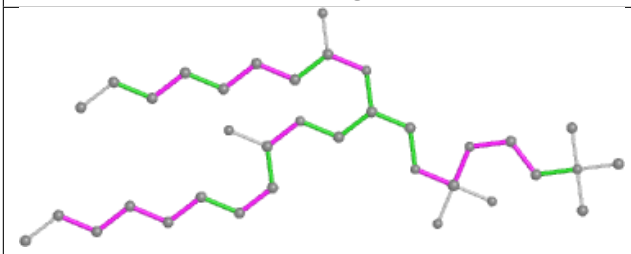
Ligand PC1 1J 202



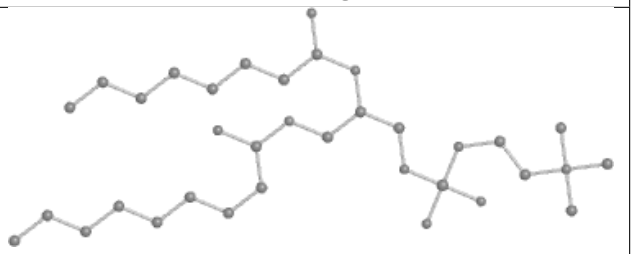
Bond lengths



Bond angles

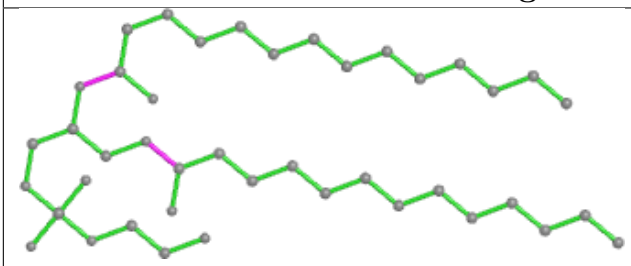


Torsions

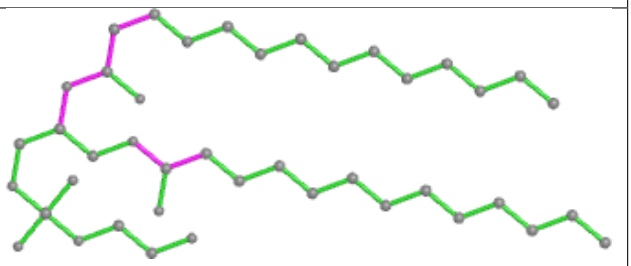


Rings

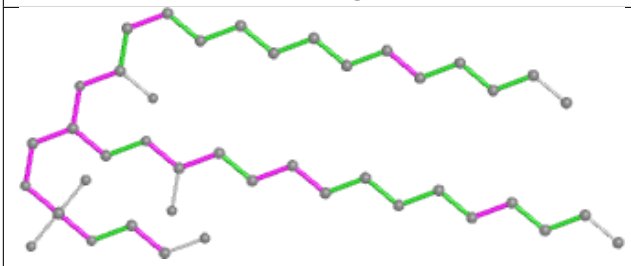
Ligand 3PE 1Y 209



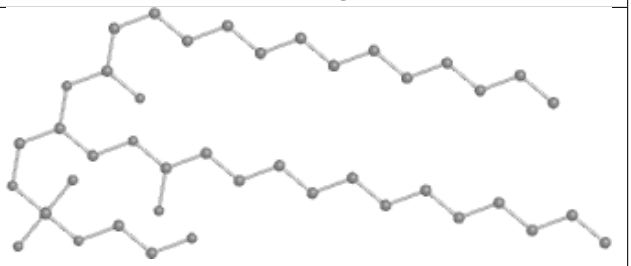
Bond lengths



Bond angles

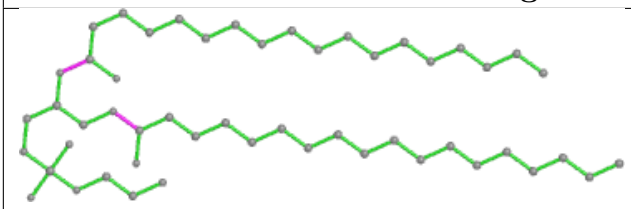


Torsions

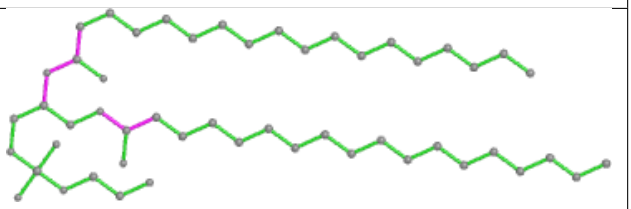


Rings

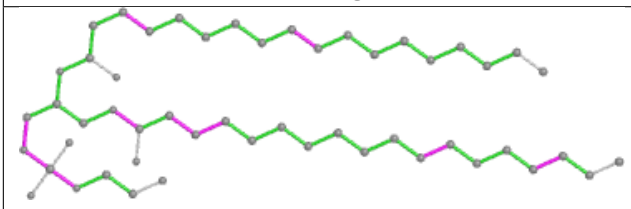
Ligand 3PE 3P 516



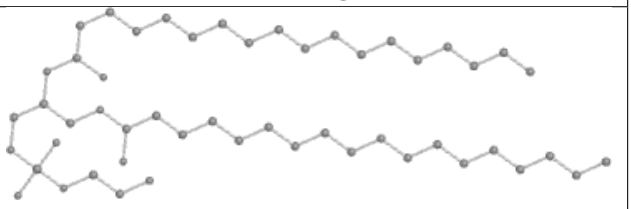
Bond lengths



Bond angles

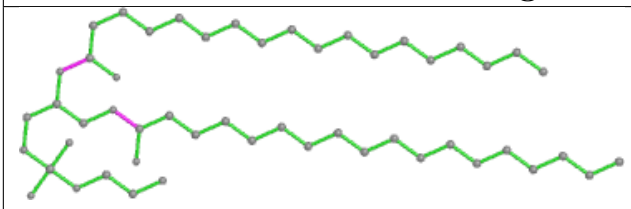


Torsions



Rings

Ligand 3PE 1Y 216



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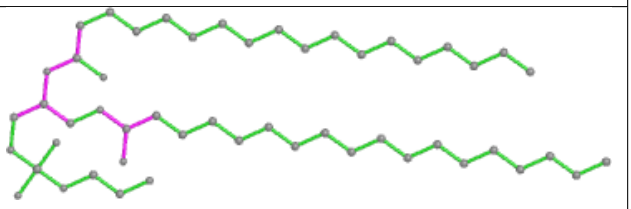
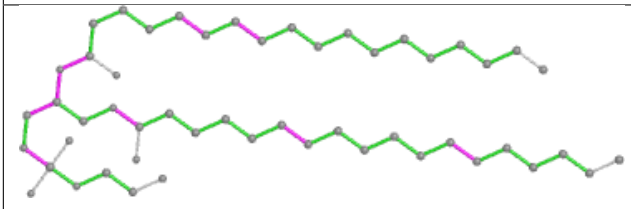
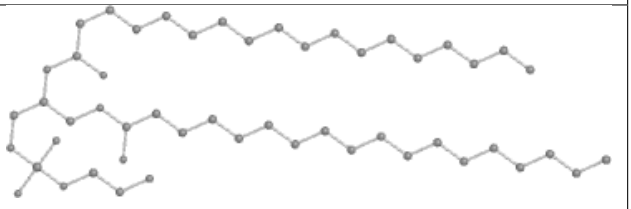


Bond angles

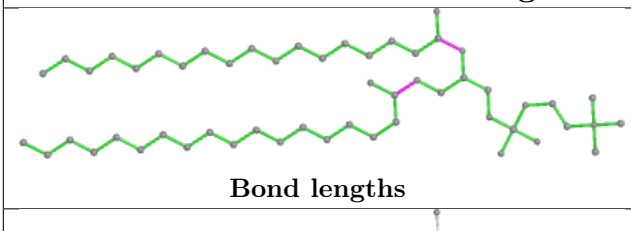


Torsions



Rings

Ligand PC1 3R 303



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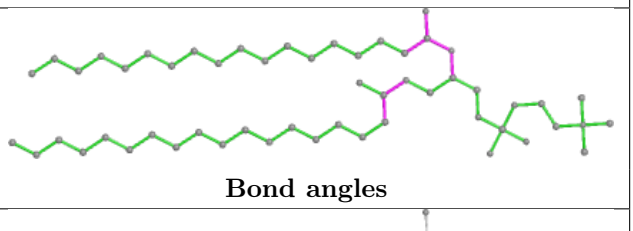
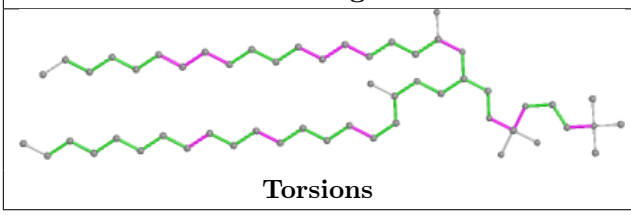


Bond angles



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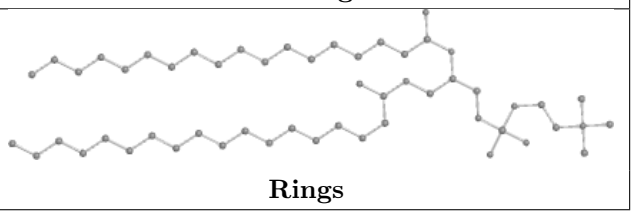
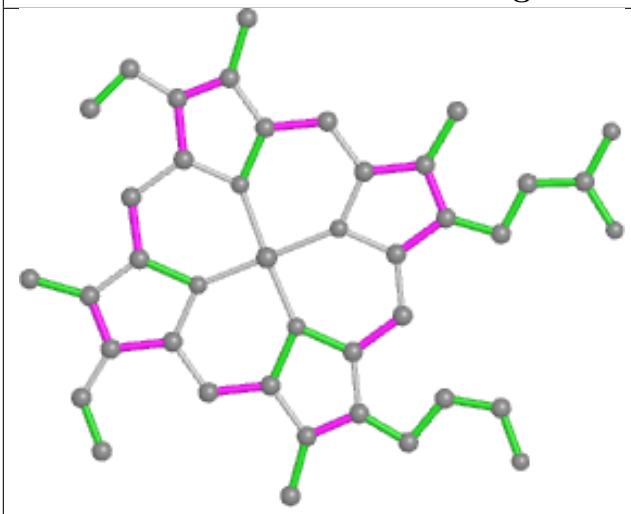


Rings

Ligand HEC 3D 501



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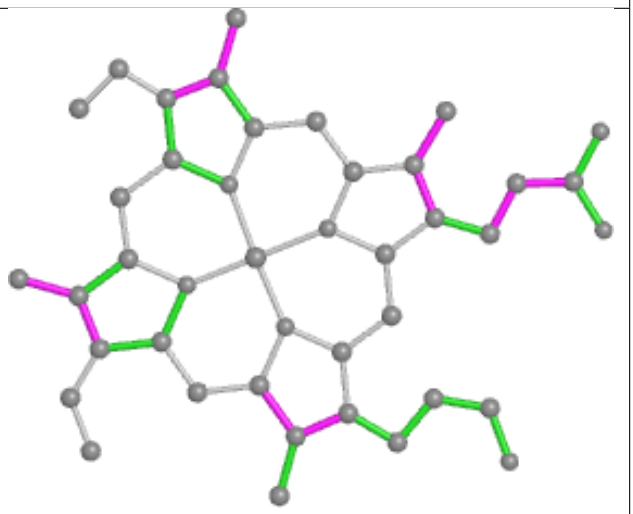
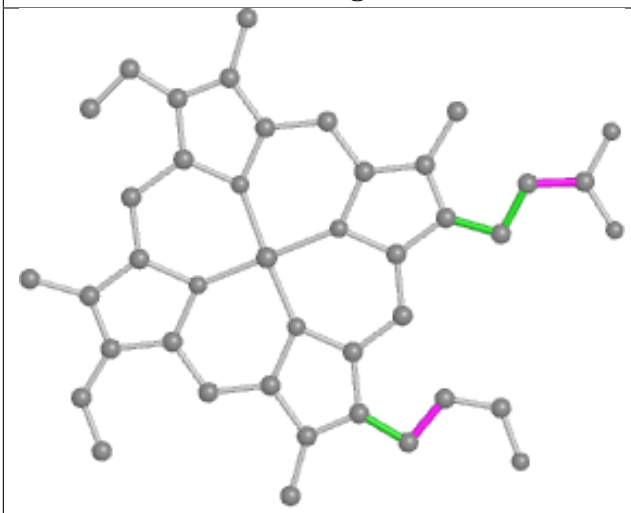


Bond angles



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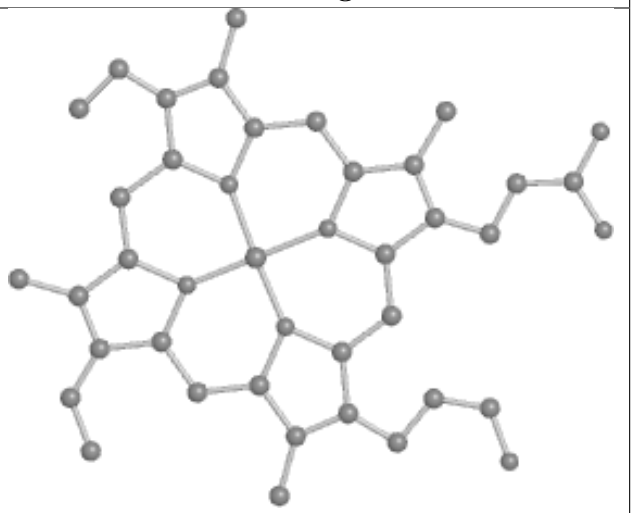
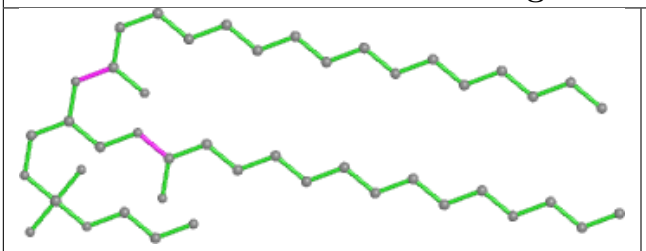


