Full wwPDB EM Validation Report ⓘ

Apr 18, 2024 – 03:04 pm BST

PDB ID	:	8PW7
EMDB ID	:	EMD-17991
Title	:	A respirasome from murine liver
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2023-07-19
Resolution	:	3.50 Å(reported)
Based on initial models	:	6g2j, 7o3c

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:

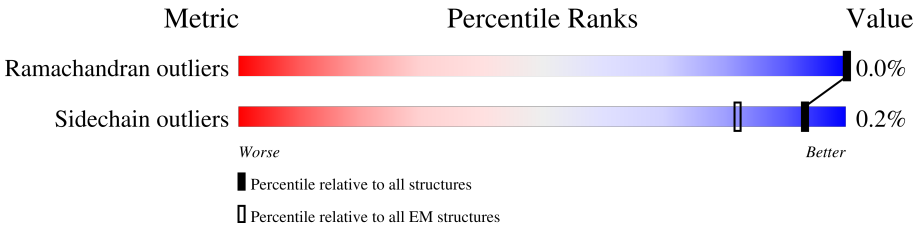
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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%

Mol	Chain	Length	Quality of chain
1	n	514	99% ·
2	o	227	99% ·
3	p	261	99%
4	q	169	81% · 18%
5	r	146	71% 29%
6	s	128	73% · 27%
7	t	97	77% 23%
8	u	86	90% · 8%
9	v	76	93% 7%
10	x	80	61% 39%

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Mol	Chain	Length	Quality of chain
11	y	63	75% 25%
12	z	70	61% 39%
13	w	83	67% 31%
14	A	480	92% 7%
14	L	480	93% 7%
15	B	453	93% 7%
15	M	453	93% 7%
16	C	381	98%
16	N	381	98%
17	D	325	73% 26%
17	O	325	74% 26%
18	E	274	72% 28%
18	P	274	71% 28%
18	T	274	28% 72%
19	F	111	90% 9%
19	Q	111	92% 8%
20	G	82	94% 6%
20	R	82	91% 6%
21	H	89	74% 26%
21	S	89	76% 24%
22	J	64	94% 6%
22	U	64	94% 6%
23	K	56	93% 7%
23	V	56	95% 5%
24	6	224	70% 30%

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Mol	Chain	Length	Quality of chain
25	C1	263	79% 21%
26	D1	463	92% 7%
27	2	248	85% 14%
28	1	464	93% 7%
29	3	727	95% 5%
30	9	212	83% 16%
31	P1	377	90% 9%
32	Q1	175	72% 28%
33	7	116	82% 17%
34	S1	99	84% 15%
35	T1	156	51% 49%
35	U1	156	56% 44%
36	V1	116	97%
37	W1	131	87% 13%
38	q1	145	100%
39	r1	113	87% 12%
40	s1	104	39% 60%
41	A1	115	97%
42	H1	318	99%
43	J1	172	100%
44	K1	98	98%
45	L1	607	100%
46	M1	459	99%
47	N1	345	100%
48	O1	355	90% 10%

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Mol	Chain	Length	Quality of chain
49	X1	172	99%
50	Y1	141	99%
51	Z1	144	97%
52	a1	70	100%
53	b1	84	96%
54	c1	76	63% 37%
55	d1	120	99%
56	e1	106	99%
57	f1	57	91% 7%
58	g1	151	67% 33%
59	h1	189	74% 26%
60	i1	128	81% 17%
61	j1	105	62% 38%
62	k1	104	73% 26%
63	l1	186	84% 16%
64	m1	129	98%
65	n1	179	99%
66	o1	137	85% 14%
67	p1	176	97%

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 115528 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	n	514	4021	2691	623	675	32	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	o	227	1817	1180	282	336	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	p	260	2118	1418	339	351	10	0	0

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	q	139	1156	745	192	212	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	r	104	842	538	141	161	2	0	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	s	94	721	449	126	138	8	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	t	75	Total	C	N	O	S	0	0
			605	392	114	96	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	u	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	z	43	Total	C	N	O	S	0	0
			311	203	51	56	1		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	w	57	Total	C	N	O	S	0	0
			435	283	71	78	3		

- Molecule 14 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
14	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 15 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
15	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 16 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
16	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 17 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		
17	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 18 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	196	Total	C	N	O	S	0	0
			1164	702	219	237	6		
18	P	196	Total	C	N	O	S	0	0
			1164	702	219	237	6		
18	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 19 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	101	Total	C	N	O	S	0	0
			894	572	159	160	3		
19	Q	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

- Molecule 20 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	77	Total	C	N	O	S	0	0
			654	424	120	109	1		
20	R	77	Total	C	N	O	S	0	0
			654	424	120	109	1		

- Molecule 21 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
21	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

- Molecule 22 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	J	60	Total	C	N	O	0	0
			495	323	86	86		
22	U	60	Total	C	N	O	0	0
			495	323	86	86		

- Molecule 23 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	52	Total	C	N	O	S	0	0
			430	287	76	66	1		
23	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	C1	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D1	430	Total	C	N	O	S	0	0
			3464	2215	595	630	24		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P1	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Q1	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S1	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 35 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T1	79	Total	C	N	O	S	0	0
			637	410	95	127	5		
35	U1	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	V1	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W1	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q1	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r1	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	s1	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A1	115	Total	C	N	O	S	0	0
			932	633	132	160	7		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	H1	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	J1	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	K1	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L1	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	M1	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	N1	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	O1	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X1	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y1	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z1	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a1	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	b1	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	c1	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	d1	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	e1	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	f1	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	g1	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	h1	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	i1	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	j1	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	k1	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	l1	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	m1	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	n1	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	o1	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	p1	170	Total	C	N	O	S	0	0
			1438	903	258	269	8		

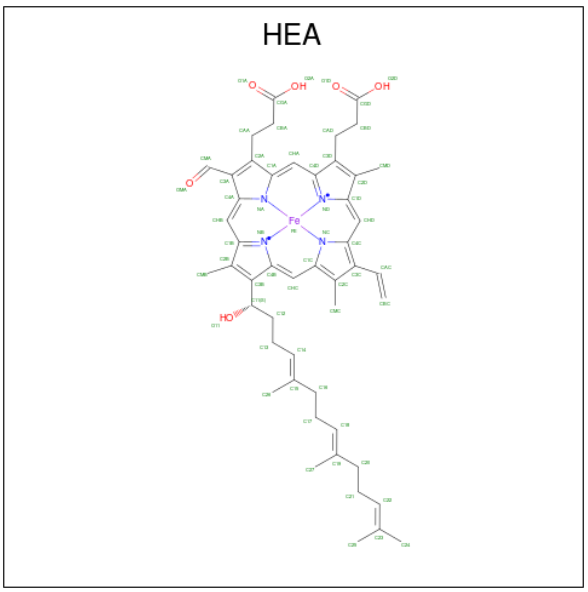
- Molecule 68 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
68	n	1	Total	Cu	0
			1	1	

- Molecule 69 is SODIUM ION (three-letter code: NA) (formula: Na).

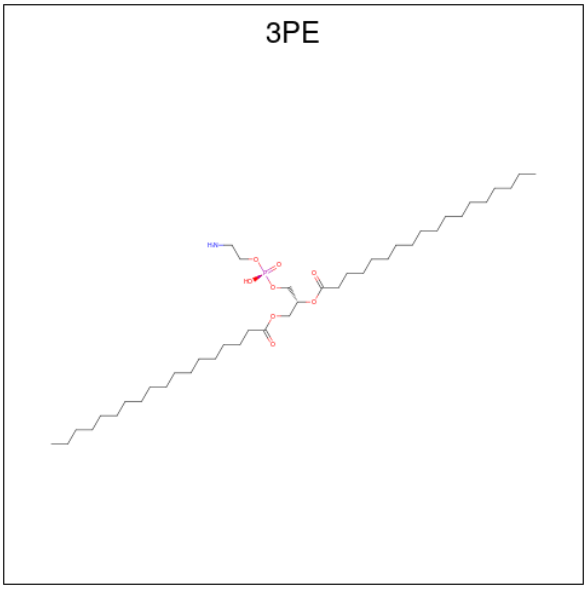
Mol	Chain	Residues	Atoms		AltConf
69	n	1	Total	Na	0
			1	1	

- Molecule 70 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 71 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
71	n	1	Total	C	N	O	P	0
			34	24	1	8	1	
71	n	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	n	1	Total	C	N	O	P	0
			27	17	1	8	1	
71	o	1	Total	C	N	O	P	0
			29	19	1	8	1	
71	p	1	Total	C	N	O	P	0
			45	35	1	8	1	
71	t	1	Total	C	N	O	P	0
			25	15	1	8	1	
71	v	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
71	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
71	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
71	N	1	Total	C	N	O	P	0
			34	24	1	8	1	
71	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
71	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	R	1	Total	C	N	O	P	0
			30	20	1	8	1	
71	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	D1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	r1	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	A1	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	H1	1	Total	C	N	O	P	0
			51	41	1	8	1	

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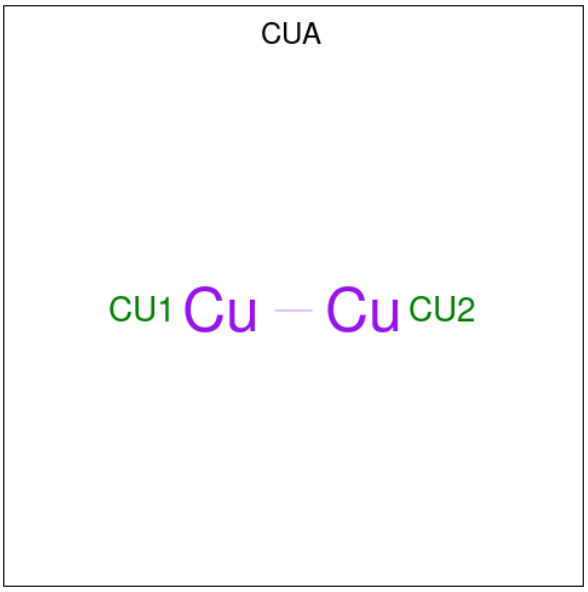
Mol	Chain	Residues	Atoms					AltConf
71	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			36	26	1	8	1	
71	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
71	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
71	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 72 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
72	o	1	Total	Mg	0
			1	1	
72	O1	1	Total	Mg	0
			1	1	

- Molecule 73 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).

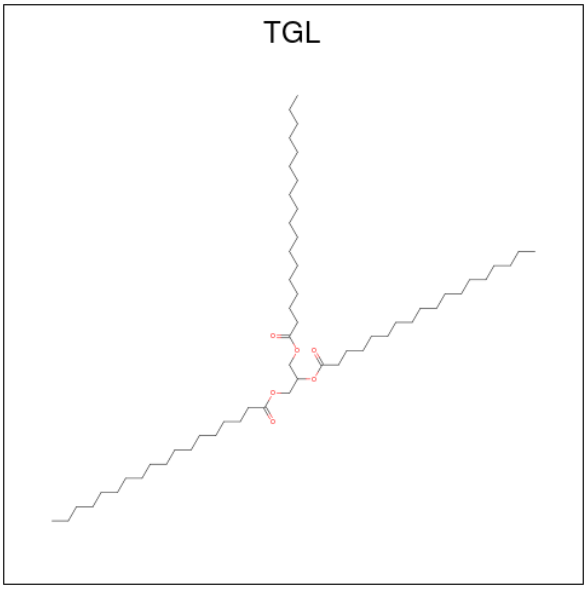


Mol	Chain	Residues	Atoms	AltConf
73	o	1	Total Cu 2 2	0

- Molecule 74 is ZINC ION (three-letter code: ZN) (formula: Zn).

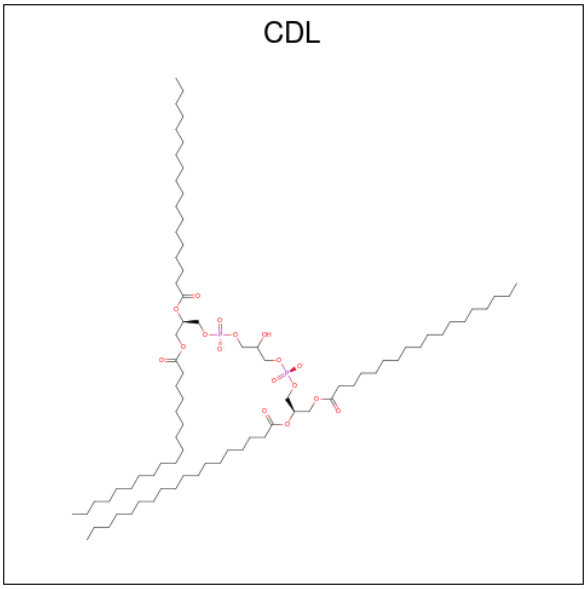
Mol	Chain	Residues	Atoms	AltConf
74	s	1	Total Zn 1 1	0
74	7	1	Total Zn 1 1	0

- Molecule 75 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms			AltConf
75	y	1	Total	C	O	0
			37	31	6	

- Molecule 76 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
76	A	1	Total	C	O	P	0
			46	27	17	2	
76	C	1	Total	C	O	P	0
			42	23	17	2	
76	G	1	Total	C	O	P	0
			56	37	17	2	
76	N	1	Total	C	O	P	0
			46	27	17	2	
76	O	1	Total	C	O	P	0
			57	38	17	2	
76	R	1	Total	C	O	P	0
			41	22	17	2	
76	R	1	Total	C	O	P	0
			57	38	17	2	
76	R	1	Total	C	O	P	0
			72	53	17	2	
76	H1	1	Total	C	O	P	0
			51	33	16	2	
76	L1	1	Total	C	O	P	0
			78	59	17	2	
76	L1	1	Total	C	O	P	0
			46	27	17	2	

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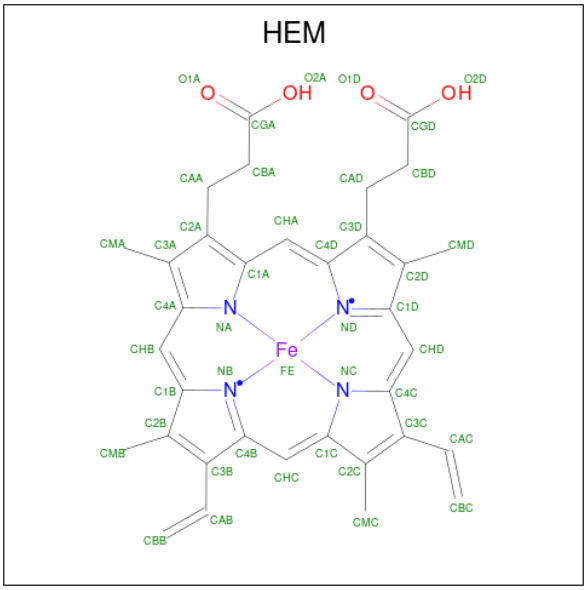
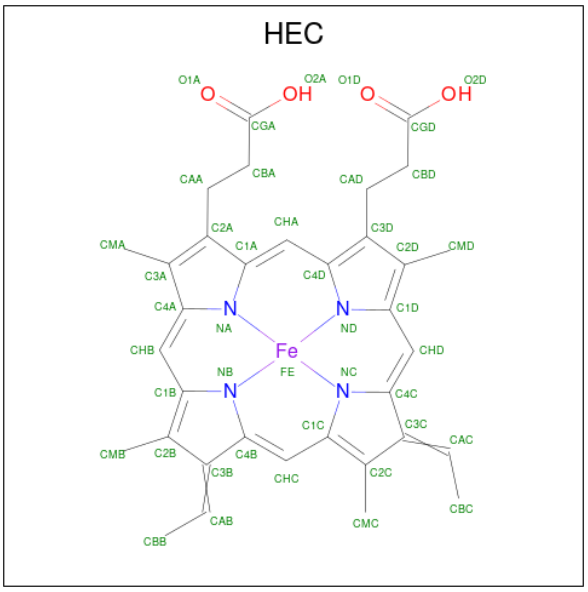
Mol	Chain	Residues	Atoms				AltConf
76	N1	1	Total	C	O	P	0
			90	71	17	2	
76	Y1	1	Total	C	O	P	0
			94	75	17	2	
76	a1	1	Total	C	O	P	0
			57	38	17	2	
76	d1	1	Total	C	O	P	0
			67	48	17	2	
76	h1	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



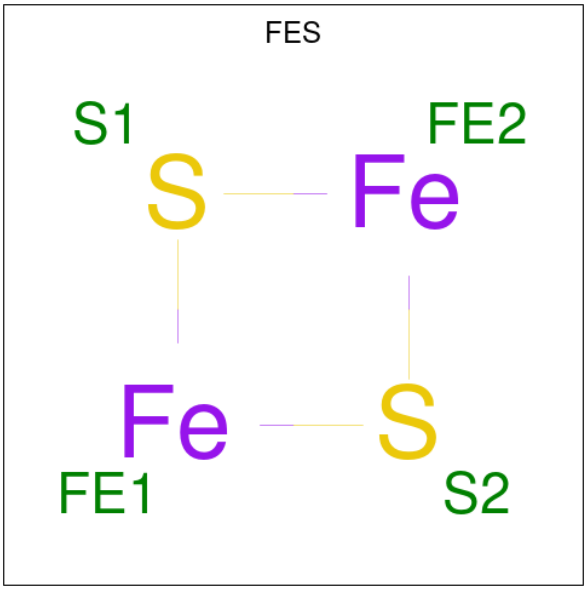
Mol	Chain	Residues	Atoms					AltConf
77	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
77	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
77	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
77	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 78 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
78	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
78	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 79 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms				AltConf
79	E	1	Total	Fe	S		0
			4	2	2		
79	P	1	Total	Fe	S		0
			4	2	2		

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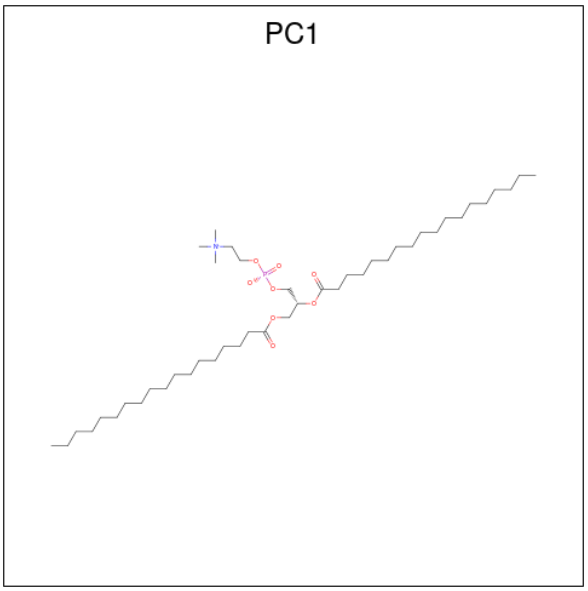
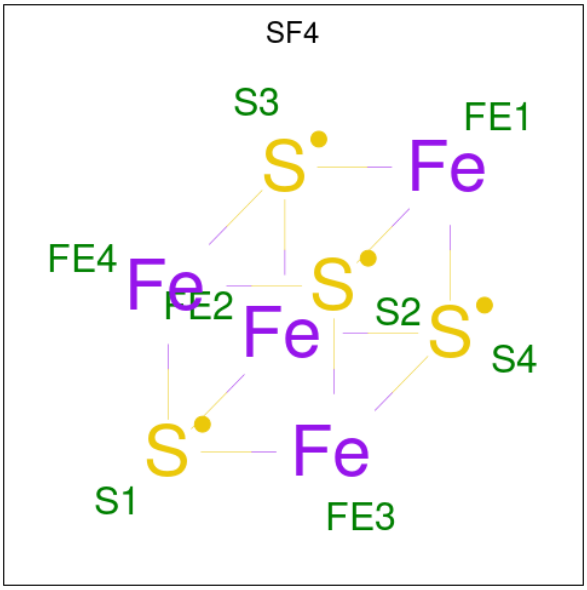
Mol	Chain	Residues	Atoms	AltConf
79	2	1	Total Fe S 4 2 2	0
79	3	1	Total Fe S 4 2 2	0

- Molecule 80 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



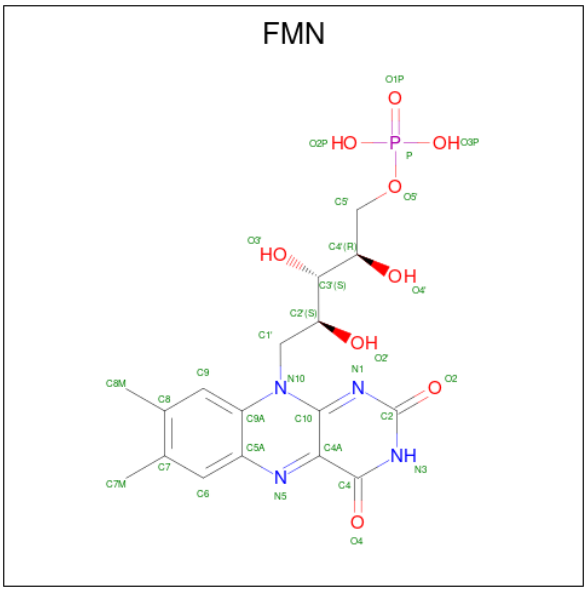
Mol	Chain	Residues	Atoms	AltConf
80	J	1	Total C N O P 35 25 1 8 1	0
80	K	1	Total C N O P 28 18 1 8 1	0
80	L	1	Total C N O P 24 14 1 8 1	0
80	V	1	Total C N O P 28 18 1 8 1	0
80	6	1	Total C N O P 43 33 1 8 1	0
80	9	1	Total C N O P 54 44 1 8 1	0
80	9	1	Total C N O P 47 37 1 8 1	0
80	P1	1	Total C N O P 31 21 1 8 1	0
80	Y1	1	Total C N O P 54 44 1 8 1	0

- Molecule 81 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
81	6	1	Total Fe S 8 4 4	0
81	1	1	Total Fe S 8 4 4	0
81	3	1	Total Fe S 8 4 4	0
81	3	1	Total Fe S 8 4 4	0
81	9	1	Total Fe S 8 4 4	0
81	9	1	Total Fe S 8 4 4	0

- Molecule 82 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

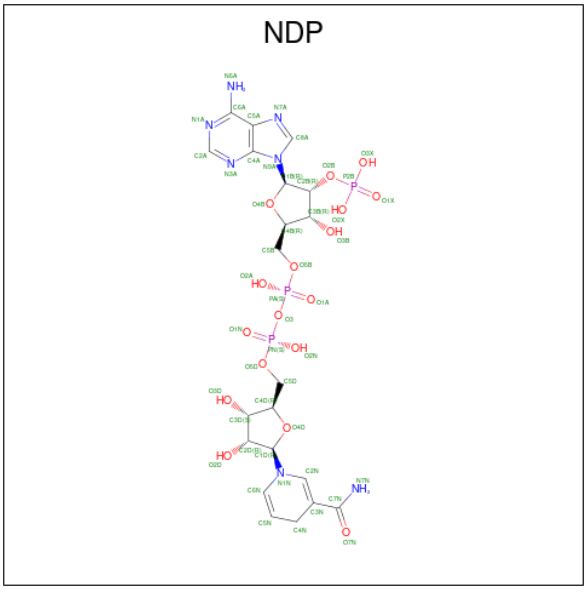


Mol	Chain	Residues	Atoms					AltConf
82	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 83 is POTASSIUM ION (three-letter code: K) (formula: K).

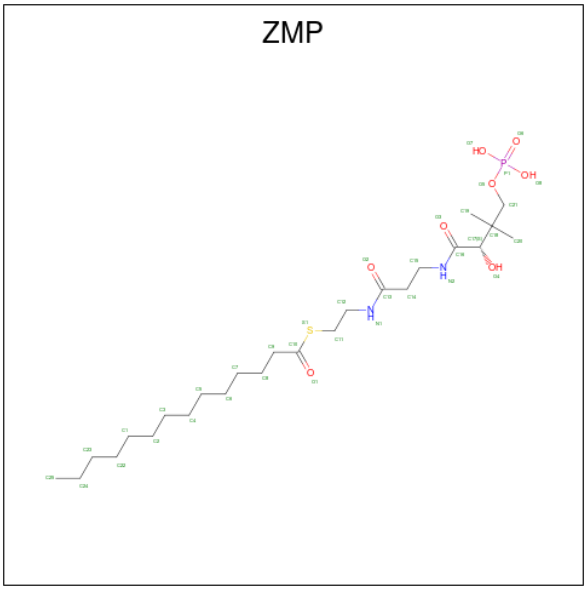
Mol	Chain	Residues	Atoms		AltConf
83	3	1	Total	K	0
			1	1	

- Molecule 84 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



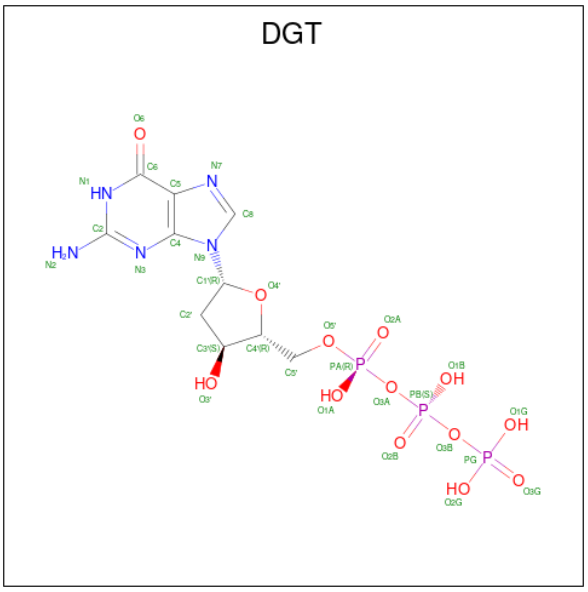
Mol	Chain	Residues	Atoms					AltConf
84	P1	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 85 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
85	W1	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
85	n1	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 86 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



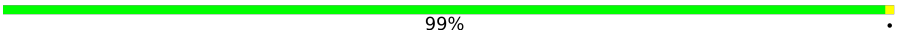
Mol	Chain	Residues	Atoms					AltConf
86	O1	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

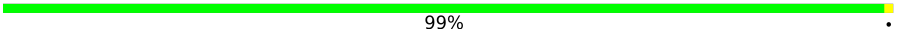
• Molecule 1: Cytochrome c oxidase subunit 1

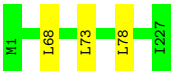
Chain n:



• Molecule 2: Cytochrome c oxidase subunit 2

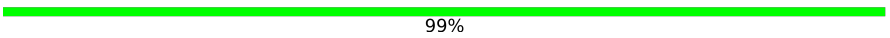
Chain o:

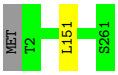




• Molecule 3: Cytochrome c oxidase subunit 3

Chain p:



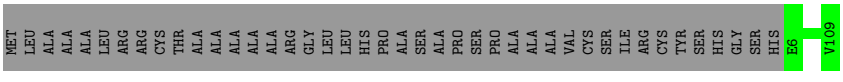


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain q:

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

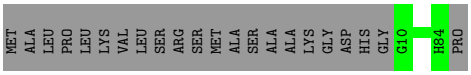
Chain r:



• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

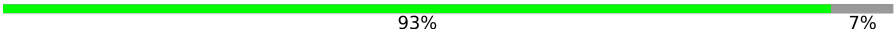
Chain s:

• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



• Molecule 8: Cytochrome c oxidase subunit 6B1

• Molecule 9: Cytochrome c oxidase subunit 6C

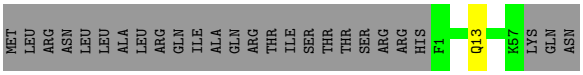


• Molecule 10: Cytochrome c oxidase subunit 7B, mitochondrial

• Molecule 11: Cytochrome c oxidase subunit 7C, mitochondrial

• Molecule 12: Cytochrome c oxidase subunit 8B, mitochondrial

• Molecule 13: Cytochrome c oxidase subunit 7A2, mitochondrial

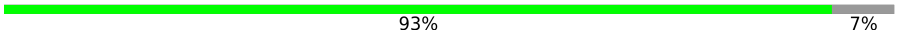


• Molecule 14: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:

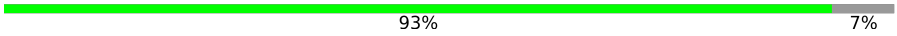
• Molecule 14: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



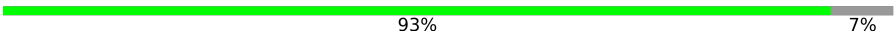
• Molecule 15: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



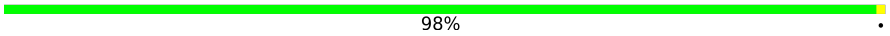
• Molecule 15: Cytochrome b-c1 complex subunit 2, mitochondrial

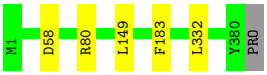
Chain M:



• Molecule 16: Cytochrome b

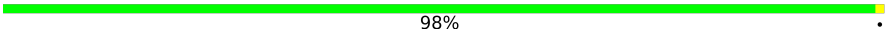
Chain C:





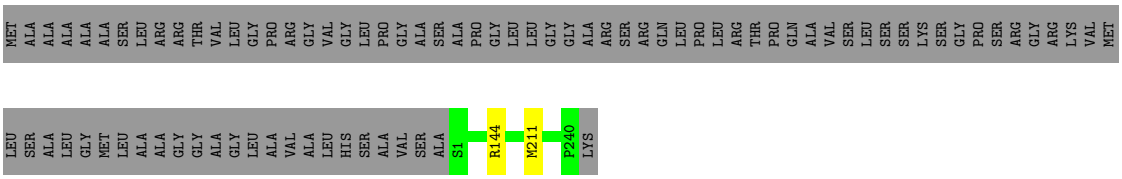
• Molecule 16: Cytochrome b

Chain N:



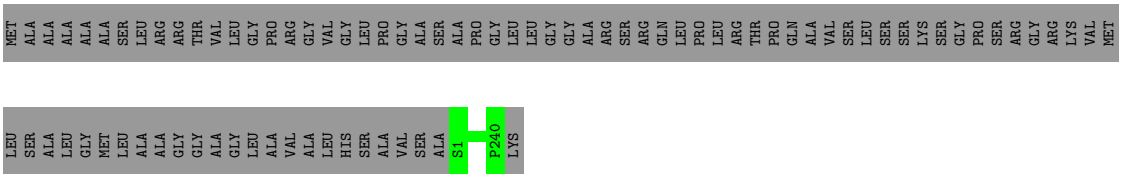
• Molecule 17: Cytochrome c1, heme protein, mitochondrial

Chain D:



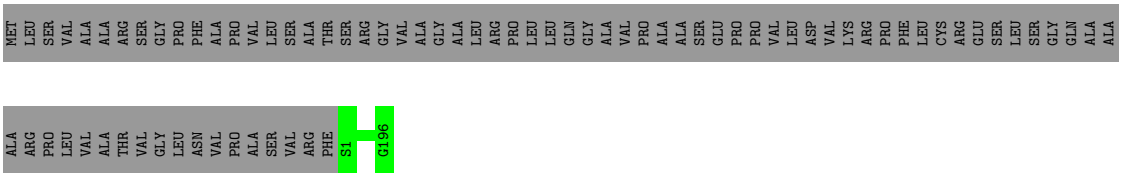
• Molecule 17: Cytochrome c1, heme protein, mitochondrial

Chain O:



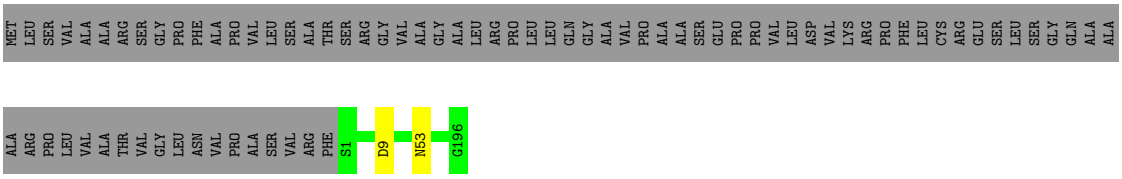
• Molecule 18: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



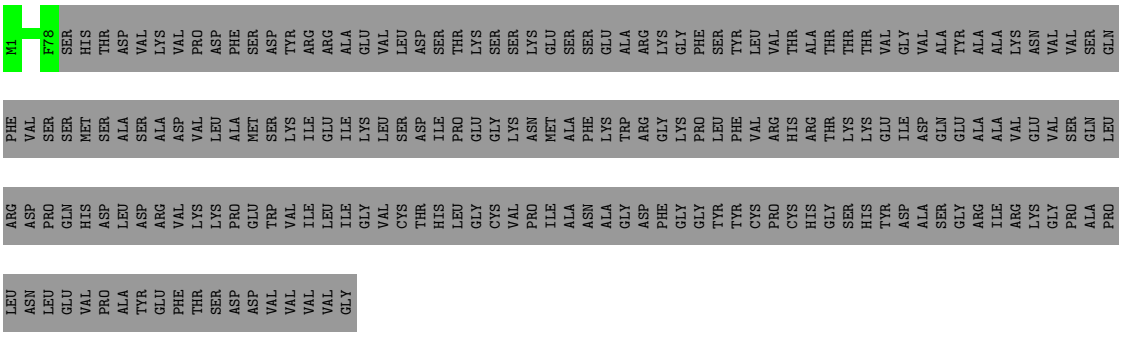
• Molecule 18: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



• Molecule 18: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain T:

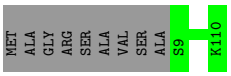


• Molecule 19: Cytochrome b-c1 complex subunit 7

Chain F:

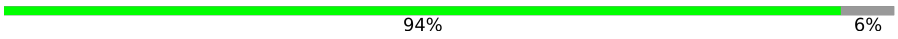
• Molecule 19: Cytochrome b-c1 complex subunit 7

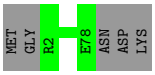
Chain Q:



• Molecule 20: Cytochrome b-c1 complex subunit 8

Chain G:





• Molecule 20: Cytochrome b-c1 complex subunit 8

Chain R:

• Molecule 21: Cytochrome b-c1 complex subunit 6, mitochondrial

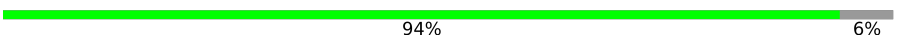
Chain H:

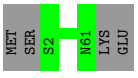
• Molecule 21: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain S:

• Molecule 22: Cytochrome b-c1 complex subunit 9

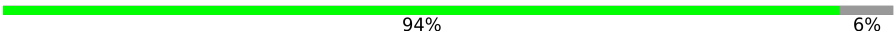
Chain J:

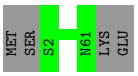




• Molecule 22: Cytochrome b-c1 complex subunit 9

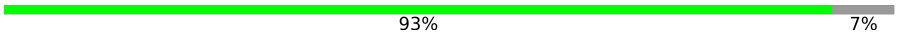
Chain U:

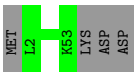




• Molecule 23: Cytochrome b-c1 complex subunit 10

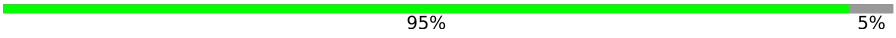
Chain K:

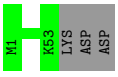




• Molecule 23: Cytochrome b-c1 complex subunit 10

Chain V:





• Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

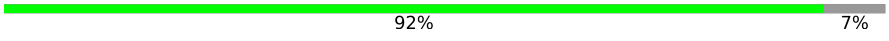
Chain 6:

• Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C1:

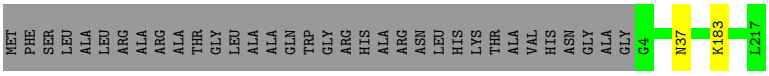
• Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D1:



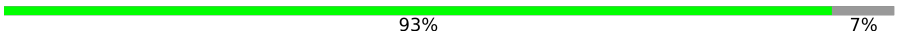
• Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

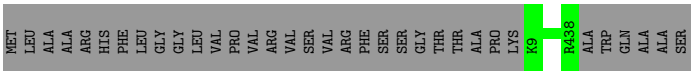
Chain 2:



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

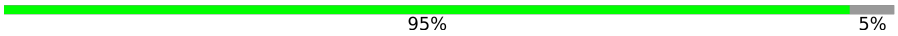
Chain 1:





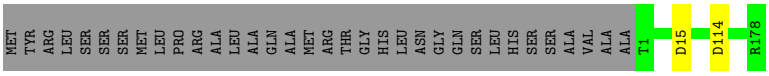
• Molecule 29: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:



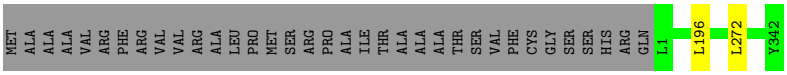
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:



• Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P1:

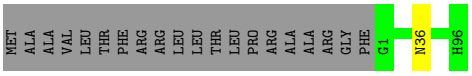


• Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q1:

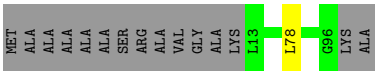
• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7:



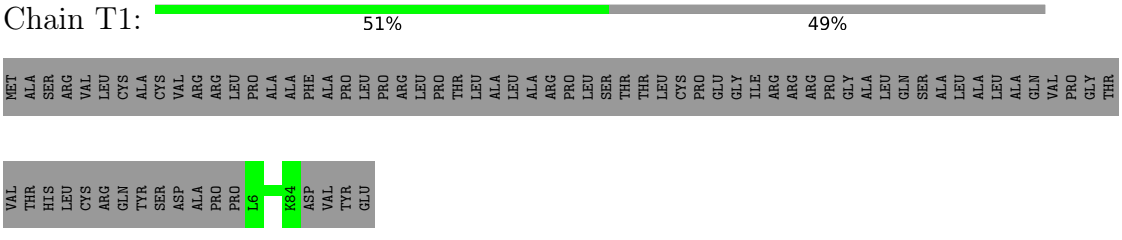
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S1:



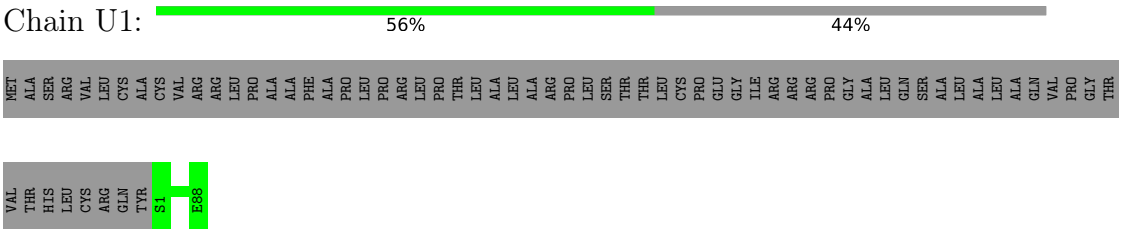
• Molecule 35: Acyl carrier protein, mitochondrial

Chain T1:



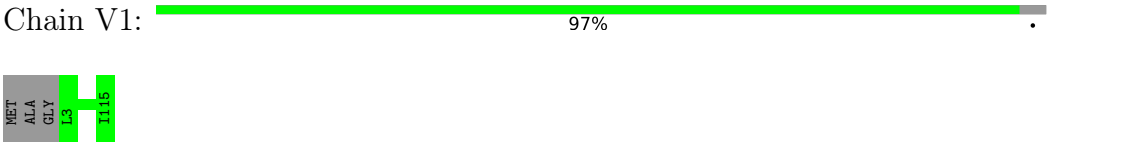
• Molecule 35: Acyl carrier protein, mitochondrial

Chain U1:



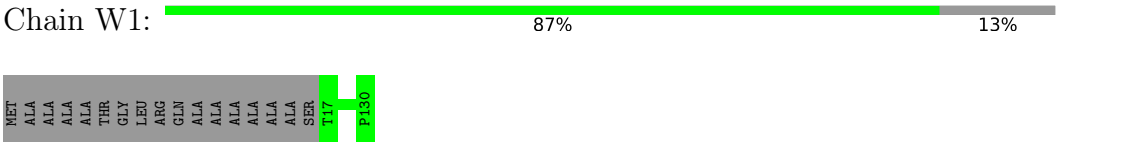
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1:



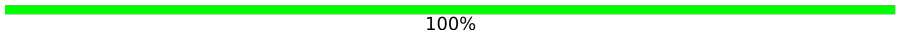
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1:



• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

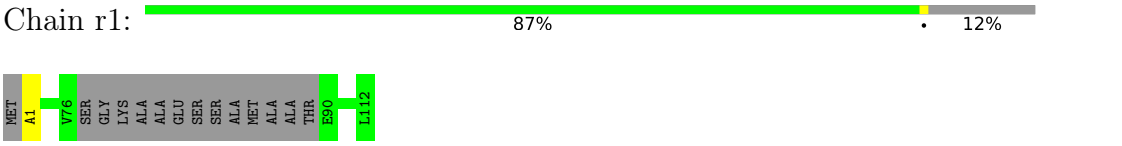
Chain q1:



There are no outlier residues recorded for this chain.

