wwPDB EM Validation Summary Report

Apr 18, 2024 – 08:18 pm BST

PDB ID	:	8PW6
EMDB ID	:	EMD-17990
Title	:	C respirasome from murine liver
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2023-07-19
Resolution	:	3.30 Å(reported)
Based on initial models	:	6g2j, 7o3c

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

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

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

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

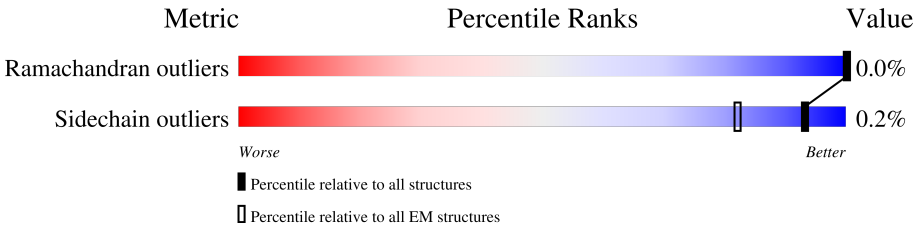
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	480	93% 7%
1	L	480	92% 7%
2	B	453	92% 8%
2	M	453	93% 7%
3	C	381	99%
3	N	381	99%
4	D	325	74% 26%
4	O	325	74% 26%
5	E	274	38% 72% 28%

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Mol	Chain	Length	Quality of chain
5	P	274	36% 72% 28%
5	T	274	5% 28% 72%
6	F	111	90% 9%
6	Q	111	92% 8%
7	G	82	94% 6%
7	R	82	6% 94% 6%
8	H	89	73% 26%
8	S	89	75% 24%
9	J	64	94% 6%
9	U	64	92% 6%
10	K	56	11% 91% 9%
10	V	56	5% 93% 7%
11	n	514	99%
12	o	227	99%
13	p	261	99%
14	q	169	82% 18%
15	r	146	71% 29%
16	s	128	5% 72% 27%
17	t	97	10% 76% 23%
18	u	86	92% 8%
19	v	76	93% 7%
20	x	80	61% 39%
21	y	63	75% 25%
22	z	70	61% 39%
23	w	83	69% 31%

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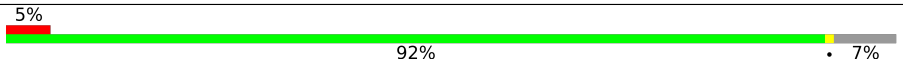
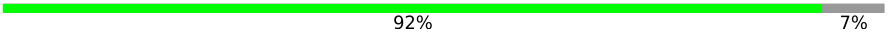
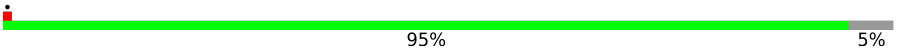
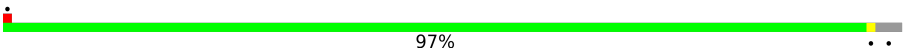
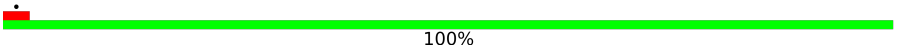
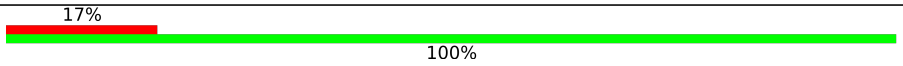
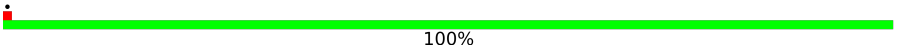
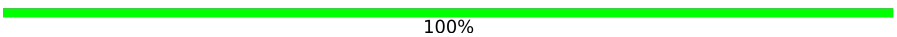
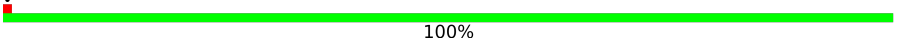
Mol	Chain	Length	Quality of chain
24	6	224	
25	C1	263	
26	D1	463	
27	2	248	
28	1	464	
29	3	727	
30	9	212	
31	P1	377	
32	Q1	175	
33	7	116	
34	S1	99	
35	T1	156	
35	U1	156	
36	V1	116	
37	W1	131	
38	q1	145	
39	r1	113	
40	s1	104	
41	A1	115	
42	H1	318	
43	J1	172	
44	K1	98	
45	L1	607	
46	M1	459	
47	N1	345	

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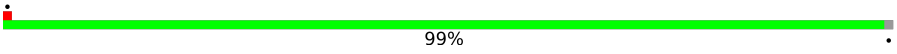
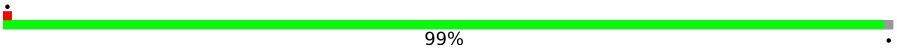
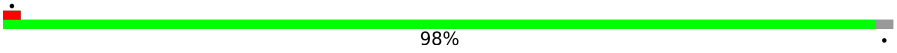
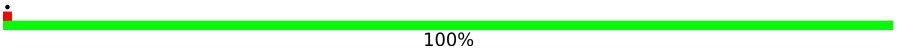
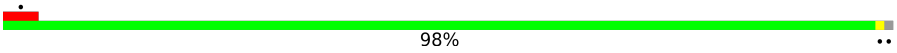
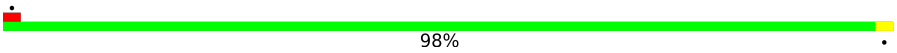
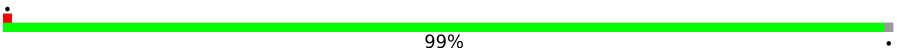
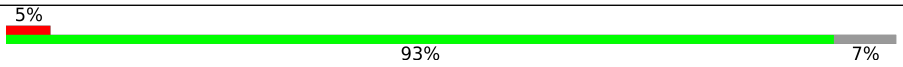
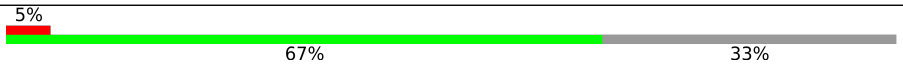
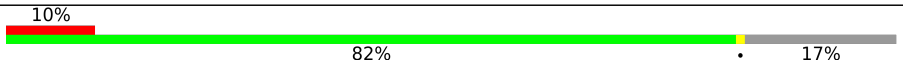
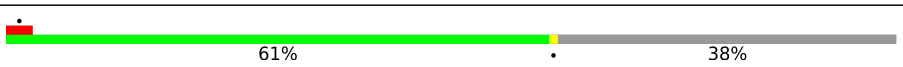
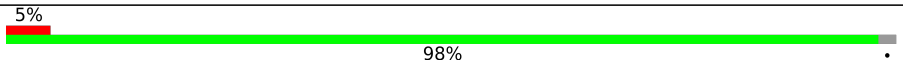
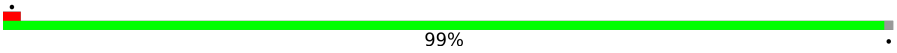
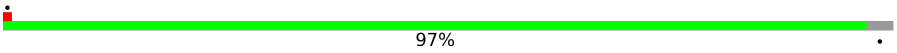
Mol	Chain	Length	Quality of chain
48	O1	355	
49	X1	172	
50	Y1	141	
51	Z1	144	
52	a1	70	
53	b1	84	
54	c1	76	
55	d1	120	
56	e1	106	
57	f1	57	
58	g1	151	
59	h1	189	
60	i1	128	
61	j1	105	
62	k1	104	
63	l1	186	
64	m1	129	
65	n1	179	
66	o1	137	
67	p1	176	

2 Entry composition (i)

There are 86 unique types of molecules in this entry. The entry contains 115643 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 b-c1 complex subunit 1, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	418	Total	C	N	O	S	0	0
			3138	1970	552	607	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1167	705	219	237	6		
5	P	196	Total	C	N	O	S	0	0
			1167	705	219	237	6		
5	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

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

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

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

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	51	Total	C	N	O	S	0	0
			422	281	75	65	1		
10	V	52	Total	C	N	O	S	0	0
			430	287	76	66	1		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	93	Total	C	N	O	S	0	0
			717	447	125	137	8		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6C.

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

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

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

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

- 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 subunit 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		

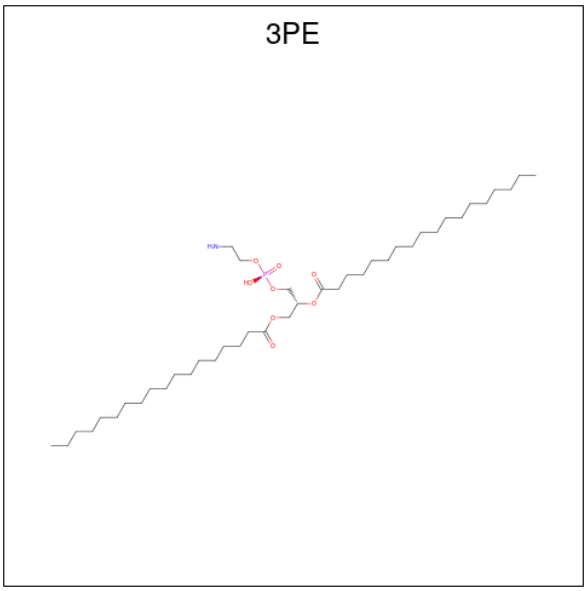
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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



Mol	Chain	Residues	Atoms					AltConf
68	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
68	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
68	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
68	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
68	N	1	Total	C	N	O	P	0
			34	24	1	8	1	
68	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
68	P	1	Total	C	N	O	P	0
			33	23	1	8	1	
68	R	1	Total	C	N	O	P	0
			30	20	1	8	1	
68	n	1	Total	C	N	O	P	0
			34	24	1	8	1	
68	n	1	Total	C	N	O	P	0
			28	18	1	8	1	
68	o	1	Total	C	N	O	P	0
			29	19	1	8	1	
68	p	1	Total	C	N	O	P	0
			45	35	1	8	1	
68	q	1	Total	C	N	O	P	0
			26	16	1	8	1	

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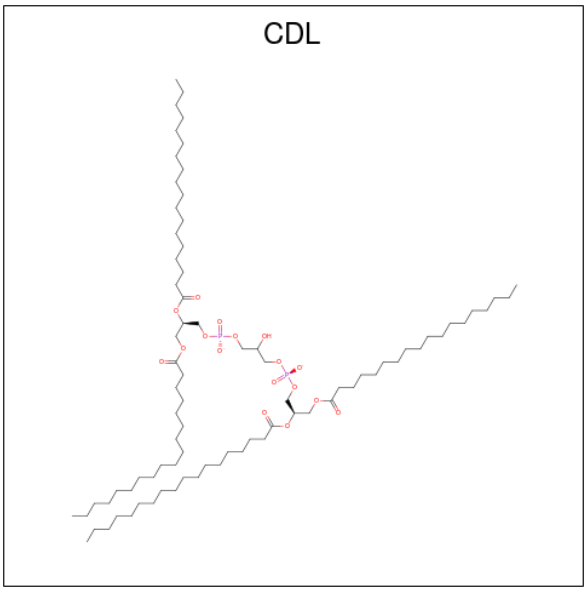
Mol	Chain	Residues	Atoms					AltConf
68	t	1	Total	C	N	O	P	0
			25	15	1	8	1	
68	v	1	Total	C	N	O	P	0
			28	18	1	8	1	
68	x	1	Total	C	N	O	P	0
			27	17	1	8	1	
68	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
68	D1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	A1	1	Total	C	N	O	P	0
			43	33	1	8	1	
68	H1	1	Total	C	N	O	P	0
			46	36	1	8	1	
68	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	
68	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	M1	1	Total	C	N	O	P	0
			36	26	1	8	1	
68	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
68	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
68	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
68	Z1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
68	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
68	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 69 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
69	A	1	Total	C	O	P	0
			46	27	17	2	
69	C	1	Total	C	O	P	0
			42	23	17	2	
69	D	1	Total	C	O	P	0
			56	37	17	2	
69	L	1	Total	C	O	P	0
			46	27	17	2	
69	R	1	Total	C	O	P	0
			57	38	17	2	
69	R	1	Total	C	O	P	0
			41	22	17	2	
69	R	1	Total	C	O	P	0
			57	38	17	2	
69	V	1	Total	C	O	P	0
			38	20	16	2	
69	H1	1	Total	C	O	P	0
			51	33	16	2	
69	L1	1	Total	C	O	P	0
			78	59	17	2	
69	L1	1	Total	C	O	P	0
			46	27	17	2	
69	N1	1	Total	C	O	P	0
			90	71	17	2	
69	Y1	1	Total	C	O	P	0
			94	75	17	2	
69	Y1	1	Total	C	O	P	0
			72	53	17	2	

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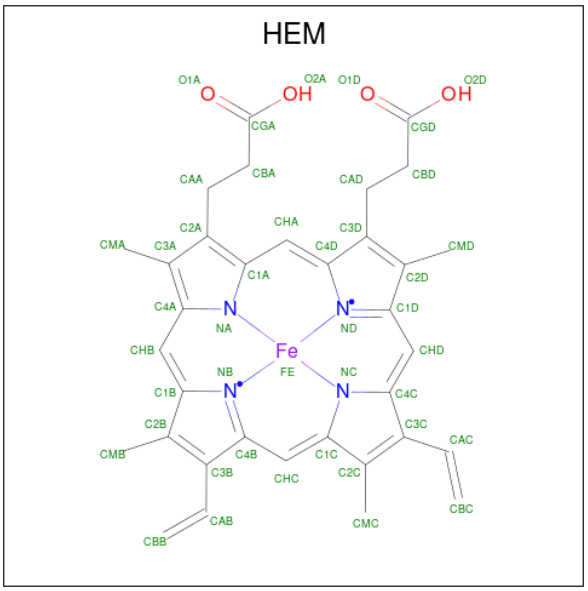
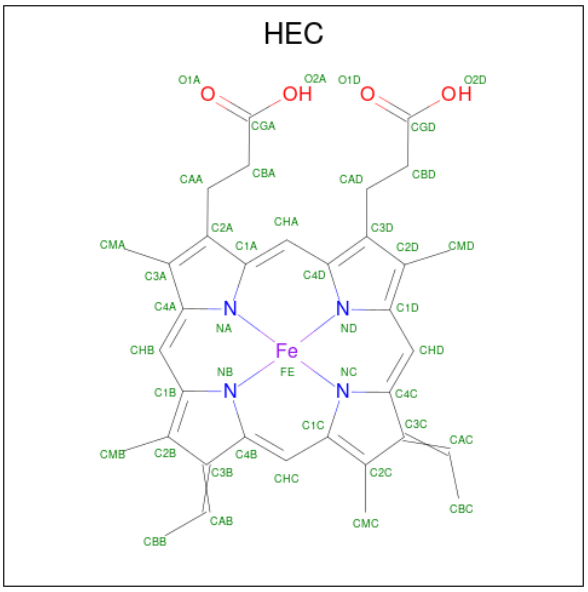
Mol	Chain	Residues	Atoms				AltConf
69	a1	1	Total	C	O	P	0
			57	38	17	2	
69	d1	1	Total	C	O	P	0
			67	48	17	2	
69	h1	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 70 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



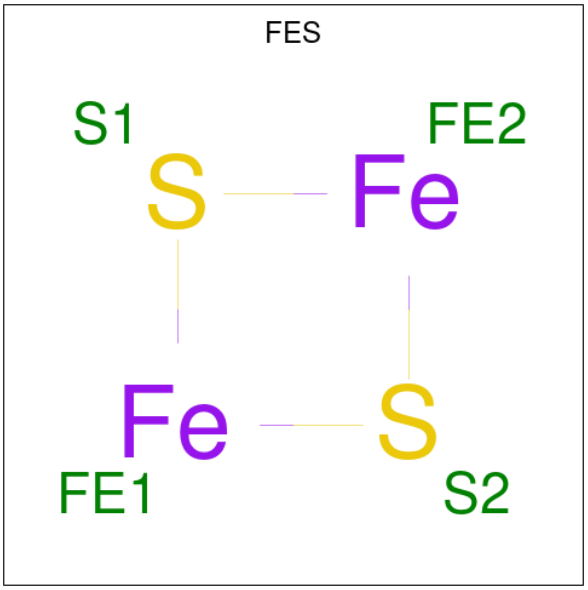
Mol	Chain	Residues	Atoms					AltConf
70	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 71 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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



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

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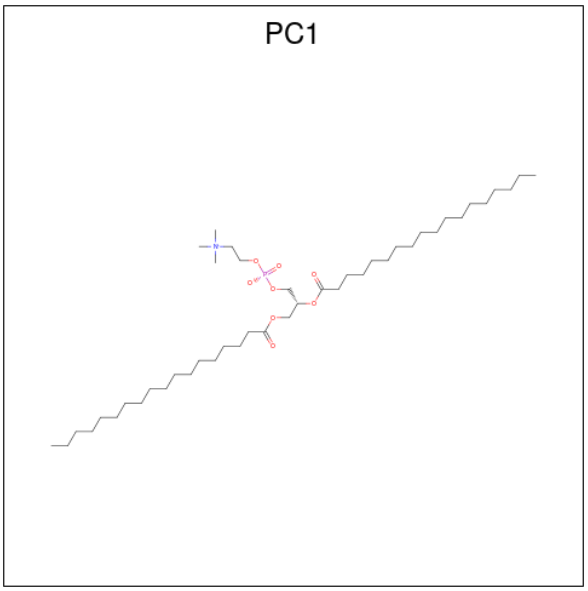
Mol	Chain	Residues	Atoms	AltConf
72	2	1	Total Fe S 4 2 2	0
72	3	1	Total Fe S 4 2 2	0

- Molecule 73 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
73	E	1	Total C N O P 35 25 1 8 1	0
73	K	1	Total C N O P 28 18 1 8 1	0
73	L	1	Total C N O P 24 14 1 8 1	0
73	V	1	Total C N O P 28 18 1 8 1	0
73	p	1	Total C N O P 35 25 1 8 1	0
73	p	1	Total C N O P 50 40 1 8 1	0
73	z	1	Total C N O P 28 18 1 8 1	0
73	6	1	Total C N O P 43 33 1 8 1	0
73	9	1	Total C N O P 54 44 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
73	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
73	A1	1	Total	C	N	O	P	0
			31	21	1	8	1	
73	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	

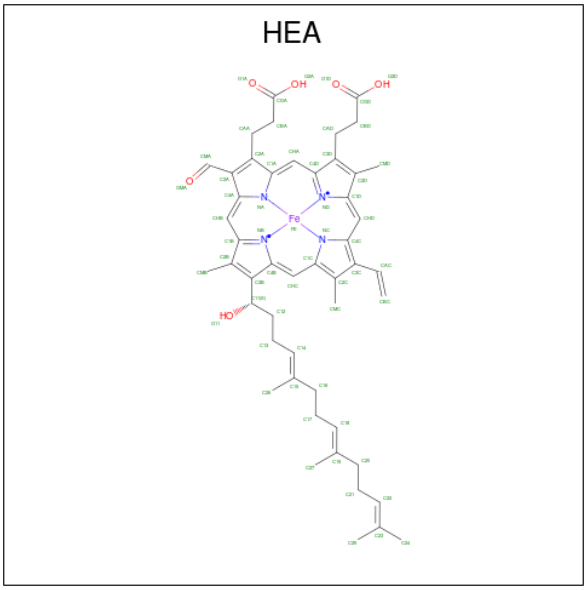
- Molecule 74 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 75 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 76 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

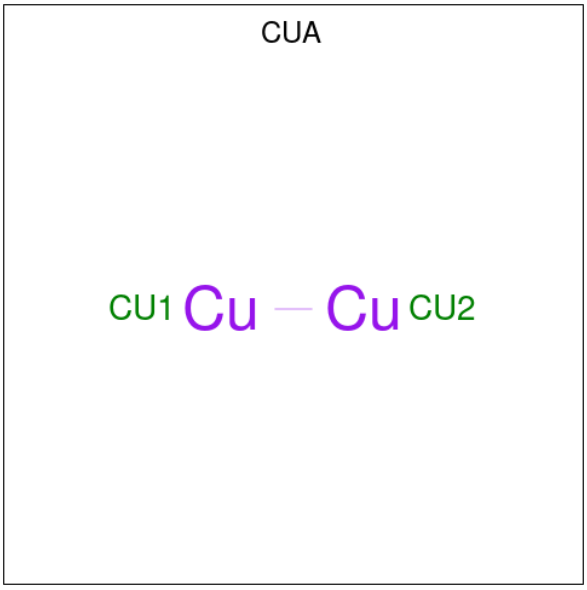


Mol	Chain	Residues	Atoms					AltConf
76	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 77 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 78 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).

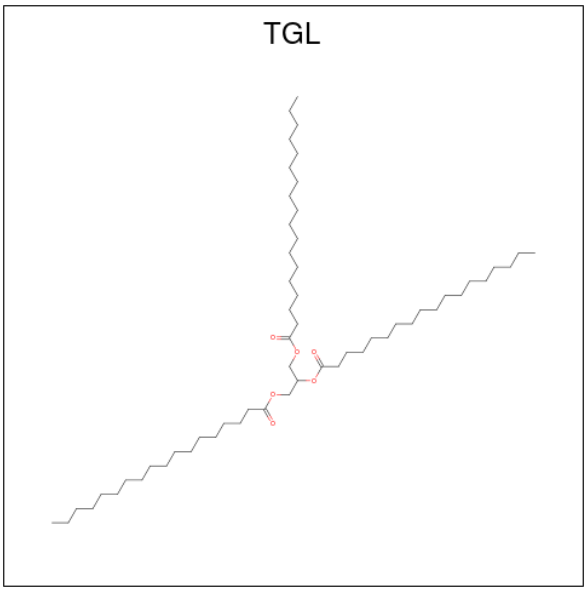


Mol	Chain	Residues	Atoms	AltConf
78	o	1	Total Cu 2 2	0

- Molecule 79 is ZINC ION (three-letter code: ZN) (formula: Zn).

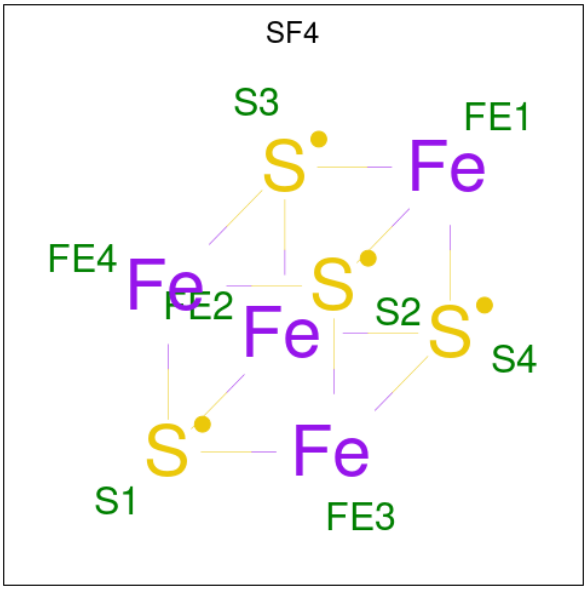
Mol	Chain	Residues	Atoms	AltConf
79	s	1	Total Zn 1 1	0
79	7	1	Total Zn 1 1	0

- Molecule 80 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



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

- 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	0
			8	4	4	
81	1	1	Total	Fe	S	0
			8	4	4	
81	3	1	Total	Fe	S	0
			8	4	4	

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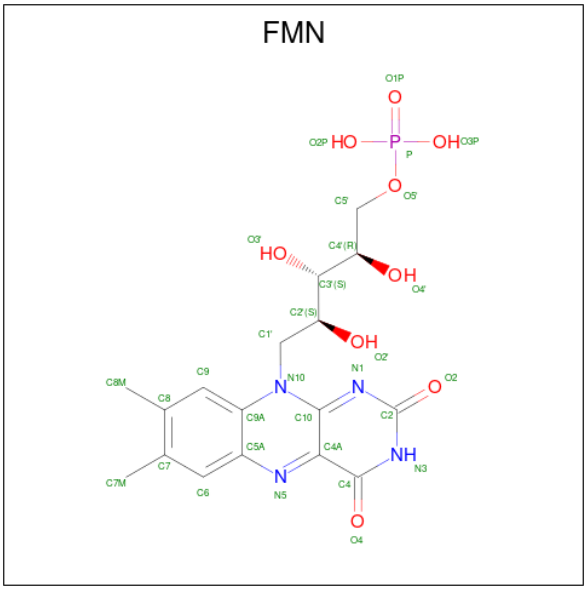
Mol	Chain	Residues	Atoms	AltConf
81	3	1	Total Fe S 8 4 4	0
81	9	1	Total Fe S 8 4 4	0
81	9	1	Total Fe S 8 4 4	0

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

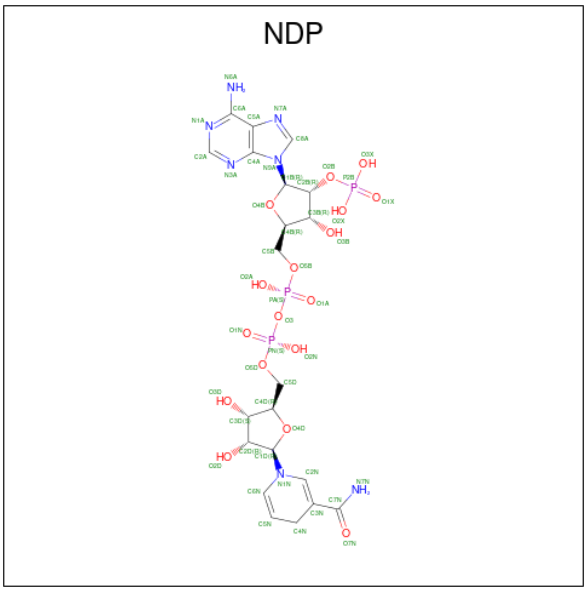


Mol	Chain	Residues	Atoms	AltConf
82	1	1	Total C N O P 31 17 4 9 1	0

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

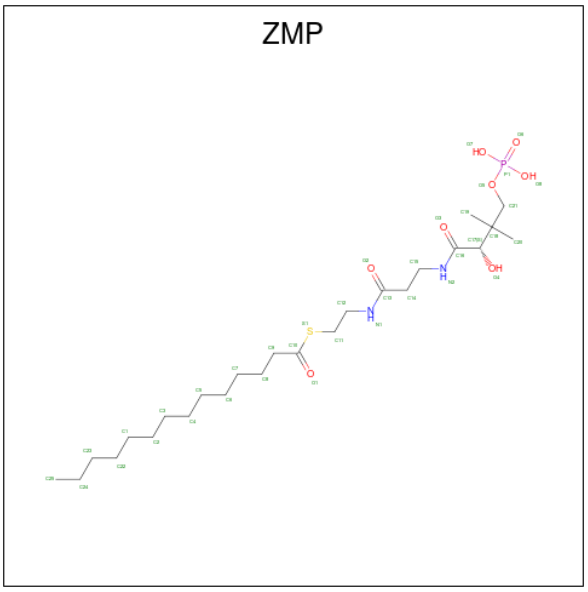
Mol	Chain	Residues	Atoms	AltConf
83	3	1	Total K 1 1	0

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



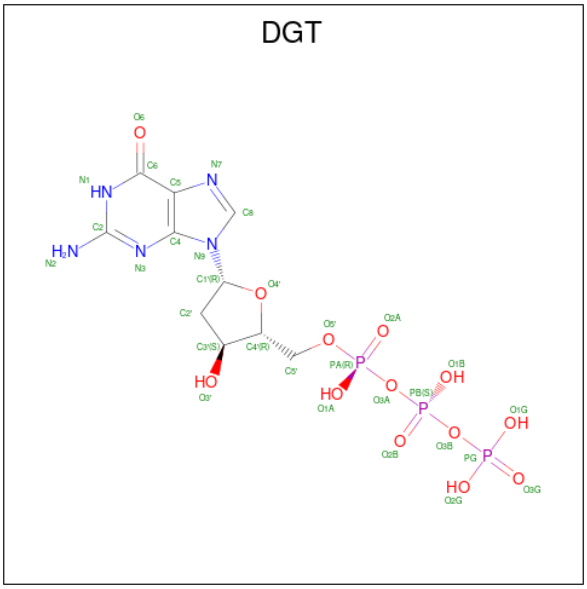
Mol	Chain	Residues	Atoms					AltConf
84	P1	1	Total	C	N	O	P	0
			48	21	7	17	3	

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



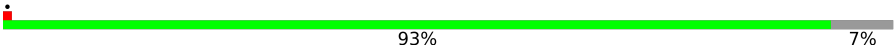
Mol	Chain	Residues	Atoms					AltConf
86	O1	1	Total	C	N	O	P	0
			31	10	5	13	3	

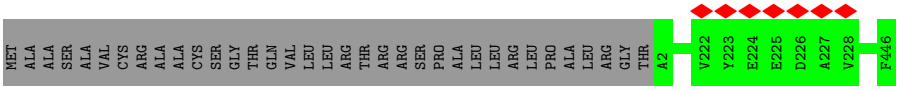
3 Residue-property plots (i)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

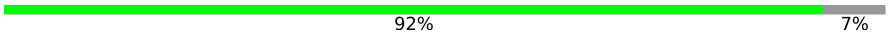
Chain A:

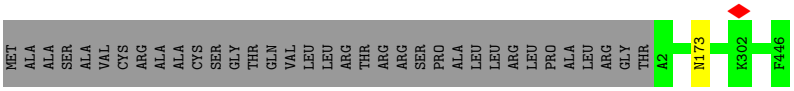




• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

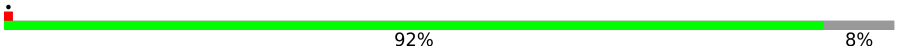
Chain L:

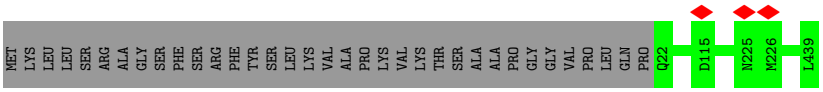




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

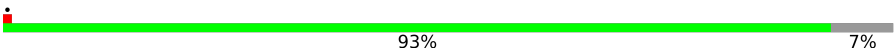
Chain B:

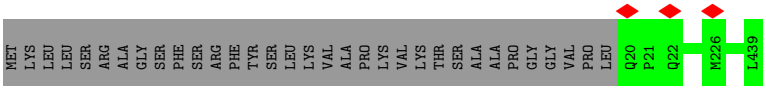




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

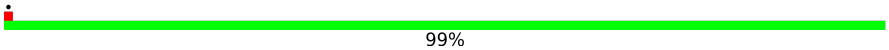
Chain M:

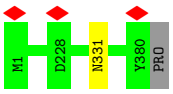




• Molecule 3: Cytochrome b

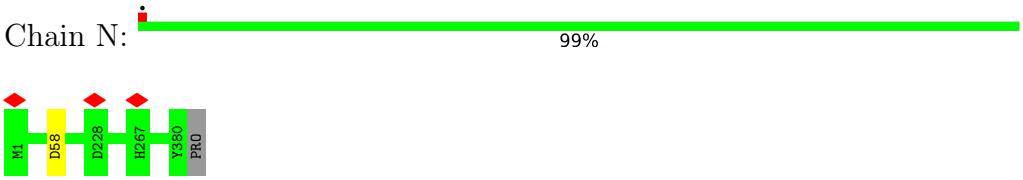
Chain C:





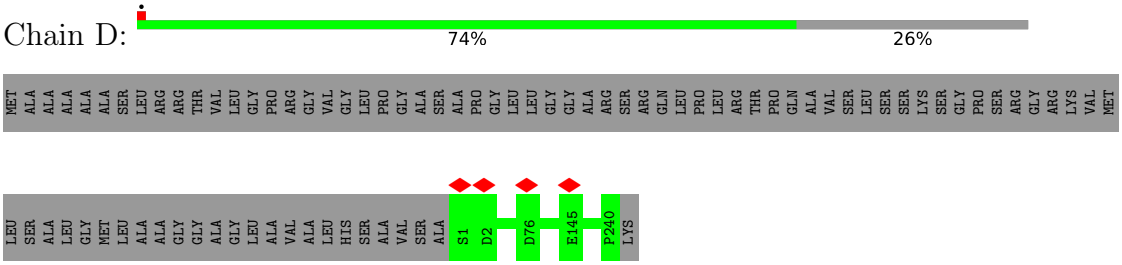
• Molecule 3: Cytochrome b

Chain N:



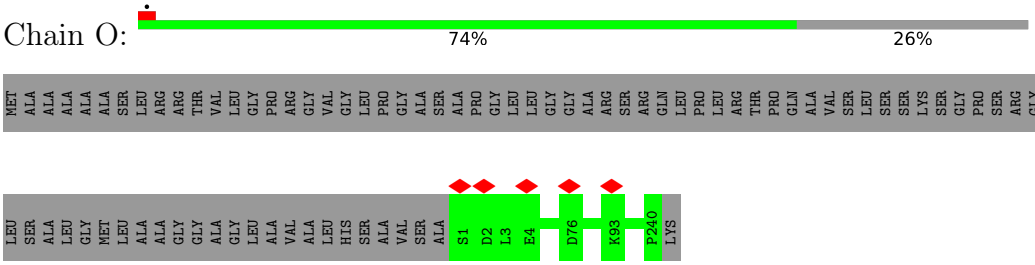
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



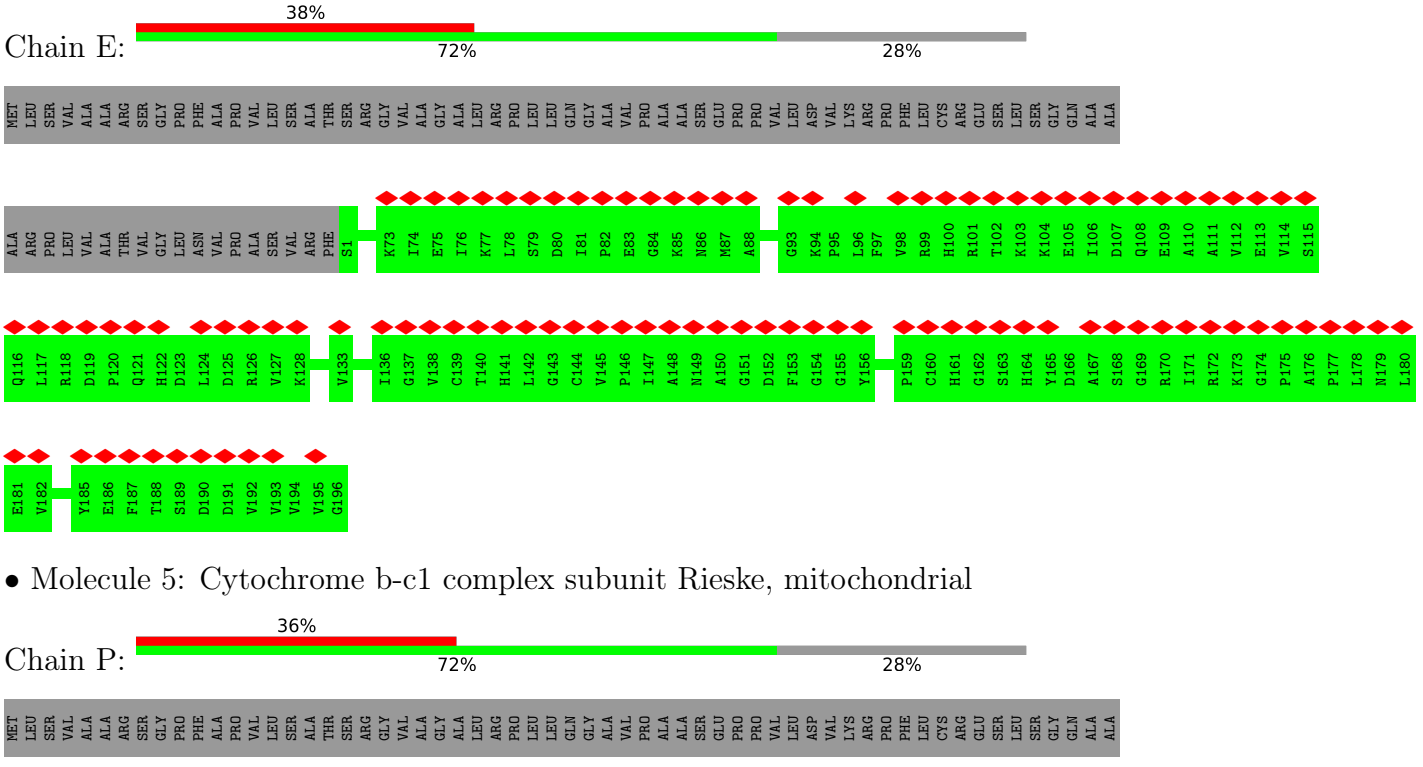
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



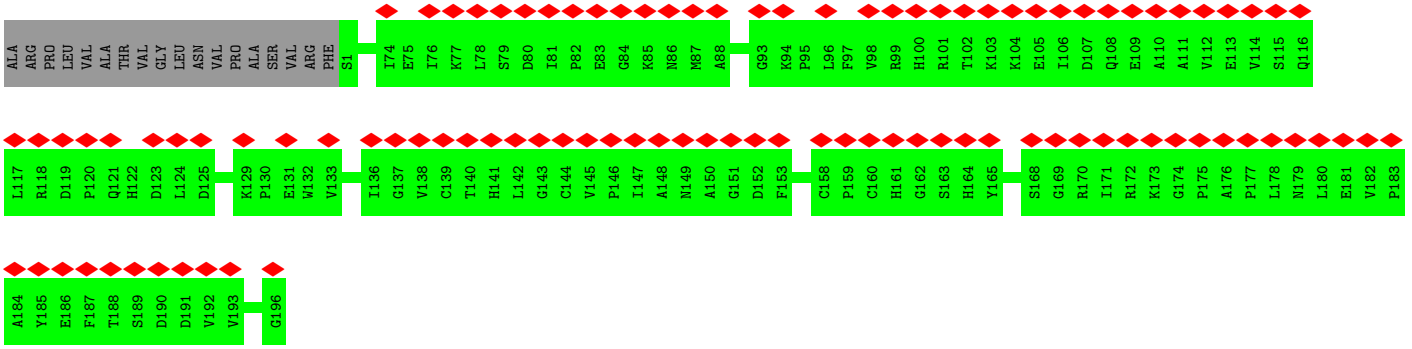
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:

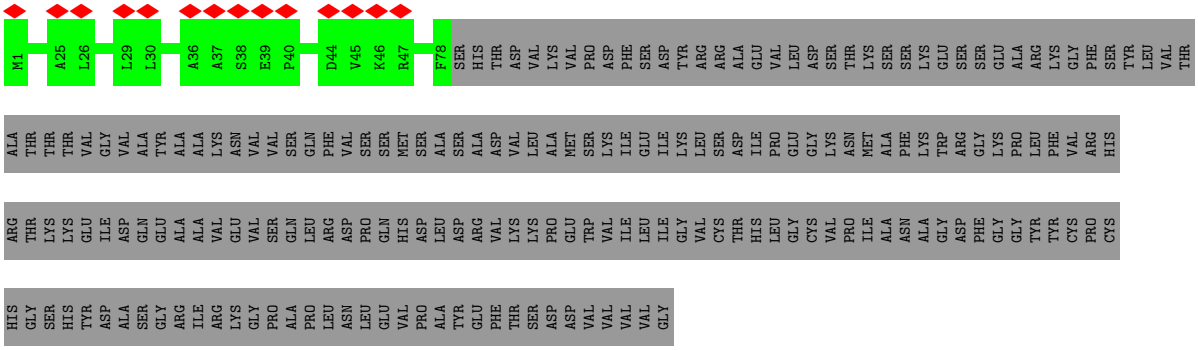


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

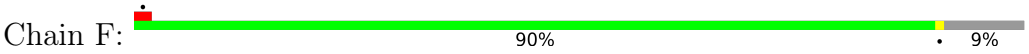
Chain P:

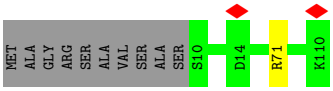


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

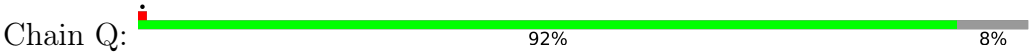


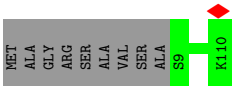
• Molecule 6: Cytochrome b-c1 complex subunit 7