Rings

Ligand 3PE 1f 101



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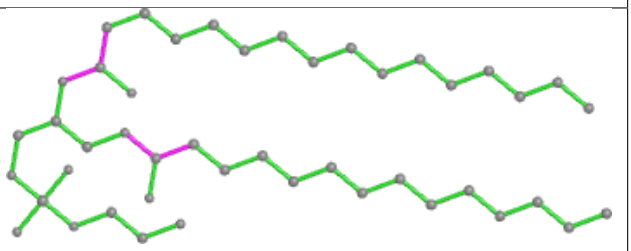
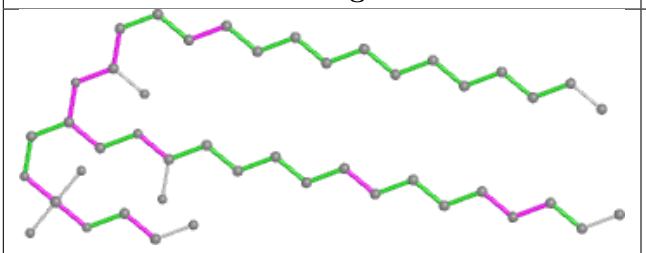


Bond angles



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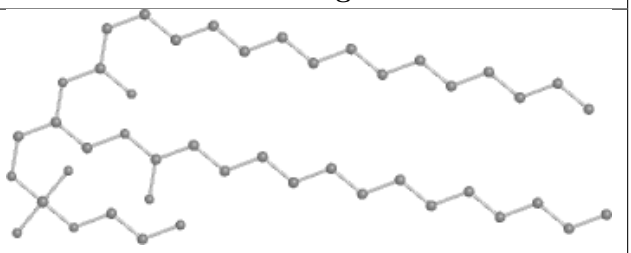
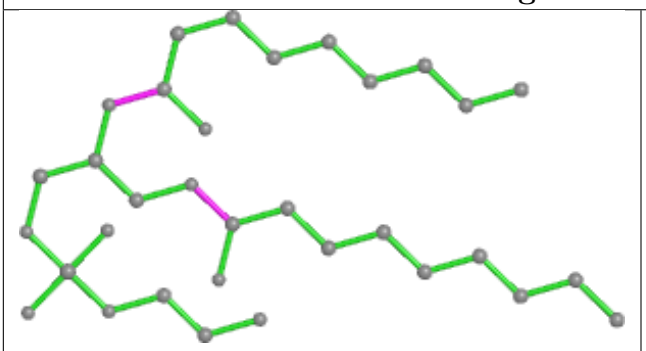


Rings

Ligand 3PE 3G 106



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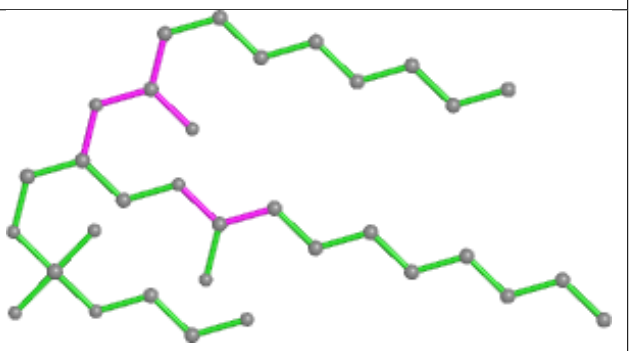
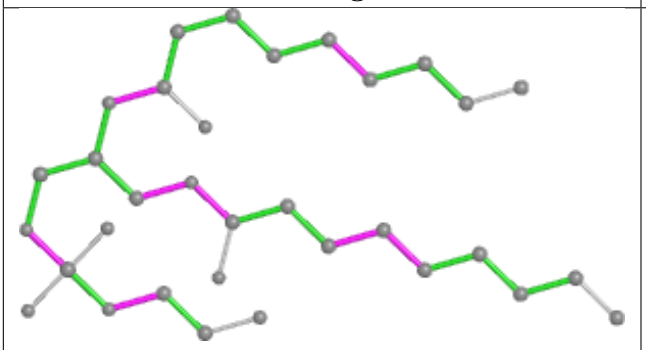
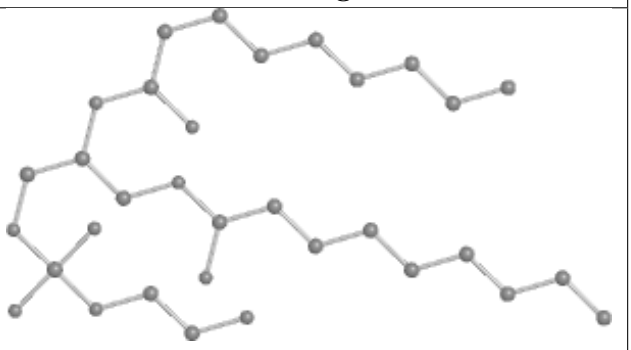


Bond angles

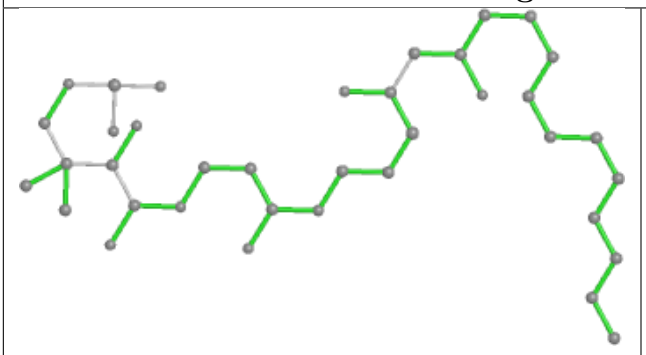


Torsions

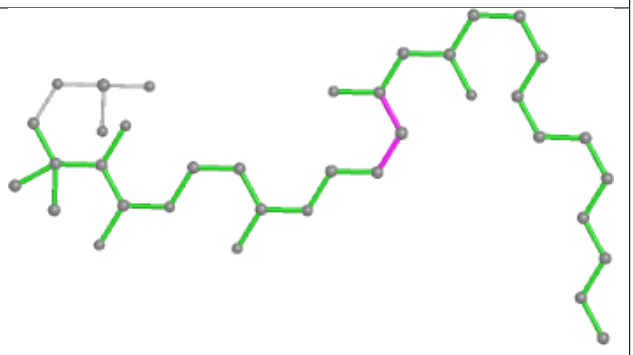


Rings

Ligand EHZ 1T 101



Bond lengths



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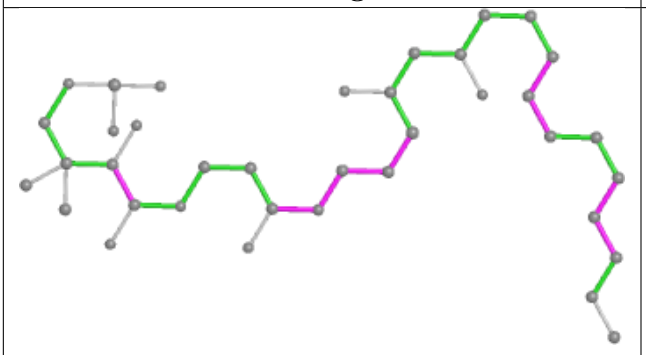

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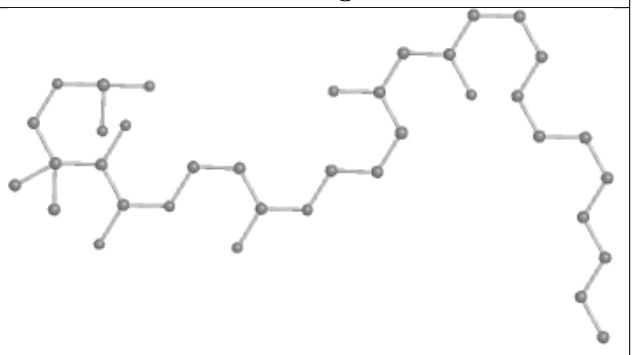
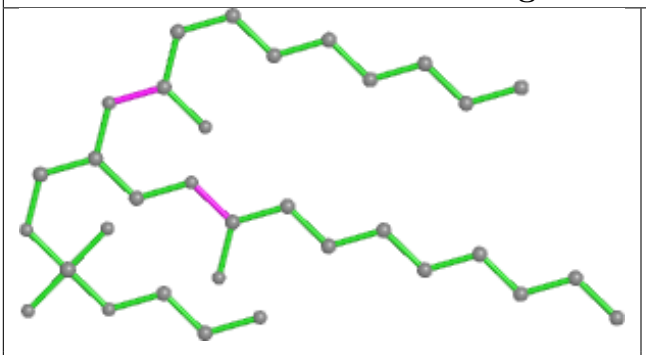
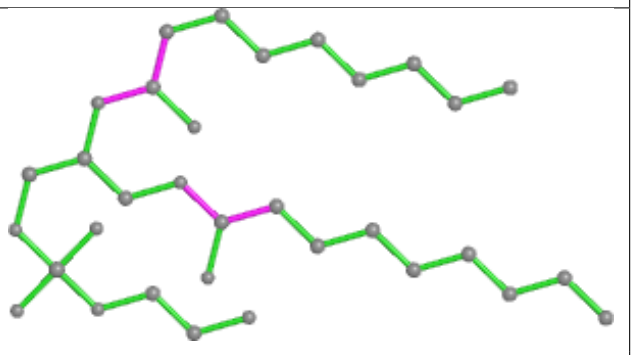


Rings

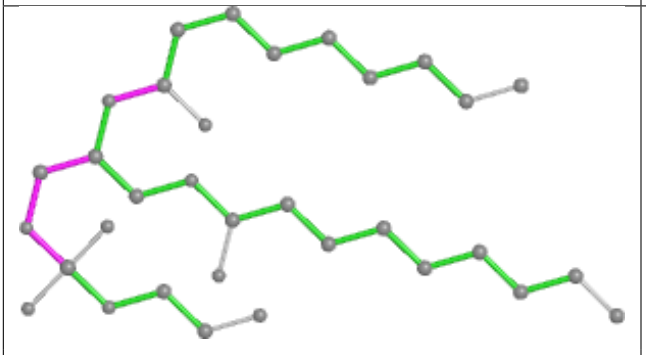
Ligand 3PE 3G 108



Bond lengths



Bond angles



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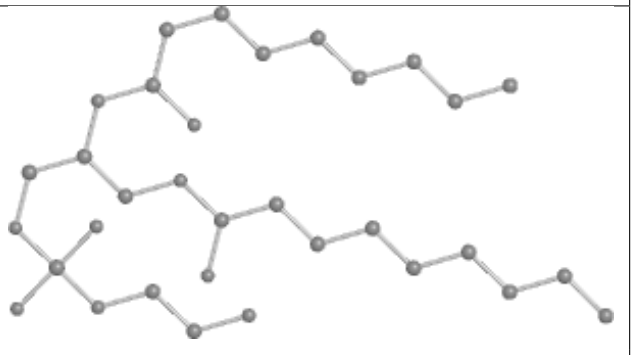
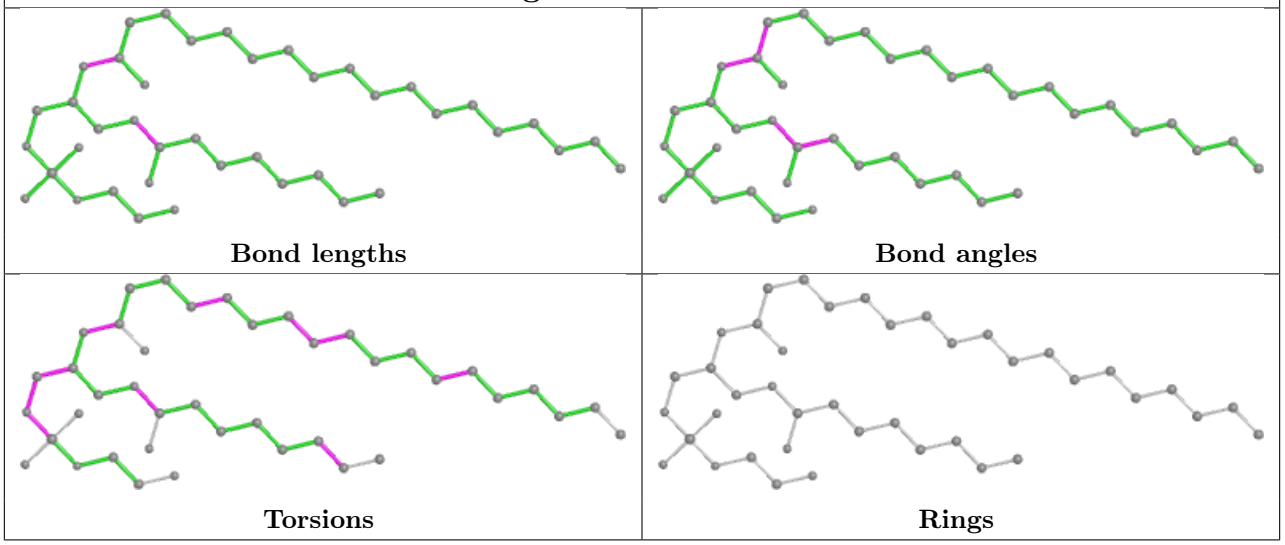
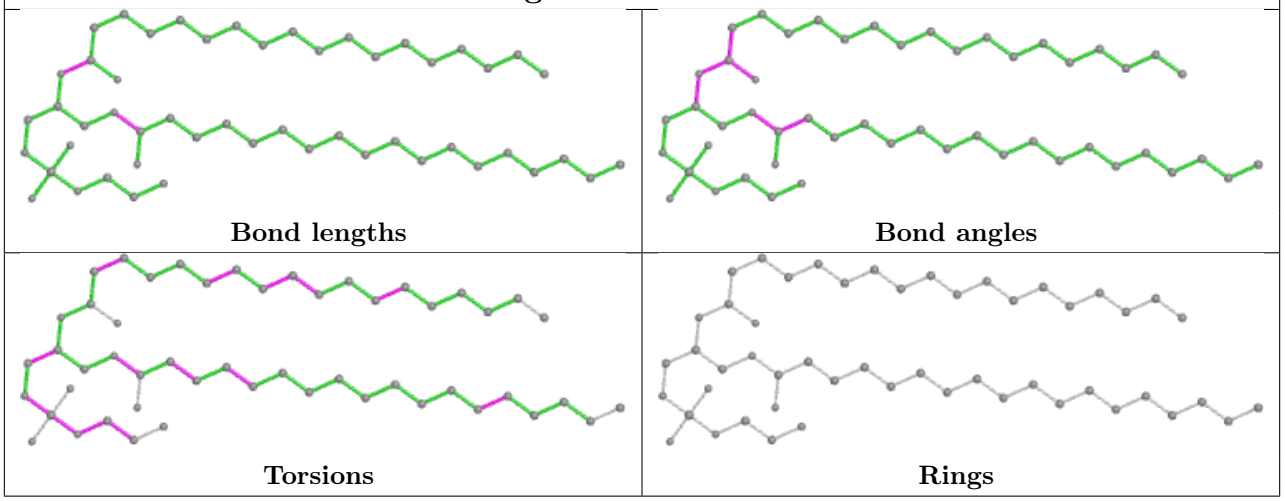


