wwPDB EM Validation Summary Report ⓘ

Apr 18, 2024 – 04:30 pm BST

PDB ID	:	8PW5
EMDB ID	:	EMD-17989
Title	:	CS respirasome from murine liver
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2023-07-19
Resolution	:	3.60 Å(reported)
Based on initial models	:	7o3c, 6g2j

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:

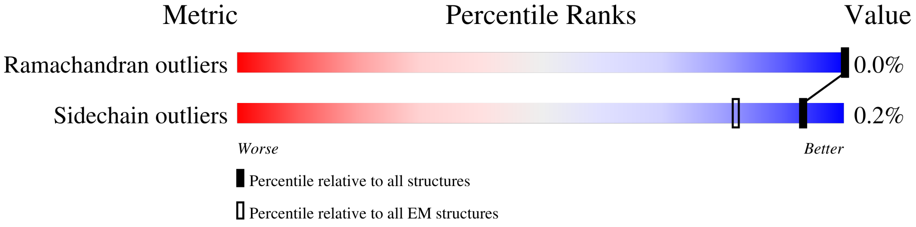
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

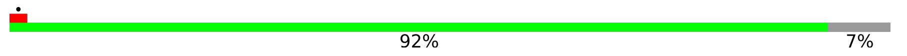
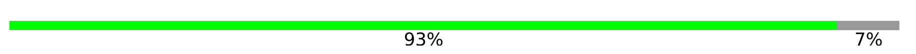
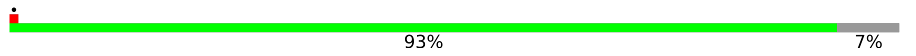
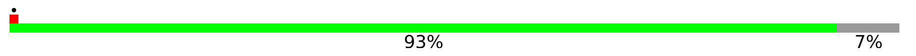
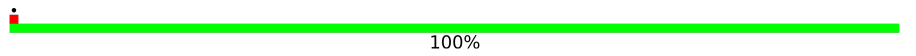
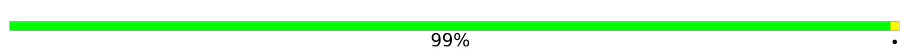
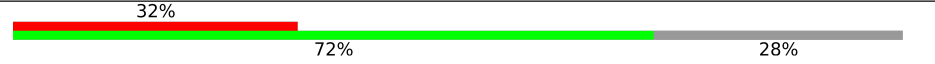
The reported resolution of this entry is 3.60 Å.

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	
1	L	480	
2	B	453	
2	M	453	
3	C	381	
3	N	381	
4	D	325	
4	O	325	
5	E	274	

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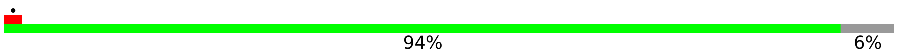
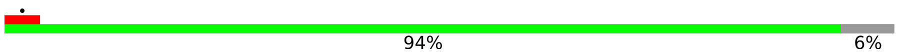
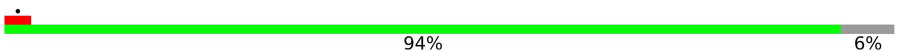
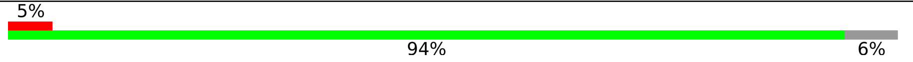
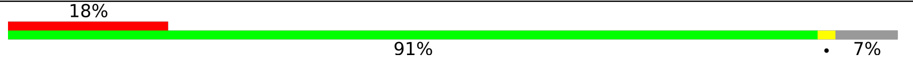
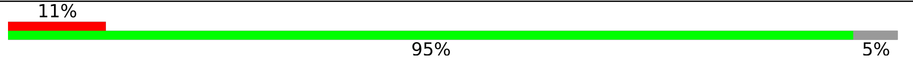
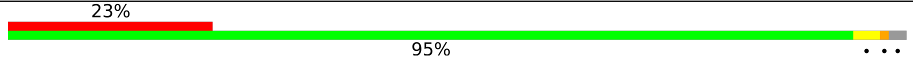
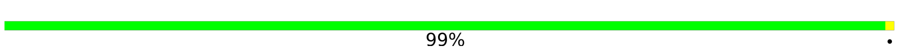
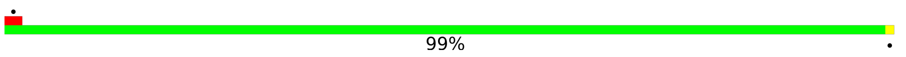
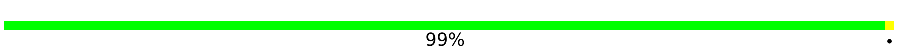
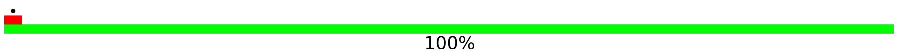
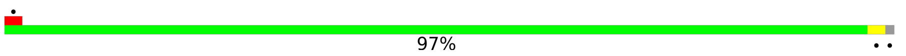
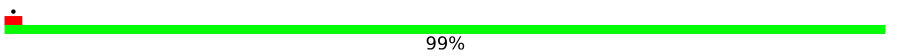
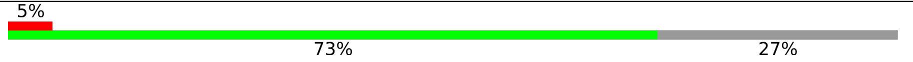
Mol	Chain	Length	Quality of chain
5	P	274	
5	T	274	
6	F	111	
6	Q	111	
7	G	82	
7	R	82	
8	H	89	
8	S	89	
9	J	64	
9	U	64	
10	K	56	
10	V	56	
11	I	113	
12	a	514	
12	n	514	
13	b	227	
13	o	227	
14	c	261	
14	p	261	
15	d	169	
15	q	169	
16	e	146	
16	r	146	
17	f	128	
17	s	128	

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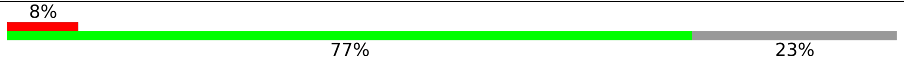
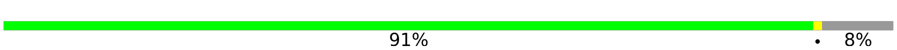
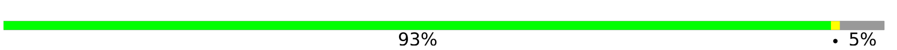
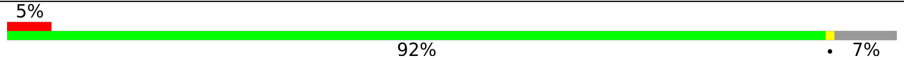
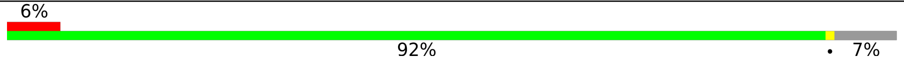
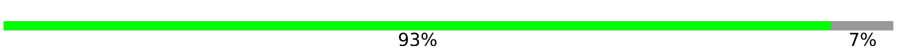
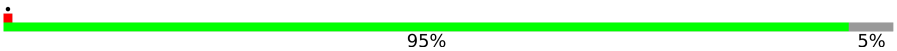
Mol	Chain	Length	Quality of chain
18	g	97	
18	t	97	
19	h	86	
19	u	86	
20	i	76	
20	v	76	
21	k	80	
21	x	80	
22	l	63	
22	y	63	
23	m	70	
23	z	70	
24	w	83	
25	6	224	
26	C1	263	
27	D1	463	
28	2	248	
29	1	464	
30	3	727	
31	9	212	
32	P1	377	
33	Q1	175	
34	7	116	
35	S1	99	
36	T1	156	

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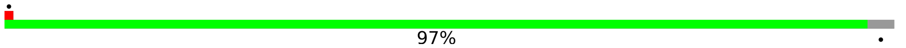
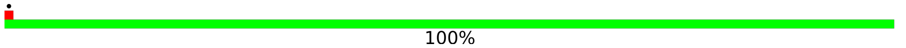
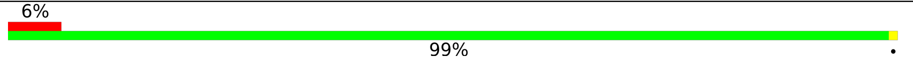
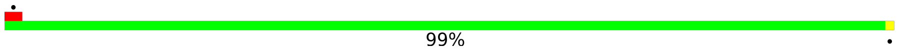
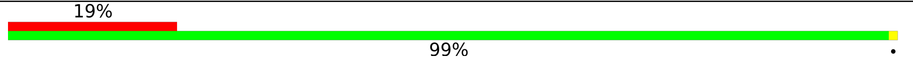
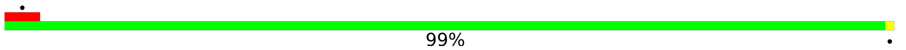
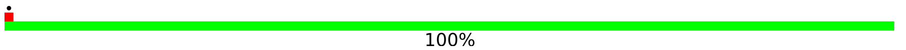
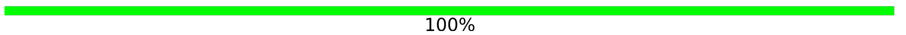
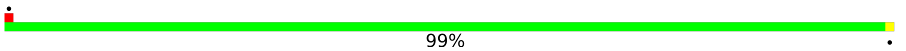
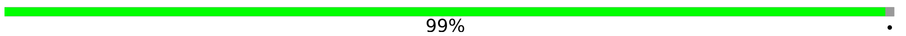
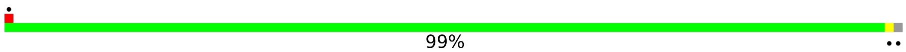
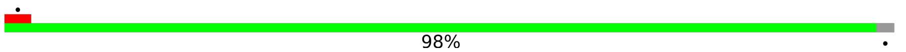
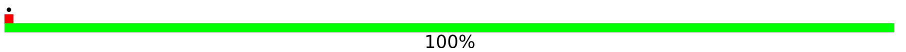
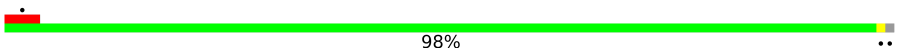
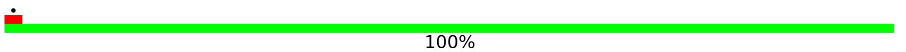
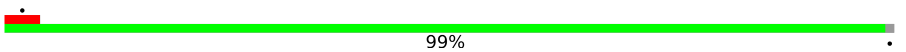
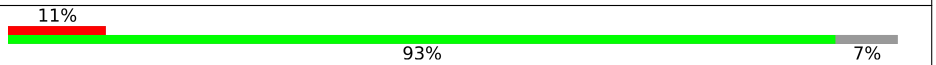
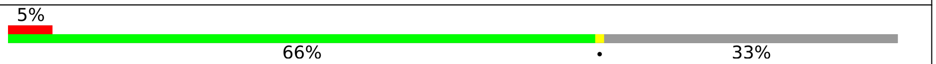
Mol	Chain	Length	Quality of chain
36	U1	156	 56% 44%
37	V1	116	 97%
38	W1	131	 87% 13%
39	q1	145	 100%
40	r1	113	 87% 12%
41	s1	104	 40% 60%
42	A1	115	 6% 99%
43	H1	318	 99%
44	J1	172	 19% 99%
45	K1	98	 99%
46	L1	607	 100%
47	M1	459	 100%
48	N1	345	 99%
49	O1	355	 90% 10%
50	X1	172	 99%
51	Y1	141	 99%
52	Z1	144	 98%
53	a1	70	 100%
54	b1	84	 98%
55	c1	76	 63% 37%
56	d1	120	 100%
57	e1	106	 99%
58	f1	57	 11% 93% 7%
59	g1	151	 5% 66% 33%
60	h1	189	 74% 26%

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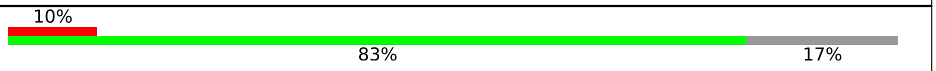
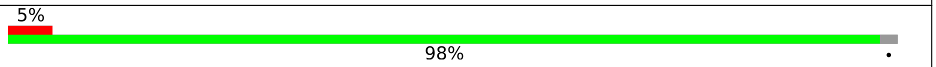
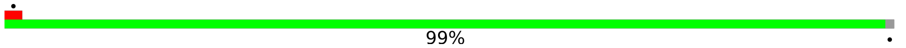
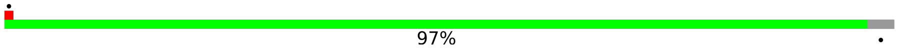
Mol	Chain	Length	Quality of chain
61	i1	128	
62	j1	105	
63	k1	104	
64	l1	186	
65	m1	129	
66	n1	179	
67	o1	137	
68	p1	176	

2 Entry composition ⓘ

There are 87 unique types of molecules in this entry. The entry contains 130520 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 3459	C 2163	N 610	O 669	S 17	0	0
1	L	445	Total 3460	C 2163	N 610	O 670	S 17	0	0

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total 1167	C 705	N 219	O 237	S 6	0	0
5	P	196	Total 1164	C 702	N 219	O 237	S 6	0	0
5	T	78	Total 554	C 352	N 103	O 97	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	98	Total 865	C 552	N 154	O 156	S 3	0	0
6	Q	102	Total 900	C 575	N 160	O 162	S 3	0	0

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	111	Total 807	C 520	N 138	O 144	S 5	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	260	Total 2118	C 1418	N 339	O 351	S 10	0	0
14	c	259	Total 2111	C 1414	N 338	O 349	S 10	0	0

- Molecule 15 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	r	104	842	538	141	161	2	0	0
16	e	103	833	533	140	158	2	0	0

- Molecule 17 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	s	94	721	449	126	138	8	0	0
17	f	93	717	447	125	137	8	0	0

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	v	71	567	369	102	93	3	0	0
20	i	72	572	372	103	94	3	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
21	x	49	Total C N O S 383 248 65 68 2	0	0
21	k	48	Total C N O S 378 245 64 67 2	0	0

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	y	47	Total C N O S 386 256 65 63 2	0	0
22	l	46	Total C N O S 380 253 64 61 2	0	0

- Molecule 23 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 24 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	6	157	Total C N O S 1258 802 227 215 14	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

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

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	2	214	1660	1056	279	314	11	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	1	430	3321	2092	596	611	22	0	0

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	3	690	5305	3326	921	1017	41	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	9	178	1431	898	245	276	12	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	7	96	758	470	141	144	3	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 36 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

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

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

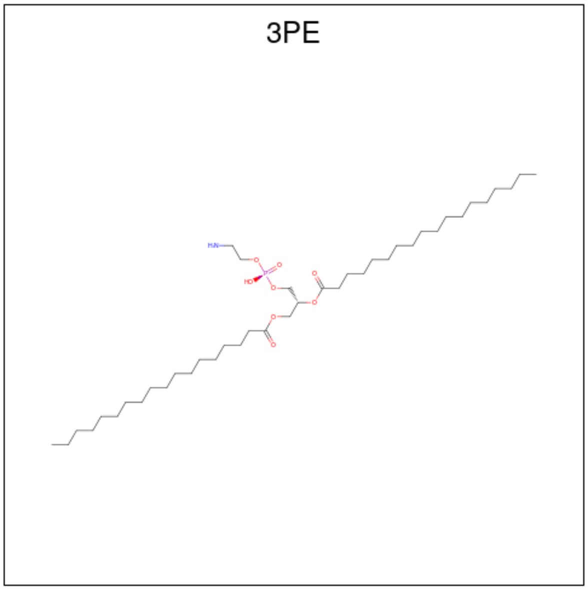
- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
69	A	1	Total C N O P 23 13 1 8 1	0
69	C	1	Total C N O P 35 25 1 8 1	0
69	C	1	Total C N O P 31 21 1 8 1	0
69	E	1	Total C N O P 32 22 1 8 1	0
69	E	1	Total C N O P 34 24 1 8 1	0
69	G	1	Total C N O P 51 41 1 8 1	0
69	L	1	Total C N O P 23 13 1 8 1	0
69	N	1	Total C N O P 37 27 1 8 1	0
69	O	1	Total C N O P 33 23 1 8 1	0
69	R	1	Total C N O P 30 20 1 8 1	0
69	n	1	Total C N O P 34 24 1 8 1	0
69	n	1	Total C N O P 28 18 1 8 1	0
69	n	1	Total C N O P 27 17 1 8 1	0
69	o	1	Total C N O P 29 19 1 8 1	0
69	p	1	Total C N O P 45 35 1 8 1	0
69	t	1	Total C N O P 25 15 1 8 1	0
69	v	1	Total C N O P 28 18 1 8 1	0
69	z	1	Total C N O P 26 16 1 8 1	0
69	6	1	Total C N O P 32 22 1 8 1	0
69	r1	1	Total C N O P 46 36 1 8 1	0
69	H1	1	Total C N O P 51 41 1 8 1	0
69	K1	1	Total C N O P 41 31 1 8 1	0

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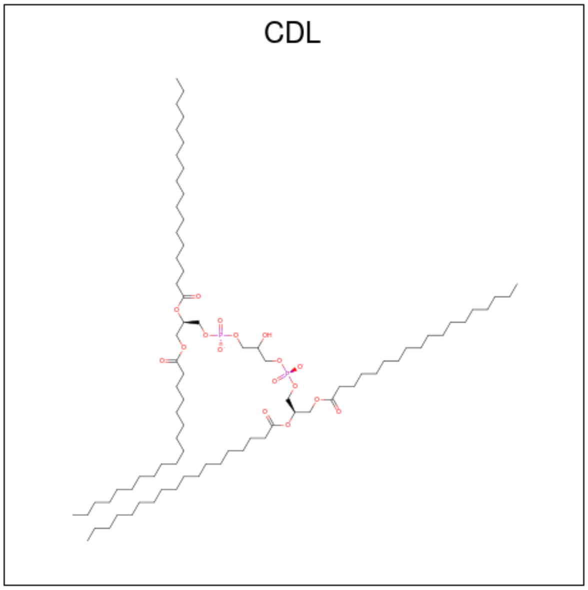
Mol	Chain	Residues	Atoms	AltConf
69	L1	1	Total C N O P 51 41 1 8 1	0
69	L1	1	Total C N O P 51 41 1 8 1	0
69	M1	1	Total C N O P 51 41 1 8 1	0
69	M1	1	Total C N O P 51 41 1 8 1	0
69	N1	1	Total C N O P 38 28 1 8 1	0
69	Y1	1	Total C N O P 28 18 1 8 1	0
69	Y1	1	Total C N O P 42 32 1 8 1	0
69	b1	1	Total C N O P 43 33 1 8 1	0
69	d1	1	Total C N O P 31 21 1 8 1	0
69	d1	1	Total C N O P 32 22 1 8 1	0
69	i1	1	Total C N O P 42 32 1 8 1	0
69	m1	1	Total C N O P 36 26 1 8 1	0
69	a	1	Total C N O P 28 18 1 8 1	0
69	a	1	Total C N O P 27 17 1 8 1	0
69	b	1	Total C N O P 29 19 1 8 1	0
69	c	1	Total C N O P 45 35 1 8 1	0
69	d	1	Total C N O P 34 24 1 8 1	0
69	g	1	Total C N O P 25 15 1 8 1	0
69	i	1	Total C N O P 28 18 1 8 1	0

- Molecule 70 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	AltConf
70	A	1	Total C O P 46 27 17 2	0
70	D	1	Total C O P 56 37 17 2	0
70	G	1	Total C O P 42 23 17 2	0
70	L	1	Total C O P 46 27 17 2	0
70	O	1	Total C O P 57 38 17 2	0
70	R	1	Total C O P 41 22 17 2	0
70	R	1	Total C O P 57 38 17 2	0
70	R	1	Total C O P 72 53 17 2	0
70	V	1	Total C O P 50 31 17 2	0
70	r1	1	Total C O P 57 38 17 2	0
70	H1	1	Total C O P 51 33 16 2	0
70	L1	1	Total C O P 78 59 17 2	0
70	L1	1	Total C O P 46 27 17 2	0
70	N1	1	Total C O P 90 71 17 2	0

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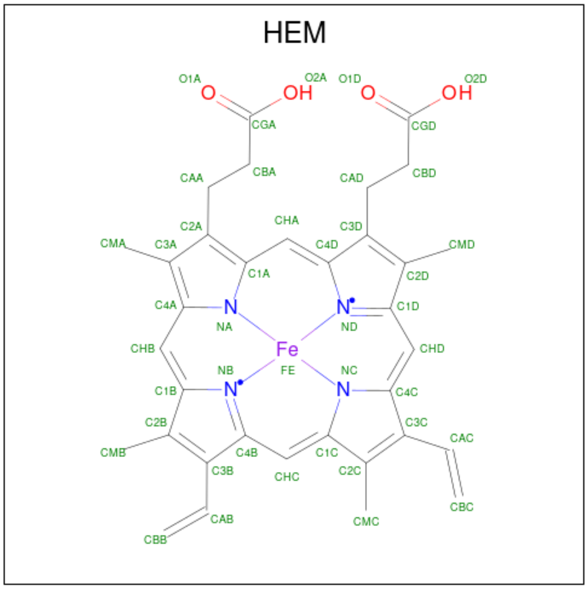
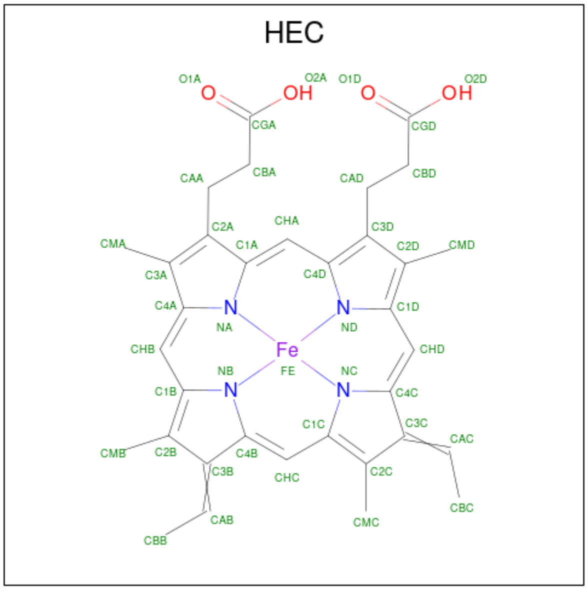
Mol	Chain	Residues	Atoms				AltConf
70	Y1	1	Total 94	C 75	O 17	P 2	0
70	d1	1	Total 67	C 48	O 17	P 2	0
70	h1	1	Total 70	C 51	O 17	P 2	0
70	g	1	Total 38	C 20	O 16	P 2	0

- Molecule 71 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



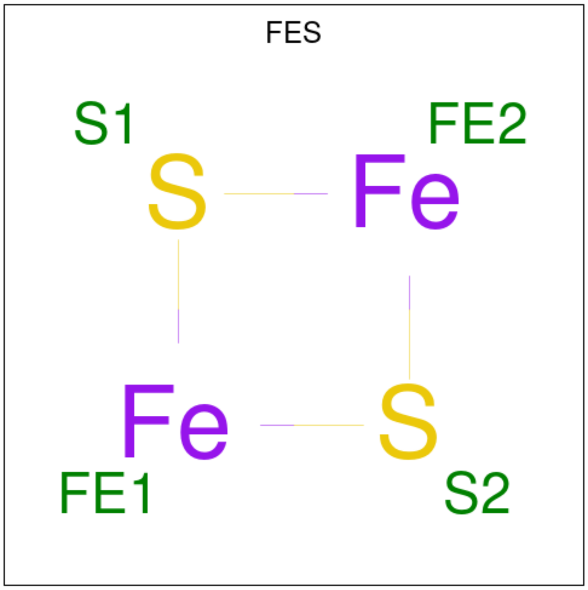
Mol	Chain	Residues	Atoms					AltConf
71	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
71	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
71	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
71	N	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 72 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 73 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

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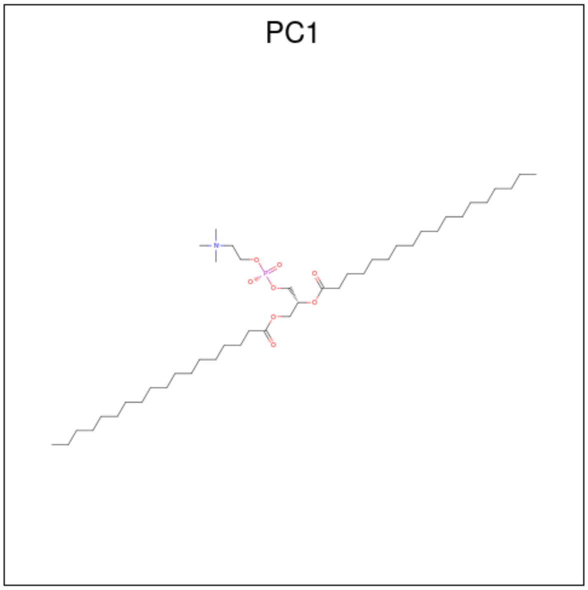
Mol	Chain	Residues	Atoms			AltConf
73	2	1	Total 4	Fe 2	S 2	0
73	3	1	Total 4	Fe 2	S 2	0

- Molecule 74 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
74	J	1	Total 35	C 25	N 1	O 8	P 1	0
74	K	1	Total 28	C 18	N 1	O 8	P 1	0
74	L	1	Total 24	C 14	N 1	O 8	P 1	0
74	V	1	Total 28	C 18	N 1	O 8	P 1	0
74	I	1	Total 50	C 40	N 1	O 8	P 1	0
74	p	1	Total 35	C 25	N 1	O 8	P 1	0
74	z	1	Total 28	C 18	N 1	O 8	P 1	0
74	6	1	Total 43	C 33	N 1	O 8	P 1	0
74	9	1	Total 54	C 44	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
74	9	1	Total 47	C 37	N 1	O 8	P 1	0
74	P1	1	Total 31	C 21	N 1	O 8	P 1	0
74	M1	1	Total 54	C 44	N 1	O 8	P 1	0
74	g	1	Total 50	C 40	N 1	O 8	P 1	0

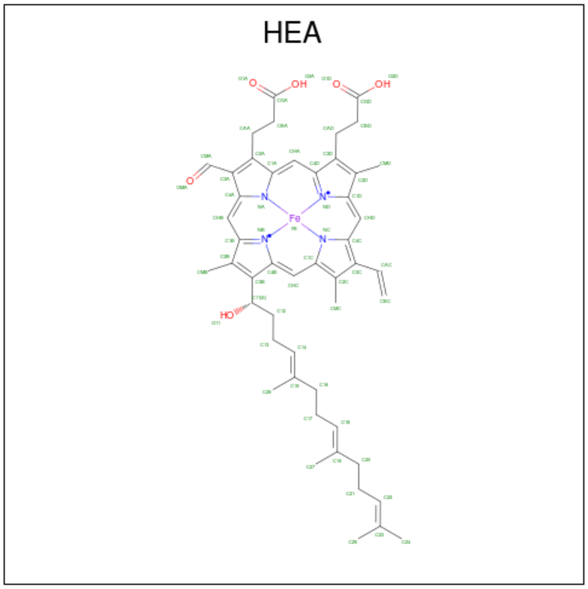
- Molecule 75 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
75	n	1	Total 1	Cu 1	0
75	a	1	Total 1	Cu 1	0

- Molecule 76 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
76	n	1	Total 1	Na 1	0
76	a	1	Total 1	Na 1	0

- Molecule 77 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

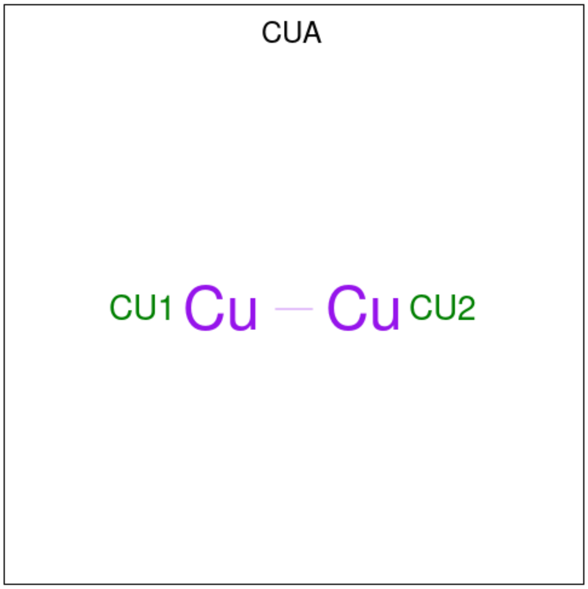


Mol	Chain	Residues	Atoms					AltConf
77	n	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	n	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

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

Mol	Chain	Residues	Atoms		AltConf
78	o	1	Total 1	Mg 1	0
78	O1	1	Total 1	Mg 1	0
78	a	1	Total 1	Mg 1	0

- Molecule 79 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).