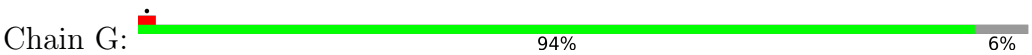


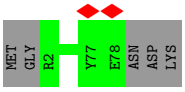
• Molecule 6: Cytochrome b-c1 complex subunit 7





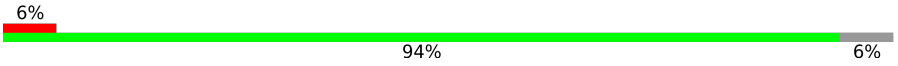
• Molecule 7: Cytochrome b-c1 complex subunit 8

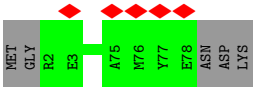




• Molecule 7: Cytochrome b-c1 complex subunit 8

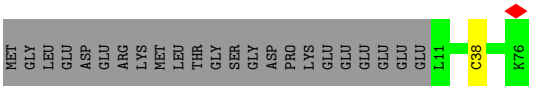
Chain R:





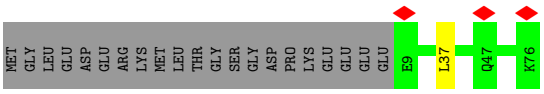
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



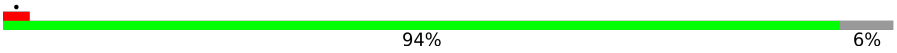
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

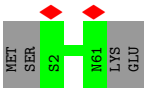
Chain S:



• Molecule 9: Cytochrome b-c1 complex subunit 9

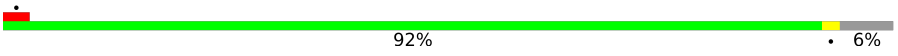
Chain J:

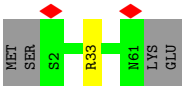




• Molecule 9: Cytochrome b-c1 complex subunit 9

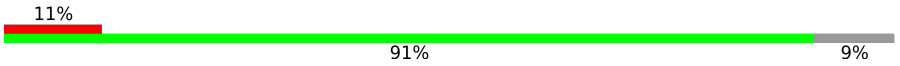
Chain U:

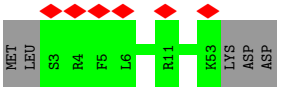




• Molecule 10: Cytochrome b-c1 complex subunit 10

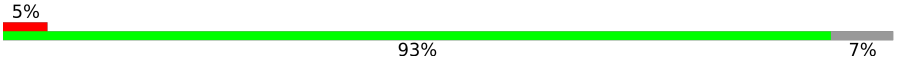
Chain K:

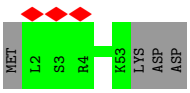




• Molecule 10: Cytochrome b-c1 complex subunit 10

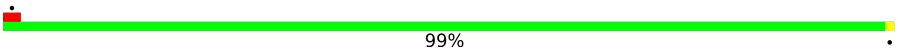
Chain V:

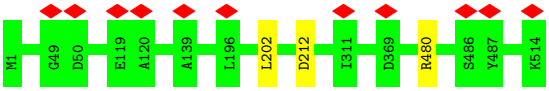




• Molecule 11: Cytochrome c oxidase subunit 1

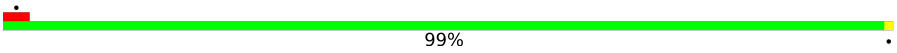
Chain n:

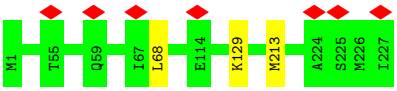




• Molecule 12: Cytochrome c oxidase subunit 2

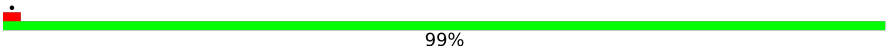
Chain o:

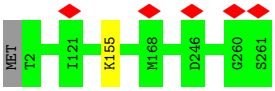




• Molecule 13: Cytochrome c oxidase subunit 3

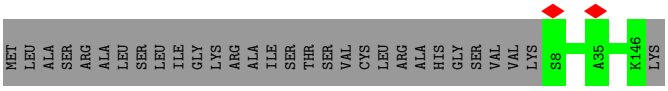
Chain p:





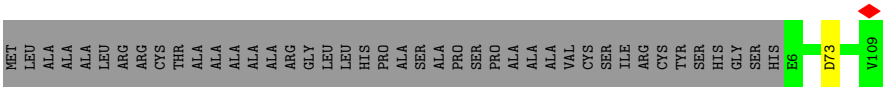
• Molecule 14: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain q:



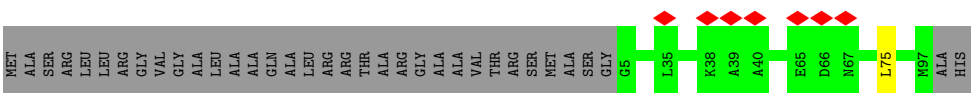
• Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial

Chain r:



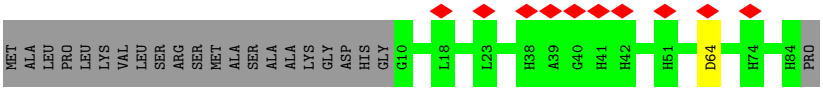
• Molecule 16: Cytochrome c oxidase subunit 5B, mitochondrial

Chain s:

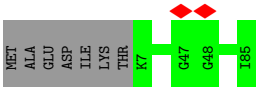


• Molecule 17: Cytochrome c oxidase subunit 6A2, mitochondrial

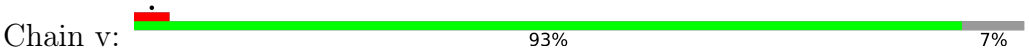
Chain t:

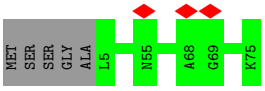


• Molecule 18: Cytochrome c oxidase subunit 6B1

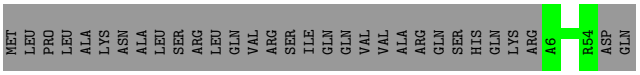


• Molecule 19: Cytochrome c oxidase subunit 6C

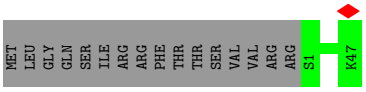




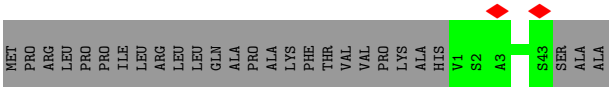
• Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial



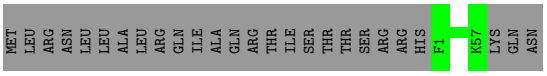
• Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial

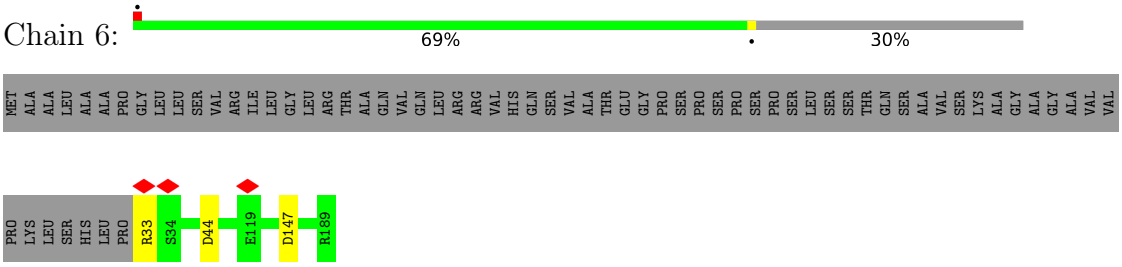


• Molecule 23: Cytochrome c oxidase subunit 7A2, mitochondrial



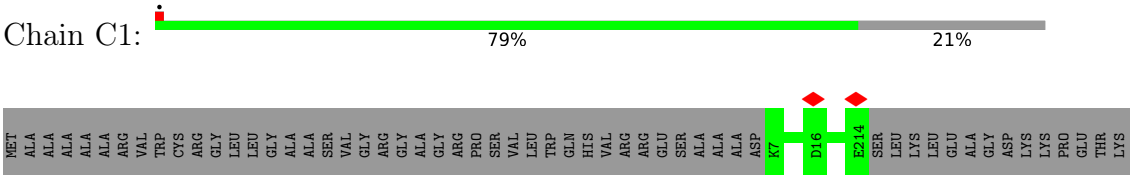
• Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:



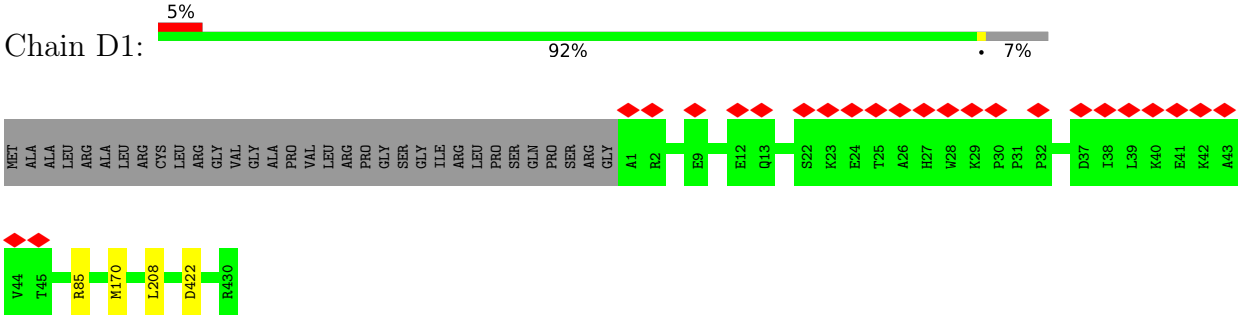
• Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C1:



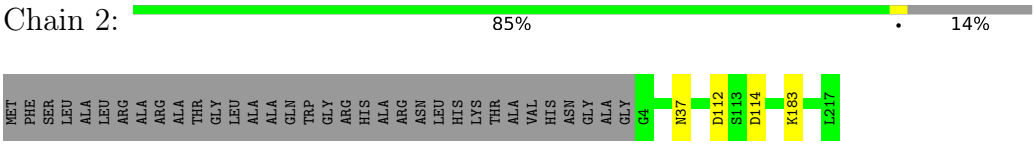
• Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D1:



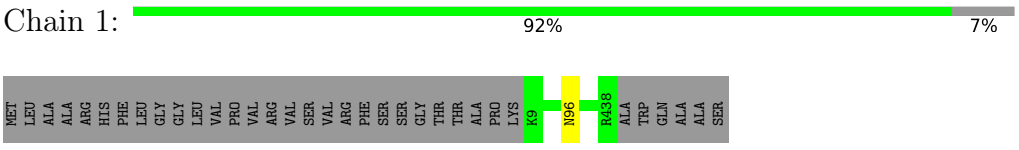
• Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2:



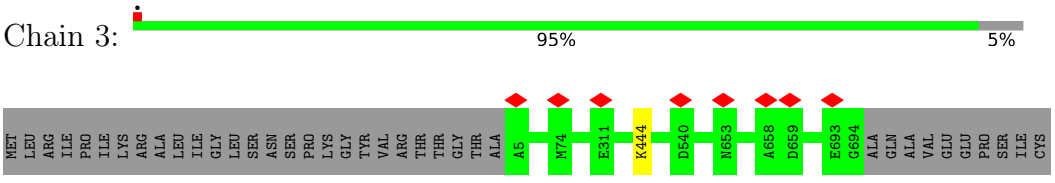
• Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



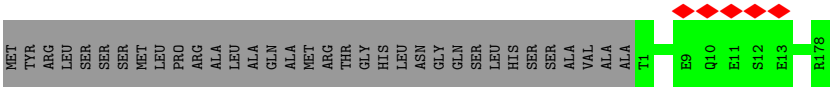
• Molecule 29: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:



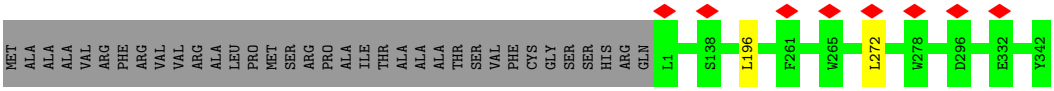
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:



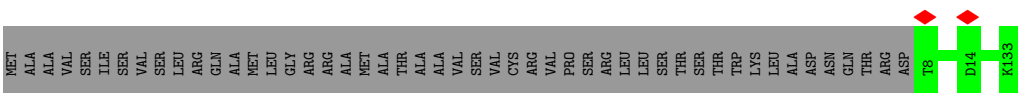
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P1:



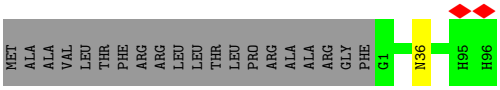
• Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q1:



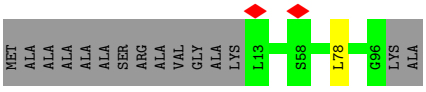
• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7:



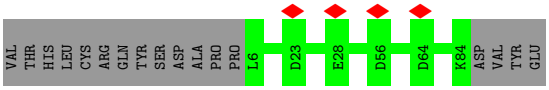
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S1:



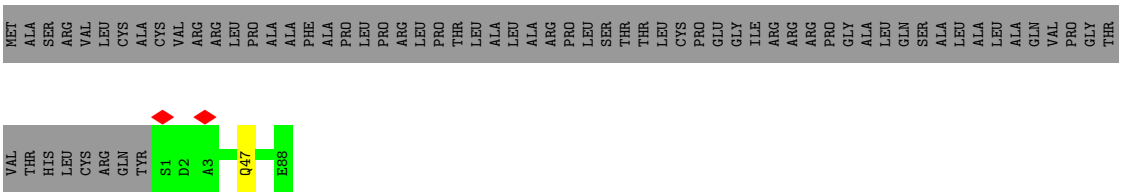
• Molecule 35: Acyl carrier protein, mitochondrial

Chain T1:



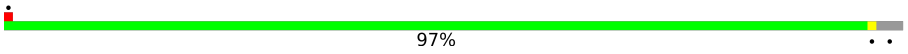
• Molecule 35: Acyl carrier protein, mitochondrial

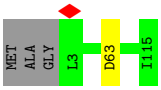
Chain U1:



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

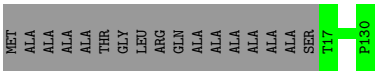
Chain V1:





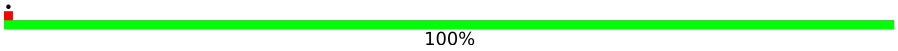
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1:



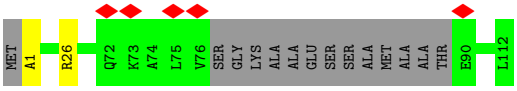
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q1:



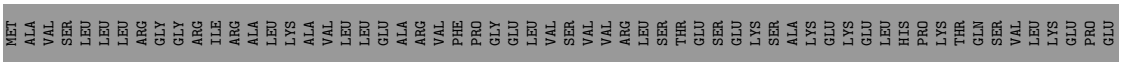
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

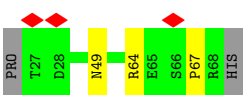
Chain r1:



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

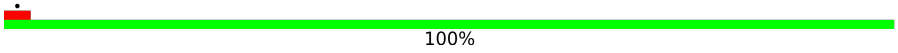
Chain s1:

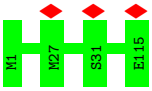




• Molecule 41: NADH-ubiquinone oxidoreductase chain 3

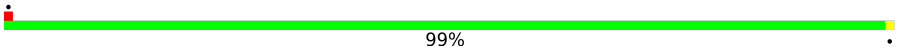
Chain A1:

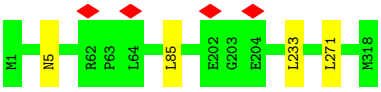




• Molecule 42: NADH-ubiquinone oxidoreductase chain 1

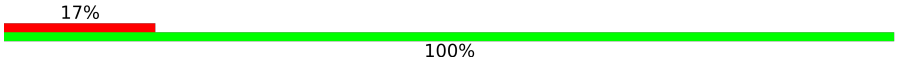
Chain H1:

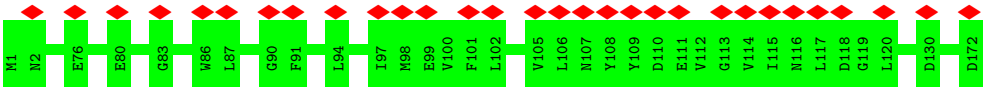




• Molecule 43: NADH-ubiquinone oxidoreductase chain 6

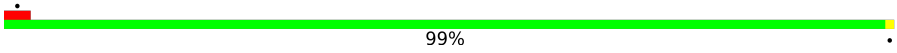
Chain J1:

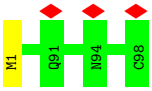




• Molecule 44: NADH-ubiquinone oxidoreductase chain 4L

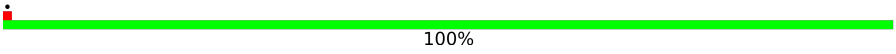
Chain K1:

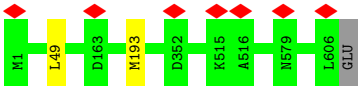




• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

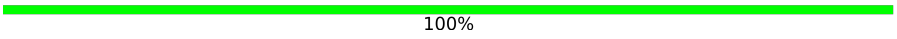
Chain L1:





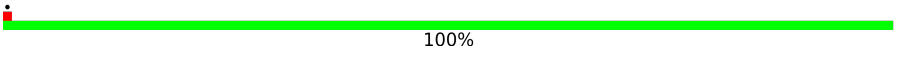
• Molecule 46: NADH-ubiquinone oxidoreductase chain 4

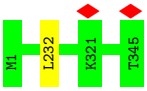
Chain M1:



• Molecule 47: NADH-ubiquinone oxidoreductase chain 2

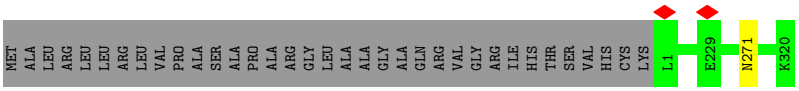
Chain N1:





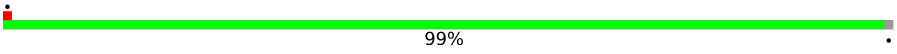
• Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

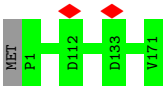
Chain O1:



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

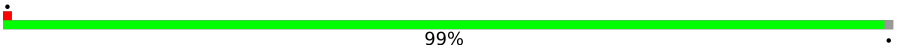
Chain X1:

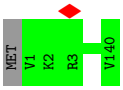




• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

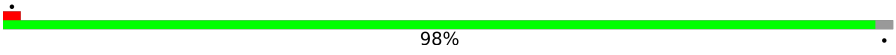
Chain Y1:

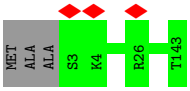




• Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

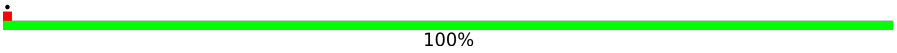
Chain Z1:





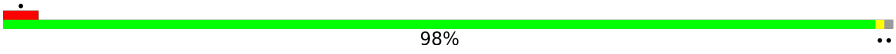
• Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

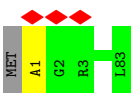
Chain a1:



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

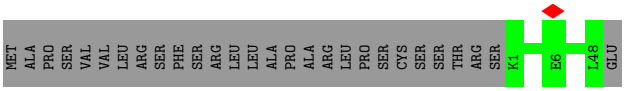
Chain b1:





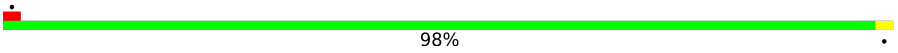
• Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

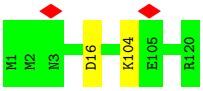
Chain c1:



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

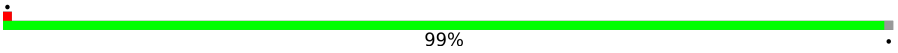
Chain d1:

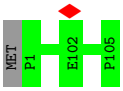




• Molecule 56: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

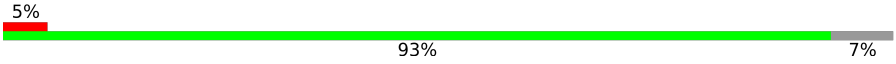
Chain e1:

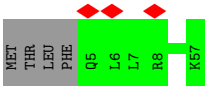




• Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

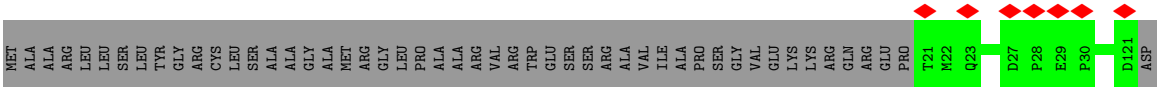
Chain f1:





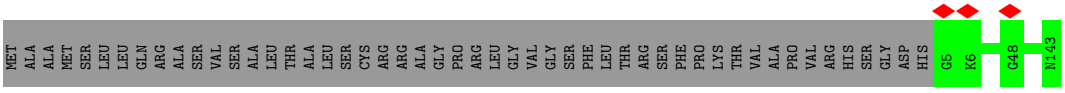
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g1:



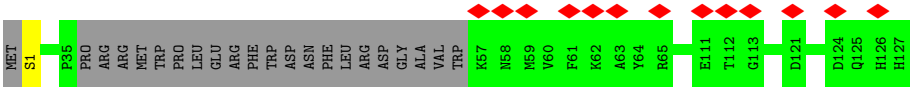
• Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h1:



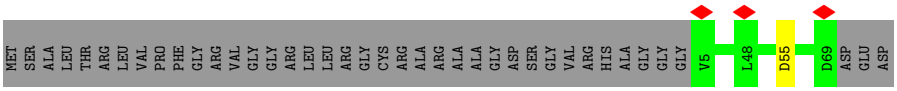
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i1:



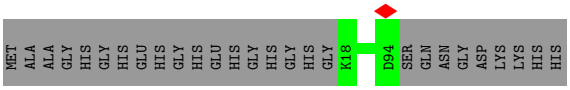
• Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j1:



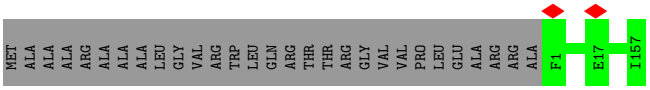
• Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k1:



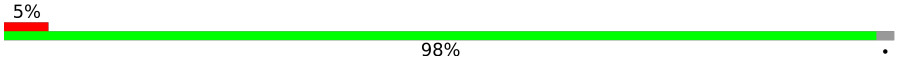
• Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

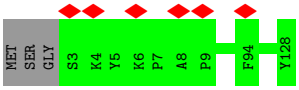
Chain l1:



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

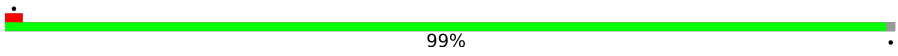
Chain m1:

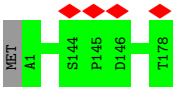




• Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

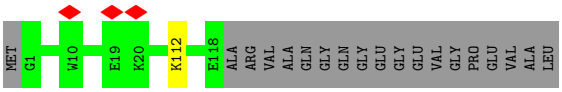
Chain n1:





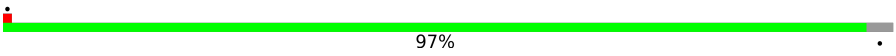
• Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

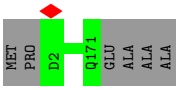
Chain o1:



• 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	103207	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
Maximum map value	0.154	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	297.86, 218.35999, 261.81998	wwPDB
Map dimensions	281, 206, 247	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CU, 2MR, AYA, MG, SAC, FME, K, DGT, SF4, TGL, CUA, FES, HEC, NDP, HEA, FMN, HEM, NA, ZN, PC1, 3PE, CDL, ZMP

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	A	0.28	0/3529	0.56	0/4793
1	L	0.28	0/3530	0.55	0/4793
2	B	0.27	0/3188	0.51	0/4308
2	M	0.28	0/3205	0.53	0/4332
3	C	0.30	0/3147	0.52	0/4297
3	N	0.29	0/3147	0.52	1/4297 (0.0%)
4	D	0.29	0/1968	0.52	0/2674
4	O	0.27	0/1968	0.50	0/2674
5	E	0.27	0/1176	0.52	0/1609
5	P	0.27	0/1176	0.49	0/1609
5	T	0.30	0/565	0.65	0/772
6	F	0.27	0/916	0.57	0/1226
6	Q	0.30	0/922	0.56	0/1234
7	G	0.34	0/673	0.62	0/909
7	R	0.36	0/673	0.66	0/909
8	H	0.35	0/552	0.76	1/739 (0.1%)
8	S	0.32	0/570	0.71	1/763 (0.1%)
9	J	0.30	0/509	0.62	0/687
9	U	0.30	0/509	0.53	0/687
10	K	0.27	0/438	0.61	0/598
10	V	0.27	0/446	0.62	0/609
11	n	0.33	0/4162	0.60	2/5686 (0.0%)
12	o	0.31	0/1863	0.67	1/2542 (0.0%)
13	p	0.30	0/2202	0.57	0/3010
14	q	0.30	0/1190	0.57	0/1609
15	r	0.31	0/860	0.67	1/1167 (0.1%)
16	s	0.28	0/734	0.56	1/996 (0.1%)
17	t	0.28	0/632	0.61	1/866 (0.1%)
18	u	0.33	0/674	0.64	0/910
19	v	0.29	0/579	0.61	0/771
20	x	0.31	0/396	0.65	0/541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
21	y	0.29	0/399	0.54	0/535
22	z	0.29	0/318	0.57	0/433
23	w	0.28	0/444	0.65	0/598
24	6	0.35	0/1289	0.71	3/1744 (0.2%)
25	C1	0.30	0/1780	0.57	0/2424
26	D1	0.32	0/3540	0.58	3/4795 (0.1%)
27	2	0.33	0/1700	0.64	2/2316 (0.1%)
28	1	0.30	0/3396	0.58	1/4586 (0.0%)
29	3	0.30	0/5392	0.57	0/7305
30	9	0.32	0/1461	0.56	0/1974
31	P1	0.29	0/2823	0.59	2/3828 (0.1%)
32	Q1	0.28	0/1045	0.54	0/1411
33	7	0.29	0/773	0.55	0/1041
34	S1	0.32	0/682	0.66	1/920 (0.1%)
35	T1	0.30	0/646	0.68	0/869
35	U1	0.33	0/718	0.52	0/970
36	V1	0.29	0/945	0.50	1/1281 (0.1%)
37	W1	0.30	0/993	0.58	0/1335
38	q1	0.31	0/1251	0.55	0/1702
39	r1	0.30	0/806	0.56	0/1090
40	s1	0.34	0/360	0.79	2/489 (0.4%)
41	A1	0.30	0/948	0.57	0/1295
42	H1	0.35	0/2607	0.65	3/3564 (0.1%)
43	J1	0.30	0/1330	0.52	0/1810
44	K1	0.29	0/738	0.58	0/1002
45	L1	0.31	0/4913	0.56	2/6686 (0.0%)
46	M1	0.29	0/3709	0.56	1/5052 (0.0%)
47	N1	0.30	0/2755	0.56	1/3751 (0.0%)
48	O1	0.28	0/2674	0.51	0/3626
49	X1	0.27	0/1434	0.51	0/1937
50	Y1	0.28	0/1061	0.49	0/1439
51	Z1	0.29	0/1198	0.56	0/1616
52	a1	0.27	0/585	0.56	0/788
53	b1	0.26	0/666	0.47	0/914
54	c1	0.29	0/409	0.52	0/555
55	d1	0.29	0/1028	0.58	1/1387 (0.1%)
56	e1	0.27	0/900	0.51	0/1199
57	f1	0.29	0/468	0.56	0/630
58	g1	0.29	0/878	0.51	0/1196
59	h1	0.28	0/1201	0.54	0/1626
60	i1	0.28	0/917	0.53	0/1243
61	j1	0.27	0/587	0.57	1/804 (0.1%)
62	k1	0.30	0/646	0.55	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	0.57	0/1463
65	n1	0.30	0/1596	0.57	0/2162
66	o1	0.31	0/1039	0.62	0/1394
67	p1	0.29	0/1471	0.52	0/1988
All	All	0.30	0/115076	0.57	33/156145 (0.0%)

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	s1	67	PRO	CA-N-CD	-9.47	98.24	111.50
24	6	44	ASP	CB-CG-OD1	8.40	125.86	118.30
27	2	114	ASP	CB-CG-OD1	8.10	125.59	118.30
12	o	68	LEU	CA-CB-CG	7.83	133.31	115.30
11	n	212	ASP	CB-CG-OD1	7.34	124.91	118.30

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	A	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
1	L	443/480 (92%)	427 (96%)	16 (4%)	0	100	100
2	B	416/453 (92%)	410 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	418/453 (92%)	400 (96%)	18 (4%)	0	100	100
3	C	378/381 (99%)	368 (97%)	10 (3%)	0	100	100
3	N	378/381 (99%)	364 (96%)	14 (4%)	0	100	100
4	D	238/325 (73%)	228 (96%)	10 (4%)	0	100	100
4	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
5	E	194/274 (71%)	188 (97%)	6 (3%)	0	100	100
5	P	194/274 (71%)	187 (96%)	7 (4%)	0	100	100
5	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
6	F	99/111 (89%)	99 (100%)	0	0	100	100
6	Q	100/111 (90%)	99 (99%)	1 (1%)	0	100	100
7	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
7	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
8	H	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
8	S	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
9	J	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
9	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
10	K	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
10	V	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
11	n	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
12	o	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
13	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
14	q	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
15	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
16	s	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
17	t	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
18	u	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
19	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
20	x	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
21	y	45/63 (71%)	45 (100%)	0	0	100	100
22	z	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
23	w	55/83 (66%)	55 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
25	C1	206/263 (78%)	198 (96%)	8 (4%)	0	100	100
26	D1	427/463 (92%)	410 (96%)	17 (4%)	0	100	100
27	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	29	61
28	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
29	3	688/727 (95%)	658 (96%)	30 (4%)	0	100	100
30	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
31	P1	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
32	Q1	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
33	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
34	S1	82/99 (83%)	77 (94%)	5 (6%)	0	100	100
35	T1	77/156 (49%)	74 (96%)	3 (4%)	0	100	100
35	U1	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
36	V1	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
37	W1	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
38	q1	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
39	r1	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
40	s1	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
41	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
42	H1	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
43	J1	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
44	K1	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
45	L1	604/607 (100%)	575 (95%)	29 (5%)	0	100	100
46	M1	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
47	N1	343/345 (99%)	333 (97%)	10 (3%)	0	100	100
48	O1	318/355 (90%)	297 (93%)	21 (7%)	0	100	100
49	X1	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
50	Y1	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
51	Z1	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
52	a1	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
53	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	c1	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
55	d1	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
56	e1	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
57	f1	51/57 (90%)	50 (98%)	1 (2%)	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%)	95 (93%)	7 (7%)	0	100	100
61	j1	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
62	k1	75/104 (72%)	74 (99%)	1 (1%)	0	100	100
63	l1	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
64	m1	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
65	n1	176/179 (98%)	170 (97%)	6 (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	13983/16116 (87%)	13472 (96%)	510 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	2	183	LYS

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	A	372/398 (94%)	372 (100%)	0	100	100
1	L	372/398 (94%)	371 (100%)	1 (0%)	92	96
2	B	328/356 (92%)	328 (100%)	0	100	100
2	M	330/356 (93%)	330 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	332/333 (100%)	331 (100%)	1 (0%)	92 96
3	N	332/333 (100%)	332 (100%)	0	100 100
4	D	205/260 (79%)	205 (100%)	0	100 100
4	O	205/260 (79%)	205 (100%)	0	100 100
5	E	69/224 (31%)	69 (100%)	0	100 100
5	P	69/224 (31%)	69 (100%)	0	100 100
5	T	58/224 (26%)	58 (100%)	0	100 100
6	F	93/99 (94%)	92 (99%)	1 (1%)	73 85
6	Q	94/99 (95%)	94 (100%)	0	100 100
7	G	70/74 (95%)	70 (100%)	0	100 100
7	R	70/74 (95%)	70 (100%)	0	100 100
8	H	63/83 (76%)	63 (100%)	0	100 100
8	S	65/83 (78%)	65 (100%)	0	100 100
9	J	51/55 (93%)	51 (100%)	0	100 100
9	U	51/55 (93%)	50 (98%)	1 (2%)	55 76
10	K	41/46 (89%)	41 (100%)	0	100 100
10	V	42/46 (91%)	42 (100%)	0	100 100
11	n	425/425 (100%)	424 (100%)	1 (0%)	93 97
12	o	210/210 (100%)	208 (99%)	2 (1%)	76 86
13	p	226/227 (100%)	225 (100%)	1 (0%)	91 95
14	q	122/146 (84%)	122 (100%)	0	100 100
15	r	91/118 (77%)	91 (100%)	0	100 100
16	s	80/101 (79%)	80 (100%)	0	100 100
17	t	62/78 (80%)	62 (100%)	0	100 100
18	u	70/76 (92%)	70 (100%)	0	100 100
19	v	54/57 (95%)	54 (100%)	0	100 100
20	x	39/67 (58%)	39 (100%)	0	100 100
21	y	40/55 (73%)	40 (100%)	0	100 100
22	z	33/55 (60%)	33 (100%)	0	100 100
23	w	43/67 (64%)	43 (100%)	0	100 100
24	6	133/185 (72%)	132 (99%)	1 (1%)	81 89

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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	93
28	1	345/370 (93%)	345 (100%)	0	100	100
29	3	580/610 (95%)	579 (100%)	1 (0%)	93	97
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	83
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%)	80 (99%)	1 (1%)	71	83
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%)	87 (99%)	1 (1%)	73	85
40	s1	41/95 (43%)	39 (95%)	2 (5%)	25	56
41	A1	103/103 (100%)	103 (100%)	0	100	100
42	H1	279/279 (100%)	278 (100%)	1 (0%)	91	95
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	97
47	N1	307/307 (100%)	307 (100%)	0	100	100
48	O1	284/309 (92%)	283 (100%)	1 (0%)	91	95
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%)	122 (100%)	0	100	100
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%)	106 (99%)	1 (1%)	78 87
56	e1	93/94 (99%)	93 (100%)	0	100 100
57	f1	49/53 (92%)	49 (100%)	0	100 100
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%)	60 (100%)	0	100 100
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%)	108 (99%)	1 (1%)	78 87
67	p1	155/158 (98%)	155 (100%)	0	100 100
All	All	12029/13709 (88%)	12008 (100%)	21 (0%)	93 97

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	s1	64	ARG
48	O1	271	ASN
66	o1	112	LYS
35	U1	47	GLN
46	M1	54	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
11	n	451	ASN
13	p	70	HIS
46	M1	366	ASN
15	r	94	ASN
8	H	65	HIS

5.3.3 RNA

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	$\#\|Z\| > 2$
46	FME	M1	1	46	8,9,10	0.97	0	7,9,11	0.79	0
60	SAC	i1	1	60	7,8,9	1.00	0	8,9,11	0.98	1 (12%)
39	AYA	r1	1	39	6,7,8	1.29	1 (16%)	5,8,10	1.29	1 (20%)
45	FME	L1	1	45	8,9,10	0.91	0	7,9,11	0.95	0
47	FME	N1	1	47	8,9,10	0.92	0	7,9,11	0.94	0
41	FME	A1	1	41	8,9,10	0.94	0	7,9,11	0.83	0
53	AYA	b1	1	53	6,7,8	1.26	1 (16%)	5,8,10	1.29	1 (20%)
26	2MR	D1	85	26	10,12,13	2.58	2 (20%)	5,13,15	2.79	2 (40%)
42	FME	H1	1	42	8,9,10	0.97	0	7,9,11	0.77	0
44	FME	K1	1	44	8,9,10	0.90	0	7,9,11	1.83	2 (28%)
43	FME	J1	1	43	8,9,10	0.94	0	7,9,11	0.86	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
46	FME	M1	1	46	-	2/7/9/11	-
60	SAC	i1	1	60	-	0/7/8/10	-
39	AYA	r1	1	39	-	0/4/6/8	-
45	FME	L1	1	45	-	3/7/9/11	-
47	FME	N1	1	47	-	4/7/9/11	-
41	FME	A1	1	41	-	1/7/9/11	-
53	AYA	b1	1	53	-	0/4/6/8	-
26	2MR	D1	85	26	-	3/10/13/15	-
42	FME	H1	1	42	-	3/7/9/11	-
44	FME	K1	1	44	-	5/7/9/11	-
43	FME	J1	1	43	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D1	85	2MR	CZ-NE	5.89	1.46	1.34
26	D1	85	2MR	CZ-NH2	5.01	1.44	1.33
39	r1	1	AYA	CA-N	-2.55	1.43	1.46
53	b1	1	AYA	CA-N	-2.35	1.44	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D1	85	2MR	CD-NE-CZ	5.27	133.27	123.41
44	K1	1	FME	C-CA-N	4.05	117.05	109.73
26	D1	85	2MR	NE-CZ-NH2	-3.00	116.73	119.48
39	r1	1	AYA	CB-CA-N	2.72	112.63	109.61
53	b1	1	AYA	CB-CA-N	2.61	112.51	109.61

There are no chirality outliers.