Rings

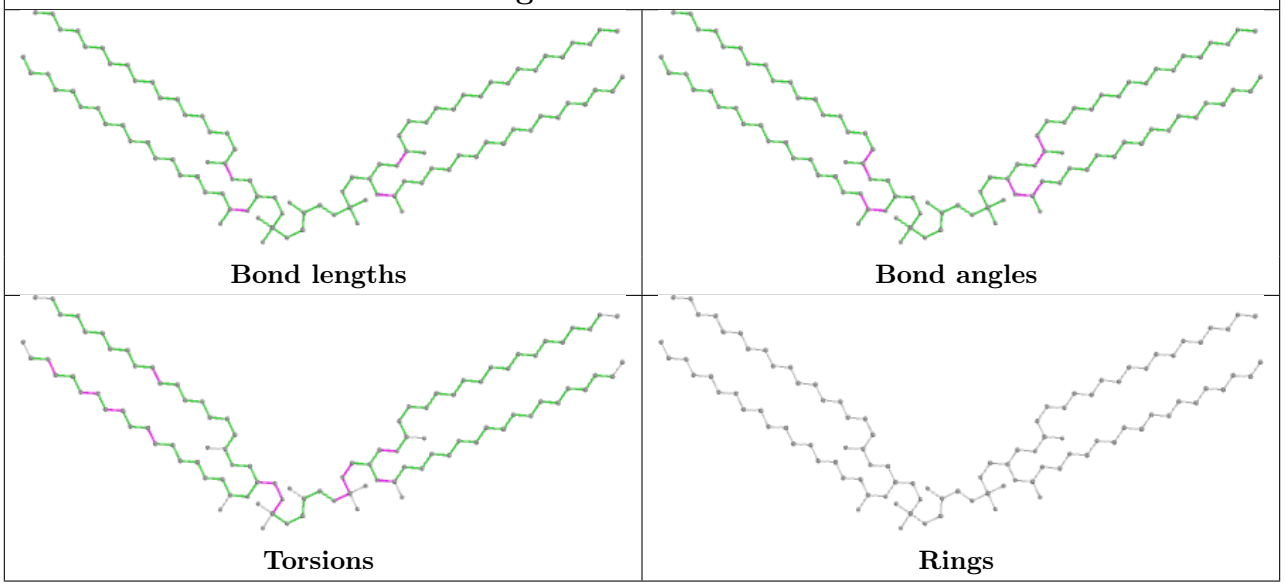
Ligand 3PE 1L 711



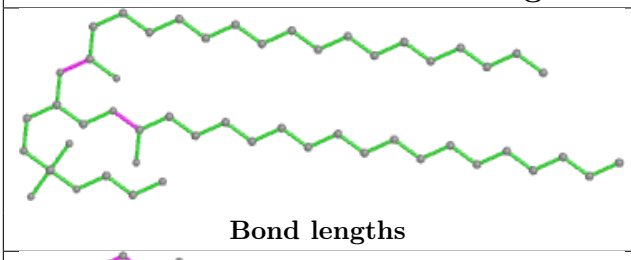
Ligand 3PE 1o 201



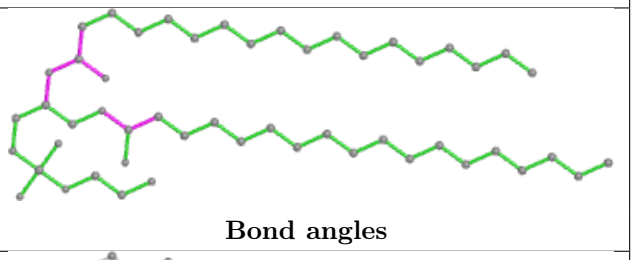
Ligand CDL 4C 307



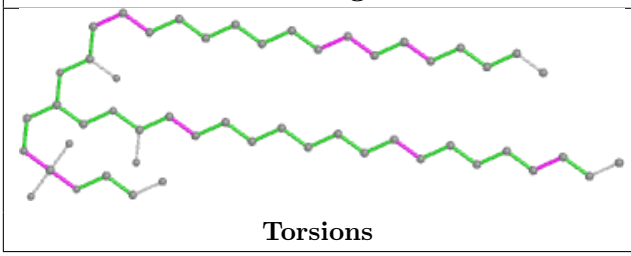
Ligand 3PE 1e 201



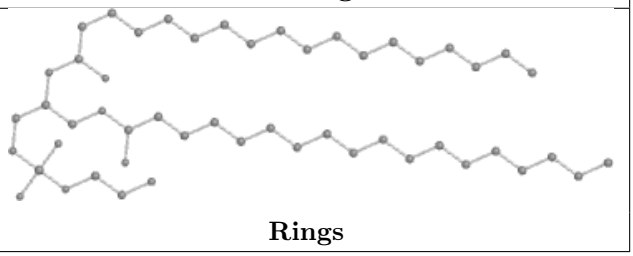
Bond lengths



Bond angles

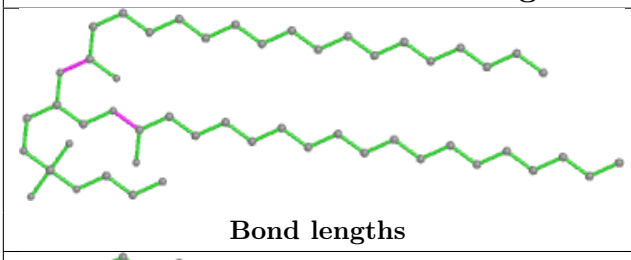


Torsions



Rings

Ligand 3PE 3X 101



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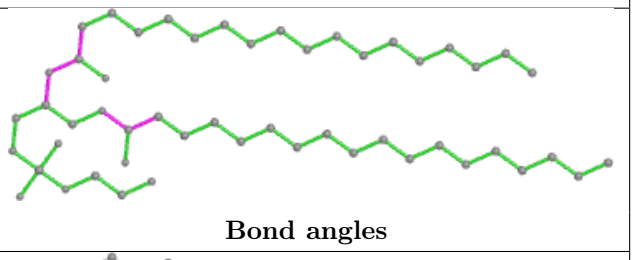
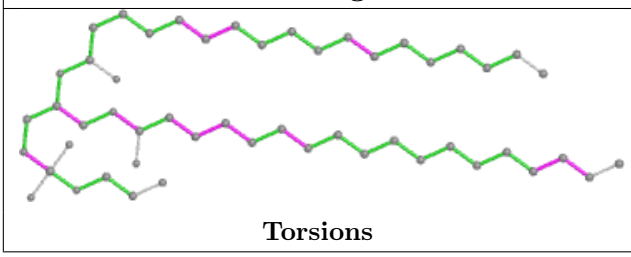


Bond angles



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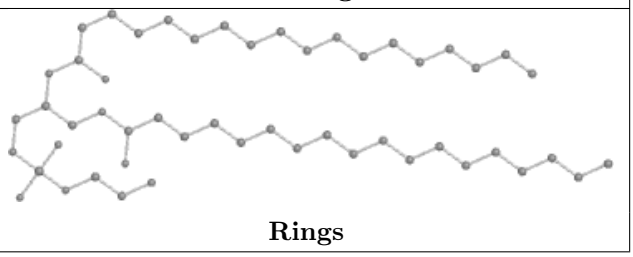
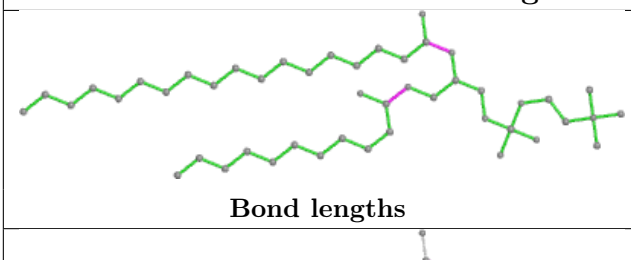


Rings

Ligand PC1 1h 202



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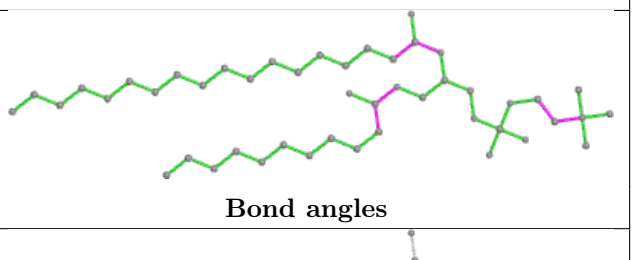
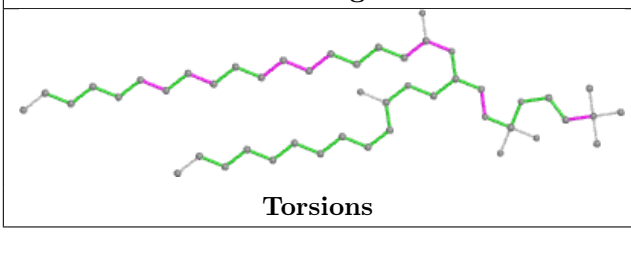


Bond angles



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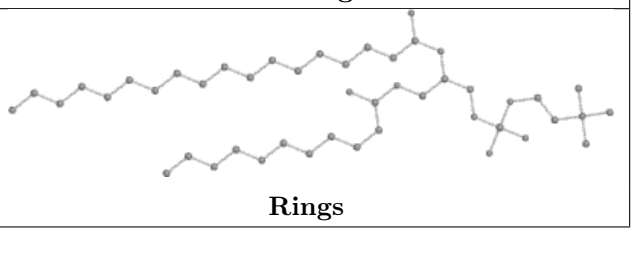
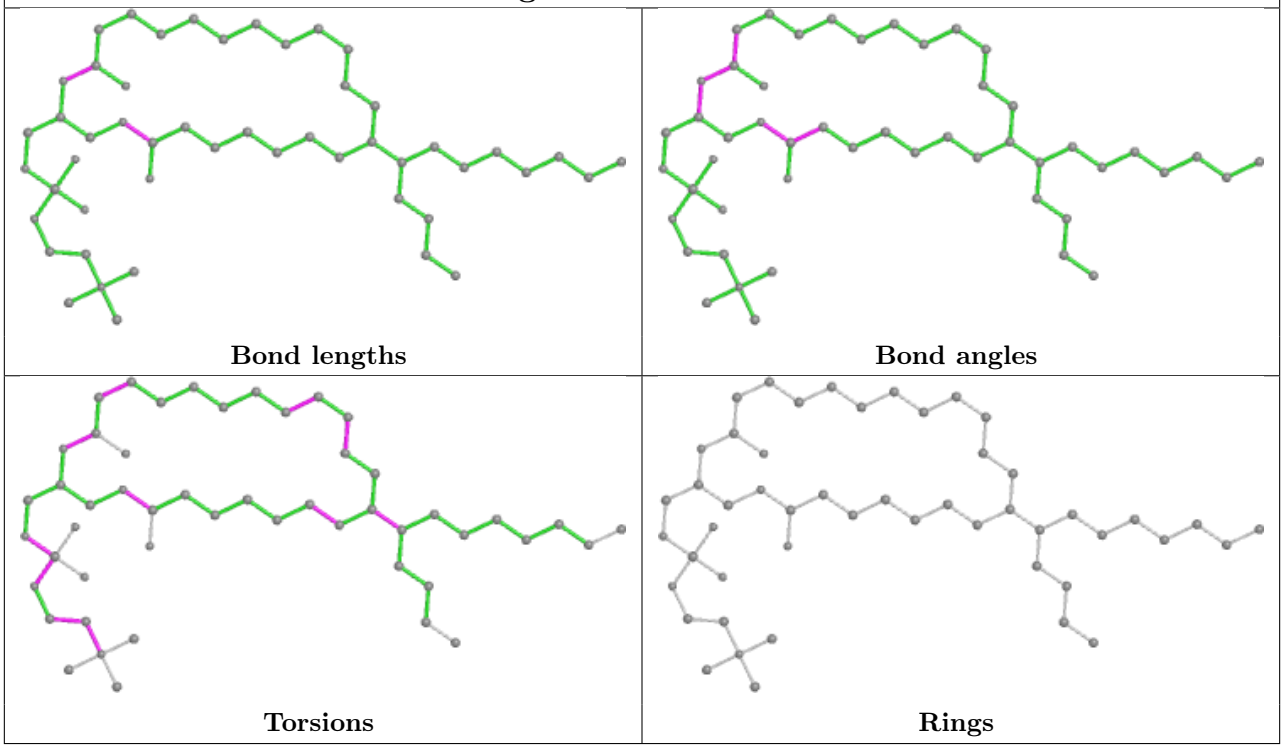
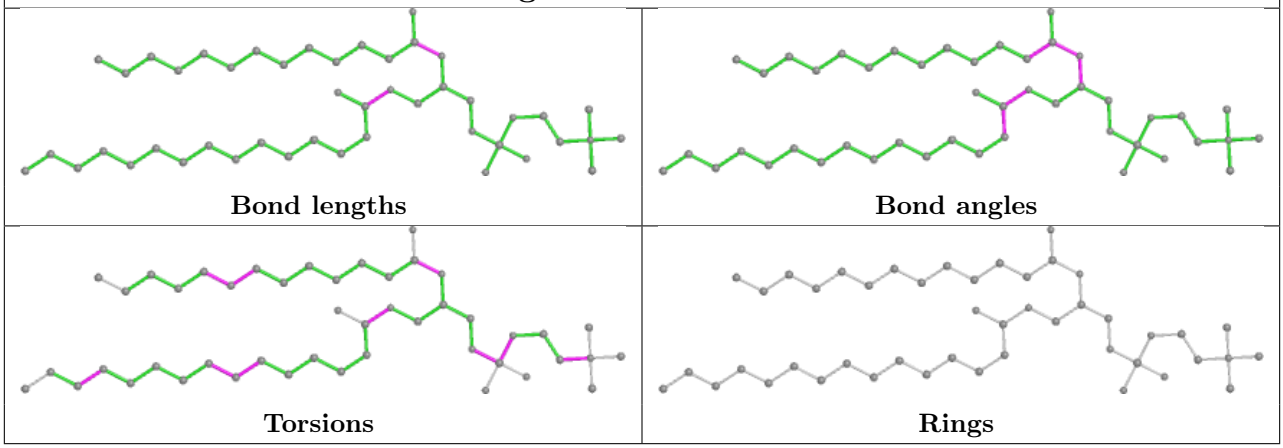