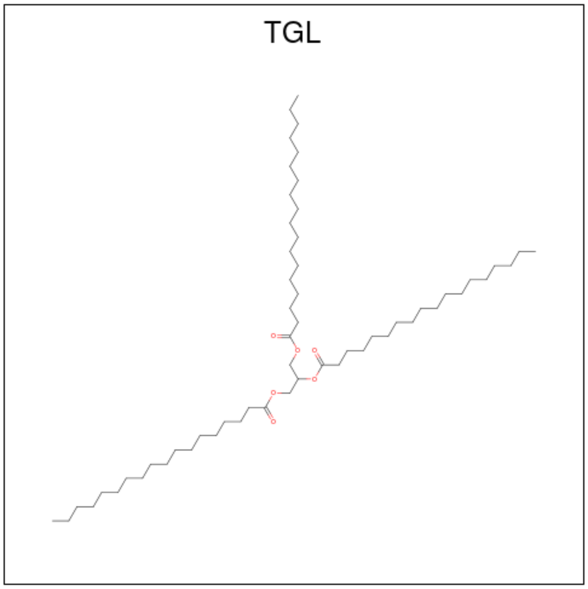


Mol	Chain	Residues	Atoms		AltConf
79	o	1	Total 2	Cu 2	0
79	b	1	Total 2	Cu 2	0

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

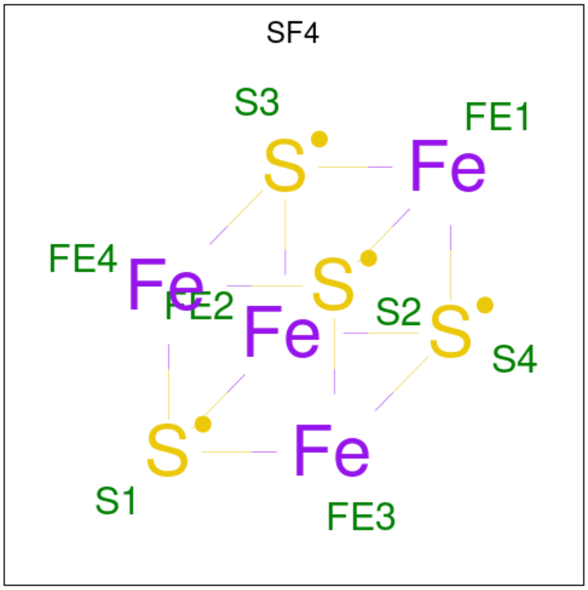
Mol	Chain	Residues	Atoms	AltConf
80	s	1	Total Zn 1 1	0
80	7	1	Total Zn 1 1	0
80	f	1	Total Zn 1 1	0

- Molecule 81 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



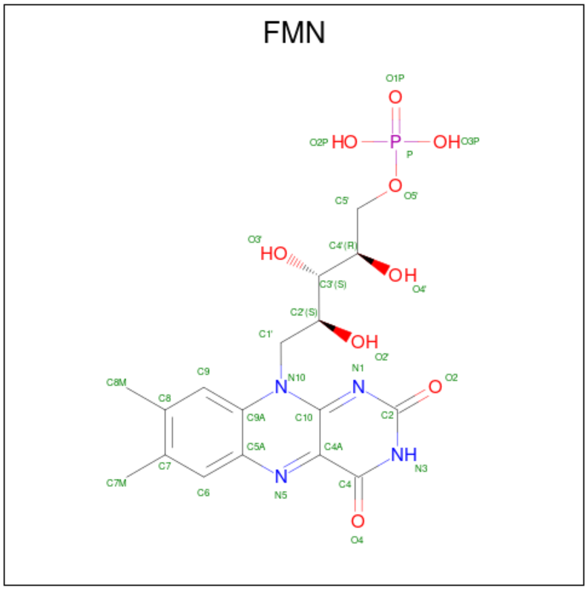
Mol	Chain	Residues	Atoms	AltConf
81	y	1	Total C O 37 31 6	0
81	l	1	Total C O 37 31 6	0

- Molecule 82 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
82	6	1	Total Fe S 8 4 4	0
82	1	1	Total Fe S 8 4 4	0
82	3	1	Total Fe S 8 4 4	0
82	3	1	Total Fe S 8 4 4	0
82	9	1	Total Fe S 8 4 4	0
82	9	1	Total Fe S 8 4 4	0

- Molecule 83 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

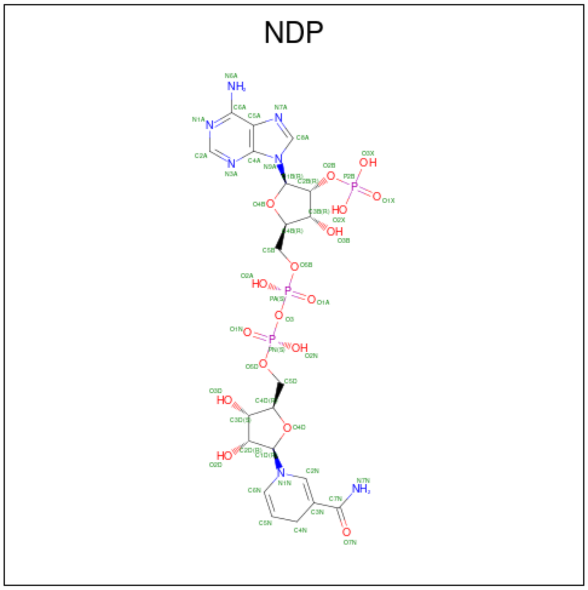


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
83	1	1	31	17	4	9	1	0

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

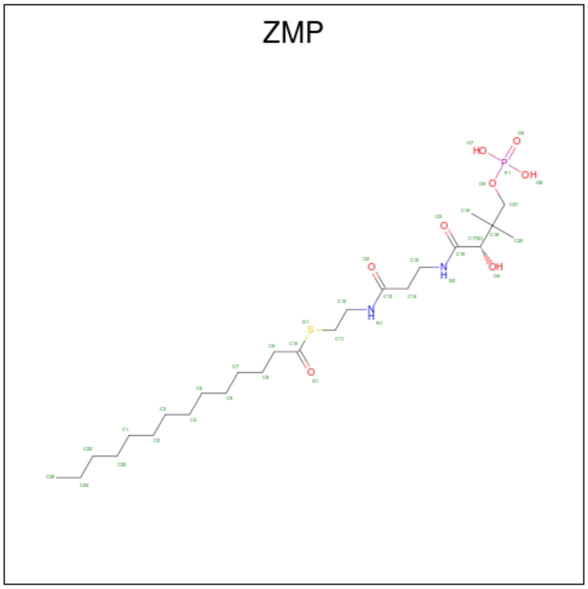
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
84	3	1	1	1	0

- Molecule 85 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



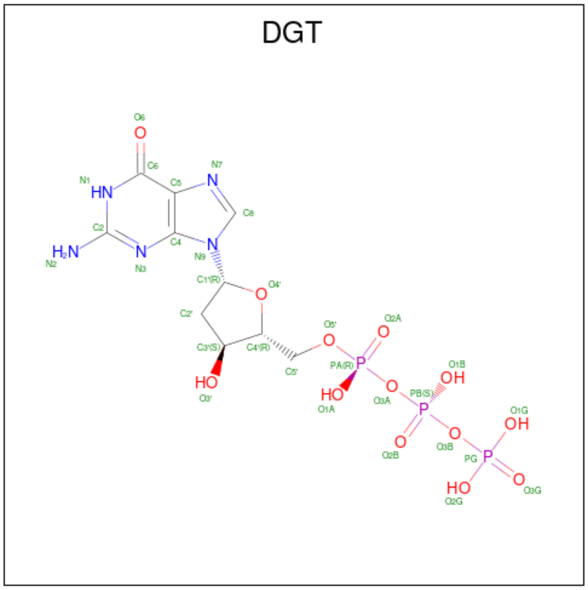
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	P1	1	48	21	7	17	3	0

- Molecule 86 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
			Total	C	N	O	P	S	
86	W1	1	34	23	2	7	1	1	0
86	n1	1	32	21	2	7	1	1	0

- Molecule 87 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

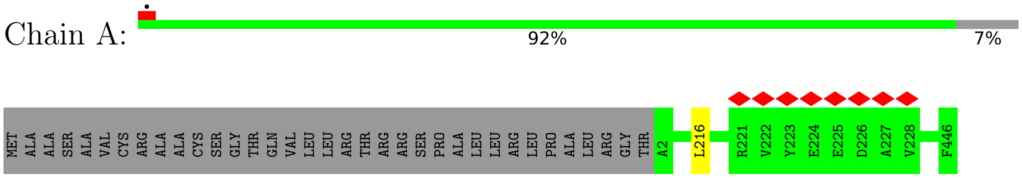


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	O1	1	31	10	5	13	3	0

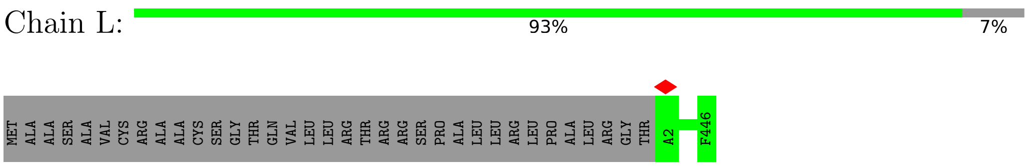
3 Residue-property plots ⓘ

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.

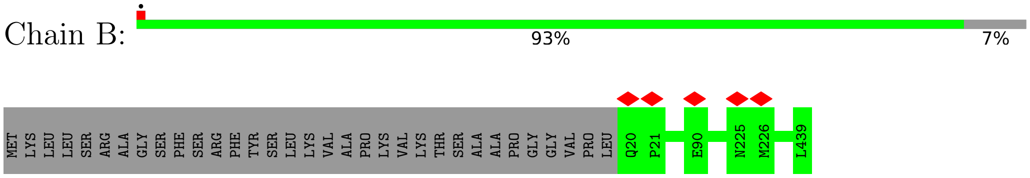
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



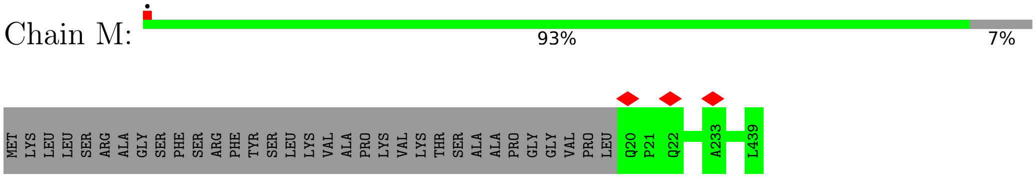
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



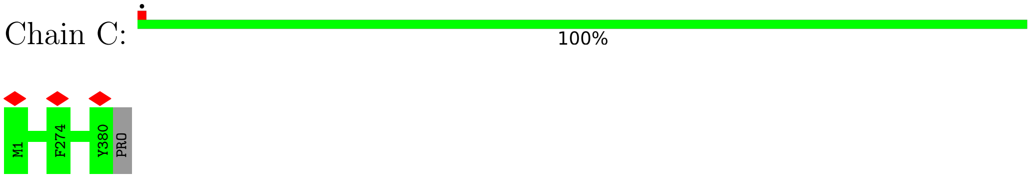
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



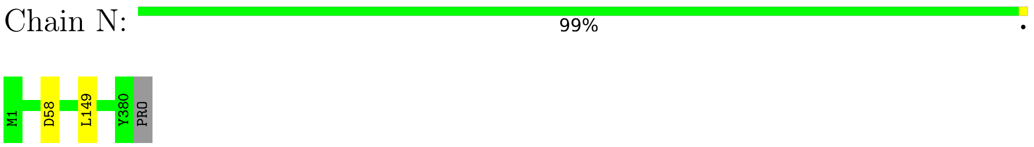
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



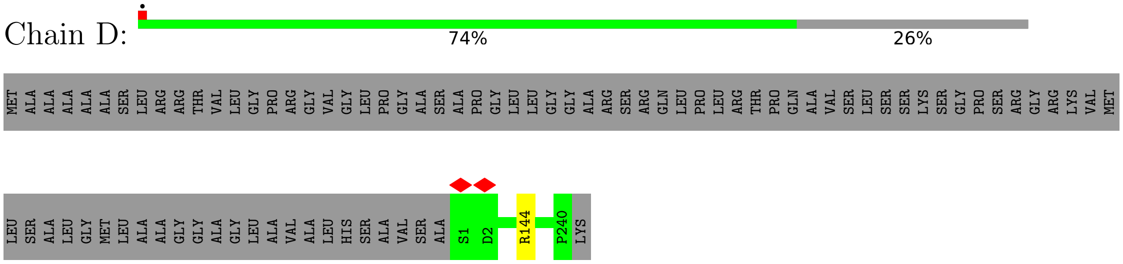
- Molecule 3: Cytochrome b



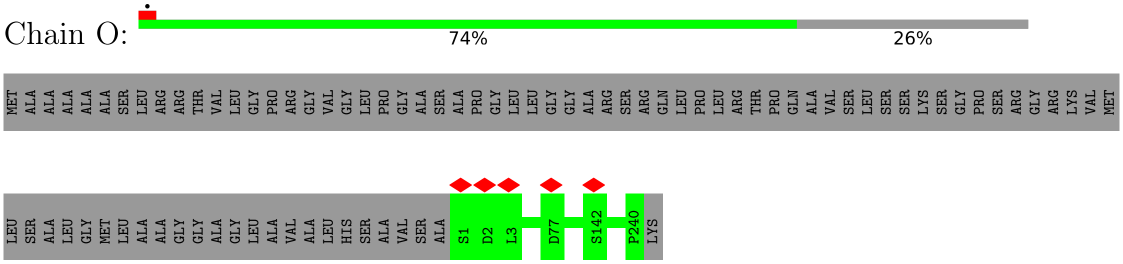
- Molecule 3: Cytochrome b



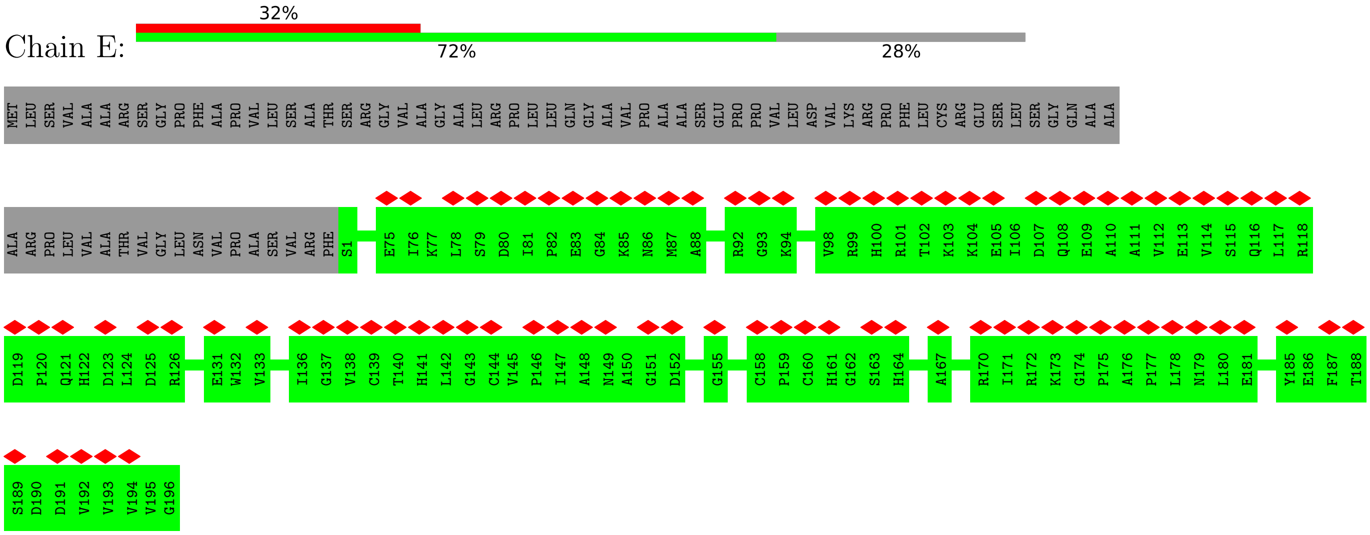
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



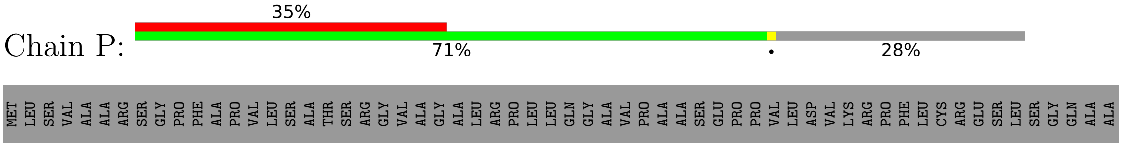
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

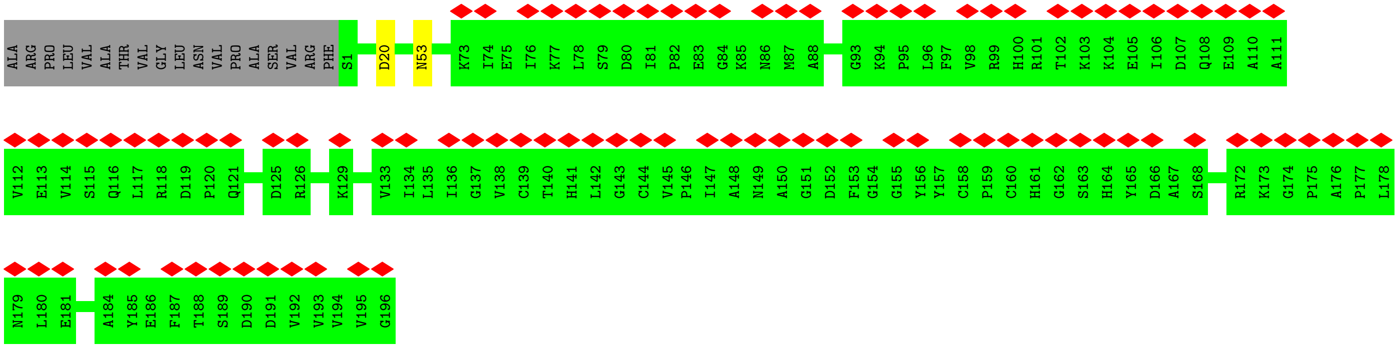


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



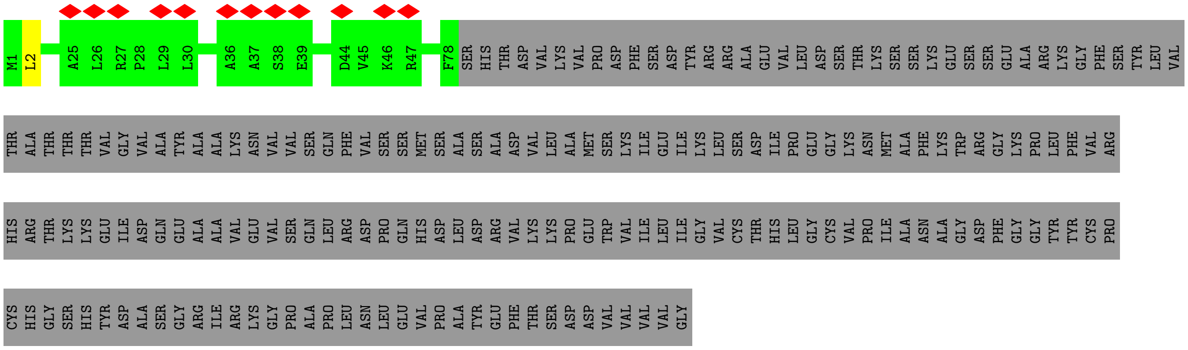
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial





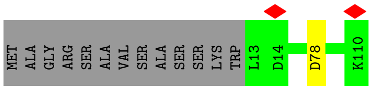
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain T:



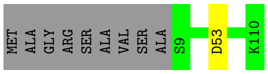
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



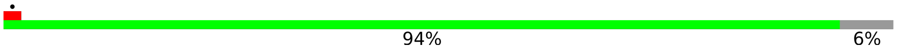
- Molecule 6: Cytochrome b-c1 complex subunit 7

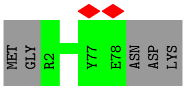
Chain Q:



- Molecule 7: Cytochrome b-c1 complex subunit 8

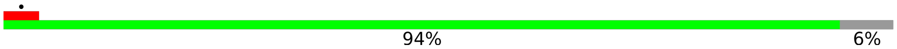
Chain G:

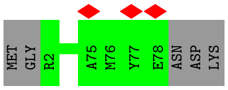




- Molecule 7: Cytochrome b-c1 complex subunit 8

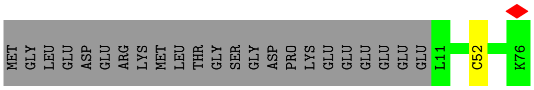
Chain R:





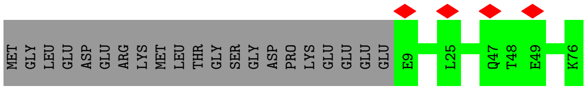
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



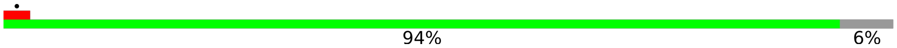
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

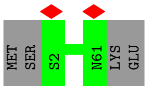
Chain S:



- Molecule 9: Cytochrome b-c1 complex subunit 9

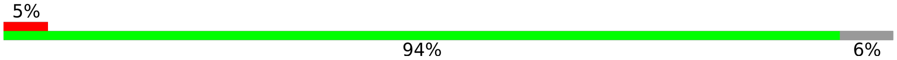
Chain J:

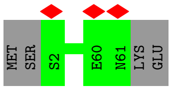




- Molecule 9: Cytochrome b-c1 complex subunit 9

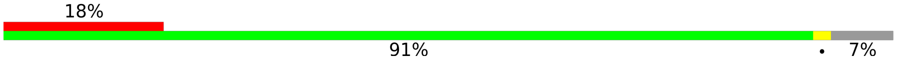
Chain U:

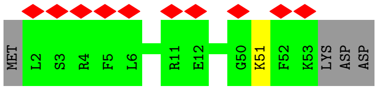




- Molecule 10: Cytochrome b-c1 complex subunit 10

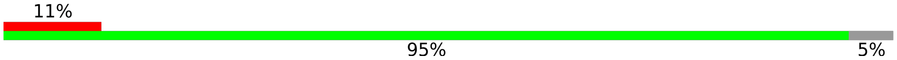
Chain K:

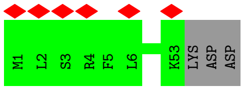




- Molecule 10: Cytochrome b-c1 complex subunit 10

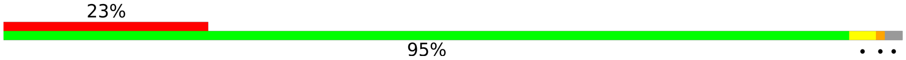
Chain V:

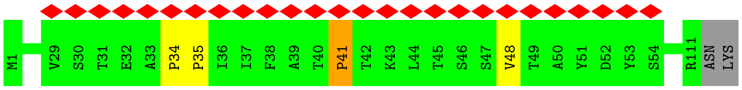




- Molecule 11: Cox7a2l protein

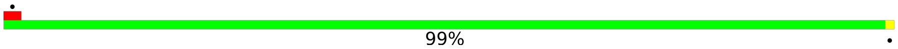
Chain I:

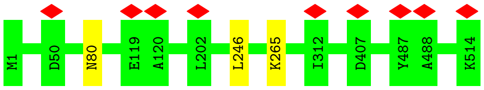




- Molecule 12: Cytochrome c oxidase subunit 1

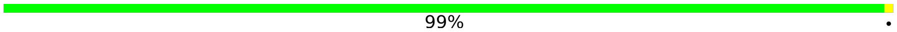
Chain n:

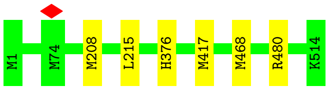




- Molecule 12: Cytochrome c oxidase subunit 1

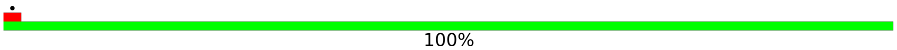
Chain a:

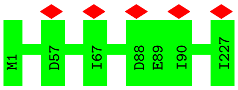




- Molecule 13: Cytochrome c oxidase subunit 2

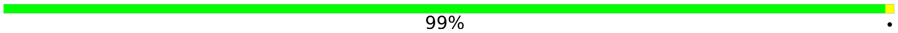
Chain o:

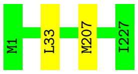




- Molecule 13: Cytochrome c oxidase subunit 2

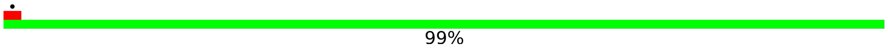
Chain b:

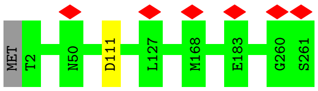




- Molecule 14: Cytochrome c oxidase subunit 3

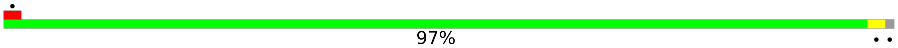
Chain p:

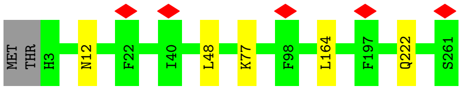




- Molecule 14: Cytochrome c oxidase subunit 3

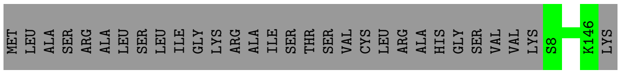
Chain c:





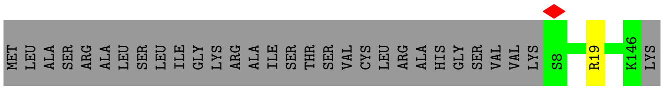
- Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain q:



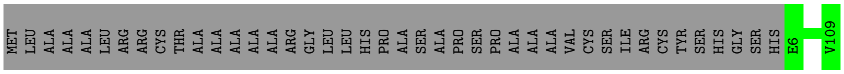
- Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain d:



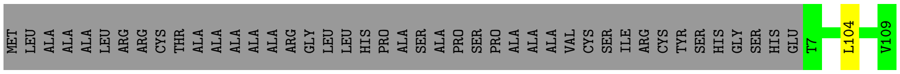
- Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial

Chain r:



- Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:



- Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial

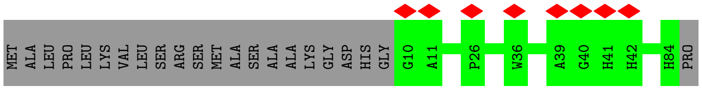
Chain s:

- Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial

Chain f:

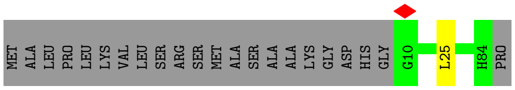
- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain t:



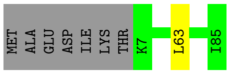
- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain g:



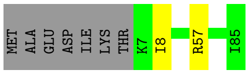
- Molecule 19: Cytochrome c oxidase subunit 6B1

Chain u:



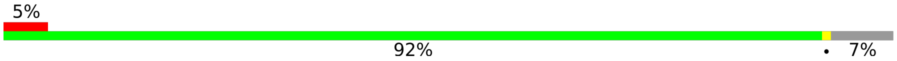
- Molecule 19: Cytochrome c oxidase subunit 6B1

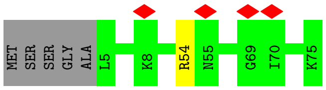
Chain h:



- Molecule 20: Cytochrome c oxidase subunit 6C

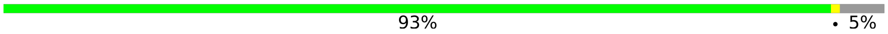
Chain v:

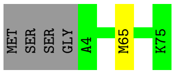




- Molecule 20: Cytochrome c oxidase subunit 6C

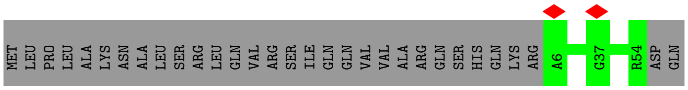
Chain i:





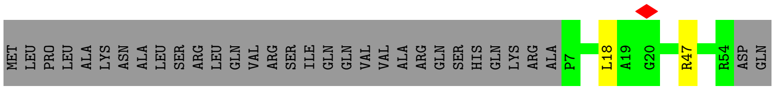
- Molecule 21: Cytochrome c oxidase subunit 7B, mitochondrial

Chain x:



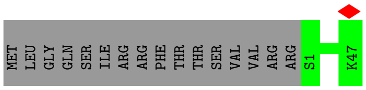
- Molecule 21: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k:



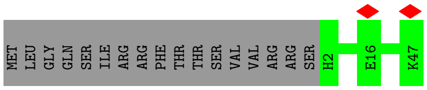
- Molecule 22: Cytochrome c oxidase subunit 7C, mitochondrial

Chain y:



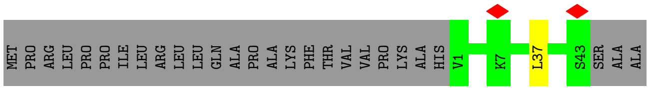
- Molecule 22: Cytochrome c oxidase subunit 7C, mitochondrial

Chain l:



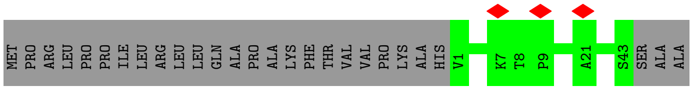
- Molecule 23: Cytochrome c oxidase subunit 8B, mitochondrial

Chain z:



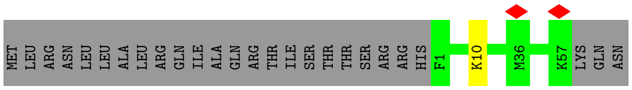
- Molecule 23: Cytochrome c oxidase subunit 8B, mitochondrial

Chain m:



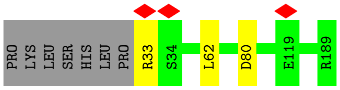
- Molecule 24: Cytochrome c oxidase subunit 7A2, mitochondrial

Chain w:



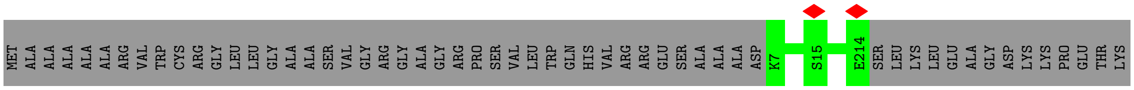
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:



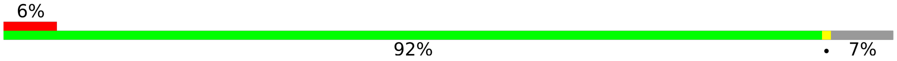
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

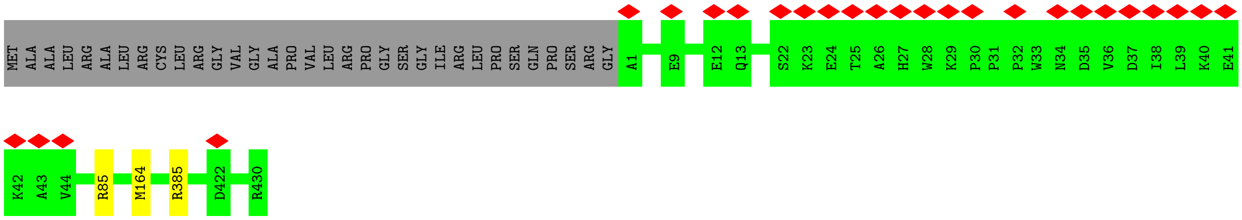
Chain C1:



- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

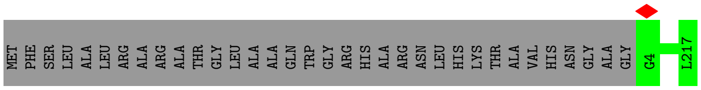
Chain D1:





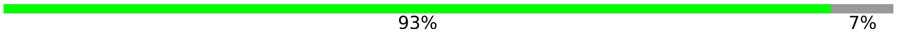
- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

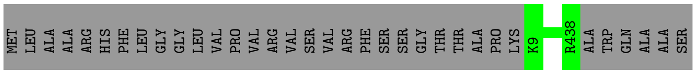
Chain 2:



- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

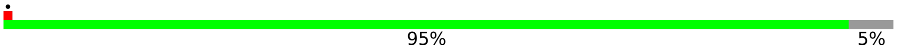
Chain 1:

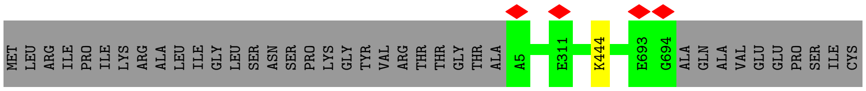




- Molecule 30: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

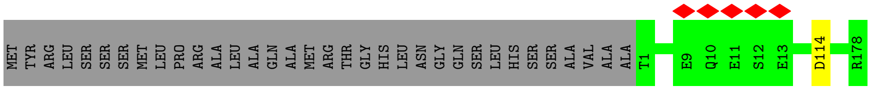
Chain 3:





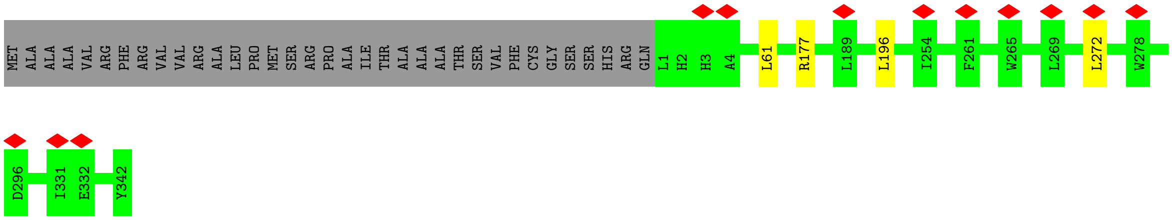
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:



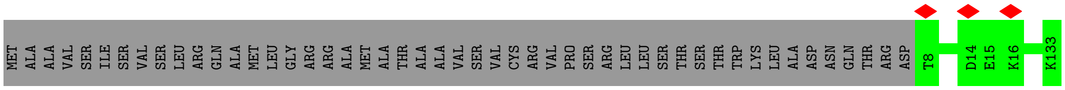
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P1:



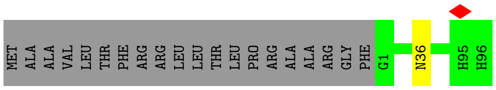
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q1:



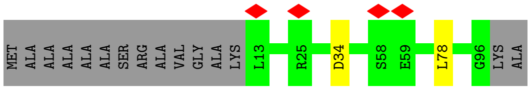
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7:



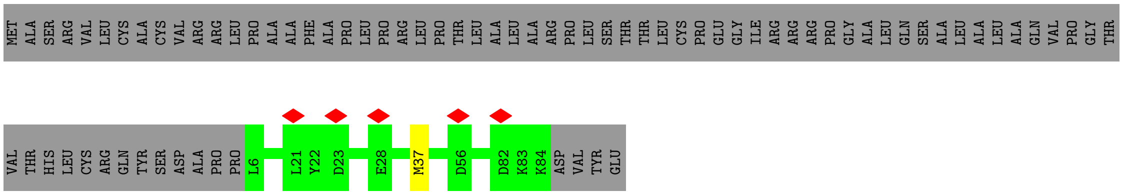
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S1:



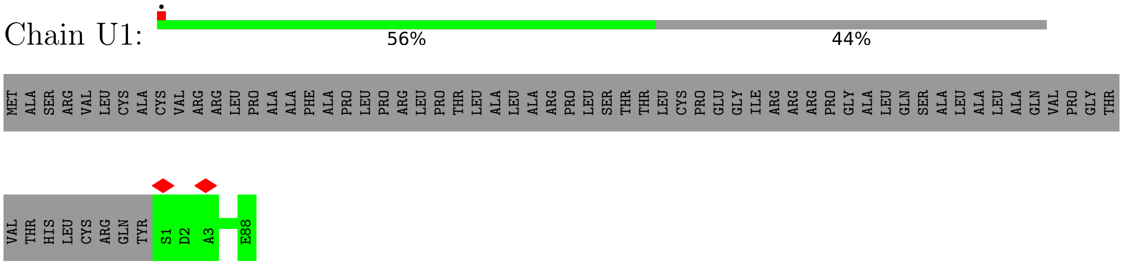
- Molecule 36: Acyl carrier protein, mitochondrial

Chain T1:



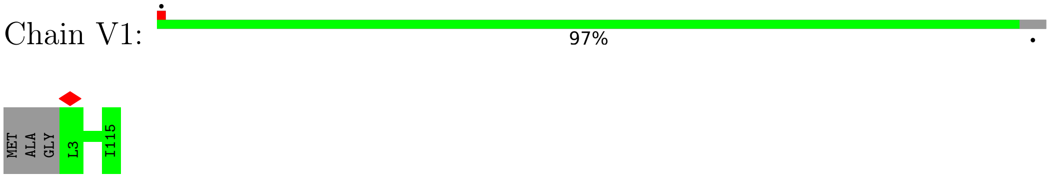
- Molecule 36: Acyl carrier protein, mitochondrial

Chain U1:



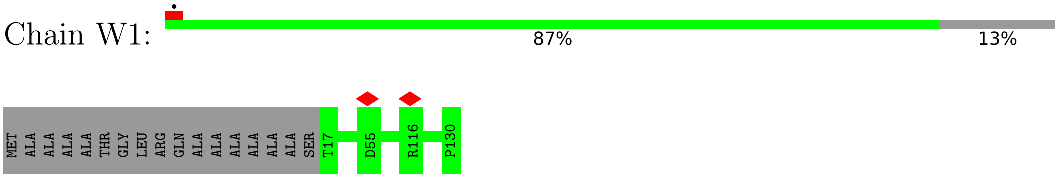
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1:



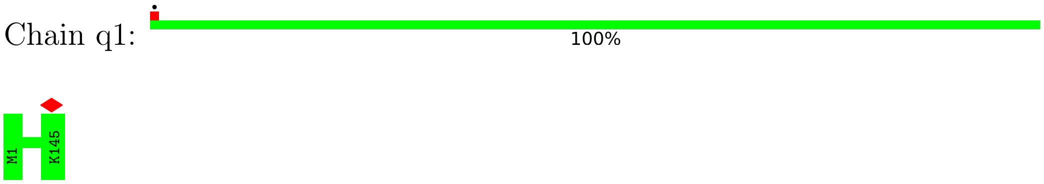
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1:



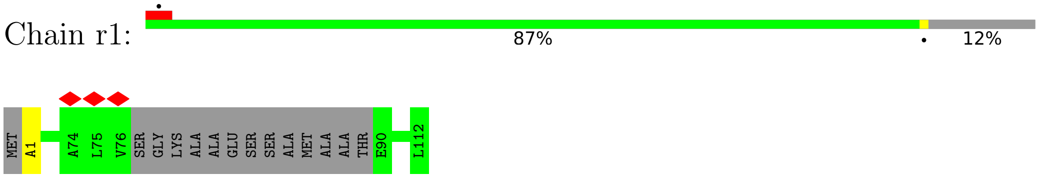
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q1:



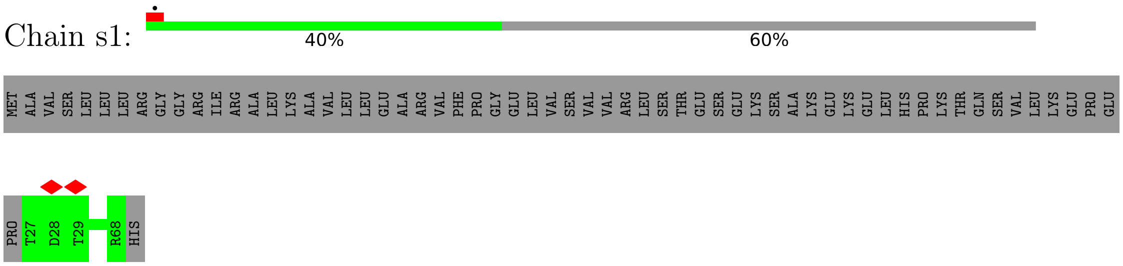
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1:

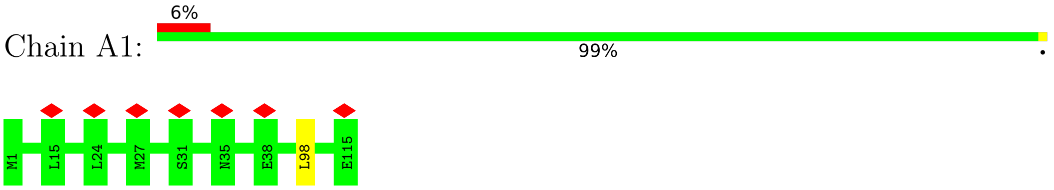


- Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

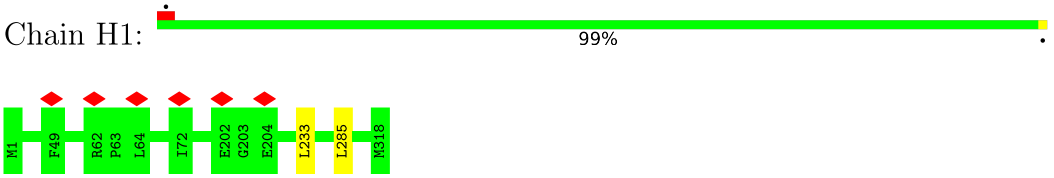
Chain s1:



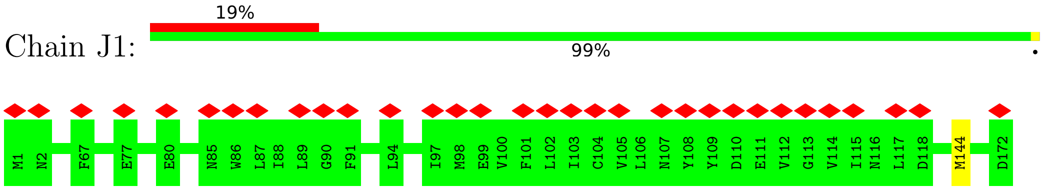
- Molecule 42: NADH-ubiquinone oxidoreductase chain 3



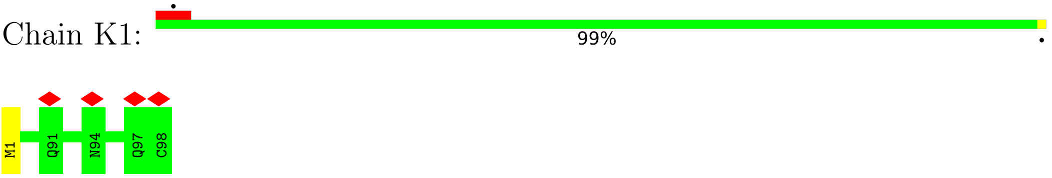
- Molecule 43: NADH-ubiquinone oxidoreductase chain 1



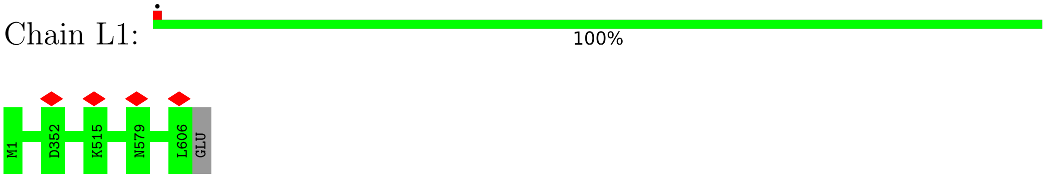
- Molecule 44: NADH-ubiquinone oxidoreductase chain 6



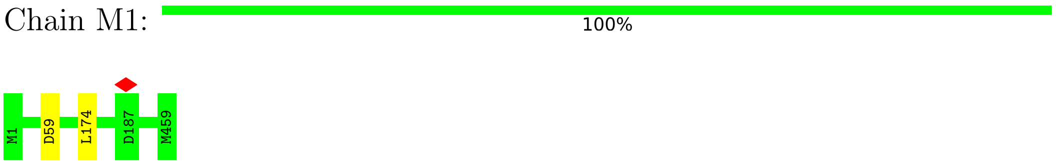
- Molecule 45: NADH-ubiquinone oxidoreductase chain 4L



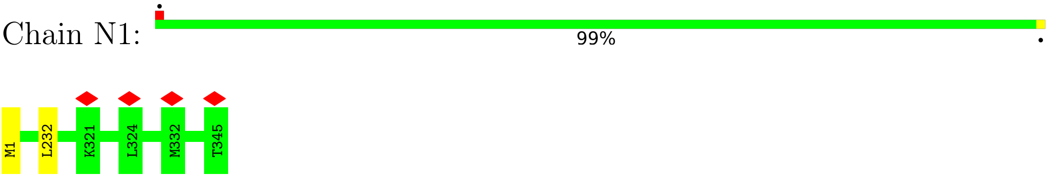
- Molecule 46: NADH-ubiquinone oxidoreductase chain 5



- Molecule 47: NADH-ubiquinone oxidoreductase chain 4

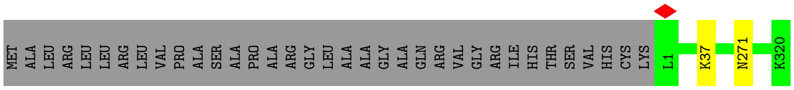


- Molecule 48: NADH-ubiquinone oxidoreductase chain 2



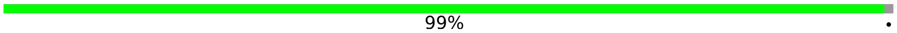
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

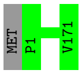
Chain O1:



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

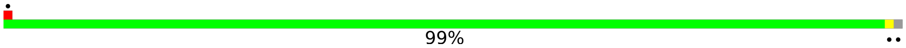
Chain X1:

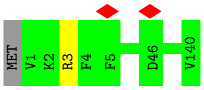




- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

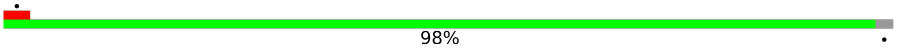
Chain Y1:

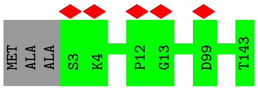




- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

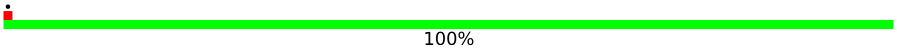
Chain Z1:

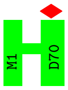




- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

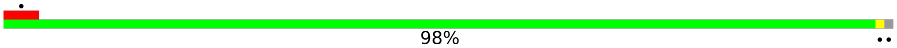
Chain a1:

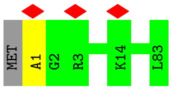




- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

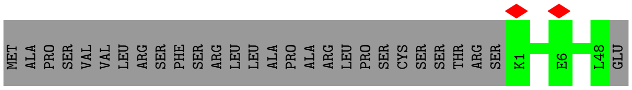
Chain b1:





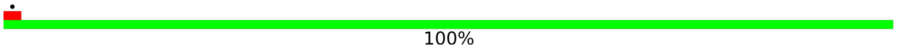
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

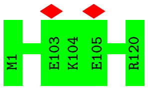
Chain c1:



- Molecule 56: NADH dehydrogenase [ubiquinone] 1 subunit C2

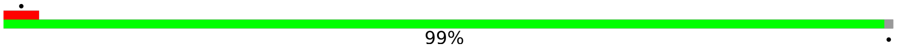
Chain d1:

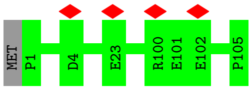




- Molecule 57: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

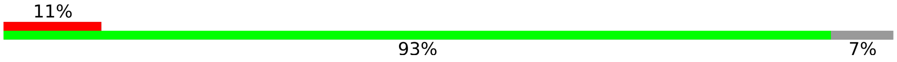
Chain e1:

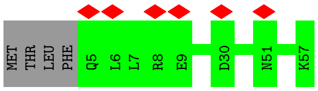




- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

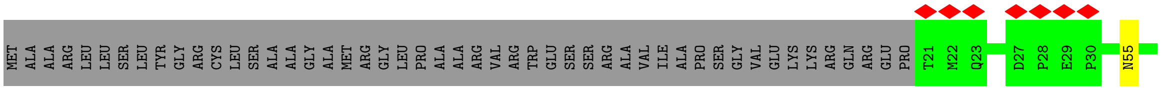
Chain f1:





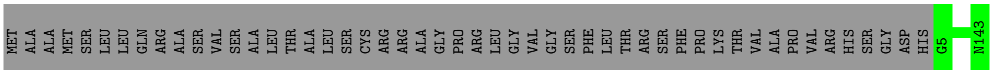
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g1:



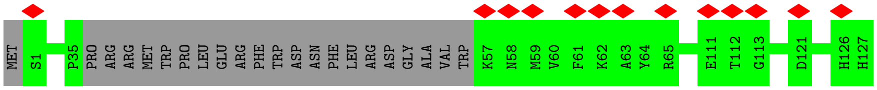
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h1:



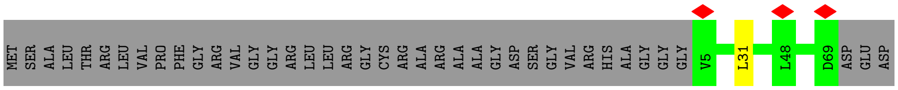
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i1:



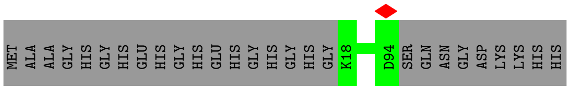
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j1:



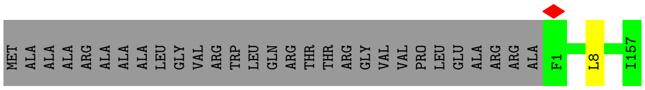
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k1:



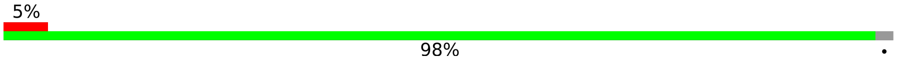
- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

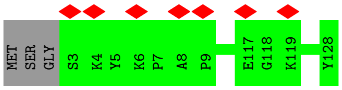
Chain l1:



- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

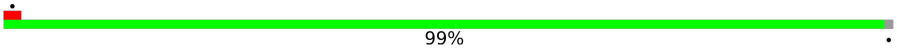
Chain m1:

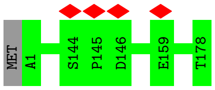




- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

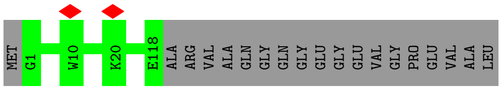
Chain n1:





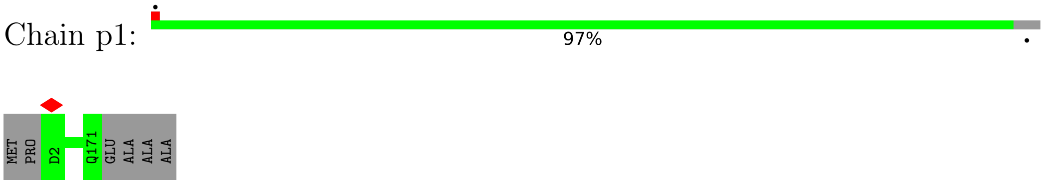
- Molecule 67: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o1:



- Molecule 68: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p1:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51488	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 $(e^{-}/\text{Å}^2)$	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	0.144	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	299.97998, 218.35999, 262.87997	wwPDB
Map dimensions	283, 206, 248	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, NA, CDL, 3PE, HEC, NDP, PC1, FES, HEM, SF4, CU, FMN, AYA, K, 2MR, HEA, FME, TGL, MG, DGT, ZN, CUA, 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	0.27	0/3529	0.56	1/4793 (0.0%)
1	L	0.28	0/3530	0.53	0/4793
2	B	0.27	0/3205	0.50	0/4332
2	M	0.27	0/3205	0.50	0/4332
3	C	0.29	0/3147	0.52	0/4297
3	N	0.30	0/3147	0.55	3/4297 (0.1%)
4	D	0.27	0/1968	0.53	0/2674
4	O	0.28	0/1968	0.53	0/2674
5	E	0.27	0/1176	0.49	0/1609
5	P	0.27	0/1173	0.52	1/1605 (0.1%)
5	T	0.28	0/565	0.66	1/772 (0.1%)
6	F	0.28	0/885	0.65	1/1184 (0.1%)
6	Q	0.29	0/922	0.60	1/1234 (0.1%)
7	G	0.31	0/673	0.63	0/909
7	R	0.32	0/673	0.63	0/909
8	H	0.35	0/552	0.76	1/739 (0.1%)
8	S	0.34	0/570	0.70	0/763
9	J	0.28	0/509	0.54	0/687
9	U	0.31	0/509	0.58	0/687
10	K	0.29	0/446	0.62	0/609
10	V	0.27	0/454	0.64	0/619
11	I	0.28	0/825	0.70	3/1119 (0.3%)
12	a	0.33	0/4162	0.68	5/5686 (0.1%)
12	n	0.33	0/4162	0.59	1/5686 (0.0%)
13	b	0.31	0/1863	0.73	2/2542 (0.1%)
13	o	0.30	0/1863	0.64	0/2542
14	c	0.29	0/2195	0.59	2/3000 (0.1%)
14	p	0.30	0/2202	0.58	1/3010 (0.0%)
15	d	0.29	0/1190	0.68	0/1609
15	q	0.31	0/1190	0.64	0/1609
16	e	0.30	0/851	0.70	1/1155 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	r	0.28	0/860	0.65	0/1167
17	f	0.30	0/734	0.64	0/996
17	s	0.30	0/738	0.60	0/1001
18	g	0.27	0/632	0.65	1/866 (0.1%)
18	t	0.28	0/632	0.57	0/866
19	h	0.32	0/674	0.74	0/910
19	u	0.34	0/674	0.69	1/910 (0.1%)
20	i	0.38	0/584	0.85	1/778 (0.1%)
20	v	0.34	0/579	0.71	0/771
21	k	0.26	0/391	0.54	1/533 (0.2%)
21	x	0.32	0/396	0.61	0/541
22	l	0.30	0/393	0.62	0/527
22	y	0.35	0/399	0.61	0/535
23	m	0.32	0/318	0.71	0/433
23	z	0.31	0/318	0.69	1/433 (0.2%)
24	w	0.28	0/444	0.55	0/598
25	6	0.34	0/1289	0.69	2/1744 (0.1%)
26	C1	0.28	0/1780	0.56	0/2424
27	D1	0.31	0/3540	0.56	0/4795
28	2	0.29	0/1700	0.51	0/2316
29	1	0.29	0/3396	0.55	0/4586
30	3	0.28	0/5392	0.54	0/7305
31	9	0.35	0/1461	0.58	1/1974 (0.1%)
32	P1	0.28	0/2823	0.60	3/3828 (0.1%)
33	Q1	0.27	0/1045	0.52	0/1411
34	7	0.28	0/773	0.52	0/1041
35	S1	0.30	0/682	0.68	2/920 (0.2%)
36	T1	0.27	0/646	0.59	0/869
36	U1	0.32	0/718	0.56	0/970
37	V1	0.25	0/945	0.41	0/1281
38	W1	0.28	0/993	0.57	0/1335
39	q1	0.28	0/1251	0.53	0/1702
40	r1	0.27	0/806	0.55	0/1090
41	s1	0.27	0/360	0.67	0/489
42	A1	0.30	0/948	0.60	1/1295 (0.1%)
43	H1	0.35	0/2607	0.63	2/3564 (0.1%)
44	J1	0.32	0/1330	0.59	1/1810 (0.1%)
45	K1	0.31	0/738	0.57	0/1002
46	L1	0.31	0/4913	0.56	0/6686
47	M1	0.30	0/3709	0.60	2/5052 (0.0%)
48	N1	0.29	0/2755	0.57	1/3751 (0.0%)
49	O1	0.28	0/2674	0.51	0/3626
50	X1	0.27	0/1434	0.55	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
51	Y1	0.28	0/1061	0.56	0/1439
52	Z1	0.27	0/1198	0.56	0/1616
53	a1	0.32	0/585	0.61	0/788
54	b1	0.28	0/666	0.55	0/914
55	c1	0.27	0/409	0.53	0/555
56	d1	0.29	0/1028	0.55	0/1387
57	e1	0.29	0/900	0.54	0/1199
58	f1	0.28	0/468	0.65	0/630
59	g1	0.28	0/878	0.51	0/1196
60	h1	0.29	0/1201	0.55	0/1626
61	i1	0.27	0/917	0.54	0/1243
62	j1	0.30	0/587	0.64	1/804 (0.1%)
63	k1	0.30	0/646	0.60	0/873
64	l1	0.29	0/1379	0.55	1/1882 (0.1%)
65	m1	0.33	0/1079	0.64	0/1463
66	n1	0.28	0/1596	0.53	0/2162
67	o1	0.29	0/1039	0.59	0/1394
68	p1	0.28	0/1471	0.52	0/1988
All	All	0.30	0/129891	0.58	46/176303 (0.0%)

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	468	MET	CG-SD-CE	9.76	115.81	100.20
32	P1	196	LEU	CA-CB-CG	7.44	132.41	115.30
25	6	80	ASP	CB-CG-OD1	6.95	124.55	118.30
6	Q	53	ASP	CB-CG-OD1	6.53	124.18	118.30
32	P1	272	LEU	CA-CB-CG	6.49	130.22	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
1	L	443/480 (92%)	429 (97%)	14 (3%)	0	100	100
2	B	418/453 (92%)	409 (98%)	9 (2%)	0	100	100
2	M	418/453 (92%)	403 (96%)	15 (4%)	0	100	100
3	C	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
3	N	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
4	D	238/325 (73%)	233 (98%)	5 (2%)	0	100	100
4	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
5	E	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
5	P	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
5	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
6	F	96/111 (86%)	96 (100%)	0	0	100	100
6	Q	100/111 (90%)	100 (100%)	0	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%)	64 (100%)	0	0	100	100
8	S	66/89 (74%)	63 (96%)	3 (4%)	0	100	100
9	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
9	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
10	K	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
10	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
11	I	109/113 (96%)	100 (92%)	7 (6%)	2 (2%)	8	43
12	a	512/514 (100%)	491 (96%)	20 (4%)	1 (0%)	47	79
12	n	512/514 (100%)	489 (96%)	23 (4%)	0	100	100
13	b	225/227 (99%)	212 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
14	c	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
14	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
15	d	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
15	q	137/169 (81%)	127 (93%)	10 (7%)	0	100	100
16	e	101/146 (69%)	100 (99%)	1 (1%)	0	100	100
16	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
17	f	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
17	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
18	g	73/97 (75%)	66 (90%)	7 (10%)	0	100	100
18	t	73/97 (75%)	68 (93%)	5 (7%)	0	100	100
19	h	77/86 (90%)	73 (95%)	3 (4%)	1 (1%)	12	50
19	u	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
20	i	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
20	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
21	k	46/80 (58%)	44 (96%)	2 (4%)	0	100	100
21	x	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
22	l	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
22	y	45/63 (71%)	45 (100%)	0	0	100	100
23	m	41/70 (59%)	37 (90%)	4 (10%)	0	100	100
23	z	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
24	w	55/83 (66%)	55 (100%)	0	0	100	100
25	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
26	C1	206/263 (78%)	200 (97%)	6 (3%)	0	100	100
27	D1	427/463 (92%)	412 (96%)	15 (4%)	0	100	100
28	2	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
29	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
30	3	688/727 (95%)	666 (97%)	22 (3%)	0	100	100
31	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
32	P1	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
33	Q1	124/175 (71%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
35	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
36	T1	77/156 (49%)	76 (99%)	1 (1%)	0	100	100
36	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
37	V1	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
38	W1	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
39	q1	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
40	r1	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
41	s1	40/104 (38%)	38 (95%)	2 (5%)	0	100	100
42	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
43	H1	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
44	J1	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
45	K1	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
46	L1	604/607 (100%)	567 (94%)	37 (6%)	0	100	100
47	M1	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
48	N1	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
49	O1	318/355 (90%)	300 (94%)	18 (6%)	0	100	100
50	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
51	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
52	Z1	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
53	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
54	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
55	c1	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
56	d1	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
57	e1	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
58	f1	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
59	g1	99/151 (66%)	95 (96%)	4 (4%)	0	100	100
60	h1	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
61	i1	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
62	j1	63/105 (60%)	61 (97%)	2 (3%)	0	100	100
63	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	l1	155/186 (83%)	152 (98%)	3 (2%)	0	100	100
65	m1	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
66	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
67	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
68	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	15768/18146 (87%)	15159 (96%)	605 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	h	8	ILE
12	a	376	HIS
11	I	48	VAL
11	I	41	PRO

5.3.2 Protein sidechains ⓘ

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%)	372 (100%)	0	100	100
2	B	330/356 (93%)	330 (100%)	0	100	100
2	M	330/356 (93%)	330 (100%)	0	100	100
3	C	332/333 (100%)	332 (100%)	0	100	100
3	N	332/333 (100%)	332 (100%)	0	100	100
4	D	205/260 (79%)	204 (100%)	1 (0%)	88	95
4	O	205/260 (79%)	205 (100%)	0	100	100
5	E	69/224 (31%)	69 (100%)	0	100	100
5	P	68/224 (30%)	67 (98%)	1 (2%)	65	84
5	T	58/224 (26%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	90/99 (91%)	90 (100%)	0	100	100
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%)	51 (100%)	0	100	100
10	K	42/46 (91%)	41 (98%)	1 (2%)	49	75
10	V	43/46 (94%)	43 (100%)	0	100	100
11	I	73/95 (77%)	73 (100%)	0	100	100
12	a	425/425 (100%)	424 (100%)	1 (0%)	93	98
12	n	425/425 (100%)	423 (100%)	2 (0%)	88	95
13	b	210/210 (100%)	210 (100%)	0	100	100
13	o	210/210 (100%)	210 (100%)	0	100	100
14	c	225/227 (99%)	222 (99%)	3 (1%)	69	86
14	p	226/227 (100%)	226 (100%)	0	100	100
15	d	122/146 (84%)	121 (99%)	1 (1%)	81	91
15	q	122/146 (84%)	122 (100%)	0	100	100
16	e	90/118 (76%)	90 (100%)	0	100	100
16	r	91/118 (77%)	91 (100%)	0	100	100
17	f	80/101 (79%)	80 (100%)	0	100	100
17	s	80/101 (79%)	80 (100%)	0	100	100
18	g	62/78 (80%)	62 (100%)	0	100	100
18	t	62/78 (80%)	62 (100%)	0	100	100
19	h	70/76 (92%)	69 (99%)	1 (1%)	67	85
19	u	70/76 (92%)	70 (100%)	0	100	100
20	i	54/57 (95%)	54 (100%)	0	100	100
20	v	54/57 (95%)	53 (98%)	1 (2%)	57	80
21	k	39/67 (58%)	38 (97%)	1 (3%)	46	74
21	x	39/67 (58%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	l	39/55 (71%)	39 (100%)	0	100	100
22	y	40/55 (73%)	40 (100%)	0	100	100
23	m	33/55 (60%)	33 (100%)	0	100	100
23	z	33/55 (60%)	33 (100%)	0	100	100
24	w	43/67 (64%)	42 (98%)	1 (2%)	50	76
25	6	133/185 (72%)	132 (99%)	1 (1%)	81	91
26	C1	190/227 (84%)	190 (100%)	0	100	100
27	D1	370/394 (94%)	368 (100%)	2 (0%)	88	95
28	2	184/206 (89%)	184 (100%)	0	100	100
29	1	345/370 (93%)	345 (100%)	0	100	100
30	3	580/610 (95%)	579 (100%)	1 (0%)	93	98
31	9	152/178 (85%)	152 (100%)	0	100	100
32	P1	299/325 (92%)	298 (100%)	1 (0%)	92	97
33	Q1	113/153 (74%)	113 (100%)	0	100	100
34	7	81/96 (84%)	80 (99%)	1 (1%)	71	87
35	S1	74/80 (92%)	74 (100%)	0	100	100
36	T1	73/135 (54%)	72 (99%)	1 (1%)	67	85
36	U1	81/135 (60%)	81 (100%)	0	100	100
37	V1	101/102 (99%)	101 (100%)	0	100	100
38	W1	108/114 (95%)	108 (100%)	0	100	100
39	q1	131/131 (100%)	131 (100%)	0	100	100
40	r1	88/96 (92%)	88 (100%)	0	100	100
41	s1	41/95 (43%)	41 (100%)	0	100	100
42	A1	103/103 (100%)	103 (100%)	0	100	100
43	H1	279/279 (100%)	279 (100%)	0	100	100
44	J1	137/137 (100%)	137 (100%)	0	100	100
45	K1	87/87 (100%)	87 (100%)	0	100	100
46	L1	548/549 (100%)	548 (100%)	0	100	100
47	M1	414/414 (100%)	414 (100%)	0	100	100
48	N1	307/307 (100%)	307 (100%)	0	100	100
49	O1	284/309 (92%)	282 (99%)	2 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	X1	153/154 (99%)	153 (100%)	0	100	100
51	Y1	105/106 (99%)	104 (99%)	1 (1%)	76	88
52	Z1	122/123 (99%)	122 (100%)	0	100	100
53	a1	60/60 (100%)	60 (100%)	0	100	100
54	b1	72/73 (99%)	72 (100%)	0	100	100
55	c1	42/67 (63%)	42 (100%)	0	100	100
56	d1	107/107 (100%)	107 (100%)	0	100	100
57	e1	93/94 (99%)	93 (100%)	0	100	100
58	f1	49/53 (92%)	49 (100%)	0	100	100
59	g1	92/129 (71%)	91 (99%)	1 (1%)	73	88
60	h1	123/162 (76%)	123 (100%)	0	100	100
61	i1	99/119 (83%)	99 (100%)	0	100	100
62	j1	61/87 (70%)	61 (100%)	0	100	100
63	k1	60/78 (77%)	60 (100%)	0	100	100
64	l1	142/161 (88%)	142 (100%)	0	100	100
65	m1	112/114 (98%)	112 (100%)	0	100	100
66	n1	163/164 (99%)	163 (100%)	0	100	100
67	o1	109/121 (90%)	109 (100%)	0	100	100
68	p1	155/158 (98%)	155 (100%)	0	100	100
All	All	13551/15419 (88%)	13526 (100%)	25 (0%)	93	98

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	O1	37	LYS
59	g1	55	ASN
21	k	47	ARG
51	Y1	3	ARG
12	a	480	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
12	a	98	ASN

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Mol	Chain	Res	Type
14	c	160	ASN
12	a	429	HIS
14	c	161	GLN
11	I	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
43	FME	H1	1	43	8,9,10	0.96	0	7,9,11	0.89	0
40	AYA	r1	1	40	6,7,8	1.28	1 (16%)	5,8,10	1.28	1 (20%)
47	FME	M1	1	47	8,9,10	0.96	0	7,9,11	0.76	0
54	AYA	b1	1	54	6,7,8	1.25	1 (16%)	5,8,10	1.28	1 (20%)
61	SAC	i1	1	61	7,8,9	1.02	0	8,9,11	0.81	0
44	FME	J1	1	44	8,9,10	0.95	0	7,9,11	0.85	0
46	FME	L1	1	46	8,9,10	0.92	0	7,9,11	0.91	0
45	FME	K1	1	45	8,9,10	0.94	0	7,9,11	1.66	2 (28%)
27	2MR	D1	85	27	10,12,13	2.58	2 (20%)	5,13,15	2.84	2 (40%)
42	FME	A1	1	42	8,9,10	0.94	0	7,9,11	0.79	0
48	FME	N1	1	48	8,9,10	0.96	0	7,9,11	1.04	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	FME	H1	1	43	-	3/7/9/11	-
40	AYA	r1	1	40	-	0/4/6/8	-
47	FME	M1	1	47	-	2/7/9/11	-
54	AYA	b1	1	54	-	0/4/6/8	-
61	SAC	i1	1	61	-	2/7/8/10	-
44	FME	J1	1	44	-	4/7/9/11	-
46	FME	L1	1	46	-	4/7/9/11	-
45	FME	K1	1	45	-	3/7/9/11	-
27	2MR	D1	85	27	-	4/10/13/15	-
42	FME	A1	1	42	-	1/7/9/11	-
48	FME	N1	1	48	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D1	85	2MR	CZ-NE	5.89	1.46	1.34
27	D1	85	2MR	CZ-NH2	5.11	1.44	1.33
40	r1	1	AYA	CA-N	-2.49	1.43	1.46
54	b1	1	AYA	CA-N	-2.30	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})
27	D1	85	2MR	CD-NE-CZ	4.86	132.50	123.41
27	D1	85	2MR	NE-CZ-NH2	-3.72	116.07	119.48
45	K1	1	FME	C-CA-N	3.51	116.06	109.73
40	r1	1	AYA	CB-CA-N	2.70	112.61	109.61
54	b1	1	AYA	CB-CA-N	2.57	112.47	109.61

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D1	85	2MR	O-C-CA-CB
43	H1	1	FME	N-CA-CB-CG
44	J1	1	FME	C-CA-CB-CG
44	J1	1	FME	O-C-CA-CB
45	K1	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 112 ligands modelled in this entry, 11 are monoatomic - leaving 101 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 $\lvert Z\rvert > 2$ 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
69	3PE	z	102	-	25,25,50	0.41	0	28,30,55	0.39	0
86	ZMP	W1	201	-	27,33,36	0.68	1 (3%)	32,40,45	0.93	1 (3%)
70	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
69	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.32	0
69	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.41	0
69	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.55	1 (2%)
73	FES	3	803	30	0,4,4	-	-	-		
69	3PE	b1	101	-	42,42,50	0.33	0	45,47,55	0.35	0
69	3PE	m1	601	-	35,35,50	0.36	0	38,40,55	0.30	0
82	SF4	9	202	31	0,12,12	-	-	-		
87	DGT	O1	401	78	26,33,33	0.79	1 (3%)	32,52,52	0.46	0
69	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.30	0
81	TGL	l	601	-	36,36,62	0.23	0	39,39,65	0.17	0
69	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.29	0
70	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
74	PC1	z	101	-	27,27,53	0.40	0	33,35,61	0.35	0
69	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.39	0
73	FES	2	301	28	0,4,4	-	-	-		
70	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
73	FES	P	201	5	0,4,4	-	-	-		
85	NDP	P1	501	-	45,52,52	0.52	0	53,80,80	0.60	1 (1%)
69	3PE	E	203	-	33,33,50	0.36	0	36,38,55	0.33	0
82	SF4	3	801	30	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	g	303	-	24,24,50	0.43	0	27,29,55	0.63	0
69	3PE	b	301	-	28,28,50	0.40	0	31,33,55	0.37	0
77	HEA	a	603	12	57,67,67	1.49	7 (12%)	61,103,103	2.43	23 (37%)
74	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.61	0
69	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.31	0
74	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.47	0
77	HEA	n	604	12	57,67,67	1.44	8 (14%)	61,103,103	2.48	23 (37%)
69	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.33	0
69	3PE	a	605	-	27,27,50	0.40	0	30,32,55	0.46	0
81	TGL	y	601	-	36,36,62	0.24	0	39,39,65	0.18	0
74	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.34	0
69	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
74	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
70	CDL	r1	202	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
73	FES	E	201	5	0,4,4	-	-	-		
69	3PE	C	404	-	30,30,50	0.38	0	33,35,55	0.34	0
69	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.30	0
70	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.33	0
71	HEM	C	402	3	41,50,50	1.43	5 (12%)	45,82,82	1.41	6 (13%)
69	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.37	0
71	HEM	N	401	3	41,50,50	1.46	3 (7%)	45,82,82	1.74	9 (20%)
69	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.66	0
74	PC1	g	302	-	49,49,53	0.30	0	55,57,61	0.28	0
69	3PE	Y1	402	-	27,27,50	0.39	0	30,32,55	0.37	0
77	HEA	a	604	12	57,67,67	1.41	8 (14%)	61,103,103	2.39	23 (37%)
69	3PE	i	101	-	27,27,50	0.39	0	30,32,55	0.33	0
69	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.30	0
69	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.32	0
79	CUA	b	302	13	0,1,1	-	-	-		
69	3PE	M1	503	-	50,50,50	0.30	0	53,55,55	0.27	0
70	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.42	0
69	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.60	1 (3%)
70	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.51	0
70	CDL	G	101	-	41,41,99	0.44	0	47,53,111	0.36	0
70	CDL	L1	703	-	45,45,99	0.43	0	51,57,111	0.34	0
69	3PE	L1	704	-	50,50,50	0.31	0	53,55,55	0.28	0
74	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.47	0
69	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.36	0
74	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.44	0
70	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.28	0
71	HEM	N	402	3	41,50,50	1.45	4 (9%)	45,82,82	1.58	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
70	CDL	g	301	-	34,37,99	0.37	0	37,47,111	0.53	0
77	HEA	n	603	12	57,67,67	1.40	7 (12%)	61,103,103	2.47	22 (36%)
69	3PE	a	606	-	26,26,50	0.40	0	29,31,55	0.36	0
74	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.33	0
69	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
69	3PE	d	201	-	33,33,50	0.37	0	36,38,55	0.53	0
70	CDL	Y1	401	-	93,93,99	0.31	0	99,105,111	0.28	0
82	SF4	6	201	25	0,12,12	-	-	-		
71	HEM	C	401	3	41,50,50	1.44	3 (7%)	45,82,82	1.59	7 (15%)
74	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.58	0
82	SF4	9	201	31	0,12,12	-	-	-		
69	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.33	0
69	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
70	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
82	SF4	1	502	29	0,12,12	-	-	-		
74	PC1	V	101	-	27,27,53	0.40	0	33,35,61	0.35	0
70	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
86	ZMP	n1	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.93	1 (3%)
69	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
74	PC1	I	201	-	49,49,53	0.32	0	55,57,61	0.52	1 (1%)
69	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.34	0
69	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.30	0
72	HEC	O	303	4	32,50,50	2.17	4 (12%)	24,82,82	1.60	3 (12%)
74	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.36	0
69	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.34	0
69	3PE	G	102	-	50,50,50	0.31	0	53,55,55	0.28	0
69	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.32	0
70	CDL	V	102	-	49,49,99	0.42	0	55,61,111	0.50	1 (1%)
70	CDL	R	101	-	40,40,99	0.45	0	46,52,111	0.53	0
72	HEC	D	301	4	32,50,50	2.23	3 (9%)	24,82,82	1.63	5 (20%)
83	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.47	1 (2%)
70	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.38	0
69	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.34	0
79	CUA	o	303	13	0,1,1	-	-	-		
82	SF4	3	802	30	0,12,12	-	-	-		
69	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
70	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.43	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	z	102	-	-	1/29/29/54	-
86	ZMP	W1	201	-	-	5/38/40/43	-
70	CDL	O	301	-	-	15/67/67/110	-
69	3PE	c	301	-	-	10/48/48/54	-
69	3PE	n	606	-	-	9/31/31/54	-
69	3PE	n	605	-	-	10/37/37/54	-
73	FES	3	803	30	-	-	0/1/1/1
69	3PE	b1	101	-	-	10/46/46/54	-
69	3PE	m1	601	-	-	13/39/39/54	-
82	SF4	9	202	31	-	-	0/6/5/5
87	DGT	O1	401	78	-	1/18/34/34	0/3/3/3
69	3PE	K1	201	-	-	12/44/44/54	-
81	TGL	l	601	-	-	0/39/39/65	-
69	3PE	r1	201	-	-	8/49/49/54	-
70	CDL	R	102	-	-	17/67/67/110	-
74	PC1	z	101	-	-	6/31/31/57	-
69	3PE	L	501	-	-	6/26/26/54	-
73	FES	2	301	28	-	-	0/1/1/1
70	CDL	A	502	-	-	13/56/56/110	-
73	FES	P	201	5	-	-	0/1/1/1
85	NDP	P1	501	-	-	5/30/77/77	0/5/5/5
69	3PE	E	203	-	-	9/37/37/54	-
82	SF4	3	801	30	-	-	0/6/5/5
69	3PE	g	303	-	-	9/28/28/54	-
69	3PE	b	301	-	-	9/32/32/54	-
77	HEA	a	603	12	-	13/32/76/76	-
74	PC1	L	503	-	-	9/27/27/57	-
69	3PE	N	403	-	-	7/40/40/54	-
74	PC1	K	101	-	-	4/31/31/57	-
77	HEA	n	604	12	-	7/32/76/76	-
69	3PE	6	202	-	-	4/35/35/54	-
69	3PE	a	605	-	-	6/31/31/54	-
81	TGL	y	601	-	-	3/39/39/65	-
74	PC1	J	101	-	-	7/38/38/57	-
69	3PE	N1	402	-	-	6/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	PC1	9	204	-	-	10/50/50/57	-
70	CDL	r1	202	-	-	13/67/67/110	-
73	FES	E	201	5	-	-	0/1/1/1
69	3PE	C	404	-	-	4/34/34/54	-
69	3PE	M1	502	-	-	17/54/54/54	-
70	CDL	D	302	-	-	19/66/66/110	-
71	HEM	C	402	3	-	1/12/54/54	-
69	3PE	d1	203	-	-	7/35/35/54	-
71	HEM	N	401	3	-	3/12/54/54	-
69	3PE	A	501	-	-	9/26/26/54	-
74	PC1	g	302	-	-	8/53/53/57	-
69	3PE	Y1	402	-	-	4/31/31/54	-
77	HEA	a	604	12	-	11/32/76/76	-
69	3PE	i	101	-	-	8/31/31/54	-
69	3PE	p	301	-	-	12/48/48/54	-
69	3PE	E	202	-	-	9/35/35/54	-
69	3PE	M1	503	-	-	14/54/54/54	-
70	CDL	h1	201	-	-	20/80/80/110	-
69	3PE	t	101	-	-	7/28/28/54	-
70	CDL	L	502	-	-	9/56/56/110	-
70	CDL	G	101	-	-	13/52/52/110	-
70	CDL	L1	703	-	-	15/56/56/110	-
69	3PE	L1	704	-	-	7/54/54/54	-
74	PC1	6	203	-	-	12/46/46/57	-
69	3PE	n	607	-	-	8/30/30/54	-
74	PC1	9	203	-	-	12/57/57/57	-
70	CDL	L1	702	-	-	15/88/88/110	-
71	HEM	N	402	3	-	4/12/54/54	-
70	CDL	g	301	-	-	9/41/45/110	-
77	HEA	n	603	12	-	9/32/76/76	-
69	3PE	a	606	-	-	9/30/30/54	-
74	PC1	p	302	-	-	10/38/38/57	-
69	3PE	H1	401	-	-	9/54/54/54	-
69	3PE	d	201	-	-	6/37/37/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	CDL	Y1	401	-	-	11/104/104/110	-
82	SF4	6	201	25	-	-	0/6/5/5
71	HEM	C	401	3	-	1/12/54/54	-
74	PC1	P1	502	-	-	15/34/34/57	-
82	SF4	9	201	31	-	-	0/6/5/5
69	3PE	v	101	-	-	7/31/31/54	-
69	3PE	o	302	-	-	10/32/32/54	-
70	CDL	H1	402	-	-	12/59/59/110	-
82	SF4	1	502	29	-	-	0/6/5/5
74	PC1	V	101	-	-	4/31/31/57	-
70	CDL	d1	201	-	-	16/77/77/110	-
86	ZMP	n1	201	-	-	20/36/38/43	-
69	3PE	L1	701	-	-	9/54/54/54	-
74	PC1	I	201	-	-	9/53/53/57	-
69	3PE	R	104	-	-	5/33/33/54	-
69	3PE	i1	201	-	-	6/45/45/54	-
72	HEC	O	303	4	-	4/10/54/54	-
74	PC1	M1	501	-	-	9/57/57/57	-
69	3PE	O	302	-	-	9/36/36/54	-
69	3PE	G	102	-	-	11/54/54/54	-
69	3PE	Y1	403	-	-	7/45/45/54	-
70	CDL	V	102	-	-	18/60/60/110	-
70	CDL	R	101	-	-	15/51/51/110	-
72	HEC	D	301	4	-	2/10/54/54	-
83	FMN	1	501	-	-	5/18/18/18	0/3/3/3
70	CDL	N1	401	-	-	21/100/100/110	-
69	3PE	d1	202	-	-	7/34/34/54	-
82	SF4	3	802	30	-	-	0/6/5/5
69	3PE	C	403	-	-	9/38/38/54	-
70	CDL	R	103	-	-	19/82/82/110	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	D	301	HEC	C2B-C3B	-6.73	1.33	1.40
72	D	301	HEC	C3C-C2C	-6.41	1.34	1.40
72	O	303	HEC	C2B-C3B	-6.33	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	O	303	HEC	C3C-C2C	-6.09	1.34	1.40
72	D	301	HEC	C3D-C2D	5.45	1.53	1.37