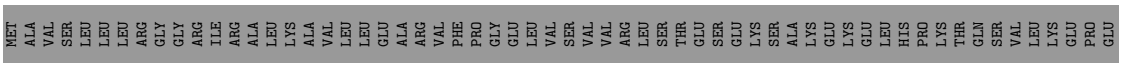
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1:



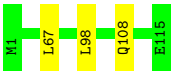
• Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s1:



• Molecule 41: NADH-ubiquinone oxidoreductase chain 3

Chain A1: 97%



• Molecule 42: NADH-ubiquinone oxidoreductase chain 1

Chain H1: 99%

• Molecule 43: NADH-ubiquinone oxidoreductase chain 6

Chain J1: 100%

There are no outlier residues recorded for this chain.

• Molecule 44: NADH-ubiquinone oxidoreductase chain 4L

Chain K1: 98%

• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain L1: 100%

• Molecule 46: NADH-ubiquinone oxidoreductase chain 4

Chain M1: 99%

• Molecule 47: NADH-ubiquinone oxidoreductase chain 2

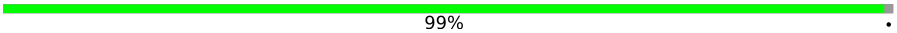
Chain N1: 100%

• Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1:

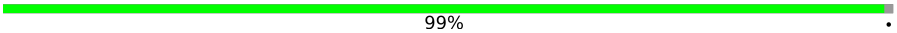
• Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1:



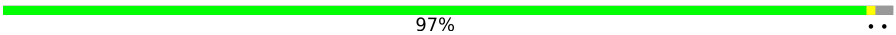
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

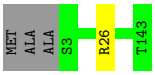
Chain Y1:



• Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

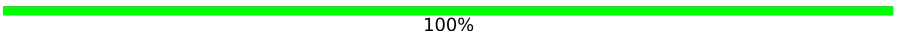
Chain Z1:





• Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

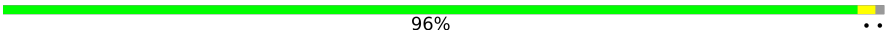
Chain a1:

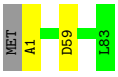


There are no outlier residues recorded for this chain.

• Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

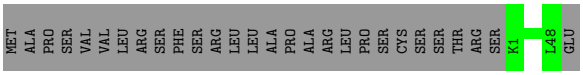
Chain b1:





• Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

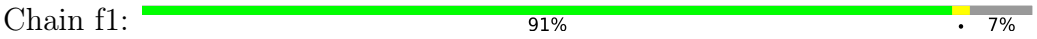
Chain c1:

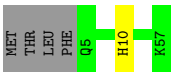


• Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C2

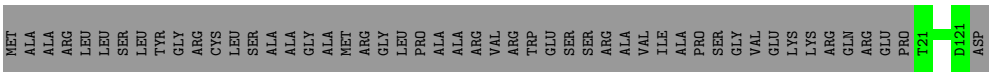
• Molecule 56: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

• Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

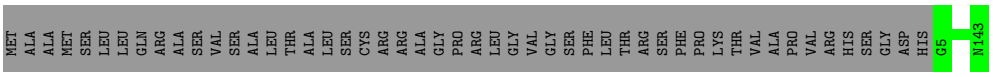




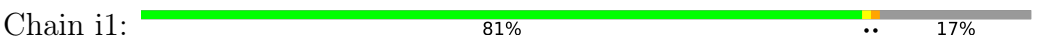
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



• Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

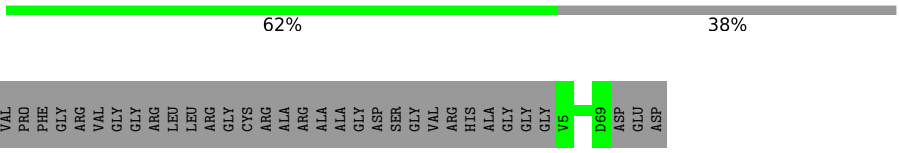


• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



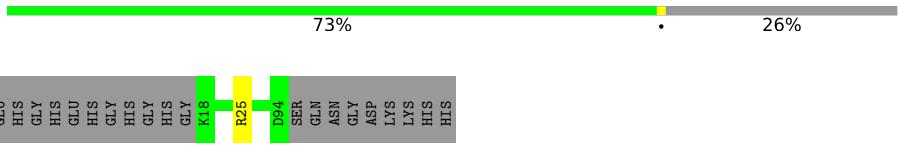
• Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j1:



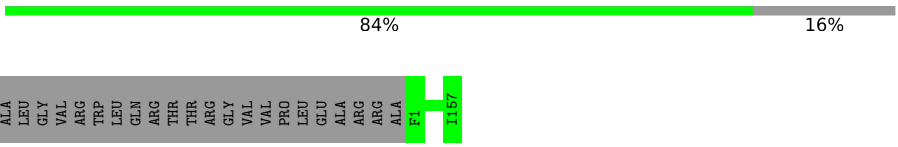
• Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k1:



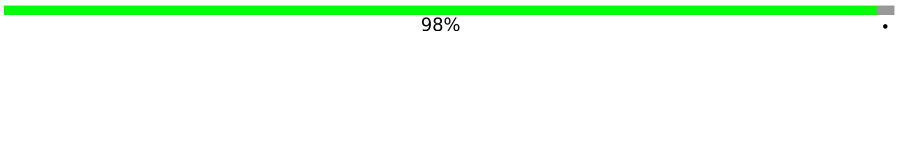
• Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l1:



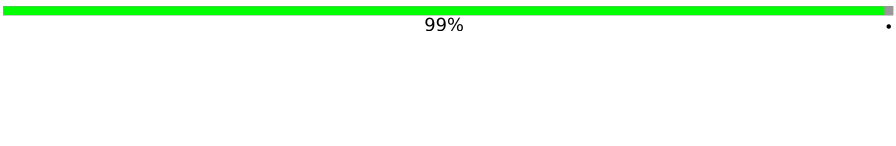
• Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m1:



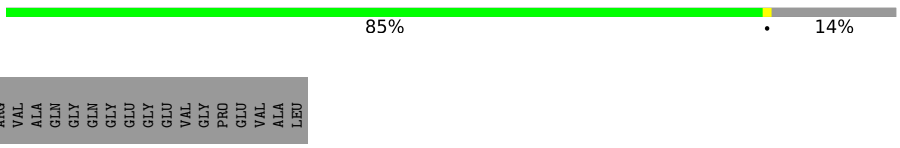
• Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n1:



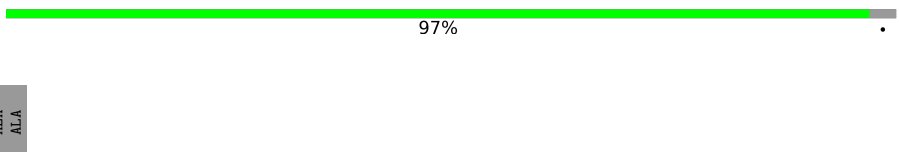
• Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o1:



• Molecule 67: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57506	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2MR, FMN, NA, HEC, SF4, 3PE, CU, CUA, ZMP, HEM, DGT, TGL, FES, FME, K, ZN, SAC, HEA, CDL, PC1, AYA, NDP

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	n	0.32	0/4162	0.65	6/5686 (0.1%)
2	o	0.31	0/1863	0.75	3/2542 (0.1%)
3	p	0.31	0/2202	0.68	1/3010 (0.0%)
4	q	0.31	0/1190	0.67	2/1609 (0.1%)
5	r	0.30	0/860	0.67	0/1167
6	s	0.29	0/738	0.67	1/1001 (0.1%)
7	t	0.27	0/632	0.62	0/866
8	u	0.33	0/674	0.67	1/910 (0.1%)
9	v	0.33	0/579	0.76	0/771
10	x	0.29	0/396	0.60	0/541
11	y	0.30	0/399	0.62	0/535
12	z	0.28	0/318	0.63	0/433
13	w	0.27	0/444	0.62	0/598
14	A	0.27	0/3529	0.56	2/4793 (0.0%)
14	L	0.28	0/3530	0.56	0/4793
15	B	0.27	0/3205	0.53	0/4332
15	M	0.27	0/3205	0.51	0/4332
16	C	0.29	0/3147	0.57	3/4297 (0.1%)
16	N	0.29	0/3147	0.56	4/4297 (0.1%)
17	D	0.28	0/1968	0.55	1/2674 (0.0%)
17	O	0.28	0/1968	0.55	0/2674
18	E	0.28	0/1173	0.52	0/1605
18	P	0.28	0/1173	0.51	1/1605 (0.1%)
18	T	0.29	0/565	0.64	0/772
19	F	0.26	0/916	0.61	1/1226 (0.1%)
19	Q	0.27	0/922	0.54	0/1234
20	G	0.34	0/673	0.67	0/909
20	R	0.33	0/673	0.60	0/909
21	H	0.32	0/552	0.69	0/739
21	S	0.30	0/570	0.67	0/763
22	J	0.28	0/509	0.56	0/687

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
22	U	0.27	0/509	0.50	0/687
23	K	0.27	0/446	0.63	0/609
23	V	0.25	0/454	0.59	0/619
24	6	0.35	0/1289	0.67	0/1744
25	C1	0.29	0/1780	0.56	1/2424 (0.0%)
26	D1	0.29	0/3540	0.54	1/4795 (0.0%)
27	2	0.29	0/1700	0.54	0/2316
28	1	0.29	0/3396	0.57	0/4586
29	3	0.28	0/5392	0.54	0/7305
30	9	0.30	0/1461	0.59	2/1974 (0.1%)
31	P1	0.28	0/2823	0.59	2/3828 (0.1%)
32	Q1	0.27	0/1045	0.55	0/1411
33	7	0.28	0/773	0.51	0/1041
34	S1	0.28	0/682	0.64	1/920 (0.1%)
35	T1	0.30	0/646	0.62	0/869
35	U1	0.30	0/718	0.53	0/970
36	V1	0.26	0/945	0.44	0/1281
37	W1	0.29	0/993	0.60	0/1335
38	q1	0.29	0/1251	0.58	0/1702
39	r1	0.28	0/806	0.57	0/1090
40	s1	0.26	0/360	0.54	0/489
41	A1	0.31	0/948	0.66	2/1295 (0.2%)
42	H1	0.34	0/2607	0.70	4/3564 (0.1%)
43	J1	0.33	0/1330	0.60	0/1810
44	K1	0.31	0/738	0.66	2/1002 (0.2%)
45	L1	0.31	0/4913	0.57	0/6686
46	M1	0.30	0/3709	0.62	2/5052 (0.0%)
47	N1	0.30	0/2755	0.60	1/3751 (0.0%)
48	O1	0.28	0/2674	0.51	0/3626
49	X1	0.29	0/1434	0.55	0/1937
50	Y1	0.30	0/1061	0.58	0/1439
51	Z1	0.28	0/1198	0.61	0/1616
52	a1	0.29	0/585	0.63	0/788
53	b1	0.29	0/666	0.58	1/914 (0.1%)
54	c1	0.31	0/409	0.55	0/555
55	d1	0.29	0/1028	0.61	1/1387 (0.1%)
56	e1	0.27	0/900	0.53	0/1199
57	f1	0.29	0/468	0.60	0/630
58	g1	0.28	0/878	0.52	0/1196
59	h1	0.30	0/1201	0.55	0/1626
60	i1	0.28	0/917	0.54	1/1243 (0.1%)
61	j1	0.27	0/587	0.51	0/804
62	k1	0.27	0/646	0.52	0/873

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
63	l1	0.28	0/1379	0.54	0/1882
64	m1	0.30	0/1079	0.59	0/1463
65	n1	0.28	0/1596	0.55	0/2162
66	o1	0.33	0/1039	0.65	1/1394 (0.1%)
67	p1	0.28	0/1471	0.53	0/1988
All	All	0.29	0/115107	0.58	48/156187 (0.0%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	n	195	LEU	CA-CB-CG	11.02	140.66	115.30
41	A1	98	LEU	CA-CB-CG	8.11	133.96	115.30
16	C	332	LEU	CA-CB-CG	8.05	133.81	115.30
6	s	46	ASP	CB-CG-OD1	7.98	125.48	118.30
44	K1	38	LEU	CA-CB-CG	7.77	133.18	115.30
31	P1	272	LEU	CA-CB-CG	7.62	132.82	115.30
2	o	78	LEU	CA-CB-CG	7.25	131.98	115.30
42	H1	233	LEU	CB-CG-CD1	-7.03	99.06	111.00
2	o	68	LEU	CA-CB-CG	6.96	131.32	115.30
66	o1	56	ASP	CB-CG-OD1	6.76	124.39	118.30
46	M1	174	LEU	CA-CB-CG	6.36	129.94	115.30
16	N	252	ASP	CB-CG-OD1	6.31	123.98	118.30
18	P	9	ASP	CB-CG-OD1	6.08	123.78	118.30
53	b1	59	ASP	CB-CG-OD1	6.02	123.72	118.30
16	N	58	ASP	CB-CG-OD1	5.95	123.65	118.30
47	N1	232	LEU	CA-CB-CG	5.92	128.91	115.30
14	A	20	ASP	CB-CG-OD1	5.90	123.61	118.30
1	n	209	LEU	CA-CB-CG	5.87	128.81	115.30
17	D	211	MET	CG-SD-CE	5.87	109.60	100.20
16	C	149	LEU	CA-CB-CG	5.86	128.79	115.30
60	i1	59	MET	CA-CB-CG	5.83	123.22	113.30
41	A1	67	LEU	CB-CG-CD2	-5.72	101.27	111.00
31	P1	196	LEU	CA-CB-CG	5.69	128.39	115.30
26	D1	83	LEU	CA-CB-CG	5.67	128.33	115.30
19	F	53	ASP	CB-CG-OD1	5.60	123.34	118.30
1	n	435	GLY	C-N-CA	-5.59	107.71	121.70
30	9	15	ASP	CB-CG-OD1	5.59	123.33	118.30
3	p	151	LEU	CA-CB-CG	5.59	128.15	115.30
55	d1	28	ASP	CB-CG-OD1	5.58	123.33	118.30
1	n	246	LEU	CA-CB-CG	5.57	128.10	115.30
4	q	58	GLN	CA-CB-CG	5.56	125.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	149	LEU	CA-CB-CG	5.55	128.07	115.30
14	A	327	ASP	CB-CG-OD1	5.51	123.26	118.30
8	u	8	ILE	CG1-CB-CG2	-5.42	99.47	111.40
42	H1	276	SER	C-N-CA	-5.40	108.21	121.70
1	n	283	LEU	CA-CB-CG	5.39	127.70	115.30
42	H1	251	LEU	CA-CB-CG	5.35	127.60	115.30
30	9	114	ASP	CB-CG-OD1	5.35	123.11	118.30
25	C1	77	ASP	CB-CG-OD1	5.34	123.10	118.30
34	S1	78	LEU	CA-CB-CG	5.22	127.31	115.30
16	N	303	LEU	CA-CB-CG	5.21	127.29	115.30
42	H1	85	LEU	CA-CB-CG	5.18	127.21	115.30
4	q	59	LEU	CA-CB-CG	5.13	127.11	115.30
16	C	58	ASP	CB-CG-OD1	5.12	122.91	118.30
2	o	73	LEU	CA-CB-CG	5.12	127.07	115.30
44	K1	38	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	n	195	LEU	CB-CG-CD2	5.06	119.60	111.00
46	M1	115	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	512/514 (100%)	490 (96%)	22 (4%)	0	100	100
2	o	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
3	p	258/261 (99%)	248 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	q	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
5	r	102/146 (70%)	98 (96%)	4 (4%)	0	100	100
6	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
7	t	73/97 (75%)	68 (93%)	5 (7%)	0	100	100
8	u	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
9	v	69/76 (91%)	65 (94%)	4 (6%)	0	100	100
10	x	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
11	y	45/63 (71%)	43 (96%)	2 (4%)	0	100	100
12	z	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
13	w	55/83 (66%)	54 (98%)	1 (2%)	0	100	100
14	A	443/480 (92%)	431 (97%)	12 (3%)	0	100	100
14	L	443/480 (92%)	431 (97%)	12 (3%)	0	100	100
15	B	418/453 (92%)	408 (98%)	10 (2%)	0	100	100
15	M	418/453 (92%)	399 (96%)	19 (4%)	0	100	100
16	C	378/381 (99%)	369 (98%)	9 (2%)	0	100	100
16	N	378/381 (99%)	369 (98%)	9 (2%)	0	100	100
17	D	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
17	O	238/325 (73%)	226 (95%)	12 (5%)	0	100	100
18	E	194/274 (71%)	184 (95%)	10 (5%)	0	100	100
18	P	194/274 (71%)	185 (95%)	9 (5%)	0	100	100
18	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
19	F	99/111 (89%)	97 (98%)	2 (2%)	0	100	100
19	Q	100/111 (90%)	100 (100%)	0	0	100	100
20	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
20	R	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
21	H	64/89 (72%)	64 (100%)	0	0	100	100
21	S	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
22	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
22	U	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
23	K	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
23	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	6	155/224 (69%)	149 (96%)	6 (4%)	0	100	100
25	C1	206/263 (78%)	197 (96%)	9 (4%)	0	100	100
26	D1	427/463 (92%)	413 (97%)	14 (3%)	0	100	100
27	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	29	68
28	1	428/464 (92%)	412 (96%)	16 (4%)	0	100	100
29	3	688/727 (95%)	659 (96%)	29 (4%)	0	100	100
30	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
31	P1	340/377 (90%)	327 (96%)	13 (4%)	0	100	100
32	Q1	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
33	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
34	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
35	T1	77/156 (49%)	77 (100%)	0	0	100	100
35	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
36	V1	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
37	W1	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
38	q1	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
39	r1	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
40	s1	40/104 (38%)	40 (100%)	0	0	100	100
41	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
42	H1	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
43	J1	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
44	K1	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
45	L1	604/607 (100%)	566 (94%)	38 (6%)	0	100	100
46	M1	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
47	N1	343/345 (99%)	330 (96%)	13 (4%)	0	100	100
48	O1	318/355 (90%)	298 (94%)	20 (6%)	0	100	100
49	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
50	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
51	Z1	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
52	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
53	b1	81/84 (96%)	76 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	c1	46/76 (60%)	46 (100%)	0	0	100	100
55	d1	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
56	e1	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
57	f1	51/57 (90%)	51 (100%)	0	0	100	100
58	g1	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
59	h1	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
60	i1	102/128 (80%)	98 (96%)	3 (3%)	1 (1%)	15	54
61	j1	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
62	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
63	l1	155/186 (83%)	153 (99%)	2 (1%)	0	100	100
64	m1	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
65	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
66	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
67	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	13988/16116 (87%)	13466 (96%)	520 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	2	183	LYS
60	i1	59	MET

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	n	425/425 (100%)	425 (100%)	0	100	100
2	o	210/210 (100%)	210 (100%)	0	100	100
3	p	226/227 (100%)	226 (100%)	0	100	100
4	q	122/146 (84%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	r	91/118 (77%)	91 (100%)	0	100 100
6	s	80/101 (79%)	80 (100%)	0	100 100
7	t	62/78 (80%)	62 (100%)	0	100 100
8	u	70/76 (92%)	69 (99%)	1 (1%)	67 85
9	v	54/57 (95%)	54 (100%)	0	100 100
10	x	39/67 (58%)	39 (100%)	0	100 100
11	y	40/55 (73%)	40 (100%)	0	100 100
12	z	33/55 (60%)	33 (100%)	0	100 100
13	w	43/67 (64%)	42 (98%)	1 (2%)	50 77
14	A	372/398 (94%)	371 (100%)	1 (0%)	92 97
14	L	372/398 (94%)	372 (100%)	0	100 100
15	B	330/356 (93%)	330 (100%)	0	100 100
15	M	330/356 (93%)	330 (100%)	0	100 100
16	C	332/333 (100%)	330 (99%)	2 (1%)	86 94
16	N	332/333 (100%)	331 (100%)	1 (0%)	92 97
17	D	205/260 (79%)	204 (100%)	1 (0%)	88 94
17	O	205/260 (79%)	205 (100%)	0	100 100
18	E	68/224 (30%)	68 (100%)	0	100 100
18	P	68/224 (30%)	67 (98%)	1 (2%)	65 84
18	T	58/224 (26%)	58 (100%)	0	100 100
19	F	93/99 (94%)	93 (100%)	0	100 100
19	Q	94/99 (95%)	94 (100%)	0	100 100
20	G	70/74 (95%)	70 (100%)	0	100 100
20	R	70/74 (95%)	68 (97%)	2 (3%)	42 71
21	H	63/83 (76%)	63 (100%)	0	100 100
21	S	65/83 (78%)	65 (100%)	0	100 100
22	J	51/55 (93%)	51 (100%)	0	100 100
22	U	51/55 (93%)	51 (100%)	0	100 100
23	K	42/46 (91%)	42 (100%)	0	100 100
23	V	43/46 (94%)	43 (100%)	0	100 100
24	6	133/185 (72%)	132 (99%)	1 (1%)	81 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	C1	190/227 (84%)	190 (100%)	0	100	100
26	D1	370/394 (94%)	370 (100%)	0	100	100
27	2	184/206 (89%)	183 (100%)	1 (0%)	88	94
28	1	345/370 (93%)	345 (100%)	0	100	100
29	3	580/610 (95%)	579 (100%)	1 (0%)	93	98
30	9	152/178 (85%)	152 (100%)	0	100	100
31	P1	299/325 (92%)	299 (100%)	0	100	100
32	Q1	113/153 (74%)	113 (100%)	0	100	100
33	7	81/96 (84%)	80 (99%)	1 (1%)	71	87
34	S1	74/80 (92%)	74 (100%)	0	100	100
35	T1	73/135 (54%)	73 (100%)	0	100	100
35	U1	81/135 (60%)	81 (100%)	0	100	100
36	V1	101/102 (99%)	101 (100%)	0	100	100
37	W1	108/114 (95%)	108 (100%)	0	100	100
38	q1	131/131 (100%)	131 (100%)	0	100	100
39	r1	88/96 (92%)	88 (100%)	0	100	100
40	s1	41/95 (43%)	40 (98%)	1 (2%)	49	76
41	A1	103/103 (100%)	102 (99%)	1 (1%)	76	88
42	H1	279/279 (100%)	279 (100%)	0	100	100
43	J1	137/137 (100%)	137 (100%)	0	100	100
44	K1	87/87 (100%)	87 (100%)	0	100	100
45	L1	548/549 (100%)	548 (100%)	0	100	100
46	M1	414/414 (100%)	413 (100%)	1 (0%)	93	98
47	N1	307/307 (100%)	307 (100%)	0	100	100
48	O1	284/309 (92%)	283 (100%)	1 (0%)	91	96
49	X1	153/154 (99%)	153 (100%)	0	100	100
50	Y1	105/106 (99%)	105 (100%)	0	100	100
51	Z1	122/123 (99%)	121 (99%)	1 (1%)	81	91
52	a1	60/60 (100%)	60 (100%)	0	100	100
53	b1	72/73 (99%)	72 (100%)	0	100	100
54	c1	42/67 (63%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	d1	107/107 (100%)	107 (100%)	0	100 100
56	e1	93/94 (99%)	93 (100%)	0	100 100
57	f1	49/53 (92%)	48 (98%)	1 (2%)	55 79
58	g1	92/129 (71%)	92 (100%)	0	100 100
59	h1	123/162 (76%)	123 (100%)	0	100 100
60	i1	99/119 (83%)	99 (100%)	0	100 100
61	j1	61/87 (70%)	61 (100%)	0	100 100
62	k1	60/78 (77%)	59 (98%)	1 (2%)	60 82
63	l1	142/161 (88%)	142 (100%)	0	100 100
64	m1	112/114 (98%)	112 (100%)	0	100 100
65	n1	163/164 (99%)	163 (100%)	0	100 100
66	o1	109/121 (90%)	109 (100%)	0	100 100
67	p1	155/158 (98%)	155 (100%)	0	100 100
All	All	12031/13709 (88%)	12010 (100%)	21 (0%)	93 98

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	u	57	ARG
13	w	13	GLN
14	A	53	ASN
16	C	80	ARG
16	C	183	PHE
17	D	144	ARG
16	N	1	MET
18	P	53	ASN
20	R	6	ASN
20	R	72	LYS
24	6	33	ARG
27	2	37	ASN
29	3	444	LYS
33	7	36	ASN
40	s1	49	ASN
41	A1	108	GLN
46	M1	421	ASN
48	O1	271	ASN
51	Z1	26	ARG

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Mol	Chain	Res	Type
57	f1	10	HIS
62	k1	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	n	80	ASN
1	n	451	ASN
6	s	67	ASN
7	t	38	HIS
11	y	10	ASN
14	A	339	GLN
15	B	153	GLN
31	P1	136	ASN
41	A1	108	GLN
46	M1	421	ASN
59	h1	44	ASN
59	h1	108	GLN
63	l1	131	GLN
67	p1	106	GLN
67	p1	123	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\| > 2$
26	2MR	D1	85	26	10,12,13	2.60	2 (20%)	5,13,15	2.77	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	AYA	b1	1	53	6,7,8	1.22	1 (16%)	5,8,10	1.30	1 (20%)
46	FME	M1	1	46	8,9,10	0.95	0	7,9,11	0.77	0
60	SAC	i1	1	60	7,8,9	1.02	0	8,9,11	0.85	1 (12%)
45	FME	L1	1	45	8,9,10	0.92	0	7,9,11	0.96	0
47	FME	N1	1	47	8,9,10	0.93	0	7,9,11	0.90	0
42	FME	H1	1	42	8,9,10	0.95	0	7,9,11	0.89	0
41	FME	A1	1	41	8,9,10	0.94	0	7,9,11	0.82	0
39	AYA	r1	1	39	6,7,8	1.27	1 (16%)	5,8,10	1.40	1 (20%)
44	FME	K1	1	44	8,9,10	0.88	0	7,9,11	2.22	2 (28%)
43	FME	J1	1	43	8,9,10	0.91	0	7,9,11	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	2MR	D1	85	26	-	2/10/13/15	-
53	AYA	b1	1	53	-	0/4/6/8	-
46	FME	M1	1	46	-	1/7/9/11	-
60	SAC	i1	1	60	-	2/7/8/10	-
45	FME	L1	1	45	-	4/7/9/11	-
47	FME	N1	1	47	-	4/7/9/11	-
42	FME	H1	1	42	-	2/7/9/11	-
41	FME	A1	1	41	-	1/7/9/11	-
39	AYA	r1	1	39	-	0/4/6/8	-
44	FME	K1	1	44	-	4/7/9/11	-
43	FME	J1	1	43	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D1	85	2MR	CZ-NE	5.93	1.47	1.34
26	D1	85	2MR	CZ-NH2	5.15	1.44	1.33
39	r1	1	AYA	CA-N	-2.43	1.44	1.46
53	b1	1	AYA	CA-N	-2.23	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	K1	1	FME	C-CA-N	4.96	118.69	109.73
26	D1	85	2MR	CD-NE-CZ	4.81	132.41	123.41
26	D1	85	2MR	NE-CZ-NH2	-3.53	116.24	119.48
39	r1	1	AYA	CB-CA-N	2.96	112.90	109.61
53	b1	1	AYA	CB-CA-N	2.70	112.61	109.61
44	K1	1	FME	O-C-CA	-2.31	118.72	124.78
60	i1	1	SAC	OG-CB-CA	-2.08	105.67	110.97

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	H1	1	FME	N-CA-CB-CG
43	J1	1	FME	C-CA-CB-CG
43	J1	1	FME	O-C-CA-CB
44	K1	1	FME	O1-CN-N-CA
44	K1	1	FME	N-CA-CB-CG
44	K1	1	FME	CA-CB-CG-SD
45	L1	1	FME	N-CA-CB-CG
47	N1	1	FME	C-CA-CB-CG
60	i1	1	SAC	C-CA-CB-OG
26	D1	85	2MR	NE-CD-CG-CB
44	K1	1	FME	CB-CG-SD-CE
60	i1	1	SAC	N-CA-CB-OG
43	J1	1	FME	N-CA-CB-CG
47	N1	1	FME	N-CA-CB-CG
47	N1	1	FME	CB-CG-SD-CE
45	L1	1	FME	CB-CG-SD-CE
43	J1	1	FME	CA-CB-CG-SD
41	A1	1	FME	N-CA-CB-CG
26	D1	85	2MR	CA-CB-CG-CD
42	H1	1	FME	C-CA-CB-CG
45	L1	1	FME	C-CA-CB-CG
46	M1	1	FME	N-CA-CB-CG
45	L1	1	FME	CB-CA-N-CN
47	N1	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 90 ligands modelled in this entry, 7 are monoatomic - leaving 83 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	$\#\|Z\| > 2$
71	3PE	M1	501	-	50,50,50	0.30	0	53,55,55	0.30	0
71	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.28	0
80	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.56	0
71	3PE	Y1	203	-	27,27,50	0.40	0	30,32,55	0.34	0
80	PC1	V	101	-	27,27,53	0.40	0	33,35,61	0.34	0
71	3PE	N	401	-	33,33,50	0.36	0	36,38,55	0.34	0
76	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.43	0
71	3PE	K1	201	-	40,40,50	0.34	0	43,45,55	0.29	0
77	HEM	C	402	16	41,50,50	1.47	4 (9%)	45,82,82	1.60	9 (20%)
75	TGL	y	601	-	36,36,62	0.23	0	39,39,65	0.18	0
71	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.55	1 (2%)
70	HEA	n	603	1	57,67,67	1.45	8 (14%)	61,103,103	2.36	22 (36%)
76	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
76	CDL	N	405	-	45,45,99	0.44	0	51,57,111	0.51	0
70	HEA	n	604	1	57,67,67	1.48	8 (14%)	61,103,103	2.52	22 (36%)
85	ZMP	W1	201	-	27,33,36	0.66	1 (3%)	32,40,45	1.03	2 (6%)
76	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
71	3PE	M1	503	-	35,35,50	0.36	0	38,40,55	0.30	0
76	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
76	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.40	1 (1%)
71	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.38	0
71	3PE	N	404	-	36,36,50	0.35	0	39,41,55	0.31	0
81	SF4	1	502	28	0,12,12	-	-	-		
71	3PE	v	101	-	27,27,50	0.39	0	30,32,55	0.34	0
71	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.34	0
71	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	NDP	P1	501	-	45,52,52	0.52	0	53,80,80	0.59	1 (1%)
79	FES	E	201	18	0,4,4	-	-	-		
86	DGT	O1	401	72	26,33,33	0.79	1 (3%)	32,52,52	0.47	0
81	SF4	9	201	30	0,12,12	-	-	-		
76	CDL	G	101	-	55,55,99	0.39	0	61,67,111	0.32	0
71	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.35	0
81	SF4	3	802	29	0,12,12	-	-	-		
71	3PE	D1	501	-	50,50,50	0.31	0	53,55,55	0.29	0
71	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.31	0
71	3PE	p	301	-	44,44,50	0.33	0	47,49,55	0.30	0
80	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.33	0
71	3PE	Y1	204	-	41,41,50	0.33	0	44,46,55	0.32	0
81	SF4	9	202	30	0,12,12	-	-	-		
76	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.42	1 (1%)
73	CUA	o	303	2	0,1,1	-	-	-		
80	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.49	0
71	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.27	0
80	PC1	9	203	-	53,53,53	0.29	0	59,61,61	0.44	0
71	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.34	0
71	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
76	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.36	0
80	PC1	L	502	-	23,23,53	0.44	0	29,31,61	0.61	0
71	3PE	L	501	-	22,22,50	0.44	0	25,27,55	0.36	0
79	FES	P	201	18	0,4,4	-	-	-		
77	HEM	N	403	16	41,50,50	1.45	4 (9%)	45,82,82	1.56	8 (17%)
82	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.46	1 (2%)
76	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
81	SF4	3	801	29	0,12,12	-	-	-		
76	CDL	Y1	202	-	93,93,99	0.31	0	99,105,111	0.27	0
80	PC1	Y1	201	-	53,53,53	0.30	0	59,61,61	0.32	0
85	ZMP	n1	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.96	1 (3%)
71	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.65	0
77	HEM	N	402	16	41,50,50	1.43	3 (7%)	45,82,82	1.59	10 (22%)
80	PC1	K	101	-	27,27,53	0.40	0	33,35,61	0.37	0
76	CDL	R	101	-	40,40,99	0.46	0	46,52,111	0.54	0
79	FES	2	301	27	0,4,4	-	-	-		
71	3PE	C	405	-	30,30,50	0.38	0	33,35,55	0.35	0
76	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
71	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.32	0
76	CDL	a1	101	-	56,56,99	0.40	0	62,68,111	0.46	0
71	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
78	HEC	O	303	17	32,50,50	2.19	3 (9%)	24,82,82	1.60	4 (16%)
71	3PE	G	102	-	50,50,50	0.30	0	53,55,55	0.28	0
71	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.44	0
78	HEC	D	301	17	32,50,50	2.19	4 (12%)	24,82,82	1.57	3 (12%)
71	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.35	0
76	CDL	L1	702	-	77,77,99	0.34	0	83,89,111	0.29	0
80	PC1	9	204	-	46,46,53	0.31	0	52,54,61	0.28	0
77	HEM	C	401	16	41,50,50	1.42	3 (7%)	45,82,82	1.52	9 (20%)
71	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.32	0
76	CDL	L1	703	-	45,45,99	0.42	0	51,57,111	0.35	0
79	FES	3	803	29	0,4,4	-	-	-		
71	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
71	3PE	A1	201	-	42,42,50	0.32	0	45,47,55	0.33	0
71	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.35	0
81	SF4	6	201	24	0,12,12	-	-	-		
71	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	3PE	M1	501	-	-	12/54/54/54	-
71	3PE	r1	201	-	-	6/49/49/54	-
80	PC1	P1	502	-	-	16/34/34/57	-
71	3PE	Y1	203	-	-	7/31/31/54	-
80	PC1	V	101	-	-	4/31/31/57	-
71	3PE	N	401	-	-	5/37/37/54	-
76	CDL	h1	201	-	-	21/80/80/110	-
71	3PE	K1	201	-	-	10/44/44/54	-
77	HEM	C	402	16	-	2/12/54/54	-
75	TGL	y	601	-	-	2/39/39/65	-
71	3PE	n	605	-	-	9/37/37/54	-
70	HEA	n	603	1	-	10/32/76/76	-
76	CDL	A	502	-	-	21/56/56/110	-
76	CDL	N	405	-	-	10/56/56/110	-
70	HEA	n	604	1	-	7/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	ZMP	W1	201	-	-	6/38/40/43	-
76	CDL	O	301	-	-	14/67/67/110	-
71	3PE	M1	503	-	-	9/39/39/54	-
76	CDL	R	102	-	-	20/67/67/110	-
76	CDL	N1	401	-	-	18/100/100/110	-
71	3PE	o	302	-	-	9/32/32/54	-
71	3PE	N	404	-	-	5/40/40/54	-
81	SF4	1	502	28	-	-	0/6/5/5
71	3PE	v	101	-	-	10/31/31/54	-
71	3PE	n	607	-	-	5/30/30/54	-
71	3PE	d1	202	-	-	8/34/34/54	-
79	FES	E	201	18	-	-	0/1/1/1
86	DGT	O1	401	72	-	7/18/34/34	0/3/3/3
81	SF4	9	201	30	-	-	0/6/5/5
76	CDL	G	101	-	-	14/66/66/110	-
71	3PE	O	302	-	-	6/36/36/54	-
81	SF4	3	802	29	-	-	0/6/5/5
71	3PE	D1	501	-	-	9/54/54/54	-
71	3PE	i1	201	-	-	6/45/45/54	-
71	3PE	p	301	-	-	8/48/48/54	-
80	PC1	J	101	-	-	7/38/38/57	-
71	3PE	Y1	204	-	-	8/45/45/54	-
81	SF4	9	202	30	-	-	0/6/5/5
76	CDL	R	103	-	-	17/82/82/110	-
80	PC1	6	203	-	-	11/46/46/57	-
71	3PE	M1	502	-	-	12/54/54/54	-
80	PC1	9	203	-	-	10/57/57/57	-
71	3PE	N1	402	-	-	7/41/41/54	-
71	3PE	C	403	-	-	11/38/38/54	-
76	CDL	C	404	-	-	13/52/52/110	-
80	PC1	L	502	-	-	7/27/27/57	-
71	3PE	L	501	-	-	7/26/26/54	-
79	FES	P	201	18	-	-	0/1/1/1
77	HEM	N	403	16	-	4/12/54/54	-
82	FMN	1	501	-	-	5/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	CDL	H1	402	-	-	12/59/59/110	-
81	SF4	3	801	29	-	-	0/6/5/5
76	CDL	Y1	202	-	-	16/104/104/110	-
80	PC1	Y1	201	-	-	14/57/57/57	-
85	ZMP	n1	201	-	-	17/36/38/43	-
71	3PE	A	501	-	-	9/26/26/54	-
77	HEM	N	402	16	-	1/12/54/54	-
80	PC1	K	101	-	-	9/31/31/57	-
76	CDL	R	101	-	-	11/51/51/110	-
79	FES	2	301	27	-	-	0/1/1/1
71	3PE	C	405	-	-	6/34/34/54	-
76	CDL	d1	201	-	-	14/77/77/110	-
71	3PE	R	104	-	-	9/33/33/54	-
76	CDL	a1	101	-	-	13/67/67/110	-
71	3PE	t	101	-	-	6/28/28/54	-
78	HEC	O	303	17	-	0/10/54/54	-
71	3PE	G	102	-	-	10/54/54/54	-
71	3PE	n	606	-	-	13/31/31/54	-
78	HEC	D	301	17	-	2/10/54/54	-
71	3PE	d1	203	-	-	6/35/35/54	-
76	CDL	L1	702	-	-	20/88/88/110	-
80	PC1	9	204	-	-	11/50/50/57	-
77	HEM	C	401	16	-	3/12/54/54	-
71	3PE	6	202	-	-	6/35/35/54	-
76	CDL	L1	703	-	-	8/56/56/110	-
79	FES	3	803	29	-	-	0/1/1/1
71	3PE	L1	701	-	-	7/54/54/54	-
71	3PE	H1	401	-	-	10/54/54/54	-
71	3PE	A1	201	-	-	9/46/46/54	-
71	3PE	E	202	-	-	6/35/35/54	-
81	SF4	6	201	24	-	-	0/6/5/5
84	NDP	P1	501	-	-	8/30/77/77	0/5/5/5

All (40) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	O	303	HEC	C2B-C3B	-6.40	1.34	1.40
78	O	303	HEC	C3C-C2C	-6.30	1.34	1.40
78	D	301	HEC	C3C-C2C	-6.27	1.34	1.40
78	D	301	HEC	C2B-C3B	-6.14	1.34	1.40
78	D	301	HEC	C3D-C2D	5.44	1.53	1.37
78	O	303	HEC	C3D-C2D	5.41	1.53	1.37
70	n	604	HEA	C3D-C2D	4.64	1.46	1.36
70	n	603	HEA	C3B-C2B	4.45	1.44	1.34
70	n	604	HEA	C3B-C2B	4.17	1.44	1.34
70	n	603	HEA	C3D-C2D	3.98	1.45	1.36
77	N	403	HEM	C3C-CAC	3.96	1.55	1.47
77	C	401	HEM	C3C-CAC	3.94	1.55	1.47
77	C	402	HEM	C3C-CAC	3.92	1.55	1.47
77	N	402	HEM	C3C-C2C	-3.89	1.35	1.40
77	N	402	HEM	C3C-CAC	3.75	1.55	1.47
77	C	401	HEM	C3C-C2C	-3.62	1.35	1.40
70	n	604	HEA	C3A-C2A	3.56	1.45	1.40
77	C	402	HEM	C3C-C2C	-3.52	1.35	1.40
70	n	603	HEA	C3C-C2C	3.51	1.45	1.40
77	N	403	HEM	C3C-C2C	-3.51	1.35	1.40
70	n	603	HEA	C3A-C2A	3.47	1.45	1.40
70	n	604	HEA	C3C-C2C	3.44	1.45	1.40
70	n	603	HEA	C4B-C3B	3.18	1.50	1.44
77	C	401	HEM	CAB-C3B	3.13	1.56	1.47
77	N	402	HEM	CAB-C3B	3.07	1.55	1.47
77	N	403	HEM	CAB-C3B	3.01	1.55	1.47
77	C	402	HEM	CAB-C3B	2.98	1.55	1.47
70	n	604	HEA	C4B-C3B	2.78	1.49	1.44
77	C	402	HEM	FE-NB	2.71	2.10	1.96
70	n	604	HEA	C2A-C1A	2.68	1.48	1.42
70	n	603	HEA	C2A-C1A	2.55	1.48	1.42
70	n	604	HEA	C1D-C2D	2.55	1.49	1.44
70	n	603	HEA	C1D-ND	-2.47	1.36	1.40
78	D	301	HEC	C4D-ND	2.45	1.41	1.36
85	n1	201	ZMP	C9-C10	2.40	1.53	1.50
85	W1	201	ZMP	C9-C10	2.23	1.53	1.50
70	n	604	HEA	C1D-ND	-2.17	1.36	1.40
77	N	403	HEM	FE-NB	2.13	2.07	1.96
86	O1	401	DGT	C5-C6	-2.13	1.43	1.47
70	n	603	HEA	C4D-C3D	2.02	1.48	1.45