5 of 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
44	K1	1	FME	O1-CN-N-CA
44	K1	1	FME	N-CA-CB-CG
45	L1	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 94 ligands modelled in this entry, 7 are monoatomic - leaving 87 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	$\#\|Z\| > 2$
81	SF4	3	801	29	0,12,12	-	-	-		
68	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.27	0
68	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.56	1 (2%)
73	PC1	z	101	-	27,27,53	0.38	0	33,35,61	0.35	0
81	SF4	6	201	24	0,12,12	-	-	-		
68	3PE	C	405	-	50,50,50	0.31	0	53,55,55	0.28	0
68	3PE	Z1	401	-	50,50,50	0.31	0	53,55,55	0.46	1 (1%)
70	HEM	N	403	3	41,50,50	1.43	4 (9%)	45,82,82	1.38	6 (13%)
68	3PE	R	304	-	29,29,50	0.38	0	32,34,55	0.33	0
73	PC1	6	203	-	42,42,53	0.33	0	48,50,61	0.49	0
68	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
68	3PE	q	201	-	25,25,50	0.41	0	28,30,55	0.40	0
71	HEC	D	301	4	32,50,50	2.18	3 (9%)	24,82,82	1.54	5 (20%)
68	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.34	0
68	3PE	n	606	-	27,27,50	0.41	0	30,32,55	0.38	0
68	3PE	x	101	-	26,26,50	0.40	0	29,31,55	0.35	0
81	SF4	9	202	30	0,12,12	-	-	-		
73	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.45	0
73	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.33	0
70	HEM	N	402	3	41,50,50	1.44	3 (7%)	45,82,82	1.50	9 (20%)
68	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.32	0
72	FES	P	202	5	0,4,4	-	-	-		
73	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.28	0
68	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.38	0
69	CDL	L1	703	-	45,45,99	0.43	0	51,57,111	0.36	0
68	3PE	C	406	-	30,30,50	0.39	0	33,35,55	0.34	0
68	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
68	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.65	0
69	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
68	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.34	0
76	HEA	n	603	11	57,67,67	1.44	7 (12%)	61,103,103	2.45	23 (37%)
68	3PE	D1	501	-	50,50,50	0.31	0	53,55,55	0.29	0
73	PC1	A1	601	-	30,30,53	0.40	0	36,38,61	0.55	0
73	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.62	0
68	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.31	0
80	TGL	y	601	-	36,36,62	0.23	0	39,39,65	0.17	0
68	3PE	L1	704	-	50,50,50	0.30	0	53,55,55	0.31	0
81	SF4	3	802	29	0,12,12	-	-	-		
85	ZMP	W1	201	-	27,33,36	0.66	1 (3%)	32,40,45	0.98	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	HEM	C	402	3	41,50,50	1.44	4 (9%)	45,82,82	1.46	8 (17%)
68	3PE	P	201	-	32,32,50	0.37	0	35,37,55	0.34	0
68	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.31	0
84	NDP	P1	501	-	45,52,52	0.53	0	53,80,80	0.60	1 (1%)
69	CDL	Y1	404	-	71,71,99	0.36	0	77,83,111	0.44	1 (1%)
69	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.34	0
82	FMN	1	501	-	33,33,33	0.27	0	48,50,50	0.47	1 (2%)
68	3PE	H1	401	-	45,45,50	0.32	0	48,50,55	0.29	0
69	CDL	V	102	-	34,37,99	0.35	0	37,47,111	0.31	0
72	FES	E	201	5	0,4,4	-	-	-		
69	CDL	R	301	-	56,56,99	0.38	0	62,68,111	0.33	0
68	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
69	CDL	L1	702	-	77,77,99	0.34	0	83,89,111	0.29	0
68	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.60	1 (3%)
68	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.35	0
86	DGT	O1	401	77	26,33,33	0.77	1 (3%)	32,52,52	0.48	0
76	HEA	n	604	11	57,67,67	1.46	8 (14%)	61,103,103	2.39	22 (36%)
69	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.50	0
73	PC1	p	303	-	49,49,53	0.33	0	55,57,61	0.57	1 (1%)
71	HEC	O	301	4	32,50,50	2.19	3 (9%)	24,82,82	1.59	4 (16%)
69	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
69	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.35	0
73	PC1	V	101	-	27,27,53	0.39	0	33,35,61	0.34	0
73	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.36	0
68	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.33	0
68	3PE	Y1	402	-	27,27,50	0.40	0	30,32,55	0.37	0
73	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.35	0
69	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.43	0
81	SF4	9	201	30	0,12,12	-	-	-		
73	PC1	E	202	-	34,34,53	0.35	0	40,42,61	0.36	0
69	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.39	1 (1%)
70	HEM	C	401	3	41,50,50	1.42	3 (7%)	45,82,82	1.49	8 (17%)
72	FES	2	301	27	0,4,4	-	-	-		
78	CUA	o	303	12	0,1,1	-	-	-		
68	3PE	N	401	-	33,33,50	0.36	0	36,38,55	0.34	0
68	3PE	M1	503	-	35,35,50	0.36	0	38,40,55	0.31	0
81	SF4	1	502	28	0,12,12	-	-	-		
68	3PE	N	404	-	36,36,50	0.35	0	39,41,55	0.33	0
68	3PE	d1	202	-	30,30,50	0.38	0	33,35,55	0.33	0
68	3PE	A1	602	-	42,42,50	0.33	0	45,47,55	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.37	0
69	CDL	a1	101	-	56,56,99	0.40	0	62,68,111	0.46	1 (1%)
68	3PE	i1	201	-	41,41,50	0.33	0	44,46,55	0.30	0
69	CDL	R	302	-	40,40,99	0.46	0	46,52,111	0.54	0
72	FES	3	803	29	0,4,4	-	-	-		
85	ZMP	n1	201	-	25,31,36	0.76	1 (4%)	30,38,45	0.90	1 (3%)
69	CDL	R	303	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
69	CDL	Y1	401	-	93,93,99	0.31	0	99,105,111	0.27	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
81	SF4	3	801	29	-	-	0/6/5/5
68	3PE	M1	502	-	-	14/54/54/54	-
68	3PE	n	605	-	-	11/37/37/54	-
73	PC1	z	101	-	-	3/31/31/57	-
81	SF4	6	201	24	-	-	0/6/5/5
68	3PE	C	405	-	-	8/54/54/54	-
68	3PE	Z1	401	-	-	10/54/54/54	-
70	HEM	N	403	3	-	4/12/54/54	-
68	3PE	R	304	-	-	6/33/33/54	-
73	PC1	6	203	-	-	6/46/46/57	-
68	3PE	L1	701	-	-	8/54/54/54	-
68	3PE	q	201	-	-	10/29/29/54	-
71	HEC	D	301	4	-	0/10/54/54	-
68	3PE	v	101	-	-	5/31/31/54	-
68	3PE	n	606	-	-	13/31/31/54	-
68	3PE	x	101	-	-	9/30/30/54	-
81	SF4	9	202	30	-	-	0/6/5/5
73	PC1	9	203	-	-	10/57/57/57	-
73	PC1	p	302	-	-	8/38/38/57	-
70	HEM	N	402	3	-	2/12/54/54	-
68	3PE	6	202	-	-	4/35/35/54	-
72	FES	P	202	5	-	-	0/1/1/1
73	PC1	9	204	-	-	14/50/50/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	3PE	L	501	-	-	6/26/26/54	-
69	CDL	L1	703	-	-	12/56/56/110	-
68	3PE	C	406	-	-	5/34/34/54	-
68	3PE	N1	402	-	-	10/41/41/54	-
68	3PE	A	501	-	-	10/26/26/54	-
69	CDL	H1	402	-	-	14/59/59/110	-
68	3PE	d1	203	-	-	6/35/35/54	-
76	HEA	n	603	11	-	10/32/76/76	-
68	3PE	D1	501	-	-	8/54/54/54	-
73	PC1	A1	601	-	-	14/34/34/57	-
73	PC1	L	503	-	-	9/27/27/57	-
68	3PE	Y1	403	-	-	11/45/45/54	-
80	TGL	y	601	-	-	1/39/39/65	-
68	3PE	L1	704	-	-	15/54/54/54	-
85	ZMP	W1	201	-	-	5/38/40/43	-
81	SF4	3	802	29	-	-	0/6/5/5
70	HEM	C	402	3	-	1/12/54/54	-
68	3PE	P	201	-	-	5/36/36/54	-
68	3PE	p	301	-	-	9/48/48/54	-
84	NDP	P1	501	-	-	6/30/77/77	0/5/5/5
69	CDL	Y1	404	-	-	18/82/82/110	-
69	CDL	D	302	-	-	17/66/66/110	-
82	FMN	1	501	-	-	6/18/18/18	0/3/3/3
68	3PE	H1	401	-	-	11/49/49/54	-
69	CDL	V	102	-	-	8/41/45/110	-
72	FES	E	201	5	-	-	0/1/1/1
69	CDL	R	301	-	-	19/67/67/110	-
68	3PE	o	302	-	-	9/32/32/54	-
69	CDL	L1	702	-	-	19/88/88/110	-
68	3PE	t	101	-	-	10/28/28/54	-
68	3PE	C	403	-	-	10/38/38/54	-
86	DGT	O1	401	77	-	4/18/34/34	0/3/3/3
76	HEA	n	604	11	-	9/32/76/76	-
69	CDL	L	502	-	-	9/56/56/110	-
73	PC1	p	303	-	-	11/53/53/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	HEC	O	301	4	-	0/10/54/54	-
69	CDL	d1	201	-	-	16/77/77/110	-
69	CDL	C	404	-	-	12/52/52/110	-
73	PC1	V	101	-	-	6/31/31/57	-
73	PC1	K	101	-	-	10/31/31/57	-
68	3PE	K1	201	-	-	12/44/44/54	-
68	3PE	Y1	402	-	-	8/31/31/54	-
73	PC1	M1	501	-	-	13/57/57/57	-
69	CDL	h1	201	-	-	20/80/80/110	-
81	SF4	9	201	30	-	-	0/6/5/5
73	PC1	E	202	-	-	7/38/38/57	-
69	CDL	N1	401	-	-	15/100/100/110	-
70	HEM	C	401	3	-	2/12/54/54	-
72	FES	2	301	27	-	-	0/1/1/1
68	3PE	N	401	-	-	5/37/37/54	-
68	3PE	M1	503	-	-	8/39/39/54	-
81	SF4	1	502	28	-	-	0/6/5/5
68	3PE	N	404	-	-	7/40/40/54	-
68	3PE	d1	202	-	-	9/34/34/54	-
68	3PE	A1	602	-	-	9/46/46/54	-
69	CDL	A	502	-	-	14/56/56/110	-
69	CDL	a1	101	-	-	13/67/67/110	-
68	3PE	i1	201	-	-	6/45/45/54	-
69	CDL	R	302	-	-	10/51/51/110	-
72	FES	3	803	29	-	-	0/1/1/1
85	ZMP	n1	201	-	-	19/36/38/43	-
69	CDL	R	303	-	-	16/67/67/110	-
69	CDL	Y1	401	-	-	13/104/104/110	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	O	301	HEC	C2B-C3B	-6.49	1.34	1.40
71	D	301	HEC	C3C-C2C	-6.45	1.34	1.40
71	O	301	HEC	C3C-C2C	-6.39	1.34	1.40
71	D	301	HEC	C2B-C3B	-6.31	1.34	1.40
71	O	301	HEC	C3D-C2D	5.38	1.53	1.37

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	n	603	HEA	CMC-C2C-C3C	7.09	137.95	124.68
76	n	604	HEA	CMC-C2C-C3C	7.06	137.89	124.68
76	n	604	HEA	CMC-C2C-C1C	-6.32	118.76	128.46
76	n	603	HEA	CMC-C2C-C1C	-6.27	118.83	128.46
76	n	604	HEA	CMD-C2D-C1D	-4.94	117.51	125.04

There are no chirality outliers.

5 of 712 torsion outliers are listed below:

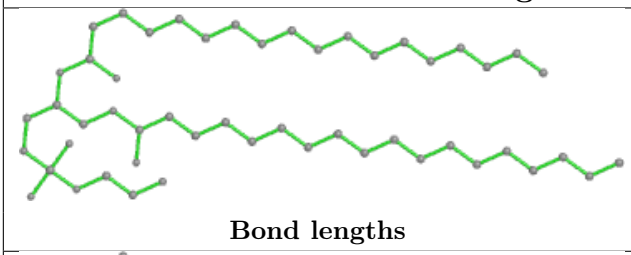
Mol	Chain	Res	Type	Atoms
68	A	501	3PE	C11-O13-P-O11
68	A	501	3PE	C11-O13-P-O12
68	A	501	3PE	C11-O13-P-O14
68	C	403	3PE	C1-O11-P-O12
68	C	403	3PE	C1-O11-P-O14

There are no ring outliers.

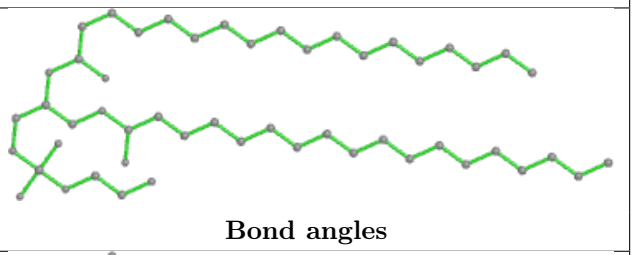
No monomer is involved in short contacts.

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.

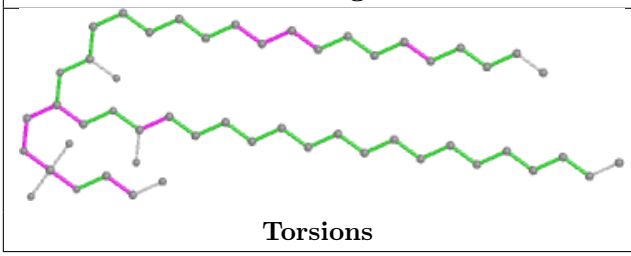
Ligand 3PE M1 502



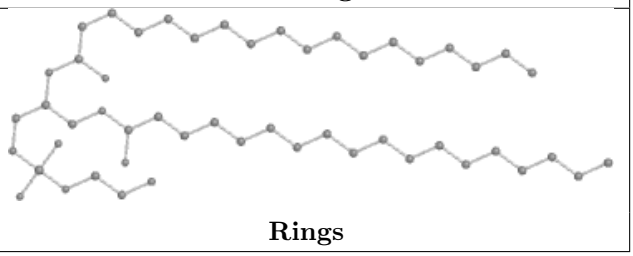
Bond lengths



Bond angles

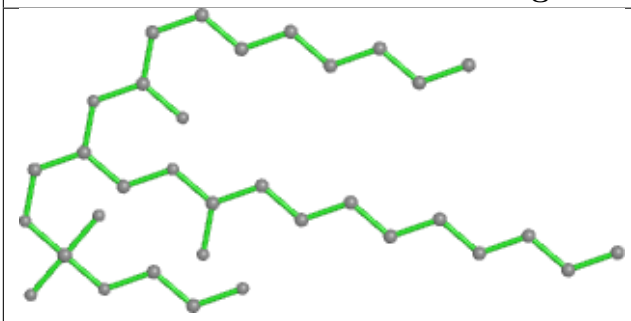


Torsions

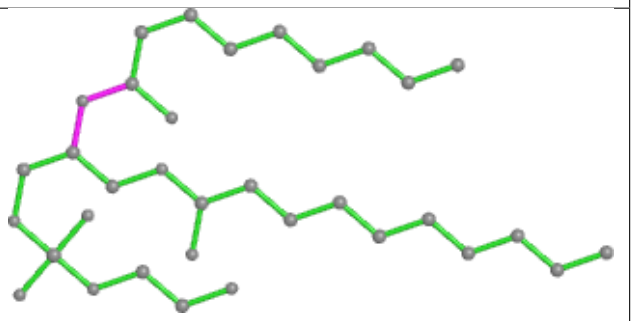


Rings

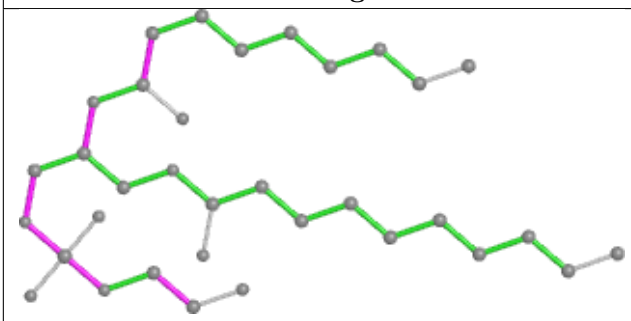
Ligand 3PE n 605



Bond lengths



Bond angles



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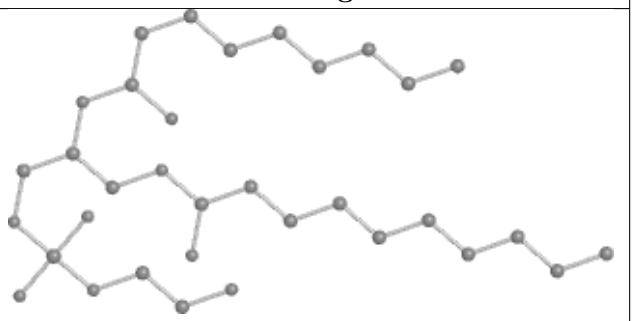
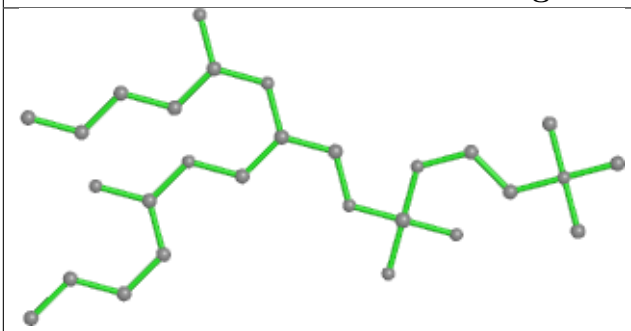
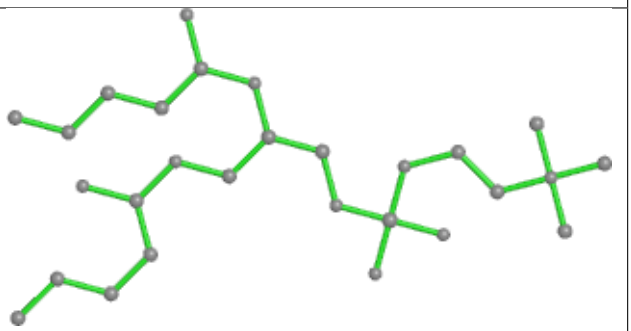


Rings

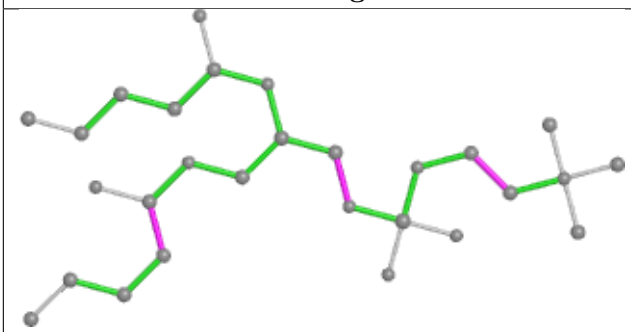
Ligand PC1 z 101



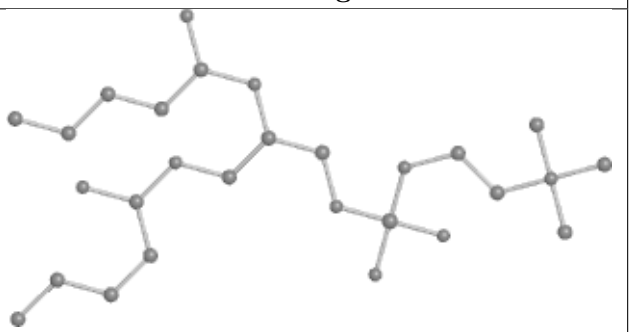
Bond lengths



Bond angles

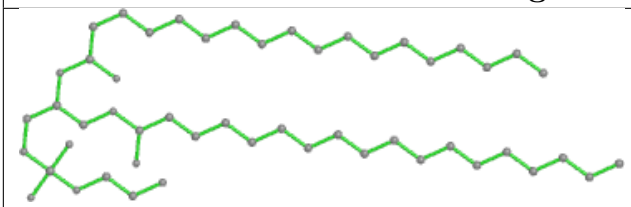


Torsions

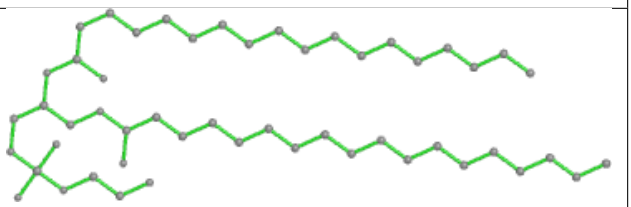


Rings

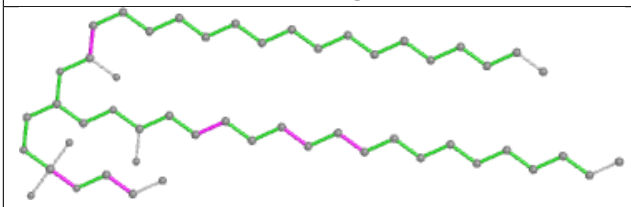
Ligand 3PE C 405



Bond lengths



Bond angles



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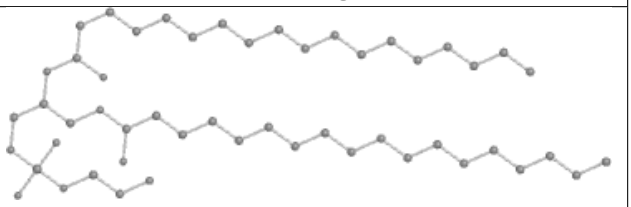
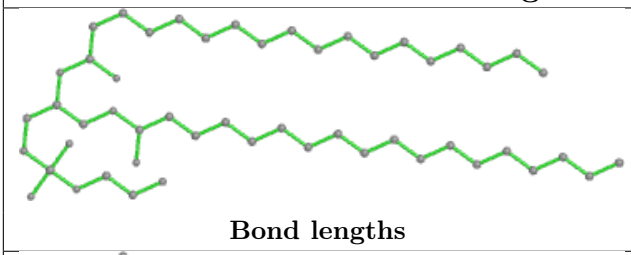


Rings

Ligand 3PE Z1 401



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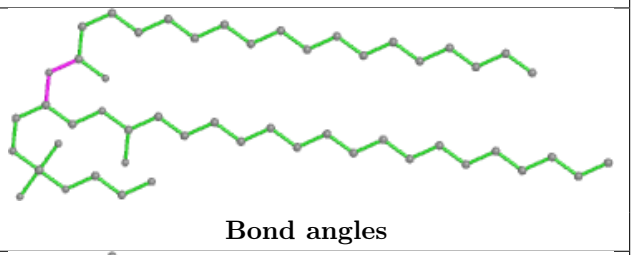

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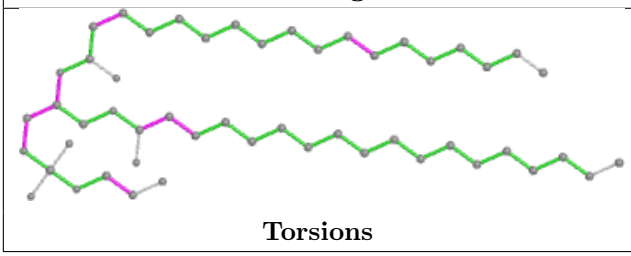

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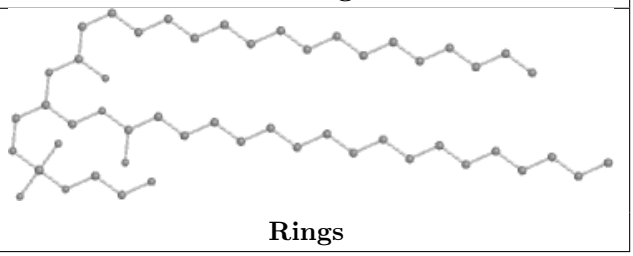
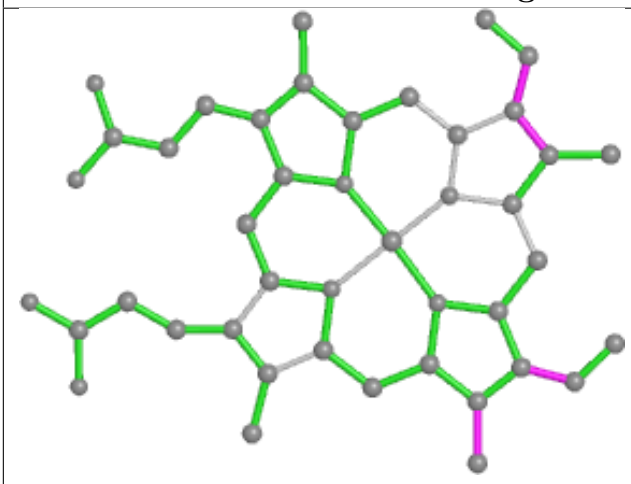


Rings

Ligand HEM N 403



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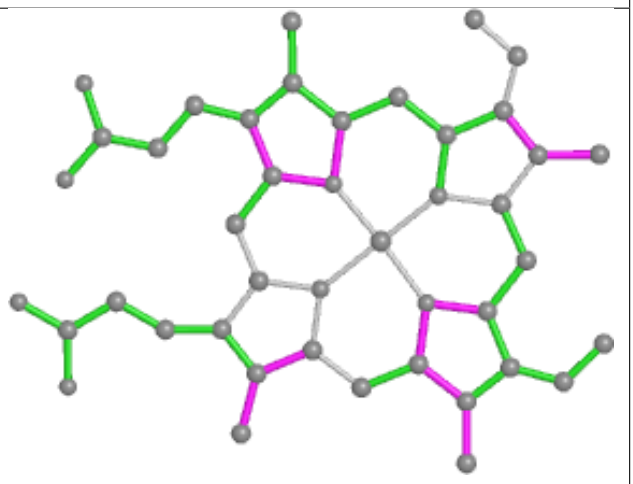

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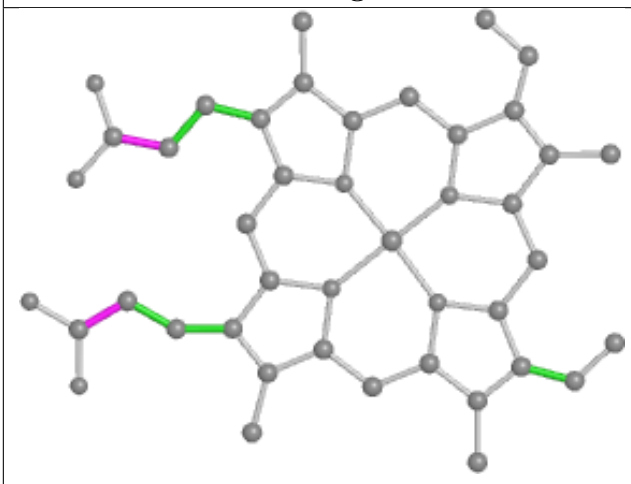
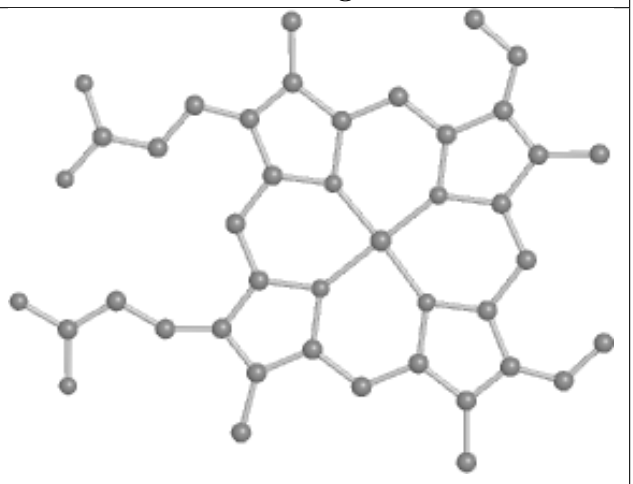


Torsions



Rings

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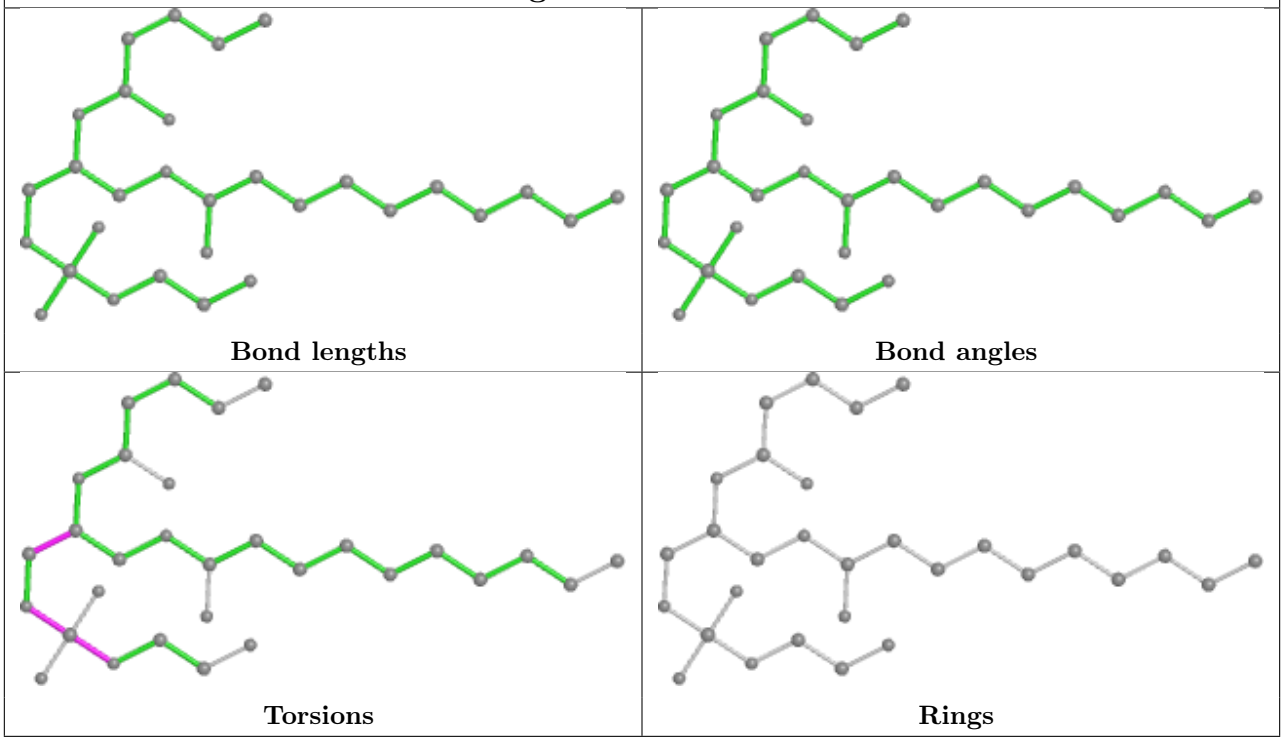
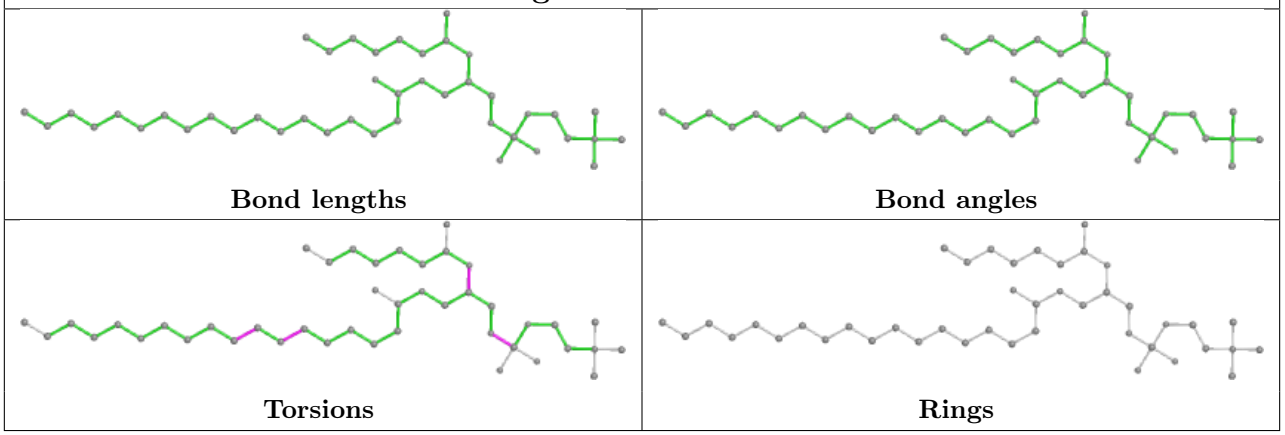


Ligand PC1 6 203



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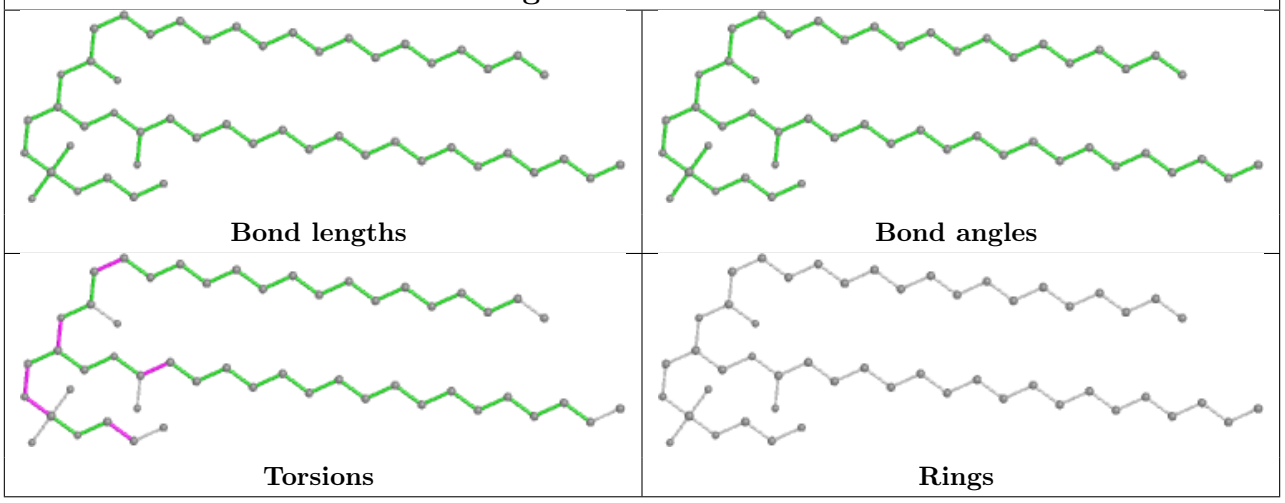
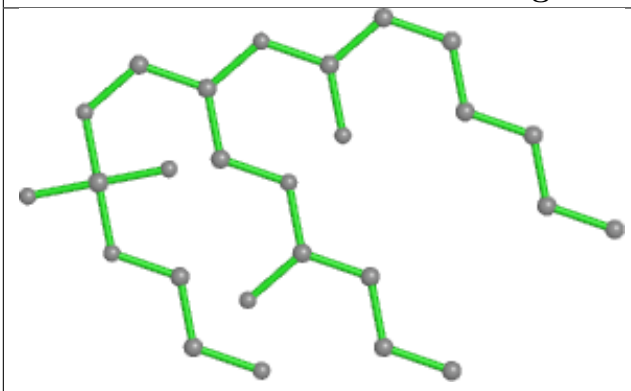


Ligand 3PE q 201



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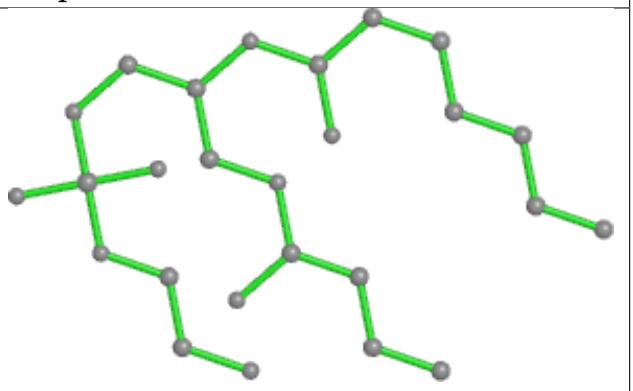
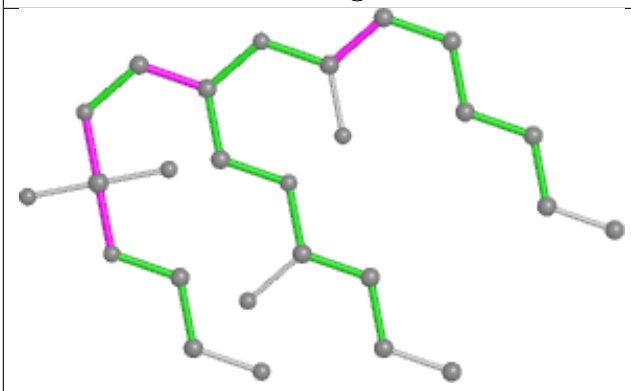
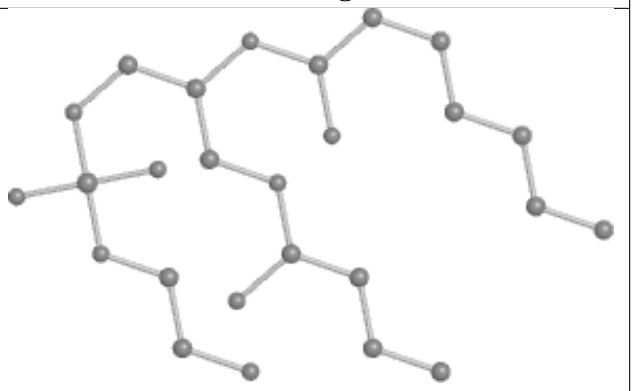


Bond angles

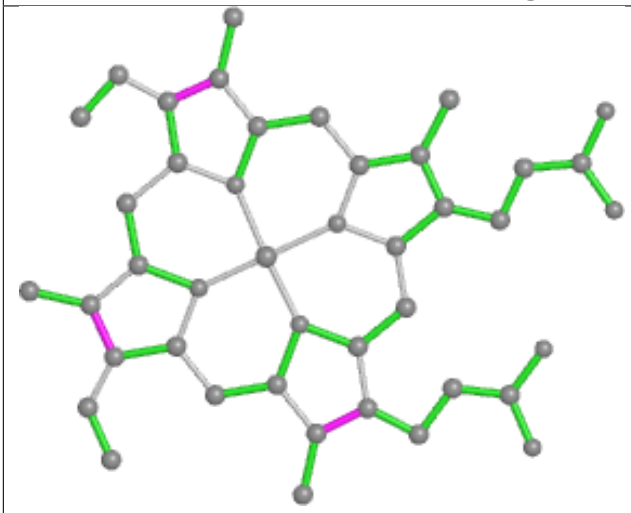


Torsions



Rings

Ligand HEC D 301



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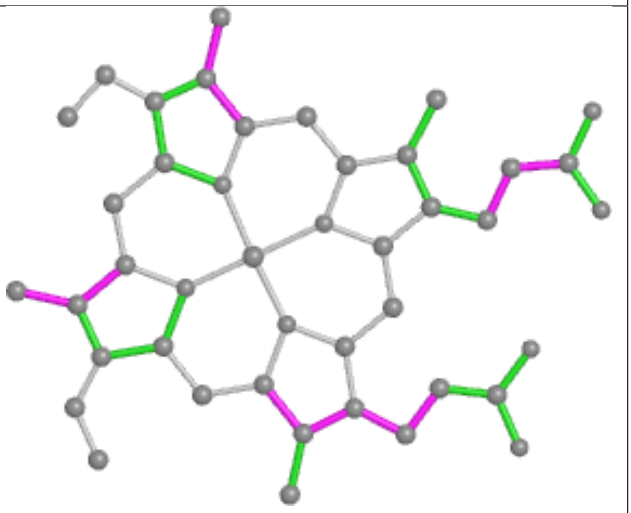
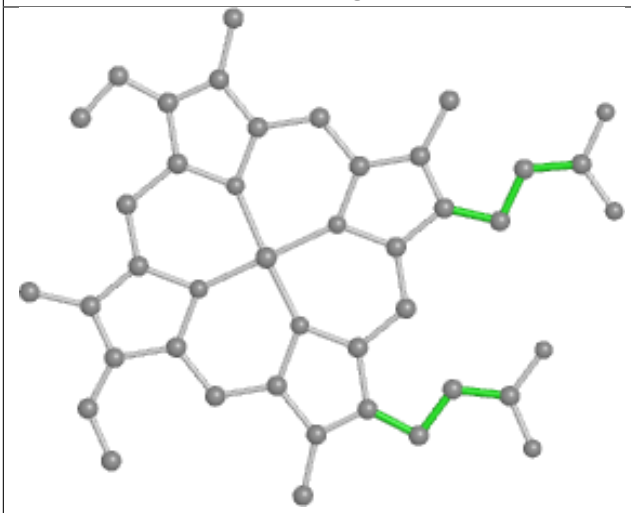


Bond angles



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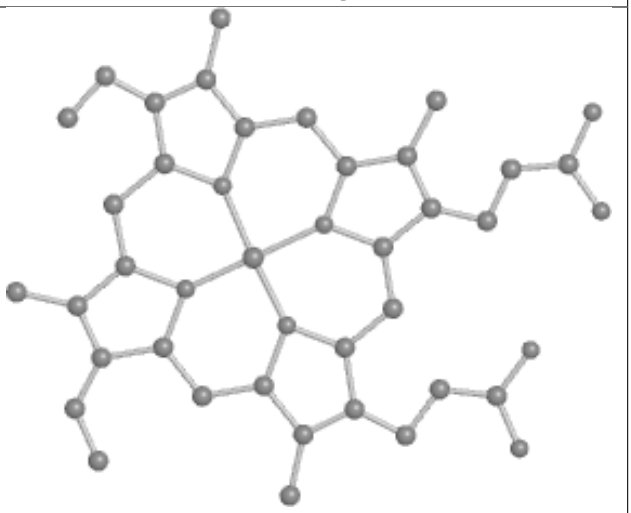
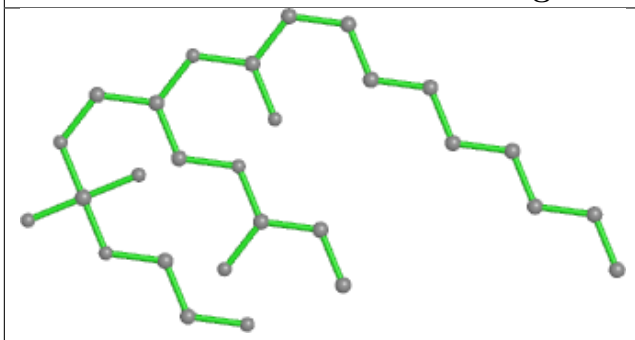