Rings

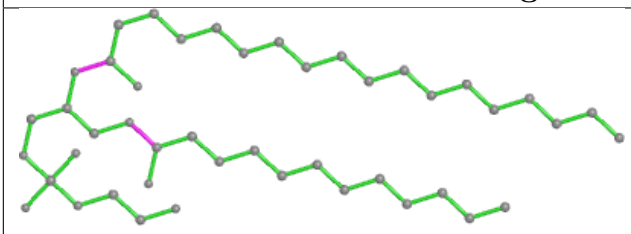
Ligand PSC 4B 303



Ligand PC1 1Y 206



Ligand 3PE 3P 511



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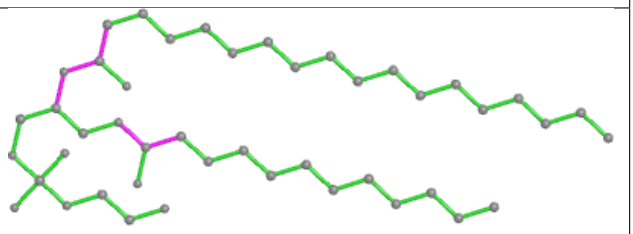
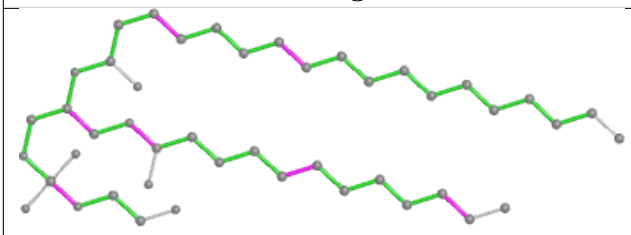
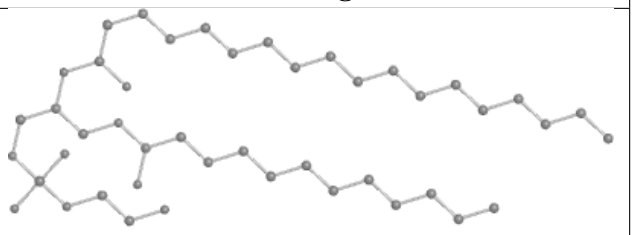


Bond angles

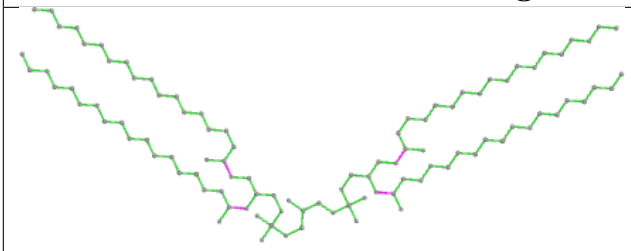


Torsions

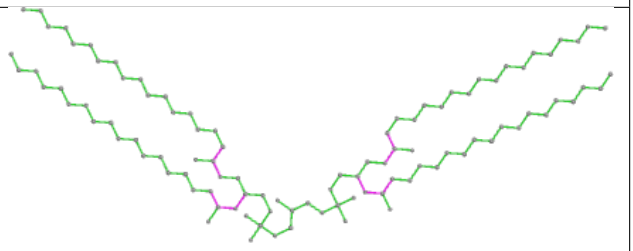


Rings

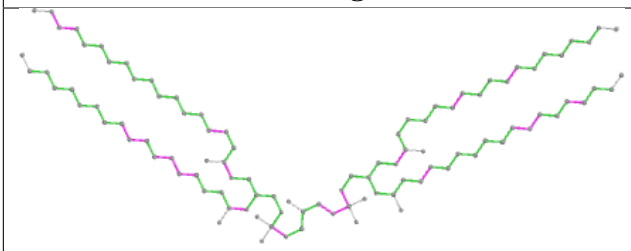
Ligand CDL 4B 302



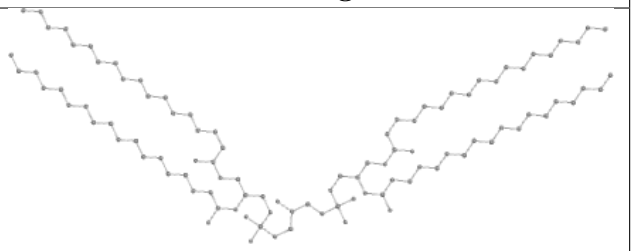
Bond lengths



Bond angles

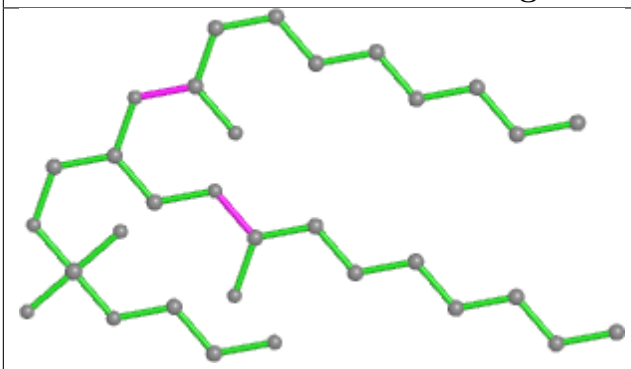


Torsions



Rings

Ligand 3PE 3C 517



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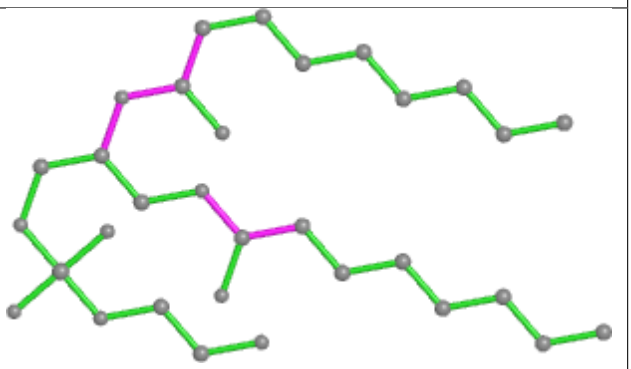
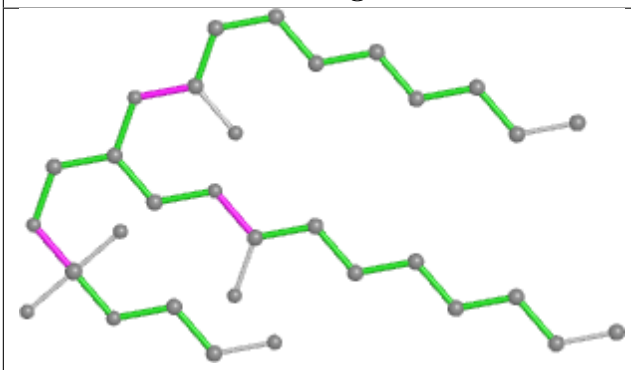
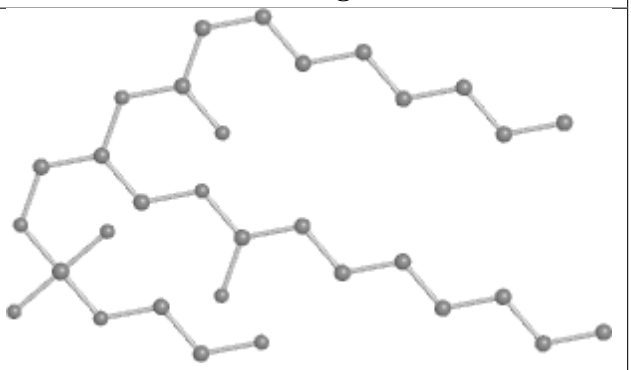


Bond angles

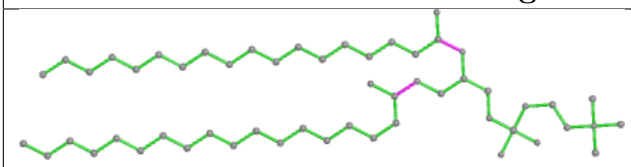


Torsions

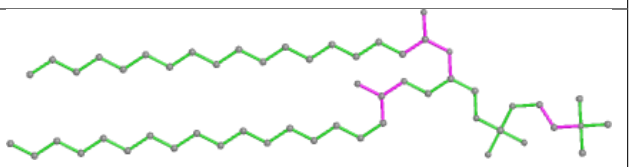


Rings

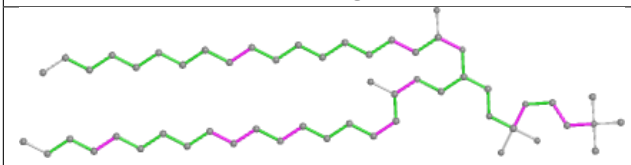
Ligand PC1 3P 509



Bond lengths



Bond angles



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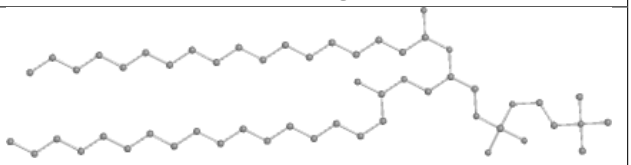
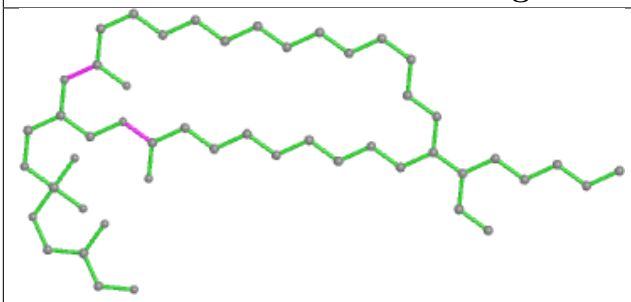
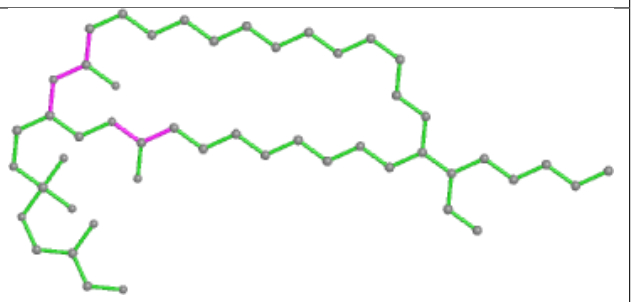