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	n	604	HEA	CMC-C2C-C3C	7.86	139.38	124.68
70	n	603	HEA	CMC-C2C-C3C	7.15	138.06	124.68
70	n	604	HEA	CMC-C2C-C1C	-7.13	117.50	128.46
70	n	603	HEA	CMC-C2C-C1C	-6.56	118.39	128.46
70	n	604	HEA	C3D-C4D-ND	5.38	115.57	110.36
70	n	604	HEA	C13-C12-C11	-4.74	107.23	114.35
70	n	603	HEA	C3D-C4D-ND	4.63	114.84	110.36
70	n	603	HEA	CMD-C2D-C1D	-4.53	118.14	125.04
70	n	604	HEA	CMD-C2D-C1D	-4.41	118.32	125.04
70	n	604	HEA	CHA-C4D-C3D	-4.41	118.36	124.84
70	n	603	HEA	CMB-C2B-C1B	-4.27	118.53	125.04
70	n	604	HEA	CMB-C2B-C1B	-4.26	118.55	125.04
70	n	604	HEA	C4D-C3D-C2D	-3.85	101.28	106.90
70	n	603	HEA	C4D-C3D-C2D	-3.83	101.31	106.90
77	N	402	HEM	C3B-C2B-C1B	3.80	109.31	106.49
70	n	603	HEA	CHA-C4D-C3D	-3.70	119.41	124.84
70	n	603	HEA	C13-C12-C11	-3.67	108.83	114.35
78	O	303	HEC	CMC-C2C-C1C	-3.64	122.87	128.46
70	n	604	HEA	CMD-C2D-C3D	3.47	135.55	126.12
77	C	401	HEM	C3B-C2B-C1B	3.35	108.97	106.49
70	n	604	HEA	CAD-C3D-C2D	3.33	134.08	127.88
77	C	402	HEM	C4D-ND-C1D	3.31	108.49	105.07
70	n	603	HEA	CMD-C2D-C3D	3.30	135.09	126.12
78	D	301	HEC	CMC-C2C-C1C	-3.26	123.45	128.46
77	C	401	HEM	CMC-C2C-C3C	3.26	130.78	124.68
77	N	403	HEM	C3B-C2B-C1B	3.13	108.81	106.49
70	n	604	HEA	C26-C15-C16	3.11	120.51	115.27
70	n	603	HEA	CMB-C2B-C3B	3.11	136.26	130.34
70	n	603	HEA	C13-C14-C15	-3.10	120.20	127.66
77	N	402	HEM	CMC-C2C-C3C	3.07	130.43	124.68
77	C	402	HEM	C3B-C2B-C1B	3.04	108.74	106.49
77	N	403	HEM	C4D-ND-C1D	3.02	108.19	105.07
78	D	301	HEC	CBD-CAD-C3D	-3.02	107.47	112.62
70	n	603	HEA	CAA-CBA-CGA	-3.00	105.34	113.76
70	n	603	HEA	CHB-C1B-C2B	-3.00	120.30	124.98
77	N	403	HEM	C1B-NB-C4B	2.98	108.15	105.07
77	C	402	HEM	CMC-C2C-C3C	2.93	130.16	124.68
77	N	403	HEM	CMC-C2C-C3C	2.91	130.13	124.68
77	N	403	HEM	C4B-CHC-C1C	2.89	126.37	122.56
77	C	401	HEM	C4D-ND-C1D	2.85	108.02	105.07
77	N	402	HEM	C4C-CHD-C1D	2.83	126.29	122.56
77	N	402	HEM	CMB-C2B-C1B	-2.78	120.81	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	n	604	HEA	C13-C14-C15	-2.78	120.97	127.66
70	n	604	HEA	CAA-CBA-CGA	-2.76	106.02	113.76
70	n	604	HEA	C27-C19-C20	2.75	119.90	115.27
77	N	402	HEM	C4D-ND-C1D	2.75	107.91	105.07
77	C	401	HEM	C4C-CHD-C1D	2.73	126.17	122.56
77	C	402	HEM	CBA-CAA-C2A	-2.73	107.97	112.62
85	W1	201	ZMP	O1-C10-C9	-2.69	120.81	123.99
70	n	604	HEA	C3B-C4B-NB	2.68	113.02	109.84
77	N	403	HEM	CHC-C4B-C3B	2.67	128.65	124.57
70	n	604	HEA	C4B-C3B-C2B	-2.65	102.88	107.41
70	n	604	HEA	C25-C23-C24	2.63	120.42	114.60
70	n	604	HEA	CMB-C2B-C3B	2.63	135.35	130.34
77	N	403	HEM	CBA-CAA-C2A	-2.62	108.15	112.62
70	n	604	HEA	CHB-C1B-C2B	-2.61	120.90	124.98
77	C	402	HEM	CHC-C4B-C3B	2.61	128.56	124.57
77	C	402	HEM	C1B-NB-C4B	2.61	107.77	105.07
70	n	603	HEA	CAD-C3D-C4D	2.60	129.20	124.66
70	n	603	HEA	C17-C18-C19	-2.59	121.43	127.66
78	O	303	HEC	C1D-C2D-C3D	-2.58	105.20	107.00
77	C	402	HEM	C4B-CHC-C1C	2.58	125.96	122.56
85	n1	201	ZMP	O1-C10-C9	-2.54	120.98	123.99
78	O	303	HEC	CMB-C2B-C1B	-2.51	124.61	128.46
78	D	301	HEC	CMB-C2B-C1B	-2.51	124.61	128.46
77	C	402	HEM	C3D-C4D-ND	-2.50	107.39	110.17
77	C	401	HEM	CAD-CBD-CGD	-2.49	108.24	113.60
70	n	603	HEA	CAD-CBD-CGD	-2.41	108.42	113.60
70	n	603	HEA	C2B-C1B-NB	2.39	112.75	109.88
70	n	603	HEA	C26-C15-C16	2.36	119.23	115.27
84	P1	501	NDP	C5A-C6A-N6A	2.35	123.92	120.35
77	N	402	HEM	CHB-C1B-NB	2.34	127.27	124.38
77	C	401	HEM	C1B-NB-C4B	2.33	107.48	105.07
70	n	604	HEA	C17-C18-C19	-2.33	122.06	127.66
70	n	603	HEA	CHB-C1B-NB	2.32	126.96	124.43
70	n	604	HEA	CHB-C1B-NB	2.32	126.95	124.43
70	n	603	HEA	C25-C23-C24	2.30	119.69	114.60
70	n	604	HEA	CAD-CBD-CGD	-2.26	108.73	113.60
85	W1	201	ZMP	C15-C14-C13	-2.20	108.69	112.36
77	N	403	HEM	C3D-C4D-ND	-2.20	107.72	110.17
77	C	401	HEM	C3D-C4D-ND	-2.18	107.74	110.17
78	O	303	HEC	CBD-CAD-C3D	-2.16	108.93	112.62
77	N	402	HEM	C3D-C4D-ND	-2.15	107.78	110.17
77	N	402	HEM	CAD-CBD-CGD	-2.14	108.99	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	N	402	HEM	C1B-NB-C4B	2.13	107.27	105.07
82	1	501	FMN	P-O5'-C5'	2.11	124.11	118.30
77	C	401	HEM	C4B-CHC-C1C	2.10	125.33	122.56
70	n	603	HEA	C4B-C3B-C2B	-2.09	103.84	107.41
77	C	402	HEM	CAB-C3B-C2B	-2.09	121.73	128.60
71	n	605	3PE	C2-O21-C21	2.08	122.92	117.79
70	n	603	HEA	C27-C19-C20	2.08	118.76	115.27
76	R	103	CDL	CA4-OA6-CA5	2.07	122.89	117.79
77	N	402	HEM	CBA-CAA-C2A	-2.05	109.12	112.62
76	R	102	CDL	CA4-OA6-CA5	2.04	122.80	117.79
77	C	401	HEM	CHD-C1D-ND	2.02	126.62	124.43
76	N1	401	CDL	CB4-OB6-CB5	2.00	122.72	117.79

There are no chirality outliers.

All (671) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	n	603	HEA	C15-C16-C17-C18
70	n	604	HEA	C2D-C3D-CAD-CBD
70	n	604	HEA	C15-C16-C17-C18
71	n	605	3PE	C11-O13-P-O12
71	n	605	3PE	C11-O13-P-O14
71	n	605	3PE	O13-C11-C12-N
71	n	606	3PE	C1-O11-P-O12
71	n	606	3PE	C1-O11-P-O14
71	n	606	3PE	O13-C11-C12-N
71	n	606	3PE	O11-C1-C2-O21
71	n	607	3PE	O13-C11-C12-N
71	o	302	3PE	C1-O11-P-O13
71	o	302	3PE	C1-O11-P-O14
71	o	302	3PE	O13-C11-C12-N
71	p	301	3PE	C1-O11-P-O12
71	p	301	3PE	C11-O13-P-O14
71	p	301	3PE	O13-C11-C12-N
71	t	101	3PE	C11-O13-P-O12
71	v	101	3PE	C1-O11-P-O12
71	v	101	3PE	C11-O13-P-O14
71	v	101	3PE	O13-C11-C12-N
71	A	501	3PE	C1-O11-P-O12
71	A	501	3PE	C1-O11-P-O13
71	A	501	3PE	C1-O11-P-O14
71	A	501	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
71	A	501	3PE	C11-O13-P-O12
71	A	501	3PE	C11-O13-P-O14
71	A	501	3PE	O13-C11-C12-N
71	C	403	3PE	C1-O11-P-O12
71	C	403	3PE	C1-O11-P-O14
71	C	403	3PE	C11-O13-P-O14
71	C	403	3PE	O13-C11-C12-N
71	E	202	3PE	O13-C11-C12-N
71	E	202	3PE	O21-C2-C3-O31
71	G	102	3PE	C1-O11-P-O14
71	G	102	3PE	O13-C11-C12-N
71	L	501	3PE	C11-O13-P-O12
71	L	501	3PE	C11-O13-P-O14
71	L	501	3PE	O13-C11-C12-N
71	N	404	3PE	C11-O13-P-O12
71	N	404	3PE	C11-O13-P-O14
71	N	404	3PE	O13-C11-C12-N
71	O	302	3PE	C11-O13-P-O11
71	O	302	3PE	C11-O13-P-O12
71	O	302	3PE	C11-O13-P-O14
71	O	302	3PE	O13-C11-C12-N
71	R	104	3PE	C1-O11-P-O14
71	R	104	3PE	C11-O13-P-O11
71	R	104	3PE	C11-O13-P-O12
71	R	104	3PE	C11-O13-P-O14
71	R	104	3PE	O13-C11-C12-N
71	6	202	3PE	C1-O11-P-O14
71	D1	501	3PE	C1-O11-P-O12
71	D1	501	3PE	O13-C11-C12-N
71	r1	201	3PE	C1-O11-P-O12
71	r1	201	3PE	C1-O11-P-O13
71	r1	201	3PE	C1-O11-P-O14
71	A1	201	3PE	C1-O11-P-O14
71	A1	201	3PE	C11-O13-P-O14
71	H1	401	3PE	C11-O13-P-O12
71	H1	401	3PE	O13-C11-C12-N
71	K1	201	3PE	C1-O11-P-O12
71	K1	201	3PE	C1-O11-P-O13
71	K1	201	3PE	C1-O11-P-O14
71	K1	201	3PE	O13-C11-C12-N
71	L1	701	3PE	C1-O11-P-O14
71	L1	701	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
71	M1	501	3PE	C11-O13-P-O12
71	M1	501	3PE	C12-C11-O13-P
71	M1	501	3PE	O13-C11-C12-N
71	M1	502	3PE	C11-O13-P-O11
71	M1	502	3PE	C11-O13-P-O12
71	M1	503	3PE	C1-O11-P-O14
71	M1	503	3PE	C11-O13-P-O12
71	M1	503	3PE	C11-O13-P-O14
71	N1	402	3PE	C1-O11-P-O12
71	N1	402	3PE	C1-O11-P-O14
71	Y1	203	3PE	C1-O11-P-O14
71	Y1	203	3PE	O13-C11-C12-N
71	Y1	204	3PE	C11-O13-P-O11
71	Y1	204	3PE	C11-O13-P-O12
71	Y1	204	3PE	C11-O13-P-O14
71	d1	202	3PE	C11-O13-P-O12
71	d1	202	3PE	O13-C11-C12-N
71	d1	203	3PE	C1-O11-P-O14
71	d1	203	3PE	O13-C11-C12-N
71	i1	201	3PE	C11-O13-P-O11
71	i1	201	3PE	C11-O13-P-O12
71	i1	201	3PE	C11-O13-P-O14
76	A	502	CDL	CA2-OA2-PA1-OA3
76	A	502	CDL	CA3-OA5-PA1-OA3
76	A	502	CDL	CB2-OB2-PB2-OB3
76	A	502	CDL	CB2-OB2-PB2-OB4
76	A	502	CDL	CB2-OB2-PB2-OB5
76	C	404	CDL	CA2-OA2-PA1-OA4
76	C	404	CDL	CB2-OB2-PB2-OB3
76	C	404	CDL	CB2-OB2-PB2-OB4
76	C	404	CDL	CB3-OB5-PB2-OB4
76	C	404	CDL	OB5-CB3-CB4-OB6
76	G	101	CDL	C1-CB2-OB2-PB2
76	G	101	CDL	CB2-OB2-PB2-OB4
76	N	405	CDL	CA3-OA5-PA1-OA3
76	O	301	CDL	CA2-OA2-PA1-OA3
76	O	301	CDL	CA2-OA2-PA1-OA4
76	O	301	CDL	CA2-OA2-PA1-OA5
76	O	301	CDL	CA3-OA5-PA1-OA2
76	O	301	CDL	CA3-OA5-PA1-OA3
76	O	301	CDL	CB2-OB2-PB2-OB3
76	O	301	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
76	O	301	CDL	CB3-OB5-PB2-OB4
76	O	301	CDL	OB5-CB3-CB4-OB6
76	R	101	CDL	CA2-OA2-PA1-OA3
76	R	101	CDL	CA2-OA2-PA1-OA4
76	R	101	CDL	CB2-OB2-PB2-OB3
76	R	102	CDL	CA2-OA2-PA1-OA4
76	R	102	CDL	CB3-OB5-PB2-OB4
76	R	103	CDL	CA2-OA2-PA1-OA3
76	R	103	CDL	CA2-OA2-PA1-OA5
76	R	103	CDL	CA3-OA5-PA1-OA2
76	R	103	CDL	CA3-OA5-PA1-OA3
76	R	103	CDL	CB2-OB2-PB2-OB3
76	R	103	CDL	CB2-OB2-PB2-OB4
76	R	103	CDL	CB2-OB2-PB2-OB5
76	R	103	CDL	CB3-OB5-PB2-OB2
76	R	103	CDL	CB3-OB5-PB2-OB3
76	R	103	CDL	CB3-OB5-PB2-OB4
76	H1	402	CDL	CA2-OA2-PA1-OA3
76	H1	402	CDL	CA2-OA2-PA1-OA4
76	H1	402	CDL	CA2-OA2-PA1-OA5
76	H1	402	CDL	CB2-OB2-PB2-OB4
76	L1	702	CDL	CA2-OA2-PA1-OA3
76	L1	702	CDL	CA2-OA2-PA1-OA4
76	L1	702	CDL	CA3-OA5-PA1-OA3
76	L1	702	CDL	CB2-OB2-PB2-OB3
76	L1	702	CDL	CB2-OB2-PB2-OB4
76	L1	702	CDL	CB2-OB2-PB2-OB5
76	L1	702	CDL	CB3-OB5-PB2-OB2
76	L1	702	CDL	CB3-OB5-PB2-OB3
76	L1	702	CDL	CB3-OB5-PB2-OB4
76	L1	703	CDL	CA2-OA2-PA1-OA3
76	L1	703	CDL	CA2-OA2-PA1-OA4
76	N1	401	CDL	CA2-OA2-PA1-OA3
76	N1	401	CDL	CA3-OA5-PA1-OA3
76	N1	401	CDL	OA6-CA4-CA6-OA8
76	N1	401	CDL	CB2-OB2-PB2-OB3
76	N1	401	CDL	CB2-OB2-PB2-OB4
76	Y1	202	CDL	CA2-OA2-PA1-OA3
76	Y1	202	CDL	CA2-OA2-PA1-OA4
76	Y1	202	CDL	CB3-OB5-PB2-OB2
76	Y1	202	CDL	CB3-OB5-PB2-OB3
76	Y1	202	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
76	a1	101	CDL	CA2-OA2-PA1-OA3
76	a1	101	CDL	CA2-OA2-PA1-OA4
76	d1	201	CDL	CA3-OA5-PA1-OA3
76	h1	201	CDL	CA2-OA2-PA1-OA3
76	h1	201	CDL	CB2-OB2-PB2-OB3
76	h1	201	CDL	CB2-OB2-PB2-OB4
76	h1	201	CDL	CB2-OB2-PB2-OB5
76	h1	201	CDL	CB3-OB5-PB2-OB4
77	C	401	HEM	C2A-CAA-CBA-CGA
80	J	101	PC1	C1-O11-P-O12
80	J	101	PC1	C1-O11-P-O14
80	J	101	PC1	C1-O11-P-O13
80	K	101	PC1	C1-O11-P-O14
80	L	502	PC1	C11-O13-P-O12
80	L	502	PC1	C1-O11-P-O12
80	L	502	PC1	C1-O11-P-O13
80	6	203	PC1	C1-O11-P-O12
80	6	203	PC1	C1-O11-P-O14
80	9	203	PC1	C11-O13-P-O11
80	9	203	PC1	C1-O11-P-O12
80	9	203	PC1	C1-O11-P-O14
80	9	203	PC1	C1-O11-P-O13
80	P1	502	PC1	C1-O11-P-O12
80	P1	502	PC1	C1-O11-P-O14
80	P1	502	PC1	C1-O11-P-O13
80	Y1	201	PC1	C11-O13-P-O12
80	Y1	201	PC1	C11-O13-P-O14
80	Y1	201	PC1	C11-O13-P-O11
82	1	501	FMN	N10-C1'-C2'-O2'
82	1	501	FMN	N10-C1'-C2'-C3'
82	1	501	FMN	C5'-O5'-P-O1P
82	1	501	FMN	C5'-O5'-P-O2P
82	1	501	FMN	C5'-O5'-P-O3P
84	P1	501	NDP	C5B-O5B-PA-O3
85	W1	201	ZMP	O1-C10-S1-C11
85	W1	201	ZMP	C9-C10-S1-C11
85	n1	201	ZMP	C17-C18-C21-O5
85	n1	201	ZMP	O4-C17-C18-C21
85	n1	201	ZMP	C16-C17-C18-C21
85	n1	201	ZMP	O4-C17-C18-C19
85	n1	201	ZMP	C16-C17-C18-C20
85	n1	201	ZMP	O3-C16-C17-O4

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Mol	Chain	Res	Type	Atoms
85	n1	201	ZMP	C17-C16-N2-C15
85	n1	201	ZMP	C13-C14-C15-N2
86	O1	401	DGT	PB-O3B-PG-O1G
86	O1	401	DGT	C5'-O5'-PA-O3A
70	n	604	HEA	C4D-C3D-CAD-CBD
85	n1	201	ZMP	O3-C16-N2-C15
76	L1	702	CDL	O1-C1-CB2-OB2
76	L1	702	CDL	CA5-C11-C12-C13
77	N	402	HEM	C2A-CAA-CBA-CGA
71	M1	501	3PE	C31-C32-C33-C34
71	p	301	3PE	C2-C1-O11-P
80	K	101	PC1	C11-C12-N-C13
70	n	603	HEA	C19-C20-C21-C22
71	M1	502	3PE	C27-C28-C29-C2A
71	n	605	3PE	C1-O11-P-O13
71	n	605	3PE	C11-O13-P-O11
71	n	606	3PE	C1-O11-P-O13
71	n	607	3PE	C1-O11-P-O13
71	o	302	3PE	C11-O13-P-O11
71	p	301	3PE	C1-O11-P-O13
71	v	101	3PE	C11-O13-P-O11
71	C	403	3PE	C1-O11-P-O13
71	C	403	3PE	C11-O13-P-O11
71	G	102	3PE	C1-O11-P-O13
71	L	501	3PE	C11-O13-P-O11
71	N	401	3PE	C11-O13-P-O11
71	N	404	3PE	C11-O13-P-O11
71	D1	501	3PE	C1-O11-P-O13
71	K1	201	3PE	C11-O13-P-O11
71	L1	701	3PE	C1-O11-P-O13
71	M1	501	3PE	C11-O13-P-O11
71	M1	503	3PE	C1-O11-P-O13
71	M1	503	3PE	C11-O13-P-O11
71	N1	402	3PE	C1-O11-P-O13
71	Y1	203	3PE	C1-O11-P-O13
71	d1	202	3PE	C1-O11-P-O13
71	d1	202	3PE	C11-O13-P-O11
71	d1	203	3PE	C1-O11-P-O13
76	A	502	CDL	CA3-OA5-PA1-OA2
76	A	502	CDL	CB3-OB5-PB2-OB2
76	C	404	CDL	CB2-OB2-PB2-OB5
76	C	404	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
76	G	101	CDL	CB2-OB2-PB2-OB5
76	G	101	CDL	CB3-OB5-PB2-OB2
76	N	405	CDL	CA3-OA5-PA1-OA2
76	O	301	CDL	CB3-OB5-PB2-OB2
76	R	101	CDL	CA2-OA2-PA1-OA5
76	R	102	CDL	CA3-OA5-PA1-OA2
76	R	102	CDL	CB2-OB2-PB2-OB5
76	R	102	CDL	CB3-OB5-PB2-OB2
76	L1	702	CDL	CA2-OA2-PA1-OA5
76	L1	702	CDL	CA3-OA5-PA1-OA2
76	L1	703	CDL	CA2-OA2-PA1-OA5
76	L1	703	CDL	CB2-OB2-PB2-OB5
76	N1	401	CDL	CB2-OB2-PB2-OB5
76	Y1	202	CDL	CA2-OA2-PA1-OA5
76	a1	101	CDL	CA2-OA2-PA1-OA5
76	a1	101	CDL	CA3-OA5-PA1-OA2
76	d1	201	CDL	CB2-OB2-PB2-OB5
76	h1	201	CDL	CA2-OA2-PA1-OA5
76	h1	201	CDL	CB3-OB5-PB2-OB2
80	J	101	PC1	C11-O13-P-O11
80	K	101	PC1	C11-O13-P-O11
80	K	101	PC1	C1-O11-P-O13
80	L	502	PC1	C11-O13-P-O11
80	6	203	PC1	C11-O13-P-O11
80	6	203	PC1	C1-O11-P-O13
80	P1	502	PC1	C11-O13-P-O11
70	n	604	HEA	C26-C15-C16-C17
80	K	101	PC1	C11-C12-N-C15
71	G	102	3PE	C32-C33-C34-C35
71	G	102	3PE	C37-C38-C39-C3A
76	N1	401	CDL	C81-C82-C83-C84
80	Y1	201	PC1	C34-C35-C36-C37
85	n1	201	ZMP	C19-C18-C21-O5
71	D1	501	3PE	C38-C39-C3A-C3B
80	Y1	201	PC1	C28-C29-C2A-C2B
85	n1	201	ZMP	C6-C7-C8-C9
71	M1	502	3PE	C28-C29-C2A-C2B
71	n	607	3PE	C2-C1-O11-P
76	R	103	CDL	OB5-CB3-CB4-OB6
80	9	204	PC1	C2A-C2B-C2C-C2D
71	M1	501	3PE	C36-C37-C38-C39
76	d1	201	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
80	Y1	201	PC1	C37-C38-C39-C3A
80	V	101	PC1	C11-C12-N-C13
80	6	203	PC1	C11-C12-N-C14
71	A1	201	3PE	C3A-C3B-C3C-C3D
71	M1	501	3PE	C23-C24-C25-C26
77	C	402	HEM	C2A-CAA-CBA-CGA
77	N	403	HEM	C2A-CAA-CBA-CGA
85	W1	201	ZMP	S1-C11-C12-N1
76	Y1	202	CDL	C73-C74-C75-C76
85	n1	201	ZMP	C5-C6-C7-C8
71	N1	402	3PE	C36-C37-C38-C39
76	d1	201	CDL	C55-C56-C57-C58
80	9	204	PC1	C11-C12-N-C15
80	P1	502	PC1	C11-C12-N-C15
71	H1	401	3PE	C21-C22-C23-C24
71	n	606	3PE	C21-C22-C23-C24
71	L1	701	3PE	C21-C22-C23-C24
76	G	101	CDL	OB5-CB3-CB4-OB6
76	d1	201	CDL	OB5-CB3-CB4-OB6
80	K	101	PC1	C11-C12-N-C14
80	V	101	PC1	C11-C12-N-C15
80	6	203	PC1	C11-C12-N-C13
71	D1	501	3PE	C32-C33-C34-C35
70	n	604	HEA	C14-C15-C16-C17
71	p	301	3PE	C11-O13-P-O11
71	t	101	3PE	C11-O13-P-O11
76	C	404	CDL	CA2-OA2-PA1-OA5
76	H1	402	CDL	CB2-OB2-PB2-OB5
76	N1	401	CDL	CA2-OA2-PA1-OA5
76	d1	201	CDL	CA3-OA5-PA1-OA2
80	P1	502	PC1	C21-C22-C23-C24
76	H1	402	CDL	C1-CB2-OB2-PB2
71	n	606	3PE	O11-C1-C2-C3
76	C	404	CDL	OB5-CB3-CB4-CB6
76	G	101	CDL	OB5-CB3-CB4-CB6
76	O	301	CDL	OB5-CB3-CB4-CB6
76	a1	101	CDL	OB5-CB3-CB4-CB6
76	d1	201	CDL	OB5-CB3-CB4-CB6
76	G	101	CDL	C74-C75-C76-C77
80	V	101	PC1	C11-C12-N-C14
80	6	203	PC1	C11-C12-N-C15
71	E	202	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
76	R	103	CDL	CB3-CB4-CB6-OB8
80	9	204	PC1	C34-C35-C36-C37
85	n1	201	ZMP	C20-C18-C21-O5
71	N	404	3PE	C25-C26-C27-C28
76	Y1	202	CDL	C24-C25-C26-C27
70	n	603	HEA	C11-C12-C13-C14
80	Y1	201	PC1	O11-C1-C2-O21
80	9	204	PC1	C11-C12-N-C14
80	P1	502	PC1	C11-C12-N-C14
76	a1	101	CDL	O1-C1-CA2-OA2
76	Y1	202	CDL	C82-C83-C84-C85
85	n1	201	ZMP	O4-C17-C18-C20
80	9	204	PC1	C11-C12-N-C13
76	A	502	CDL	OB5-CB3-CB4-CB6
76	R	103	CDL	OB5-CB3-CB4-CB6
71	t	101	3PE	O13-C11-C12-N
70	n	603	HEA	C27-C19-C20-C21
70	n	603	HEA	C18-C19-C20-C21
80	J	101	PC1	C2-C1-O11-P
71	L	501	3PE	C32-C33-C34-C35
71	n	606	3PE	C1-C2-C3-O31
76	N1	401	CDL	CA3-CA4-CA6-OA8
71	R	104	3PE	C1-O11-P-O13
71	A1	201	3PE	C1-O11-P-O13
71	A1	201	3PE	C11-O13-P-O11
71	H1	401	3PE	C11-O13-P-O11
76	A	502	CDL	CA2-OA2-PA1-OA5
76	R	102	CDL	CA2-OA2-PA1-OA5
71	o	302	3PE	O11-C1-C2-O21
71	H1	401	3PE	O11-C1-C2-O21
76	R	101	CDL	OB5-CB3-CB4-OB6
76	L1	702	CDL	OB5-CB3-CB4-OB6
80	P1	502	PC1	O11-C1-C2-O21
71	D1	501	3PE	C31-C32-C33-C34
76	R	103	CDL	OB6-CB4-CB6-OB8
76	h1	201	CDL	OB6-CB4-CB6-OB8
76	a1	101	CDL	CB2-C1-CA2-OA2
71	n	606	3PE	C2-C1-O11-P
71	M1	503	3PE	C2-C1-O11-P
71	i1	201	3PE	C2-C1-O11-P
76	G	101	CDL	C1-CA2-OA2-PA1
76	N1	401	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
80	P1	502	PC1	O21-C21-C22-C23
76	R	103	CDL	CA5-C11-C12-C13
76	N1	401	CDL	C51-C52-C53-C54
76	Y1	202	CDL	OB5-CB3-CB4-CB6
76	h1	201	CDL	OB5-CB3-CB4-CB6
80	9	203	PC1	C29-C2A-C2B-C2C
76	R	102	CDL	C31-C32-C33-C34
80	P1	502	PC1	C11-C12-N-C13
71	K1	201	3PE	C2-C1-O11-P
76	h1	201	CDL	CA4-CA3-OA5-PA1
76	h1	201	CDL	CB3-CB4-CB6-OB8
80	V	101	PC1	C2-C1-O11-P
71	L	501	3PE	O11-C1-C2-O21
76	A	502	CDL	OB5-CB3-CB4-OB6
77	C	402	HEM	C4B-C3B-CAB-CBB
77	N	403	HEM	C4B-C3B-CAB-CBB
85	n1	201	ZMP	C16-C17-C18-C19
71	n	606	3PE	O21-C2-C3-O31
80	Y1	201	PC1	C3A-C3B-C3C-C3D
84	P1	501	NDP	PN-O3-PA-O2A
86	O1	401	DGT	PB-O3A-PA-O1A
80	9	204	PC1	C35-C36-C37-C38
76	N	405	CDL	CA2-OA2-PA1-OA5
76	R	101	CDL	CB2-OB2-PB2-OB5
76	N1	401	CDL	CA3-OA5-PA1-OA2
71	t	101	3PE	C2-C1-O11-P
71	Y1	203	3PE	C2-C1-O11-P
76	C	404	CDL	C1-CA2-OA2-PA1
76	O	301	CDL	CB4-CB3-OB5-PB2
76	R	101	CDL	CA4-CA3-OA5-PA1
76	H1	402	CDL	C1-CA2-OA2-PA1
76	L1	703	CDL	C1-CA2-OA2-PA1
71	n	605	3PE	C1-O11-P-O12
71	n	605	3PE	C1-O11-P-O14
71	n	607	3PE	C1-O11-P-O14
71	o	302	3PE	C11-O13-P-O14
71	p	301	3PE	C11-O13-P-O12
71	t	101	3PE	C11-O13-P-O14
71	v	101	3PE	C1-O11-P-O14
71	v	101	3PE	C11-O13-P-O12
71	C	403	3PE	C11-O13-P-O12
71	G	102	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
71	N	401	3PE	C11-O13-P-O12
71	N	401	3PE	C11-O13-P-O14
71	H1	401	3PE	C11-O13-P-O14
71	K1	201	3PE	C11-O13-P-O14
71	L1	701	3PE	C1-O11-P-O12
71	M1	502	3PE	C11-O13-P-O14
71	M1	503	3PE	C1-O11-P-O12
71	Y1	203	3PE	C1-O11-P-O12
71	d1	202	3PE	C1-O11-P-O12
71	d1	202	3PE	C1-O11-P-O14
71	d1	202	3PE	C11-O13-P-O14
71	d1	203	3PE	C1-O11-P-O12
76	A	502	CDL	CA3-OA5-PA1-OA4
76	A	502	CDL	CB3-OB5-PB2-OB3
76	A	502	CDL	CB3-OB5-PB2-OB4
76	C	404	CDL	CA2-OA2-PA1-OA3
76	G	101	CDL	CB3-OB5-PB2-OB4
76	N	405	CDL	CA3-OA5-PA1-OA4
76	O	301	CDL	CB2-OB2-PB2-OB4
76	R	102	CDL	CA2-OA2-PA1-OA3
76	R	102	CDL	CA3-OA5-PA1-OA3
76	R	102	CDL	CB2-OB2-PB2-OB3
76	H1	402	CDL	CB2-OB2-PB2-OB3
76	L1	702	CDL	CA3-OA5-PA1-OA4
76	L1	703	CDL	CB2-OB2-PB2-OB3
76	N1	401	CDL	CA2-OA2-PA1-OA4
76	d1	201	CDL	CB2-OB2-PB2-OB3
76	h1	201	CDL	CA2-OA2-PA1-OA4
80	J	101	PC1	C11-O13-P-O14
80	K	101	PC1	C11-O13-P-O12
80	K	101	PC1	C11-O13-P-O14
80	K	101	PC1	C1-O11-P-O12
80	L	502	PC1	C1-O11-P-O14
80	6	203	PC1	C11-O13-P-O12
80	6	203	PC1	C11-O13-P-O14
80	9	203	PC1	C11-O13-P-O12
80	P1	502	PC1	C11-O13-P-O14
86	O1	401	DGT	C5'-O5'-PA-O1A
71	H1	401	3PE	O11-C1-C2-C3
76	R	101	CDL	OB5-CB3-CB4-CB6
71	6	202	3PE	O13-C11-C12-N
71	M1	502	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
80	Y1	201	PC1	C29-C2A-C2B-C2C
71	N	401	3PE	C12-C11-O13-P
80	P1	502	PC1	C12-C11-O13-P
76	a1	101	CDL	C52-C51-CB5-OB6
76	Y1	202	CDL	OB5-CB3-CB4-OB6
76	a1	101	CDL	OB5-CB3-CB4-OB6
76	h1	201	CDL	OB5-CB3-CB4-OB6
71	p	301	3PE	C23-C24-C25-C26
84	P1	501	NDP	C2D-C1D-N1N-C6N
80	J	101	PC1	O13-C11-C12-N
80	L	502	PC1	O13-C11-C12-N
80	9	203	PC1	O13-C11-C12-N
80	Y1	201	PC1	O13-C11-C12-N
76	d1	201	CDL	C59-C60-C61-C62
76	G	101	CDL	CB4-CB3-OB5-PB2
76	N	405	CDL	CB4-CB3-OB5-PB2
80	9	203	PC1	C35-C36-C37-C38
71	d1	203	3PE	C21-C22-C23-C24
71	M1	501	3PE	C3D-C3E-C3F-C3G
76	L1	702	CDL	OB5-CB3-CB4-CB6
80	Y1	201	PC1	O11-C1-C2-C3
71	o	302	3PE	C2-C1-O11-P
76	A	502	CDL	C1-CA2-OA2-PA1
76	h1	201	CDL	C1-CA2-OA2-PA1
71	R	104	3PE	O11-C1-C2-O21
71	r1	201	3PE	O31-C31-C32-C33
84	P1	501	NDP	O4D-C1D-N1N-C6N
75	y	601	TGL	CC1-CC2-CC3-CC4
71	n	606	3PE	C11-O13-P-O11
71	G	102	3PE	C11-O13-P-O11
71	N	401	3PE	C1-O11-P-O13
71	6	202	3PE	C1-O11-P-O13
71	6	202	3PE	C11-O13-P-O11
71	r1	201	3PE	C11-O13-P-O11
71	M1	502	3PE	C1-O11-P-O13
71	N1	402	3PE	C11-O13-P-O11
76	H1	402	CDL	CB3-OB5-PB2-OB2
76	a1	101	CDL	CB2-OB2-PB2-OB5
71	d1	202	3PE	C1-C2-C3-O31
71	d1	203	3PE	O21-C21-C22-C23
71	M1	501	3PE	C37-C38-C39-C3A
76	A	502	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
80	9	204	PC1	C2B-C2C-C2D-C2E
76	A	502	CDL	CB4-CB3-OB5-PB2
76	L1	702	CDL	C1-CB2-OB2-PB2
71	E	202	3PE	C21-C22-C23-C24
70	n	604	HEA	CAA-CBA-CGA-O1A
71	n	607	3PE	O21-C2-C3-O31
76	Y1	202	CDL	CB3-CB4-CB6-OB8
76	d1	201	CDL	CA3-CA4-CA6-OA8
70	n	603	HEA	CAA-CBA-CGA-O1A
70	n	603	HEA	CAD-CBD-CGD-O1D
85	W1	201	ZMP	C19-C18-C21-O5
85	W1	201	ZMP	C20-C18-C21-O5
71	E	202	3PE	C32-C33-C34-C35
70	n	604	HEA	CAA-CBA-CGA-O2A
71	A1	201	3PE	C38-C39-C3A-C3B
80	9	203	PC1	C3-C2-O21-C21
71	A1	201	3PE	C23-C24-C25-C26
76	Y1	202	CDL	C80-C81-C82-C83
71	v	101	3PE	C1-O11-P-O13
71	Y1	203	3PE	C11-O13-P-O11
80	9	204	PC1	C21-C22-C23-C24
76	A	502	CDL	C52-C51-CB5-OB7
71	R	104	3PE	O11-C1-C2-C3
85	n1	201	ZMP	C12-C11-S1-C10
71	N1	402	3PE	O21-C2-C3-O31
76	Y1	202	CDL	OB6-CB4-CB6-OB8
76	d1	201	CDL	OA6-CA4-CA6-OA8
76	G	101	CDL	CB2-C1-CA2-OA2
76	L1	702	CDL	CA2-C1-CB2-OB2
70	n	603	HEA	CAA-CBA-CGA-O2A
77	N	403	HEM	CAD-CBD-CGD-O2D
70	n	603	HEA	CAD-CBD-CGD-O2D
71	D1	501	3PE	O21-C21-C22-C23
71	N1	402	3PE	C1-C2-C3-O31
71	Y1	204	3PE	C1-C2-C3-O31
71	D1	501	3PE	C3D-C3E-C3F-C3G
76	N1	401	CDL	C80-C81-C82-C83
71	M1	502	3PE	C23-C24-C25-C26
71	L	501	3PE	O11-C1-C2-C3
71	C	405	3PE	O13-C11-C12-N
71	M1	502	3PE	C2C-C2D-C2E-C2F
76	A	502	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
76	R	101	CDL	C12-C11-CA5-OA6
76	R	101	CDL	C72-C71-CB7-OB8
71	C	405	3PE	O31-C31-C32-C33
71	L1	701	3PE	C2-C1-O11-P
80	Y1	201	PC1	C33-C34-C35-C36
85	n1	201	ZMP	N2-C16-C17-O4
77	N	403	HEM	CAD-CBD-CGD-O1D
84	P1	501	NDP	C2D-C1D-N1N-C2N
71	v	101	3PE	O32-C31-C32-C33
76	C	404	CDL	C72-C71-CB7-OB9
71	C	405	3PE	O21-C21-C22-C23
71	O	302	3PE	O21-C21-C22-C23
76	Y1	202	CDL	CB7-C71-C72-C73
76	G	101	CDL	C52-C51-CB5-OB6
76	R	102	CDL	C12-C11-CA5-OA6
71	t	101	3PE	C3-C2-O21-C21
76	a1	101	CDL	CA3-CA4-OA6-CA5
76	h1	201	CDL	CB6-CB4-OB6-CB5
80	6	203	PC1	C3-C2-O21-C21
80	Y1	201	PC1	C35-C36-C37-C38
84	P1	501	NDP	O4D-C1D-N1N-C2N
78	D	301	HEC	CAD-CBD-CGD-O2D
71	K1	201	3PE	O31-C31-C32-C33
76	R	102	CDL	C52-C51-CB5-OB6
71	H1	401	3PE	C2A-C2B-C2C-C2D
76	R	102	CDL	C32-C31-CA7-OA8
76	L1	702	CDL	C72-C71-CB7-OB8
71	D1	501	3PE	C39-C3A-C3B-C3C
76	R	102	CDL	OA5-CA3-CA4-OA6
76	A	502	CDL	C32-C31-CA7-OA8
71	i1	201	3PE	C2B-C2C-C2D-C2E
86	O1	401	DGT	PB-O3B-PG-O2G
71	M1	503	3PE	O21-C21-C22-C23
71	M1	502	3PE	O11-C1-C2-C3
76	h1	201	CDL	C32-C31-CA7-OA8
71	Y1	204	3PE	O21-C2-C3-O31
76	R	101	CDL	C72-C71-CB7-OB9
76	d1	201	CDL	C14-C15-C16-C17
76	h1	201	CDL	C12-C11-CA5-OA6
71	C	403	3PE	O21-C21-C22-C23
71	M1	501	3PE	O21-C21-C22-C23
76	R	102	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
76	h1	201	CDL	C72-C71-CB7-OB8
71	v	101	3PE	O31-C31-C32-C33
76	C	404	CDL	C72-C71-CB7-OB8
76	N	405	CDL	C52-C51-CB5-OB6
76	L1	703	CDL	C72-C71-CB7-OB8
76	H1	402	CDL	C12-C13-C14-C15
76	d1	201	CDL	C57-C58-C59-C60
71	6	202	3PE	O21-C21-C22-C23
80	9	204	PC1	O31-C31-C32-C33
84	P1	501	NDP	PN-O3-PA-O1A
78	D	301	HEC	CAD-CBD-CGD-O1D
71	Y1	204	3PE	C23-C24-C25-C26
71	C	403	3PE	O31-C31-C32-C33
76	R	102	CDL	C52-C51-CB5-OB7
71	K1	201	3PE	O32-C31-C32-C33
76	G	101	CDL	C52-C51-CB5-OB7
76	R	102	CDL	C32-C31-CA7-OA9
76	N	405	CDL	C52-C51-CB5-OB7
76	L1	703	CDL	C72-C71-CB7-OB9
71	C	405	3PE	O22-C21-C22-C23
76	A	502	CDL	C32-C31-CA7-OA9
71	o	302	3PE	C1-C2-C3-O31
71	G	102	3PE	O21-C21-C22-C23
76	O	301	CDL	CB2-OB2-PB2-OB5
80	Y1	201	PC1	C3B-C3C-C3D-C3E
71	C	405	3PE	O32-C31-C32-C33
71	E	202	3PE	C33-C34-C35-C36
71	K1	201	3PE	O21-C21-C22-C23
71	H1	401	3PE	C2-C1-O11-P
80	6	203	PC1	C21-C22-C23-C24
71	O	302	3PE	O22-C21-C22-C23
80	9	204	PC1	O32-C31-C32-C33
71	n	606	3PE	C11-O13-P-O14
71	G	102	3PE	C11-O13-P-O14
71	r1	201	3PE	C11-O13-P-O14
76	R	102	CDL	CA3-OA5-PA1-OA4
76	N1	401	CDL	CB3-OB5-PB2-OB3
76	a1	101	CDL	CA3-OA5-PA1-OA3
76	a1	101	CDL	CB2-OB2-PB2-OB3
84	P1	501	NDP	C5B-O5B-PA-O2A
86	O1	401	DGT	C5'-O5'-PA-O2A
71	M1	503	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
80	P1	502	PC1	O22-C21-C22-C23
71	o	302	3PE	O11-C1-C2-C3
77	C	401	HEM	CAA-CBA-CGA-O2A
76	L1	702	CDL	C72-C71-CB7-OB9
76	h1	201	CDL	C72-C71-CB7-OB9
86	O1	401	DGT	PB-O3B-PG-O3G
70	n	603	HEA	O11-C11-C12-C13
85	W1	201	ZMP	C2-C1-C22-C23
76	h1	201	CDL	C52-C51-CB5-OB6
71	n	605	3PE	C1-C2-O21-C21
71	n	606	3PE	C12-C11-O13-P
71	v	101	3PE	C12-C11-O13-P
71	A	501	3PE	C1-C2-O21-C21
71	C	405	3PE	C12-C11-O13-P
71	R	104	3PE	C12-C11-O13-P
71	H1	401	3PE	C3-C2-O21-C21
71	L1	701	3PE	C3-C2-O21-C21
76	N	405	CDL	CB6-CB4-OB6-CB5
76	R	102	CDL	CA6-CA4-OA6-CA5
76	R	103	CDL	CA3-CA4-OA6-CA5
76	N1	401	CDL	CB3-CB4-OB6-CB5
76	N1	401	CDL	CB6-CB4-OB6-CB5
80	L	502	PC1	C1-C2-O21-C21
80	9	204	PC1	C12-C11-O13-P
80	P1	502	PC1	C3-C2-O21-C21
71	C	403	3PE	O22-C21-C22-C23
71	M1	501	3PE	O22-C21-C22-C23
76	Y1	202	CDL	C13-C14-C15-C16
71	A1	201	3PE	O31-C31-C32-C33
76	R	102	CDL	C72-C71-CB7-OB9
71	n	605	3PE	O21-C21-C22-C23
71	A1	201	3PE	O21-C21-C22-C23
71	M1	501	3PE	O31-C31-C32-C33
76	R	103	CDL	C72-C73-C74-C75
71	M1	502	3PE	O31-C31-C32-C33
80	P1	502	PC1	O31-C31-C32-C33
71	C	403	3PE	O32-C31-C32-C33
71	M1	502	3PE	O32-C31-C32-C33
76	N	405	CDL	C12-C11-CA5-OA7
77	C	401	HEM	CAA-CBA-CGA-O1A
71	Y1	204	3PE	O31-C31-C32-C33
75	y	601	TGL	OG1-CA1-CA2-CA3