Rings

Ligand 3PE v 101



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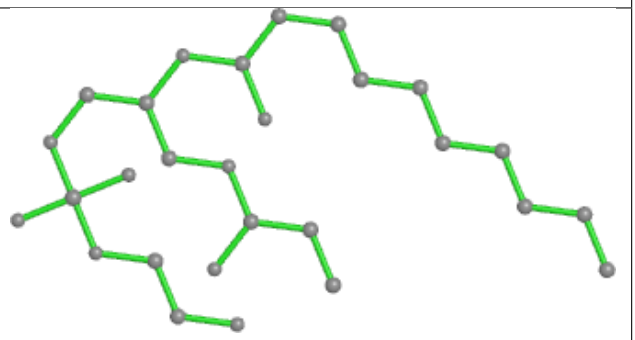
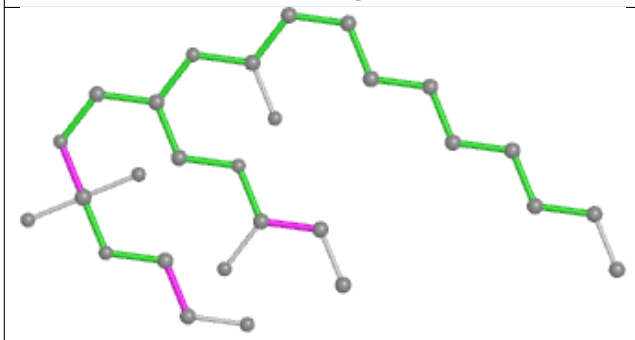


Bond angles



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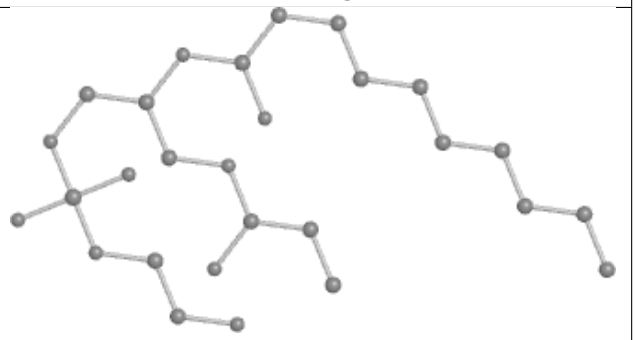
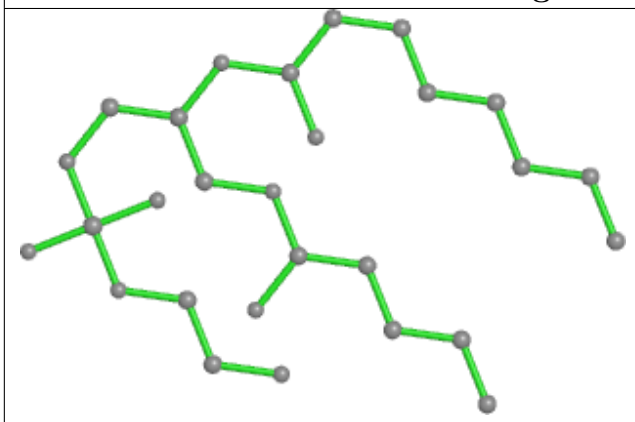


Rings

Ligand 3PE n 606



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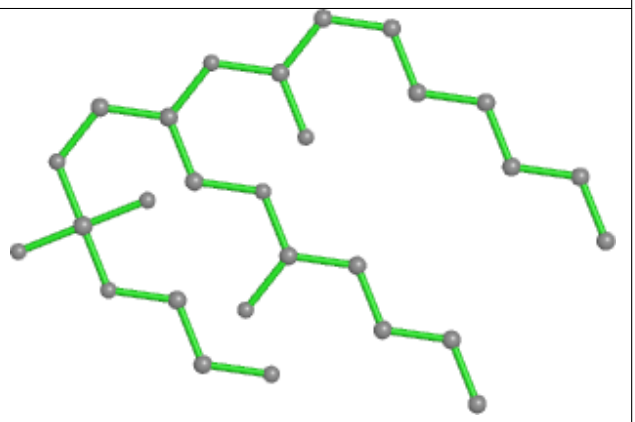
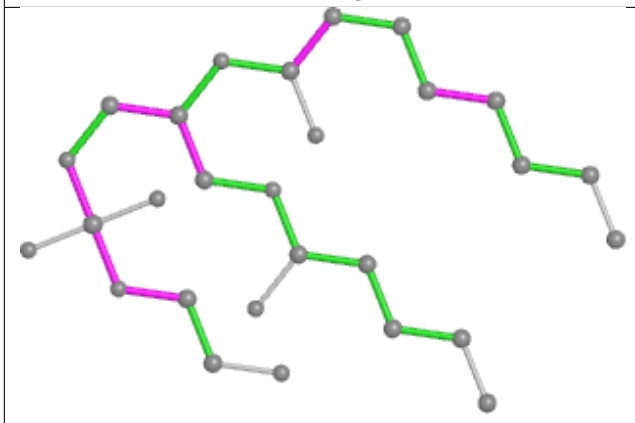


Bond angles



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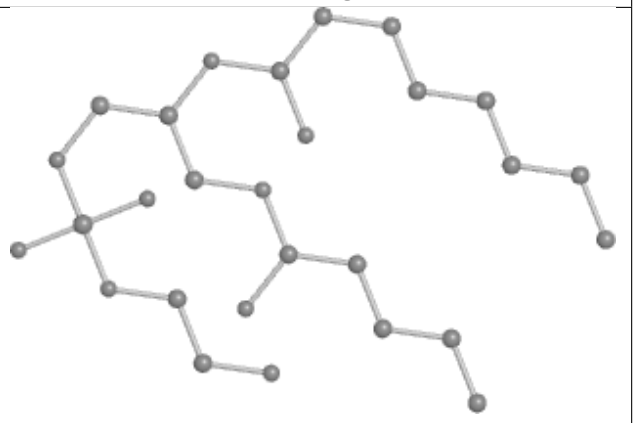
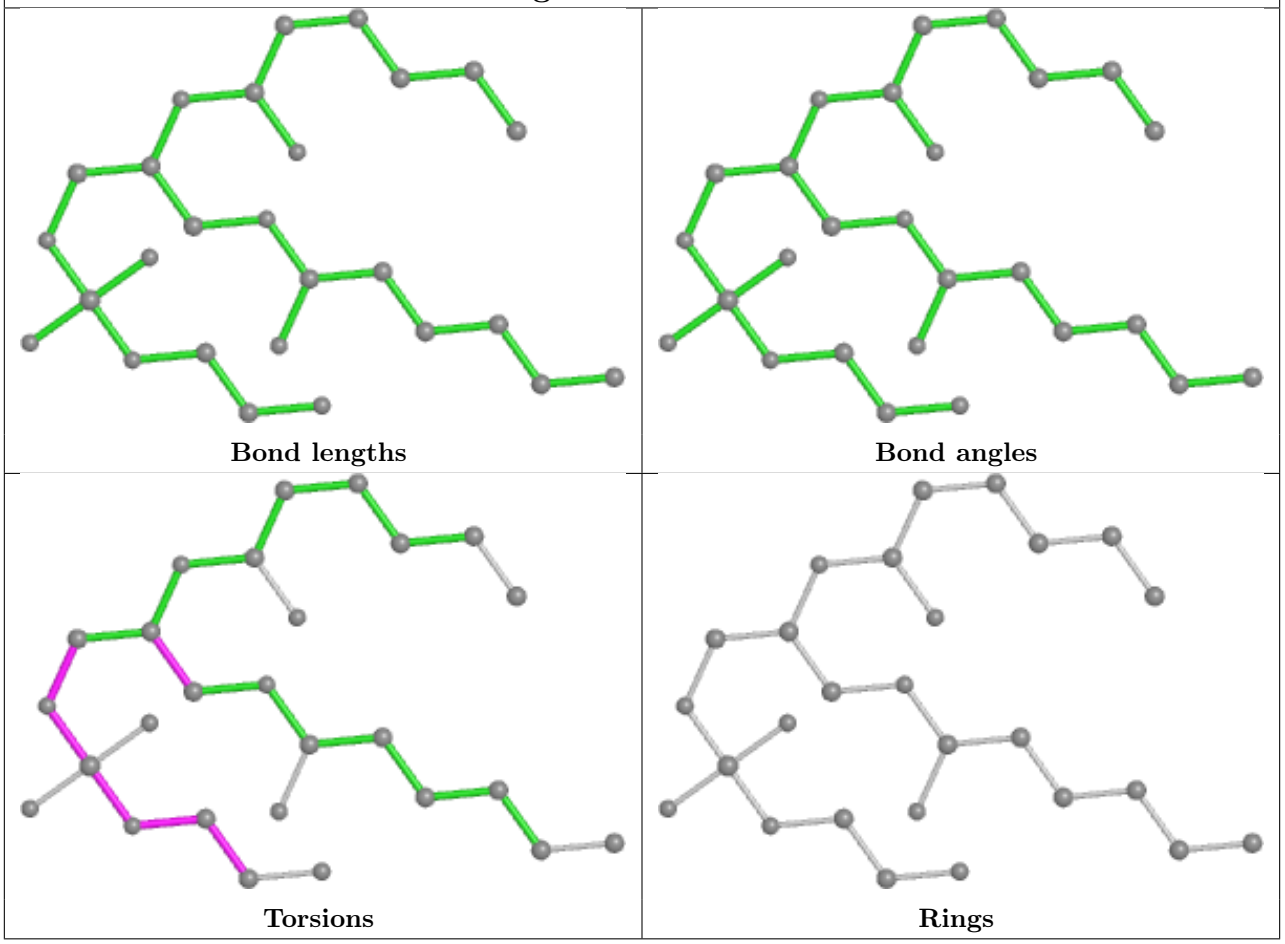
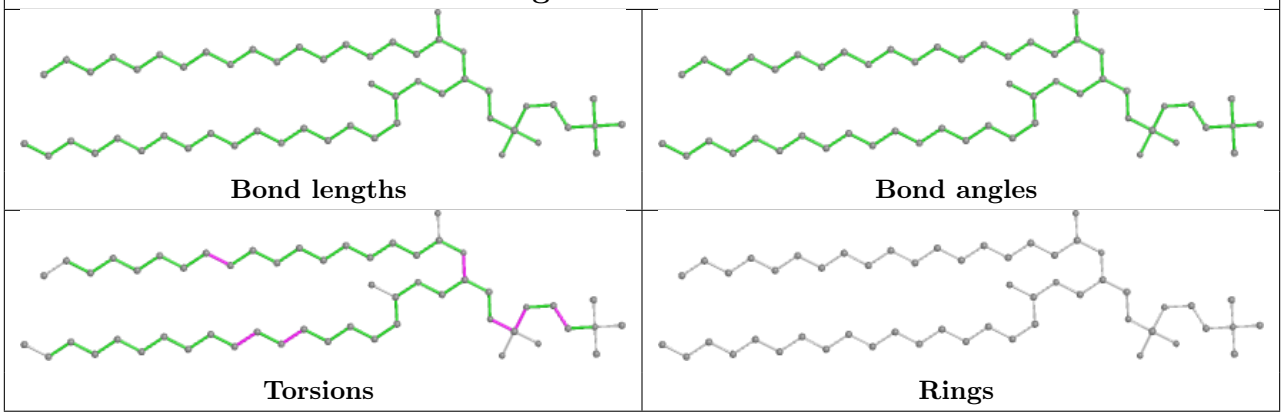


Rings

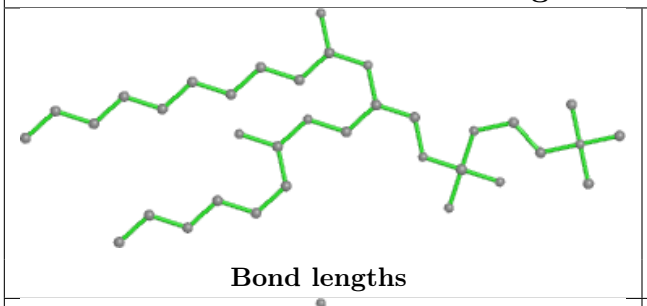
Ligand 3PE x 101



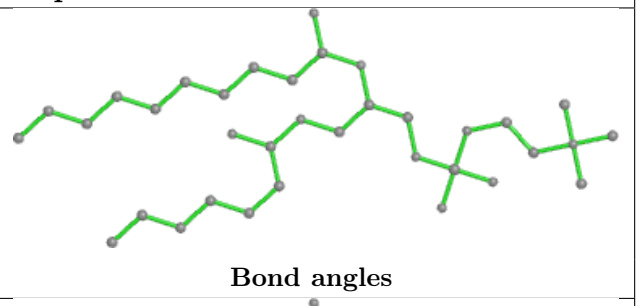
Ligand PC1 9 203



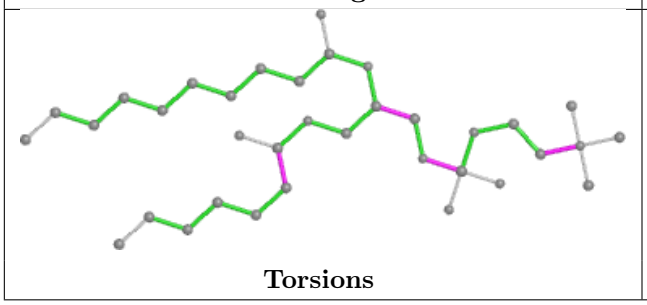
Ligand PC1 p 302



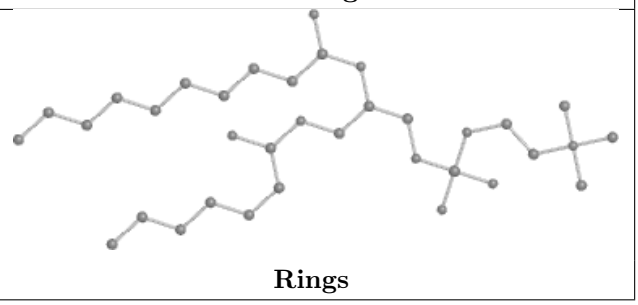
Bond lengths



Bond angles

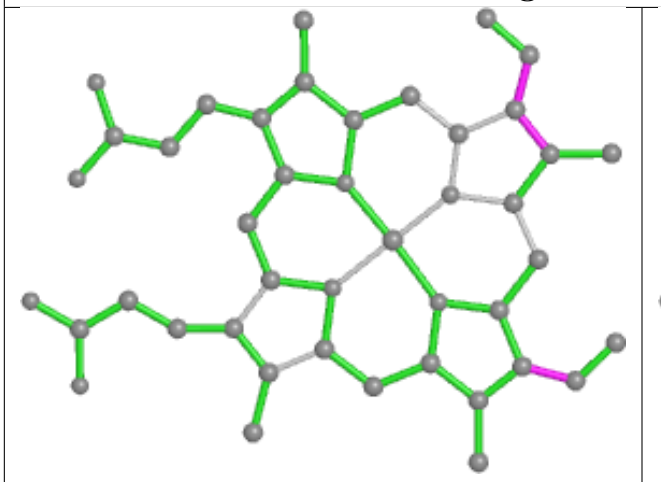


Torsions

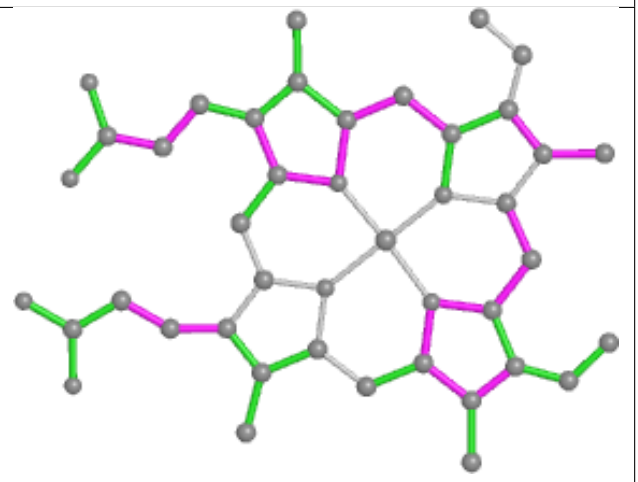


Rings

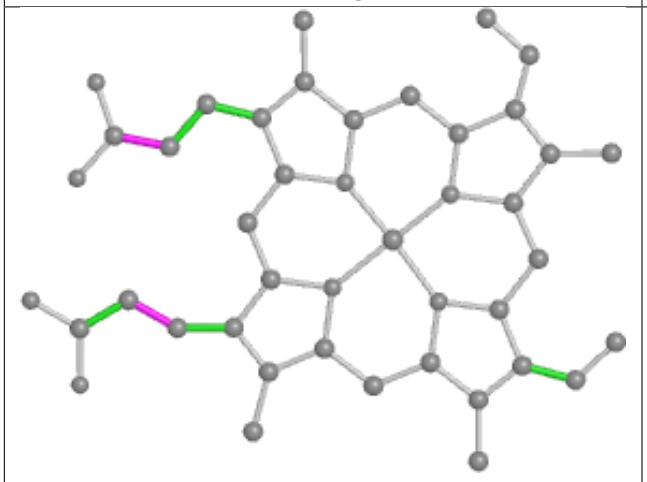
Ligand HEM N 402



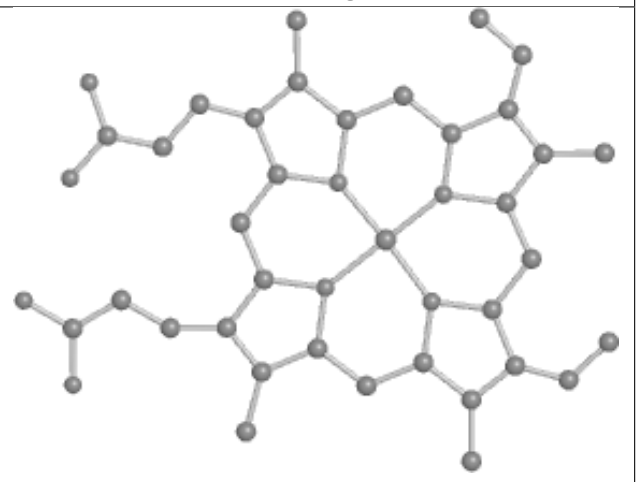
Bond lengths



Bond angles

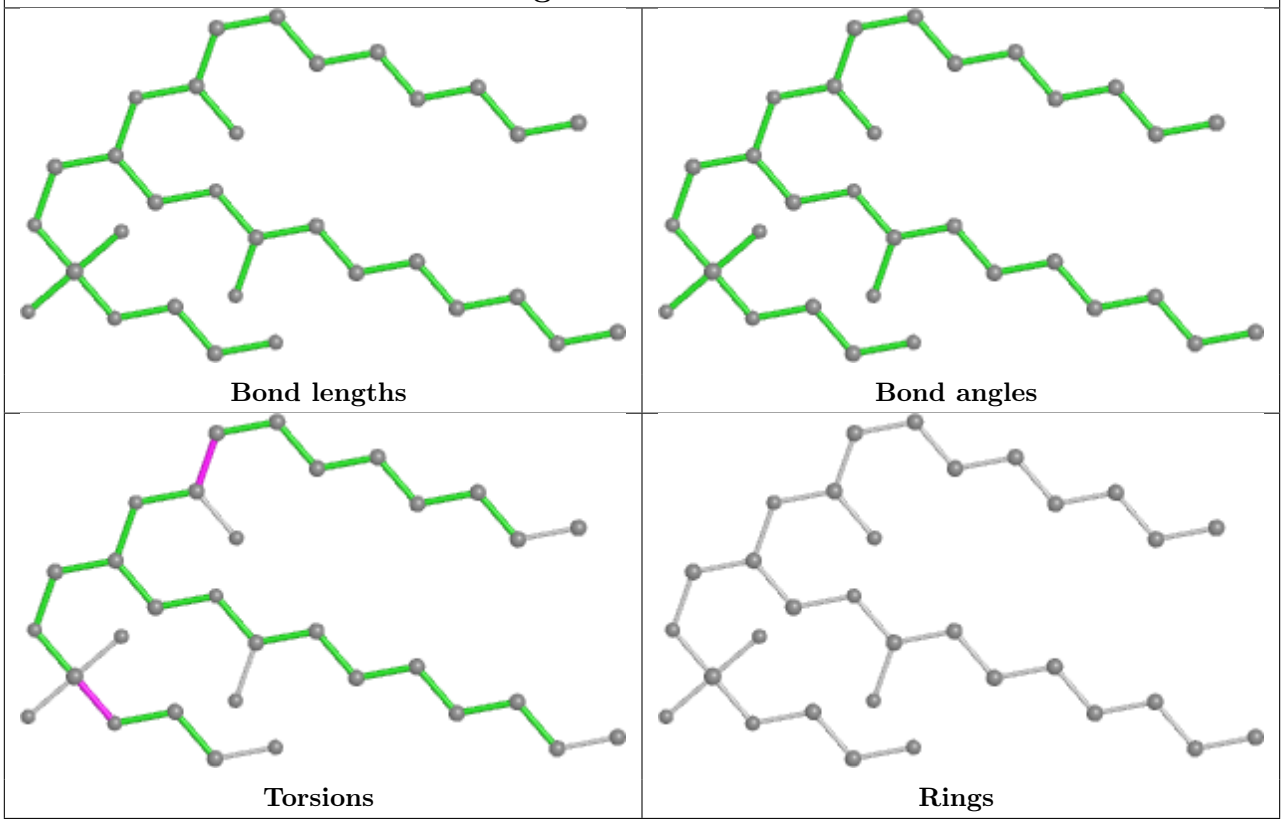


Torsions

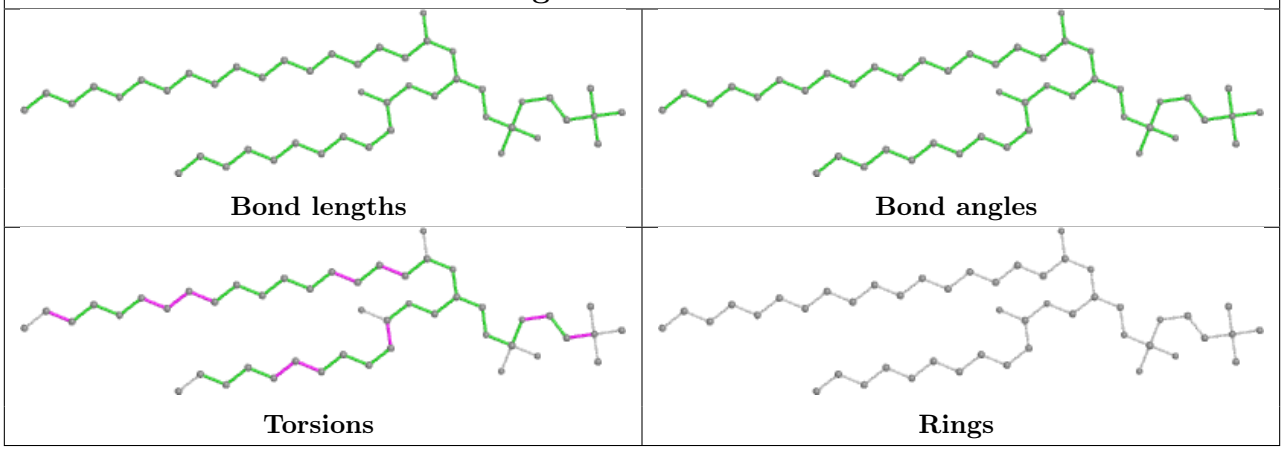


Rings

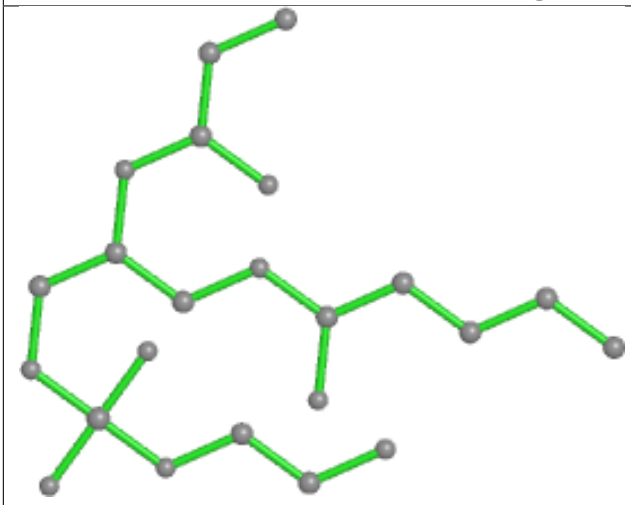
Ligand 3PE 6 202



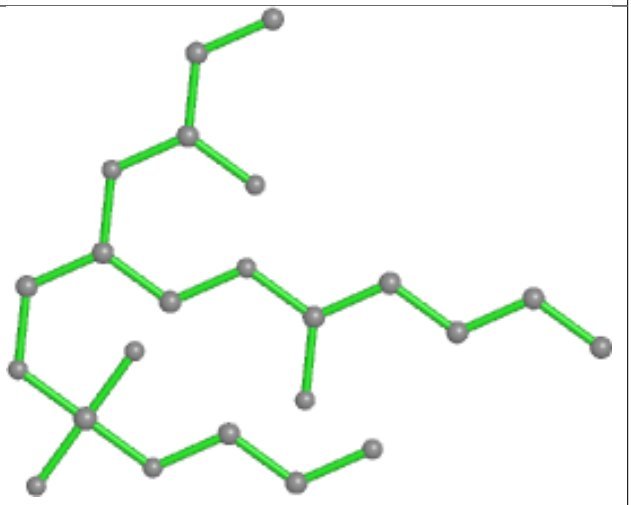
Ligand PC1 9 204



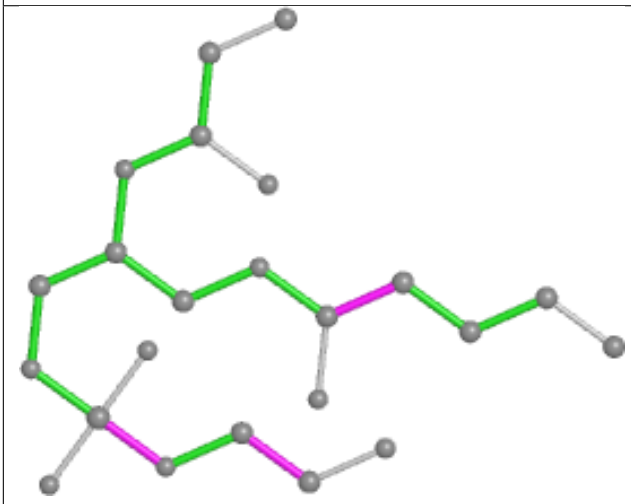
Ligand 3PE L 501



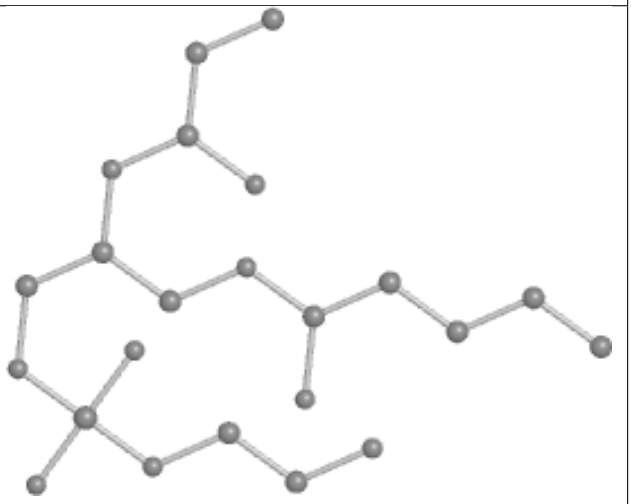
Bond lengths



Bond angles

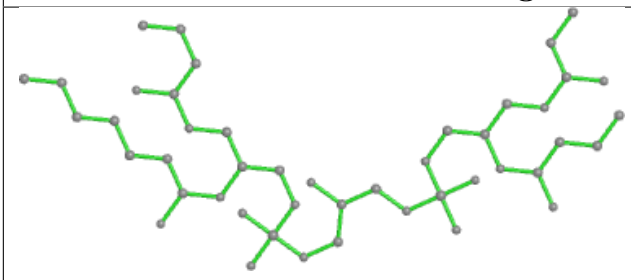


Torsions



Rings

Ligand CDL L1 703



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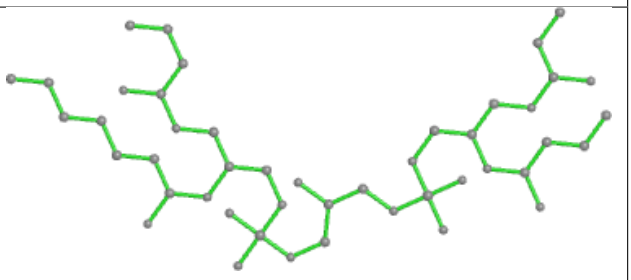
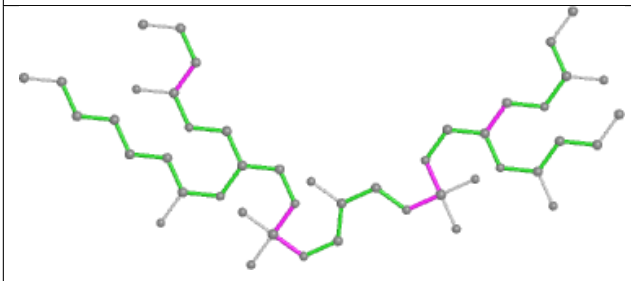
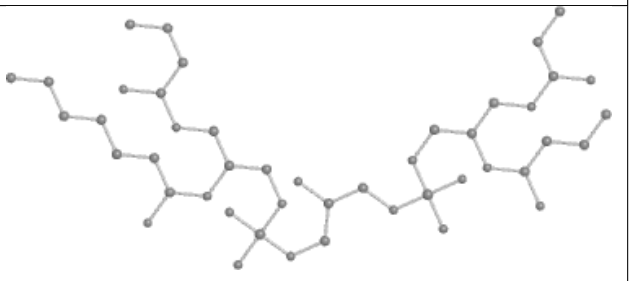


Bond angles

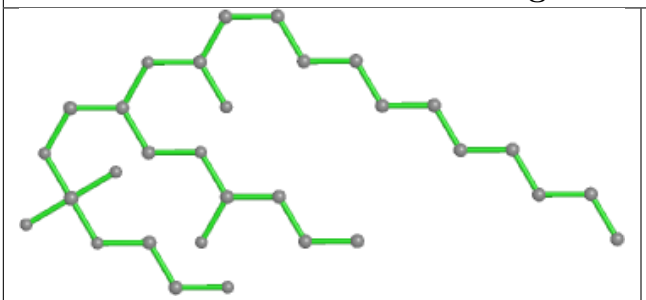


Torsions

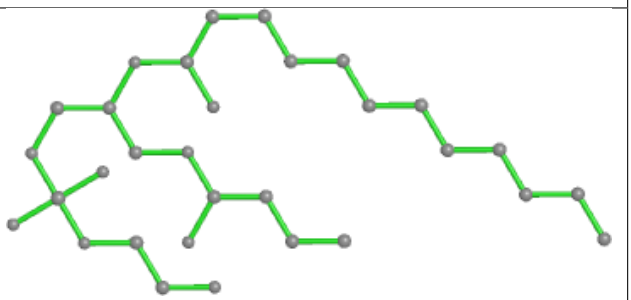


Rings

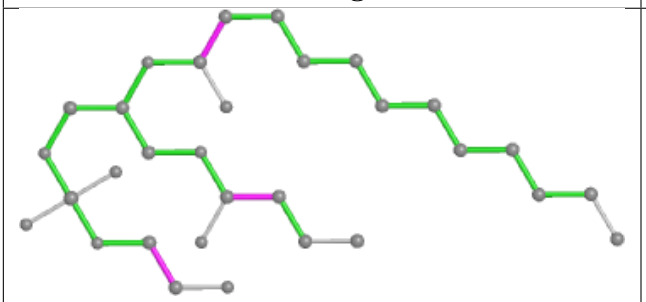
Ligand 3PE C 406



Bond lengths



Bond angles



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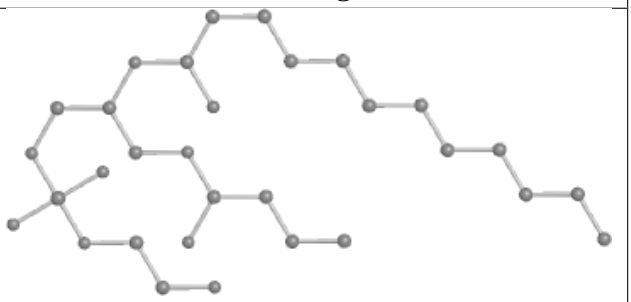
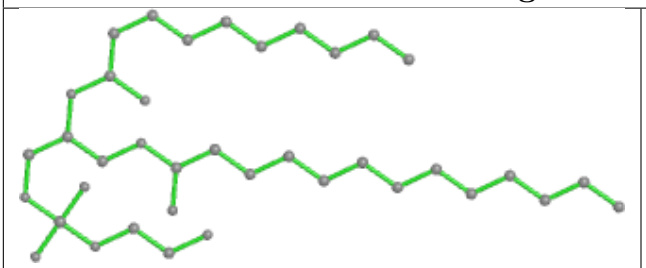
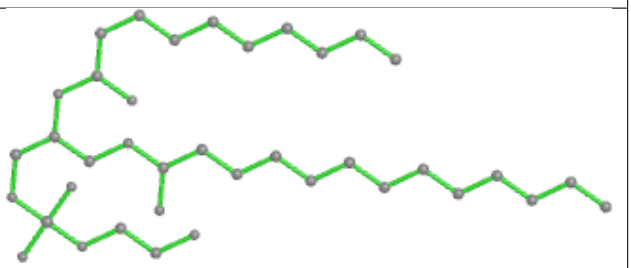


Rings

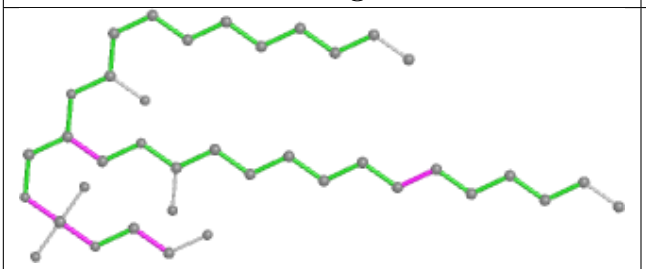
Ligand 3PE N1 402



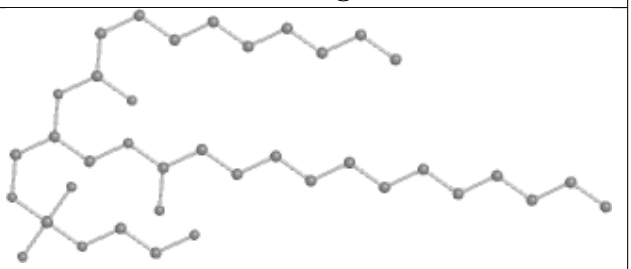
Bond lengths



Bond angles

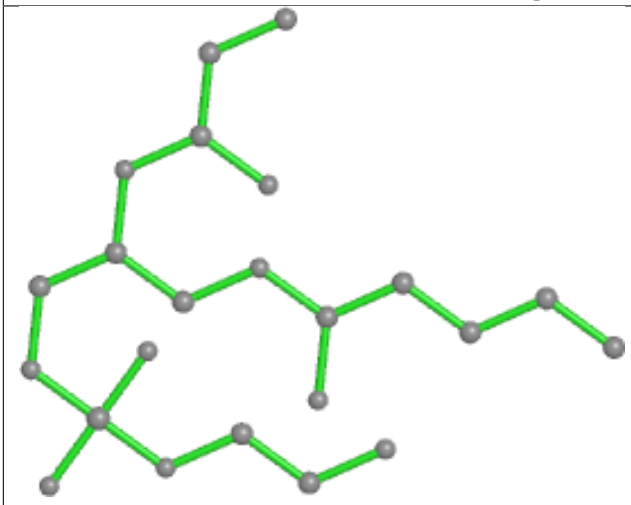


Torsions



Rings

Ligand 3PE A 501



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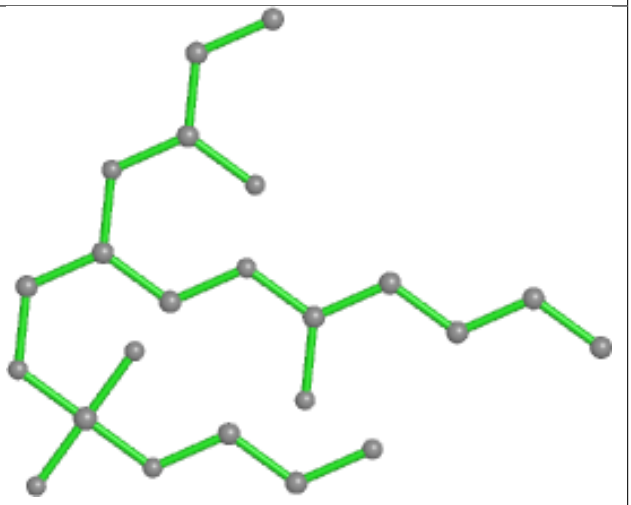
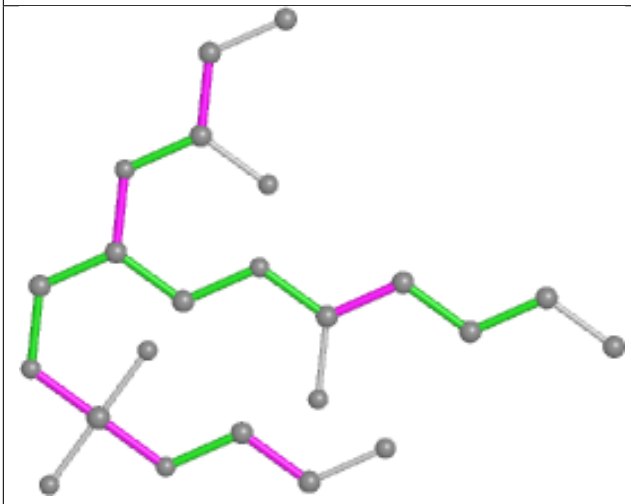


Bond angles



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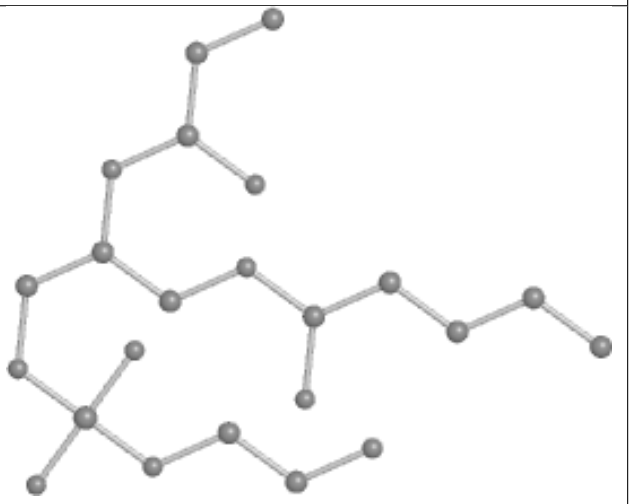
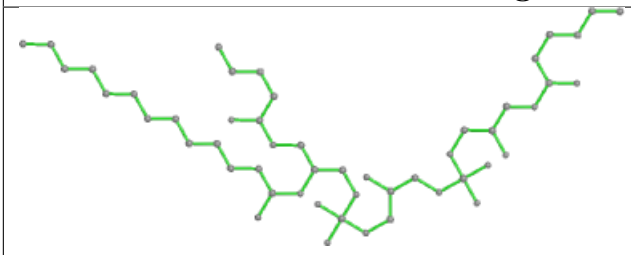