Rings

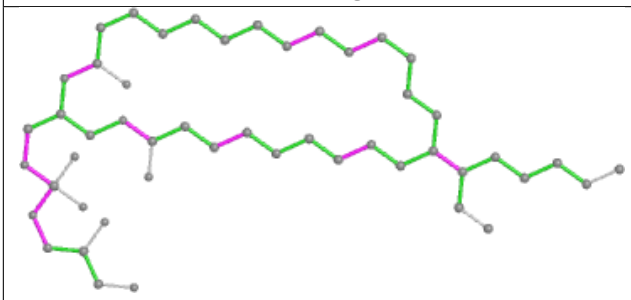
Ligand PGV 4A 607



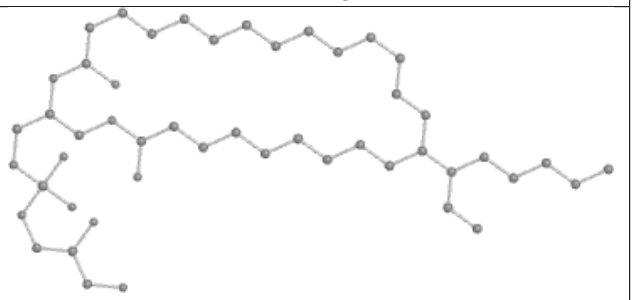
Bond lengths



Bond angles

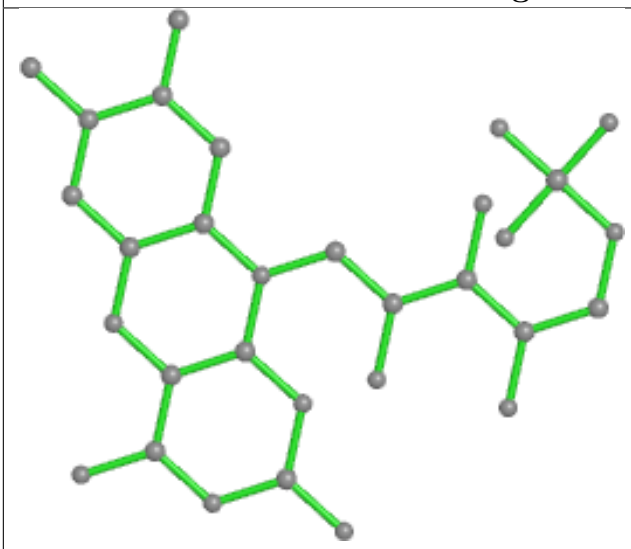


Torsions

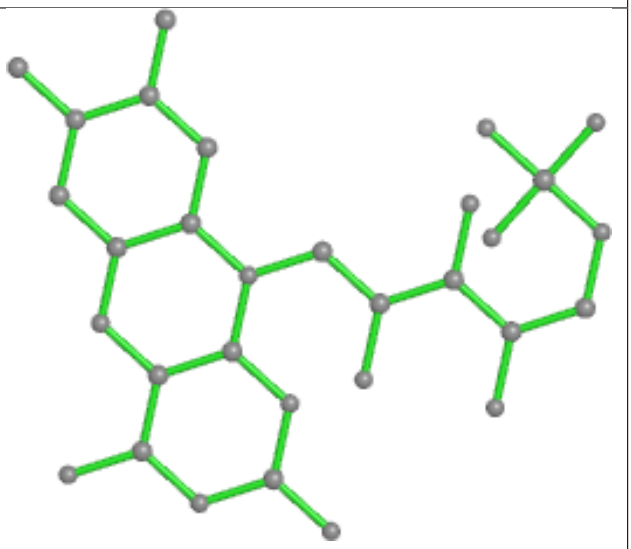


Rings

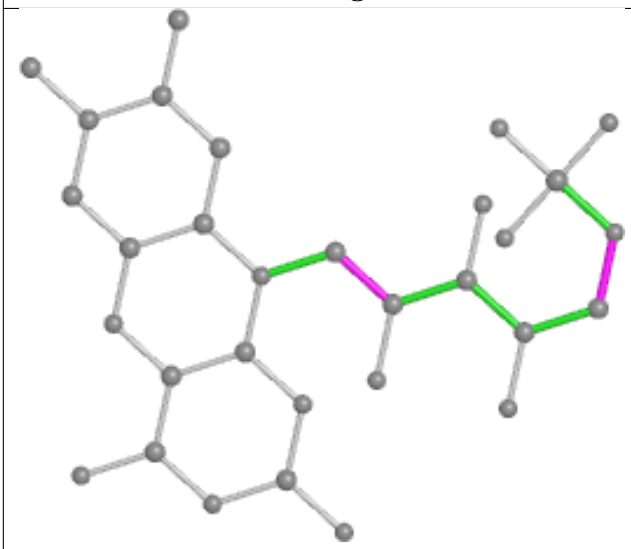
Ligand FMN 1F 501



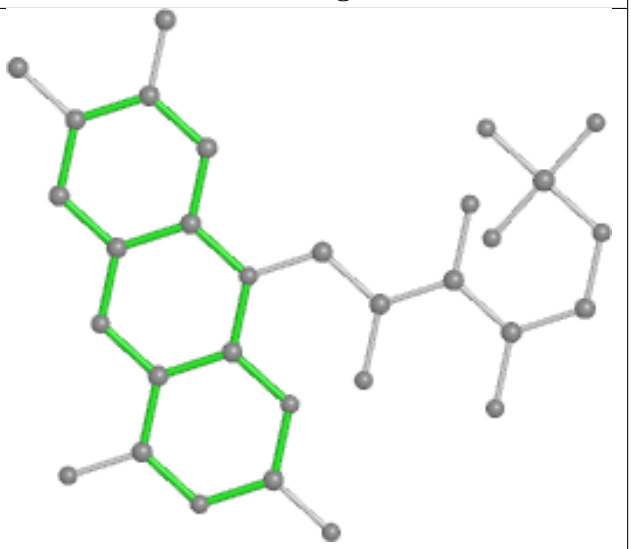
Bond lengths



Bond angles

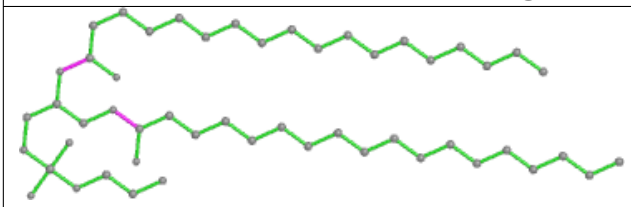


Torsions

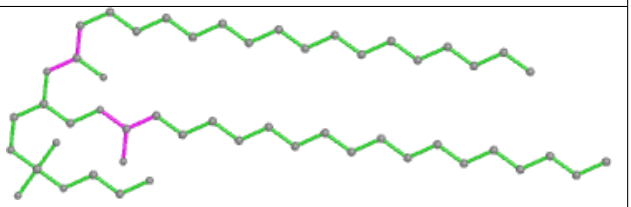


Rings

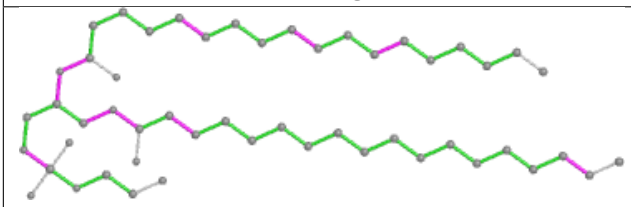
Ligand 3PE 3C 513



Bond lengths



Bond angles



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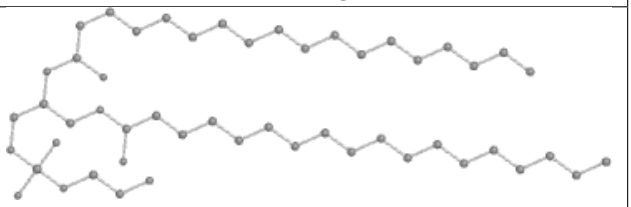
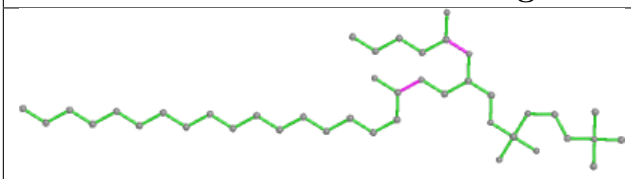
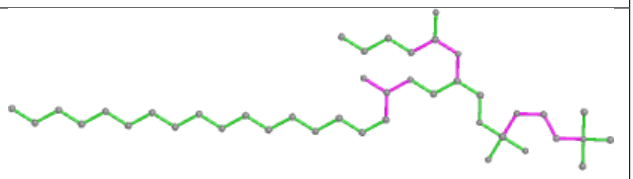


Rings

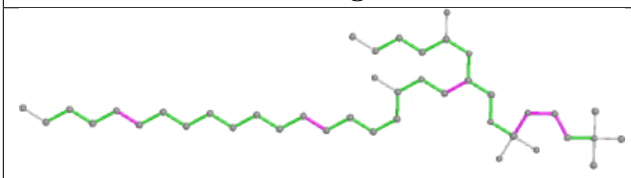
Ligand PC1 1H 404



Bond lengths



Bond angles



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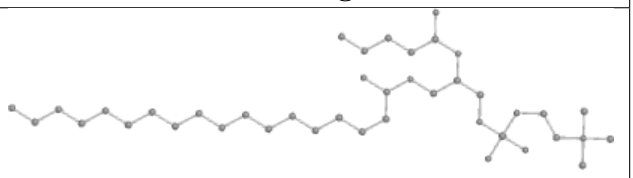
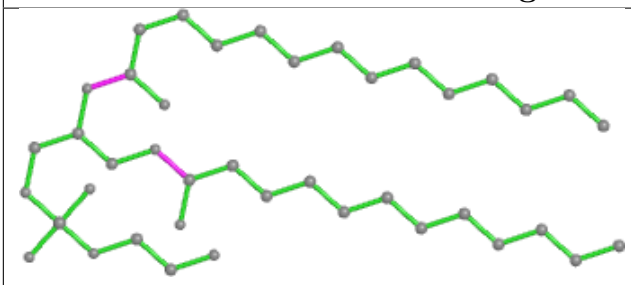
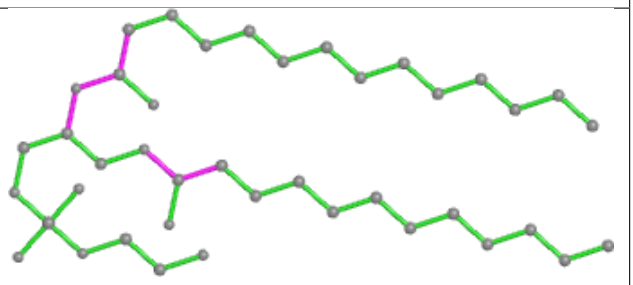


Rings

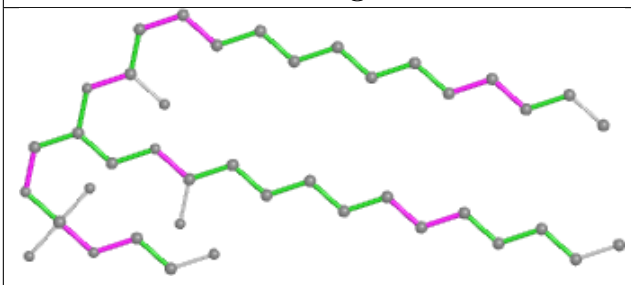
Ligand 3PE 1A 203



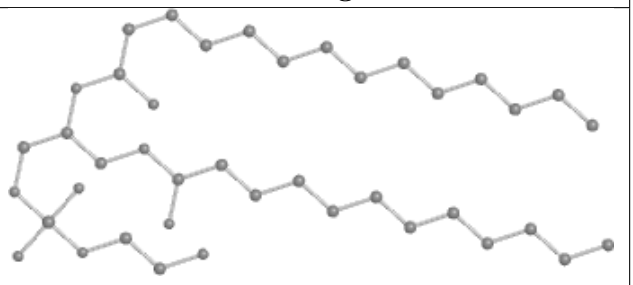
Bond lengths



Bond angles

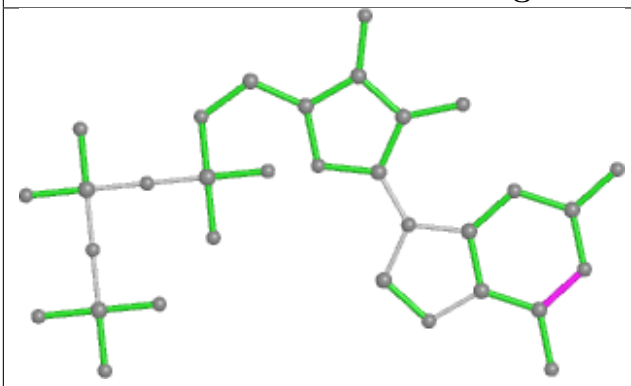


Torsions

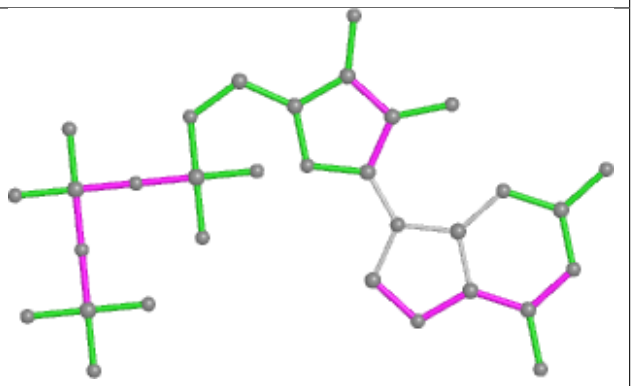


Rings

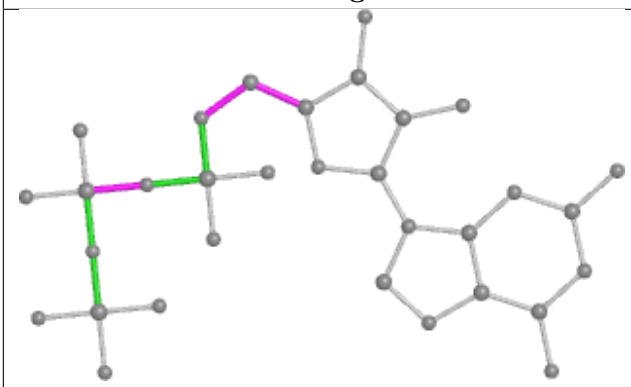
Ligand GTP 1O 401



Bond lengths



Bond angles



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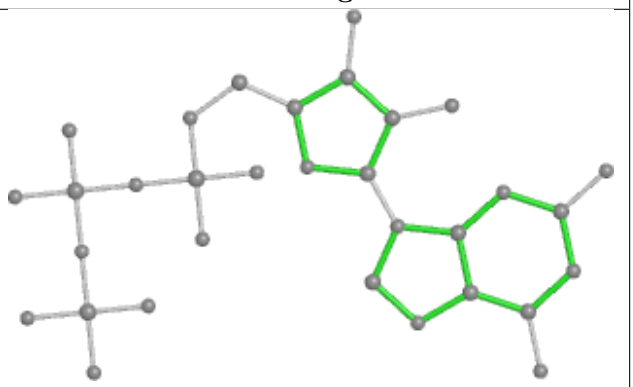
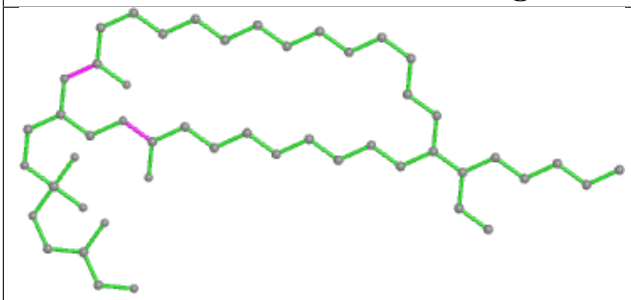
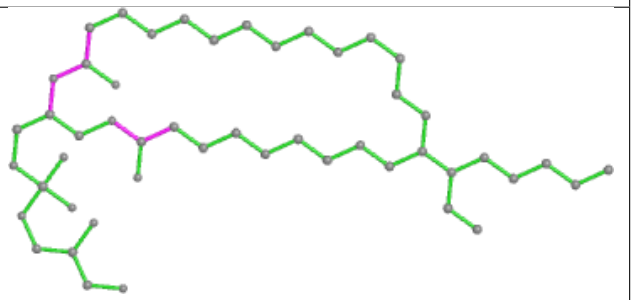