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	a	604	HEA	CMC-C2C-C3C	7.88	139.42	124.68
77	a	603	HEA	CMC-C2C-C3C	7.77	139.22	124.68
77	n	604	HEA	CMC-C2C-C3C	7.59	138.87	124.68
77	n	603	HEA	CMC-C2C-C3C	7.42	138.56	124.68
77	a	604	HEA	CMC-C2C-C1C	-6.87	117.91	128.46

There are no chirality outliers.

5 of 818 torsion outliers are listed below:

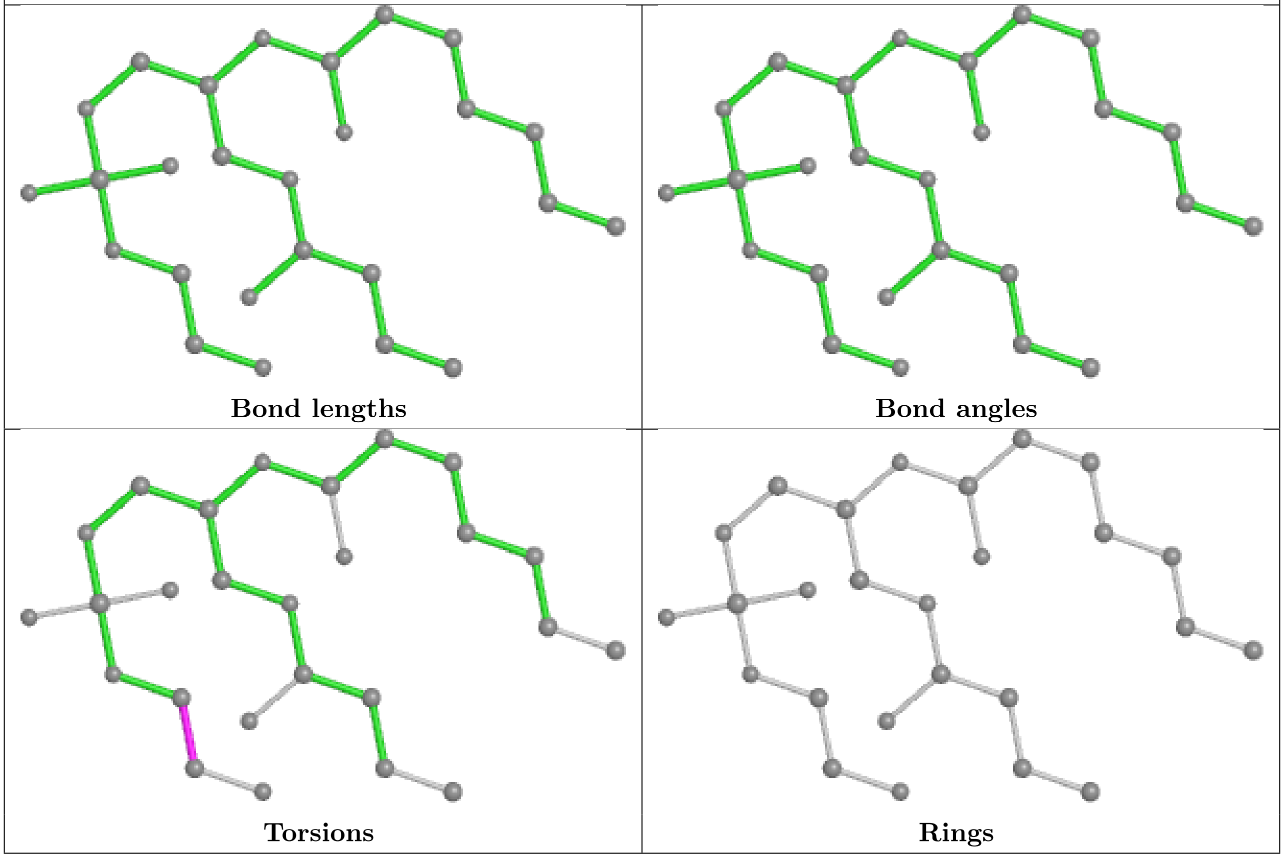
Mol	Chain	Res	Type	Atoms
69	A	501	3PE	C1-O11-P-O12
69	A	501	3PE	C1-O11-P-O13
69	A	501	3PE	C1-O11-P-O14
69	A	501	3PE	C11-O13-P-O11
69	A	501	3PE	C11-O13-P-O12

There are no ring outliers.

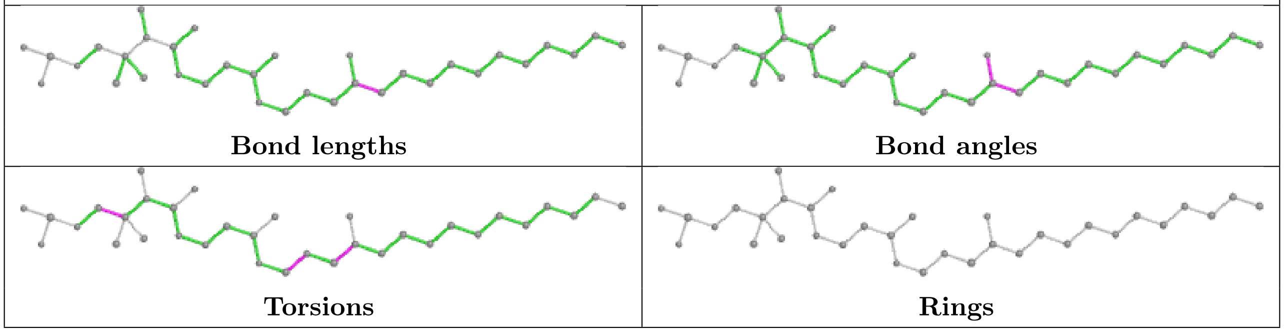
No monomer is involved in short contacts.

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.

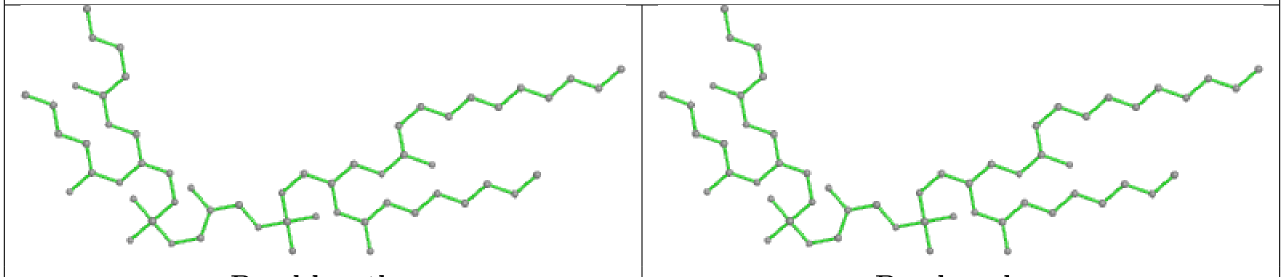
Ligand 3PE z 102



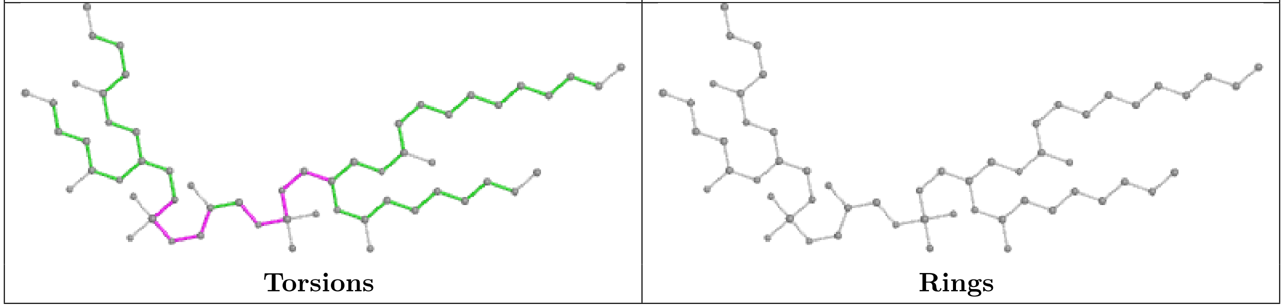
Ligand ZMP W1 201



Ligand CDL O 301

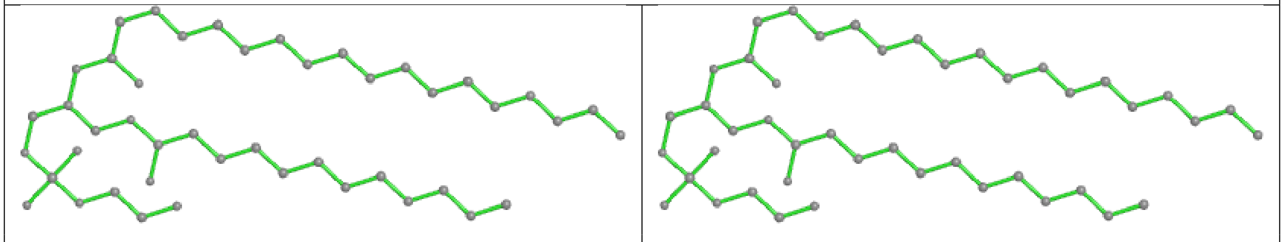


Bond lengths Bond angles

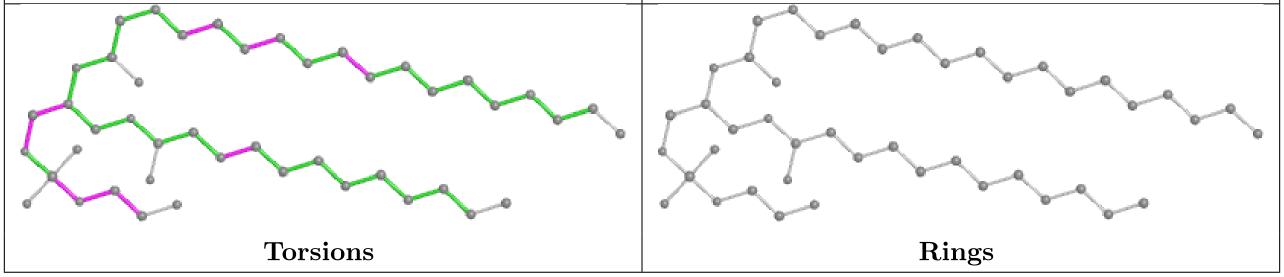


Torsions Rings

Ligand 3PE c 301

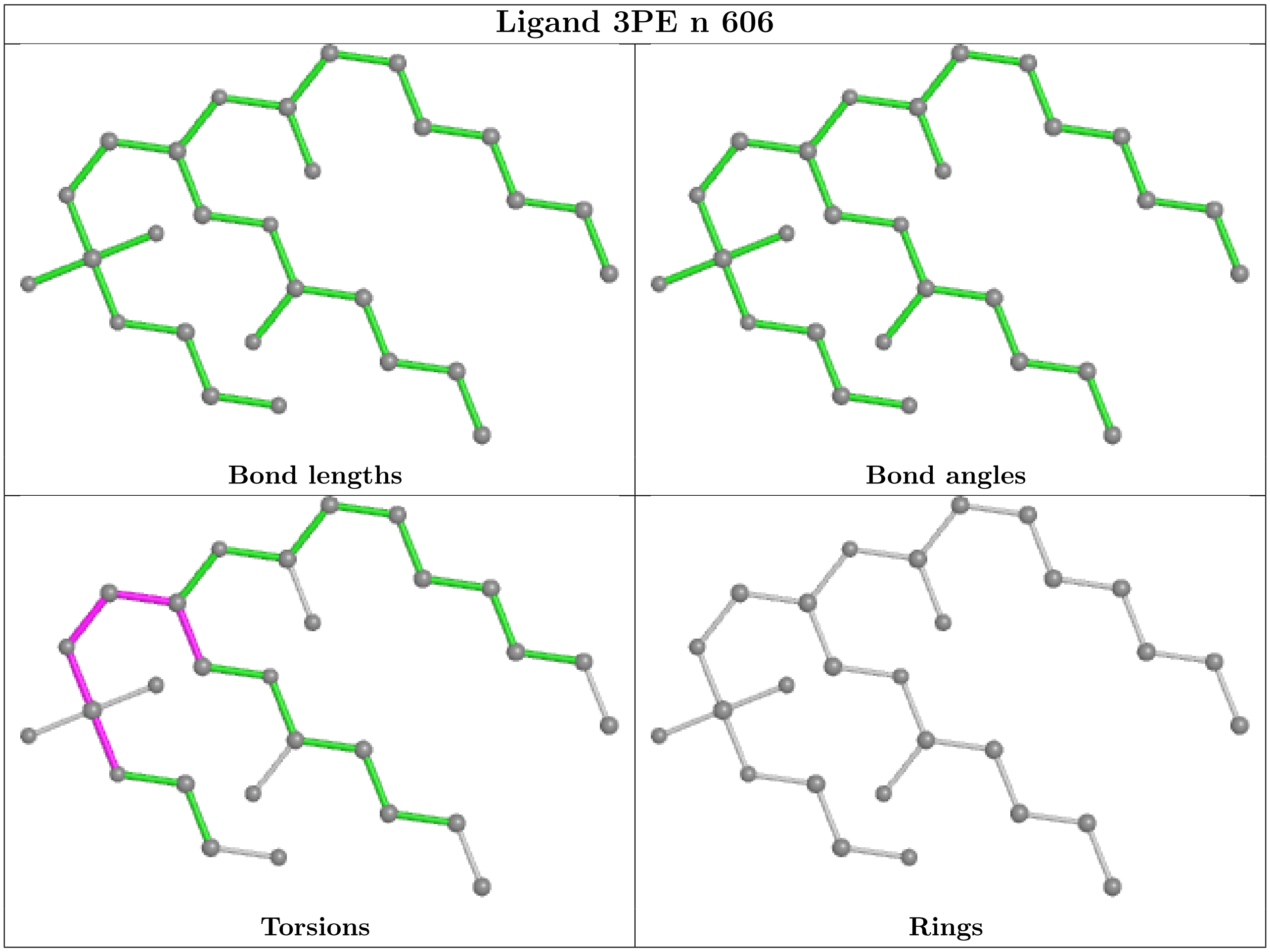


Bond lengths Bond angles



Torsions Rings

Ligand 3PE n 606



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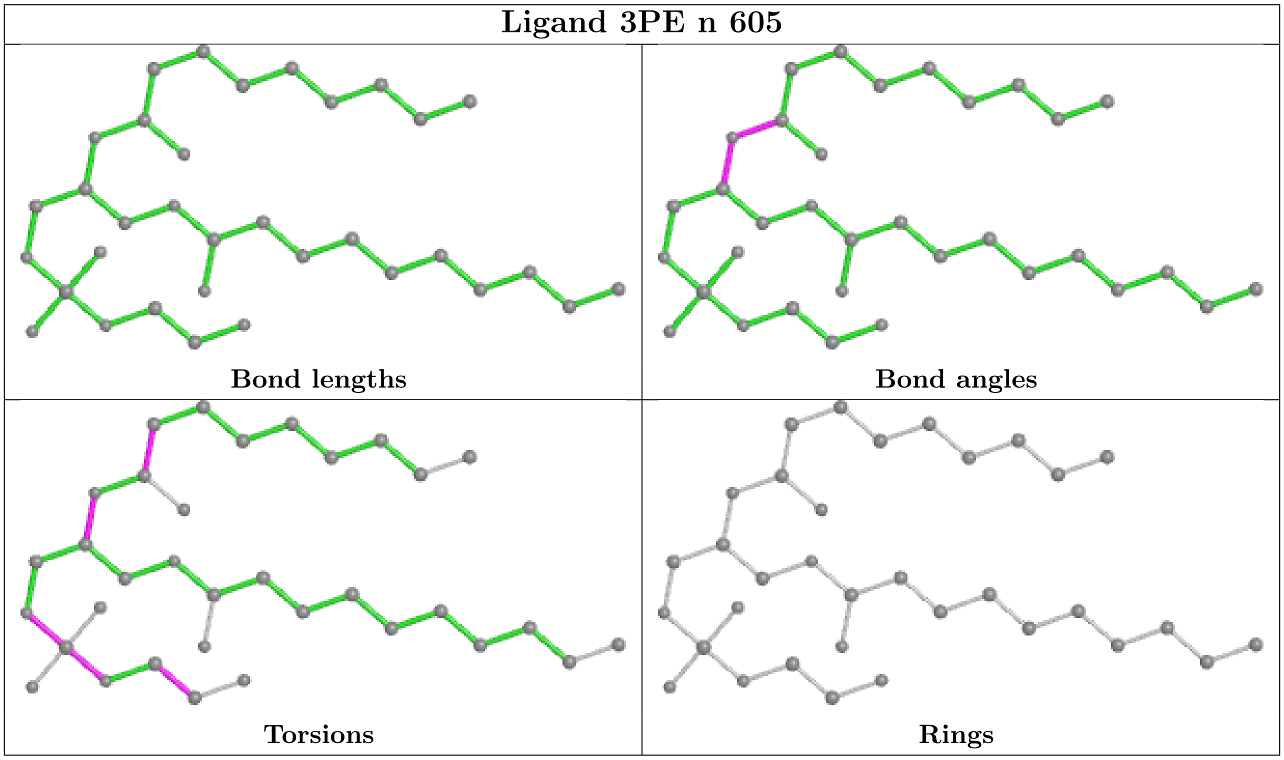
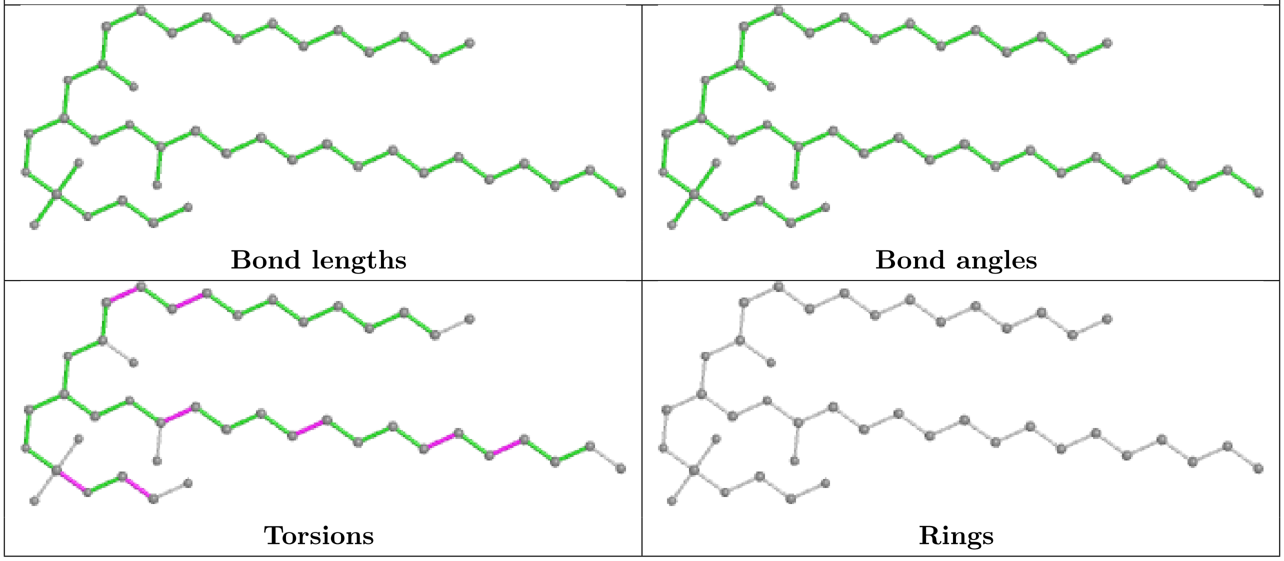