Rings

Ligand CDL H1 402



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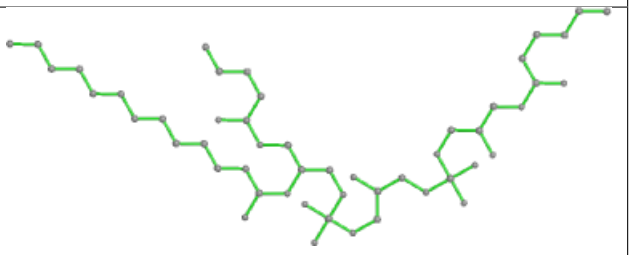
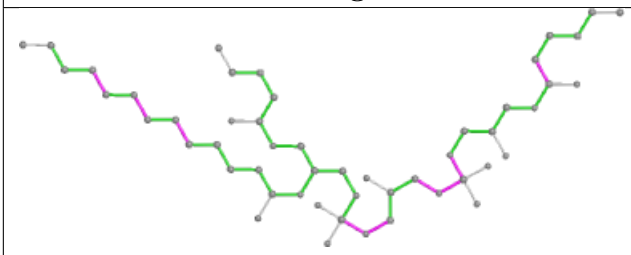
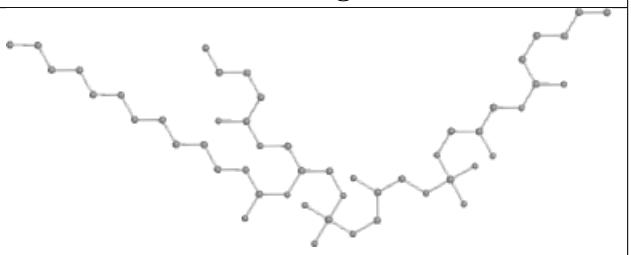


Bond angles

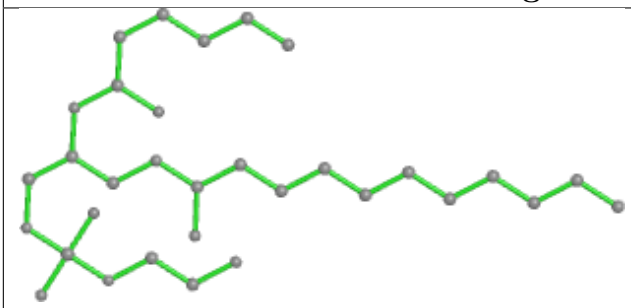


Torsions



Rings

Ligand 3PE d1 203



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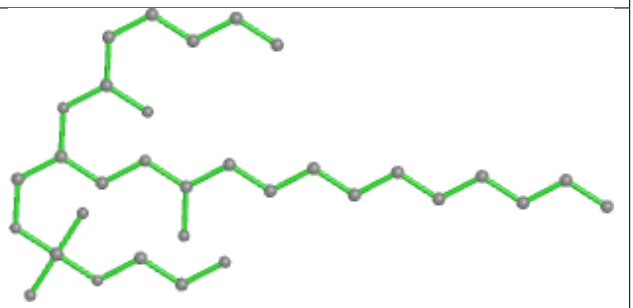
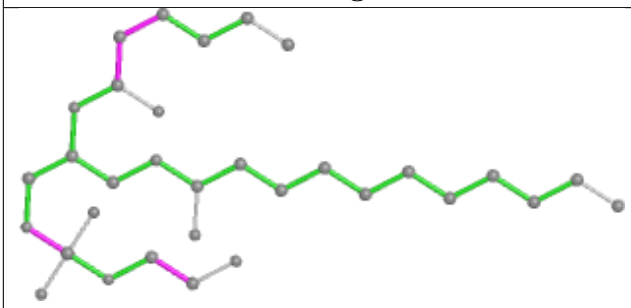
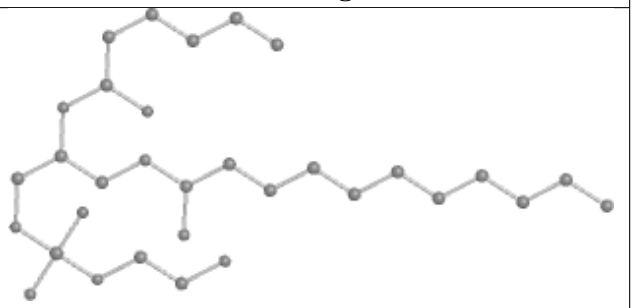


Bond angles

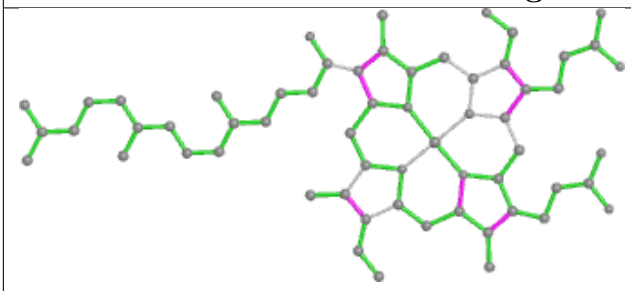


Torsions



Rings

Ligand HEA n 603



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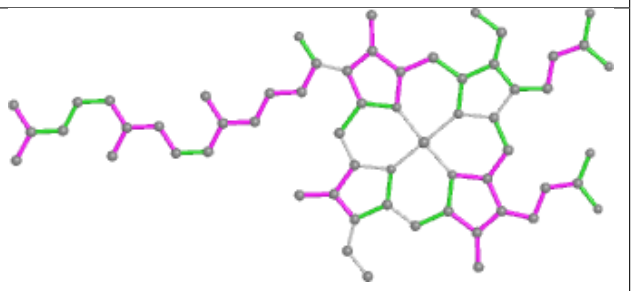
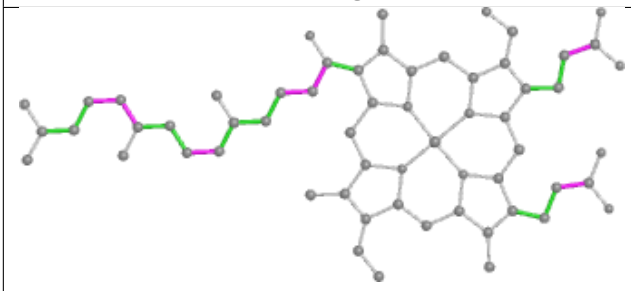
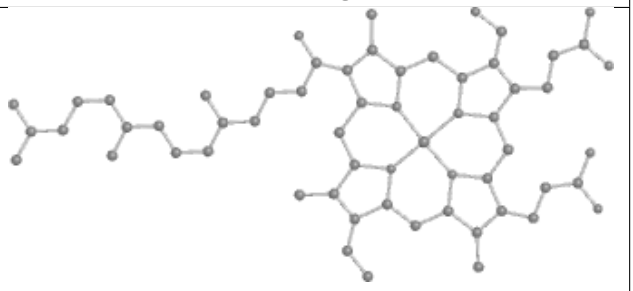


Bond angles

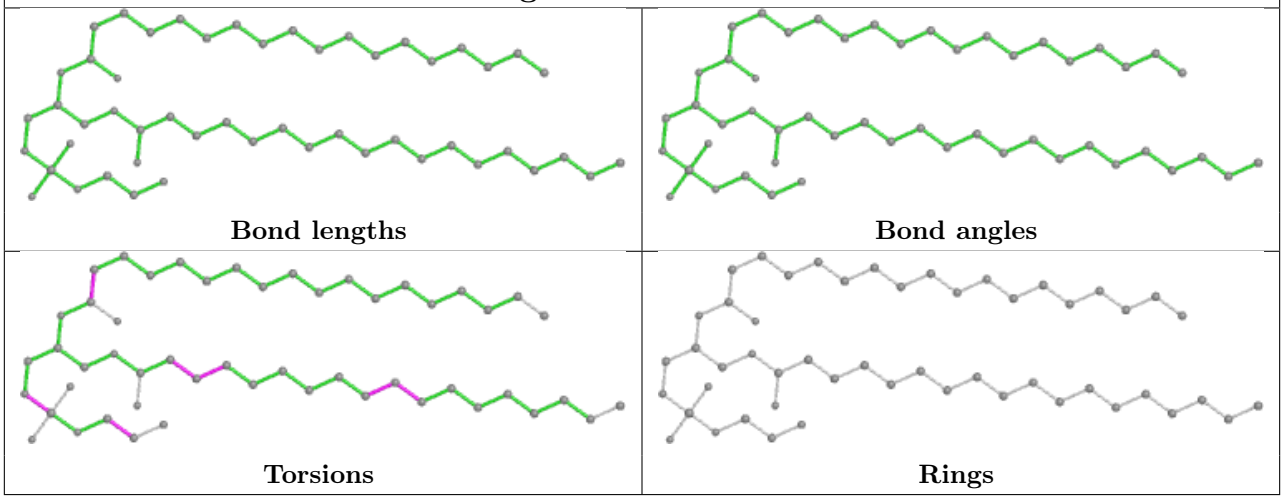


Torsions

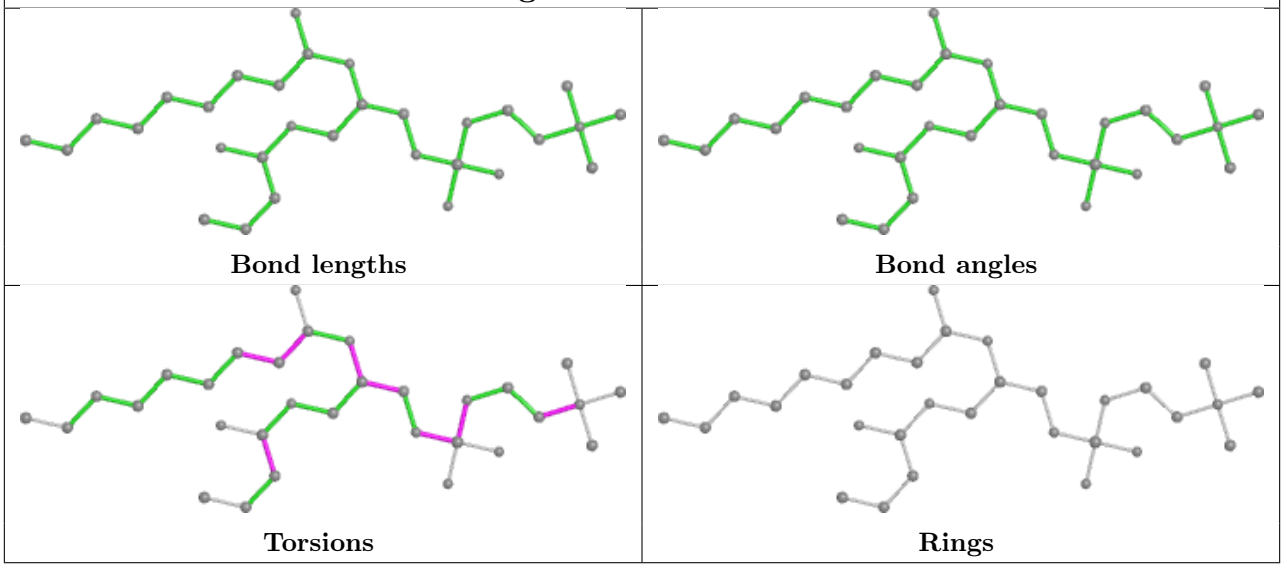


Rings

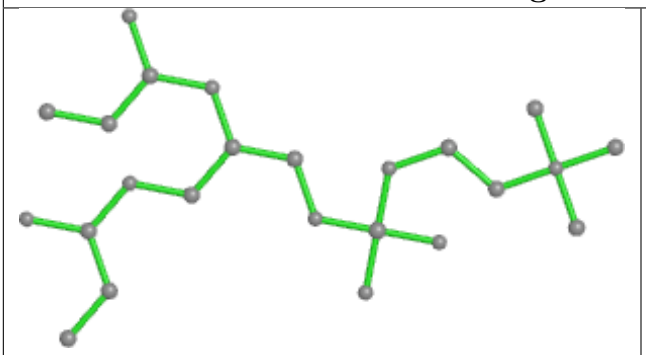
Ligand 3PE D1 501



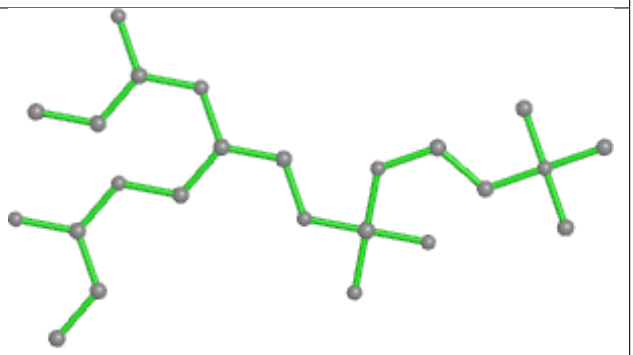
Ligand PC1 A1 601



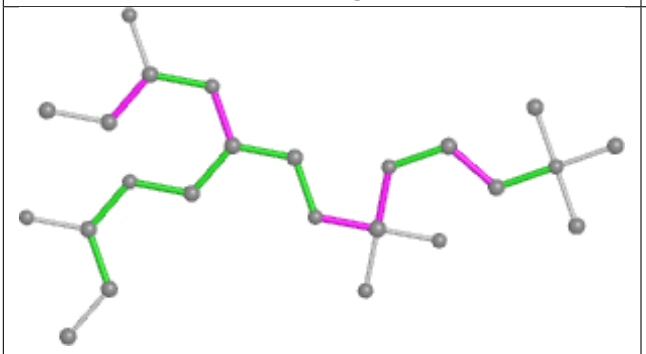
Ligand PC1 L 503



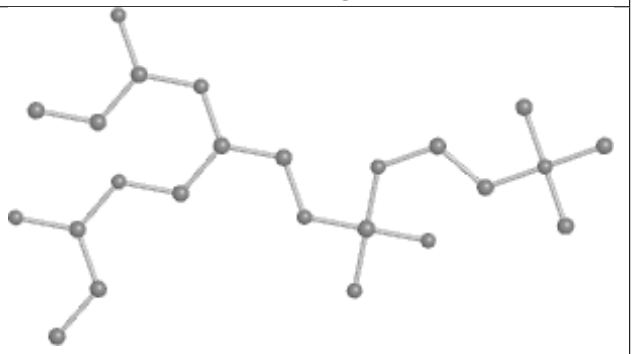
Bond lengths



Bond angles

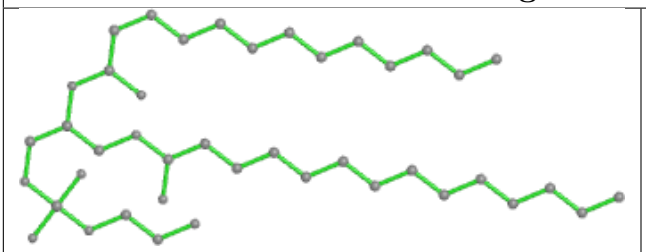


Torsions

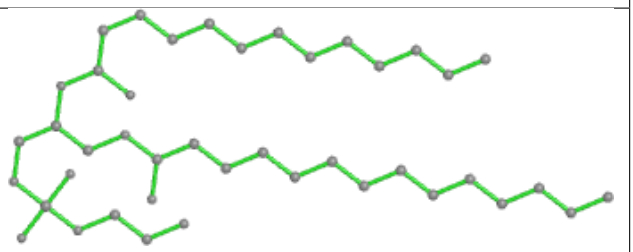


Rings

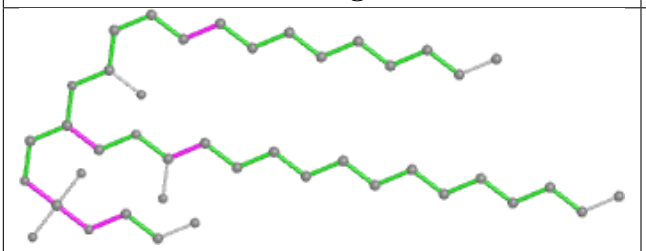
Ligand 3PE Y1 403



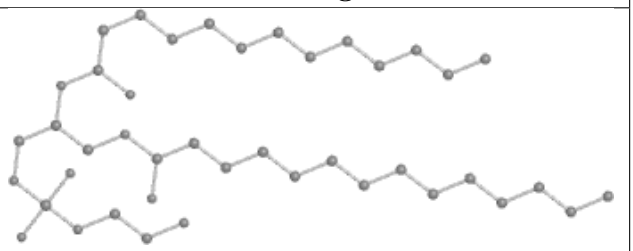
Bond lengths



Bond angles

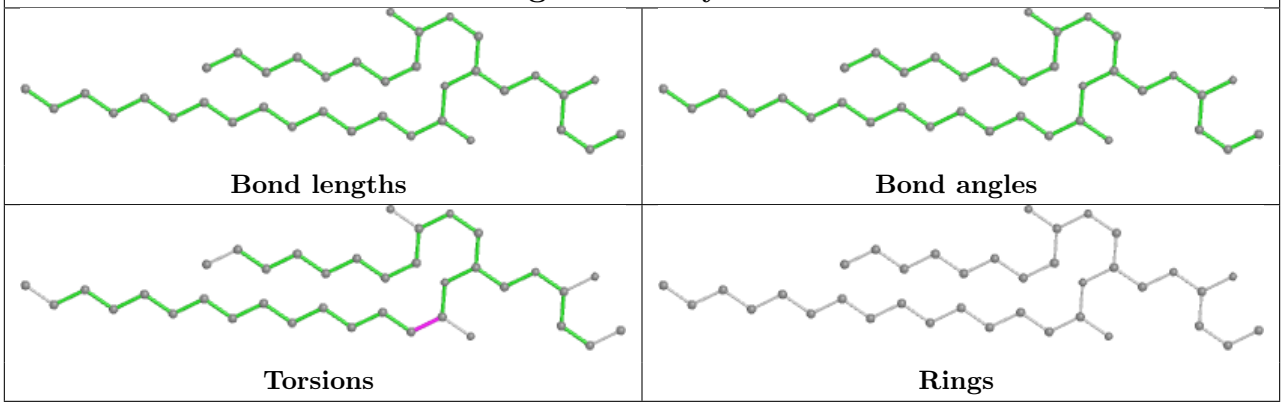


Torsions

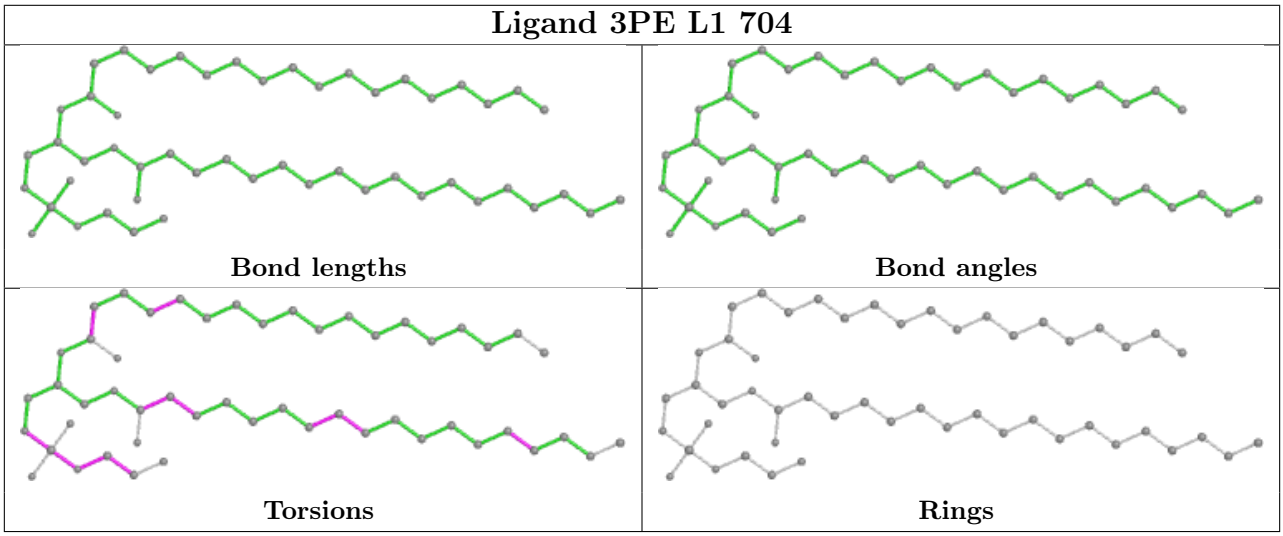


Rings

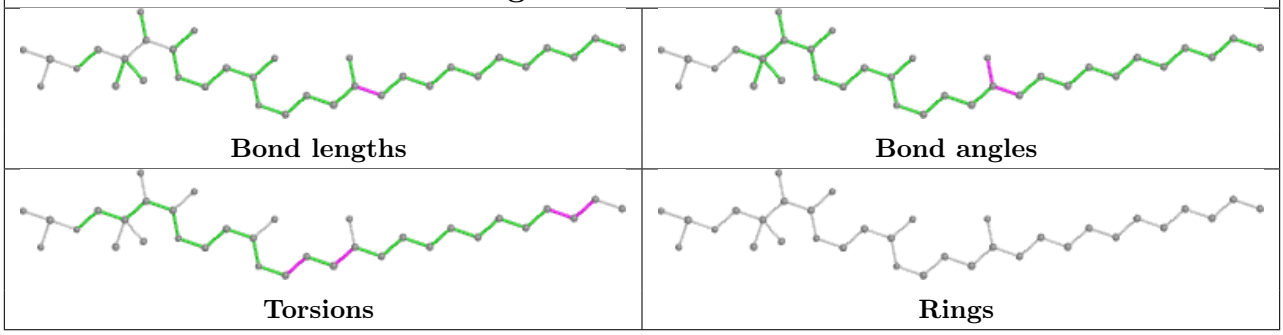
Ligand TGL y 601



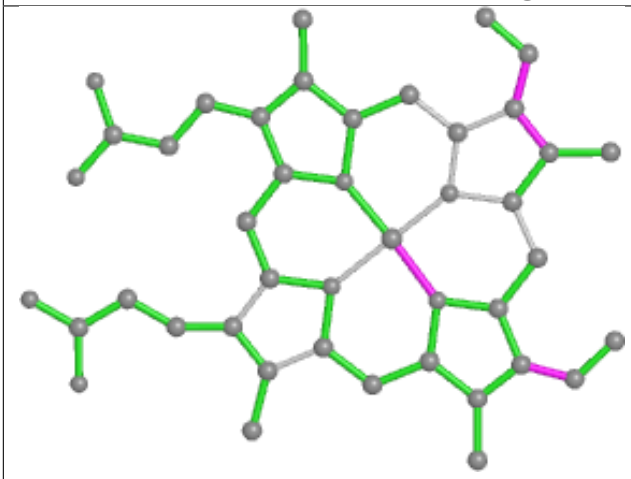
Ligand 3PE L1 704



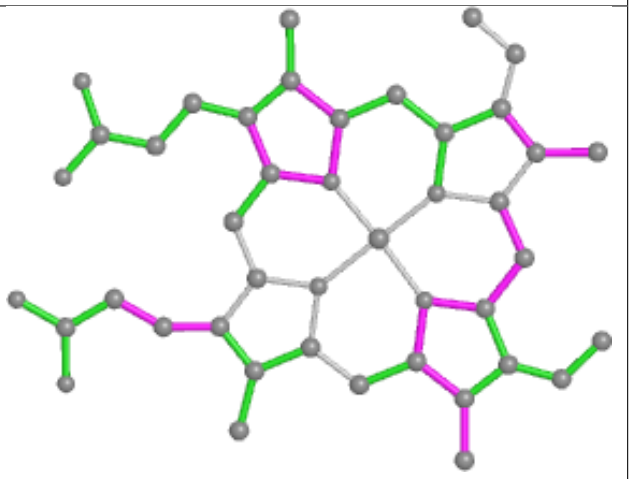
Ligand ZMP W1 201



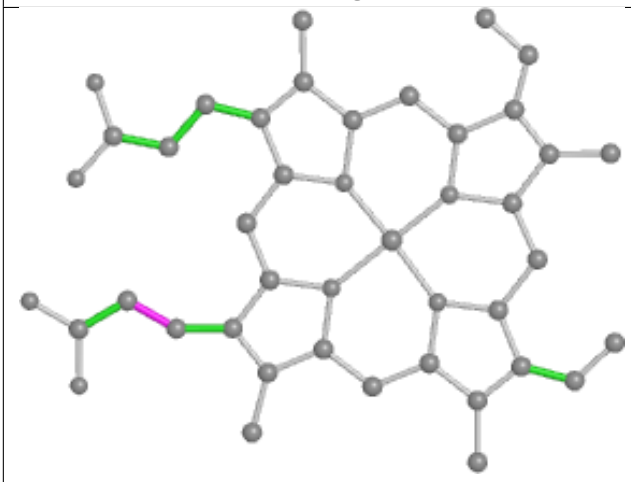
Ligand HEM C 402



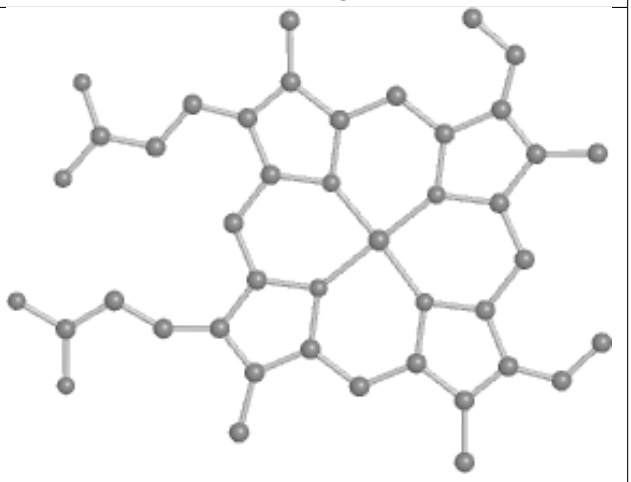
Bond lengths



Bond angles

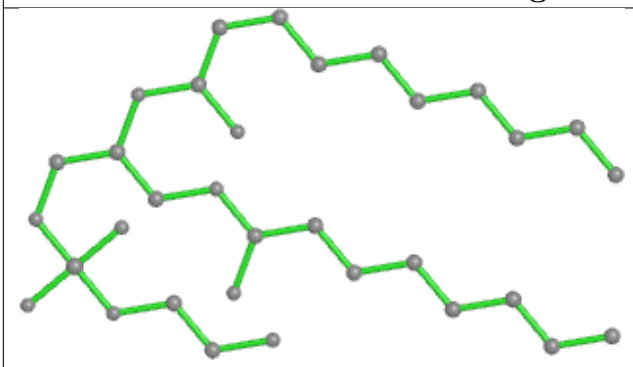


Torsions

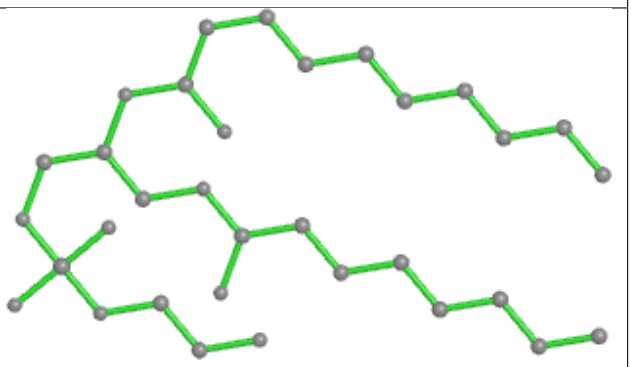


Rings

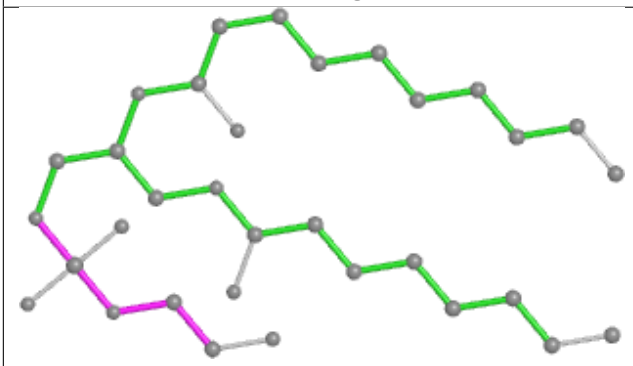
Ligand 3PE P 201



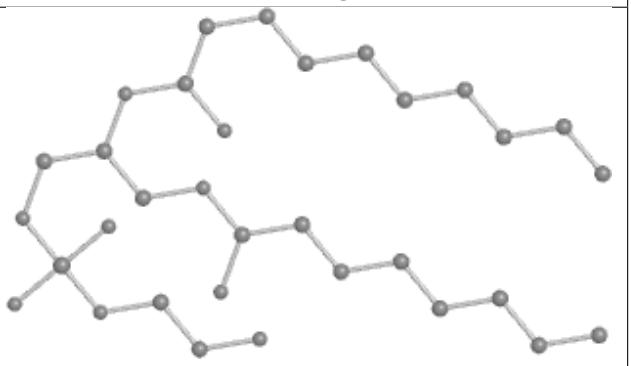
Bond lengths



Bond angles

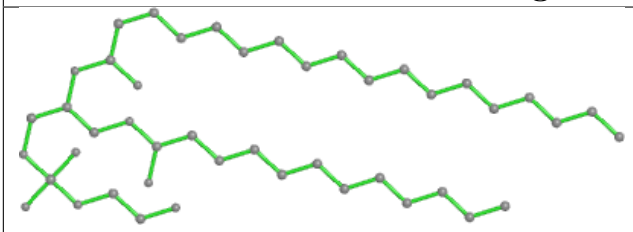


Torsions

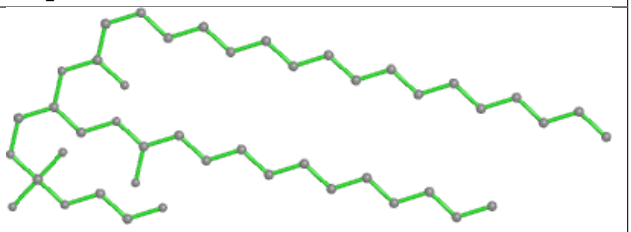


Rings

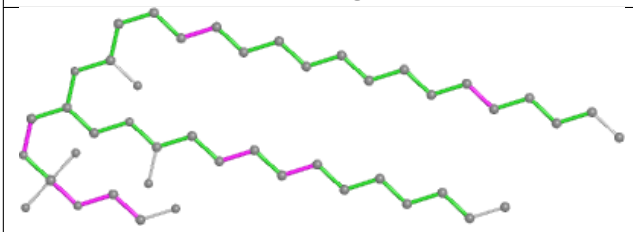
Ligand 3PE p 301



Bond lengths



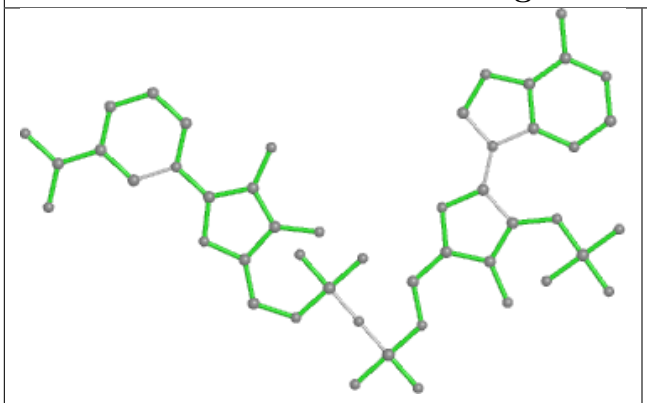
Bond angles



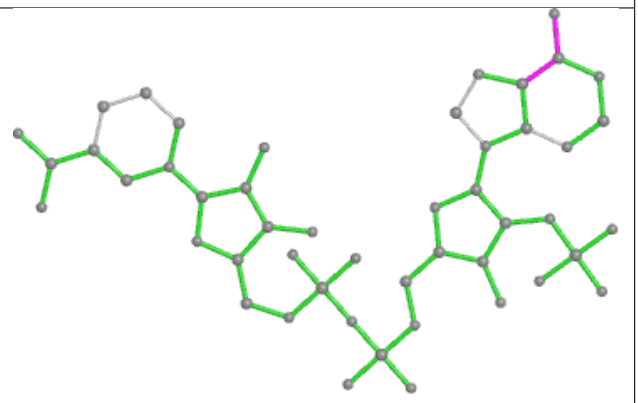
Torsions

Rings

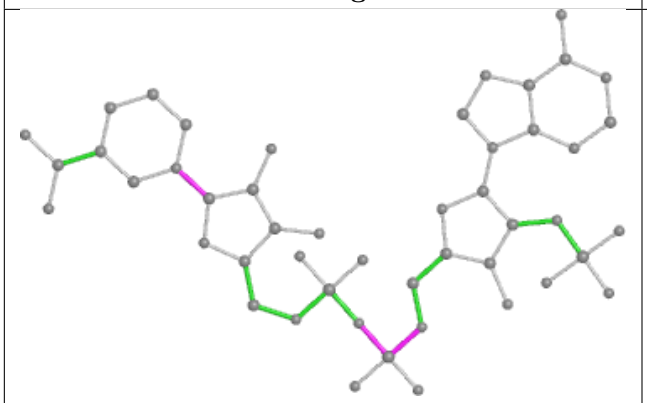
Ligand NDP P1 501



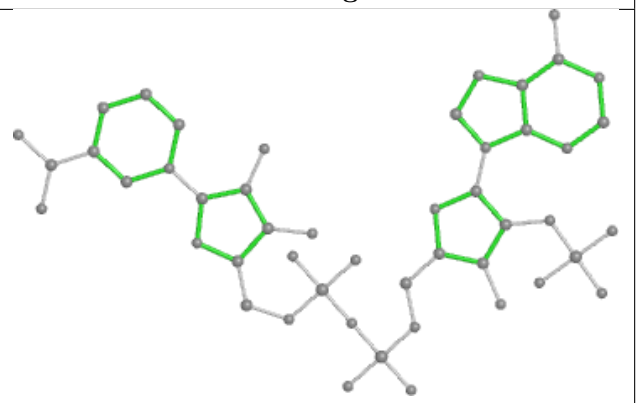
Bond lengths



Bond angles

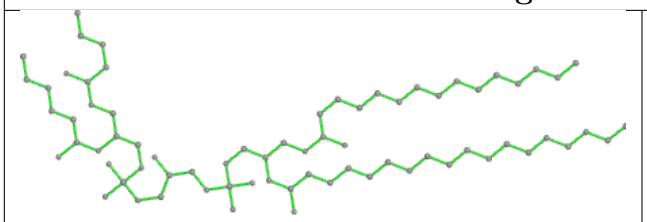


Torsions



Rings

Ligand CDL Y1 404



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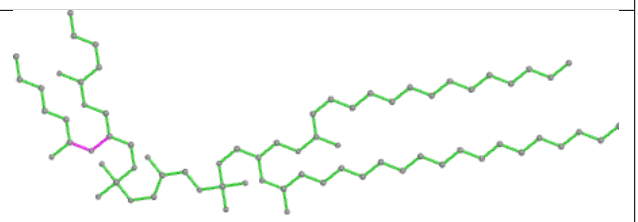

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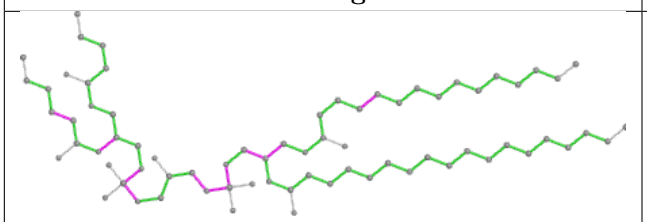

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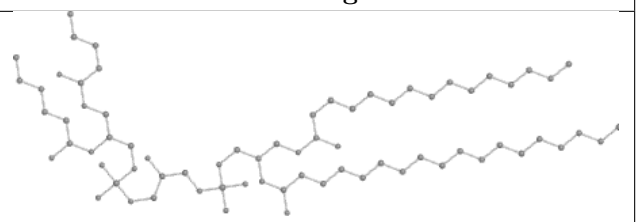
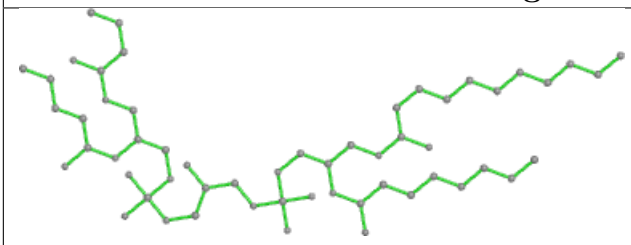


Rings

Ligand CDL D 302



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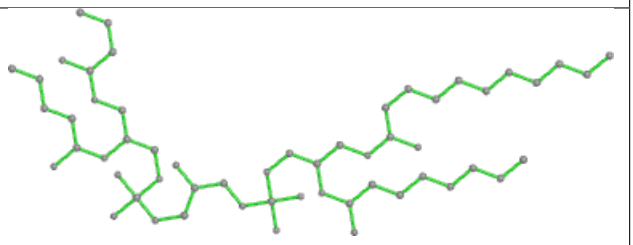

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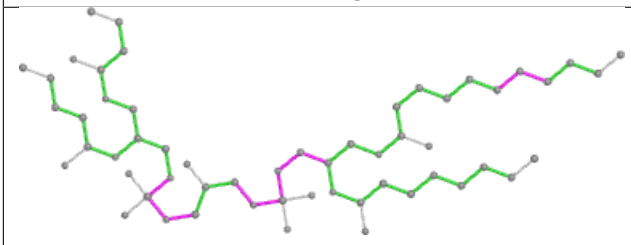

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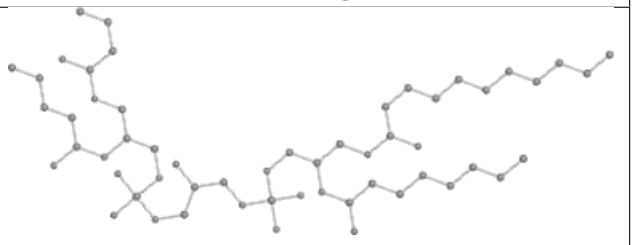
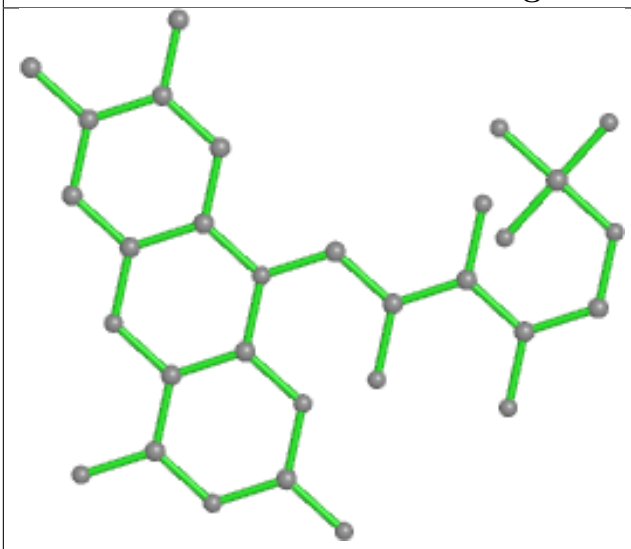


Rings

Ligand FMN 1 501



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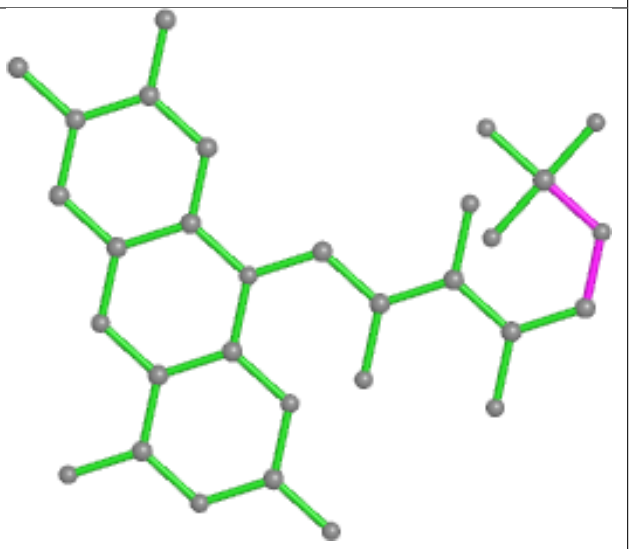