Rings

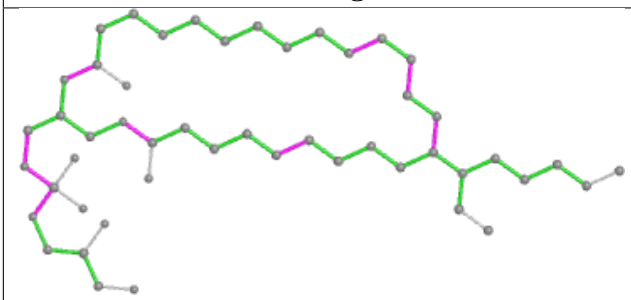
Ligand PGV 4N 101



Bond lengths



Bond angles



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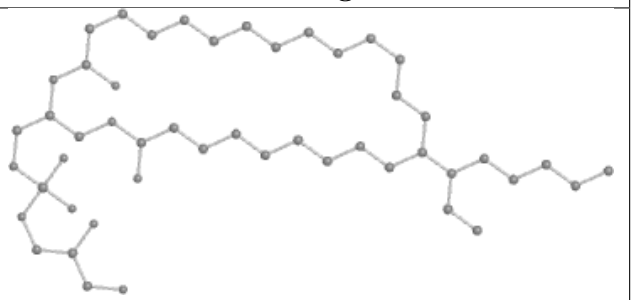
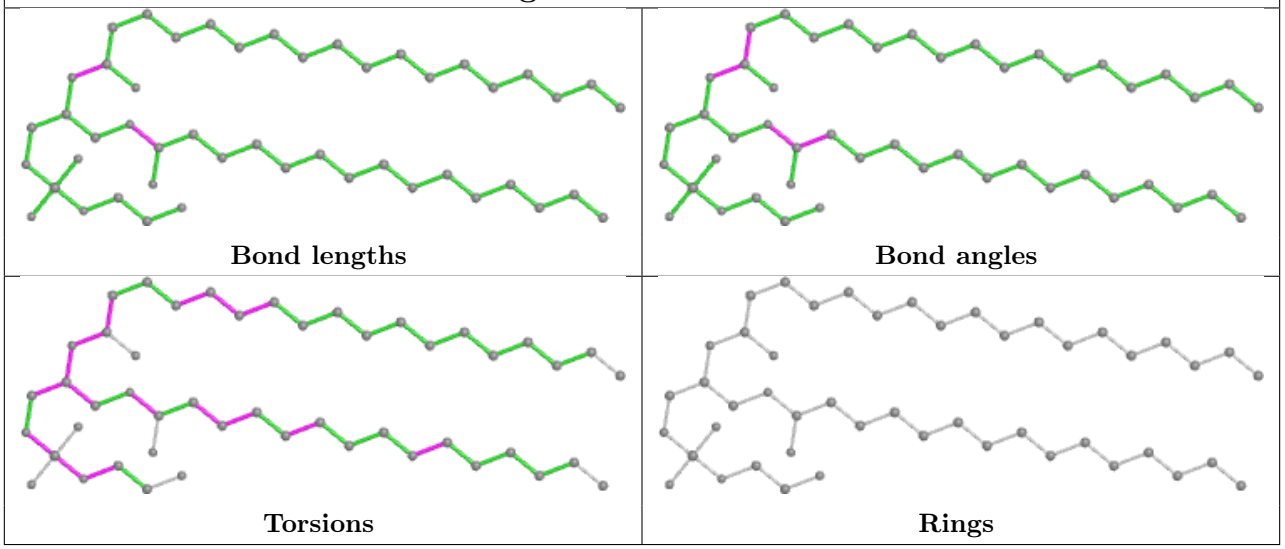
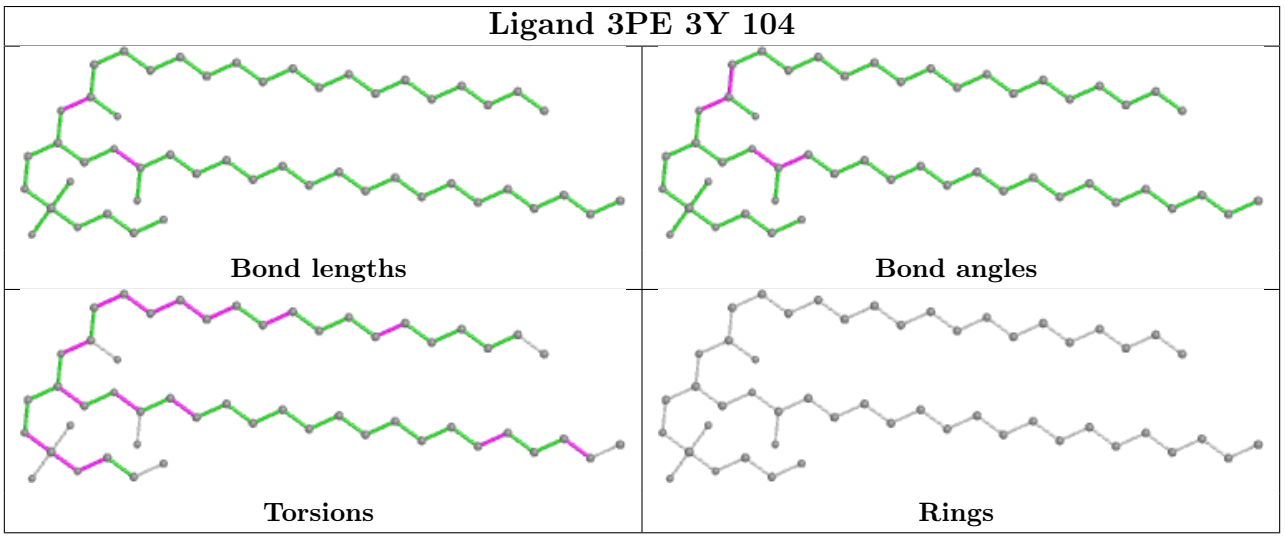


Rings

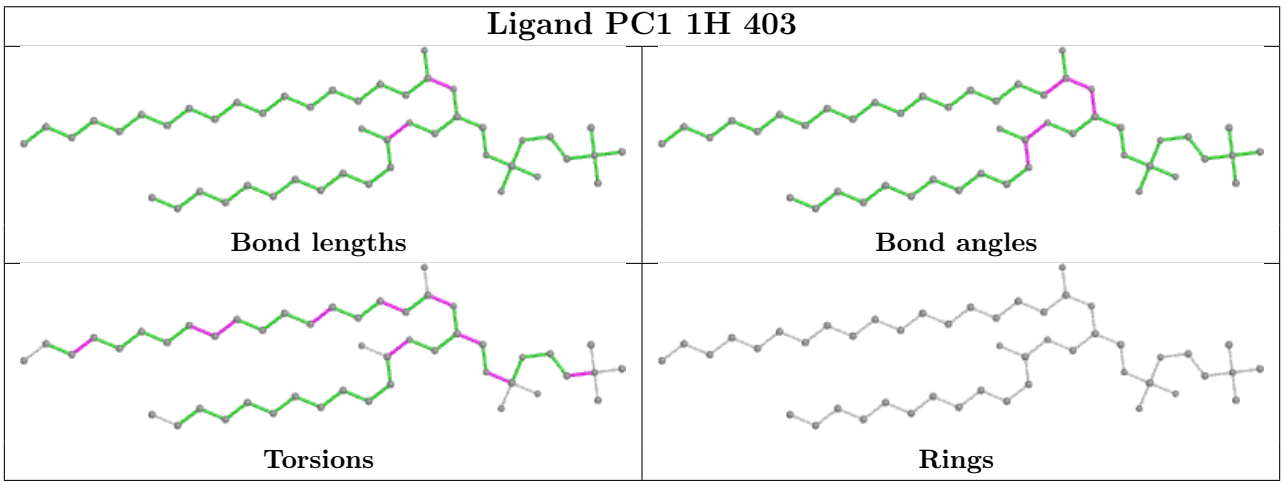
Ligand 3PE 3G 111



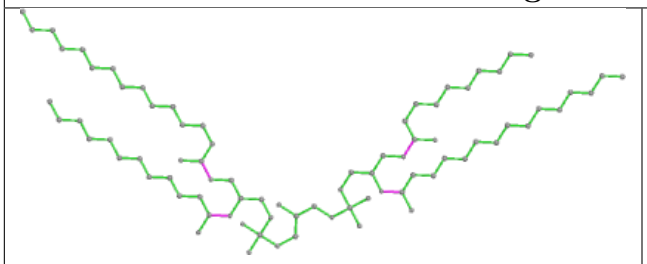
Ligand 3PE 3Y 104



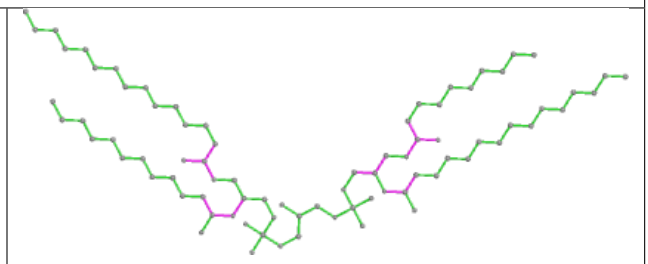
Ligand PC1 1H 403



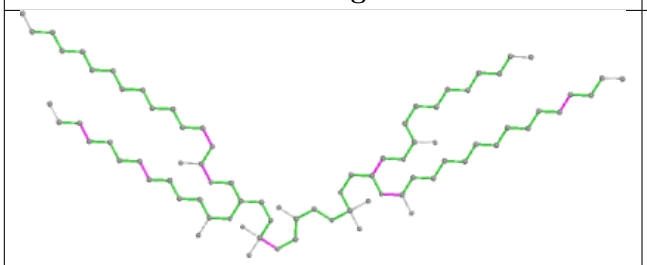
Ligand CDL 1i 201



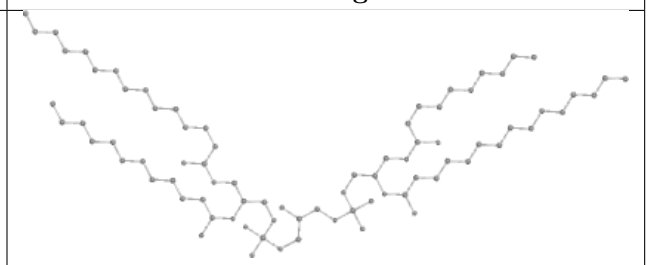
Bond lengths



Bond angles

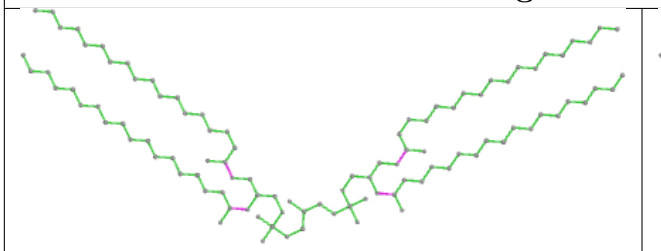


Torsions

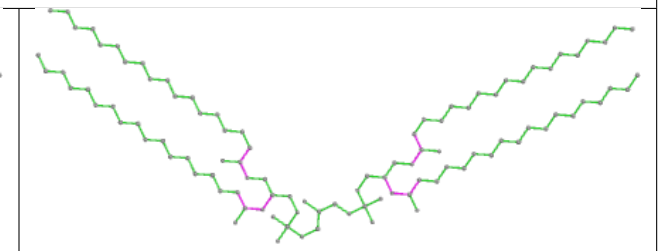


Rings

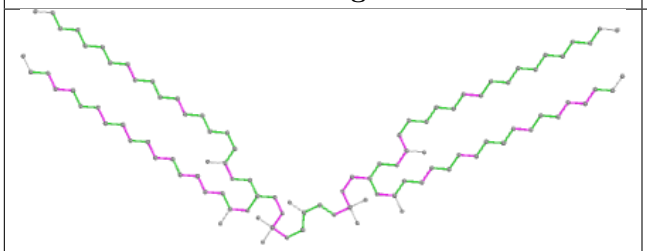
Ligand CDL 4C 306



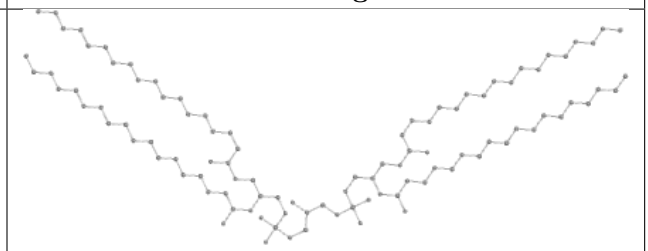
Bond lengths



Bond angles

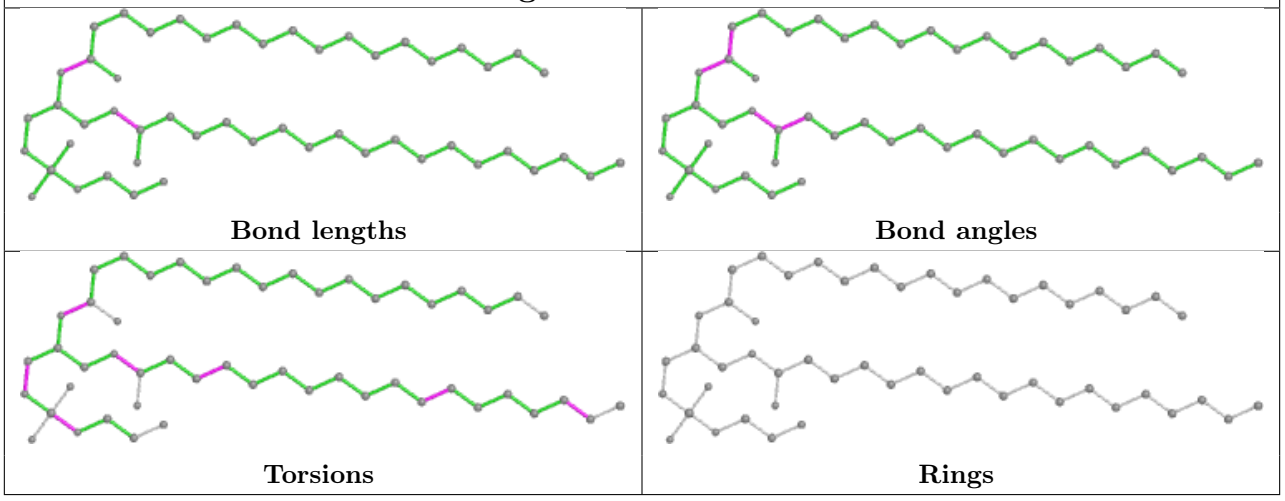


Torsions



Rings

Ligand 3PE 1m 205



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	3W	3
53	3J	2
51	3G	1
52	3H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3G	75:ASN	C	82:PRO	N	2.65
1	3H	77:GLU	C	78:ASP	N	2.52
1	3W	57:LYS	C	58:HIS	N	2.37
1	3J	59:LYS	C	60:TYR	N	1.79
1	3J	56:ILE	C	57:LYS	N	1.07
1	3W	58:HIS	C	59:LYS	N	1.02
1	3W	56:ILE	C	57:LYS	N	0.94

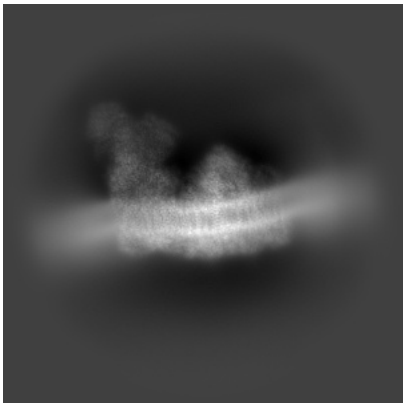
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42225. These allow visual inspection of the internal detail of the map and identification of artifacts.