Ligand 3PE b1 101



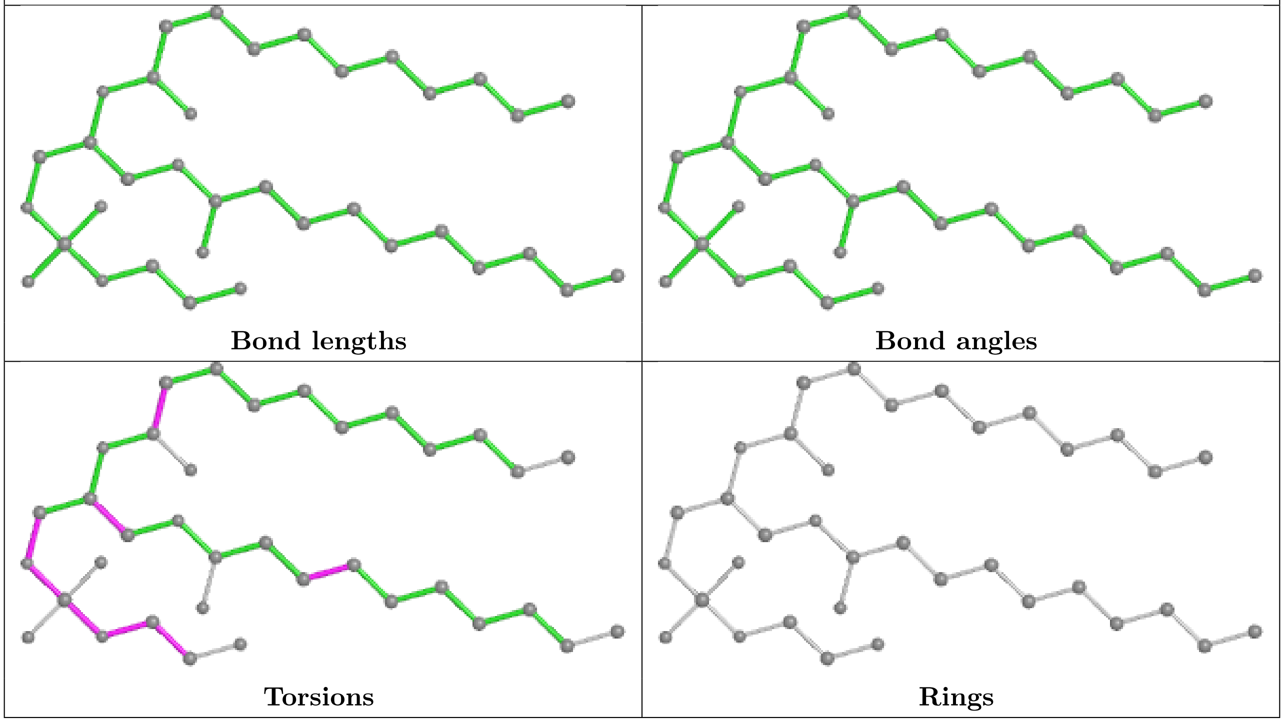
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE m1 601



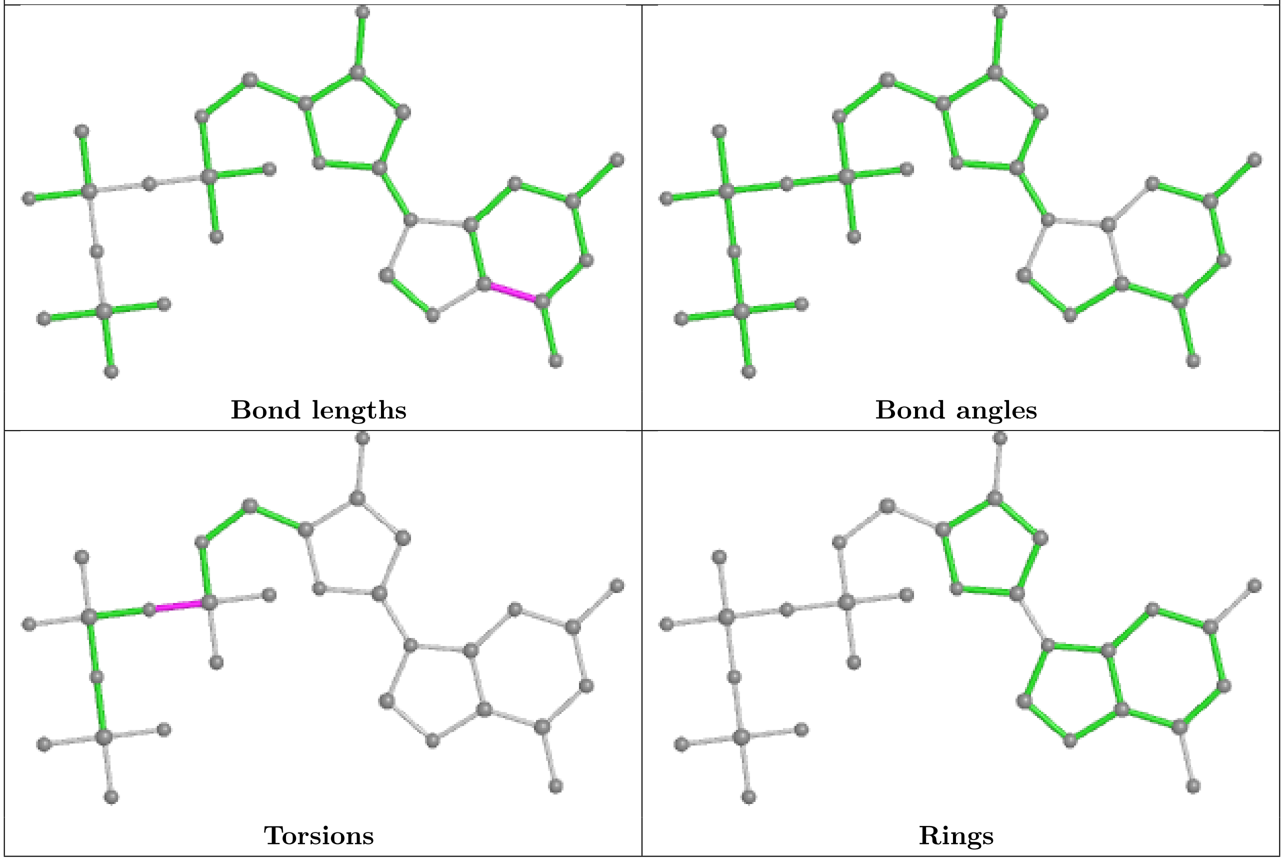
Bond lengths

Bond angles

Torsions

Rings

Ligand DGT O1 401



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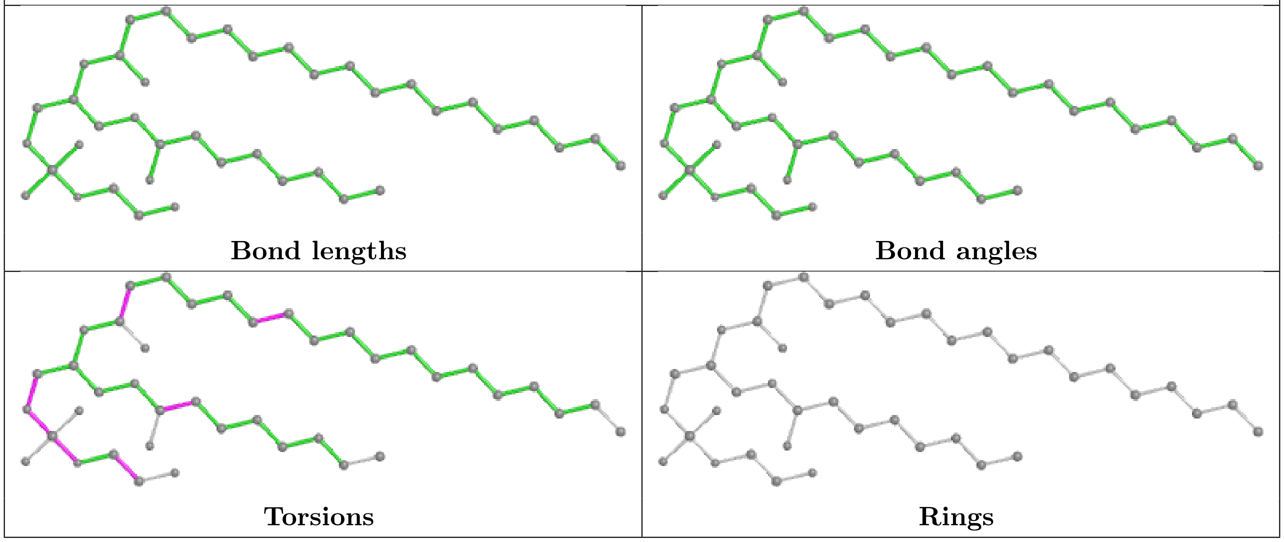
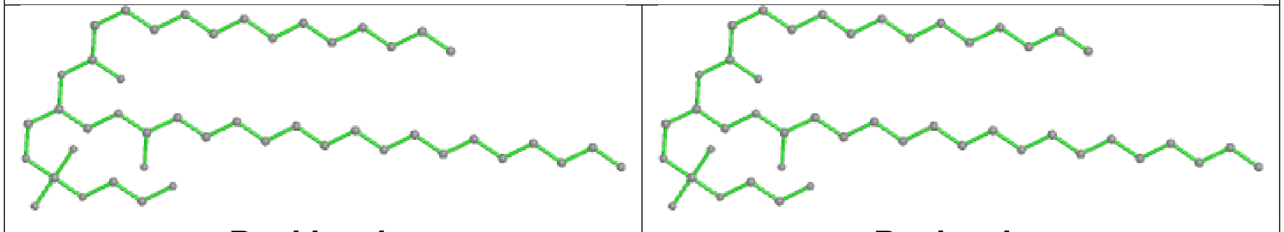
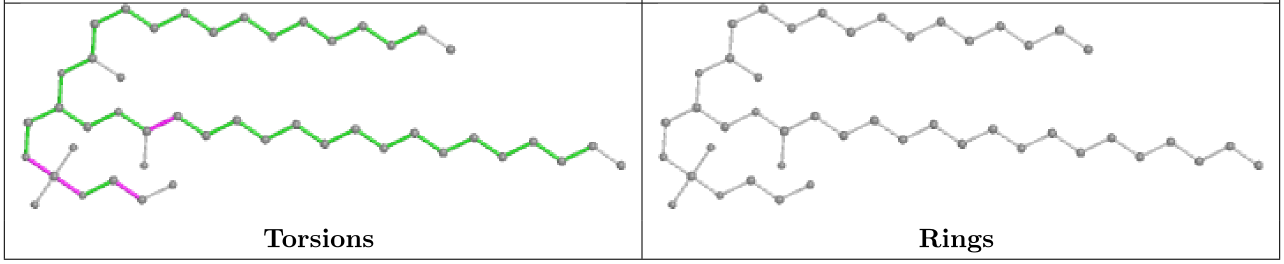


Ligand 3PE r1 201

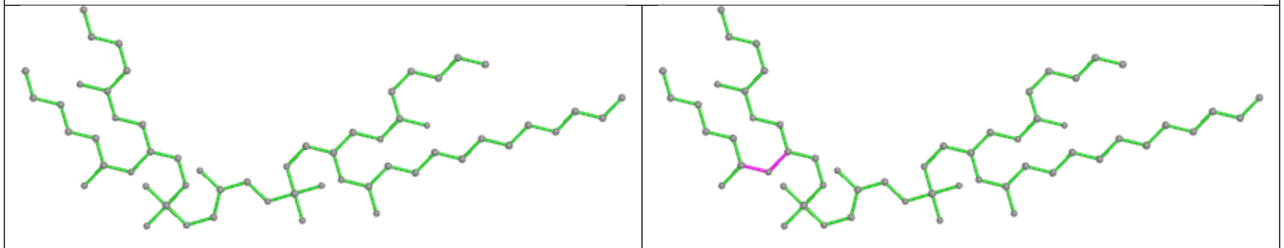


Bond lengths Bond angles

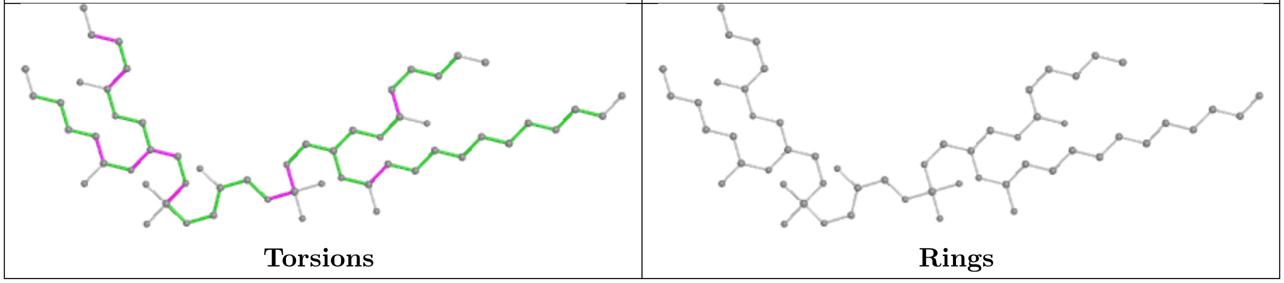


Torsions Rings

Ligand CDL R 102

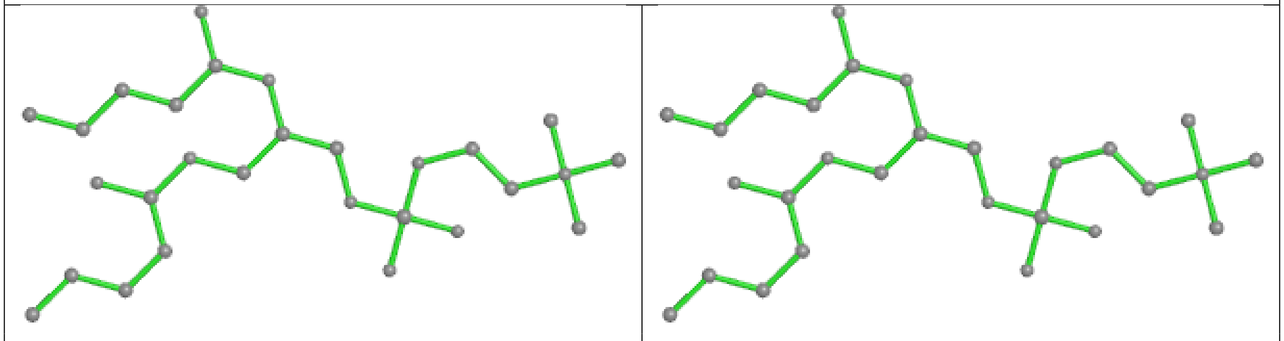


Bond lengths Bond angles



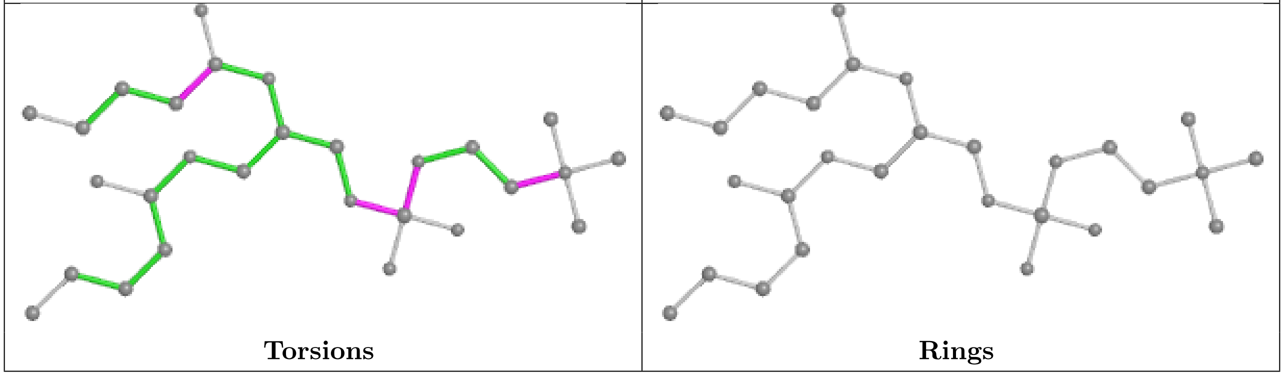
Torsions Rings

Ligand PC1 z 101



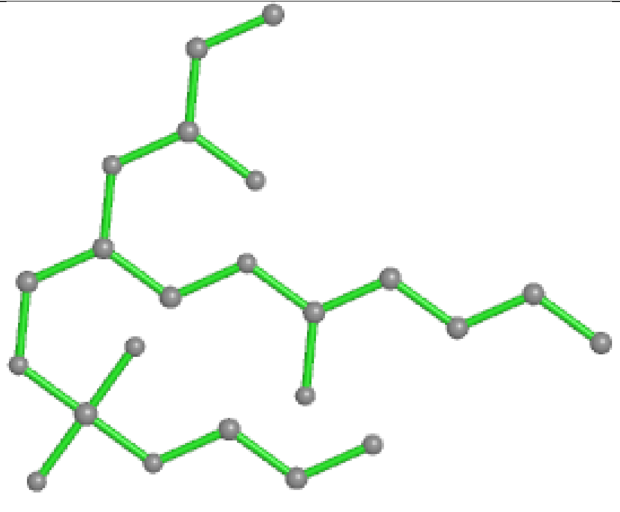
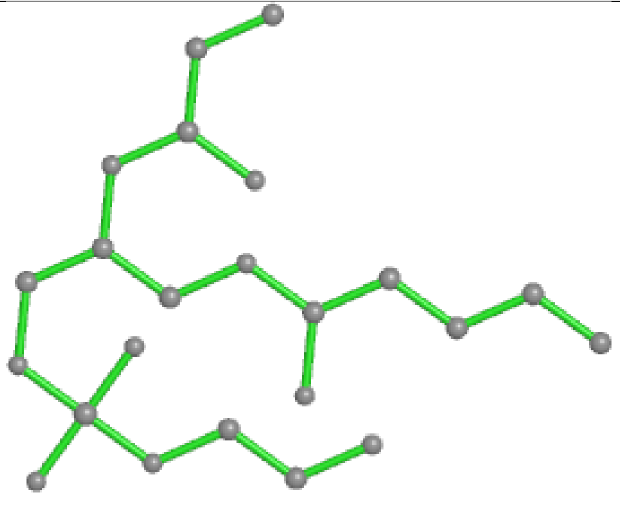
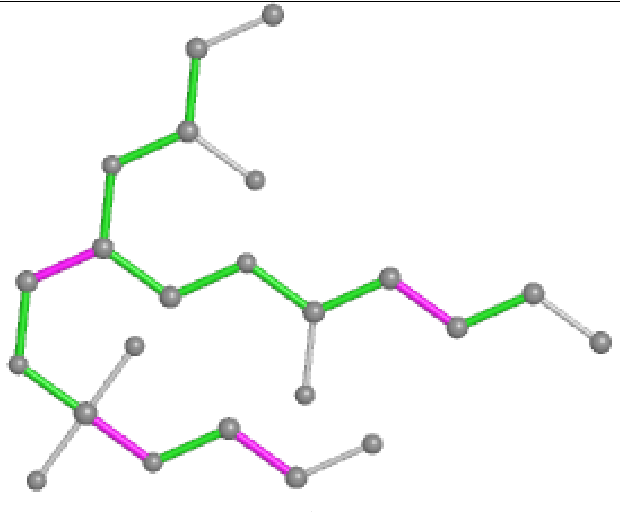
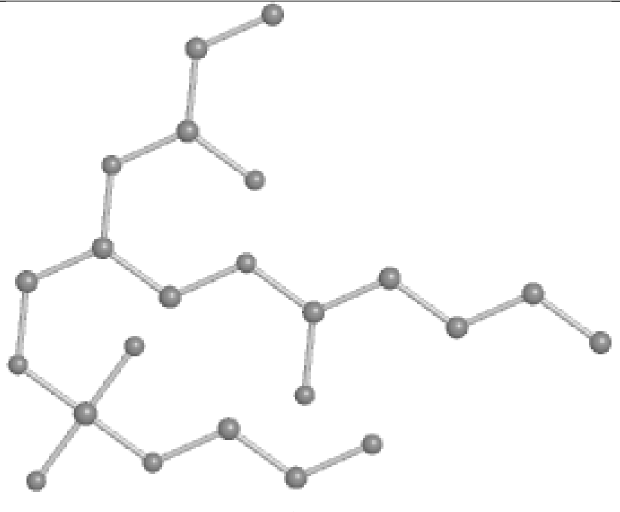
Bond lengths

Bond angles

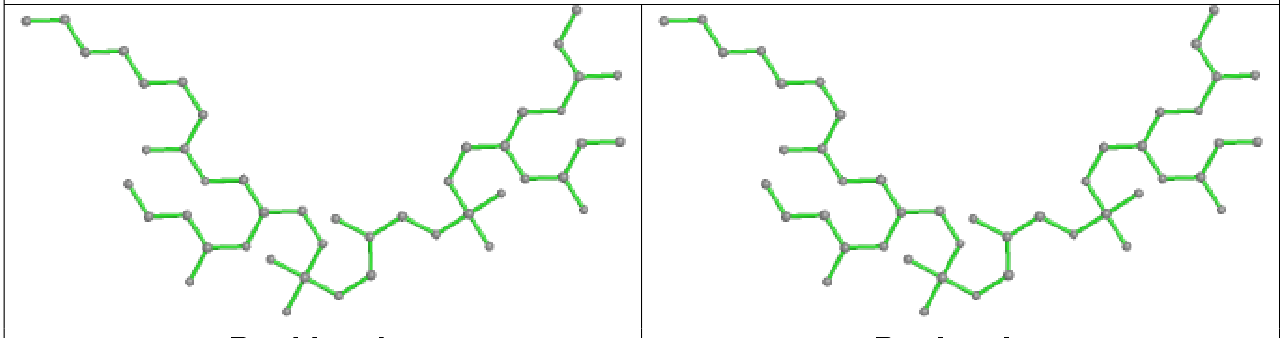


Torsions

Rings

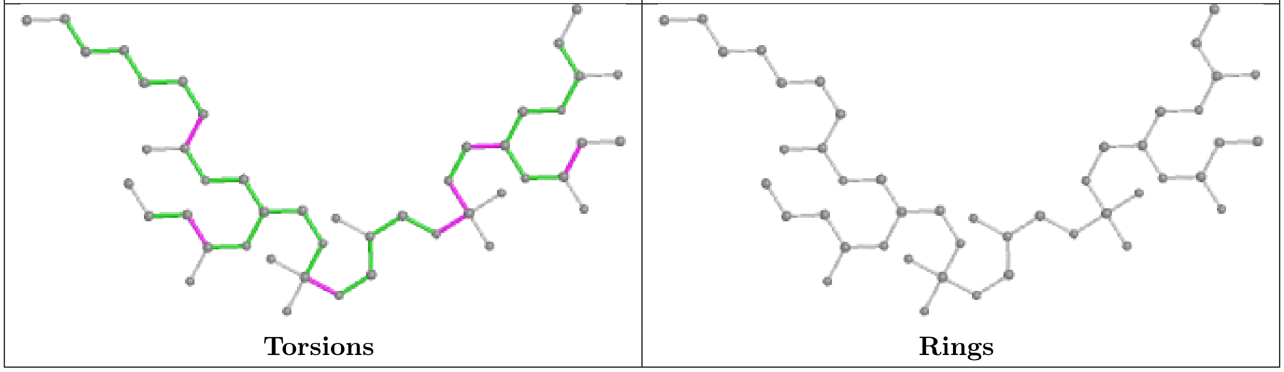
Ligand 3PE L 501	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CDL A 502