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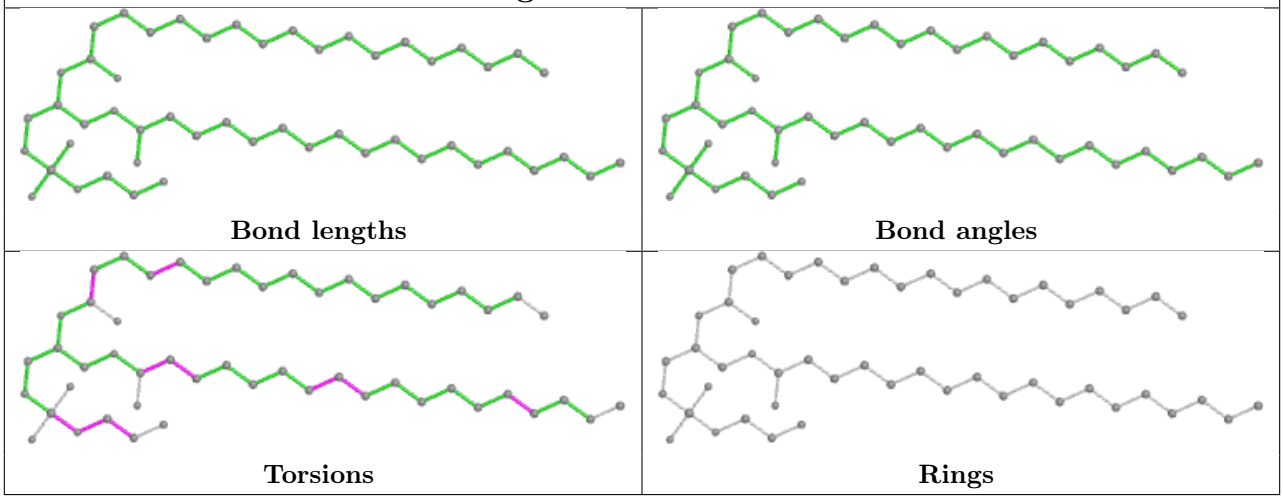
Mol	Chain	Res	Type	Atoms
76	A	502	CDL	C12-C11-CA5-OA6
76	N	405	CDL	C12-C11-CA5-OA6
76	N1	401	CDL	C52-C51-CB5-OB6
76	d1	201	CDL	C72-C71-CB7-OB8
71	i1	201	3PE	C24-C25-C26-C27
71	G	102	3PE	O22-C21-C22-C23
71	6	202	3PE	O22-C21-C22-C23
80	P1	502	PC1	O32-C31-C32-C33
76	G	101	CDL	C72-C73-C74-C75
71	Y1	203	3PE	O31-C31-C32-C33
76	H1	402	CDL	C12-C11-CA5-OA6
76	h1	201	CDL	C32-C31-CA7-OA9
80	9	203	PC1	C2D-C2E-C2F-C2G
71	A	501	3PE	O31-C31-C32-C33
71	Y1	204	3PE	O32-C31-C32-C33
76	H1	402	CDL	C13-C14-C15-C16

There are no ring outliers.

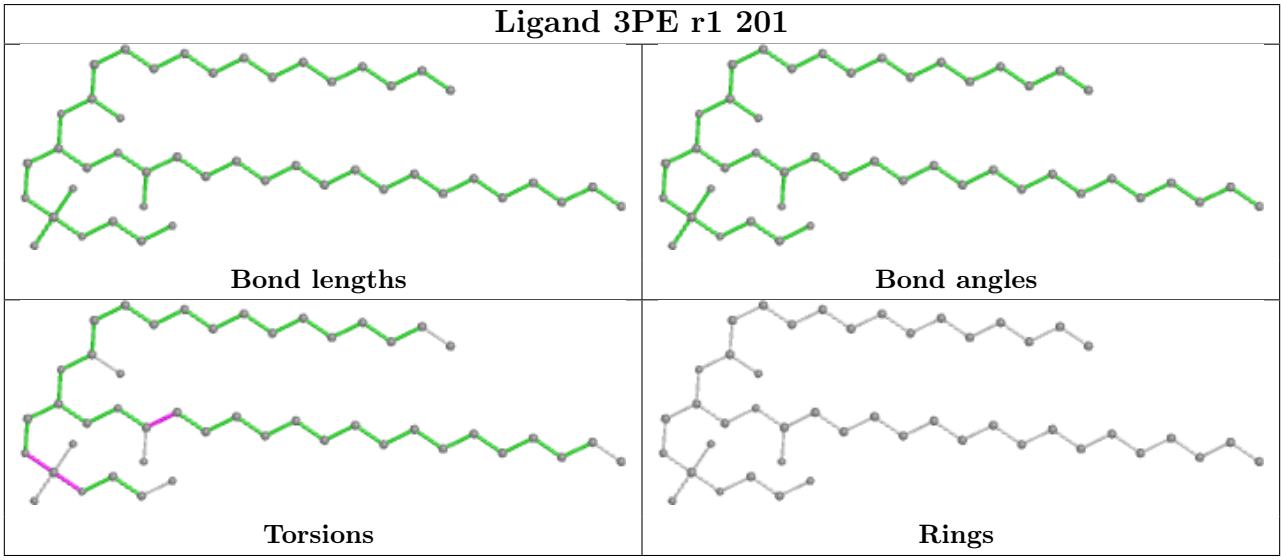
No monomer is involved in short contacts.

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.

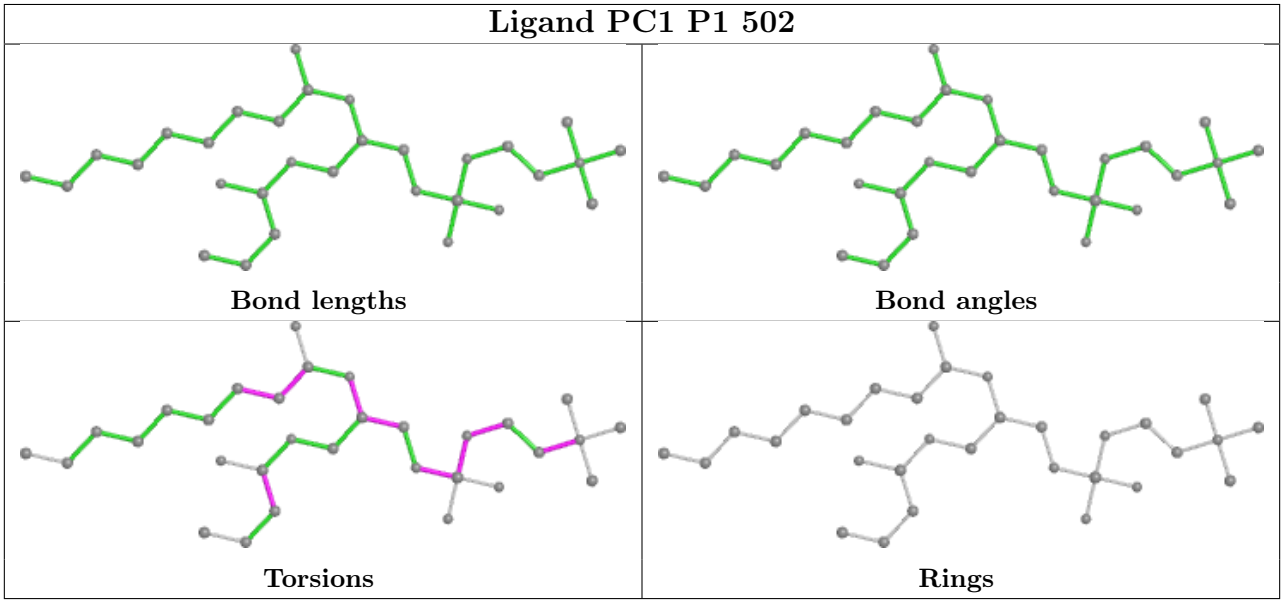
Ligand 3PE M1 501



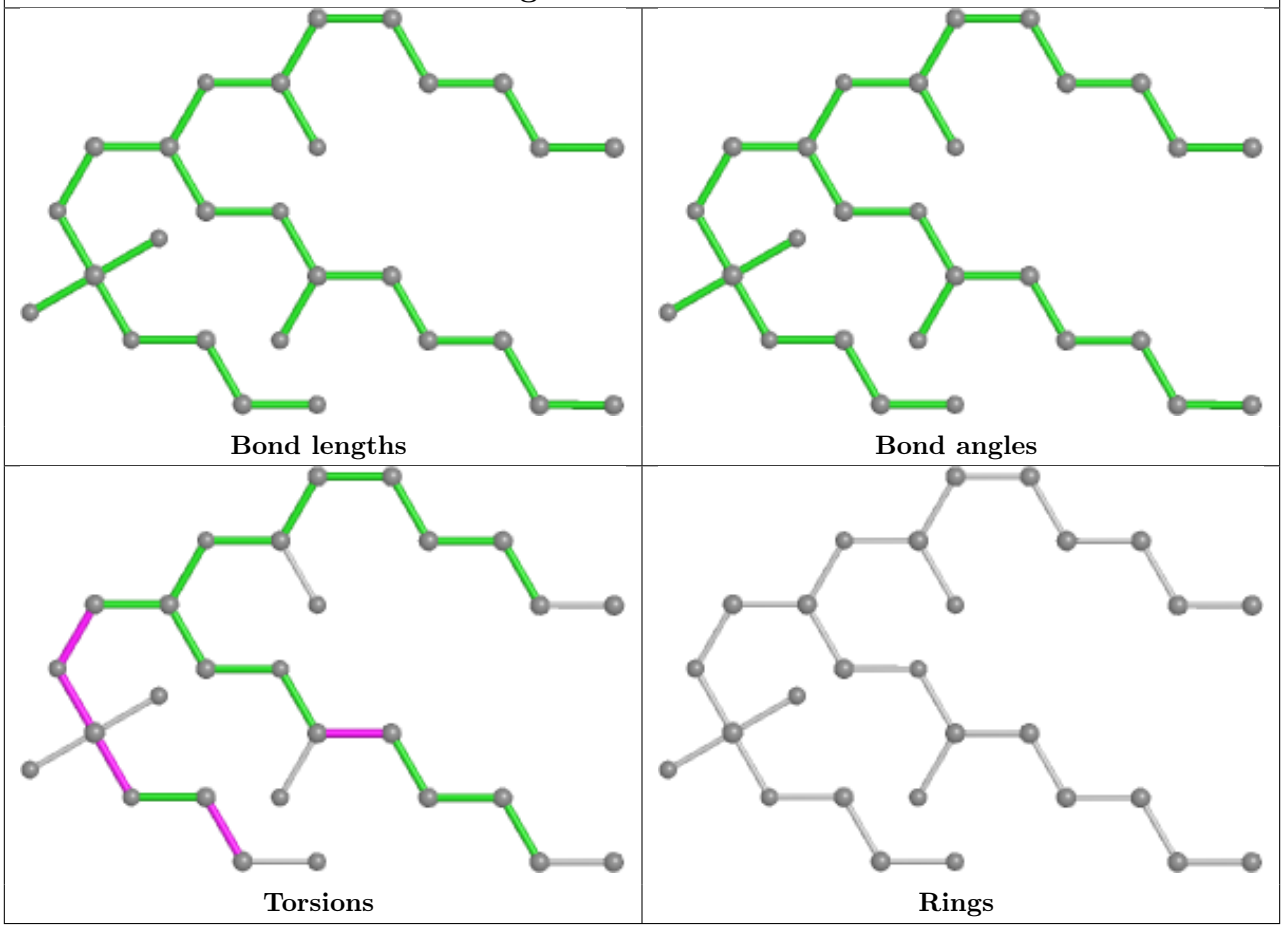
Ligand 3PE r1 201



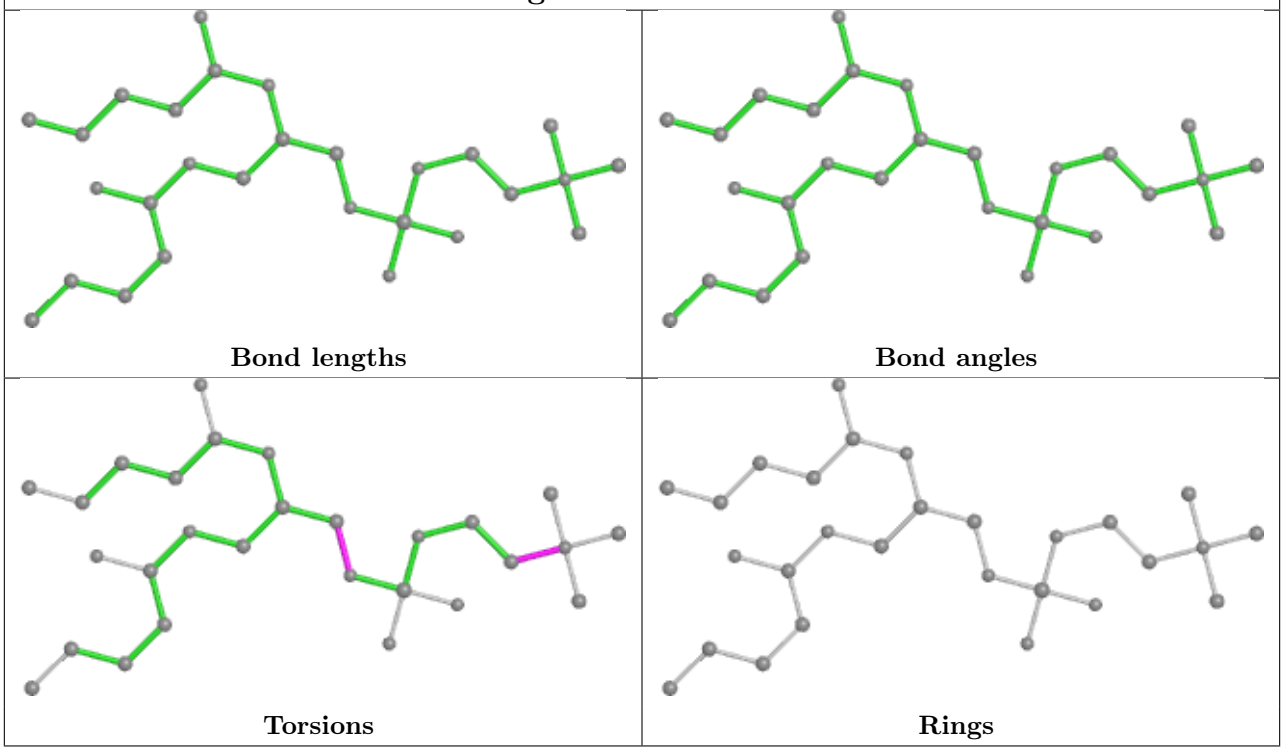
Ligand PC1 P1 502



Ligand 3PE Y1 203



Ligand PC1 V 101



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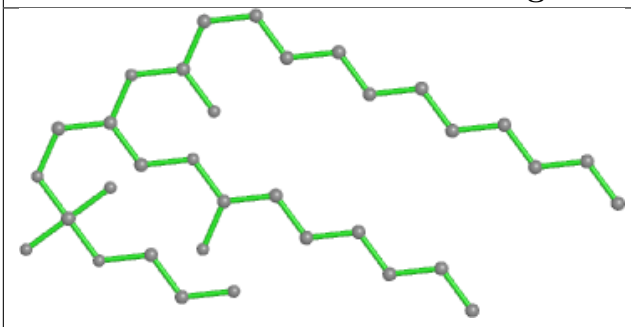
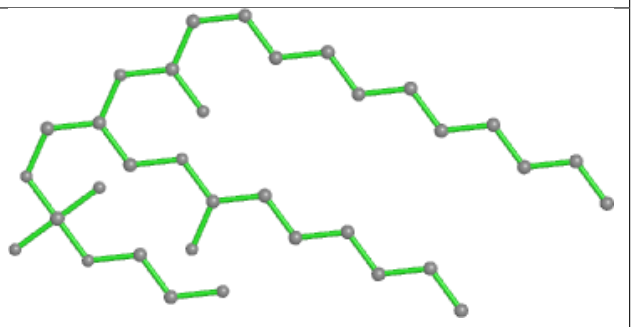
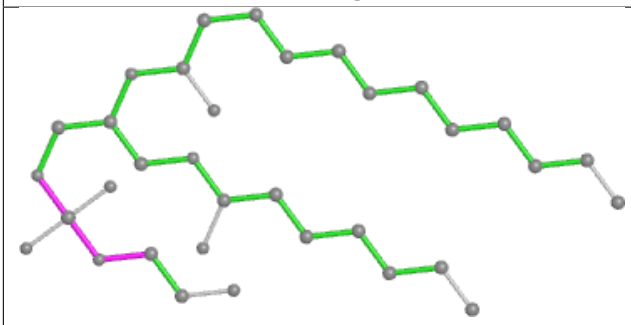


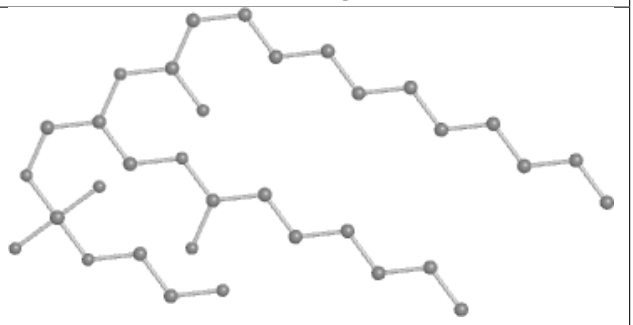
Bond lengths



Bond angles

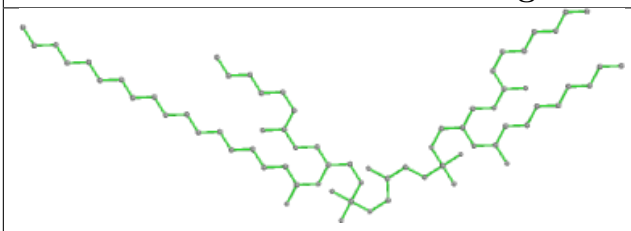


Torsions

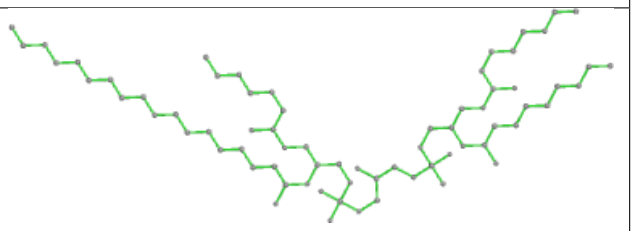


Rings

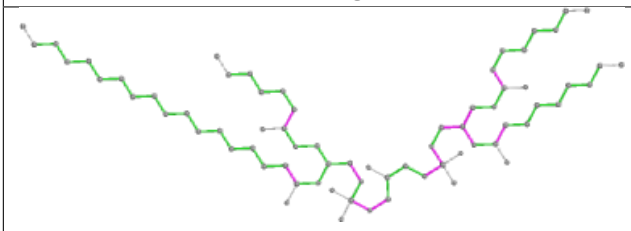
Ligand CDL h1 201



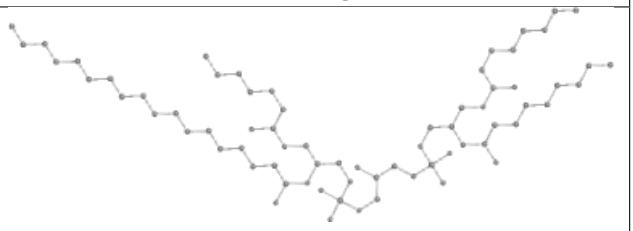
Bond lengths



Bond angles

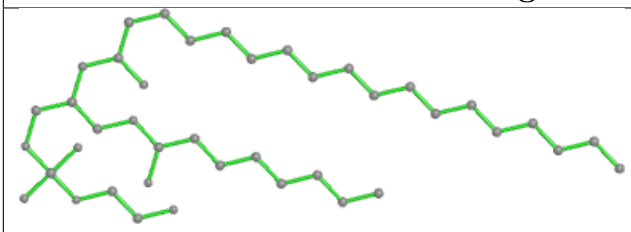


Torsions

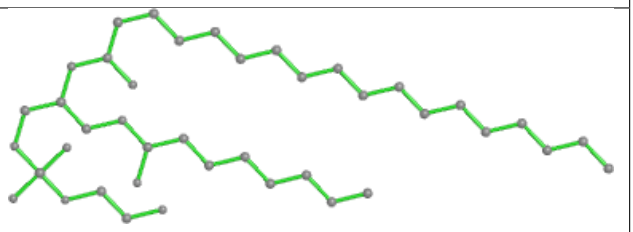


Rings

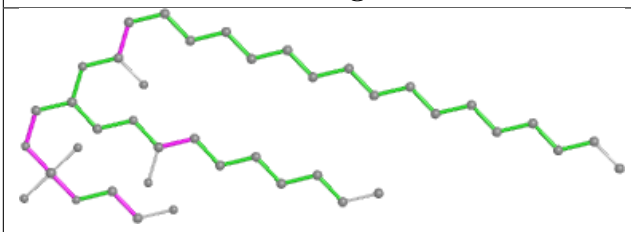
Ligand 3PE K1 201



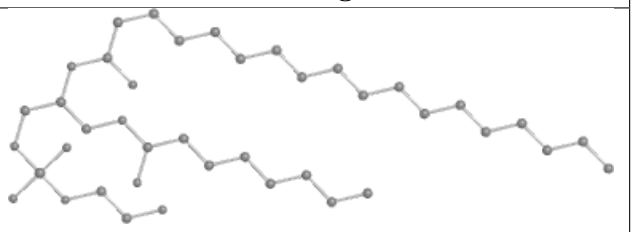
Bond lengths



Bond angles

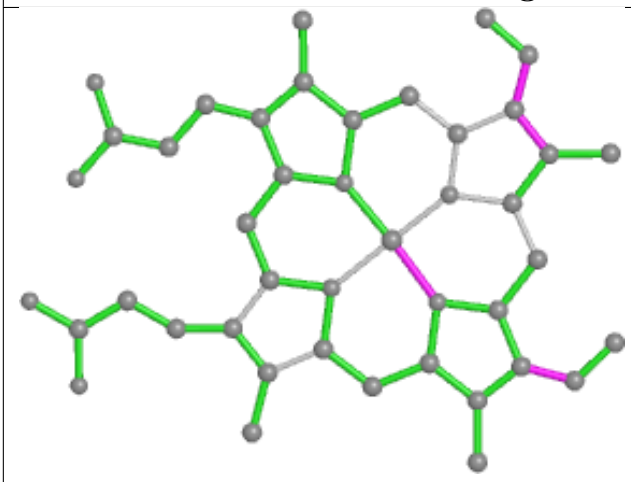


Torsions

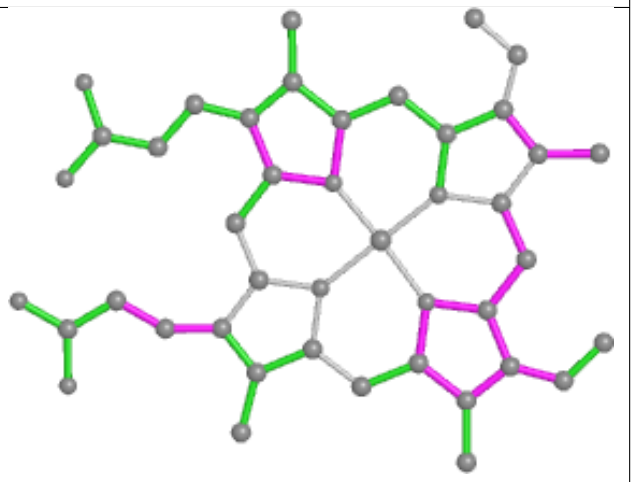


Rings

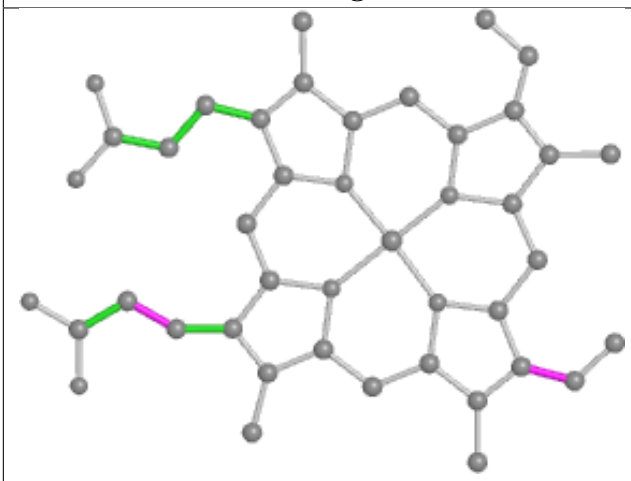
Ligand HEM C 402



Bond lengths



Bond angles



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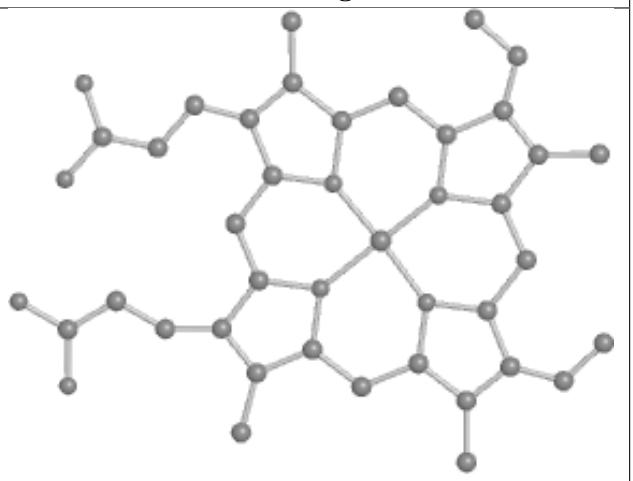
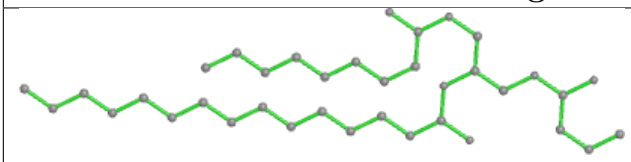
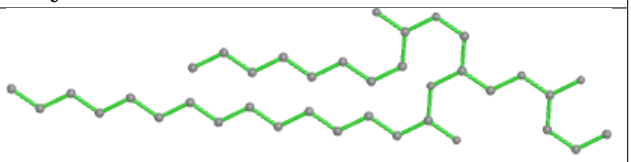


Rings

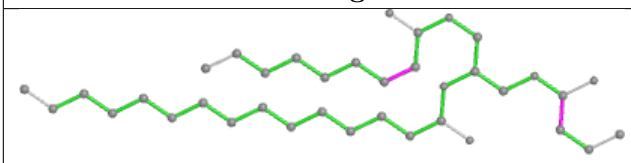
Ligand TGL y 601



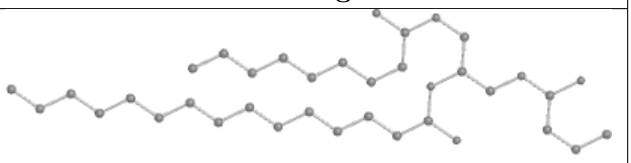
Bond lengths



Bond angles

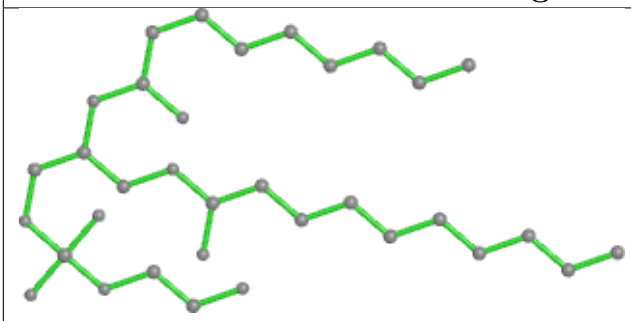


Torsions

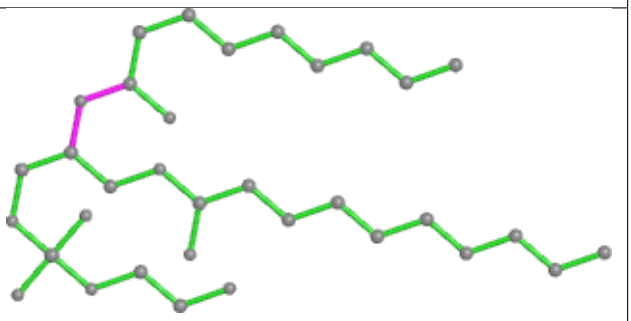


Rings

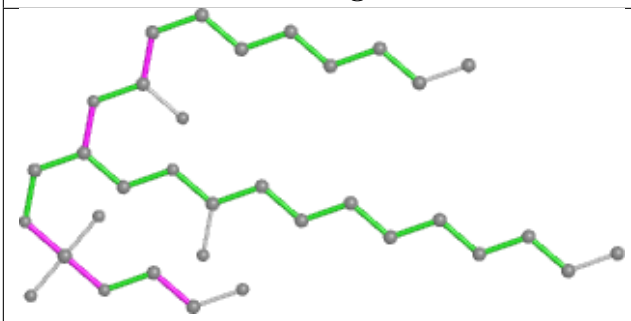
Ligand 3PE n 605



Bond lengths



Bond angles



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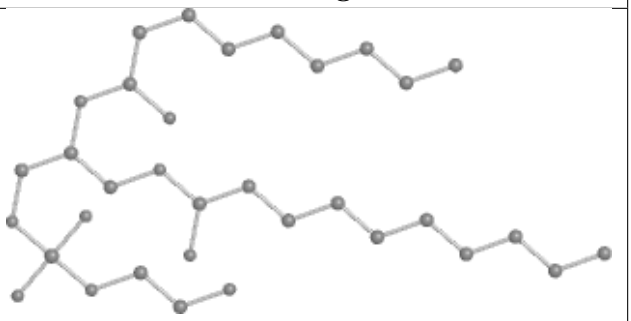
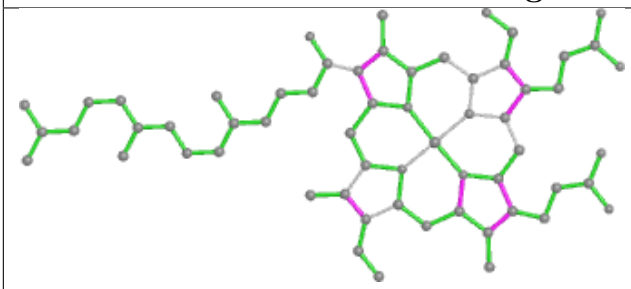
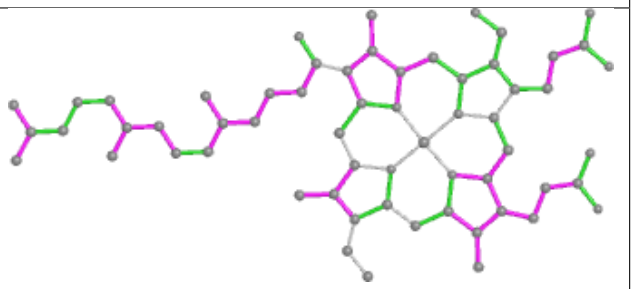


Rings

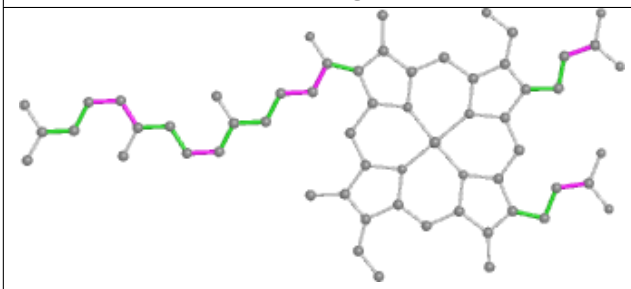
Ligand HEA n 603



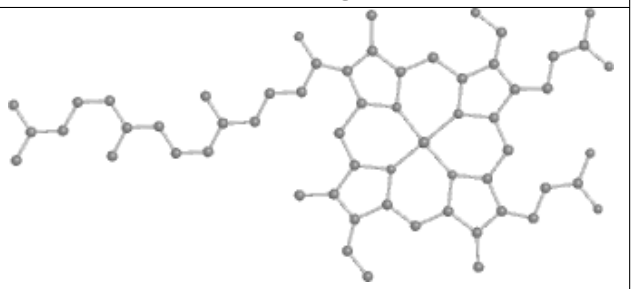
Bond lengths



Bond angles

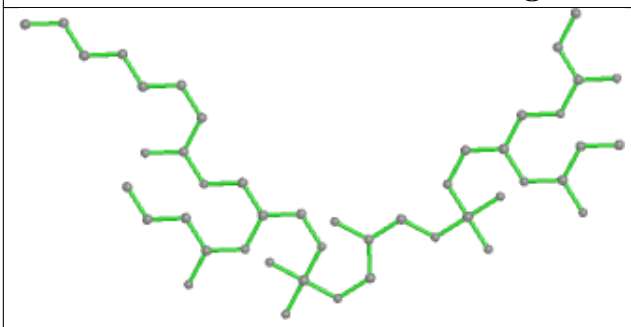


Torsions

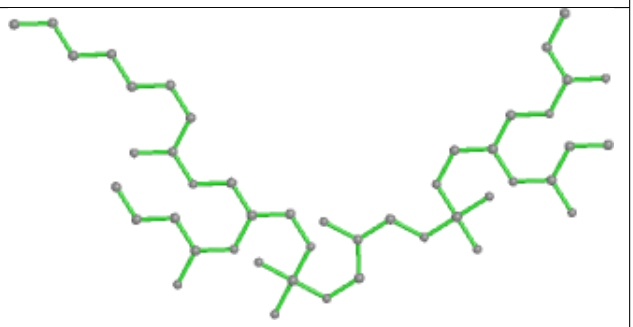


Rings

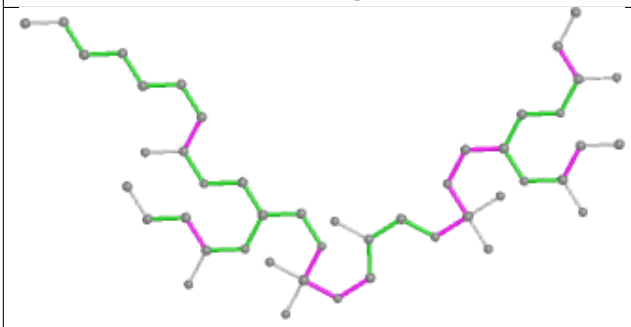
Ligand CDL A 502



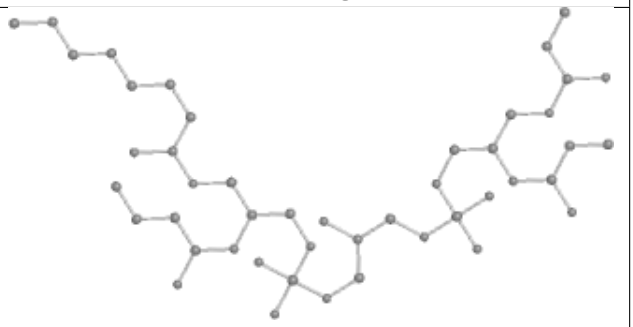
Bond lengths



Bond angles

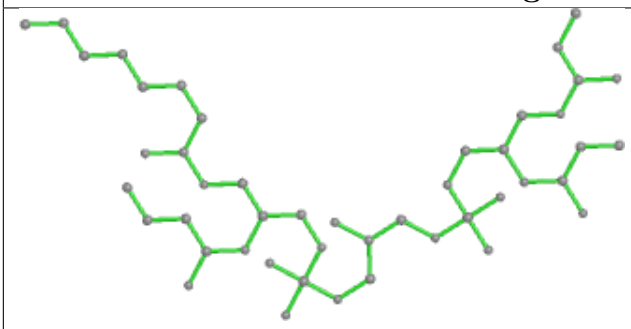


Torsions



Rings

Ligand CDL N 405



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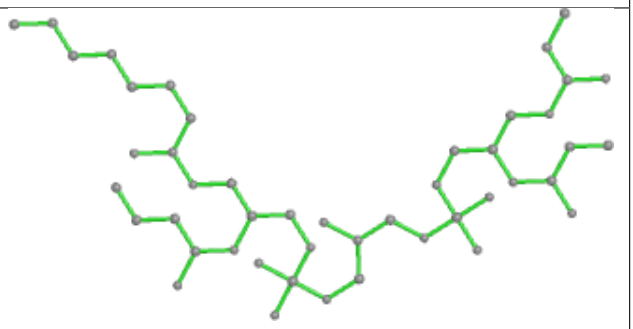
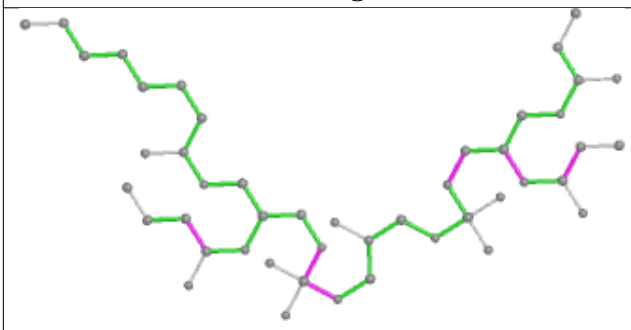
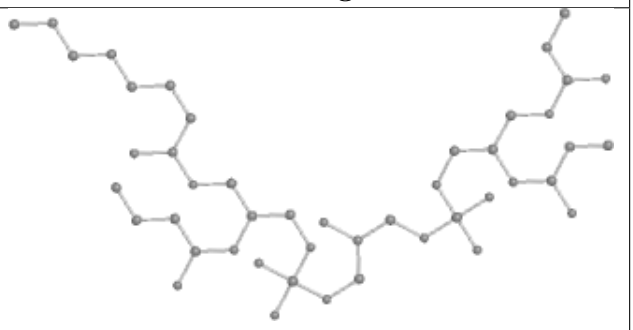