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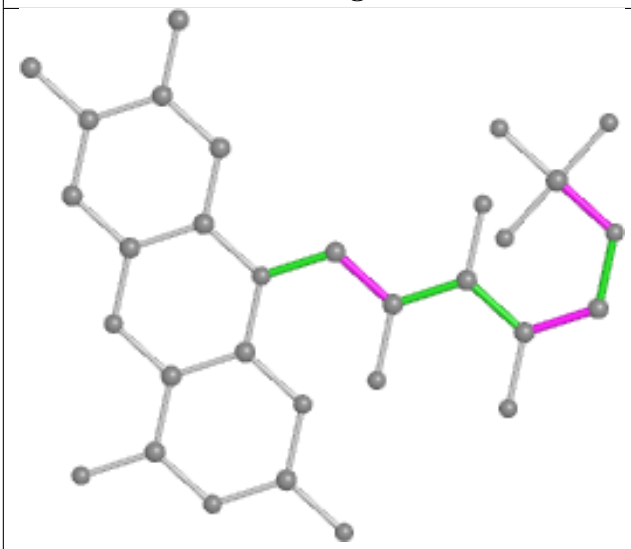

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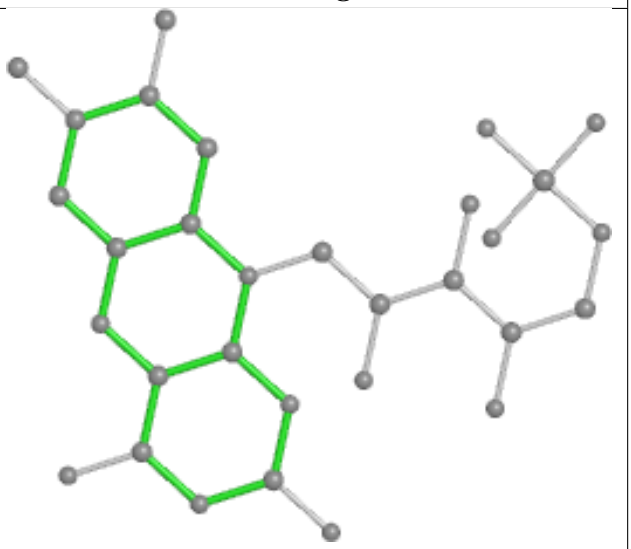
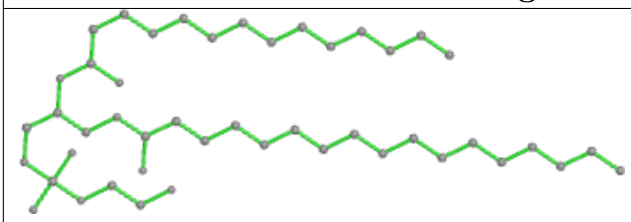


Rings

Ligand 3PE H1 401



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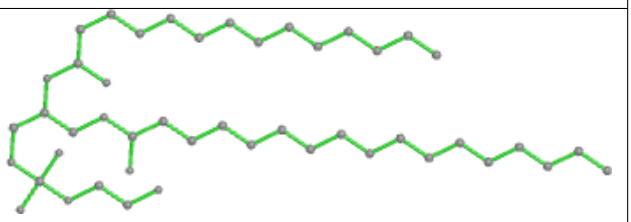

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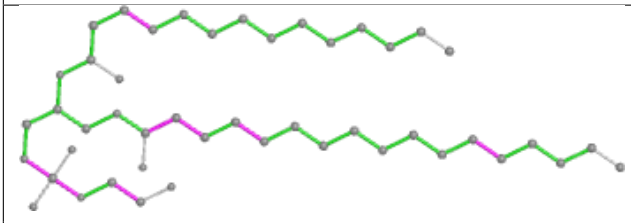

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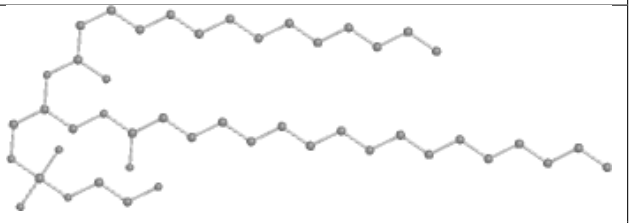
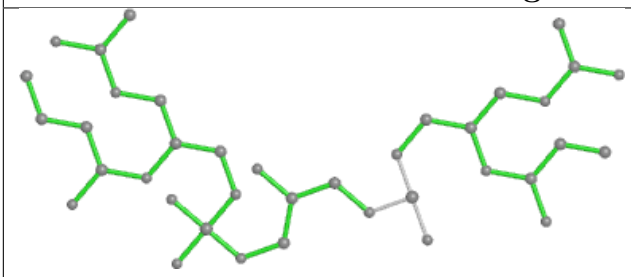


Rings

Ligand CDL V 102



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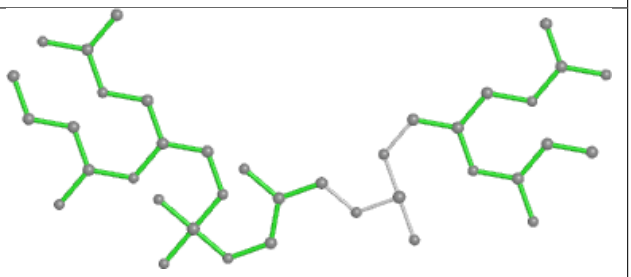

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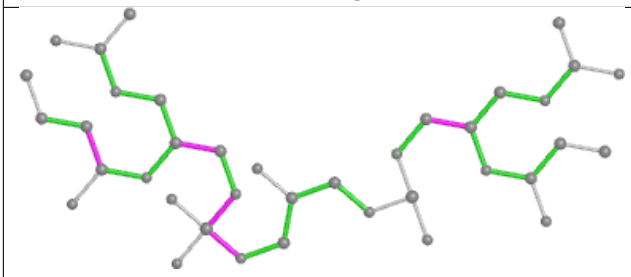

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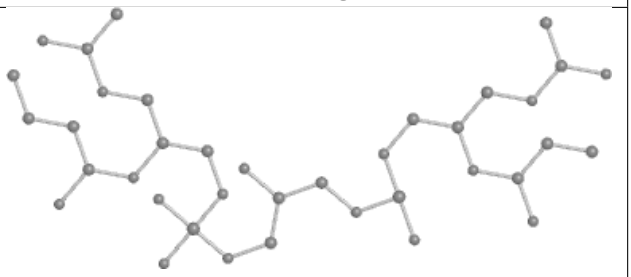
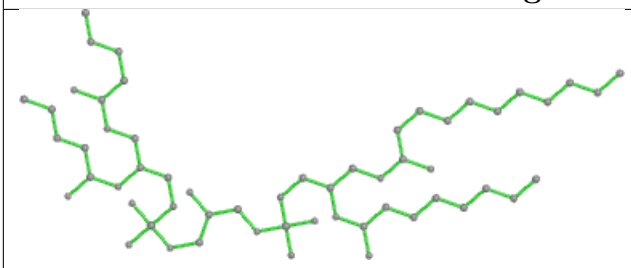


Rings

Ligand CDL R 301



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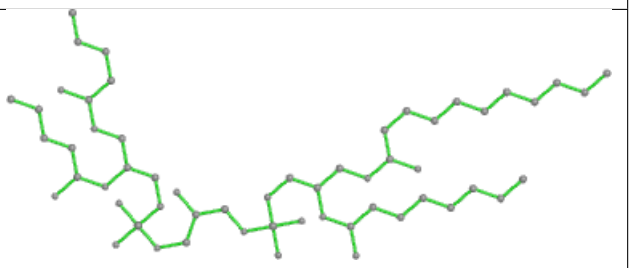

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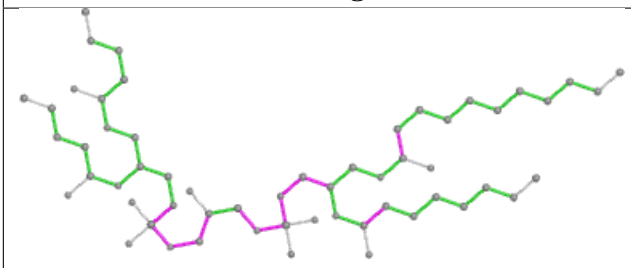

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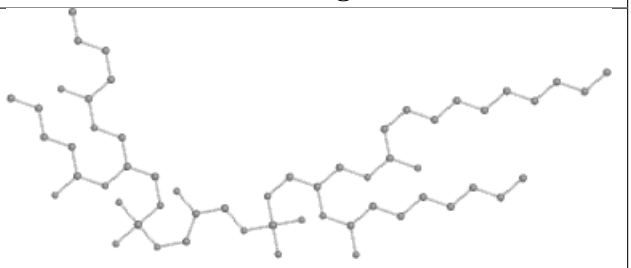
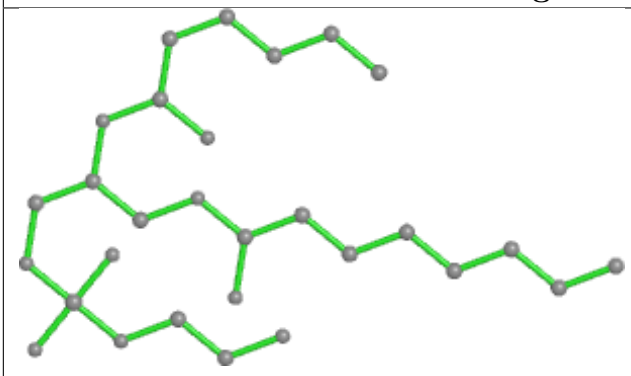


Rings

Ligand 3PE o 302



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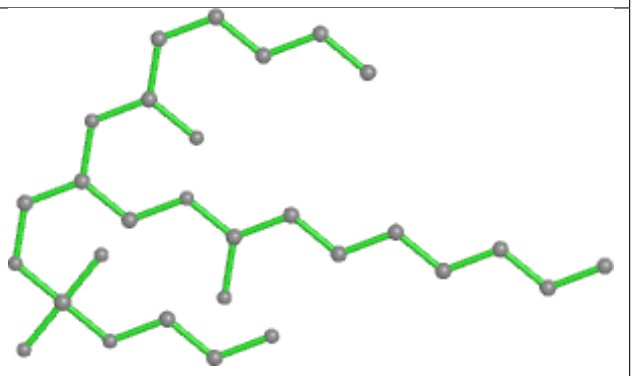

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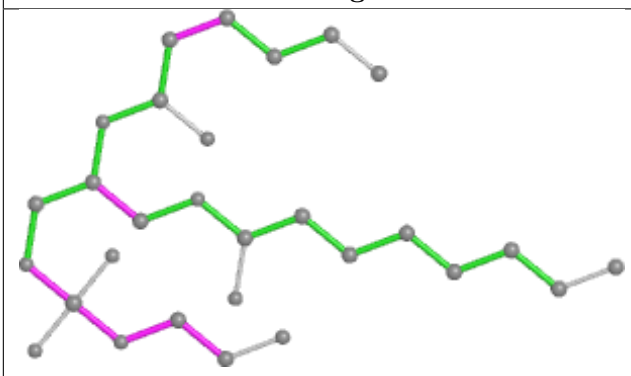

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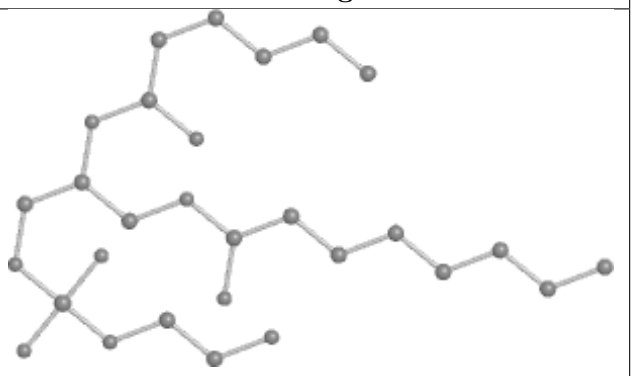
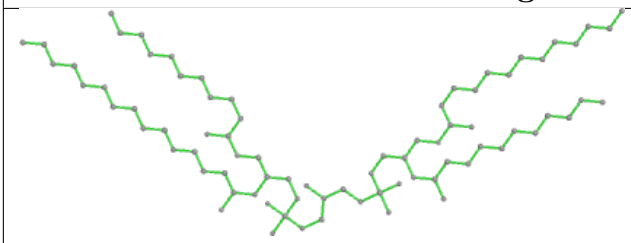


Rings

Ligand CDL L1 702



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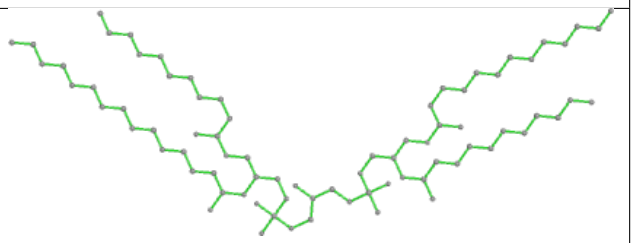

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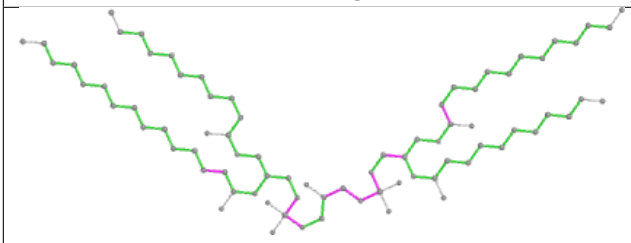

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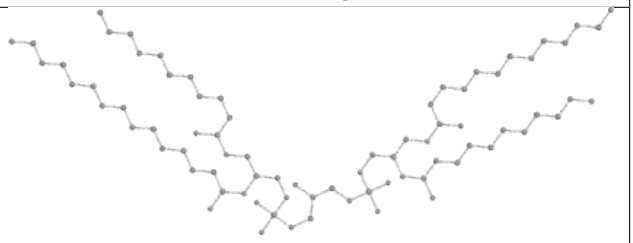
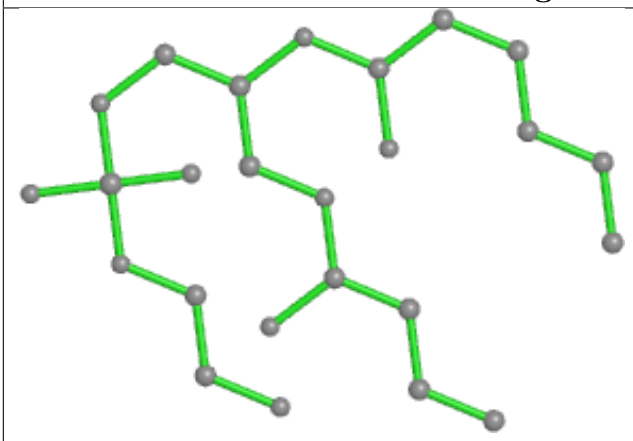


Rings

Ligand 3PE t 101



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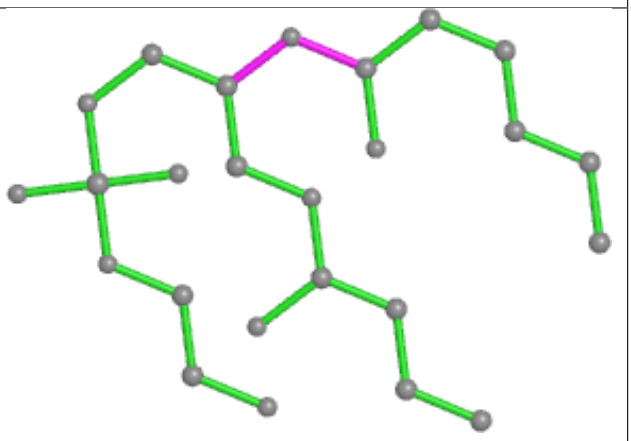
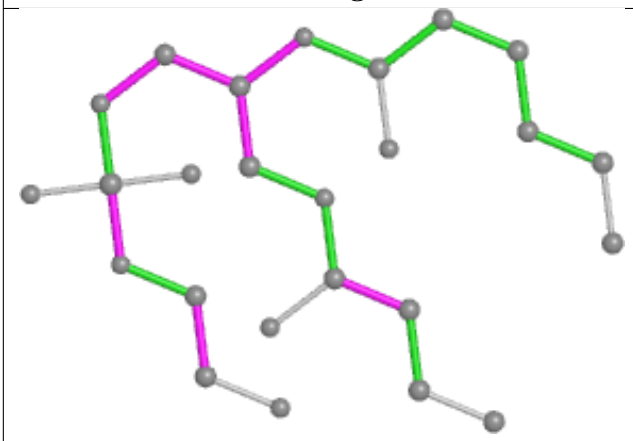


Bond angles



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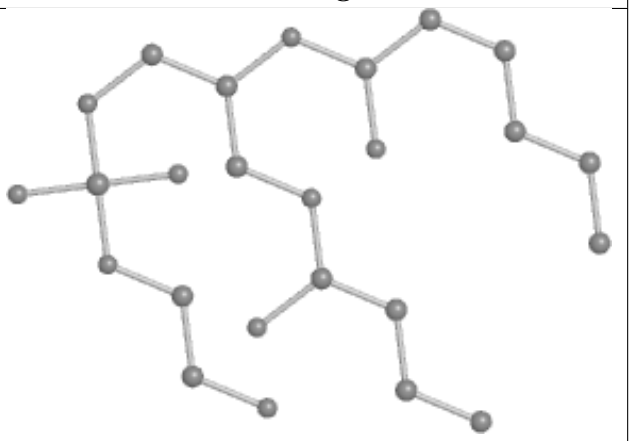
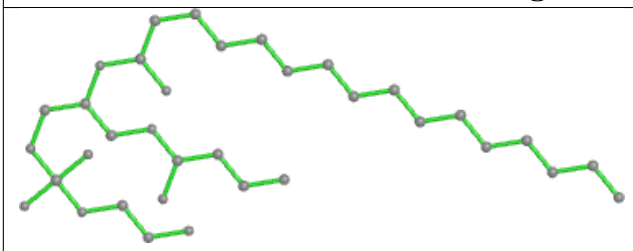


Rings

Ligand 3PE C 403



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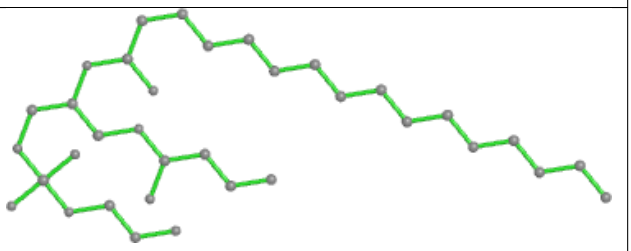
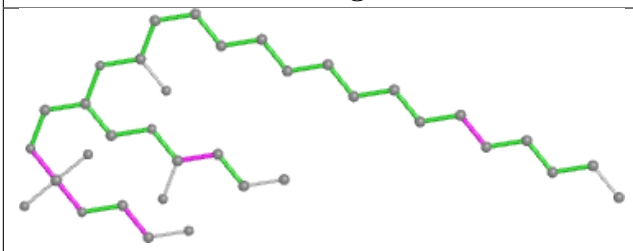


Bond angles



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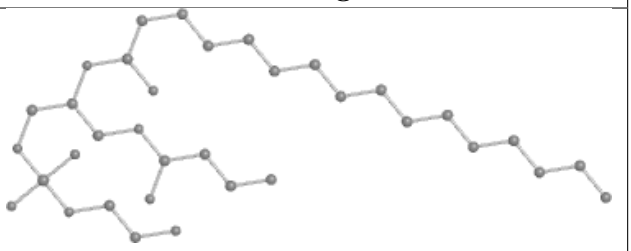
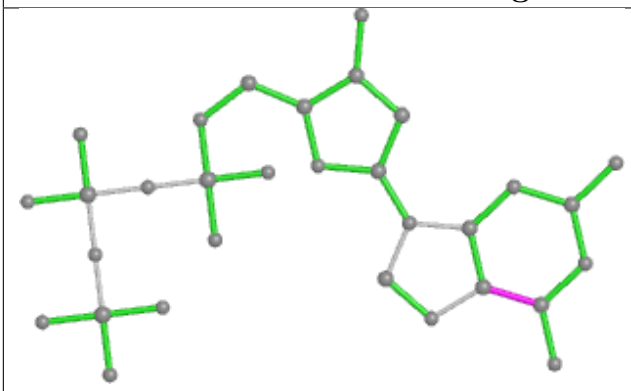


Rings

Ligand DGT O1 401



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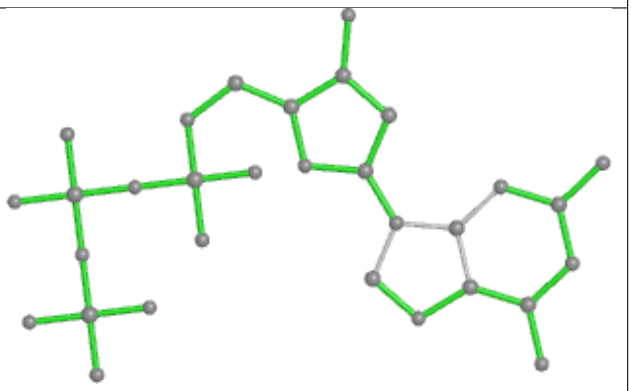
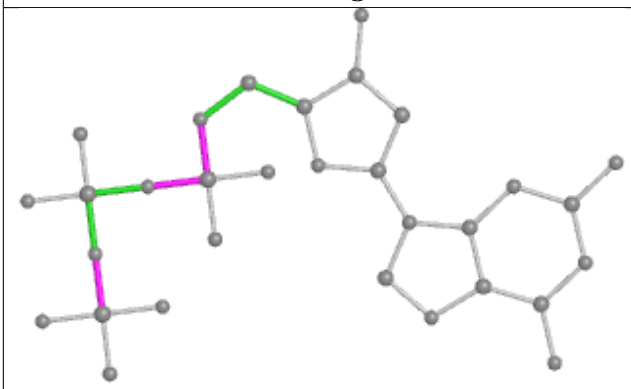


Bond angles



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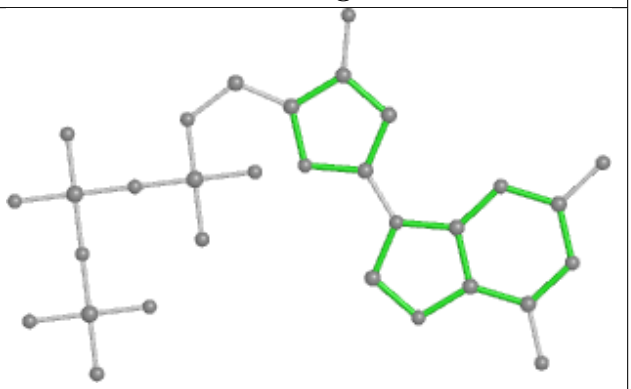
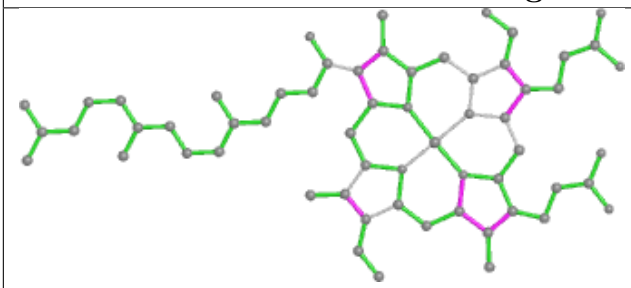


Rings

Ligand HEA n 604



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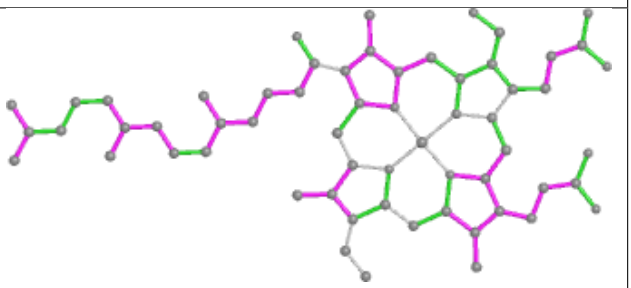
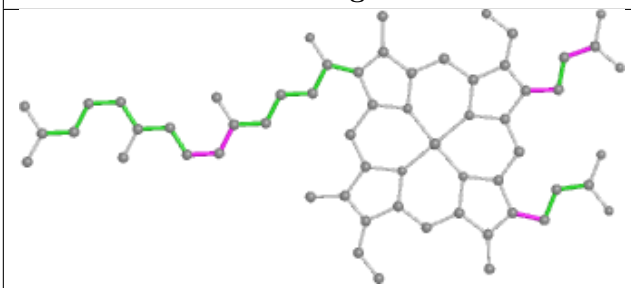


Bond angles



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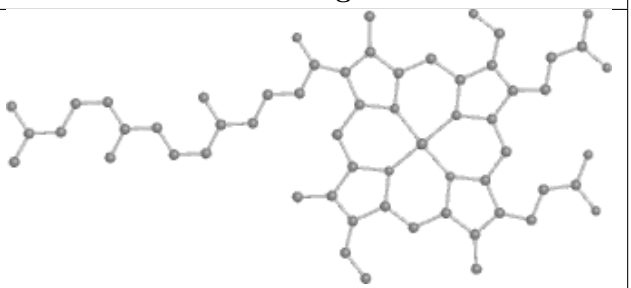
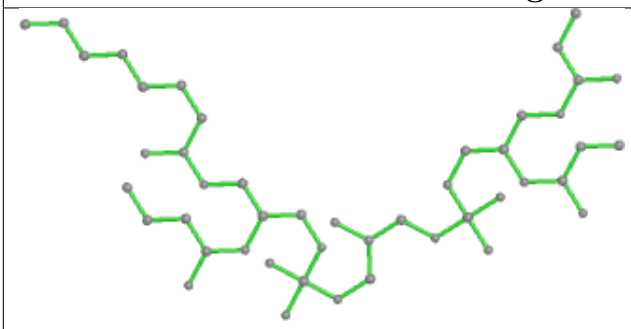


Rings

Ligand CDL L 502



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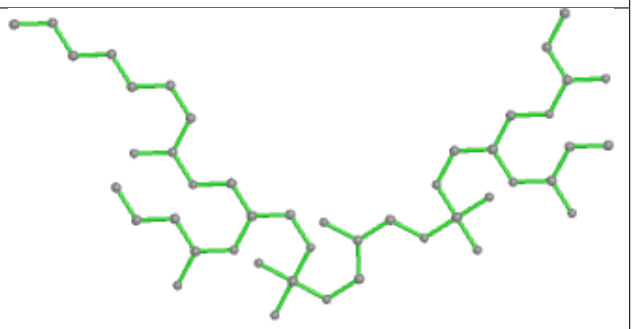
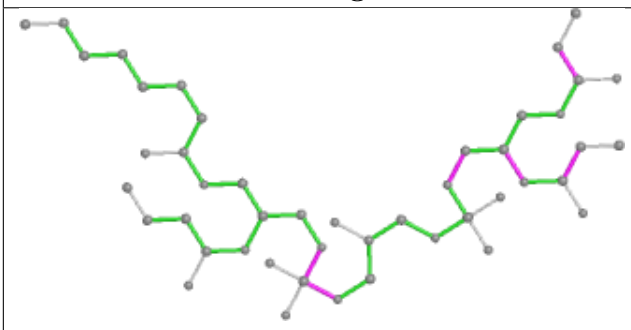


Bond angles



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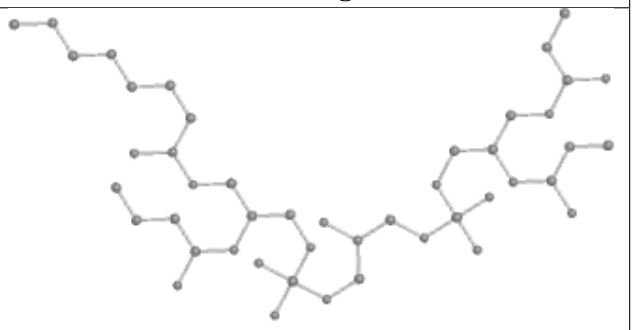
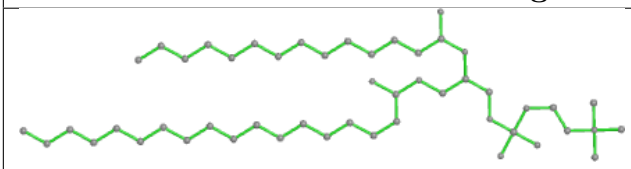


Rings

Ligand PC1 p 303



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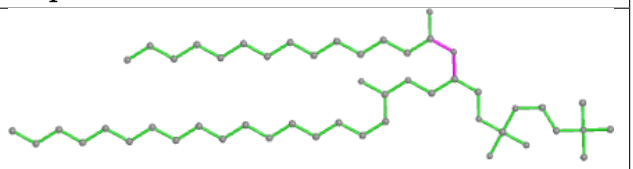
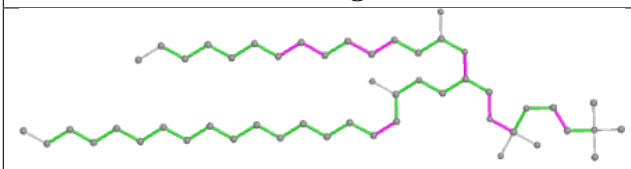
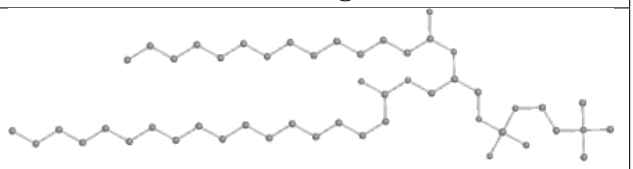


Bond angles

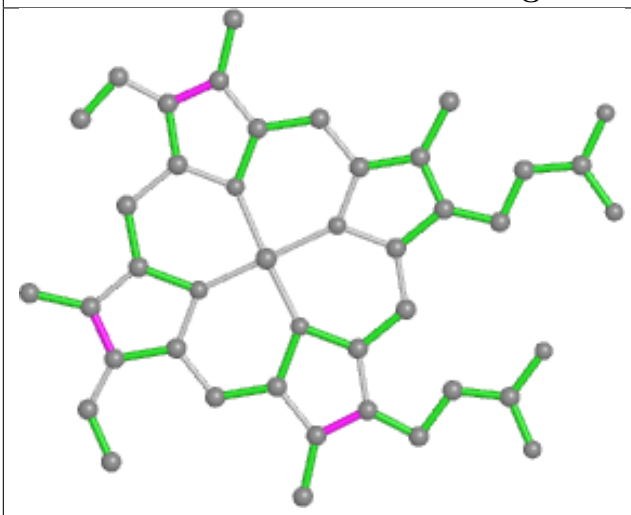


Torsions

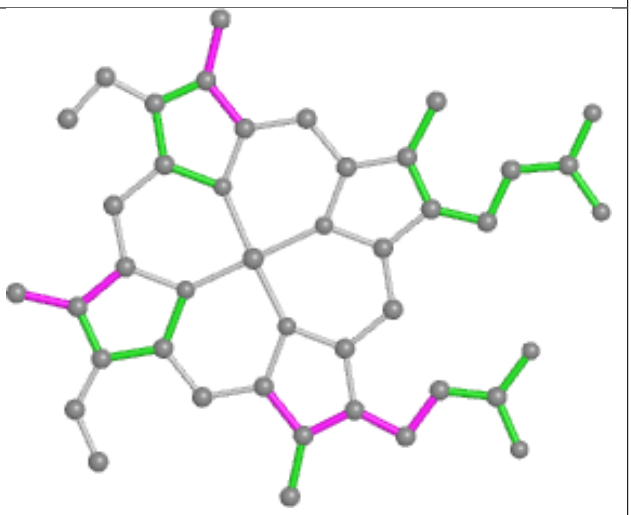


Rings

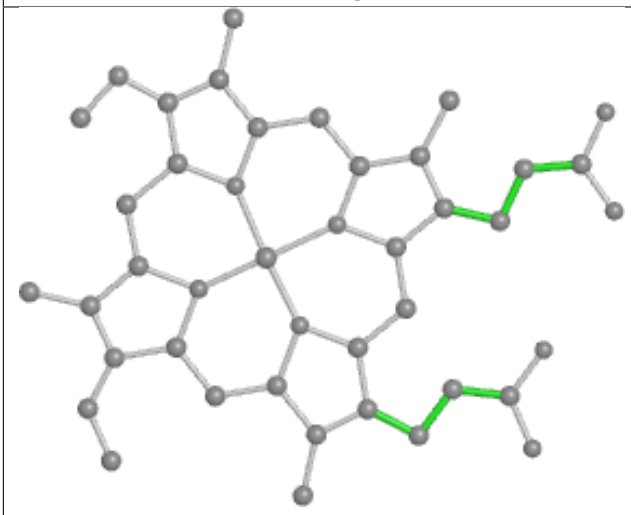
Ligand HEC O 301



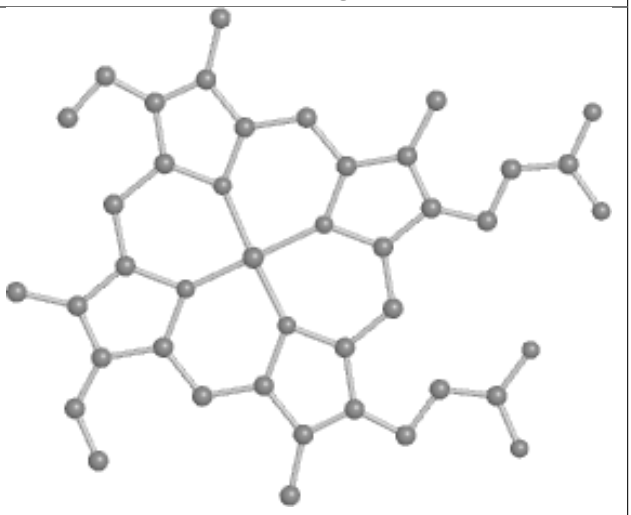
Bond lengths



Bond angles

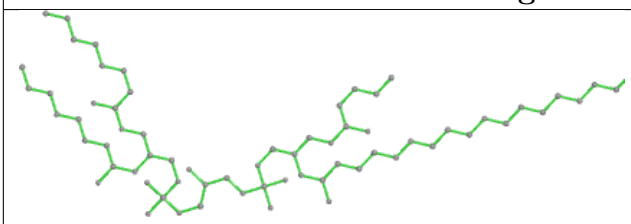


Torsions



Rings

Ligand CDL d1 201



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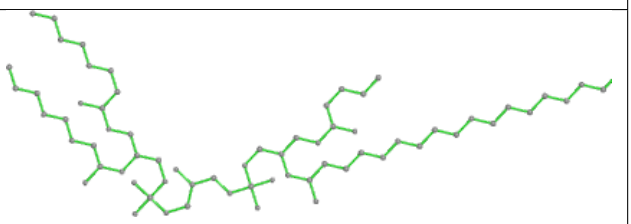
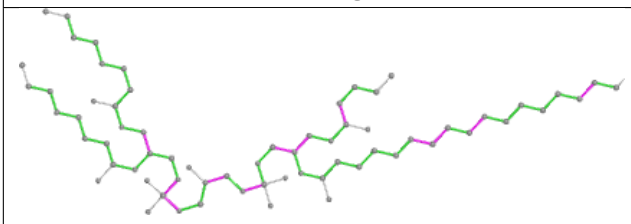
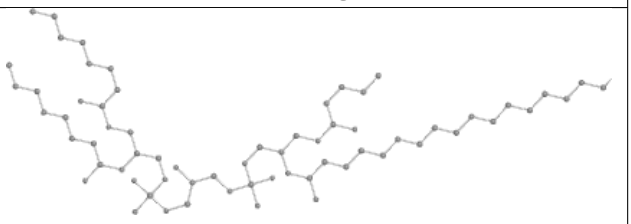


Bond angles

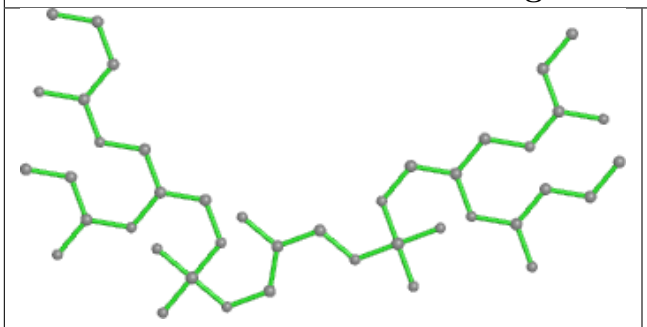


Torsions



Rings

Ligand CDL C 404



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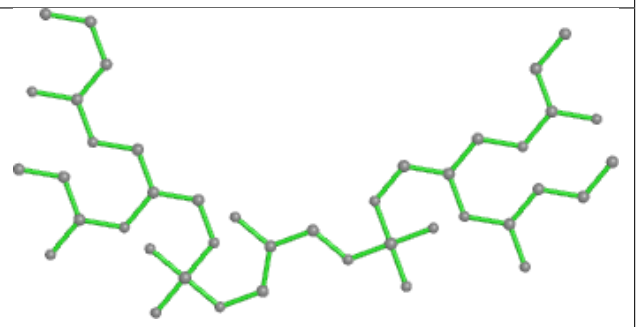
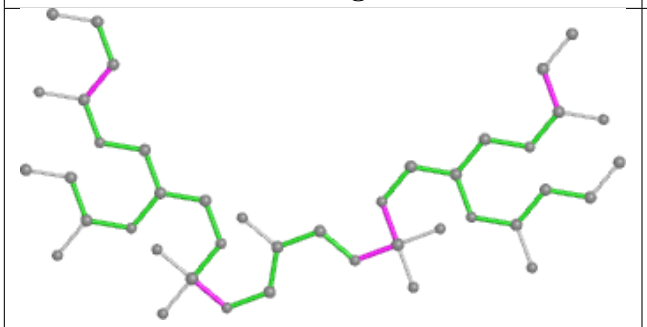
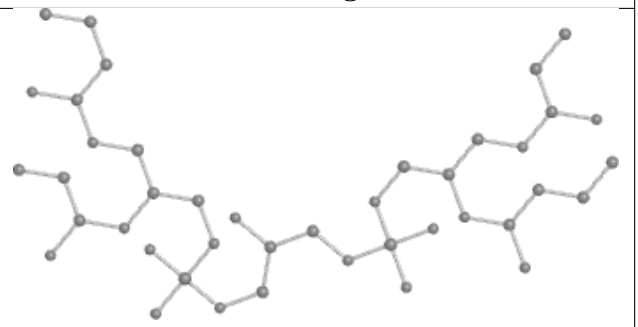


Bond angles

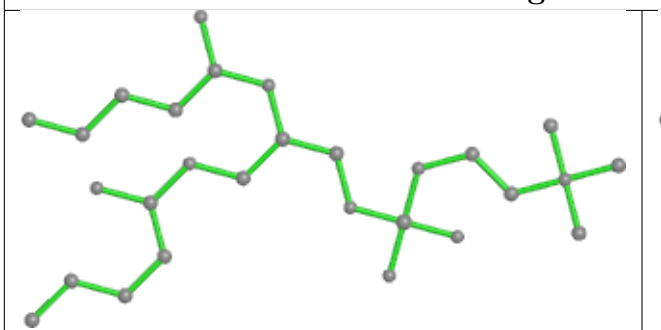


Torsions



Rings

Ligand PC1 V 101



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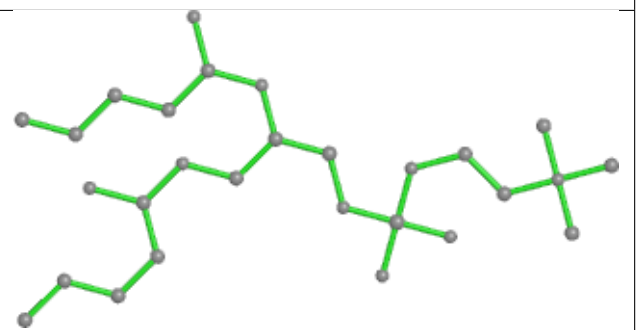