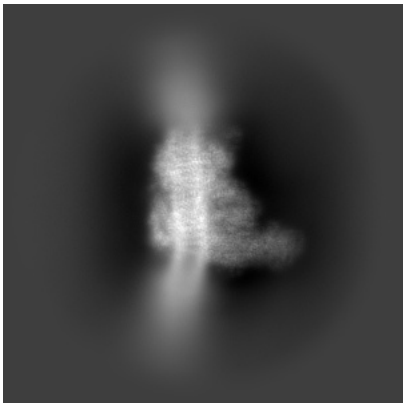
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

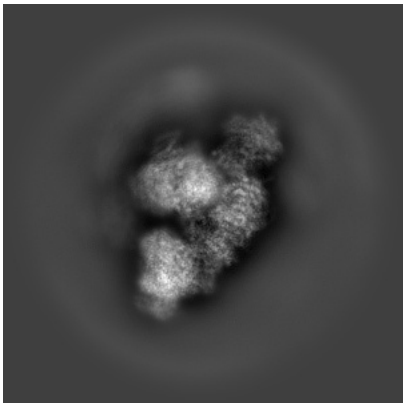
6.1.1 Primary map



X



Y

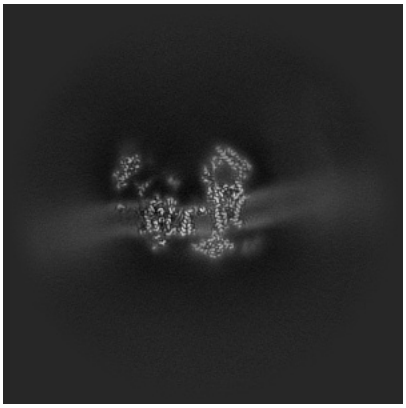


Z

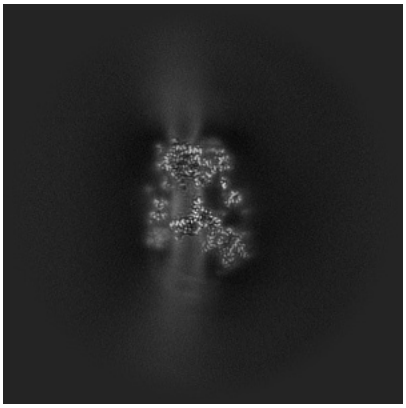
The images above show the map projected in three orthogonal directions.

6.2 Central slices

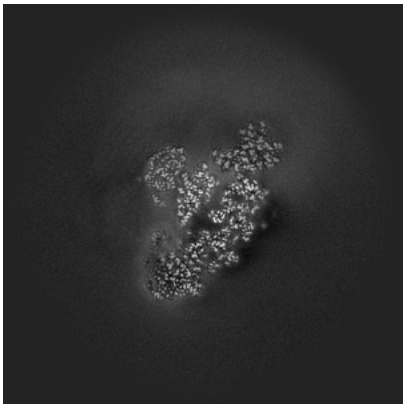
6.2.1 Primary map



X Index: 320



Y Index: 320

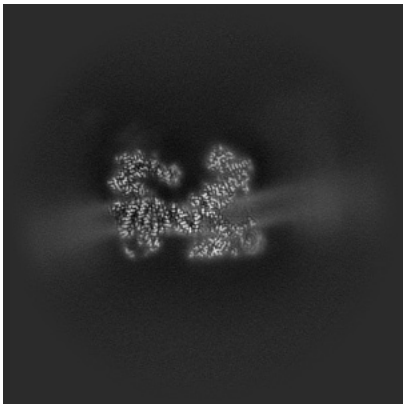


Z Index: 320

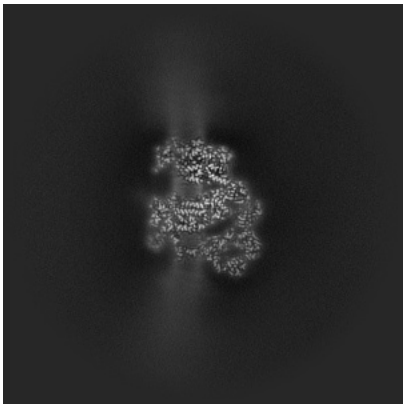
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

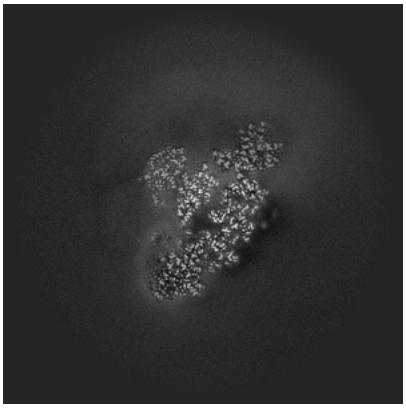
6.3.1 Primary map



X Index: 300



Y Index: 342

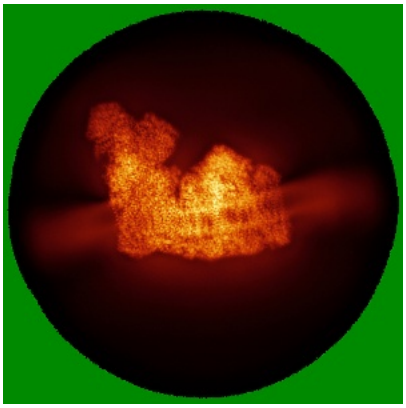


Z Index: 319

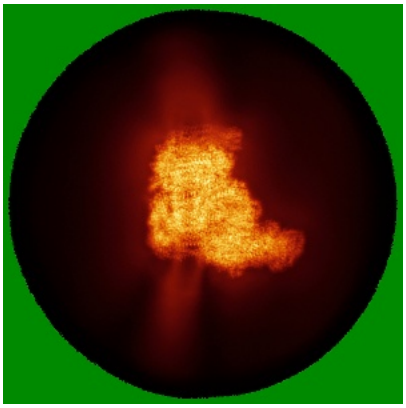
The images above show the largest variance slices of the map in three orthogonal directions.

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

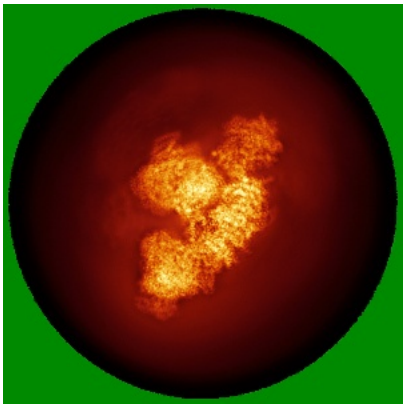
6.4.1 Primary map



X



Y



Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

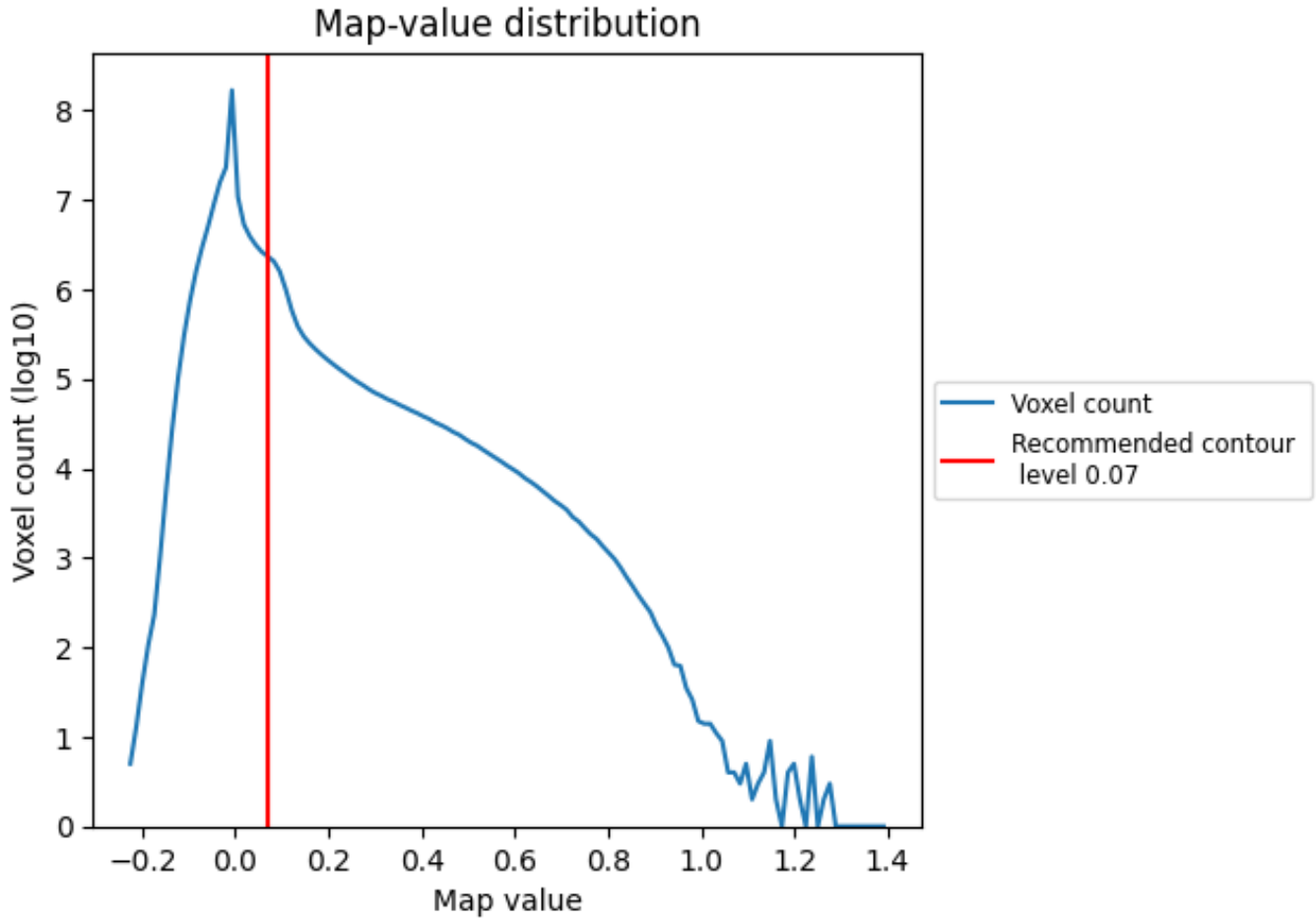
6.6 Mask visualisation (i)

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

7 Map analysis

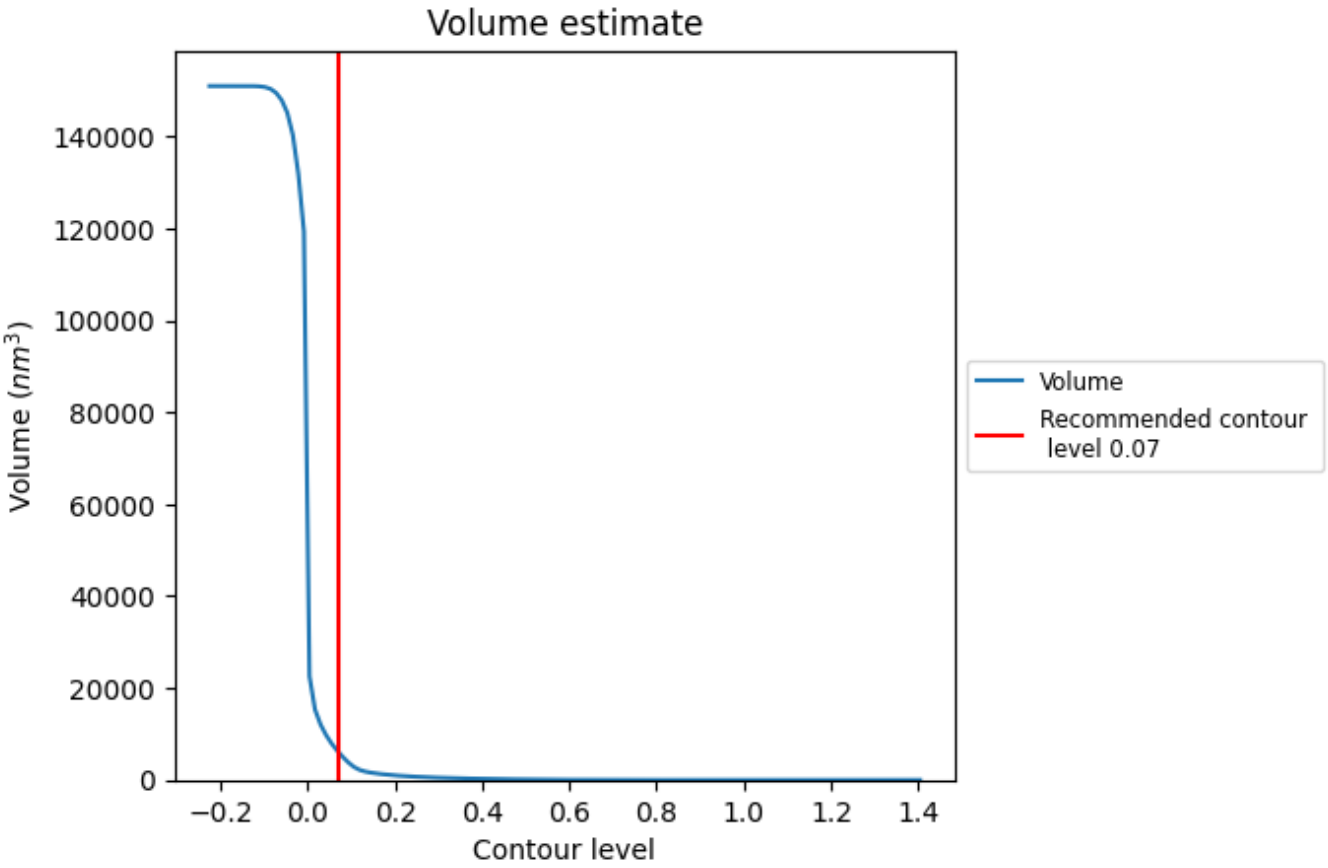
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