Bond lengths

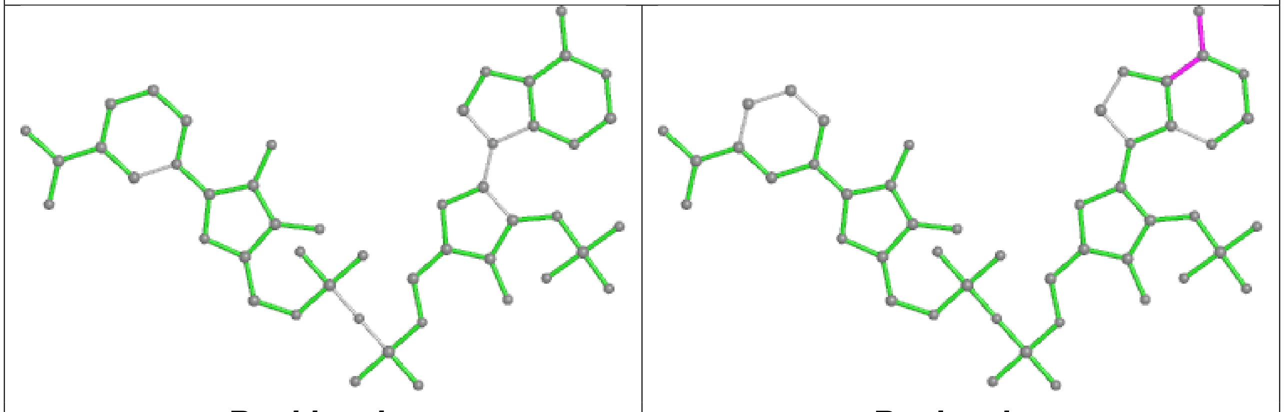
Bond angles



Torsions

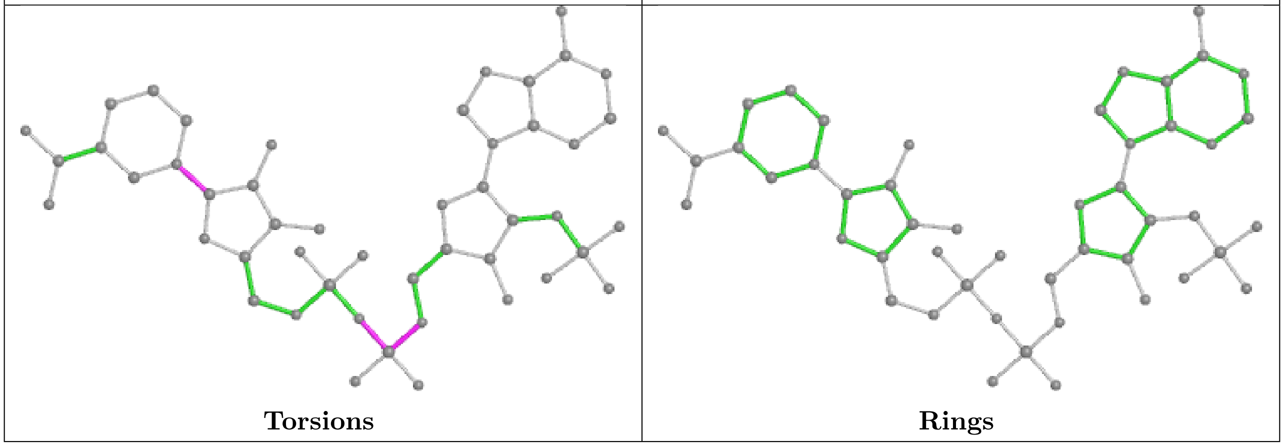
Rings

Ligand NDP P1 501



Bond lengths

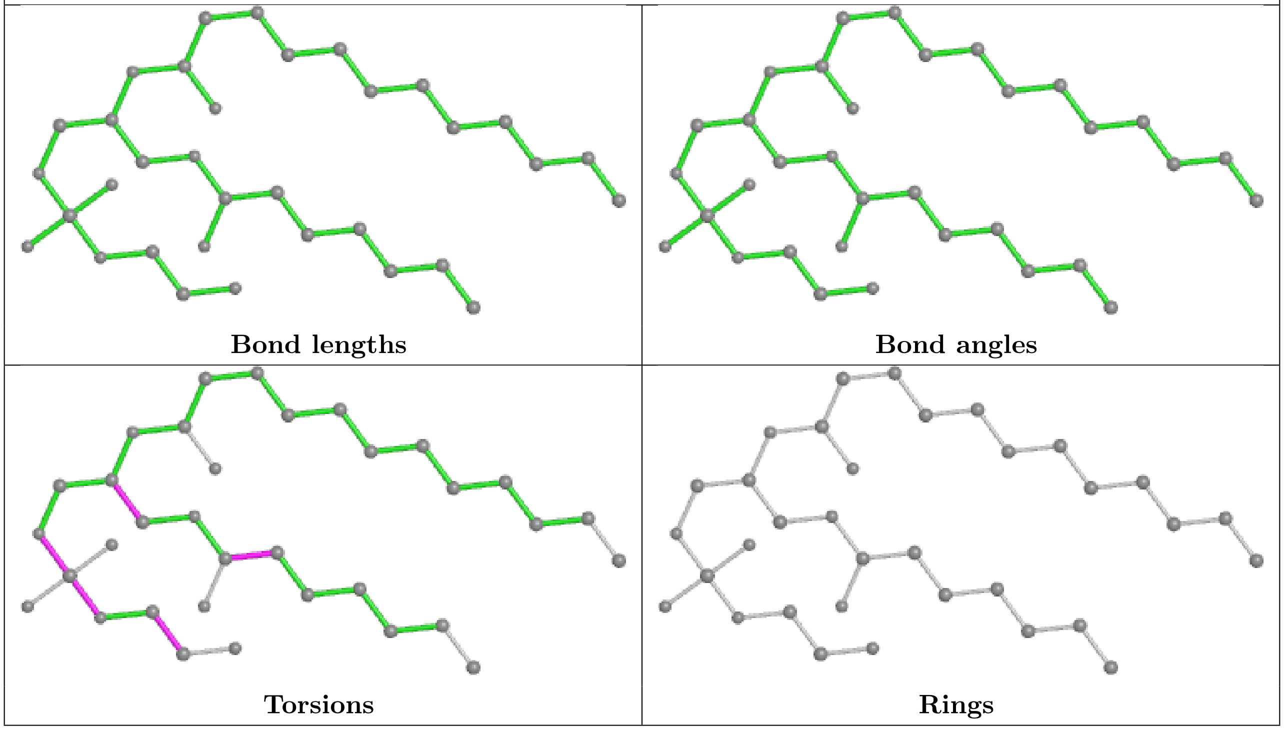
Bond angles



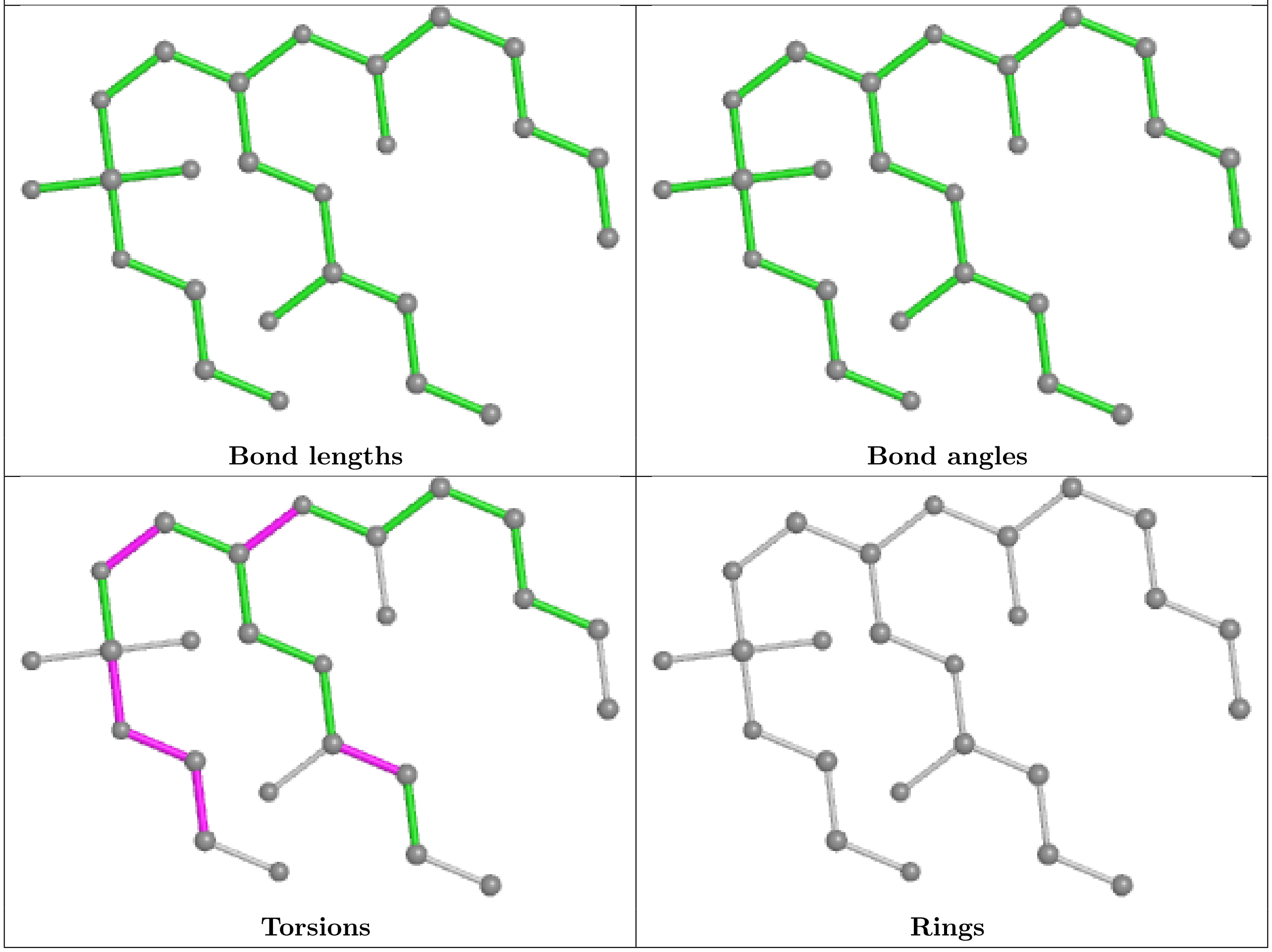
Torsions

Rings

Ligand 3PE E 203



Ligand 3PE g 303



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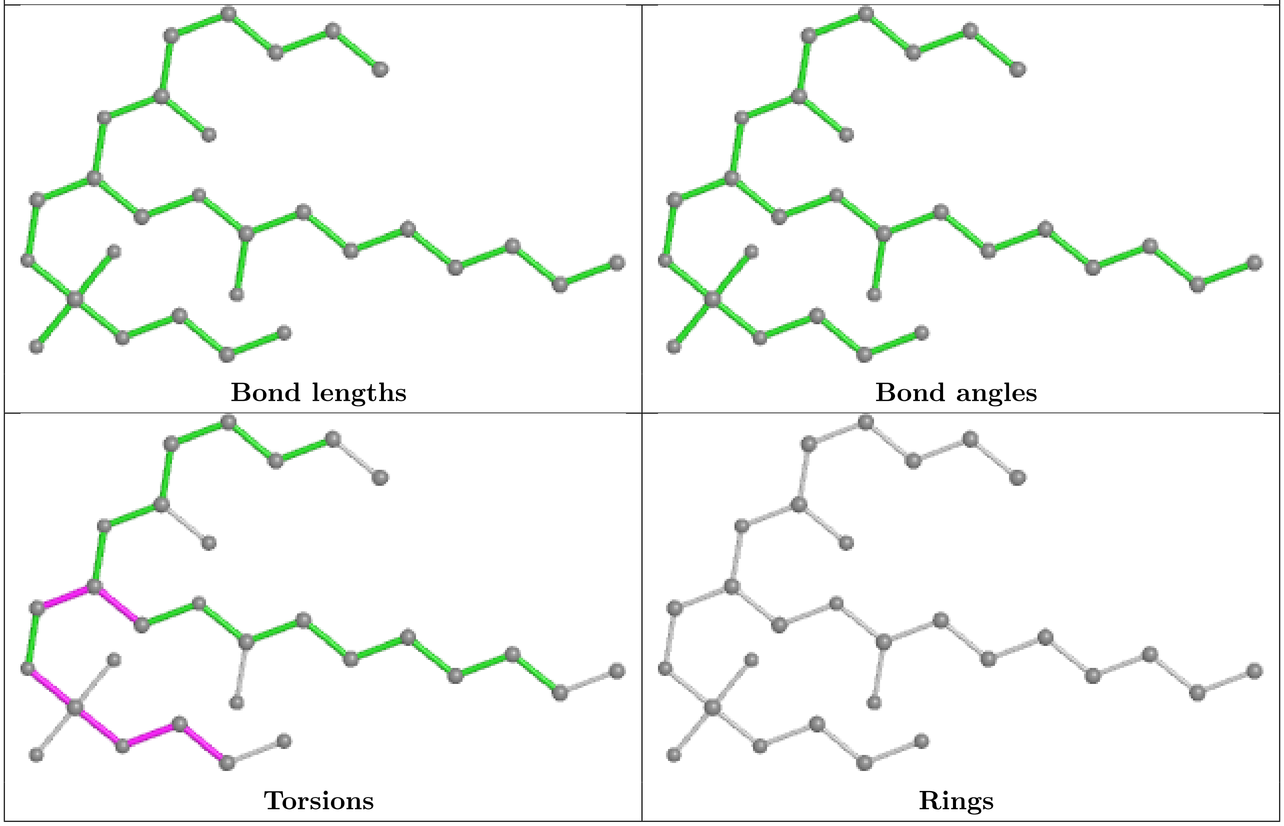


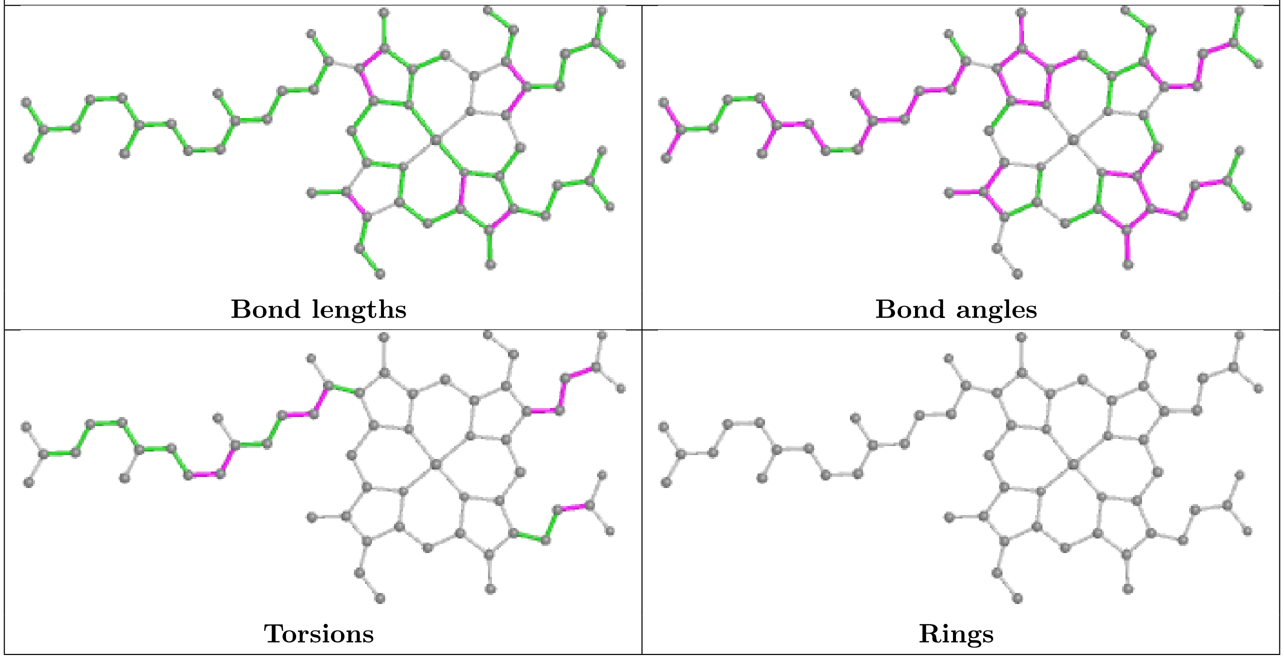
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA a 603



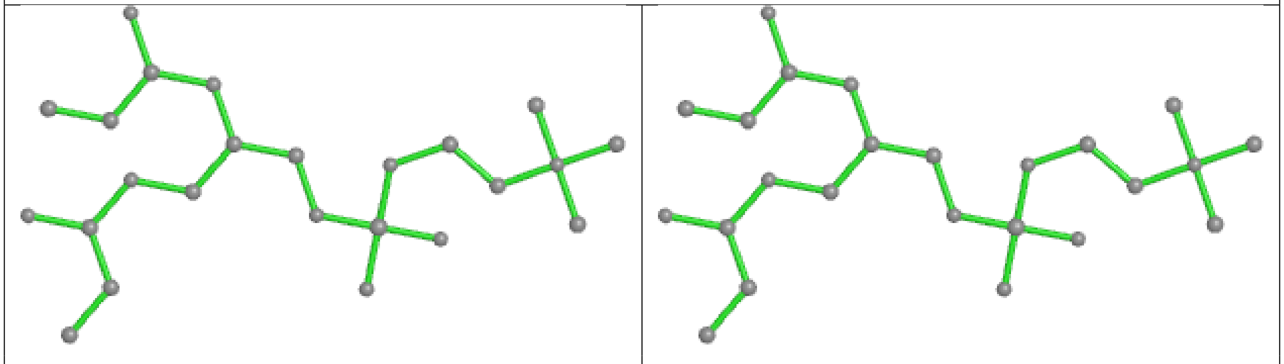
Bond lengths

Bond angles

Torsions

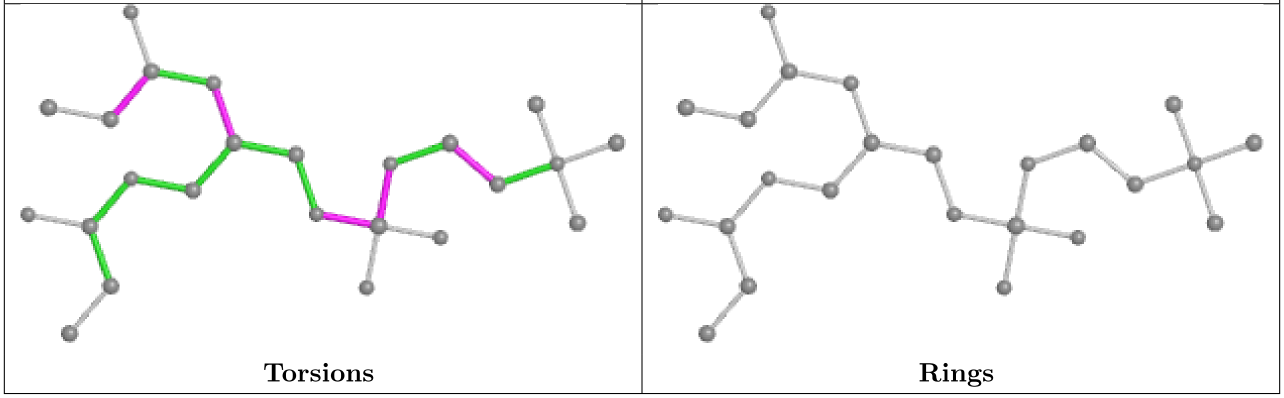
Rings

Ligand PC1 L 503



Bond lengths

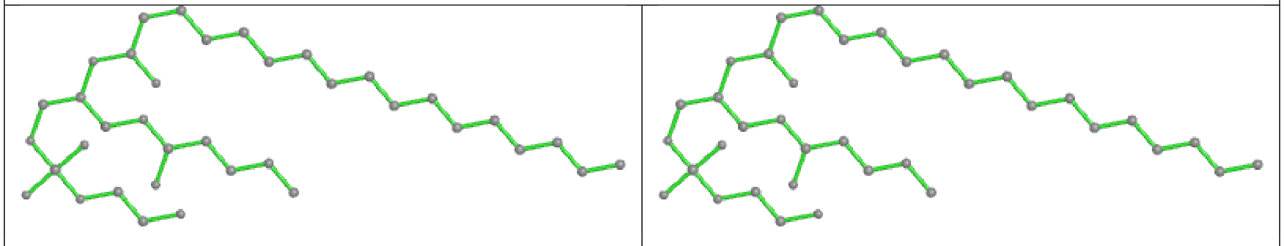
Bond angles



Torsions

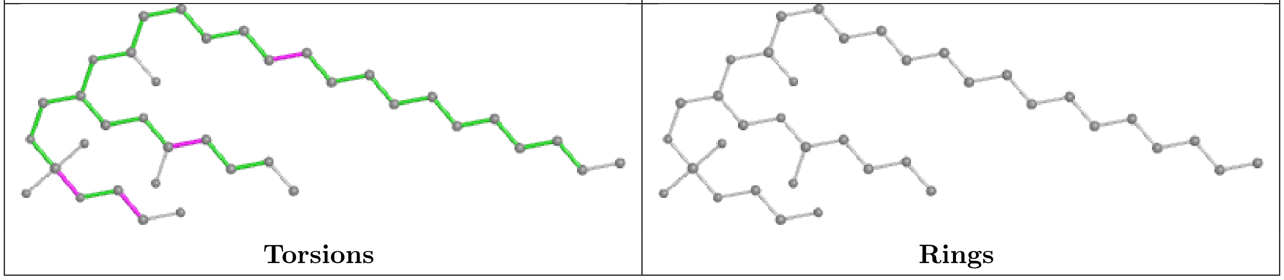
Rings

Ligand 3PE N 403



Bond lengths

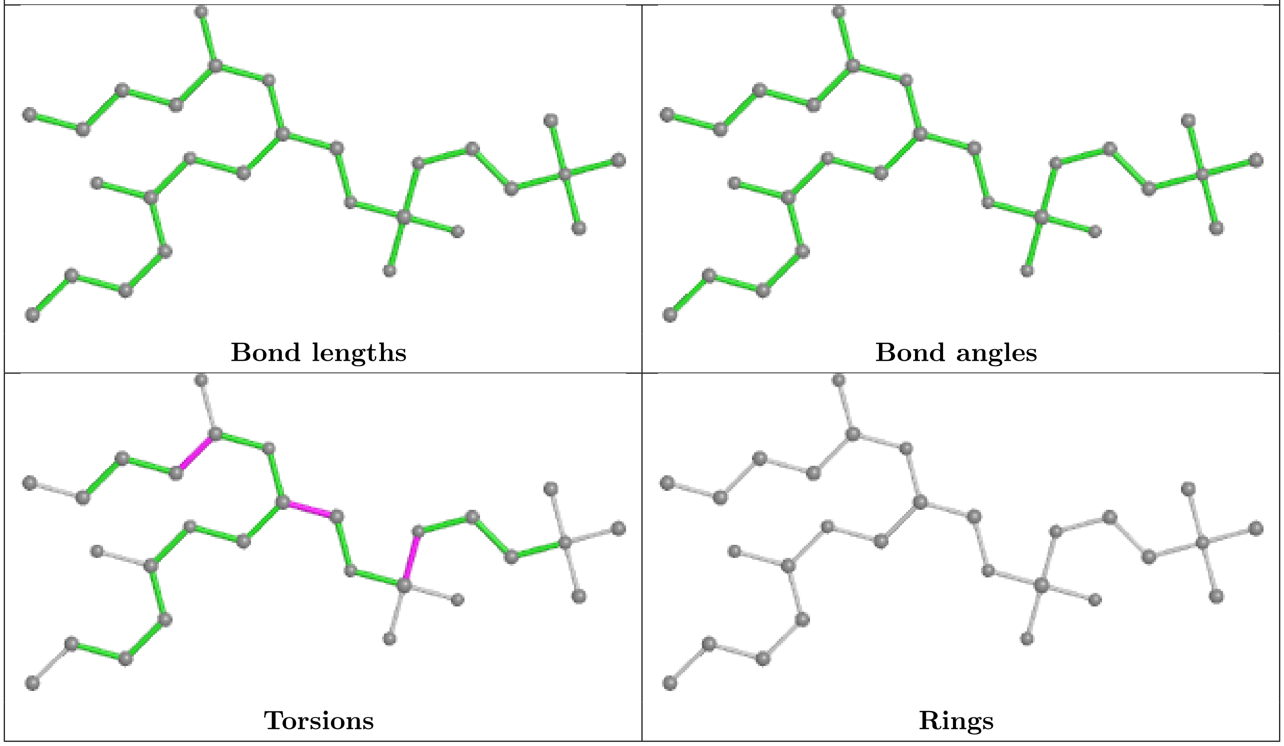
Bond angles



Torsions

Rings

Ligand PC1 K 101



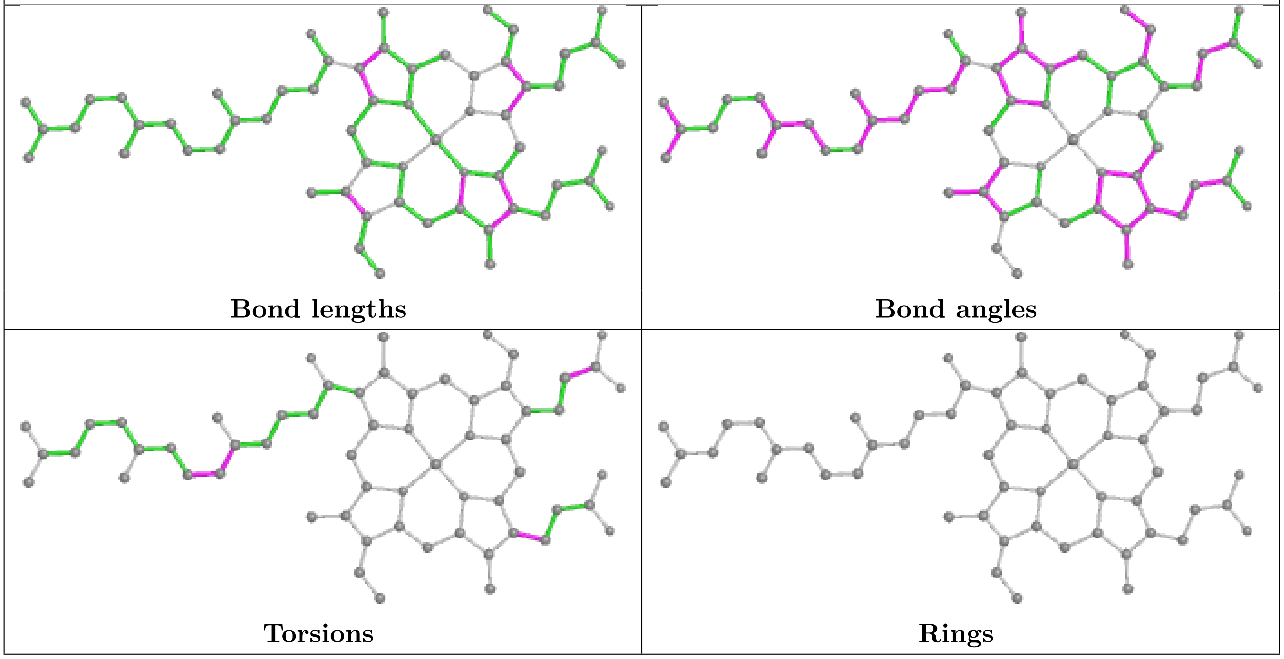
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA n 604