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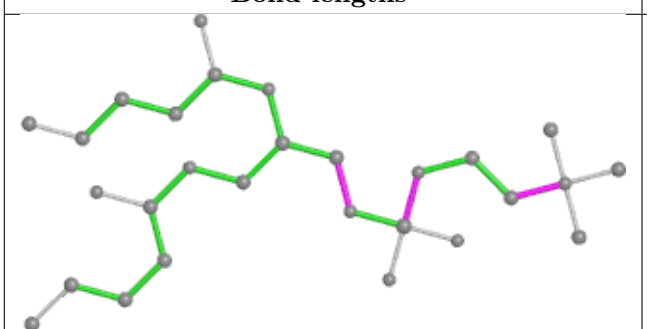

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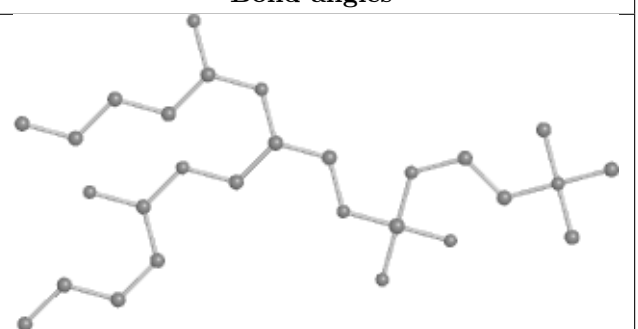
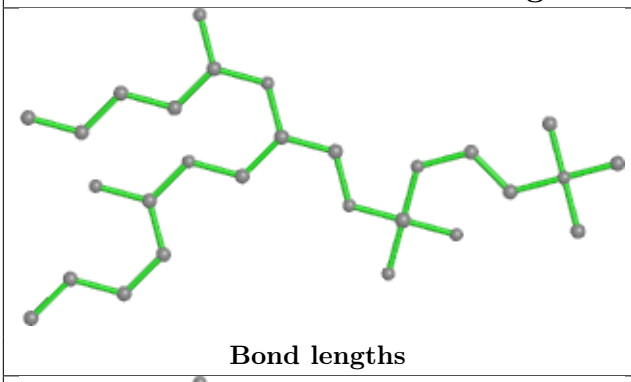


Rings

Ligand PC1 K 101



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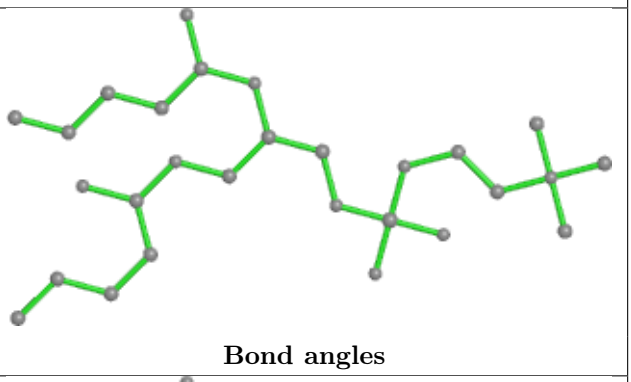
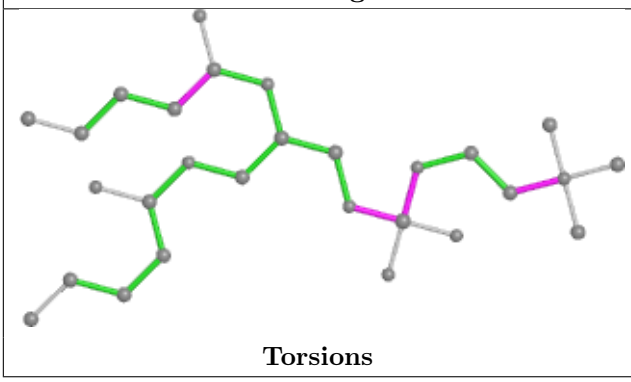


Bond angles



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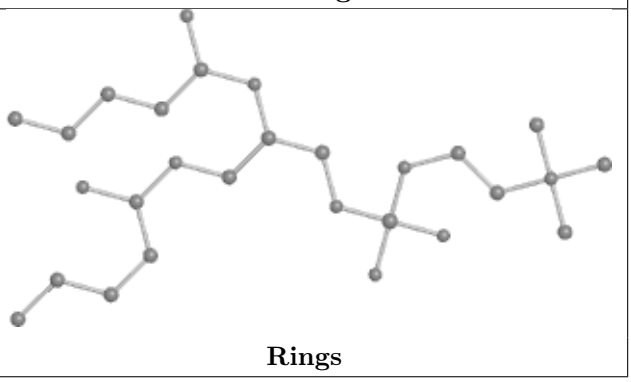
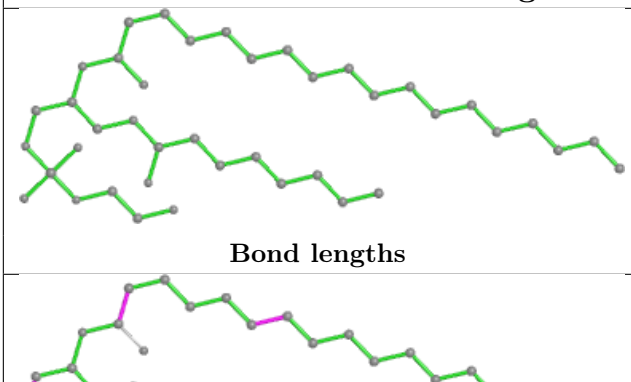


Rings

Ligand 3PE K1 201



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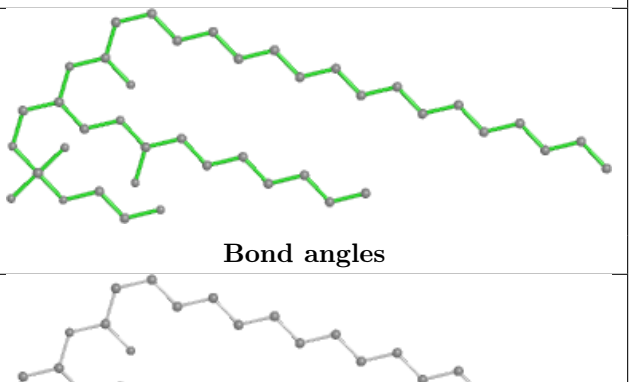

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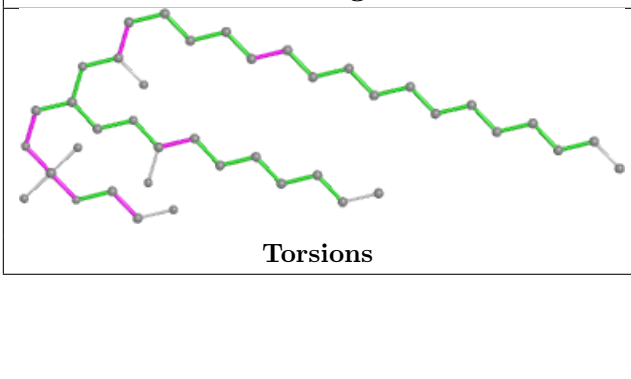

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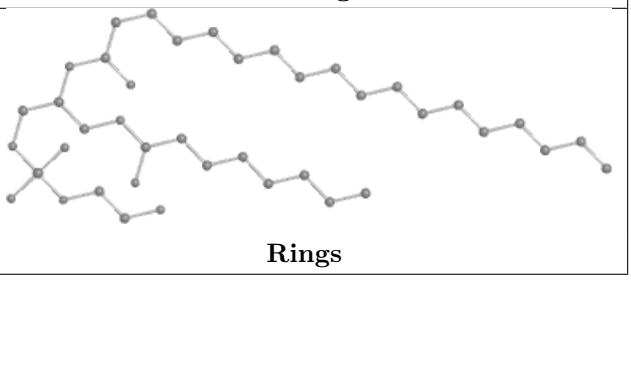
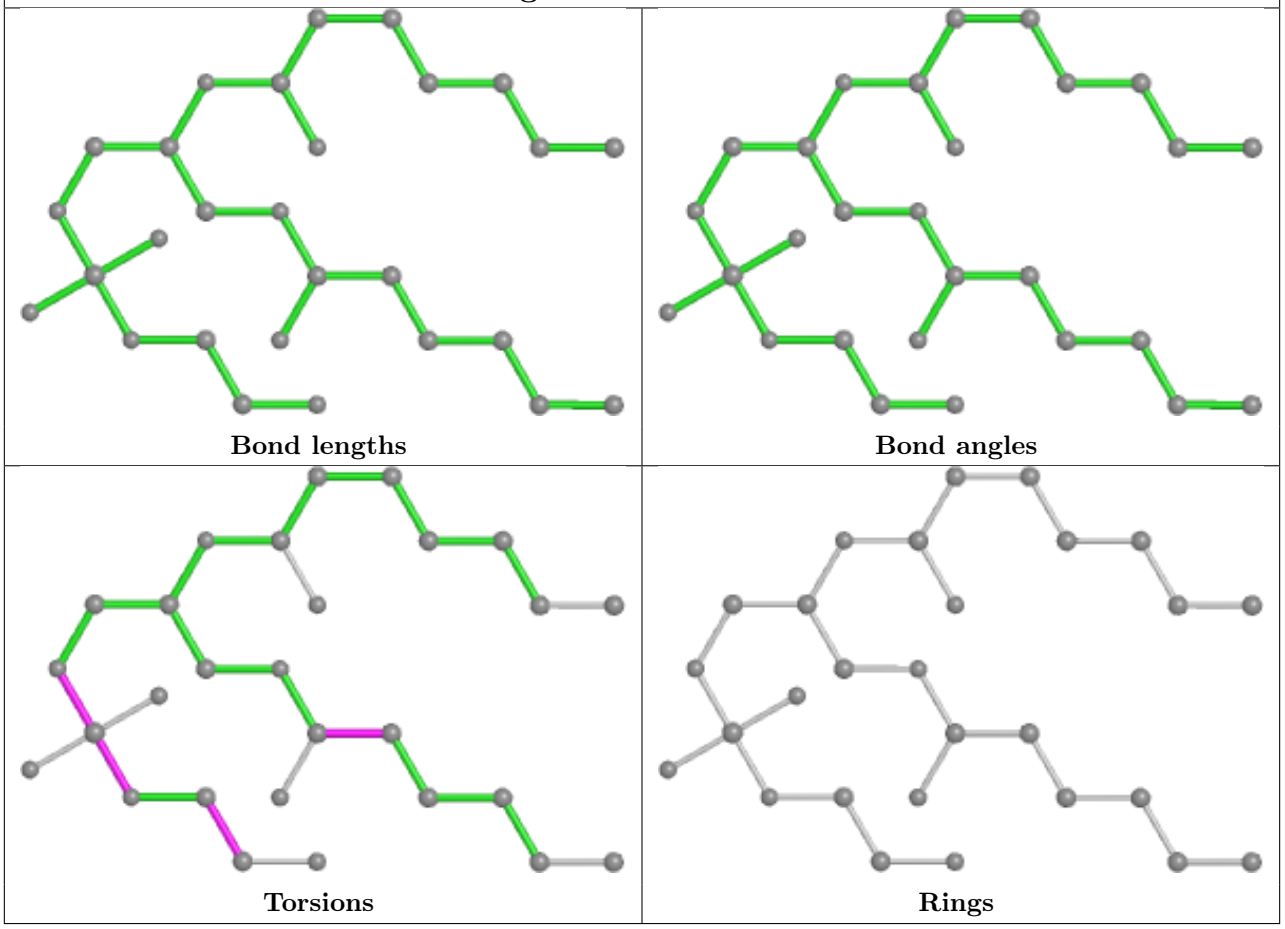
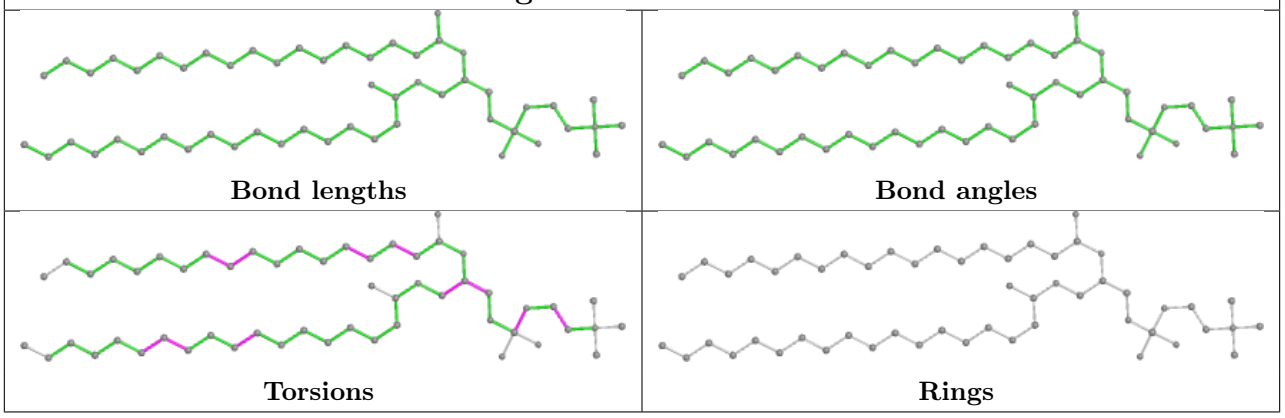


Rings

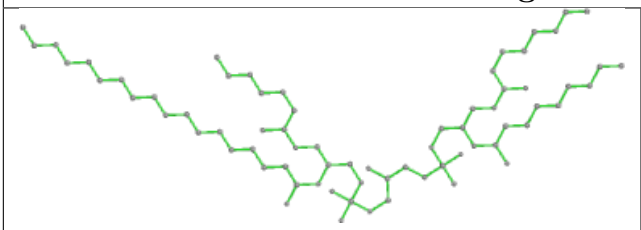
Ligand 3PE Y1 402



Ligand PC1 M1 501



Ligand CDL h1 201



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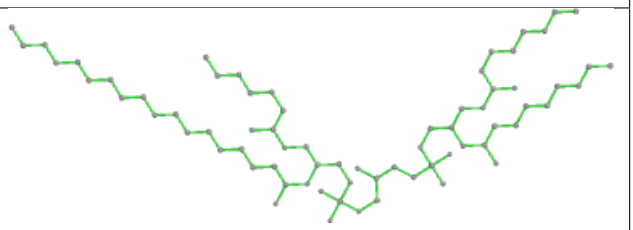
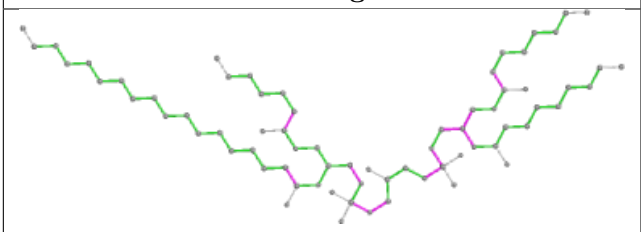


Bond angles



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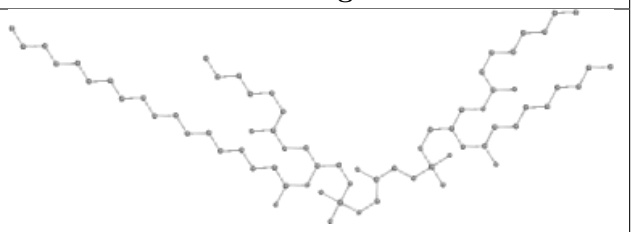
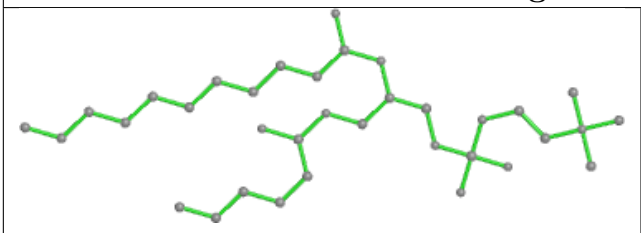


Rings

Ligand PC1 E 202



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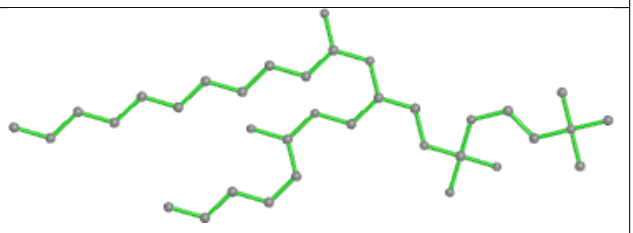

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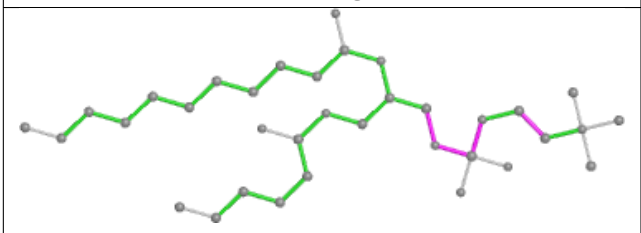

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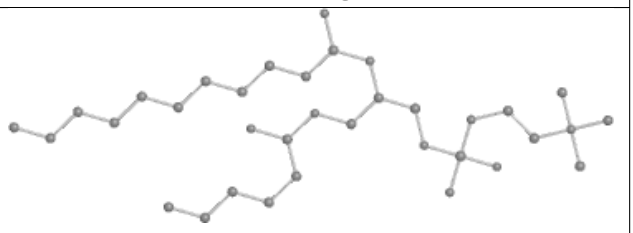
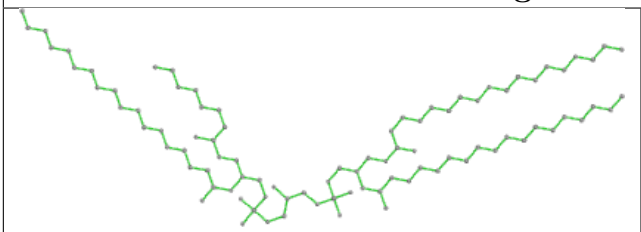


Rings

Ligand CDL N1 401



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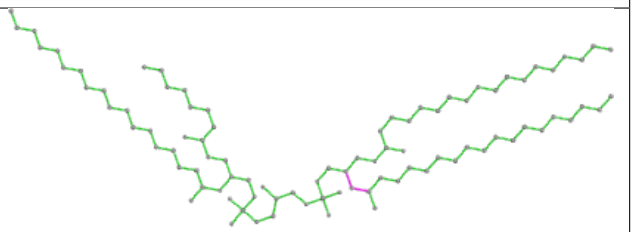
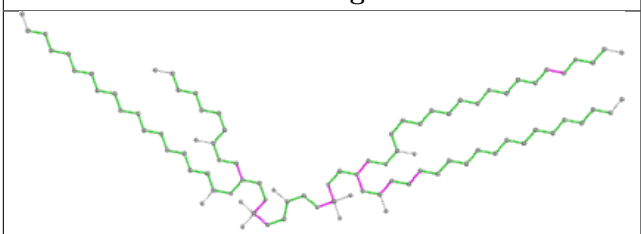


Bond angles



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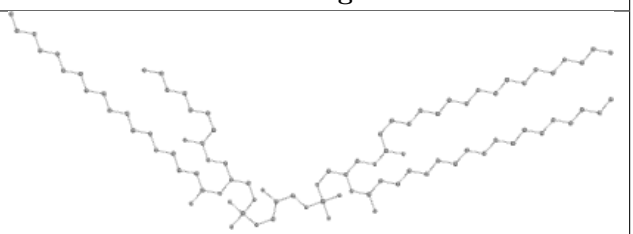
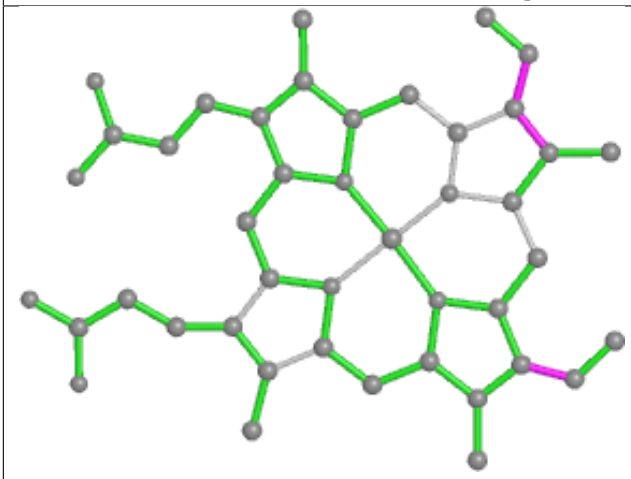


Rings

Ligand HEM C 401



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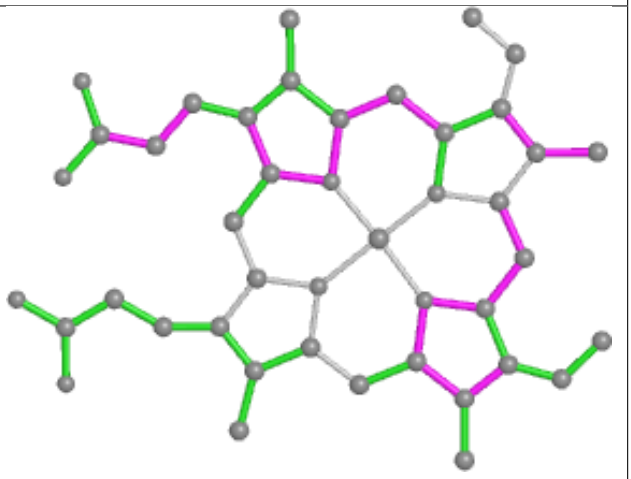
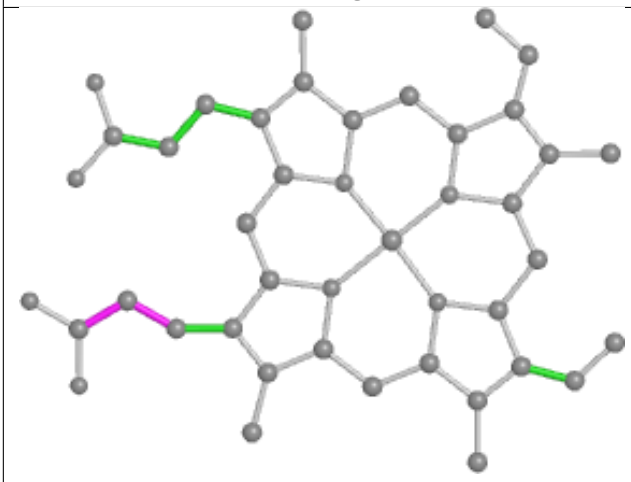
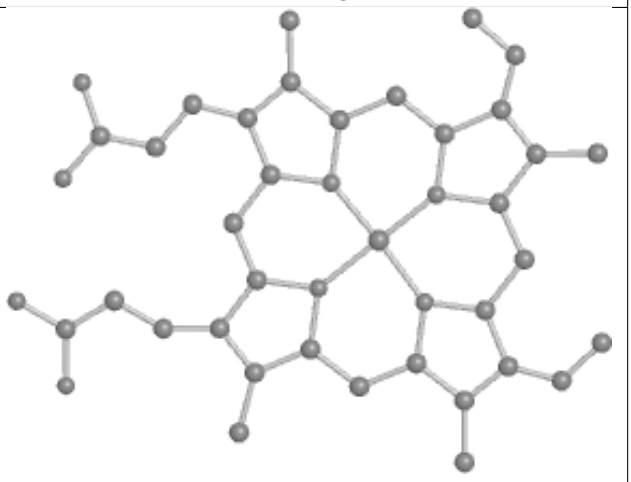


Bond angles

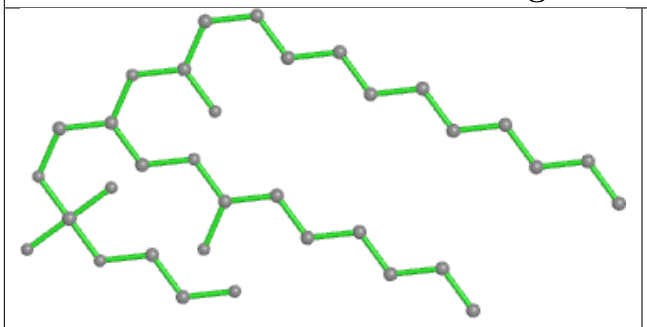


Torsions



Rings

Ligand 3PE N 401



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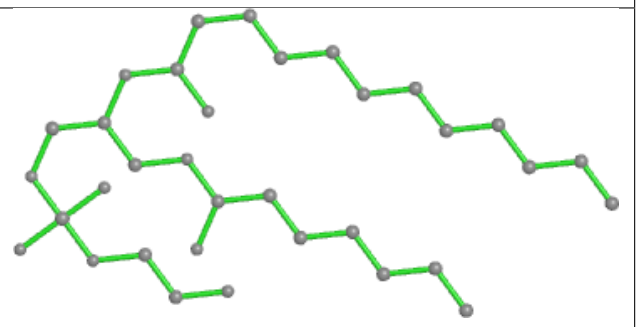

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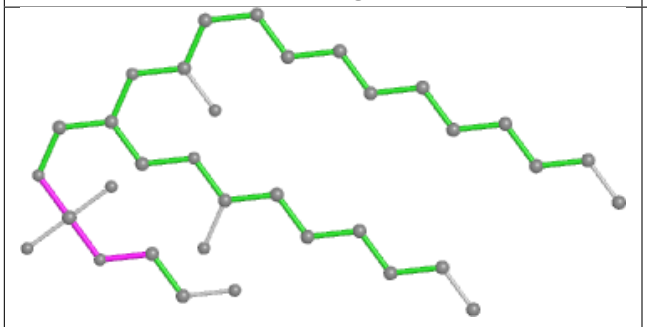
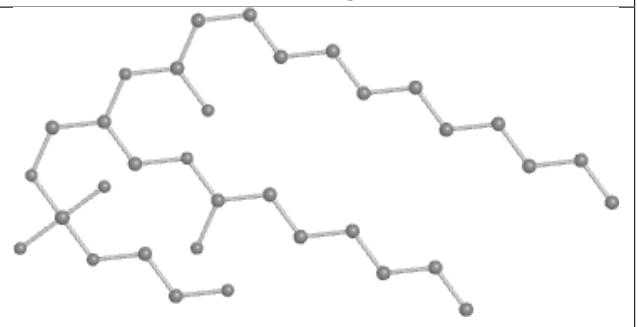
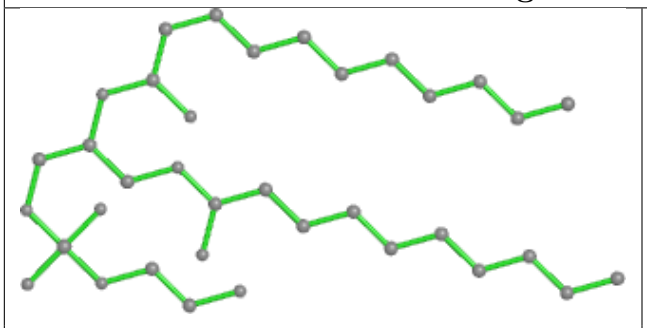


Torsions

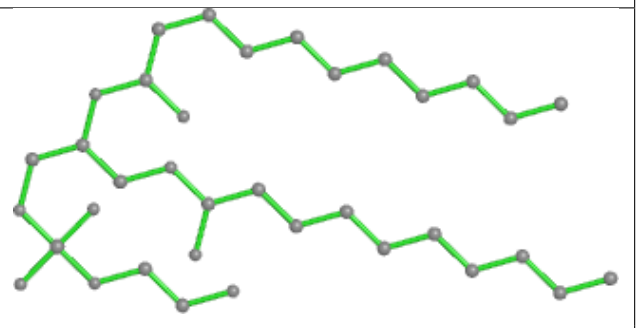


Rings

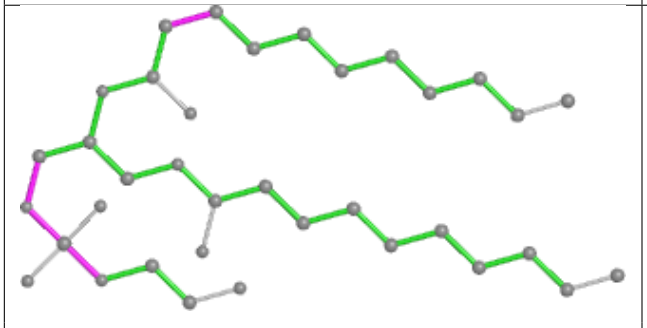
Ligand 3PE M1 503



Bond lengths



Bond angles



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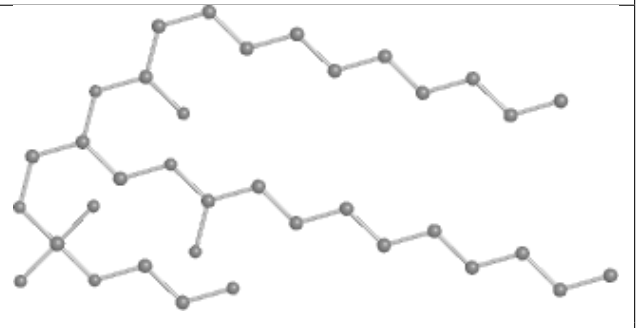
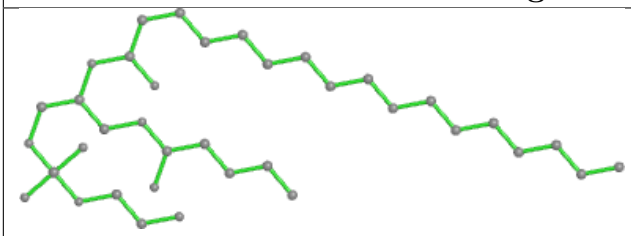
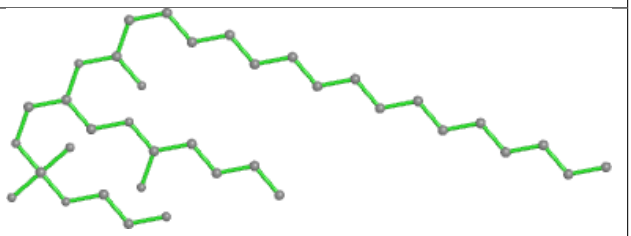


Rings

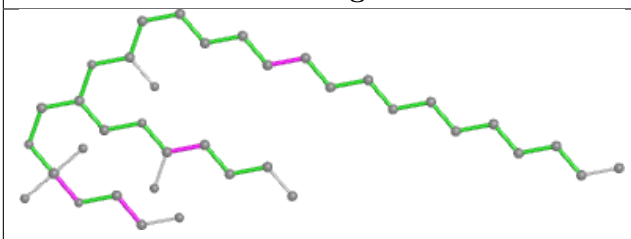
Ligand 3PE N 404



Bond lengths



Bond angles



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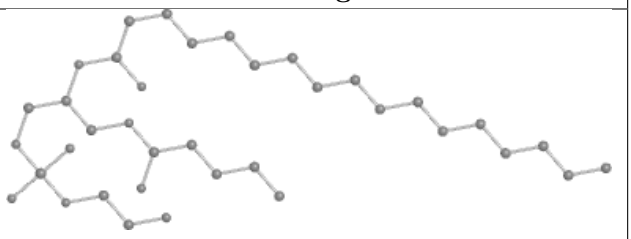
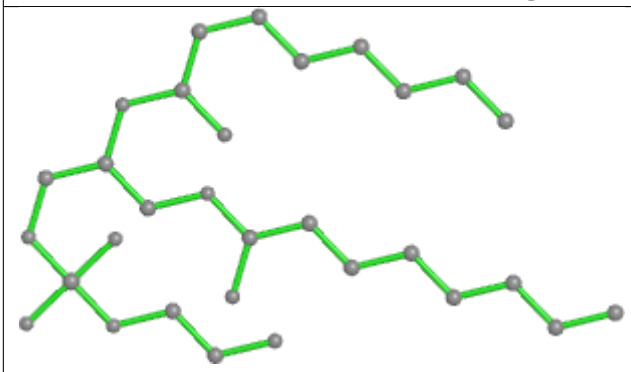
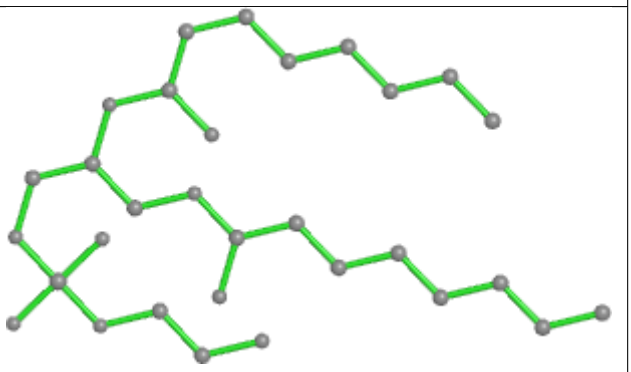