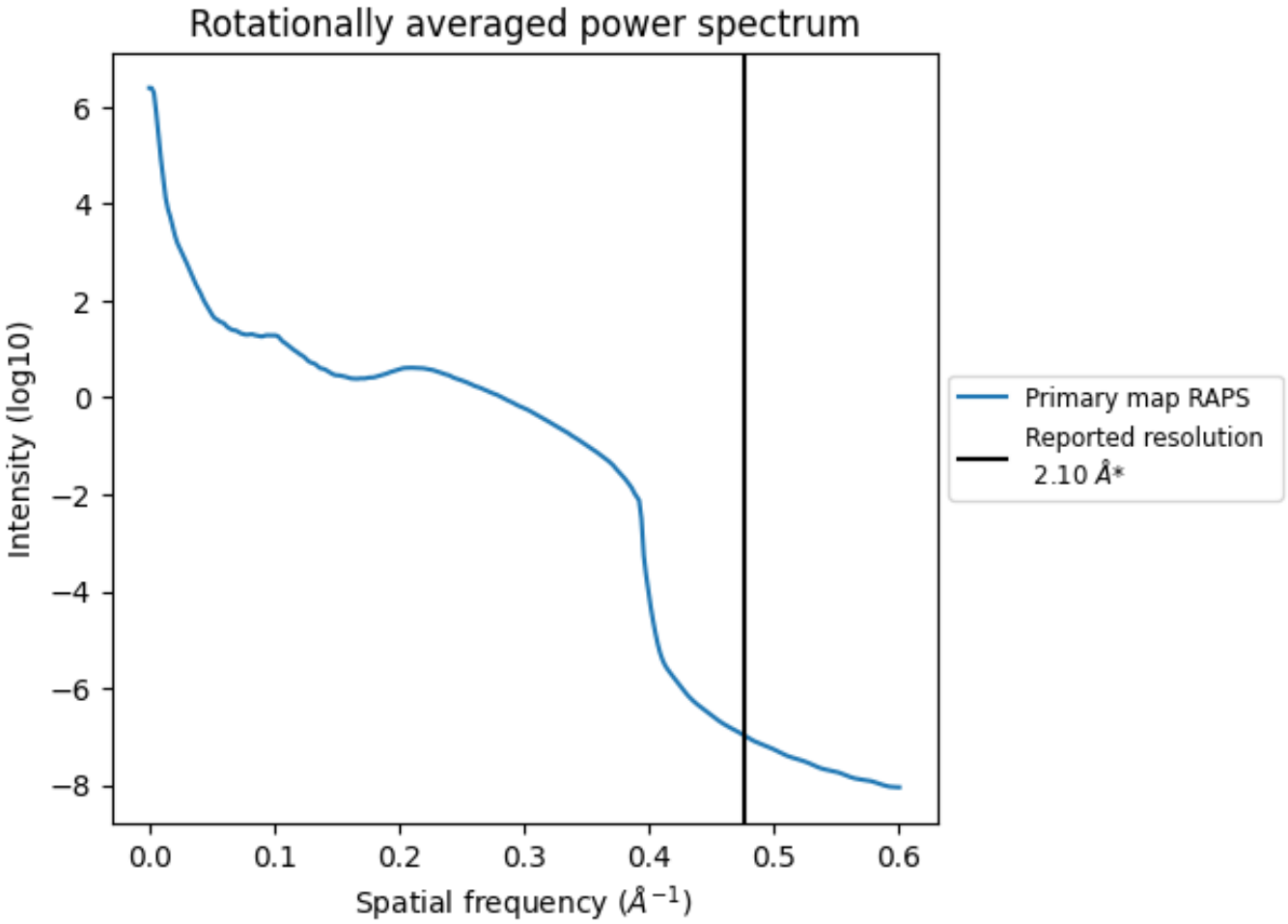
7.2 Volume estimate



The volume at the recommended contour level is 6122 nm^3; this corresponds to an approximate mass of 5530 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 0.476 Å^{-1}

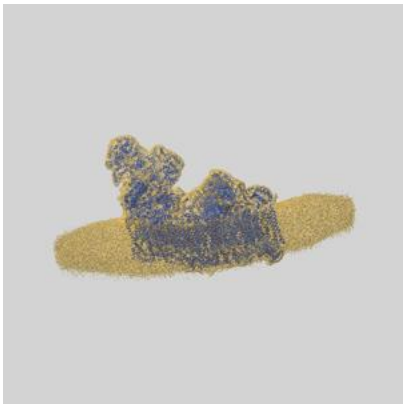
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

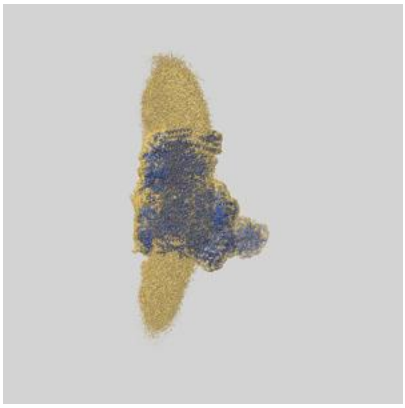
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42225 and PDB model 8UGH. Per-residue inclusion information can be found in section 3 on page 40.

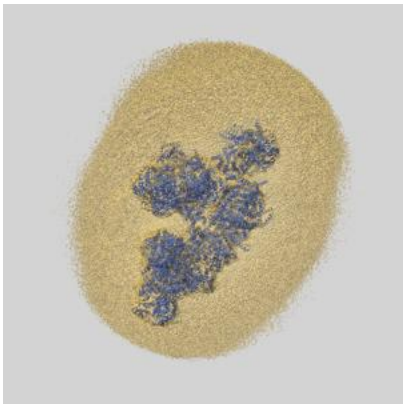
9.1 Map-model overlay



X



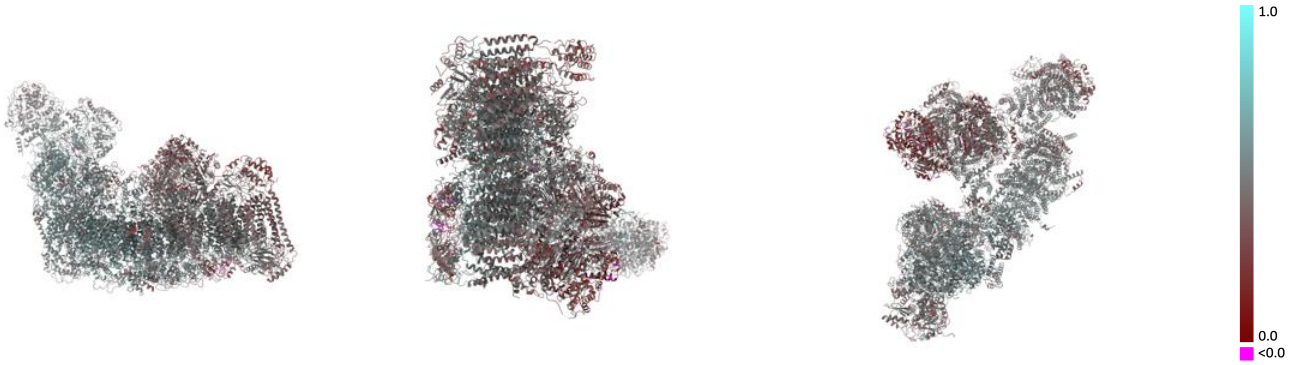
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

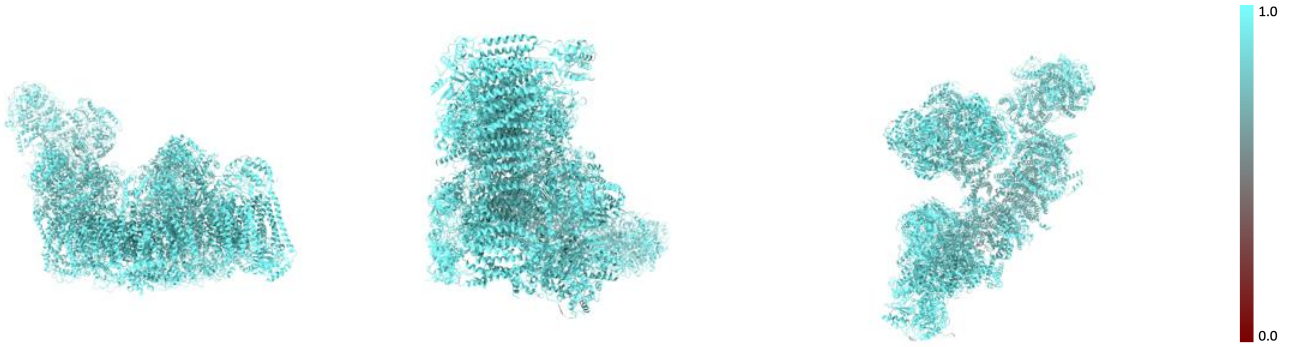
9.2 Q-score mapped to coordinate model



X Y Z

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

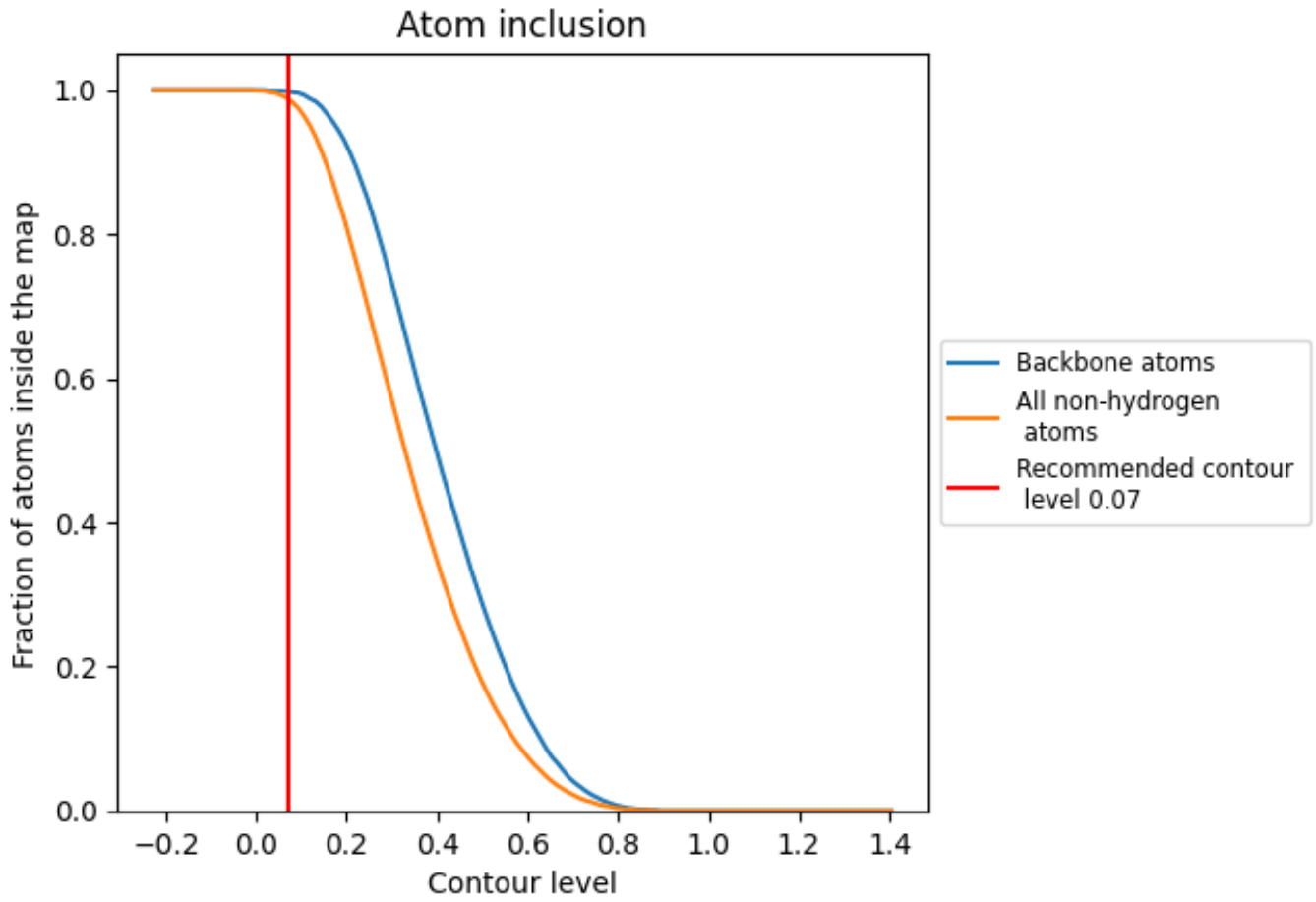
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9880	0.4640
1A	0.9850	0.4890
1B	0.9970	0.5530
1C	0.9940	0.5640
1D	0.9930	0.5690
1E	0.9740	0.4480
1F	0.9800	0.4530
1G	0.9890	0.4920
1H	0.9960	0.5470
1I	0.9970	0.5700
1J	0.9970	0.4700
1K	0.9960	0.5340
1L	0.9980	0.5100
1M	1.0000	0.5660
1N	0.9990	0.5680
1O	0.9810	0.5080
1P	0.9820	0.5060
1Q	0.9330	0.4950
1R	0.9810	0.5220
1S	0.9720	0.4570
1T	0.9580	0.3790
1U	0.9910	0.4370
1V	0.9630	0.5190
1W	0.9640	0.5210
1X	0.9960	0.5020
1Y	0.9960	0.4570
1Z	0.9950	0.5150
1a	0.9980	0.5440
1b	0.9820	0.4920
1c	0.9850	0.4660
1d	0.9970	0.5400
1e	0.9940	0.5000
1f	0.9800	0.4660
1g	0.9920	0.4970
1h	0.9980	0.5310

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Chain	Atom inclusion	Q-score
1i	0.9930	0.4440
1j	0.9930	0.4170
1k	0.9840	0.3990
1l	0.9940	0.4960
1m	0.9990	0.4860
1n	0.9970	0.4730
1o	0.9980	0.4490
1p	1.0000	0.5200
1q	0.9960	0.5390
1r	0.9930	0.5460
1s	0.9380	0.4160
3A	0.9670	0.3190
3B	0.9820	0.3030
3C	0.9940	0.4390
3D	0.9960	0.4890
3E	0.9910	0.3270
3F	0.9540	0.3590
3G	0.9070	0.3240
3H	0.9710	0.4230
3I	0.9970	0.3670
3J	0.9960	0.4200
3N	1.0000	0.4360
3O	0.9970	0.3550
3P	1.0000	0.4720
3Q	1.0000	0.5100
3R	0.9890	0.3080
3S	1.0000	0.4180
3T	0.9970	0.4580
3U	1.0000	0.4590
3V	0.9910	0.3240
3W	1.0000	0.4340
3X	1.0000	0.3610
3Y	0.9940	0.3390
4A	0.9900	0.4630
4B	0.9900	0.4110
4C	0.9900	0.4560
4D	0.9470	0.3920
4E	0.9400	0.3040
4F	0.9290	0.4000
4G	0.9940	0.4080
4H	0.9700	0.4090
4I	0.9870	0.3920

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Chain	Atom inclusion	Q-score
4J	0.9940	0.4810
4K	0.9980	0.4330
4L	0.9650	0.4530
4M	0.9850	0.4420
4N	0.9710	0.3780