Bond angles

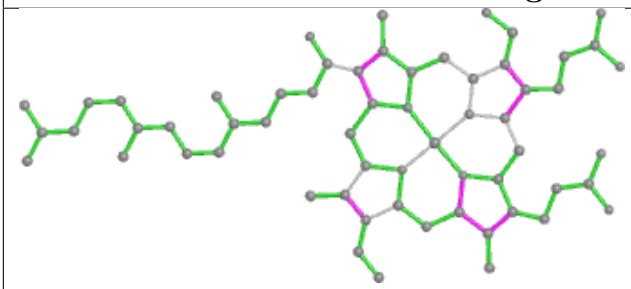


Torsions

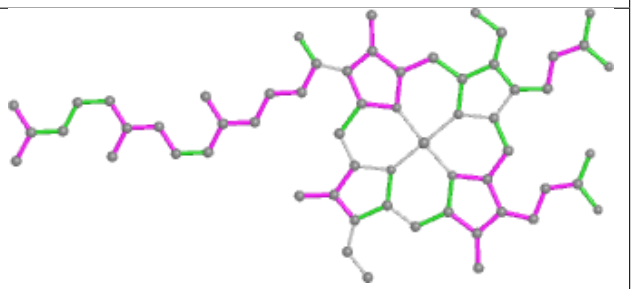


Rings

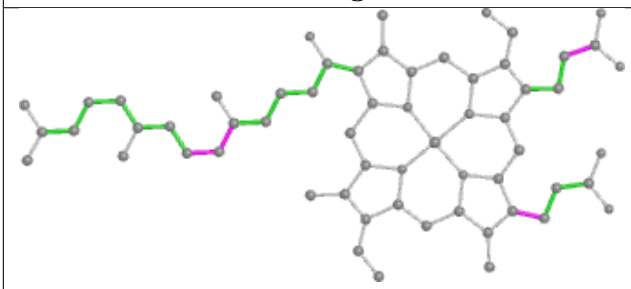
Ligand HEA n 604



Bond lengths



Bond angles



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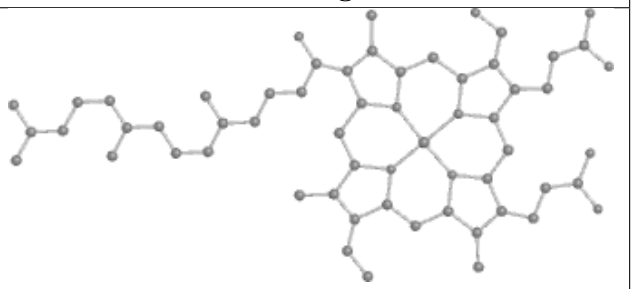
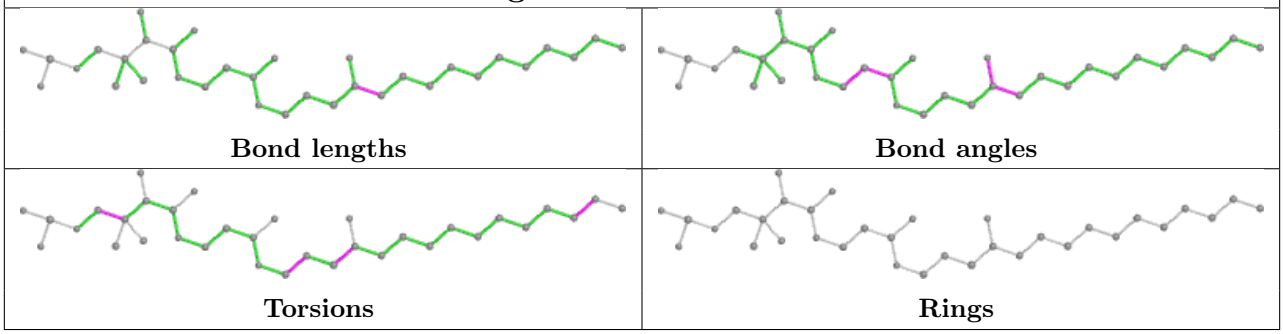
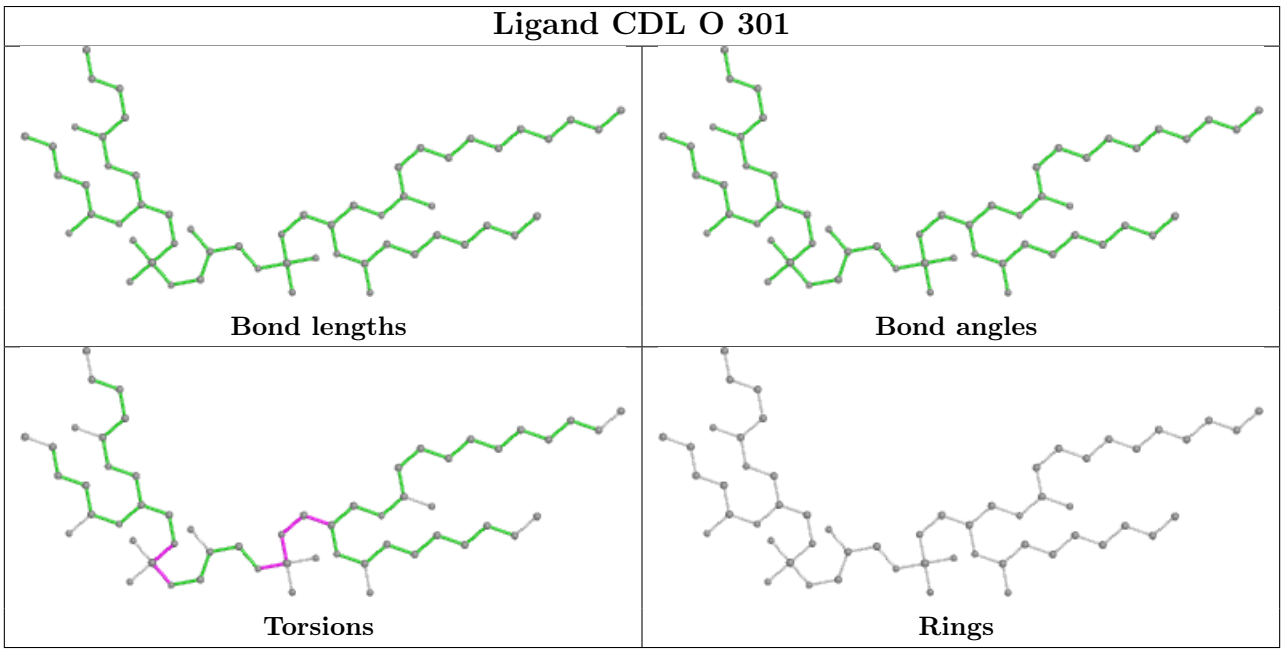


Rings

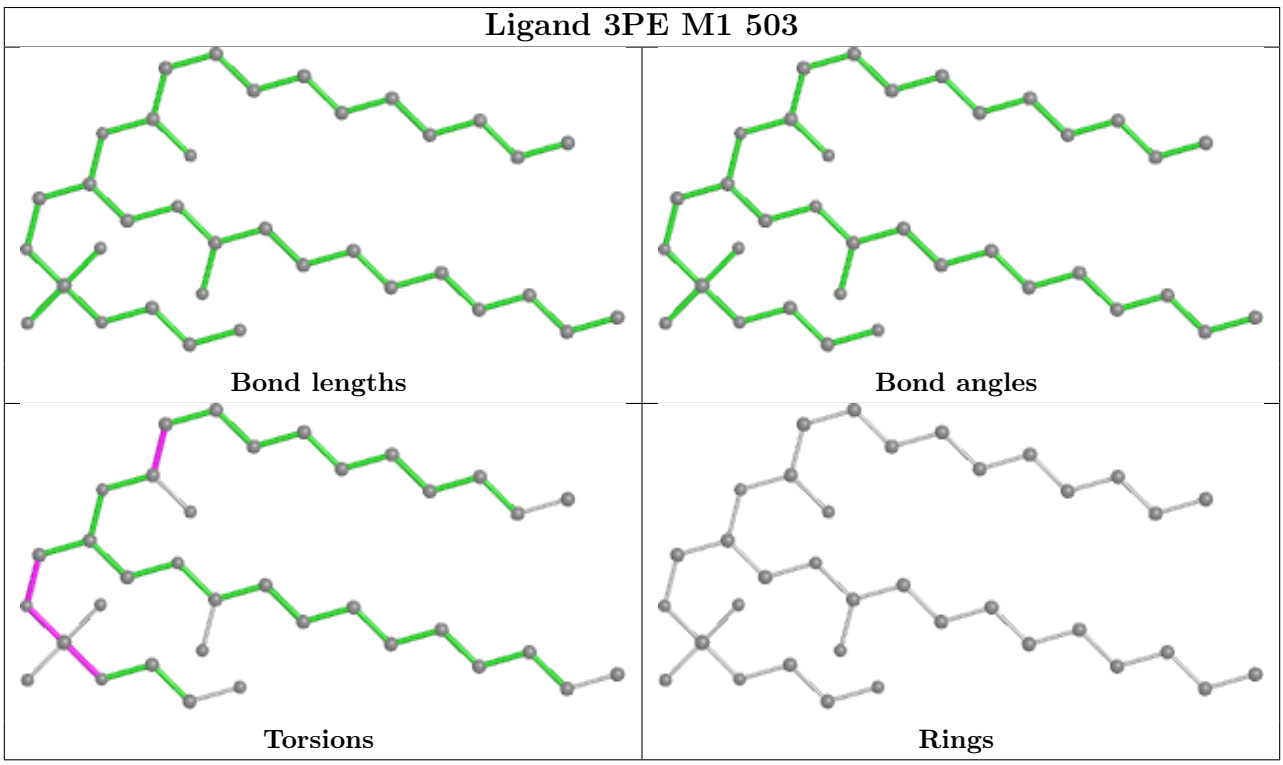
Ligand ZMP W1 201



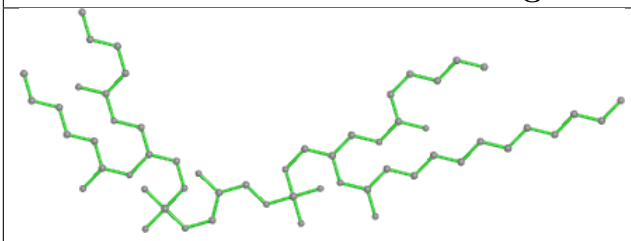
Ligand CDL O 301



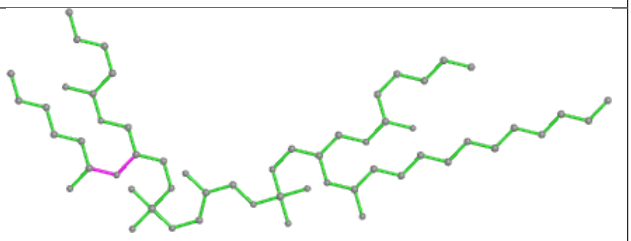
Ligand 3PE M1 503



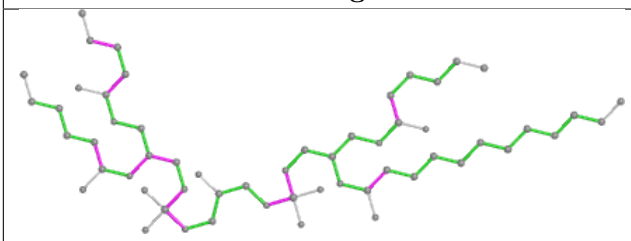
Ligand CDL R 102



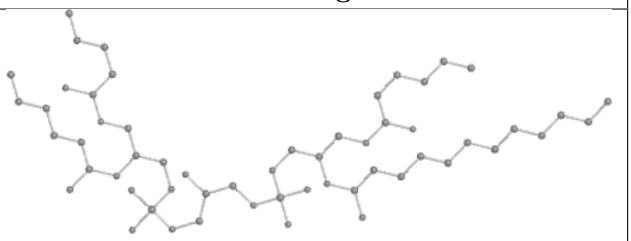
Bond lengths



Bond angles

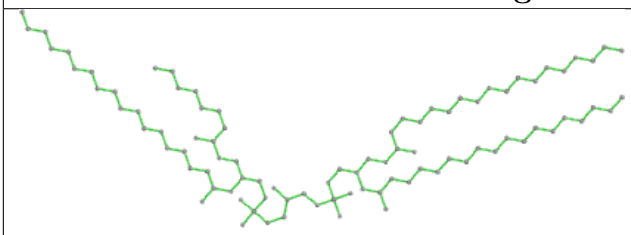


Torsions



Rings

Ligand CDL N1 401



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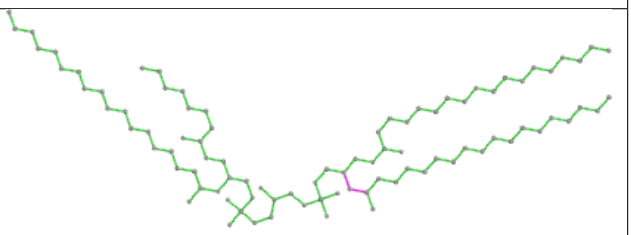
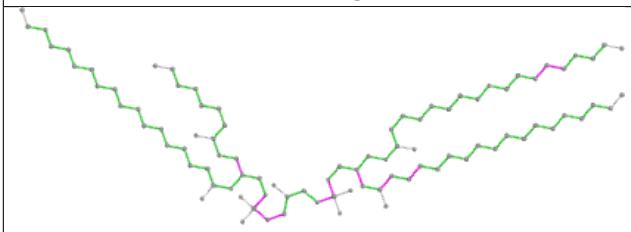
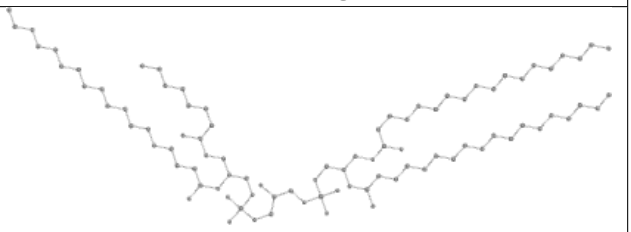


Bond angles

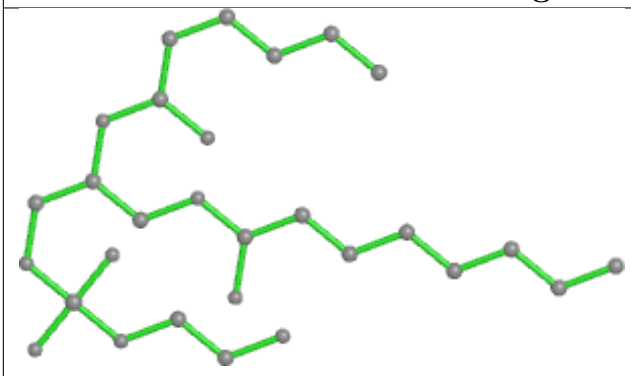


Torsions



Rings

Ligand 3PE o 302



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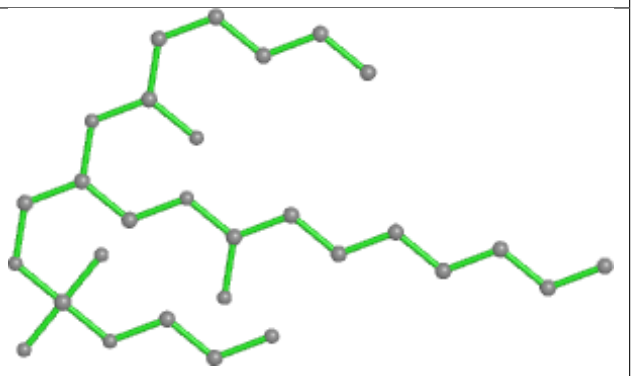
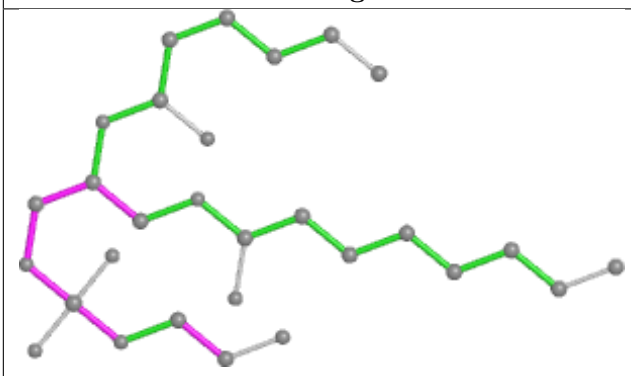


Bond angles



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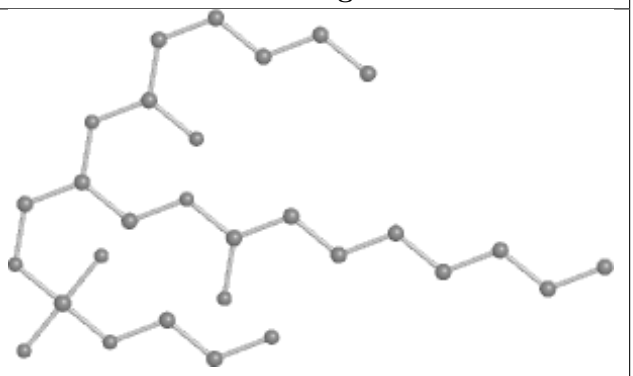
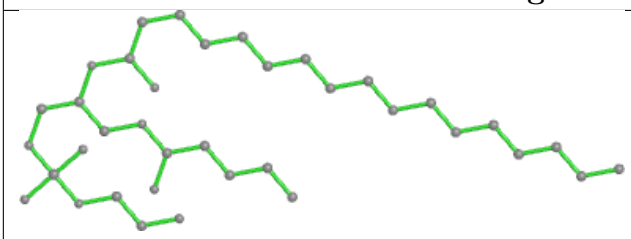
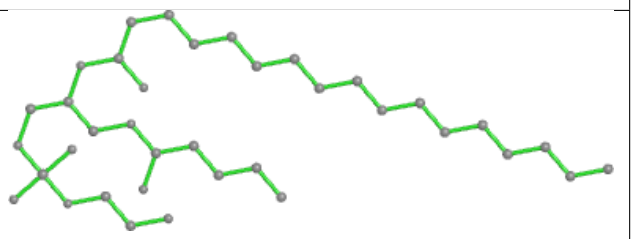