Rings

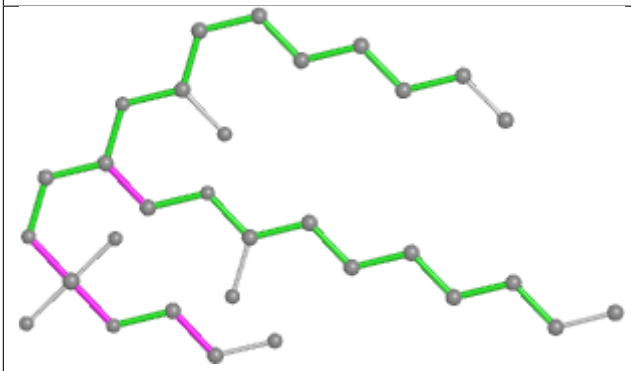
Ligand 3PE d1 202



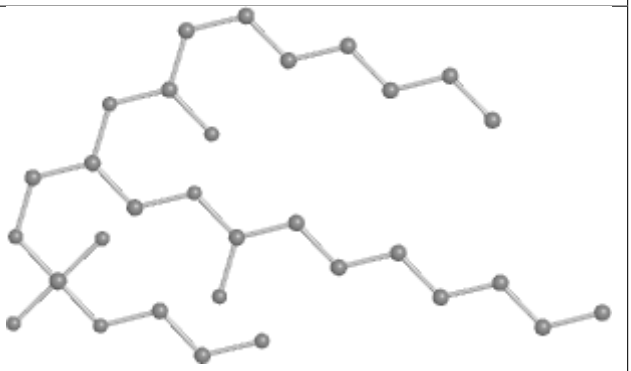
Bond lengths



Bond angles

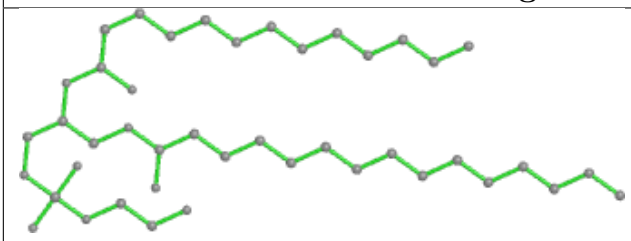


Torsions

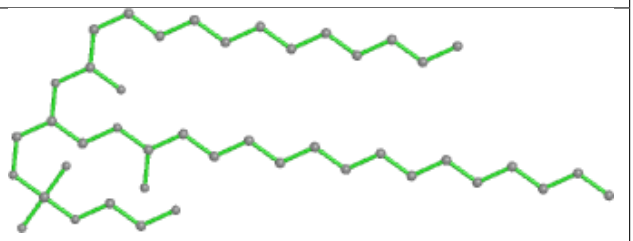


Rings

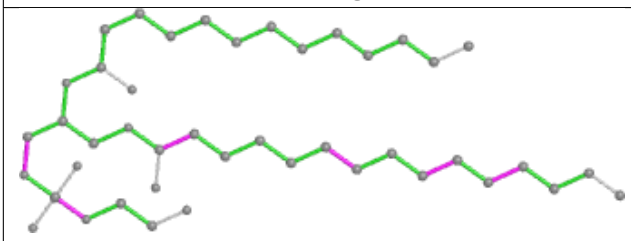
Ligand 3PE A1 602



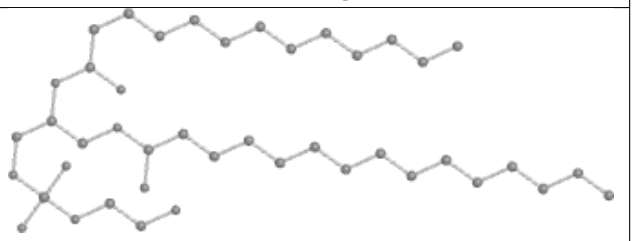
Bond lengths



Bond angles

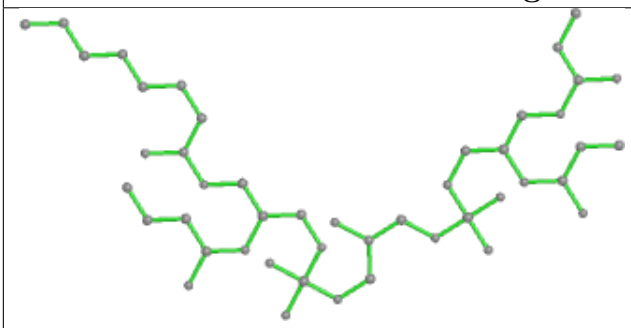


Torsions

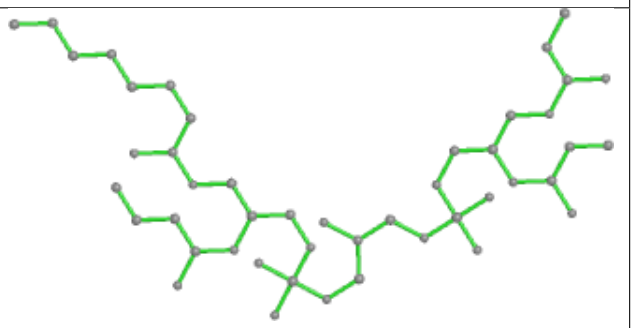


Rings

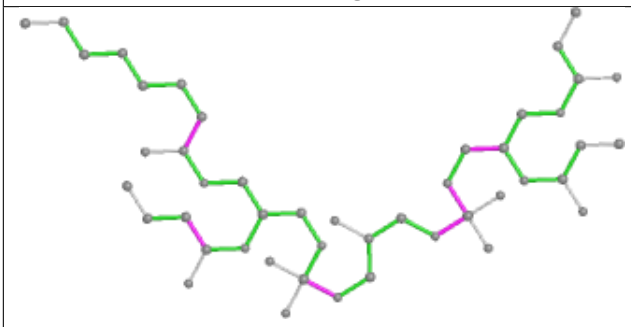
Ligand CDL A 502



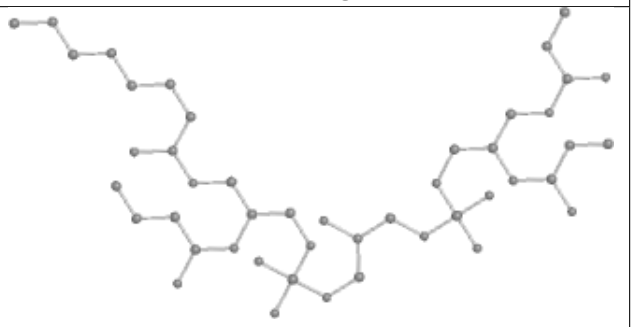
Bond lengths



Bond angles

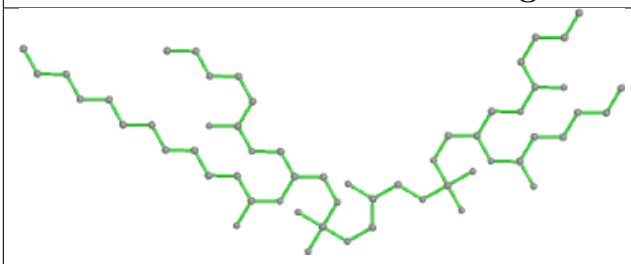


Torsions

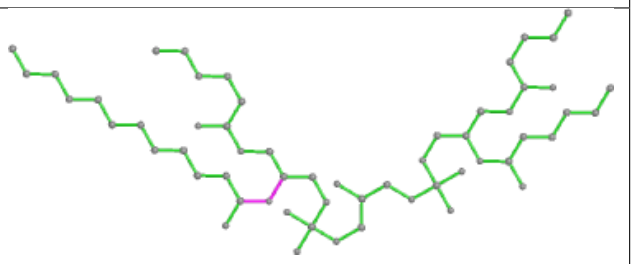


Rings

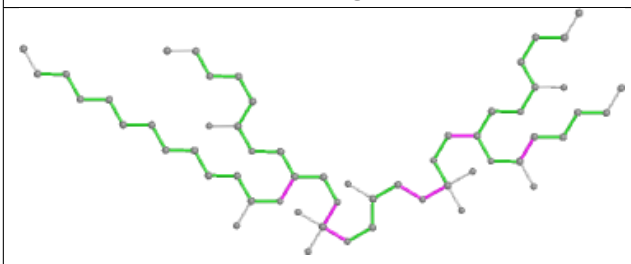
Ligand CDL a1 101



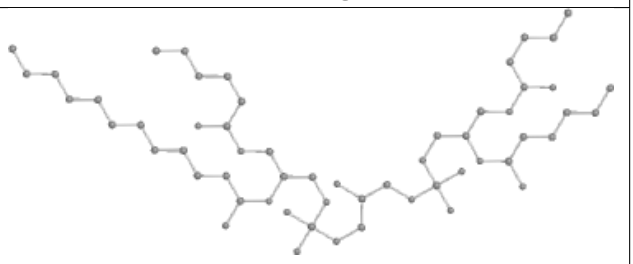
Bond lengths



Bond angles

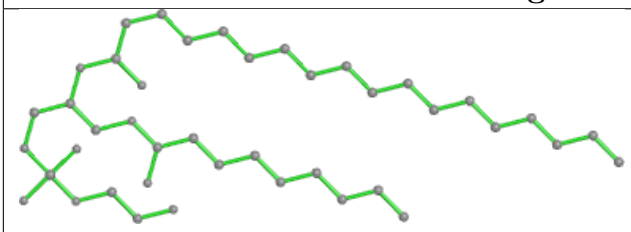


Torsions

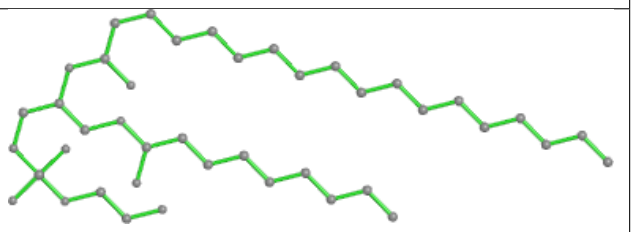


Rings

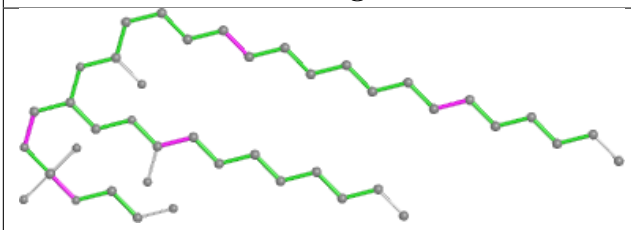
Ligand 3PE i1 201



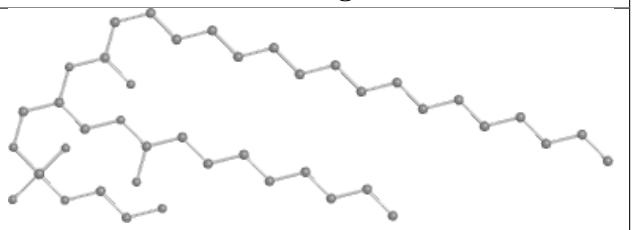
Bond lengths



Bond angles

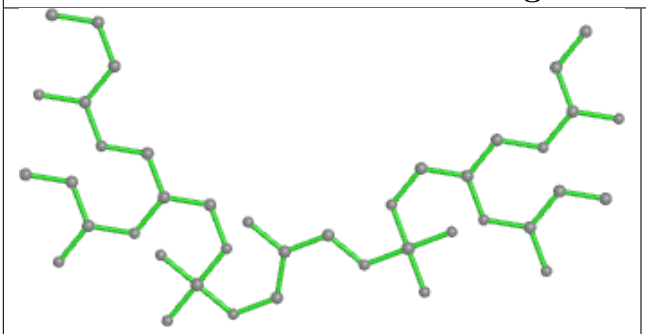


Torsions

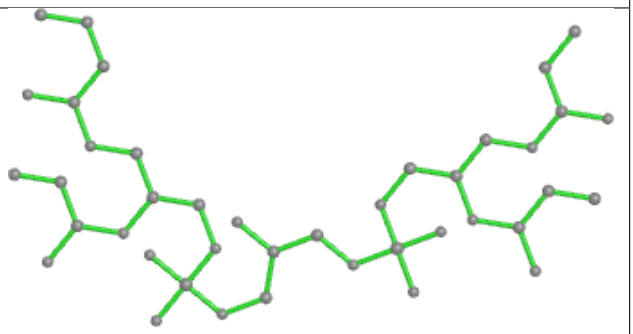


Rings

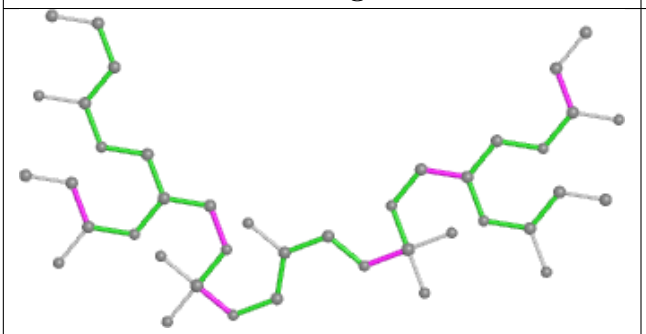
Ligand CDL R 302



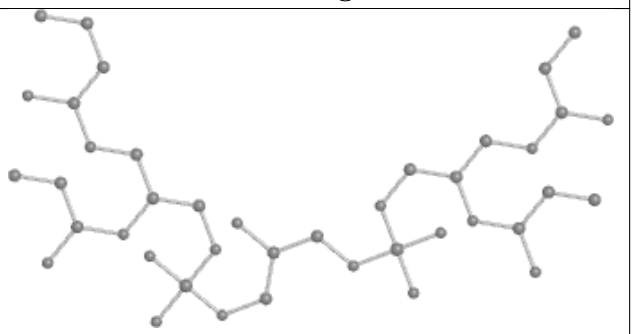
Bond lengths



Bond angles

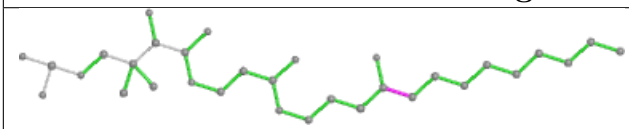


Torsions

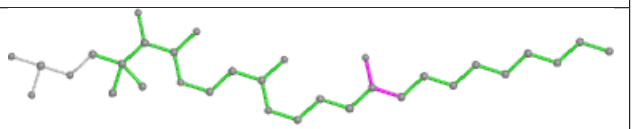


Rings

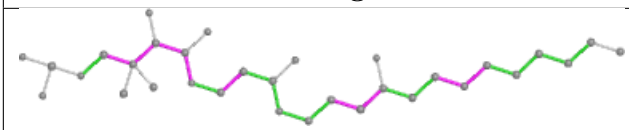
Ligand ZMP n1 201



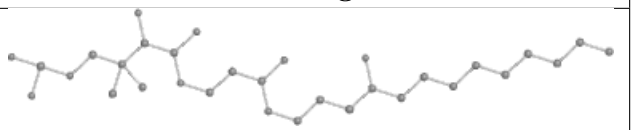
Bond lengths



Bond angles

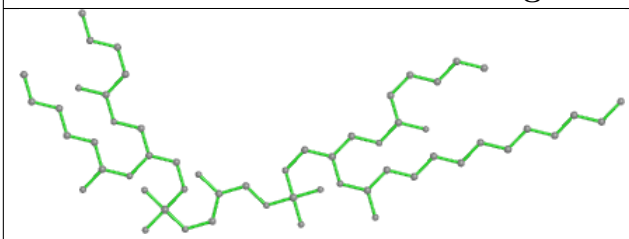


Torsions

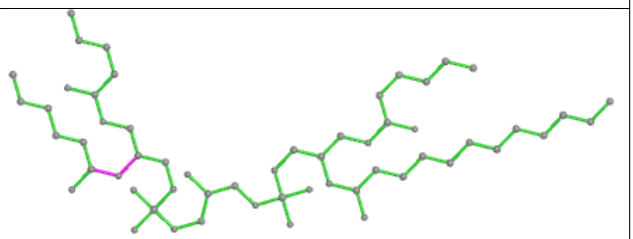


Rings

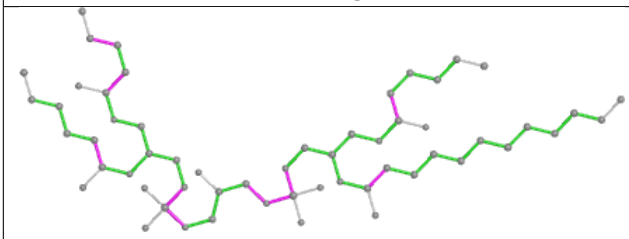
Ligand CDL R 303



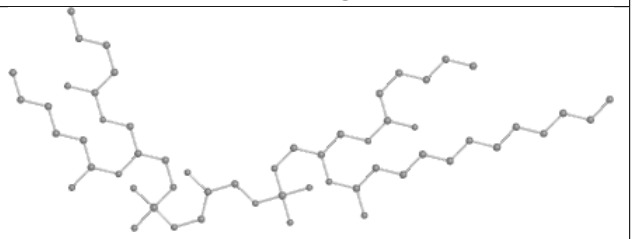
Bond lengths



Bond angles

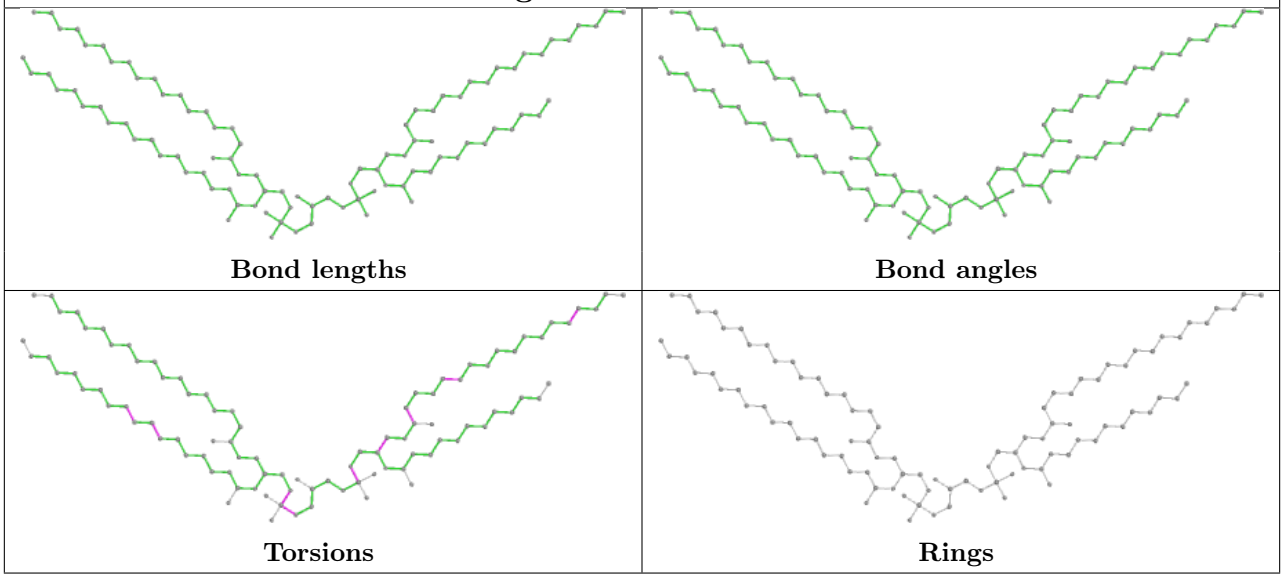


Torsions



Rings

Ligand CDL Y1 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

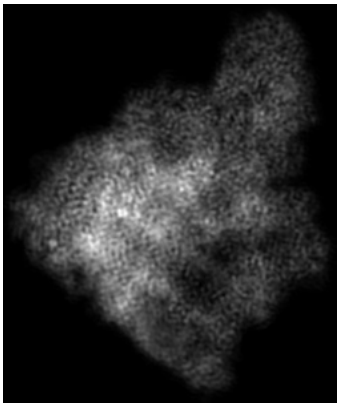
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17990. These allow visual inspection of the internal detail of the map and identification of artifacts.

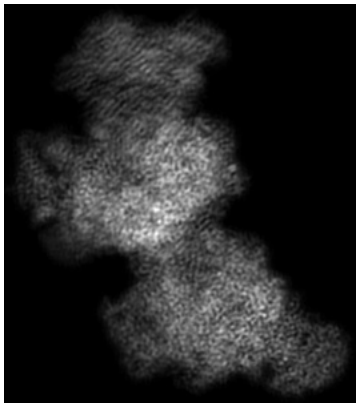
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

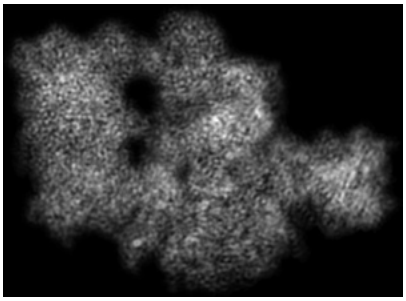
6.1.1 Primary map



X



Y



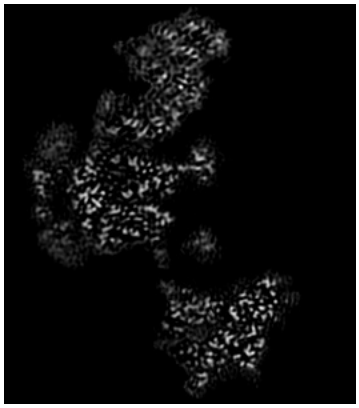
Z

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

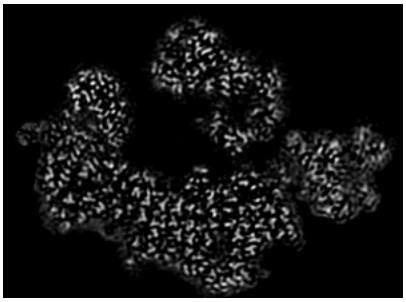
6.2 Central slices

6.2.1 Primary map

X Index: 140



Y Index: 103



Z Index: 123

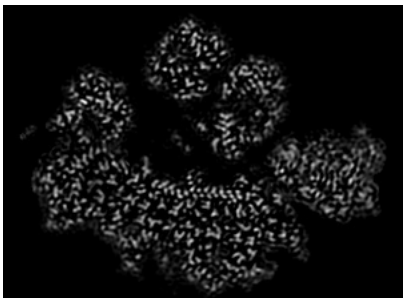
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 140

Y Index: 75

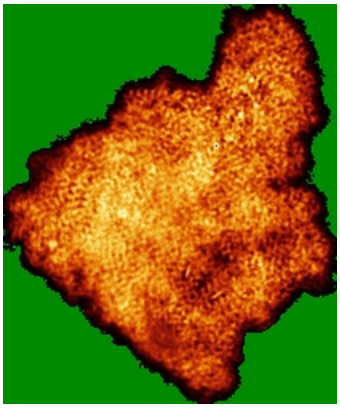


Z Index: 118

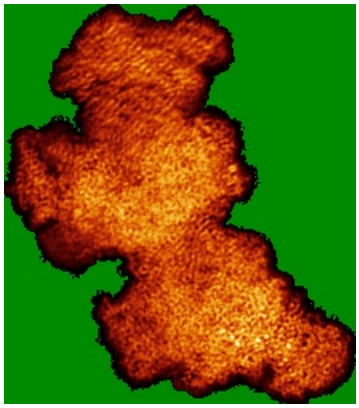
The images above show the largest variance slices of the map in three orthogonal directions.

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

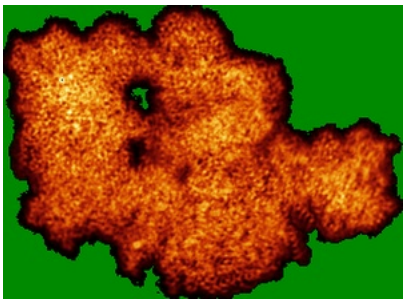
6.4.1 Primary map



X



Y

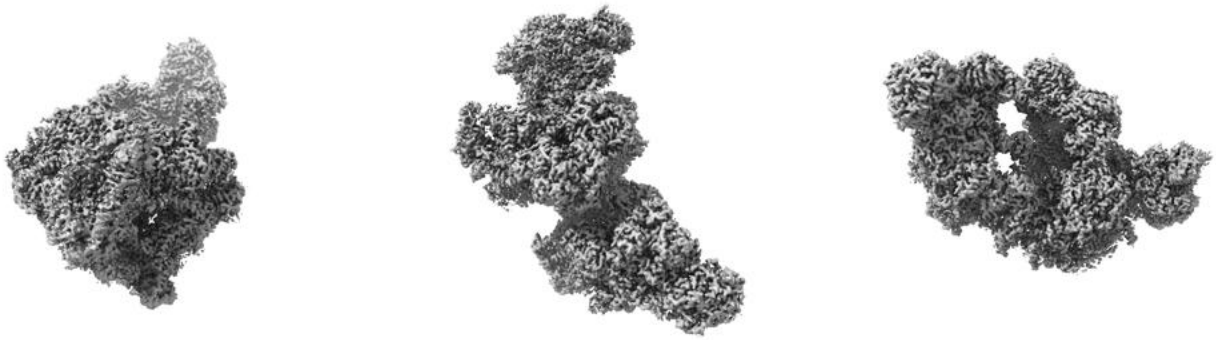


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

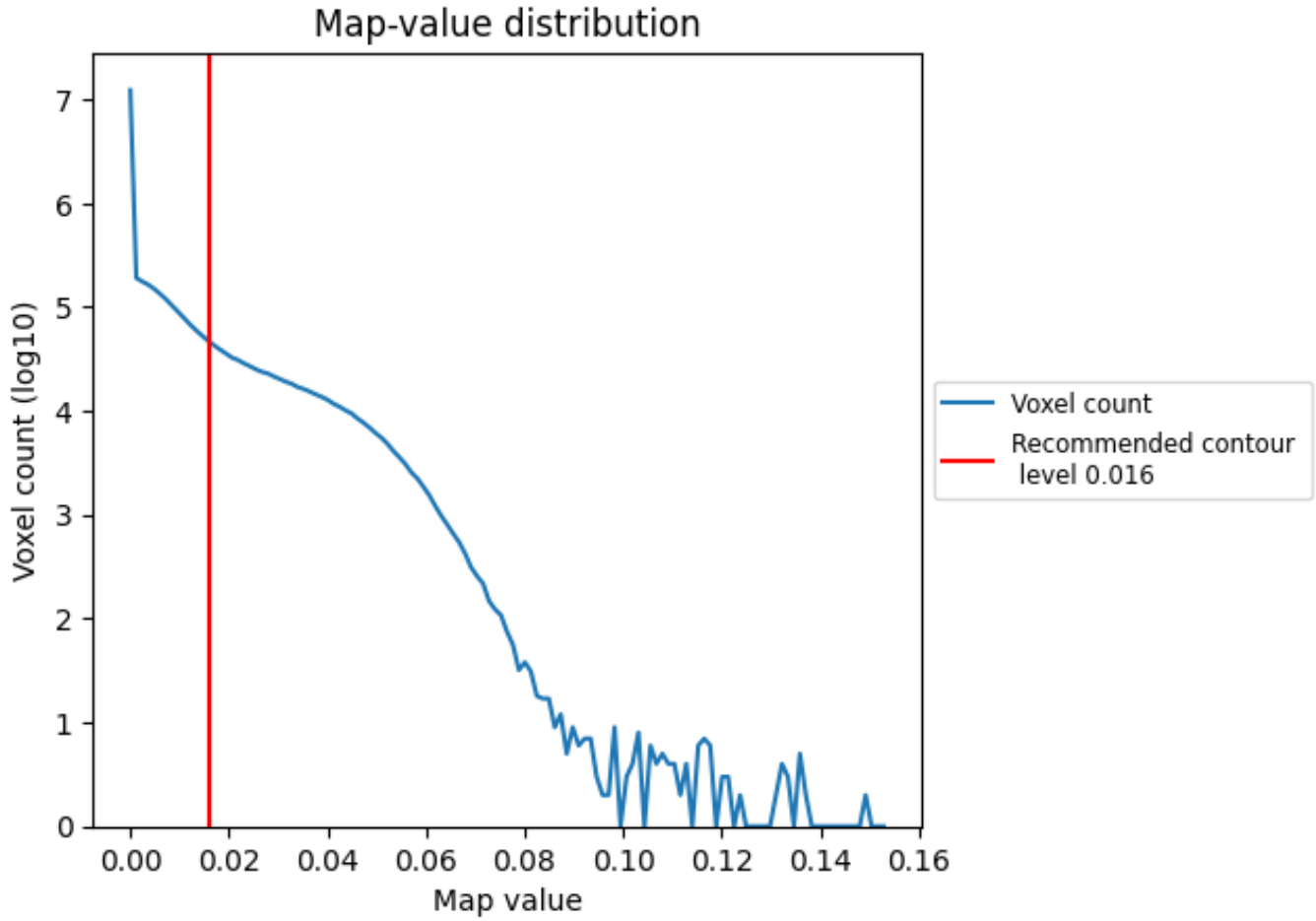
6.6 Mask visualisation (i)

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

7 Map analysis

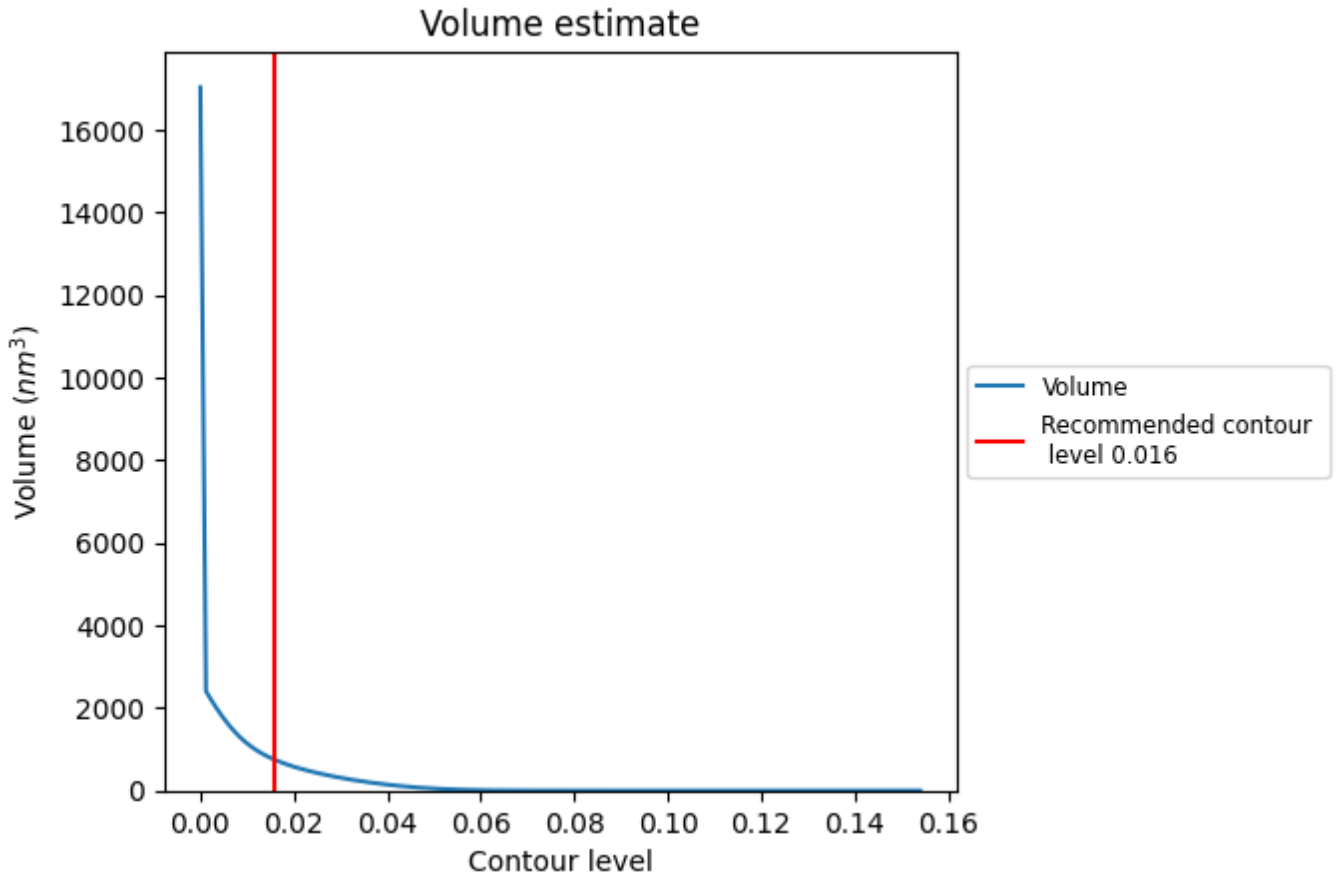
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 743 nm^3; this corresponds to an approximate mass of 671 kDa.

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

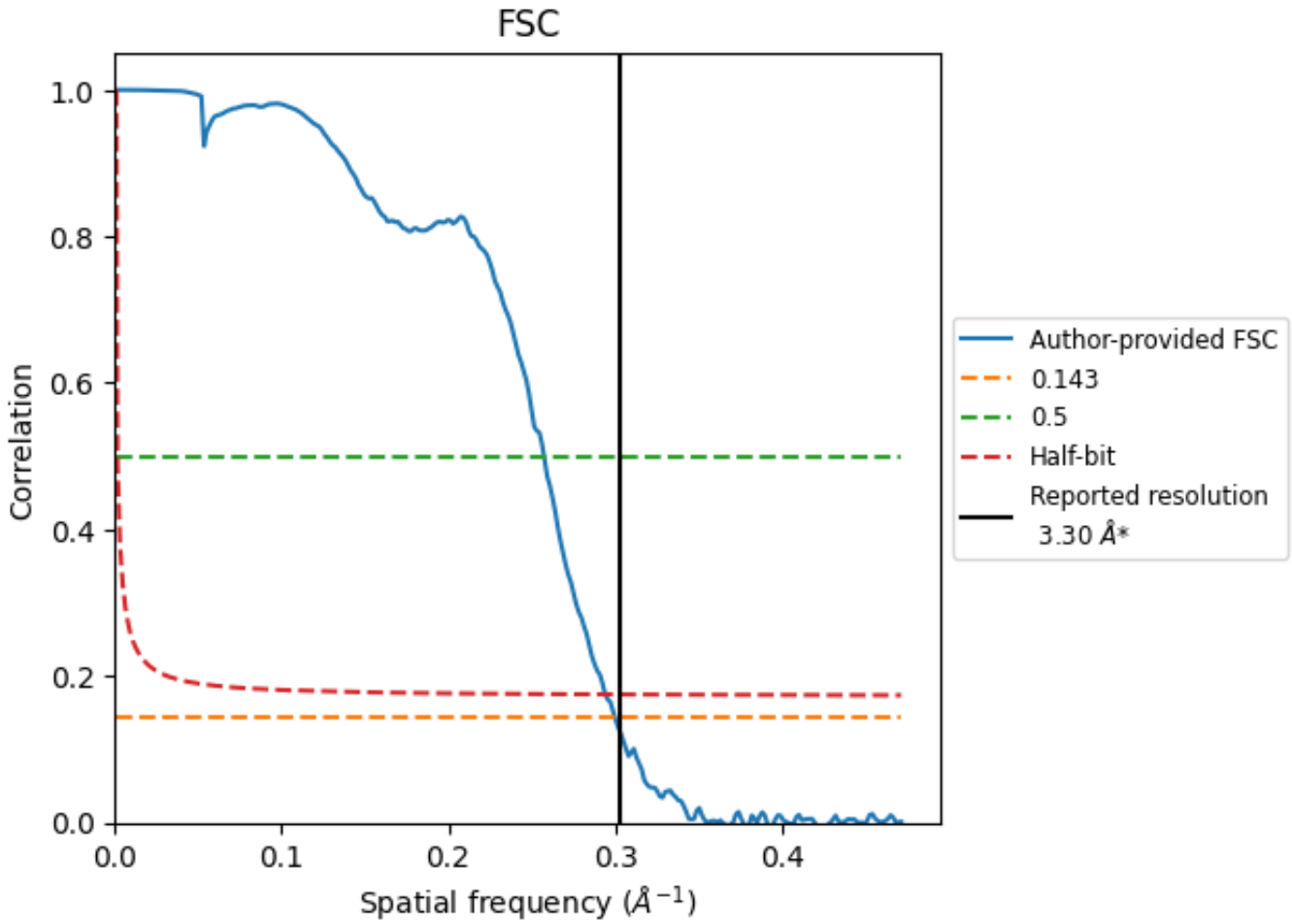
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

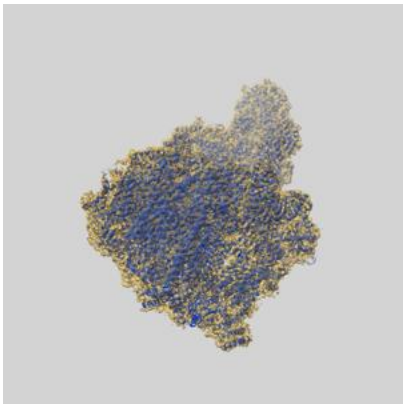
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.89	3.40
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

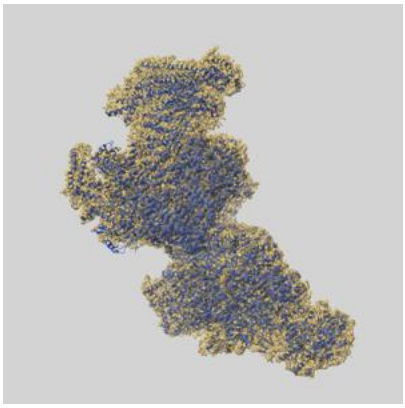
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17990 and PDB model 8PW6. Per-residue inclusion information can be found in section 3 on page 29.

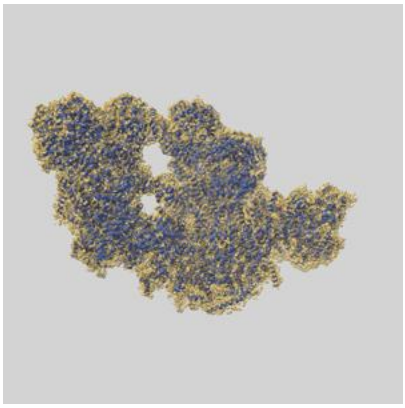
9.1 Map-model overlay



X



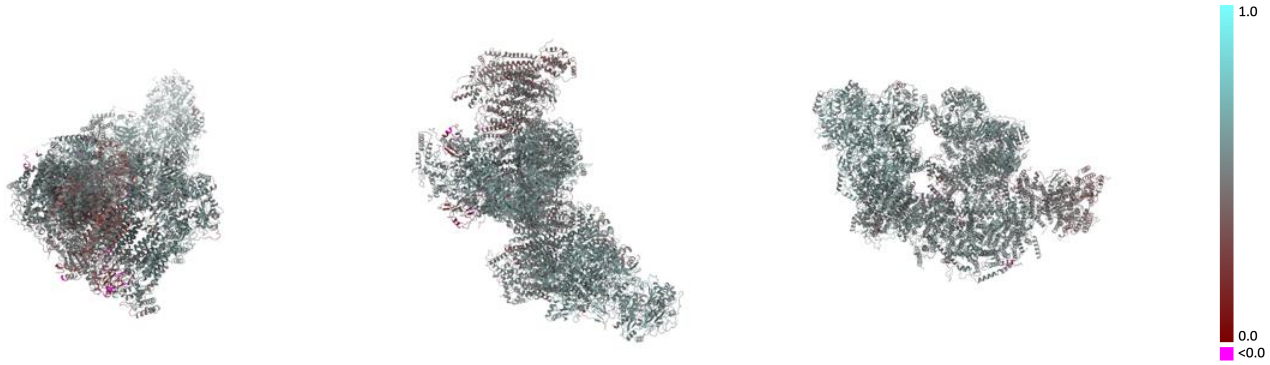
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

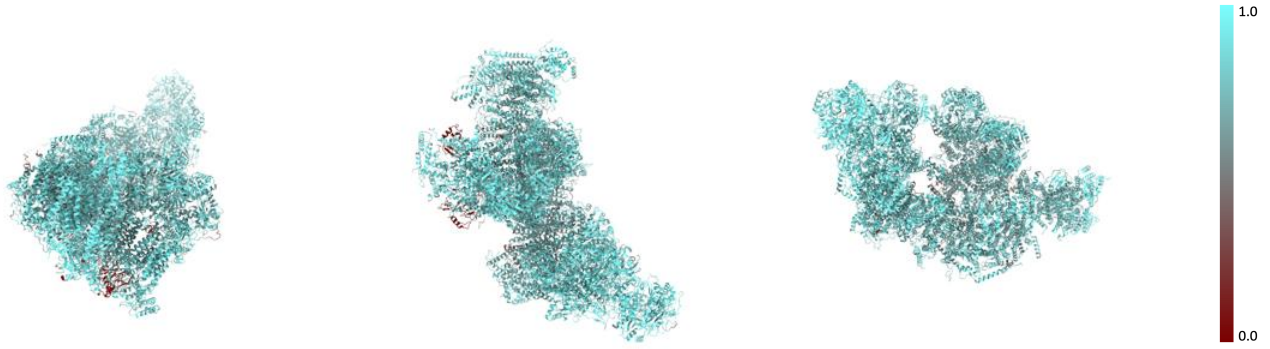
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

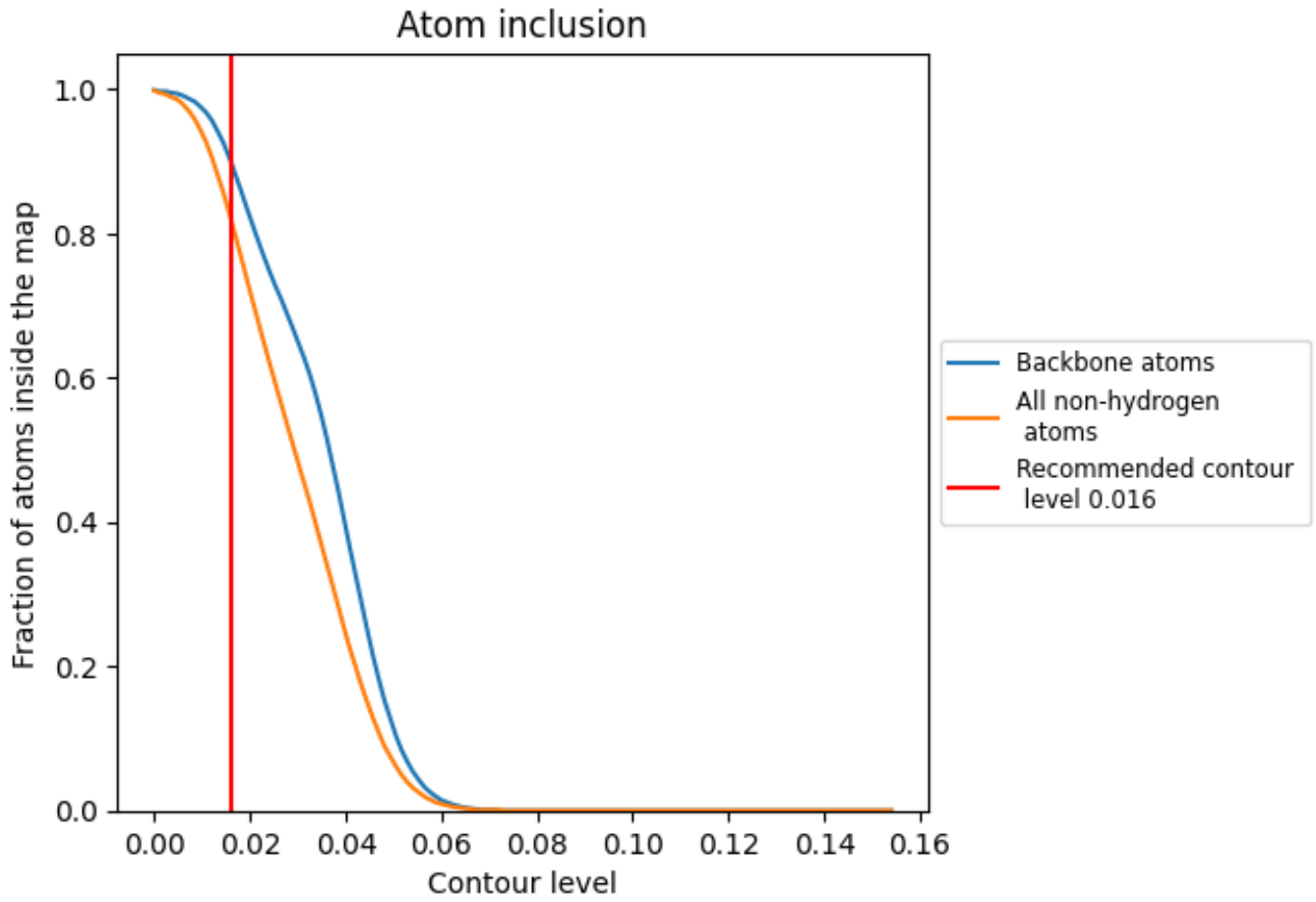
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.5140
1	0.8940	0.5550
2	0.8910	0.5520
3	0.8740	0.5540
6	0.8800	0.5540
7	0.8850	0.5510
9	0.8770	0.5580
A	0.8440	0.5370
A1	0.7500	0.4950
B	0.8410	0.5430
C	0.8390	0.5430
C1	0.9190	0.5920
D	0.8550	0.5290
D1	0.8470	0.5410
E	0.5030	0.3560
F	0.8360	0.5430
G	0.8380	0.5250
H	0.8120	0.4680
H1	0.7860	0.5100
J	0.8090	0.5140
J1	0.6690	0.4550
K	0.7000	0.5130
K1	0.7480	0.5110
L	0.8310	0.5360
L1	0.8060	0.5290
M	0.8470	0.5380
M1	0.8120	0.5330
N	0.8160	0.5330
N1	0.7890	0.5270
O	0.8390	0.5300
O1	0.8460	0.5260
P	0.5000	0.3510
P1	0.8440	0.5460
Q	0.7940	0.5400
Q1	0.8690	0.5750

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Chain	Atom inclusion	Q-score
R	0.7370	0.5110
S	0.7310	0.4490
S1	0.8740	0.5240
T	0.6040	0.4810
T1	0.7420	0.4420
U	0.7930	0.5190
U1	0.8370	0.5320
V	0.6930	0.4700
V1	0.8760	0.5540
W1	0.8700	0.5590
X1	0.8280	0.5120
Y1	0.6850	0.4810
Z1	0.8310	0.5220
a1	0.8150	0.5240
b1	0.8030	0.5000
c1	0.7850	0.5030
d1	0.7690	0.5130
e1	0.8050	0.5210
f1	0.7580	0.5040
g1	0.7910	0.5040
h1	0.8240	0.5210
i1	0.7470	0.4790
j1	0.7970	0.4950
k1	0.8290	0.5200
l1	0.8450	0.5400
m1	0.7990	0.5160
n	0.8410	0.4470
n1	0.8520	0.5310
o	0.8260	0.4160
o1	0.8130	0.4980
p	0.8070	0.4350
p1	0.8420	0.5210
q	0.8710	0.4190
q1	0.8950	0.5660
r	0.8690	0.4010
r1	0.8630	0.5580
s	0.8010	0.4170
s1	0.8040	0.5260
t	0.7290	0.3820
u	0.8570	0.4230
v	0.8050	0.3780
w	0.8160	0.4630

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Chain	Atom inclusion	Q-score
x	0.8680	0.3990
y	0.8440	0.4680
z	0.8040	0.3900