Rings

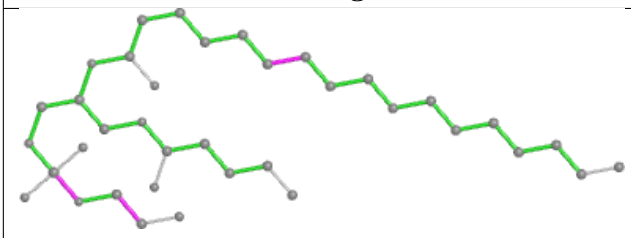
Ligand 3PE N 404



Bond lengths



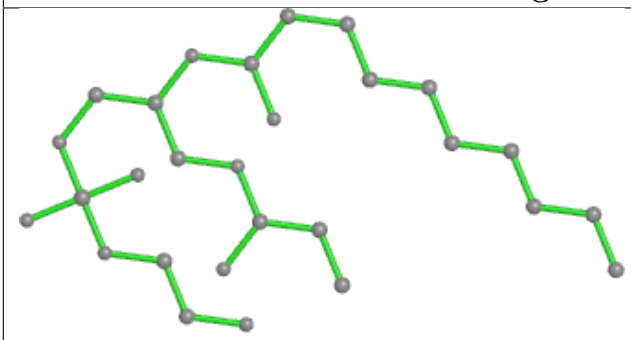
Bond angles



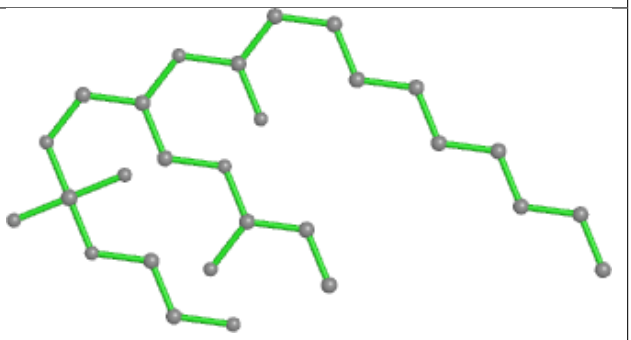
Torsions

Rings

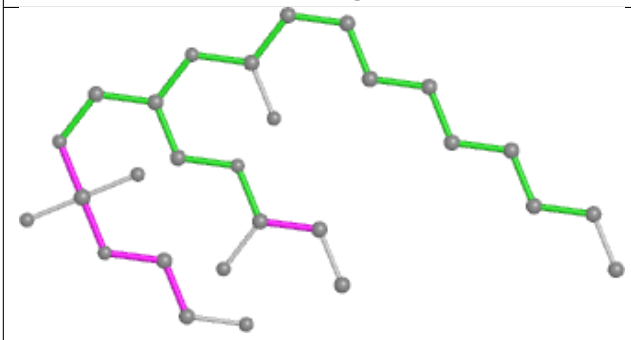
Ligand 3PE v 101



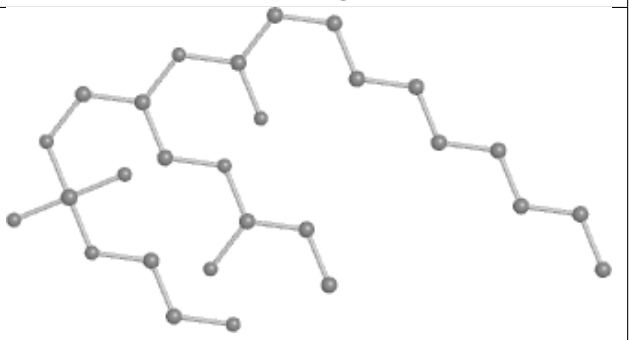
Bond lengths



Bond angles

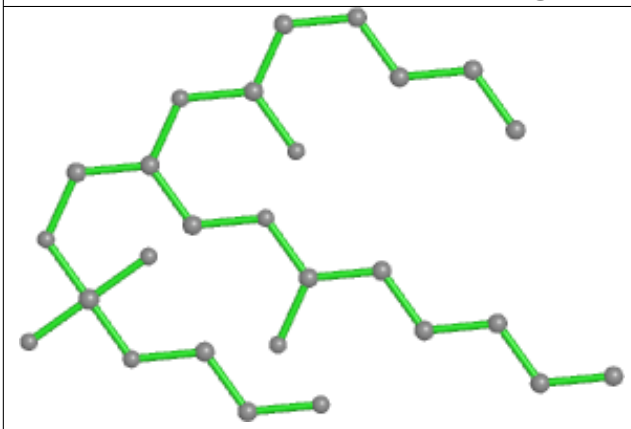


Torsions

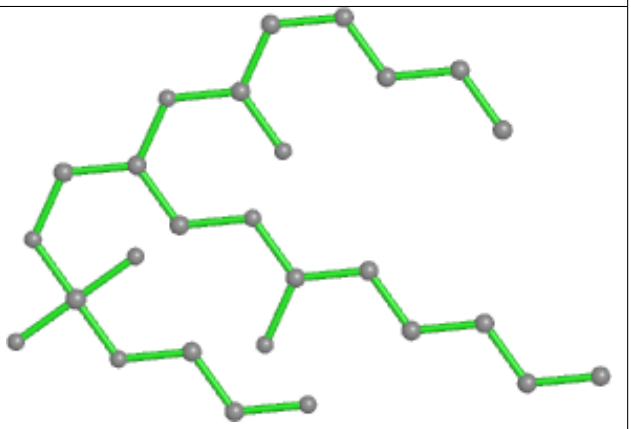


Rings

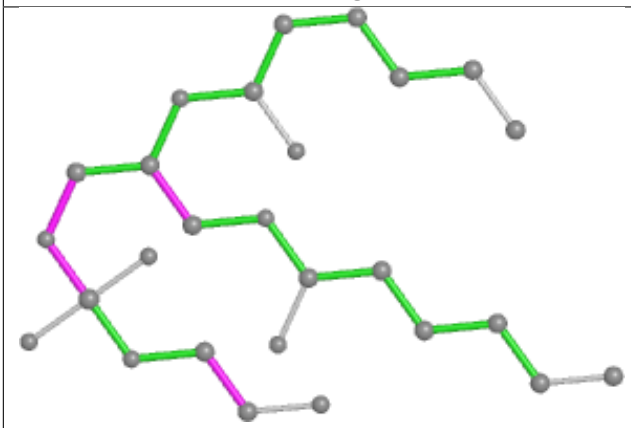
Ligand 3PE n 607



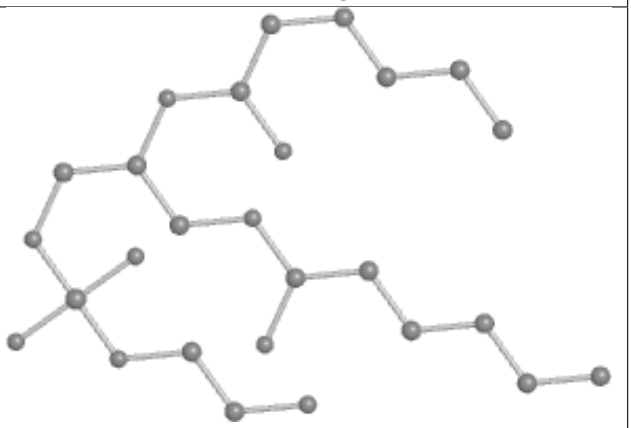
Bond lengths



Bond angles

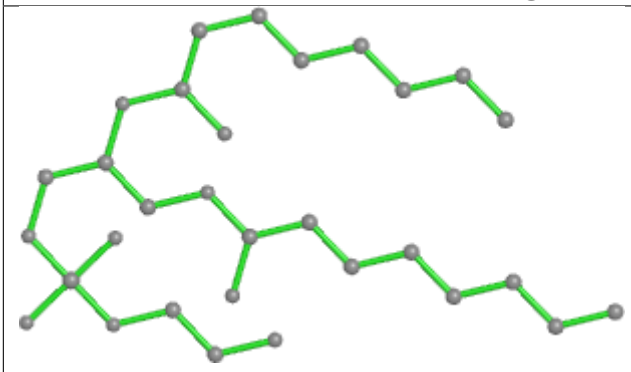


Torsions

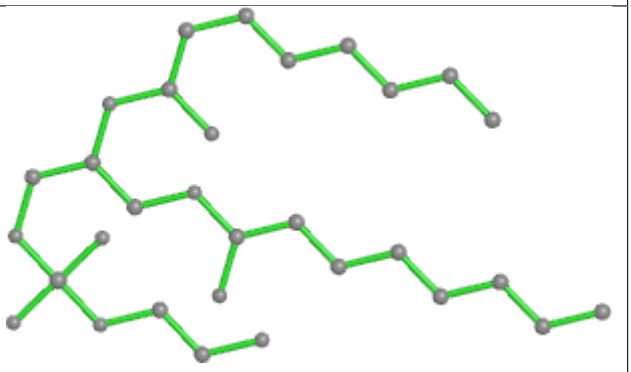


Rings

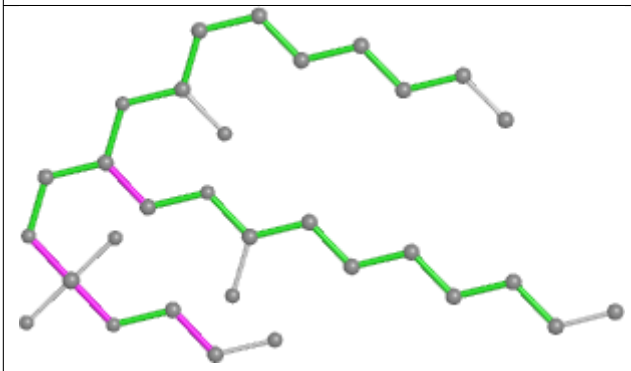
Ligand 3PE d1 202



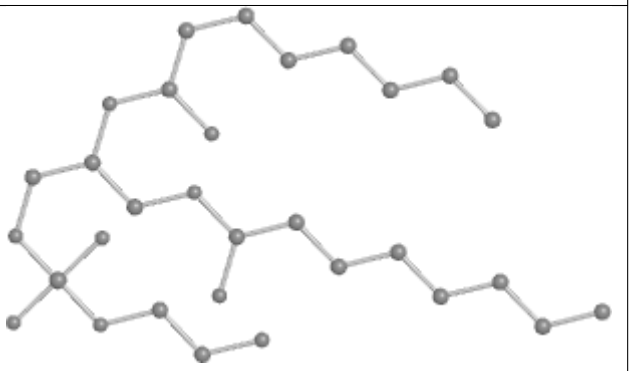
Bond lengths



Bond angles

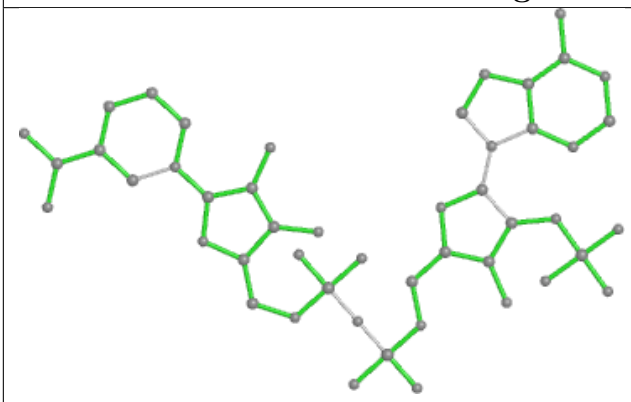


Torsions

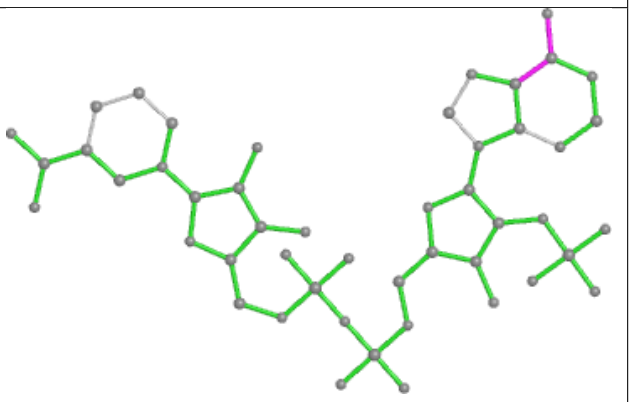


Rings

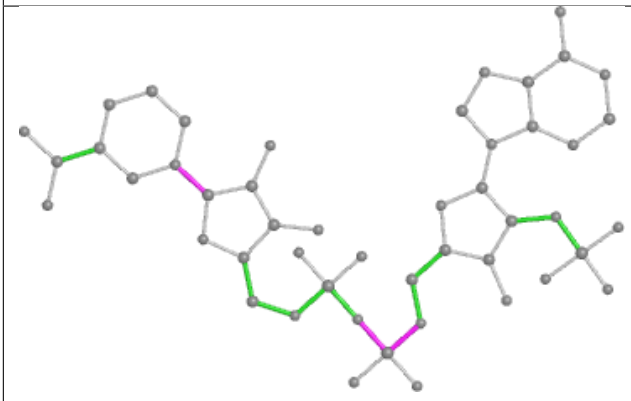
Ligand NDP P1 501



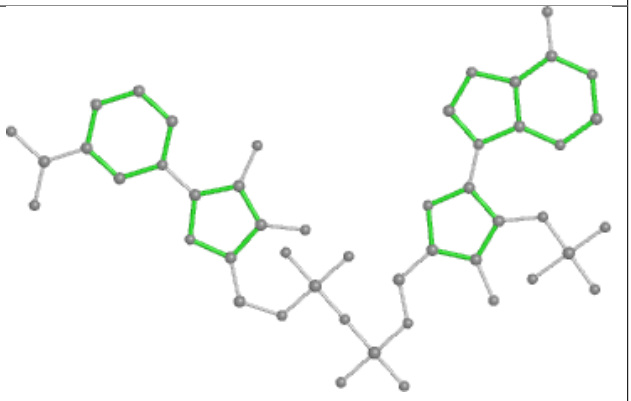
Bond lengths



Bond angles

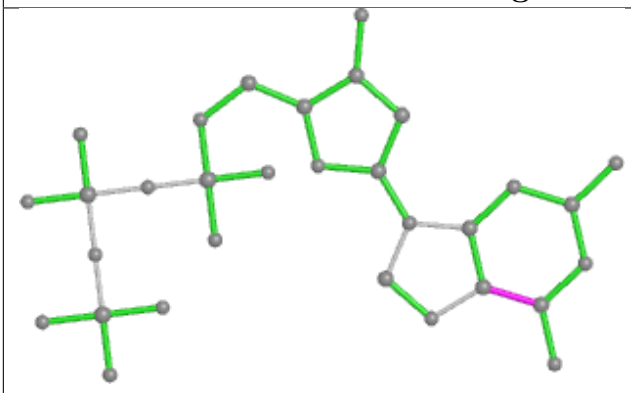


Torsions

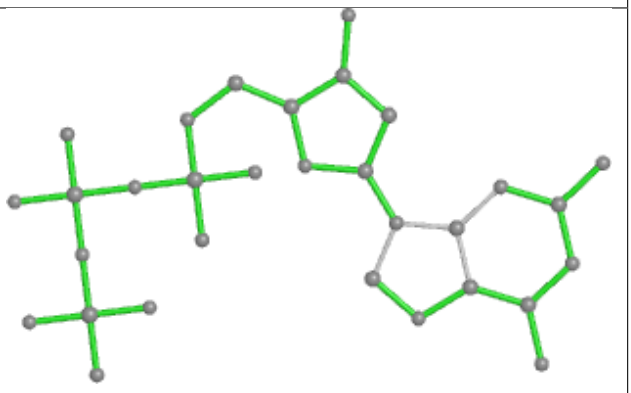


Rings

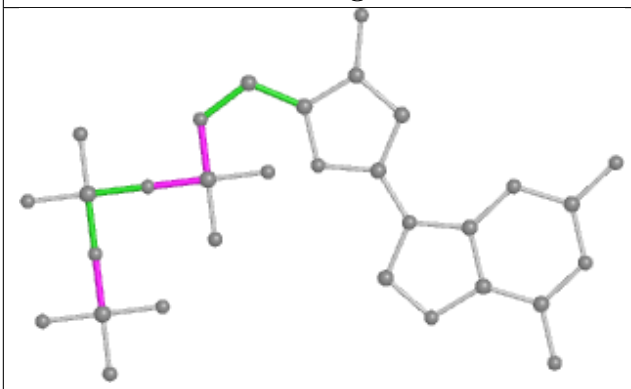
Ligand DGT O1 401



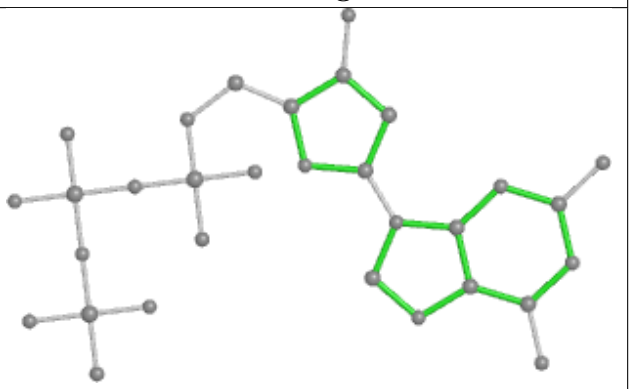
Bond lengths



Bond angles

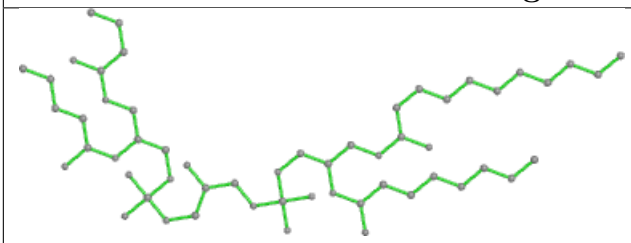


Torsions

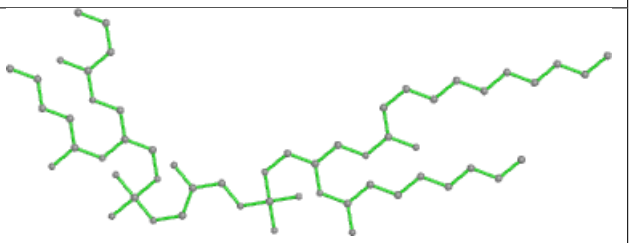


Rings

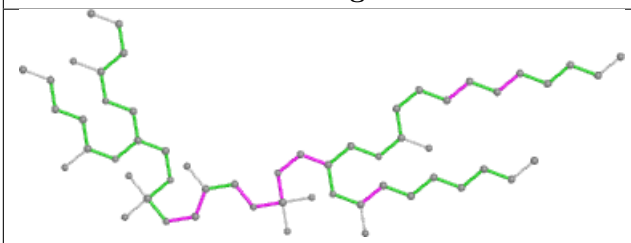
Ligand CDL G 101



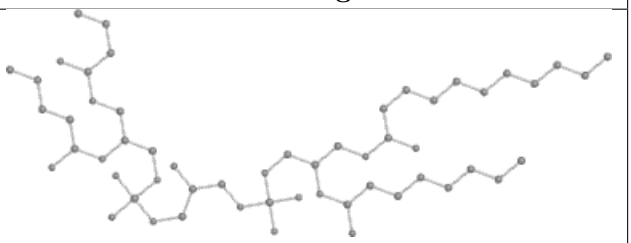
Bond lengths



Bond angles

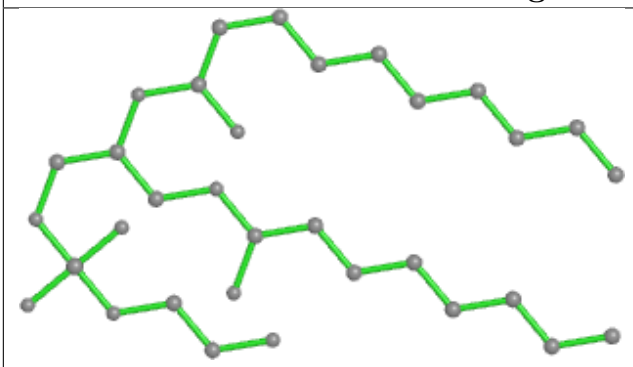


Torsions

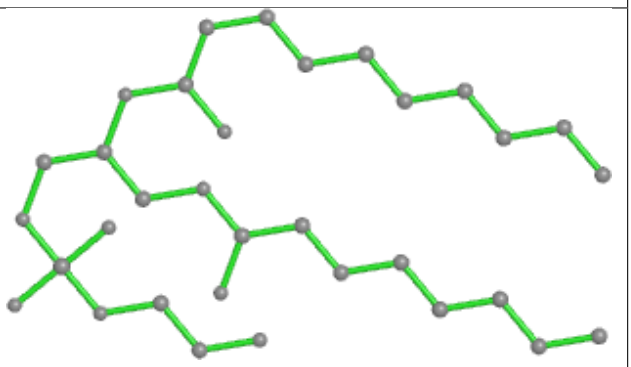


Rings

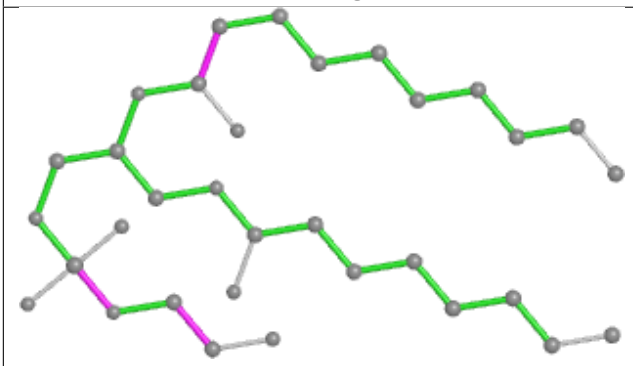
Ligand 3PE O 302



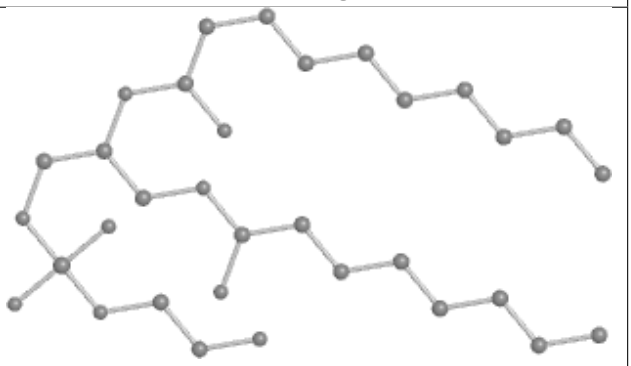
Bond lengths



Bond angles

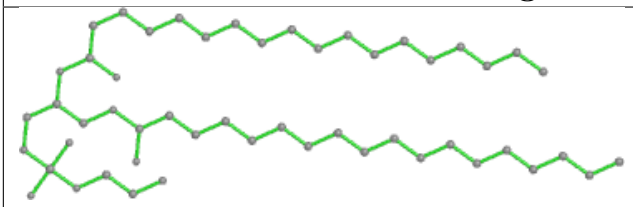


Torsions

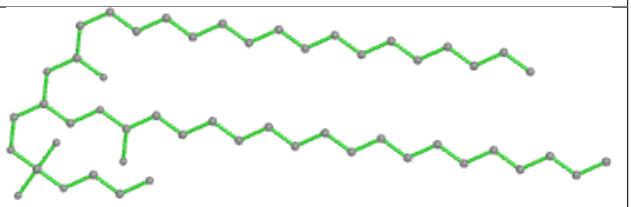


Rings

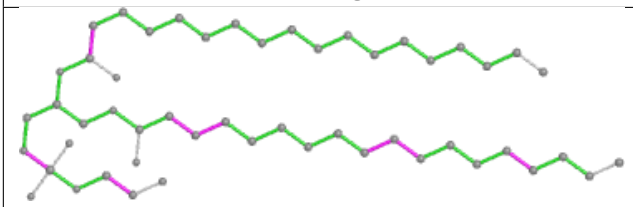
Ligand 3PE D1 501



Bond lengths



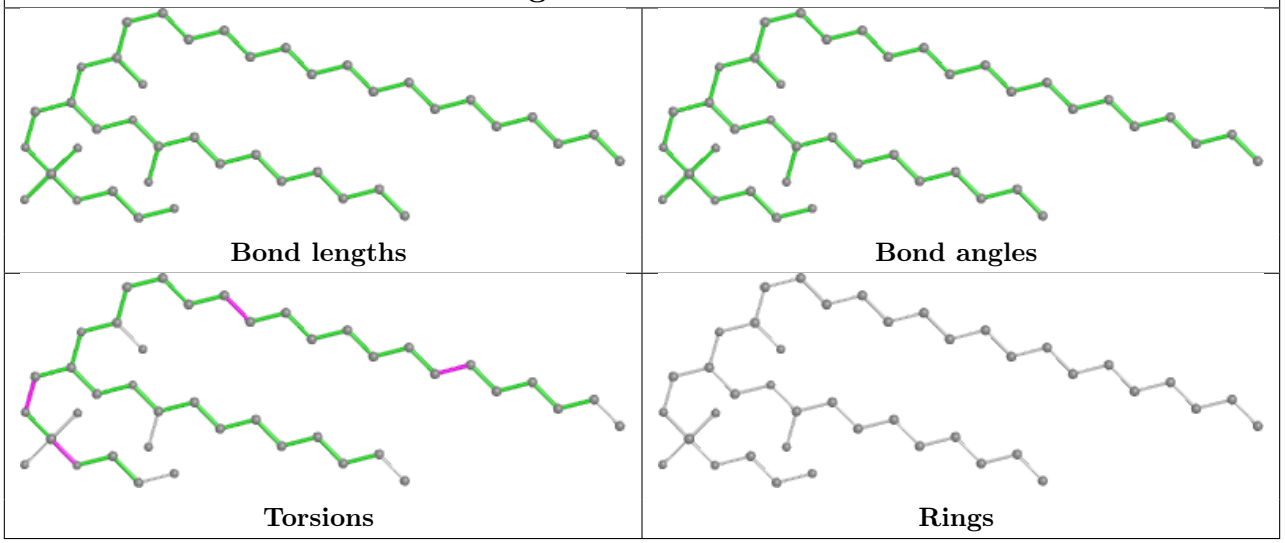
Bond angles



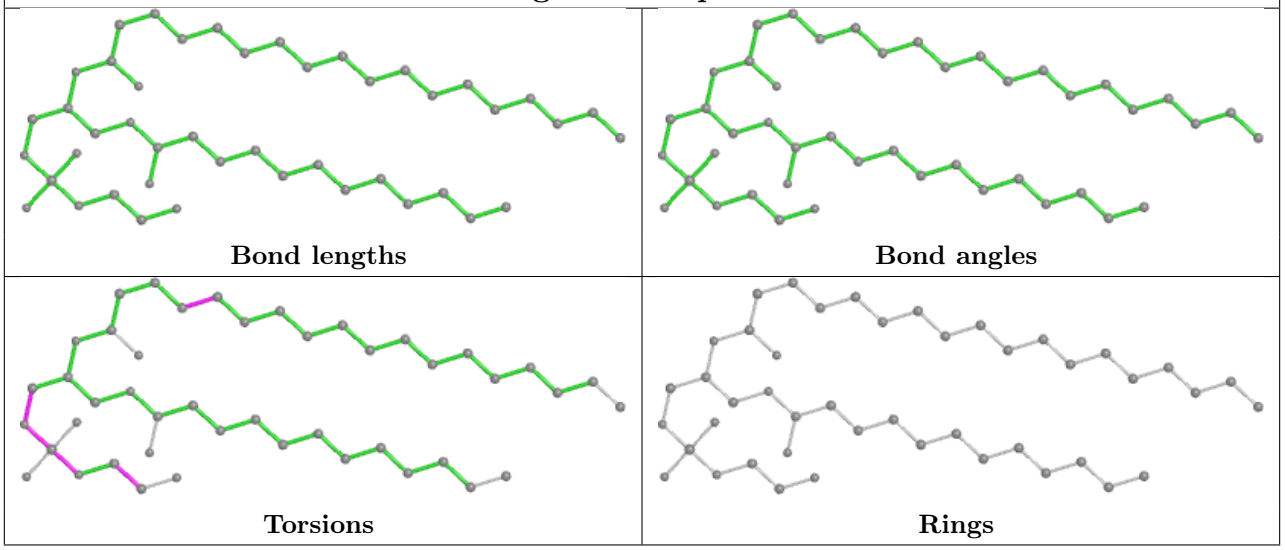
Torsions

Rings

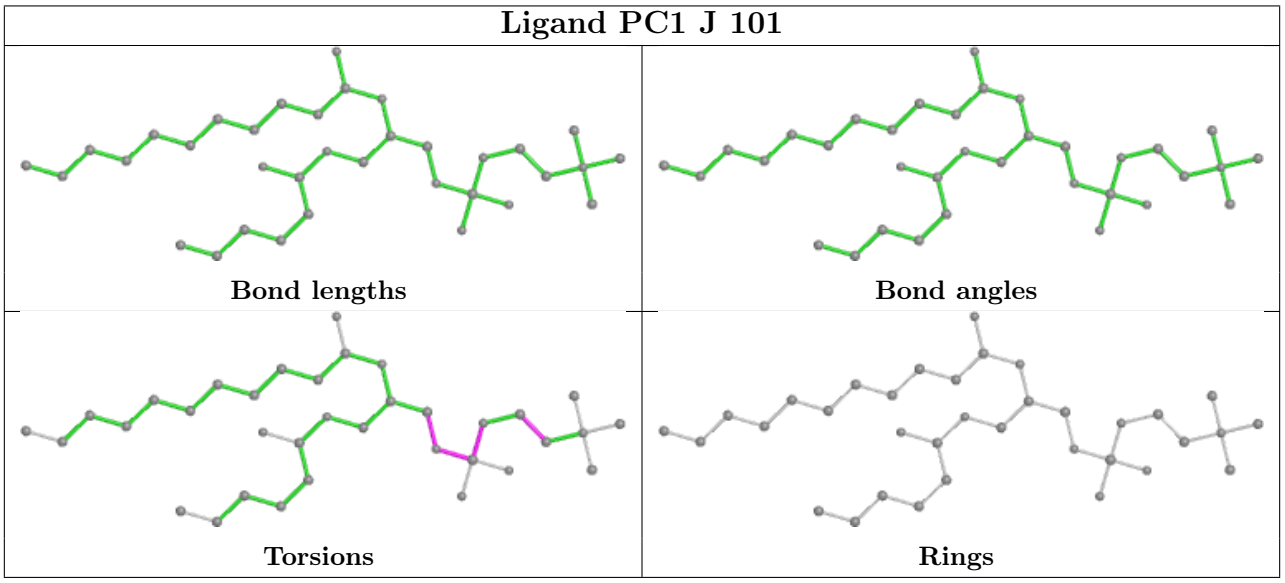
Ligand 3PE i1 201



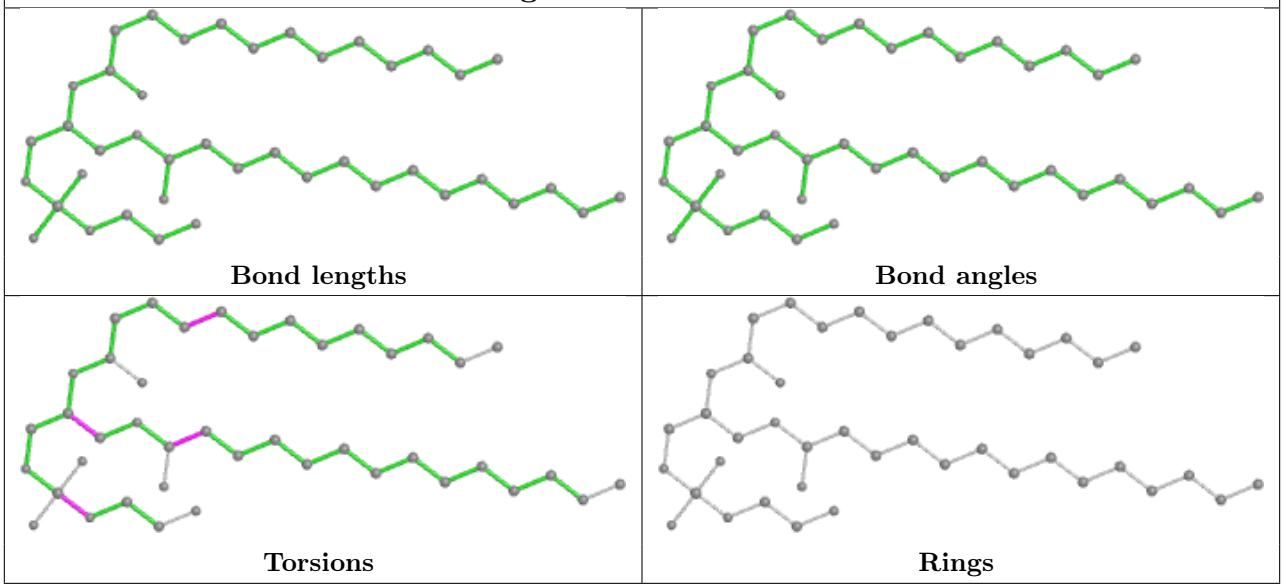
Ligand 3PE p 301



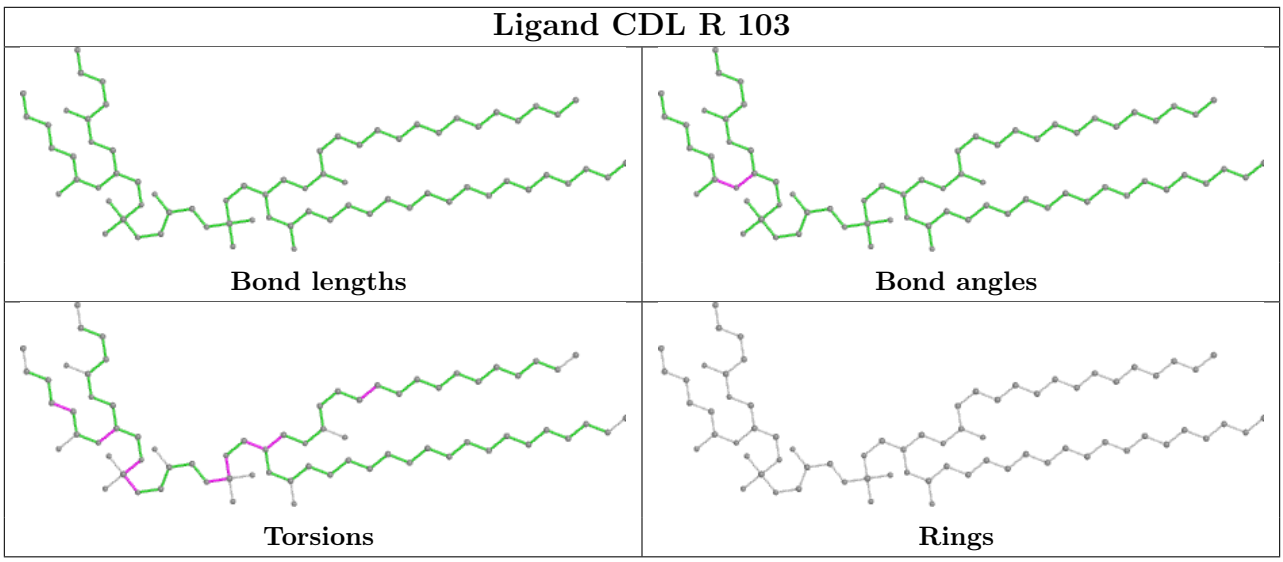
Ligand PC1 J 101



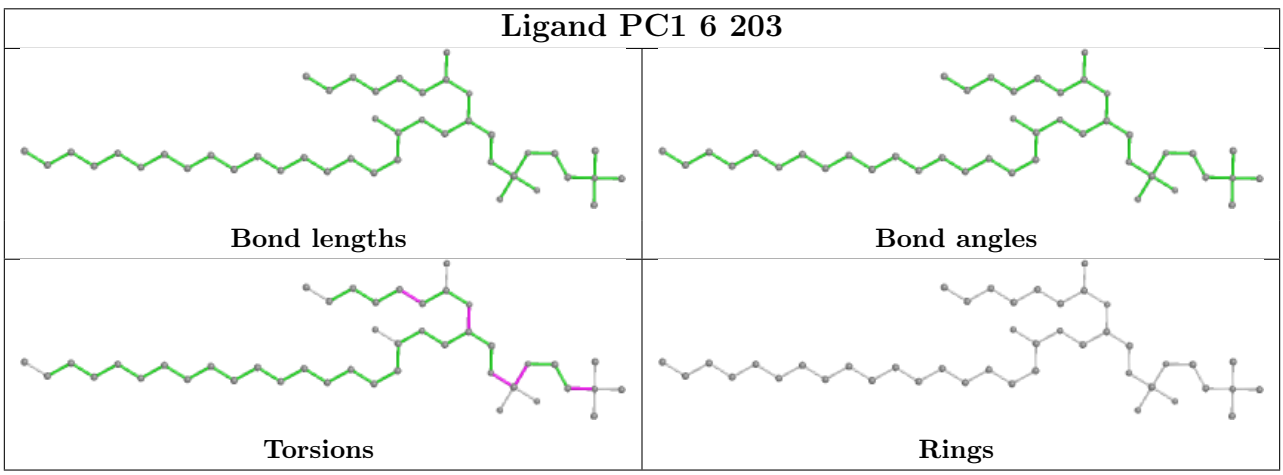
Ligand 3PE Y1 204



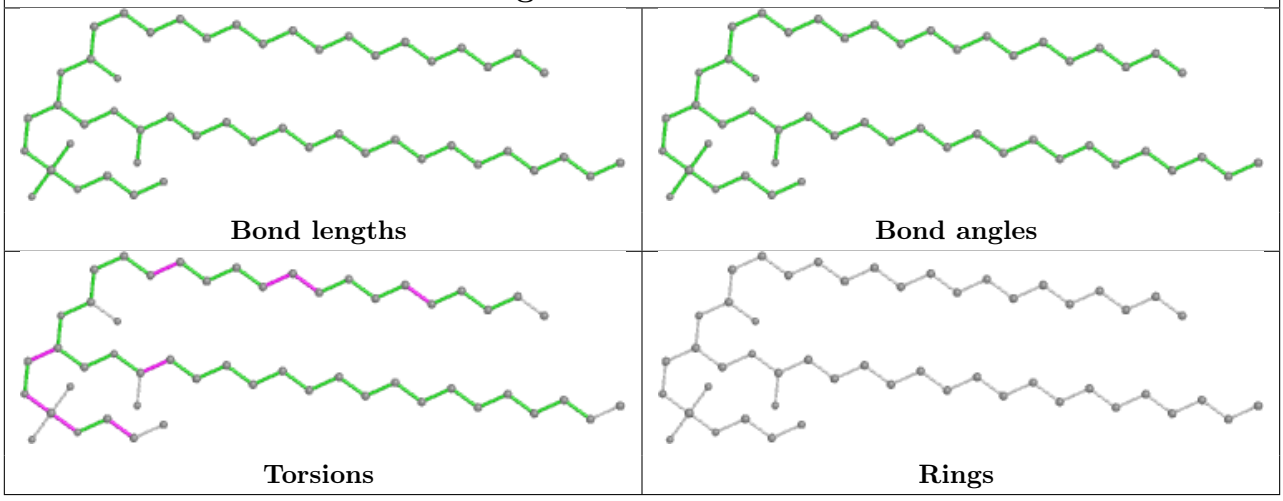
Ligand CDL R 103



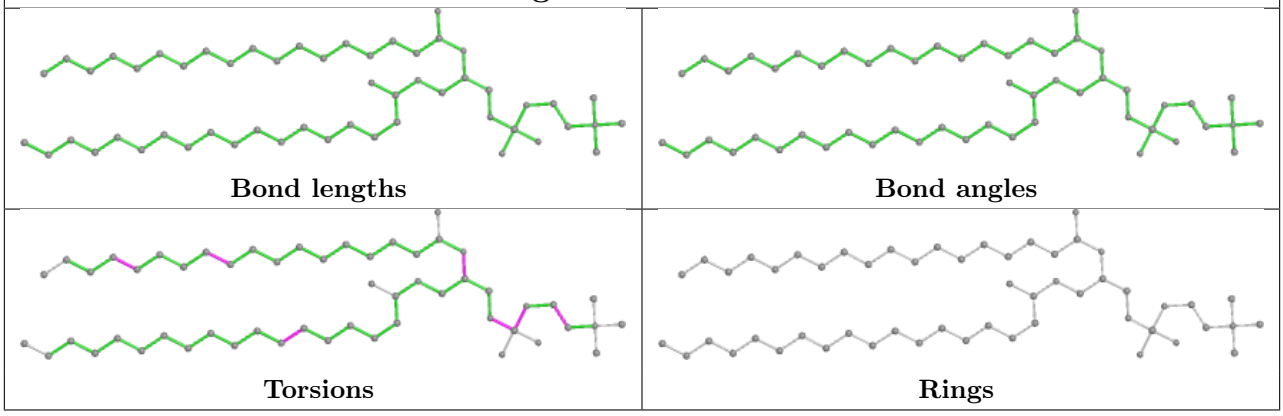
Ligand PC1 6 203



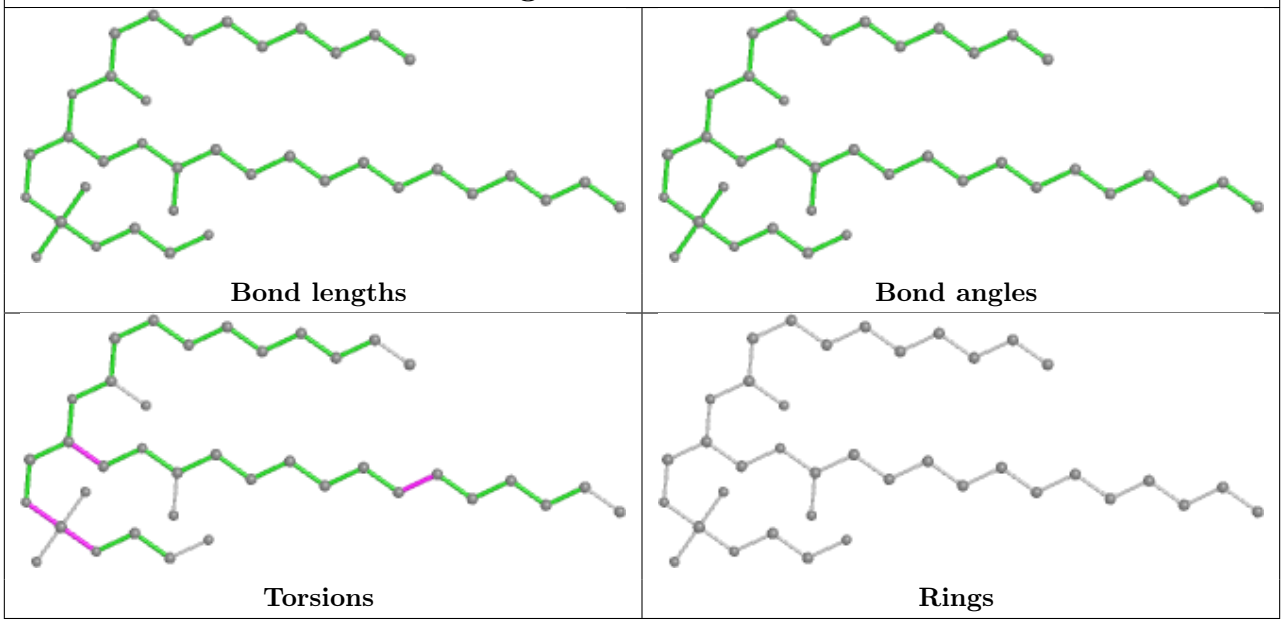
Ligand 3PE M1 502



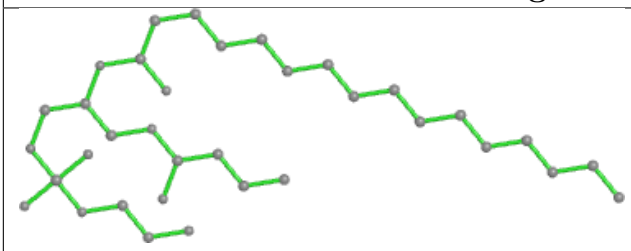
Ligand PC1 9 203



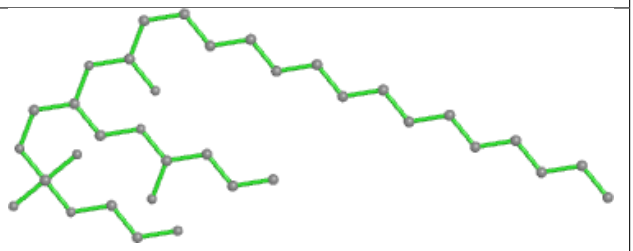
Ligand 3PE N1 402



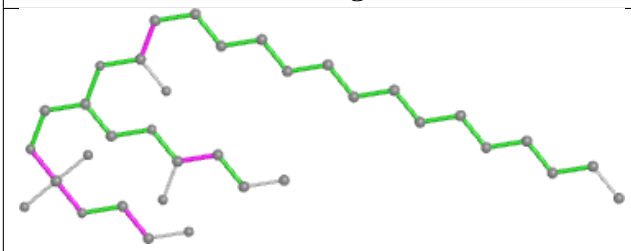
Ligand 3PE C 403



Bond lengths



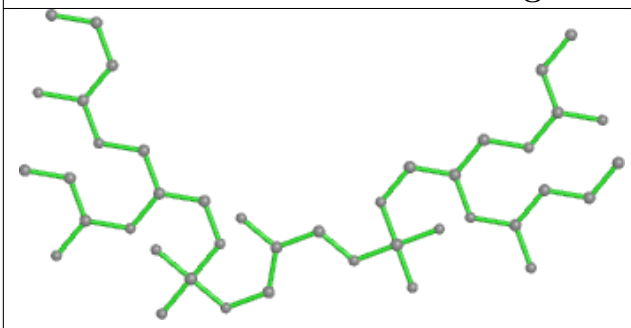
Bond angles



Torsions

Rings

Ligand CDL C 404



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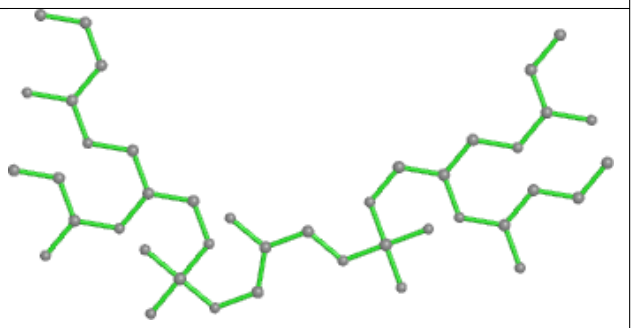
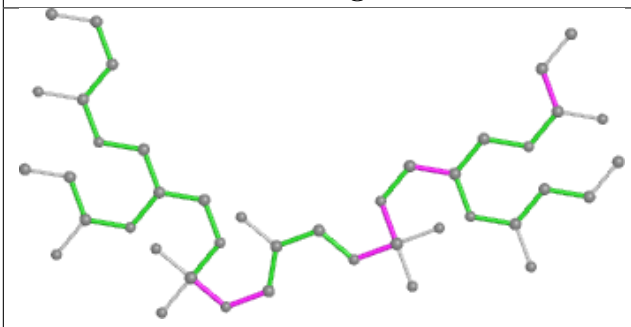


Bond angles



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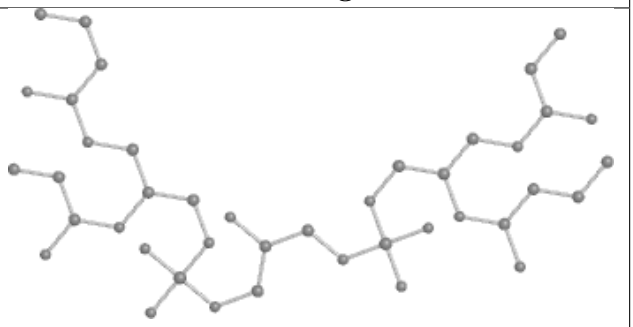
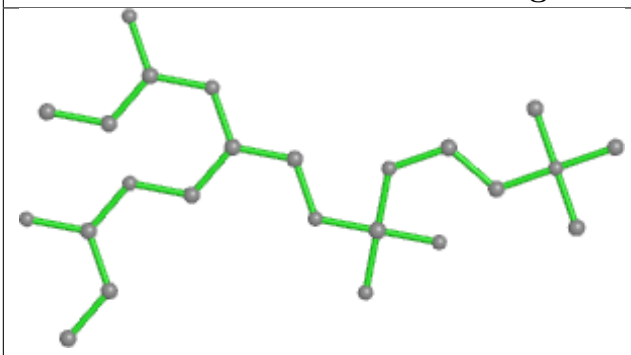
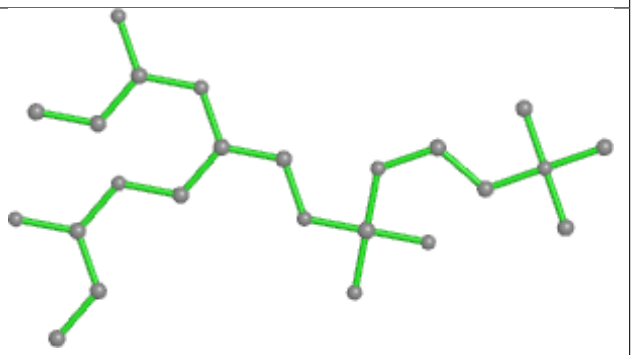


Rings

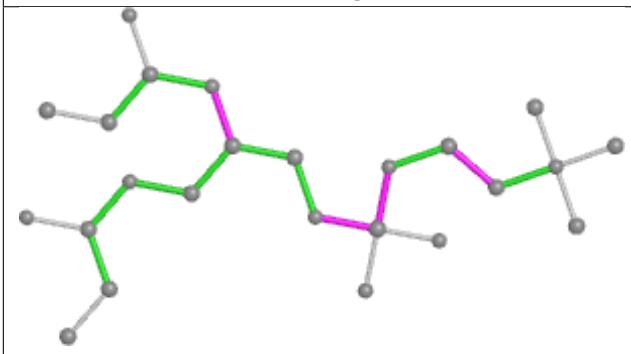
Ligand PC1 L 502



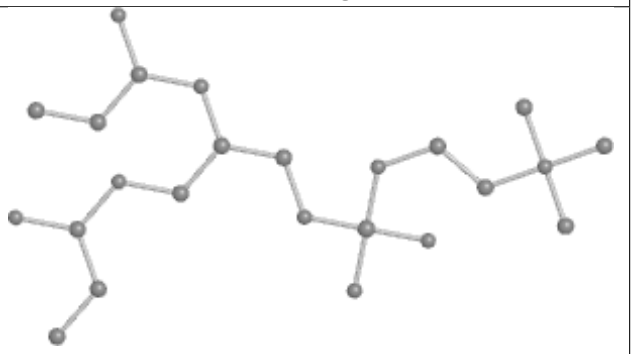
Bond lengths



Bond angles

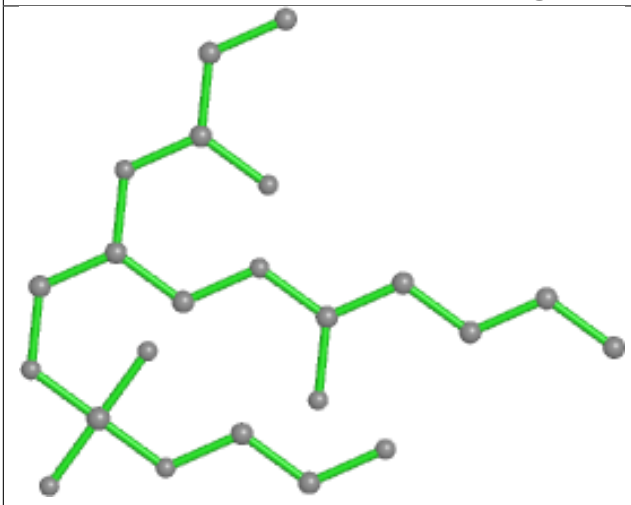


Torsions

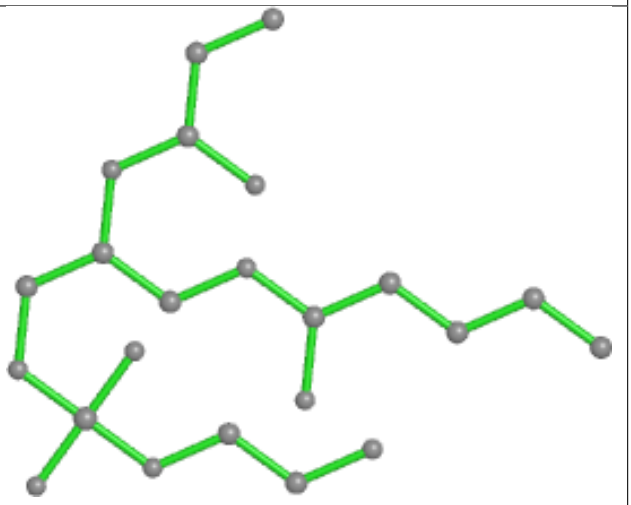


Rings

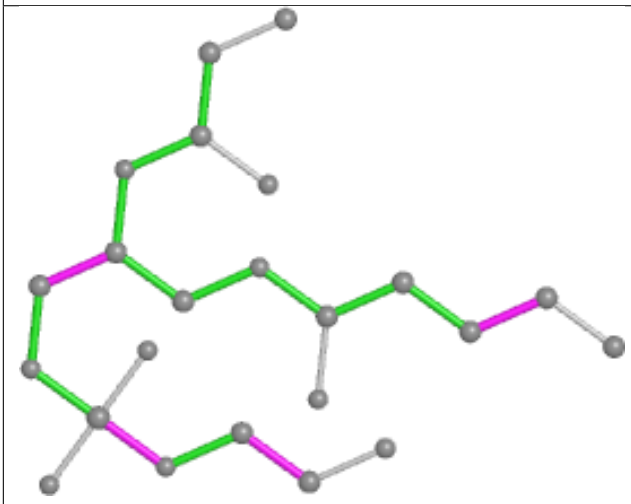
Ligand 3PE L 501



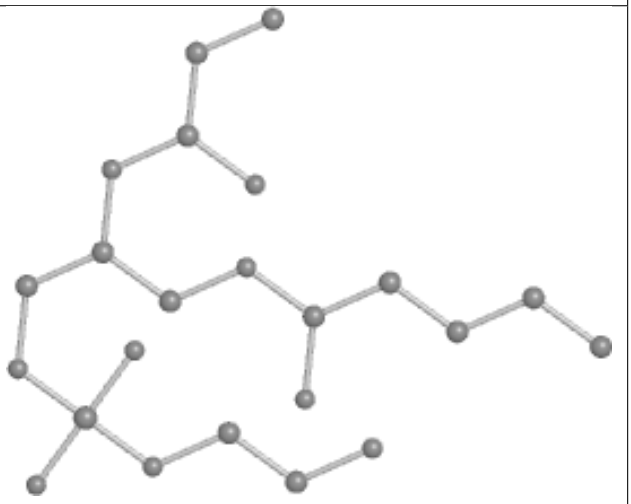
Bond lengths



Bond angles

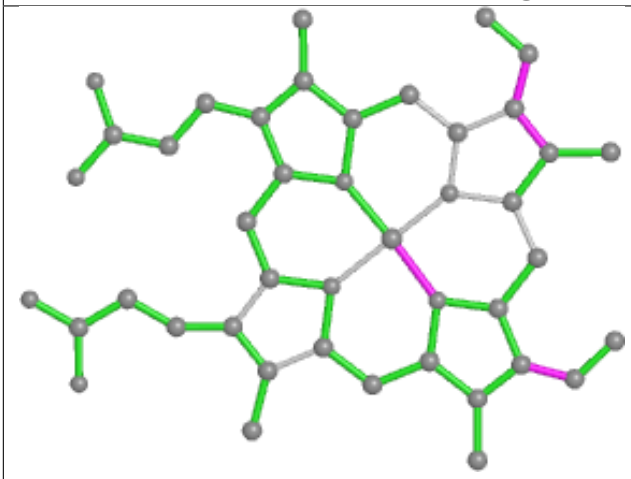


Torsions

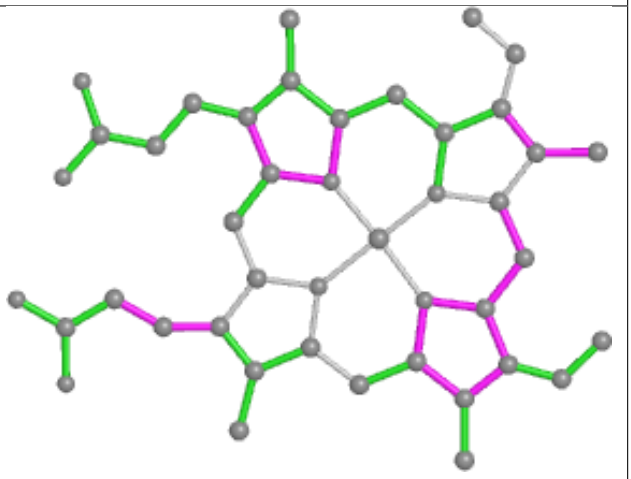


Rings

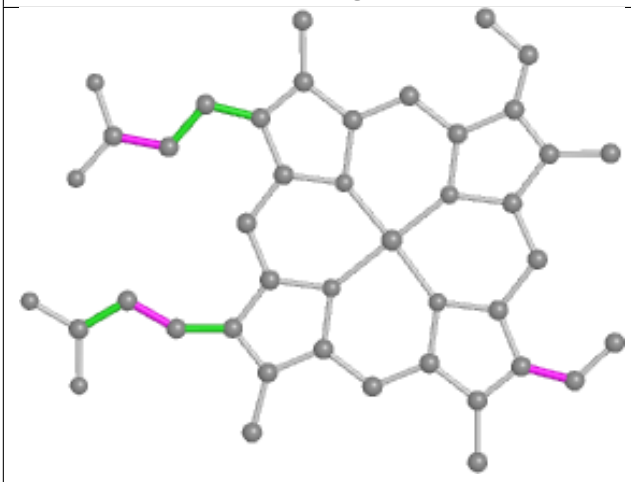
Ligand HEM N 403



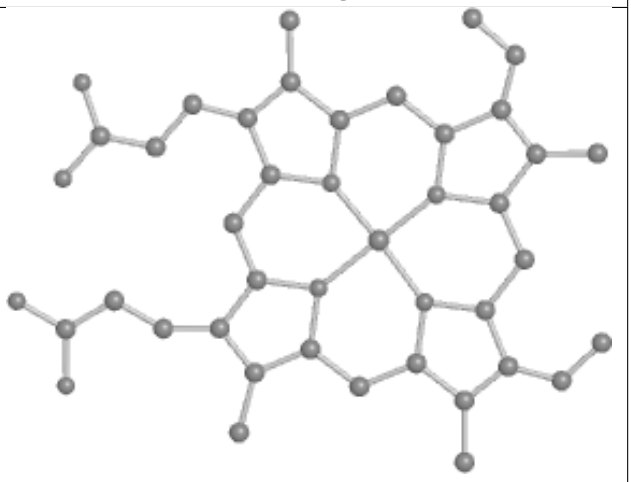
Bond lengths



Bond angles

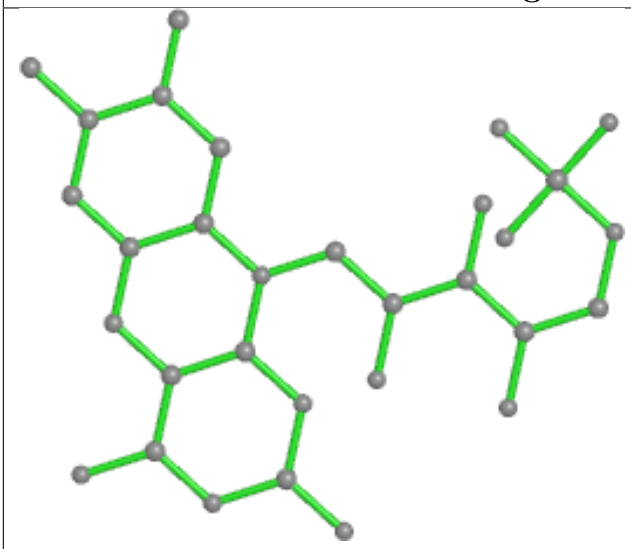


Torsions

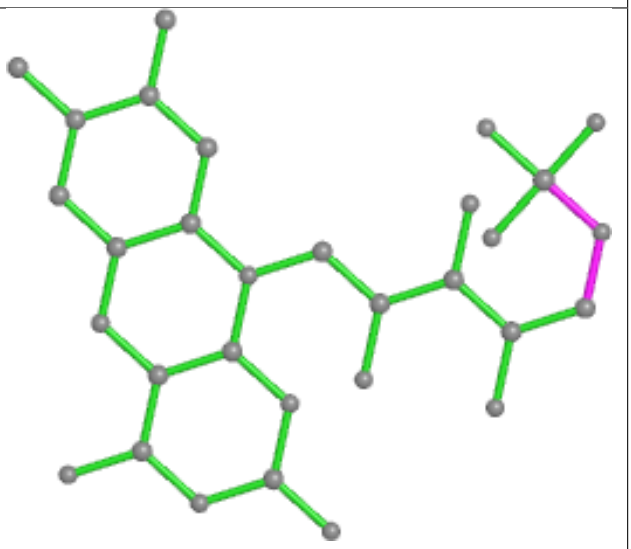


Rings

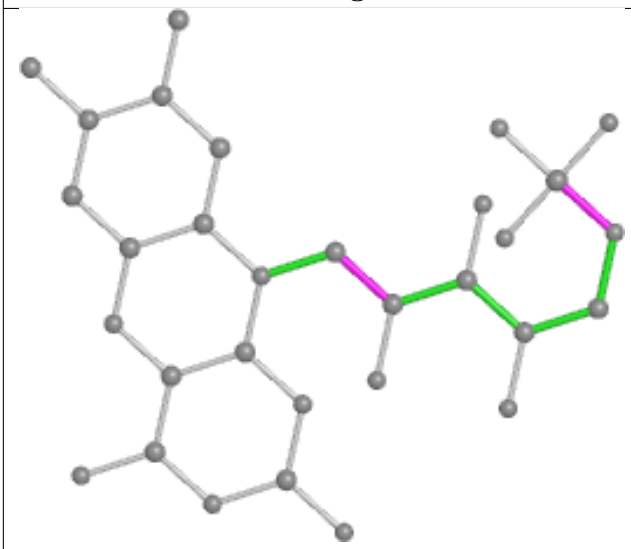
Ligand FMN 1 501



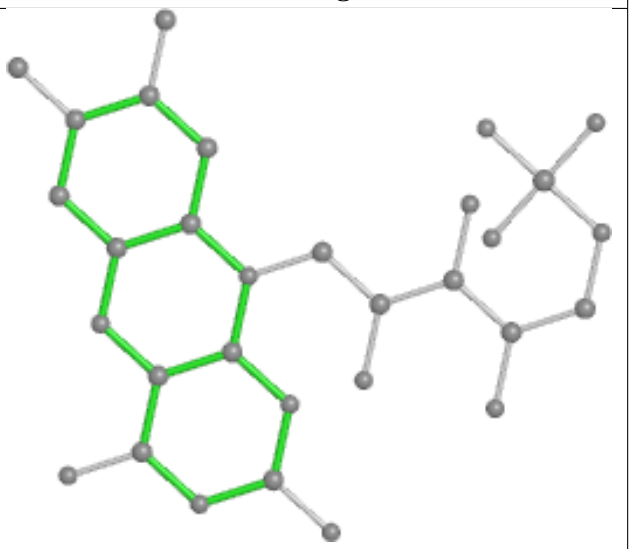
Bond lengths



Bond angles

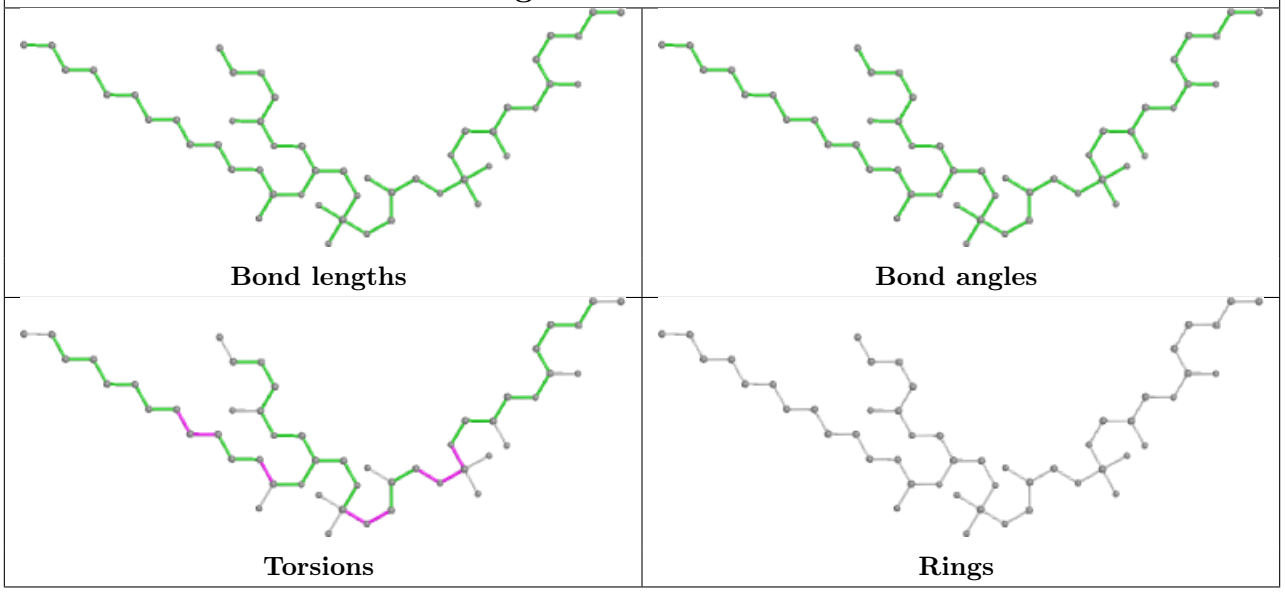


Torsions

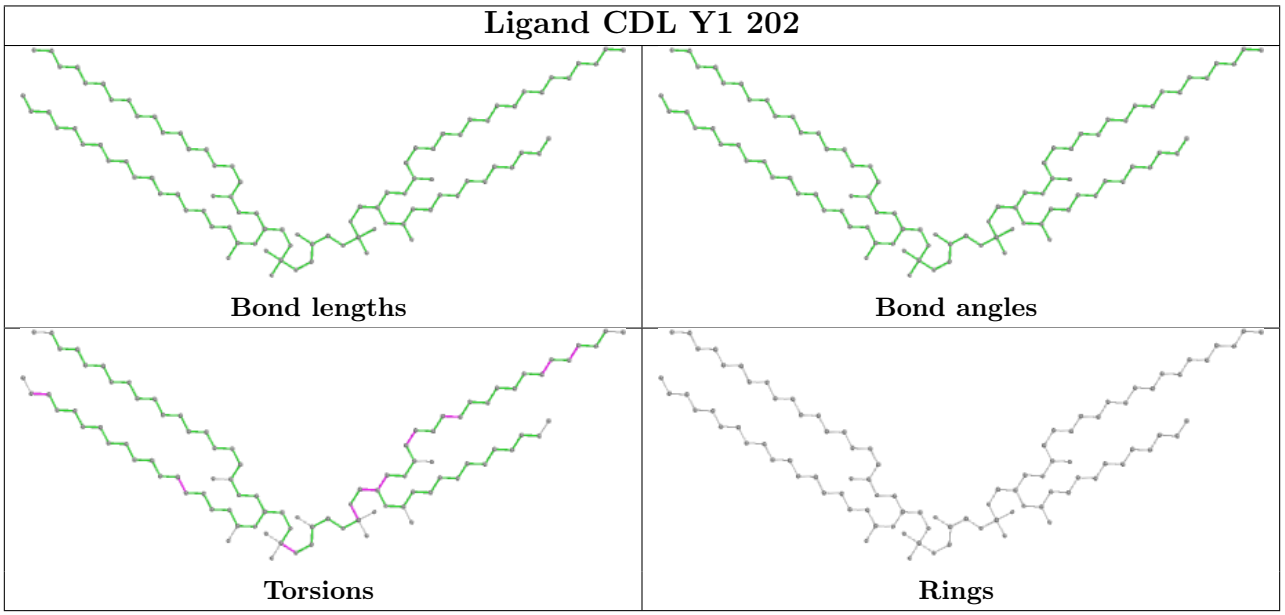


Rings

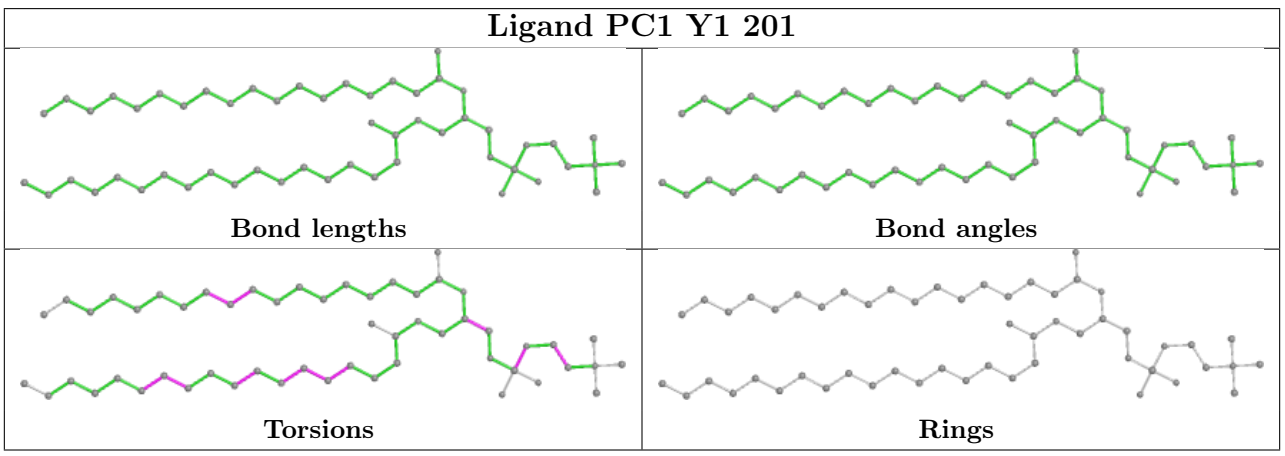
Ligand CDL H1 402

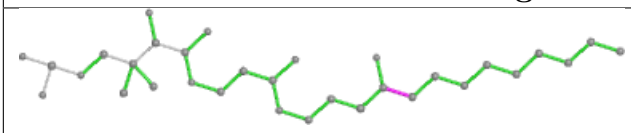
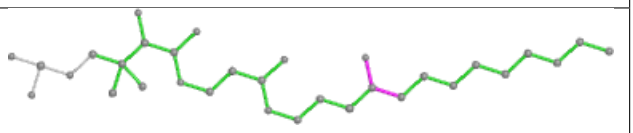
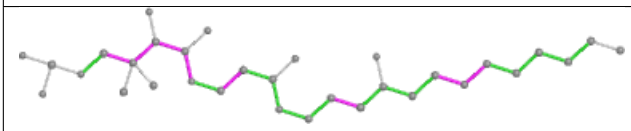
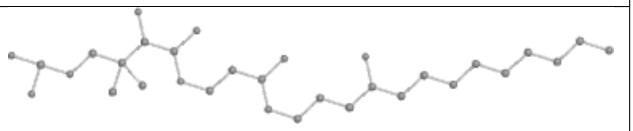


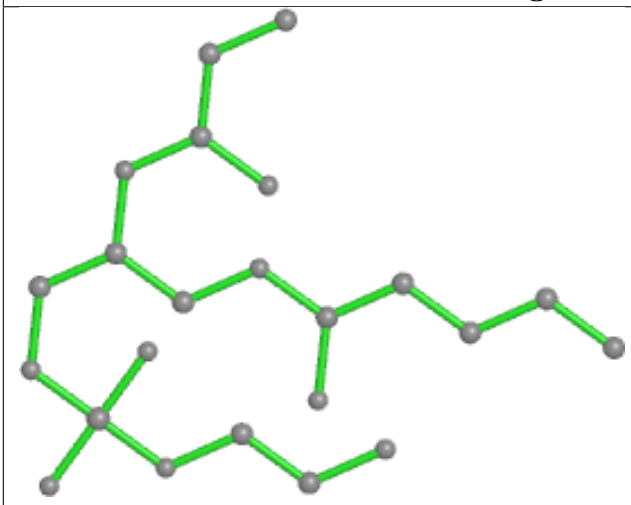
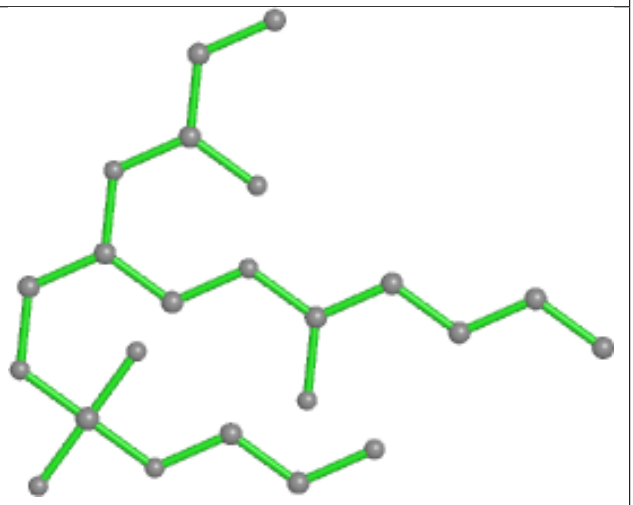
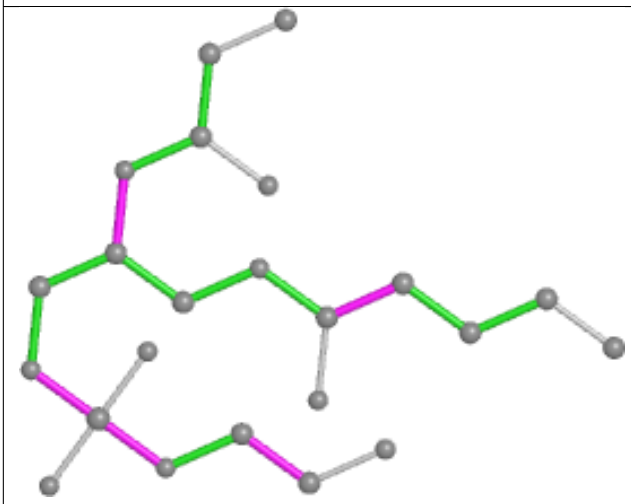
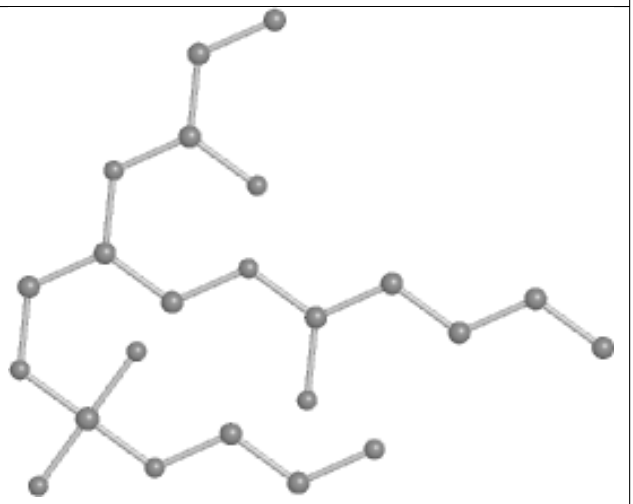
Ligand CDL Y1 202



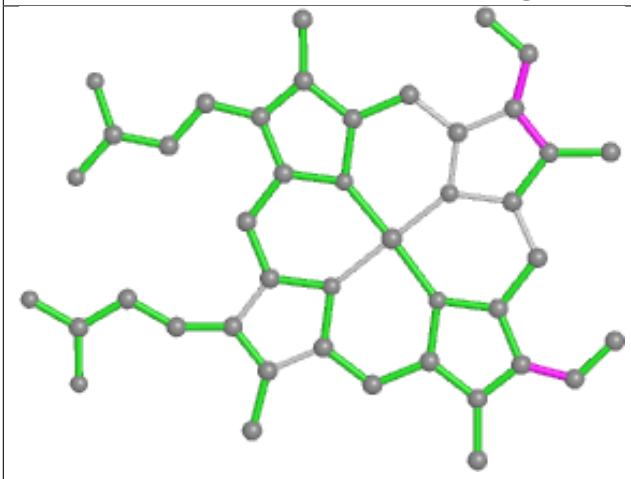
Ligand PC1 Y1 201



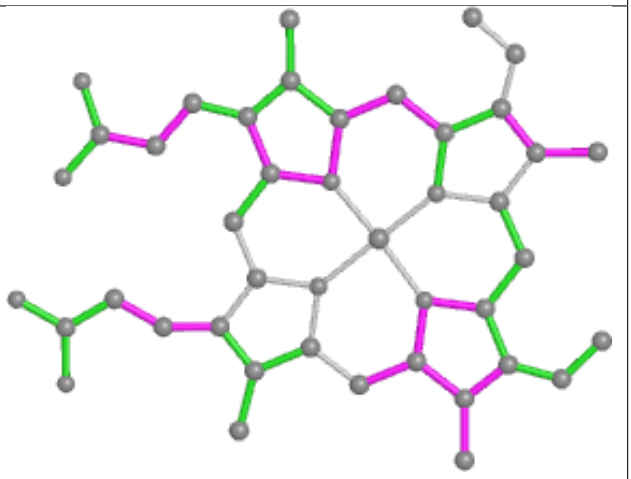
Ligand ZMP n1 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

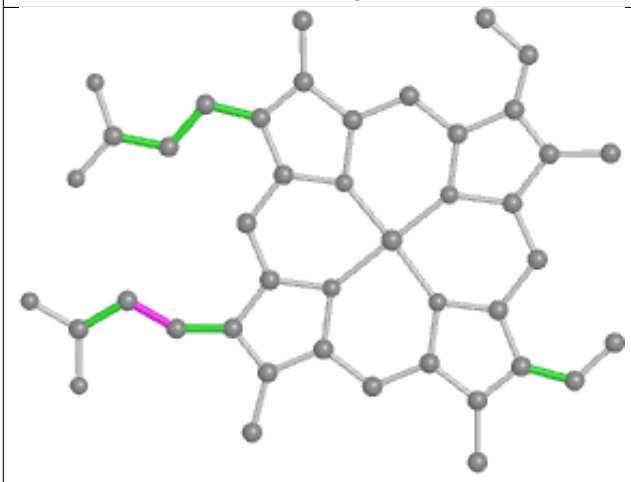
Ligand HEM N 402



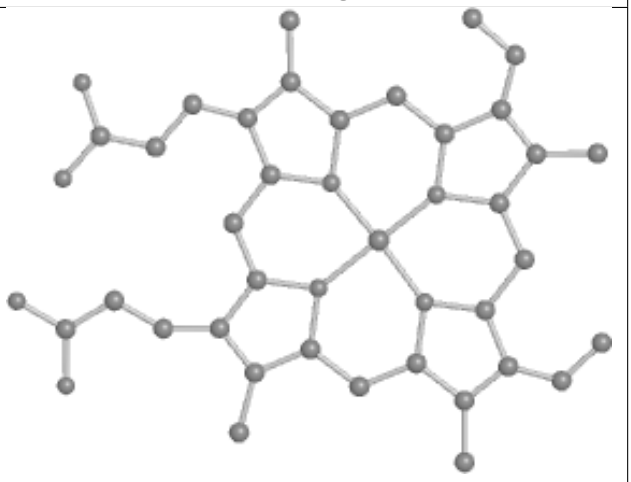
Bond lengths



Bond angles

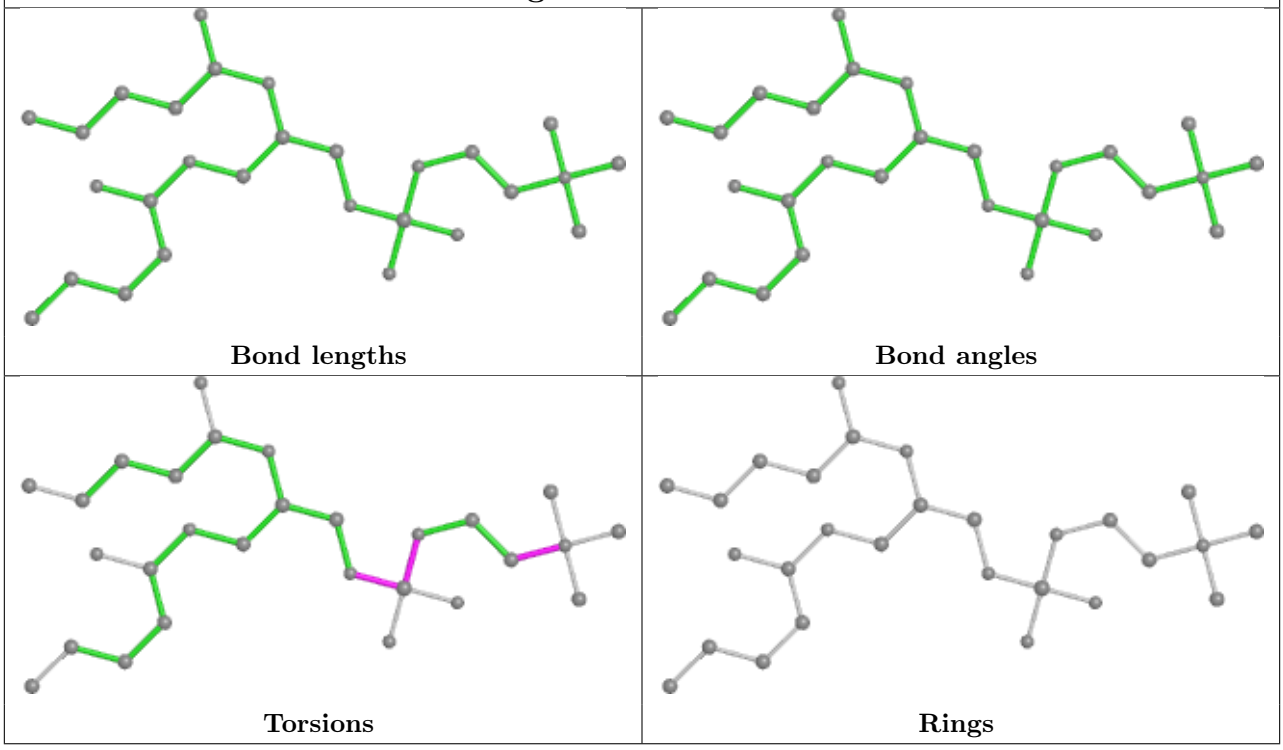


Torsions

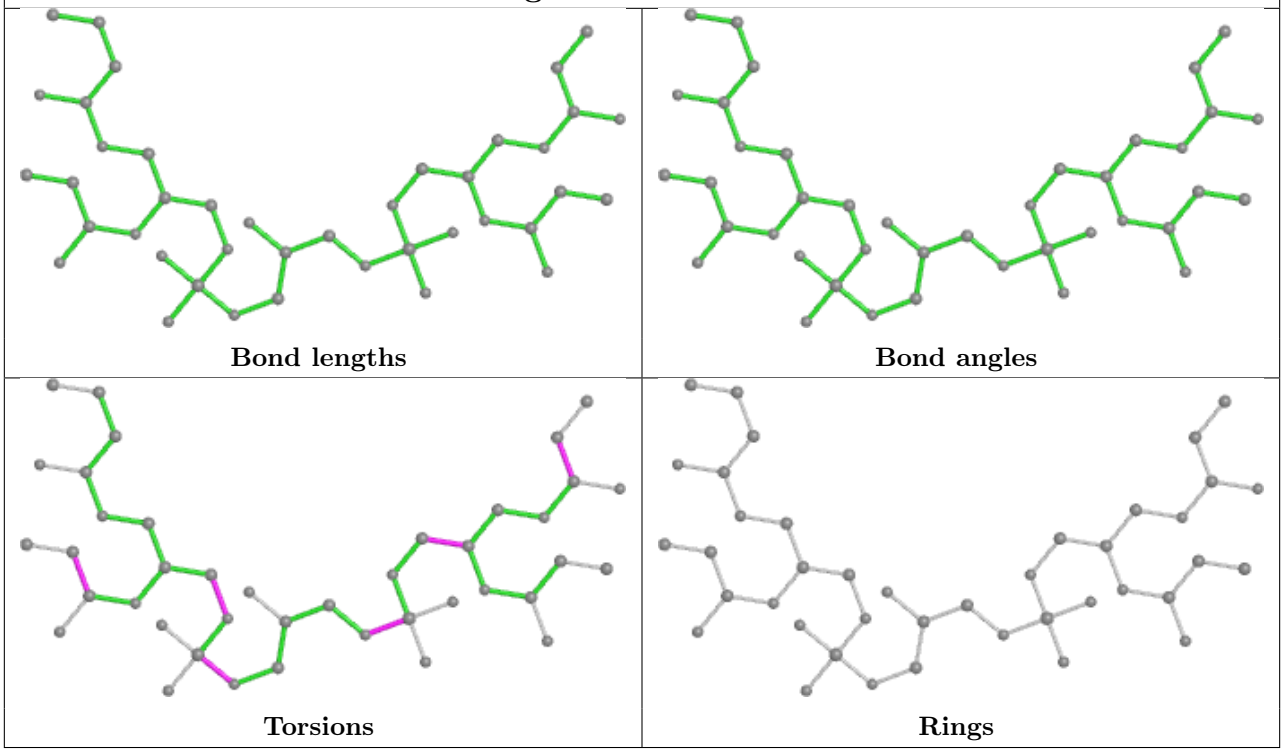


Rings

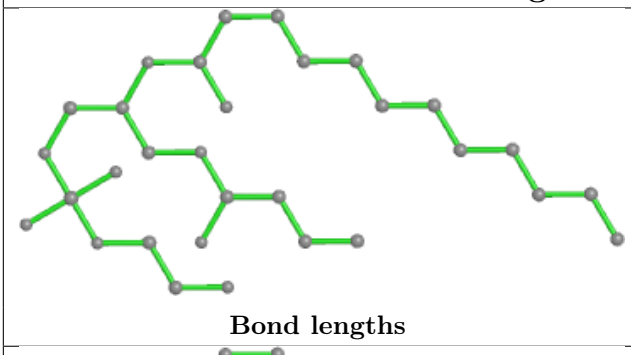
Ligand PC1 K 101



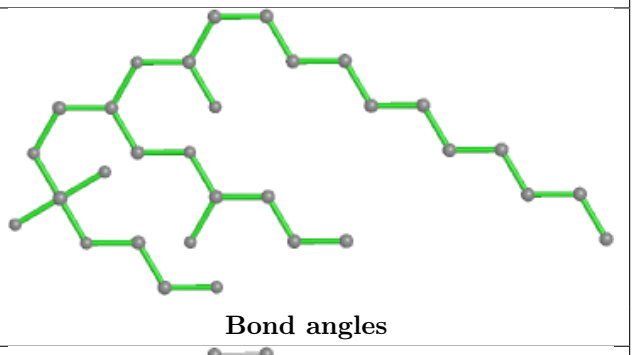
Ligand CDL R 101



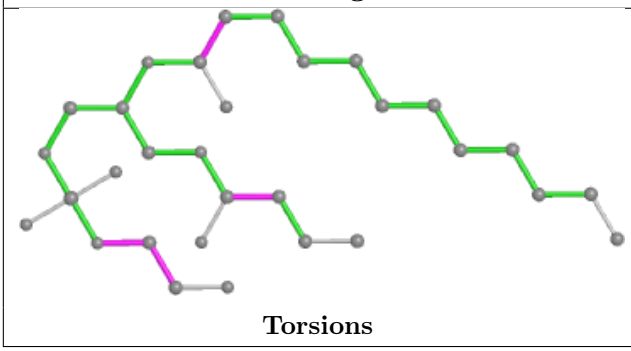
Ligand 3PE C 405



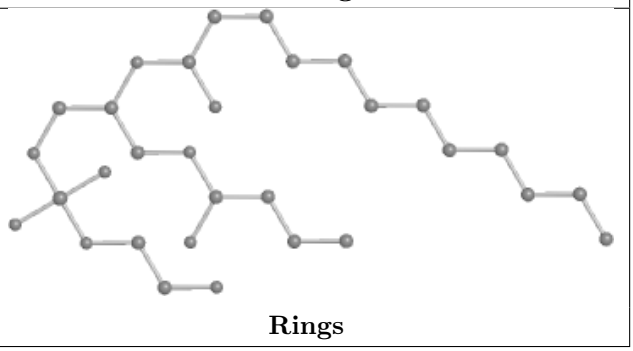
Bond lengths



Bond angles

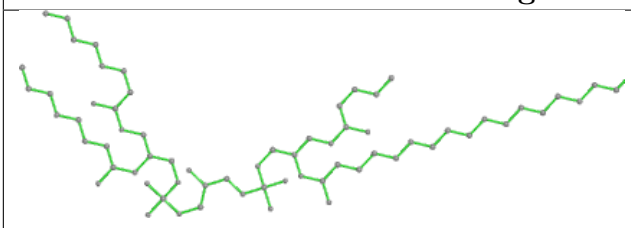


Torsions

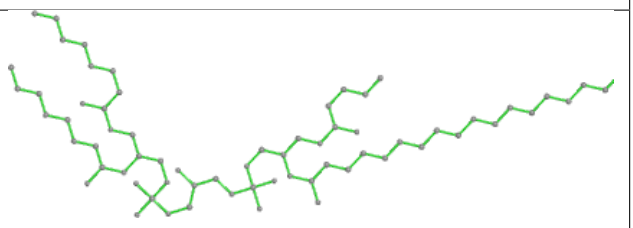


Rings

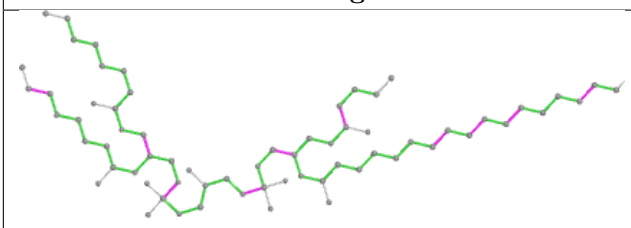
Ligand CDL d1 201



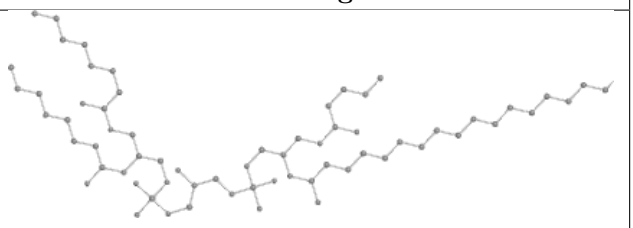
Bond lengths



Bond angles

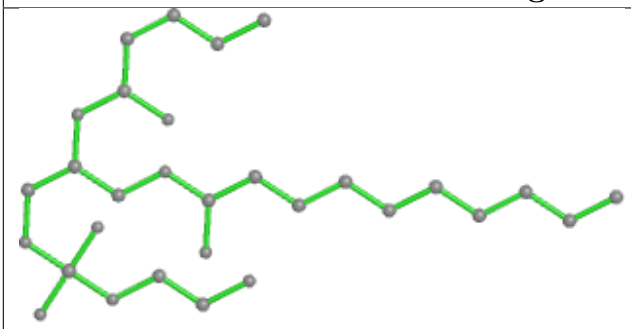


Torsions



Rings

Ligand 3PE R 104



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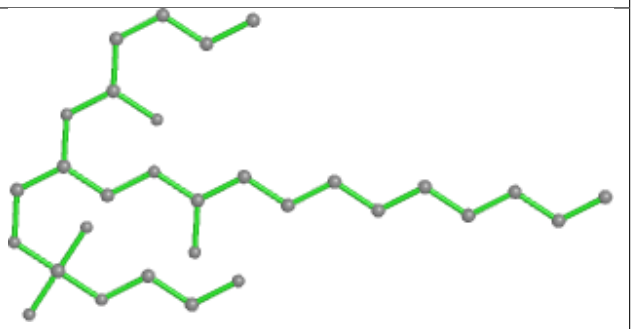
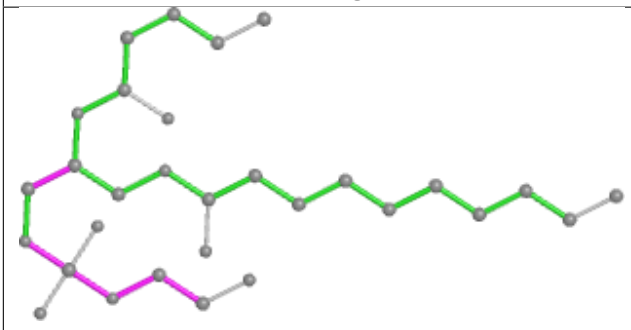


Bond angles



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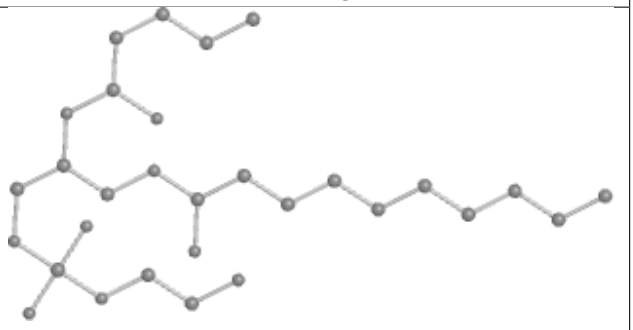
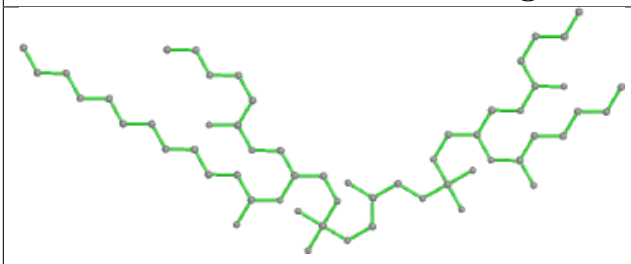


Rings

Ligand CDL a1 101



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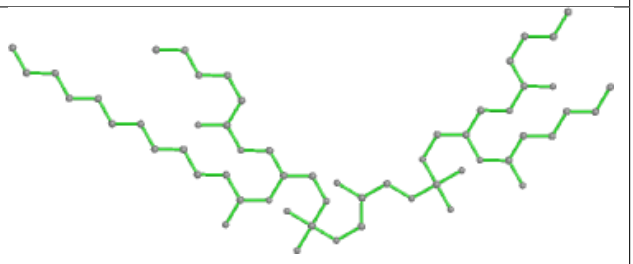
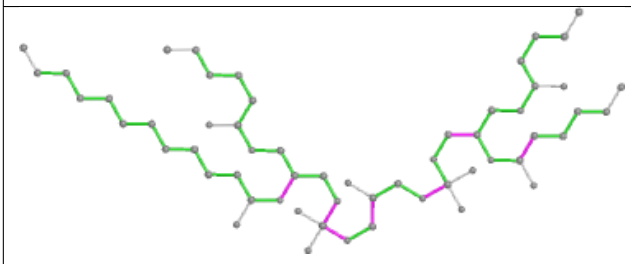


Bond angles



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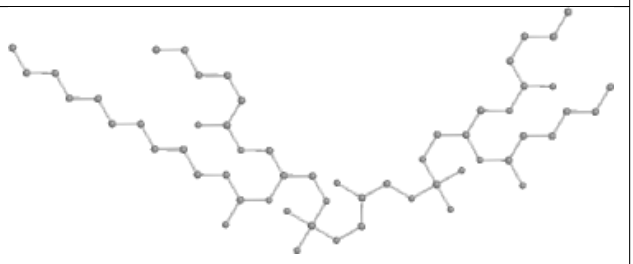
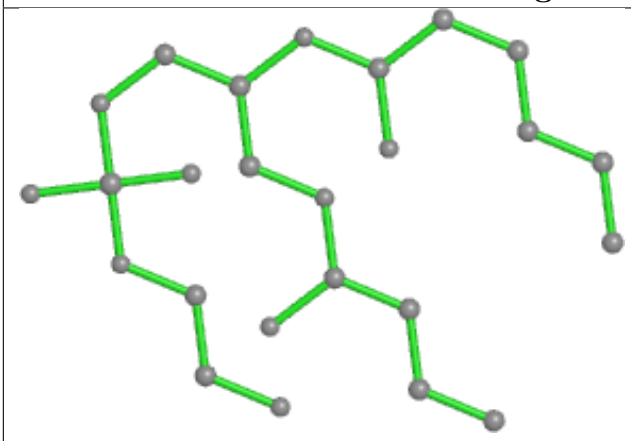


Rings

Ligand 3PE t 101



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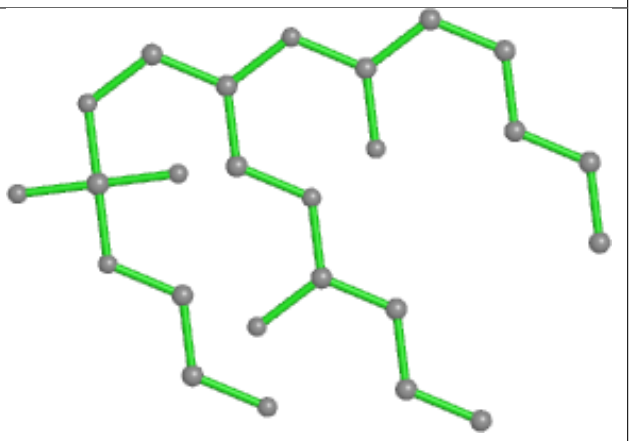
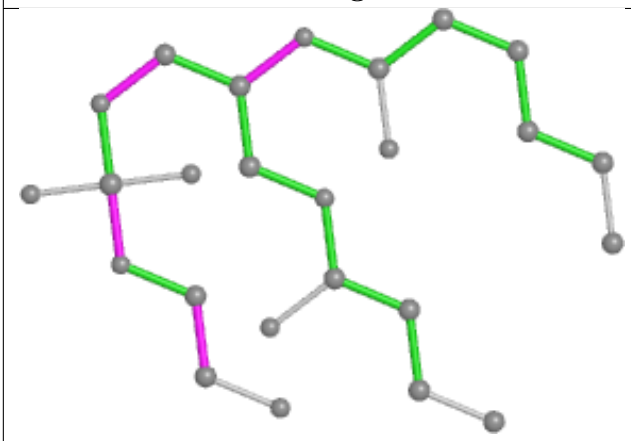


Bond angles



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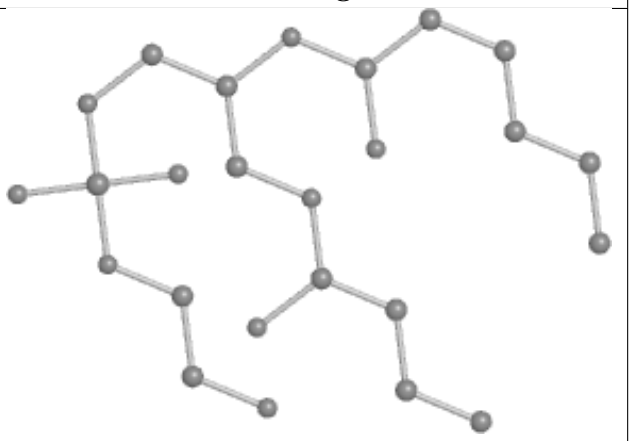
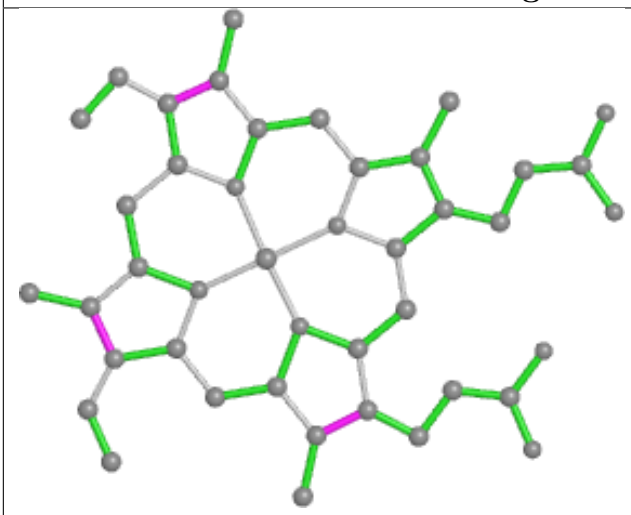


Rings

Ligand HEC O 303



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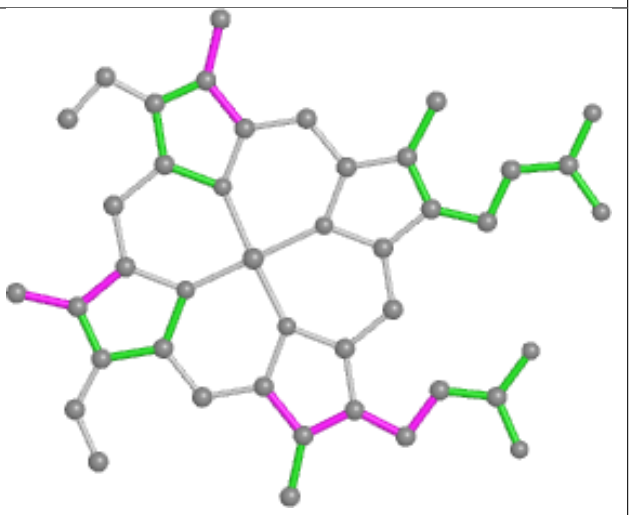
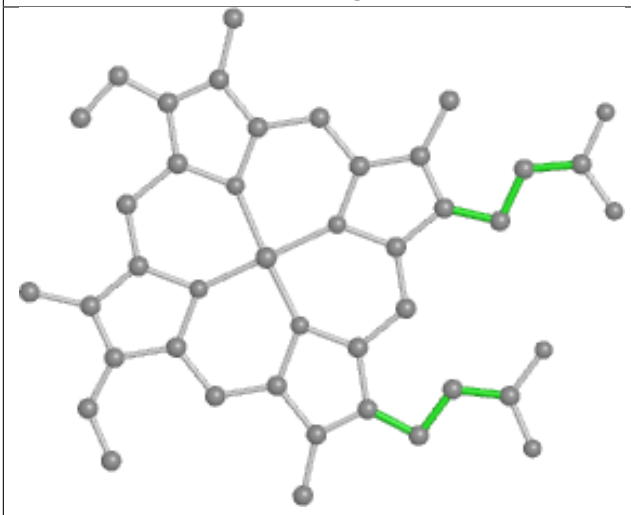


Bond angles



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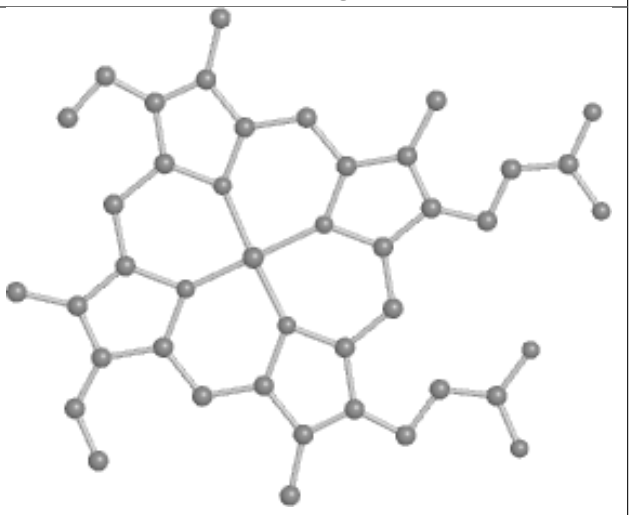
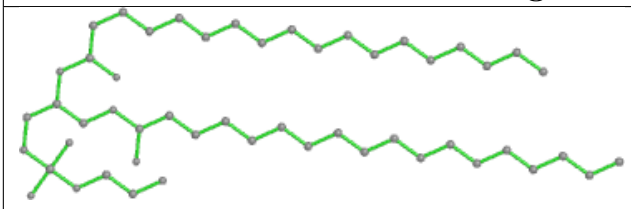


Rings

Ligand 3PE G 102



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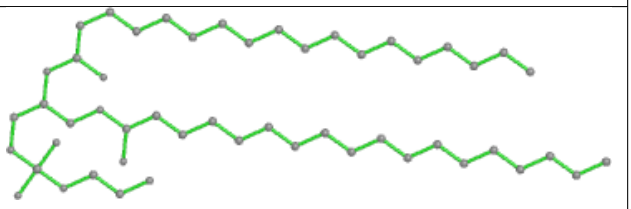
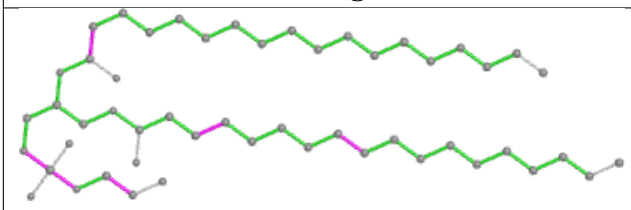


Bond angles



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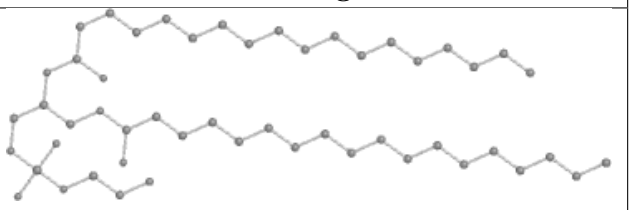
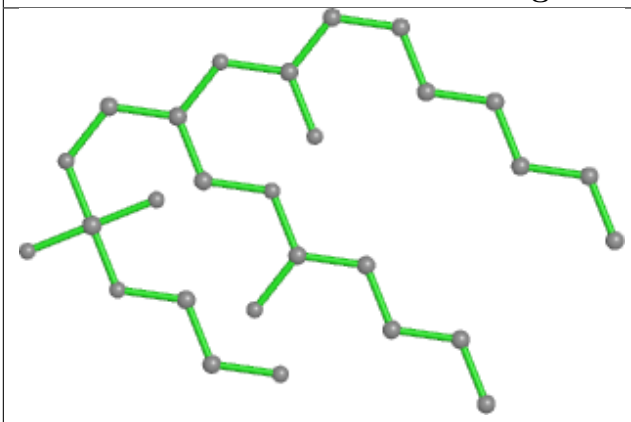


Rings

Ligand 3PE n 606



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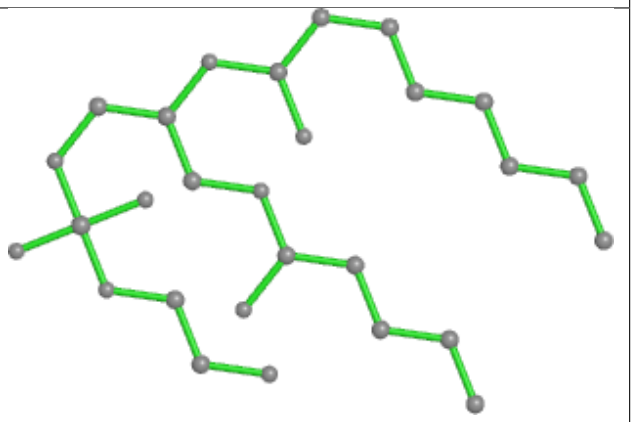
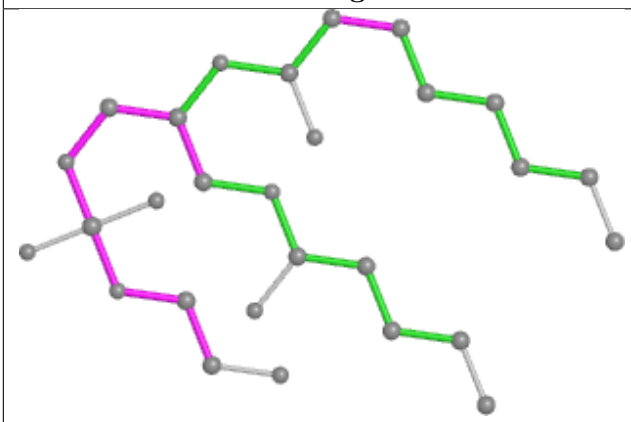


Bond angles



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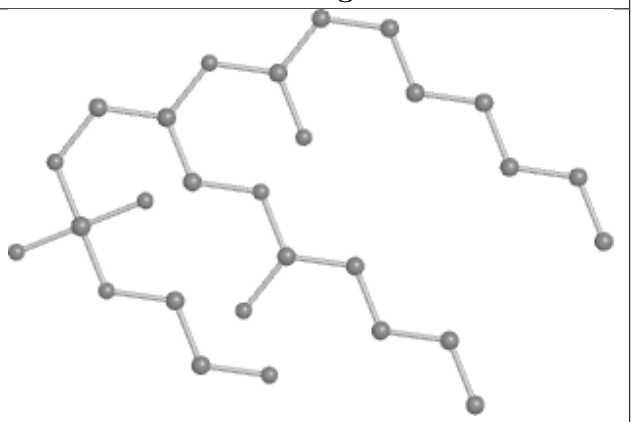
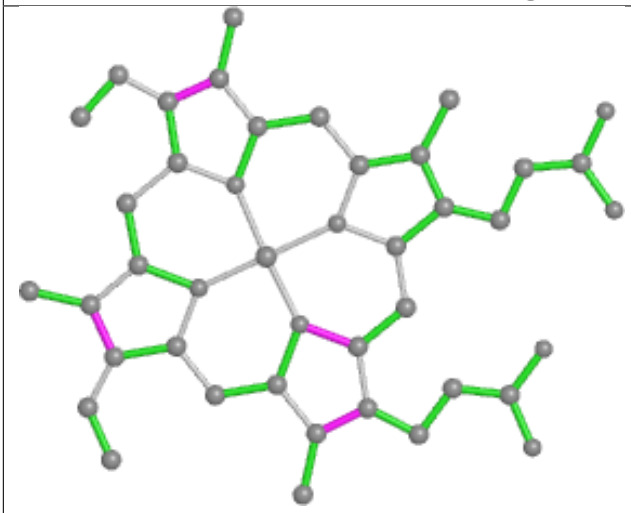


Rings

Ligand HEC D 301



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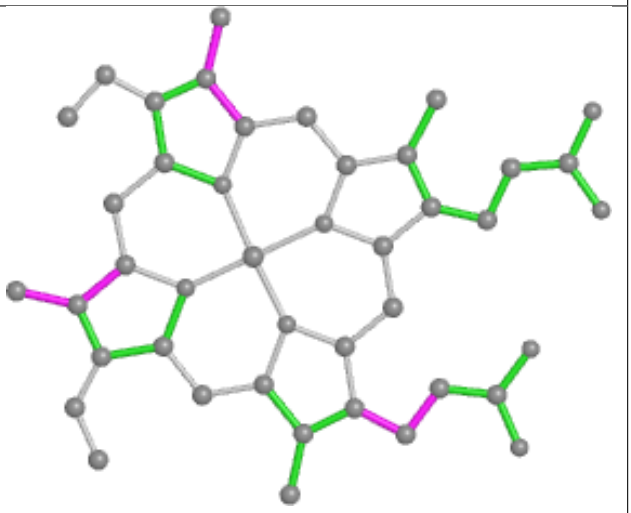
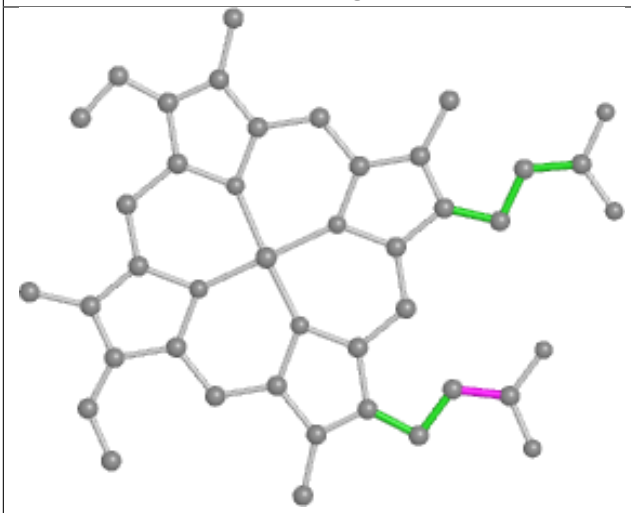


Bond angles



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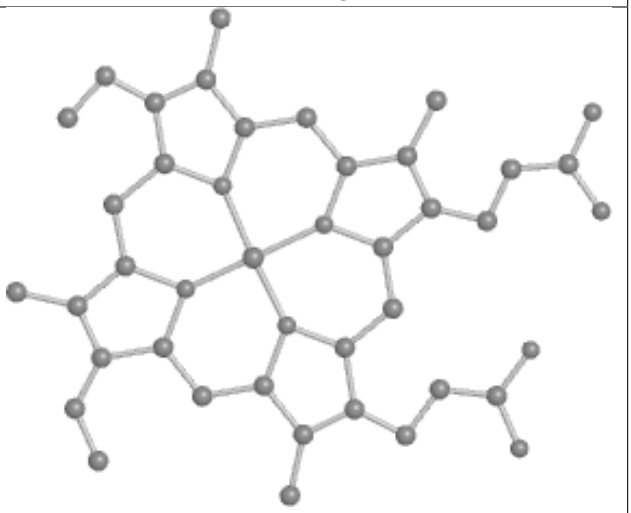
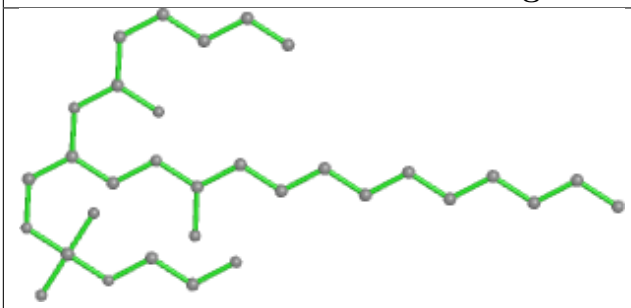


Rings

Ligand 3PE d1 203



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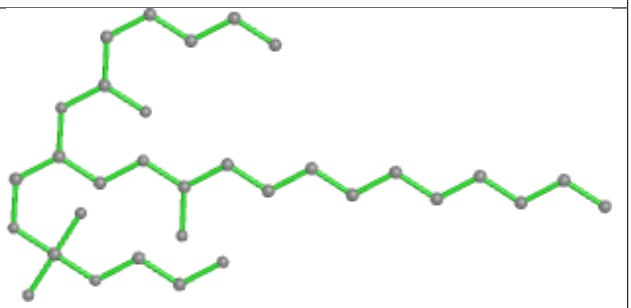
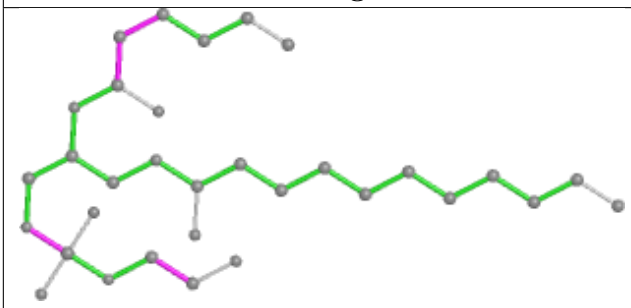


Bond angles



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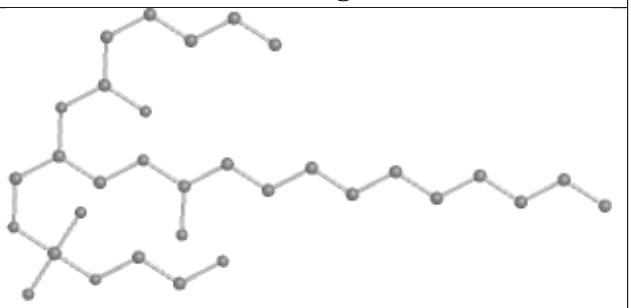
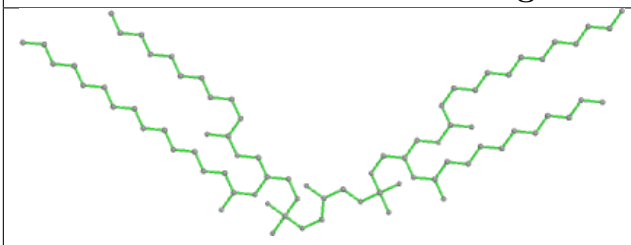


Rings

Ligand CDL L1 702



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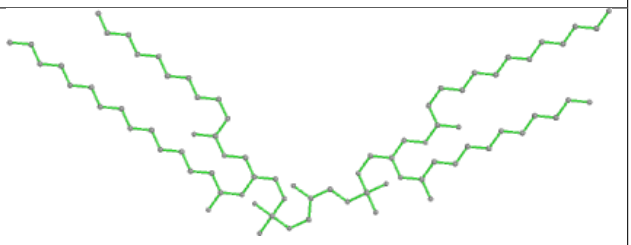
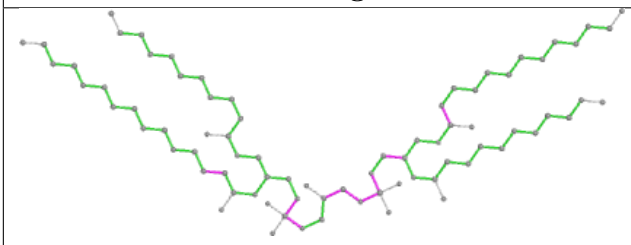


Bond angles



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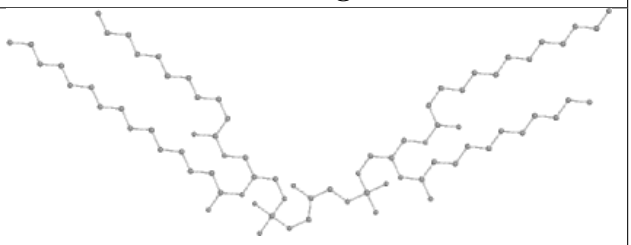
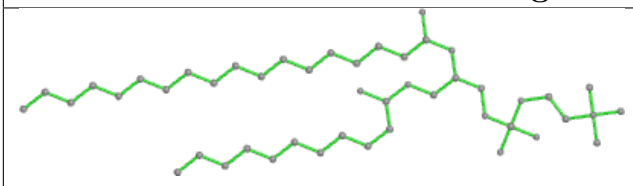
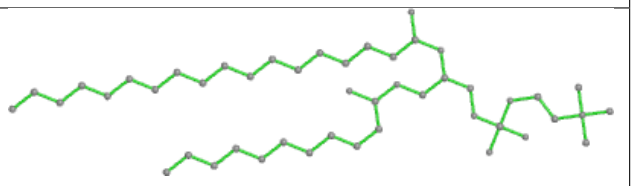


Rings

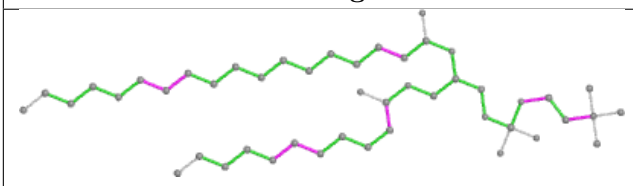
Ligand PC1 9 204



Bond lengths



Bond angles



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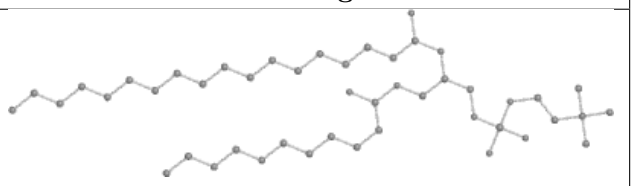
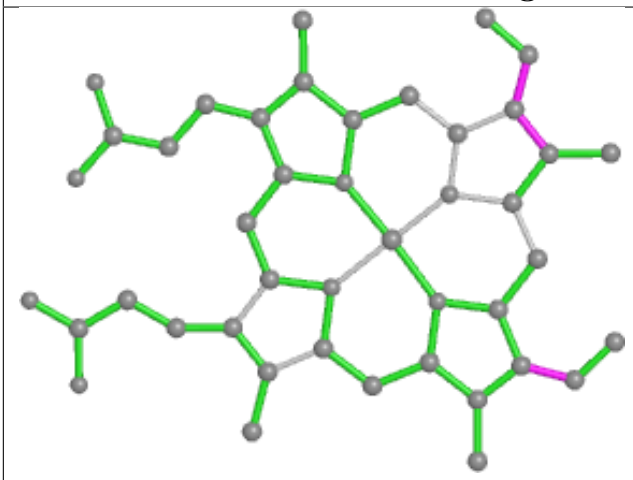


Rings

Ligand HEM C 401



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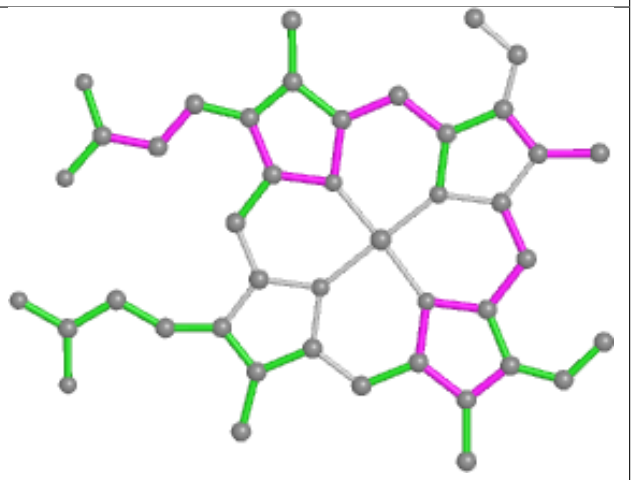
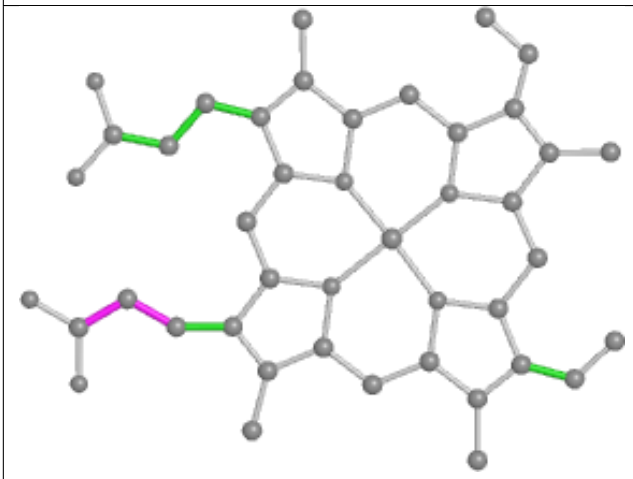
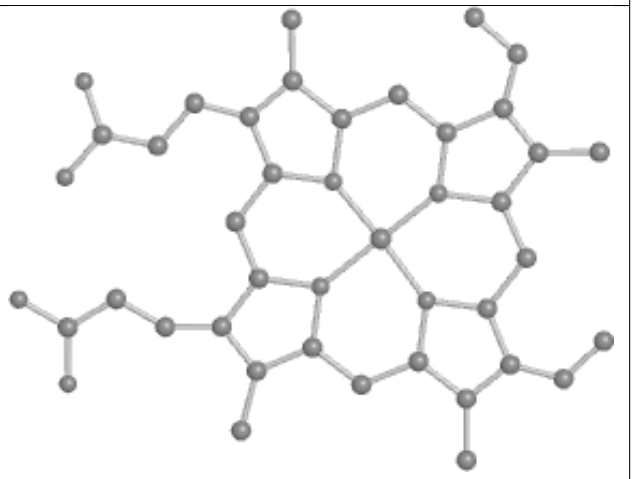


Bond angles

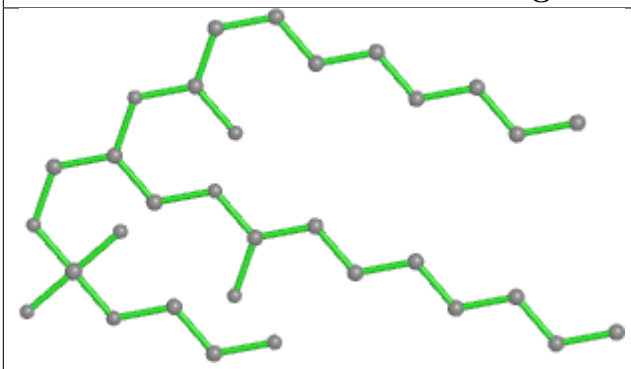


Torsions

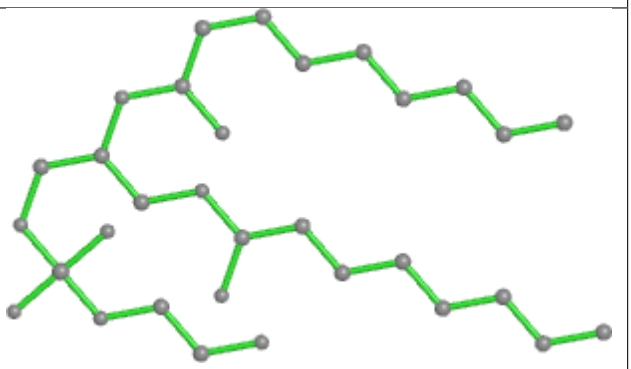


Rings

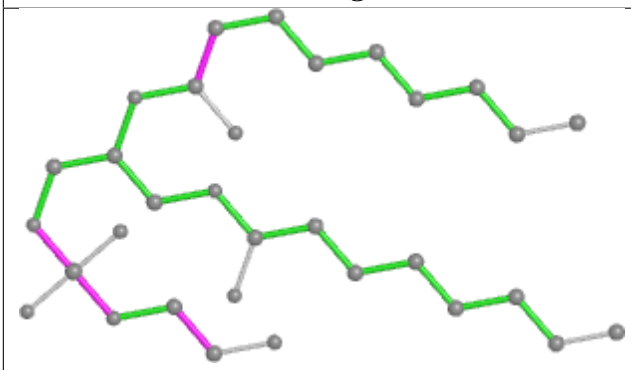
Ligand 3PE 6 202



Bond lengths



Bond angles



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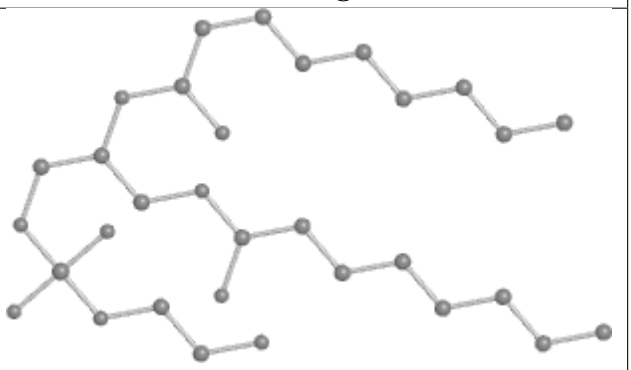
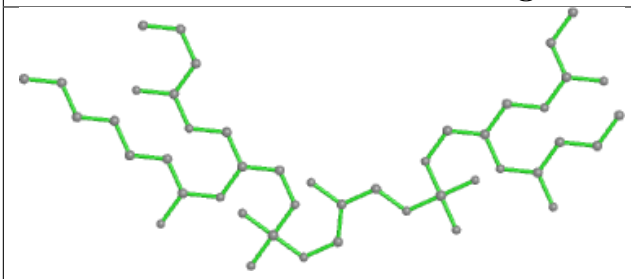
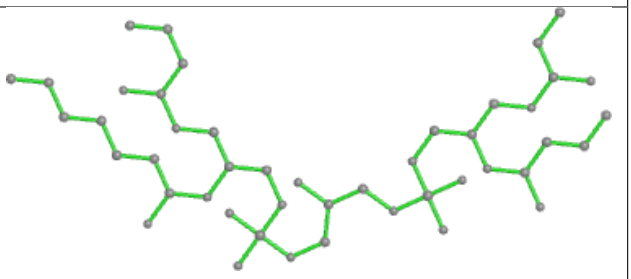


Rings

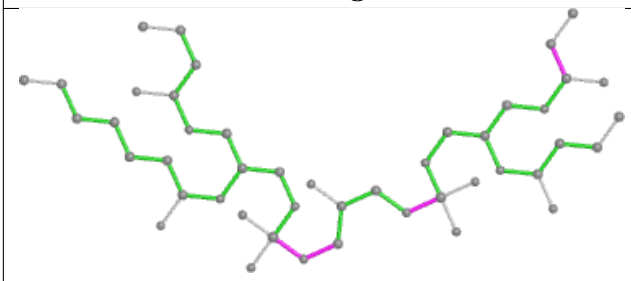
Ligand CDL L1 703



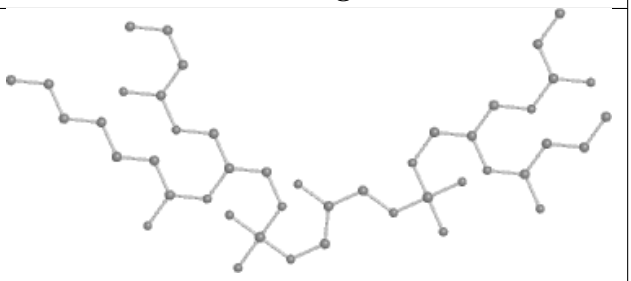
Bond lengths



Bond angles

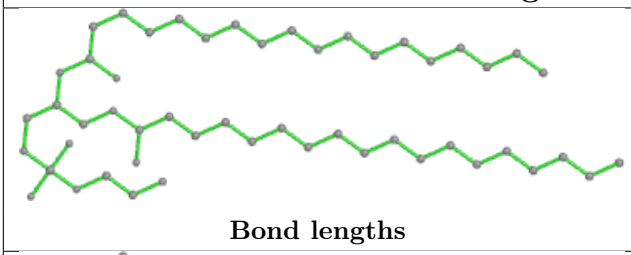


Torsions

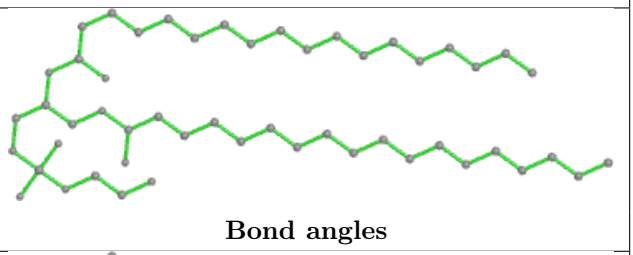


Rings

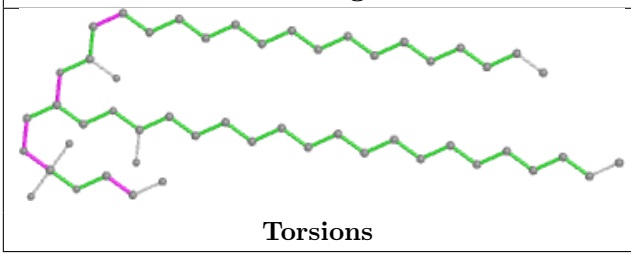
Ligand 3PE L1 701



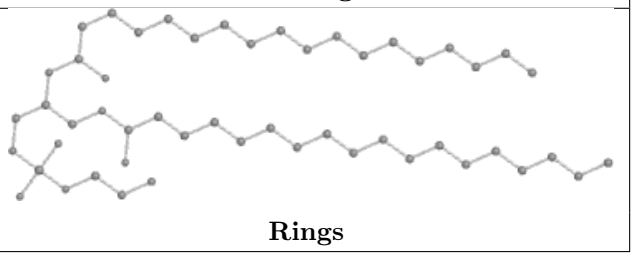
Bond lengths



Bond angles

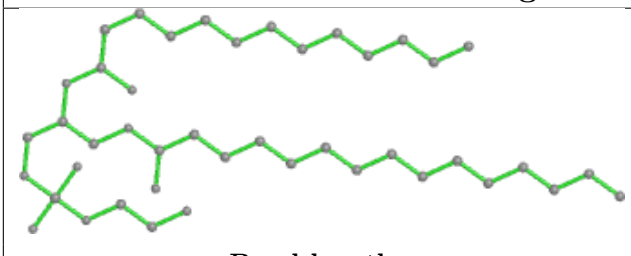


Torsions

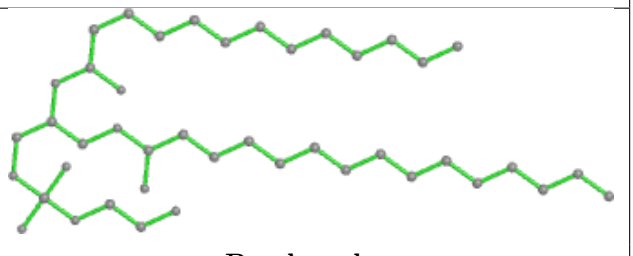


Rings

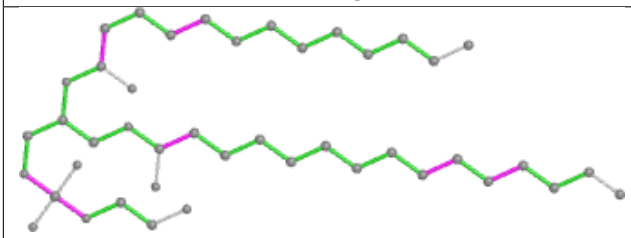
Ligand 3PE A1 201



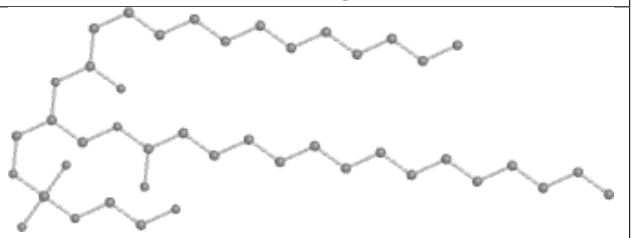
Bond lengths



Bond angles

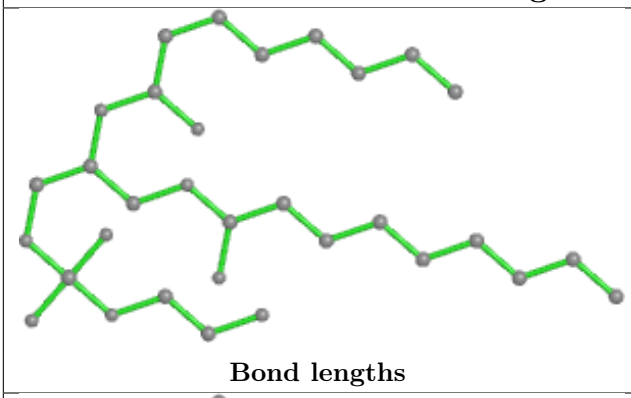


Torsions

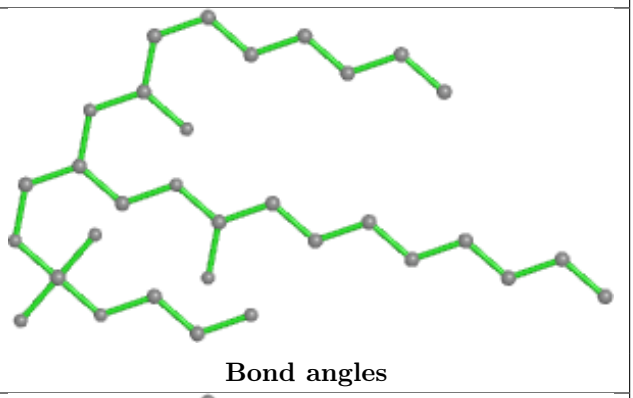


Rings

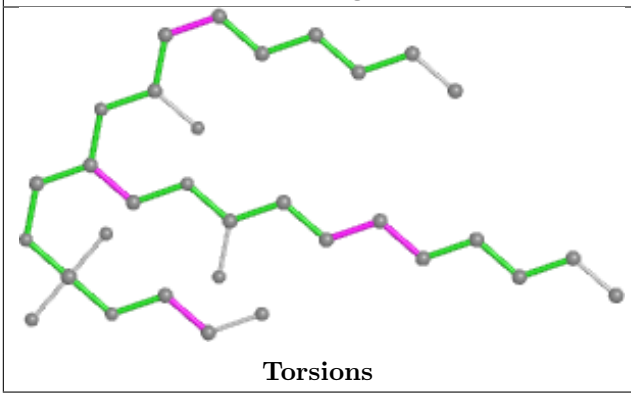
Ligand 3PE E 202



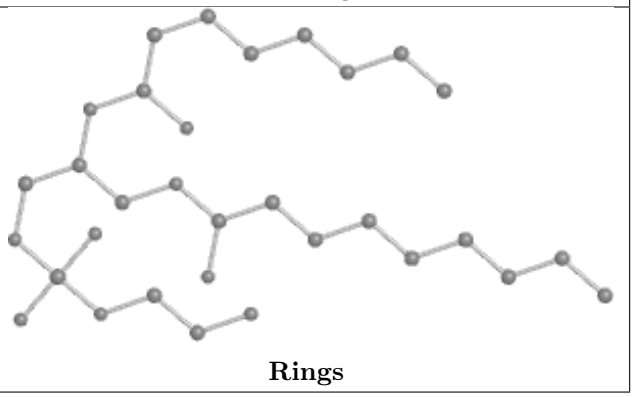
Bond lengths



Bond angles

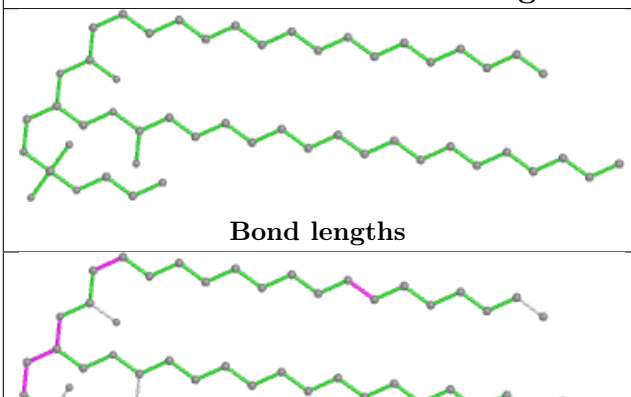


Torsions

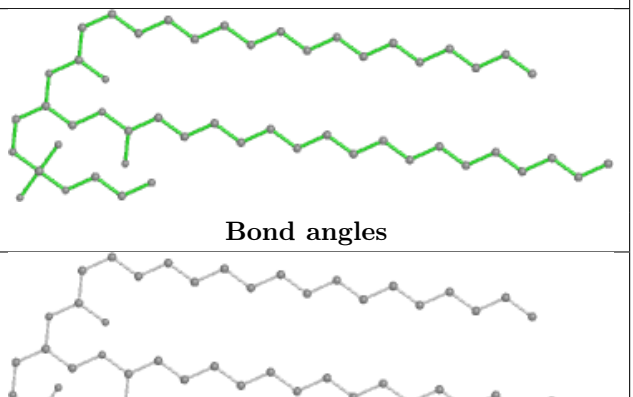


Rings

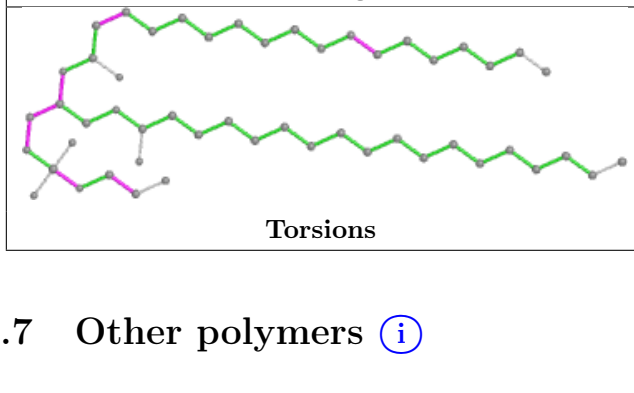
Ligand 3PE H1 401



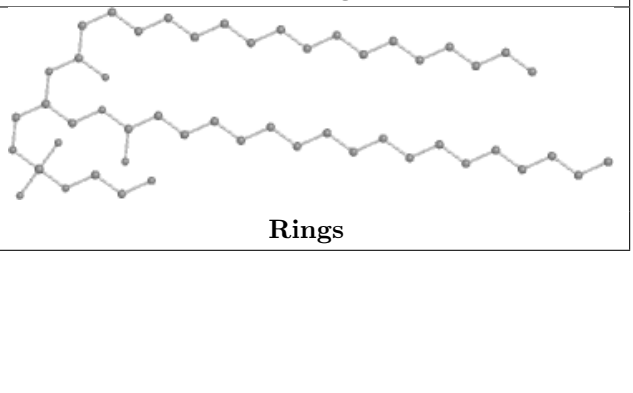
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17991. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.