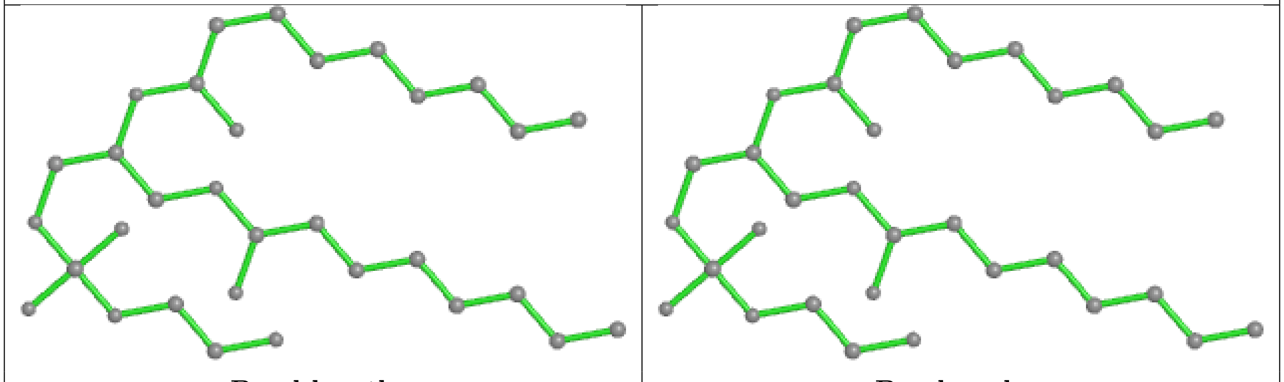
Bond lengths

Bond angles

Torsions

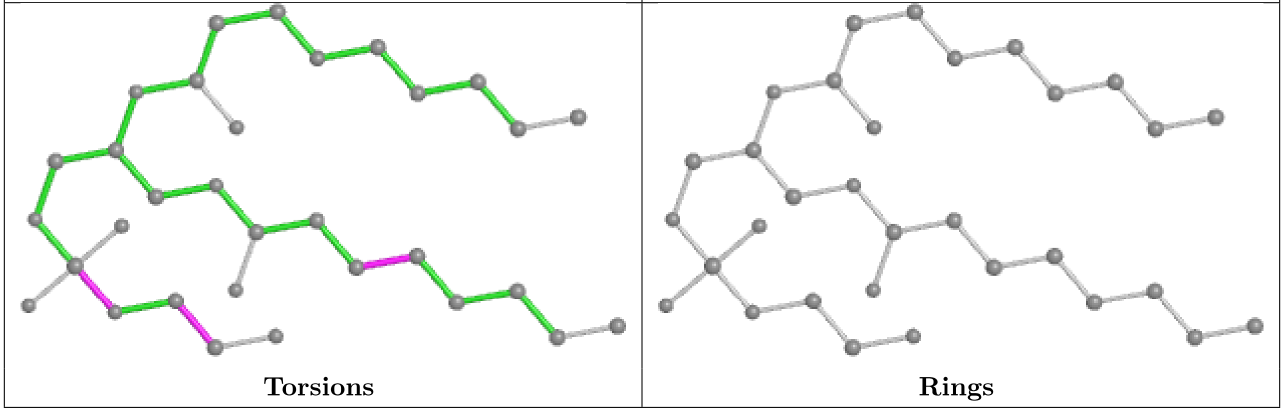
Rings

Ligand 3PE 6 202



Bond lengths

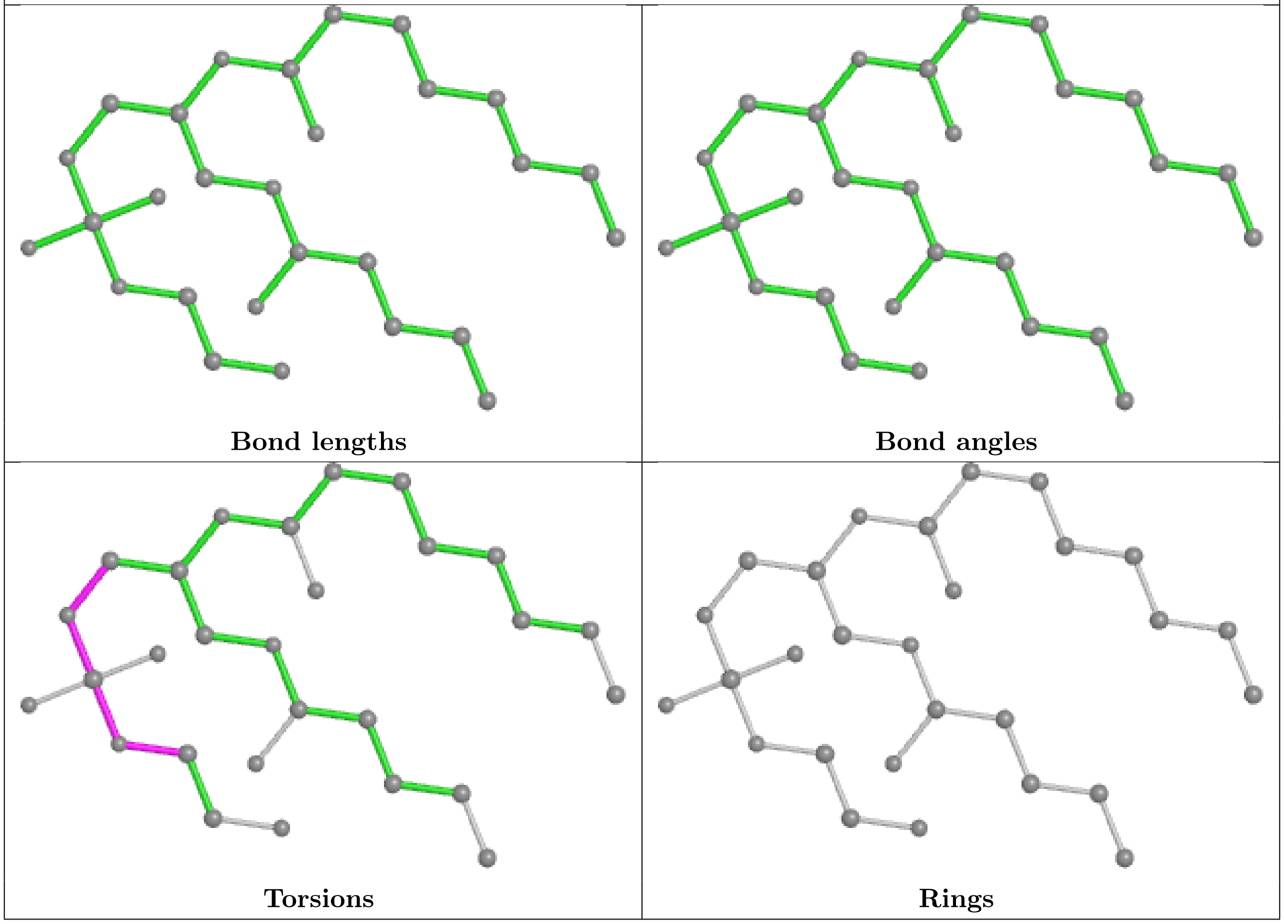
Bond angles



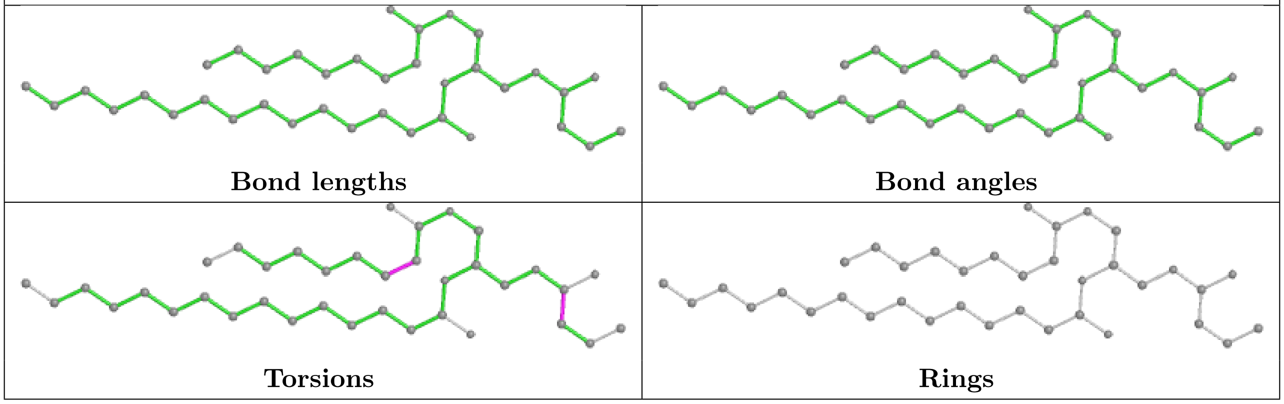
Torsions

Rings

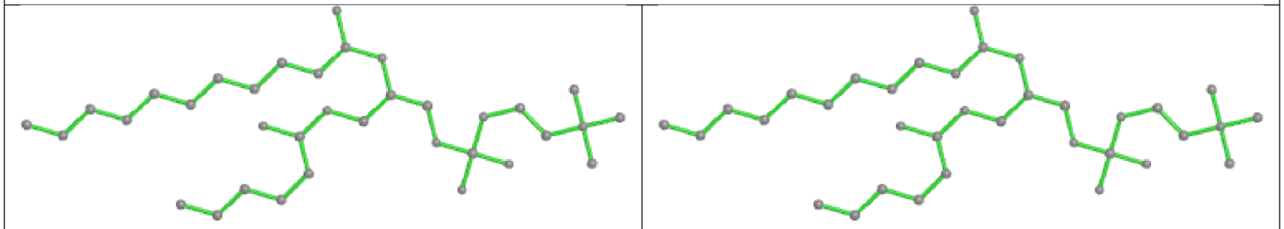
Ligand 3PE a 605


Bond lengths
Bond angles
Torsions
Rings

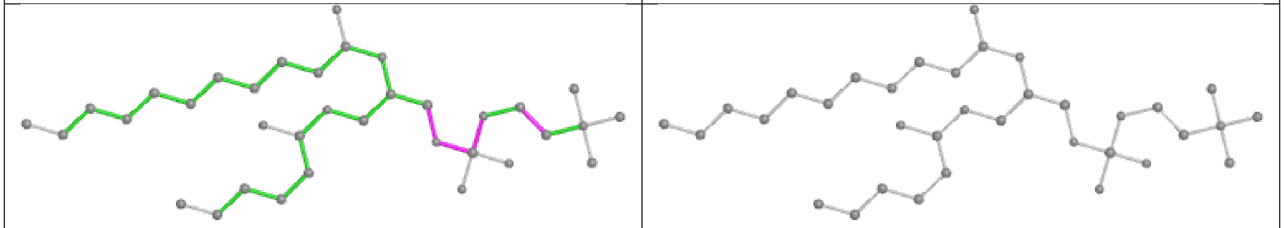
Ligand TGL y 601


Bond lengths
Bond angles
Torsions
Rings

Ligand PC1 J 101

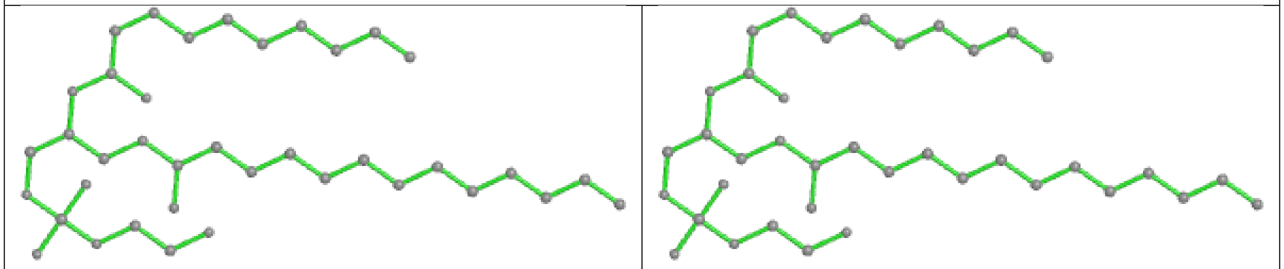


Bond lengths Bond angles

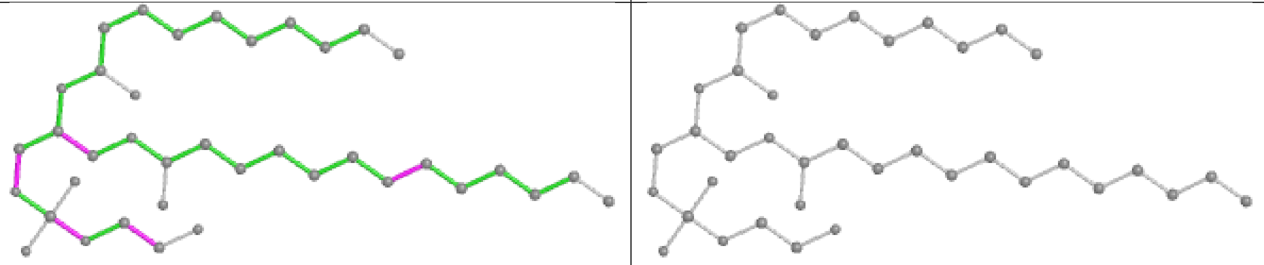


Torsions Rings

Ligand 3PE N1 402

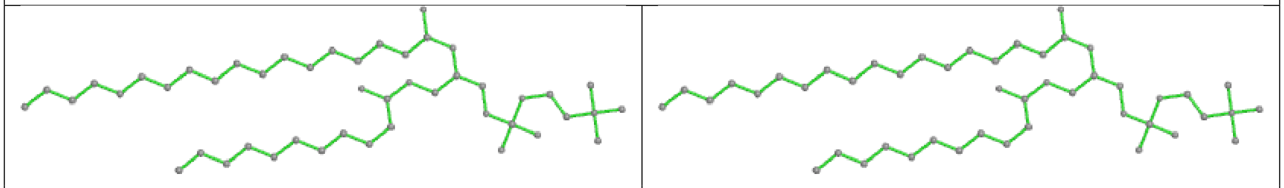


Bond lengths Bond angles

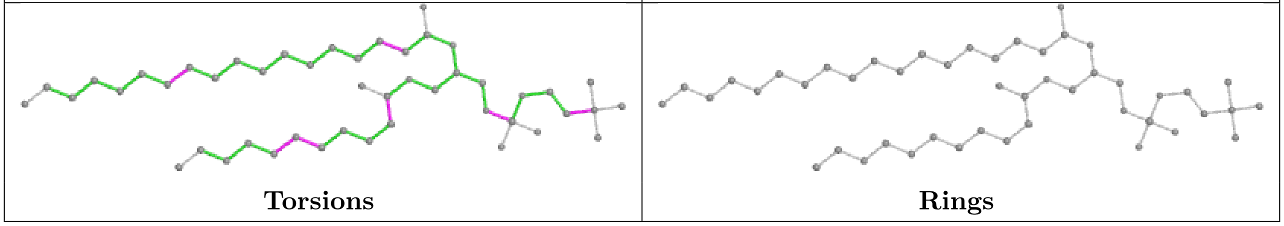


Torsions Rings

Ligand PC1 9 204

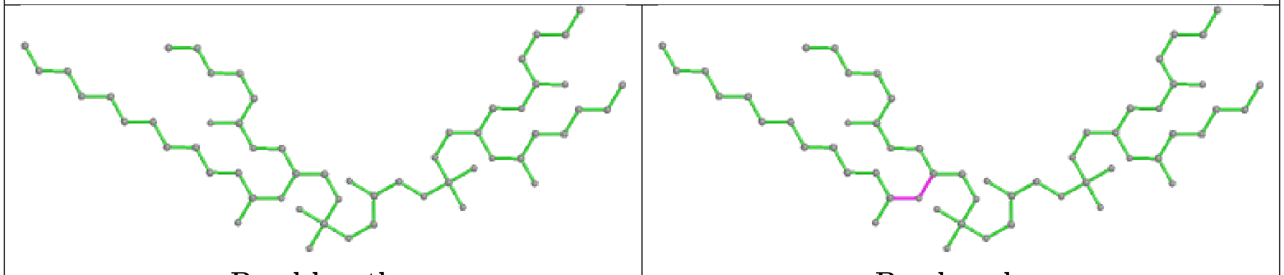


Bond lengths Bond angles



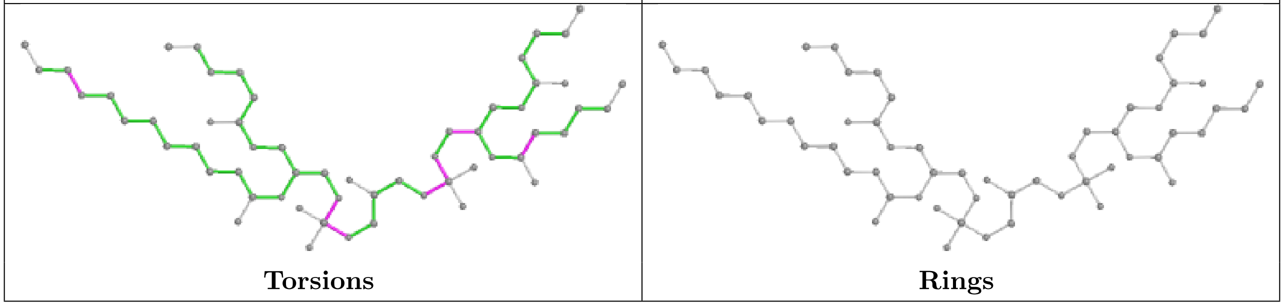
Torsions Rings

Ligand CDL r1 202



Bond lengths

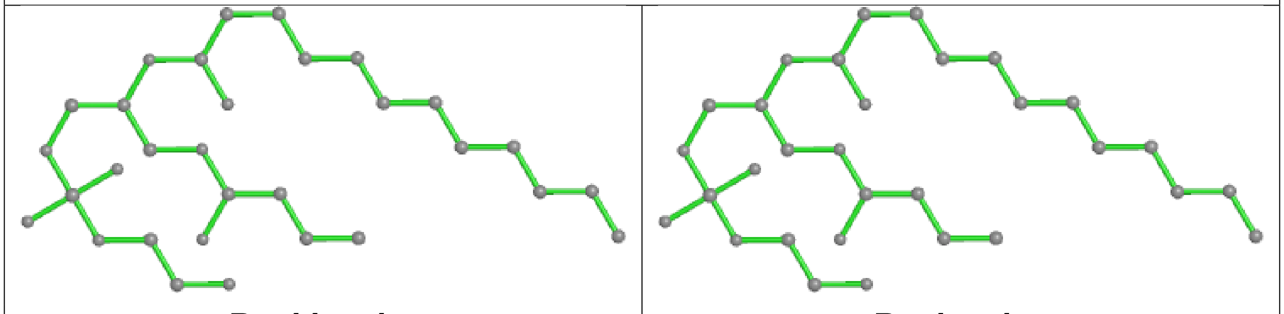
Bond angles



Torsions

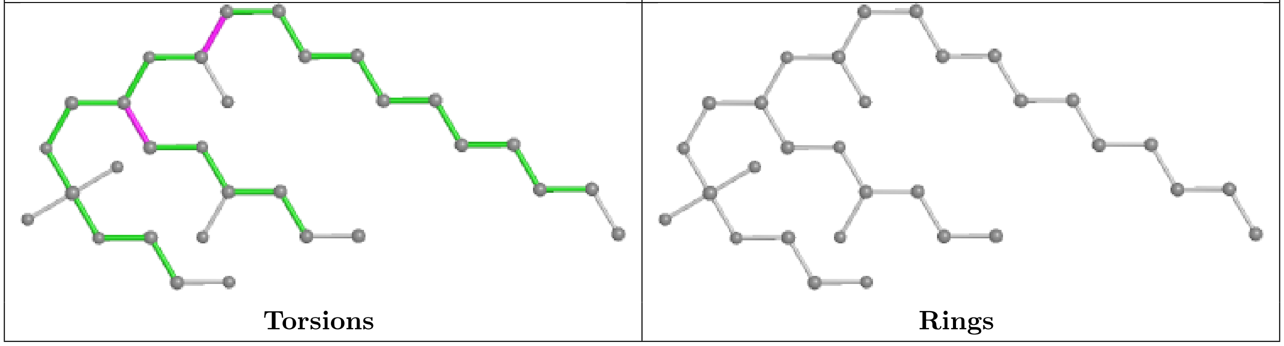
Rings

Ligand 3PE C 404



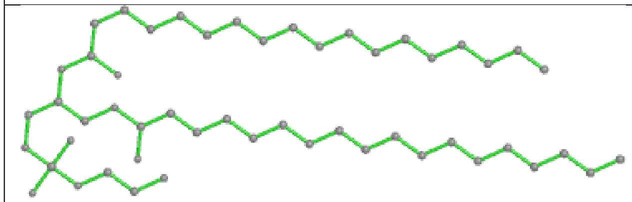
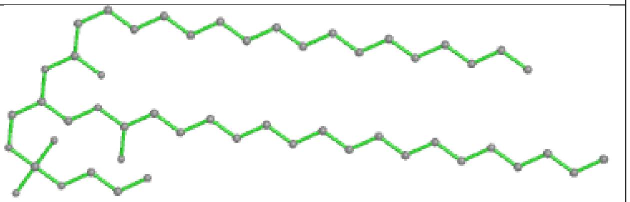
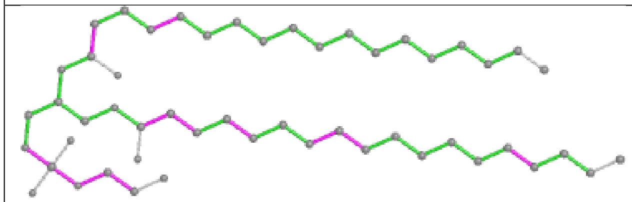
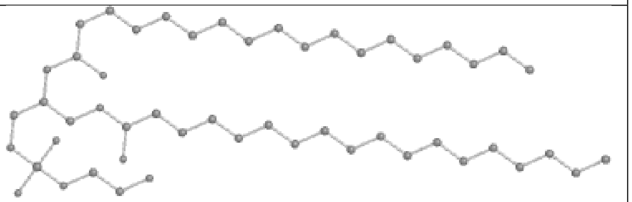
Bond lengths

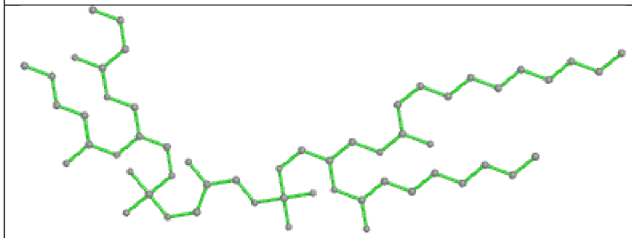
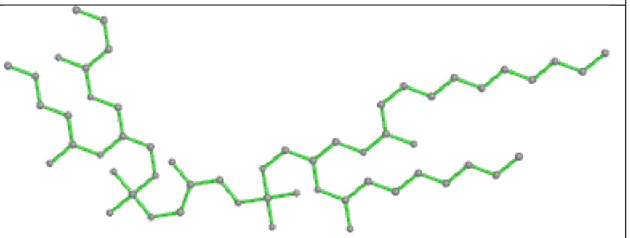
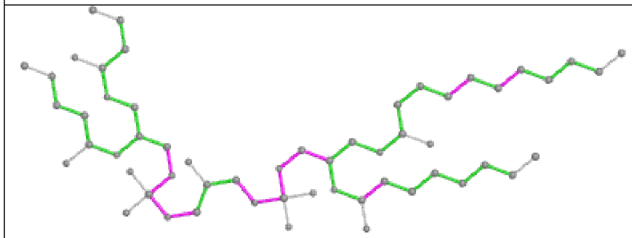
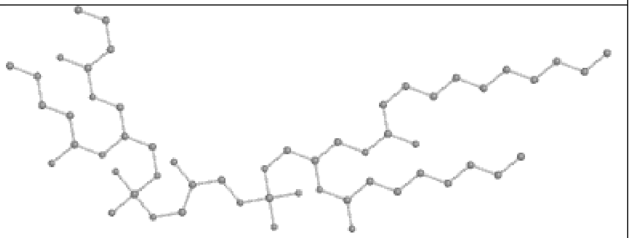
Bond angles



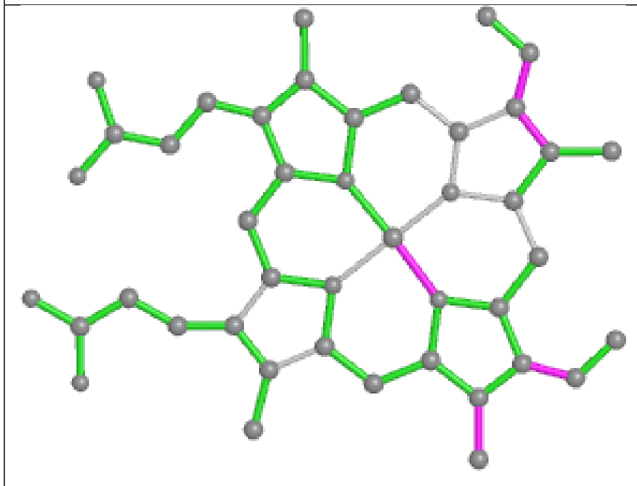
Torsions

Rings

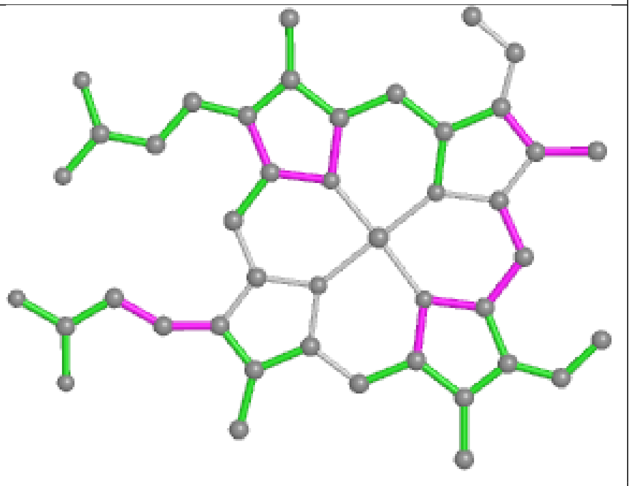
Ligand 3PE M1 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL D 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

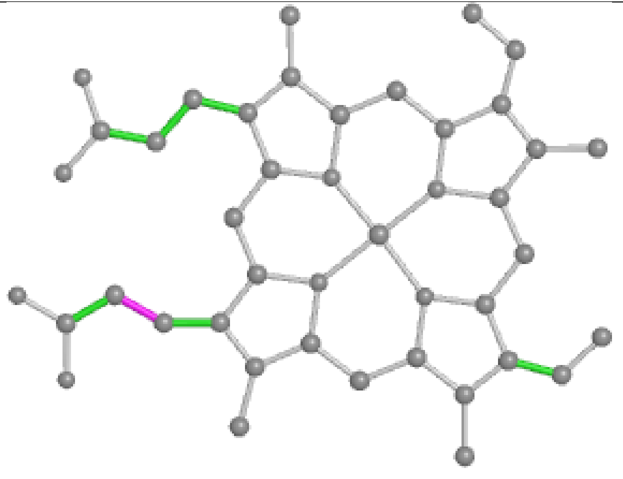
Ligand HEM C 402



Bond lengths



Bond angles



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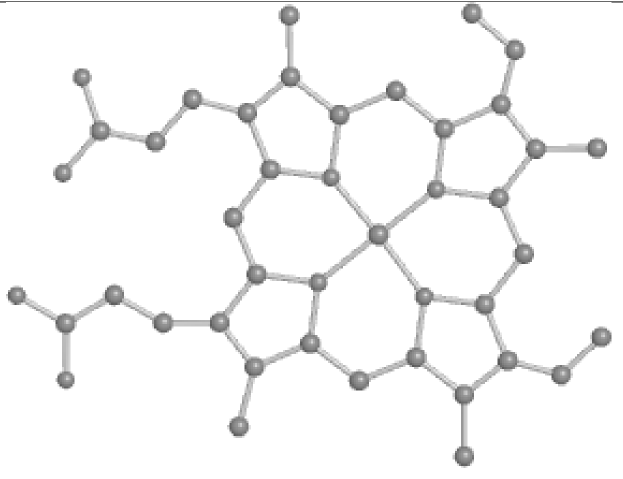
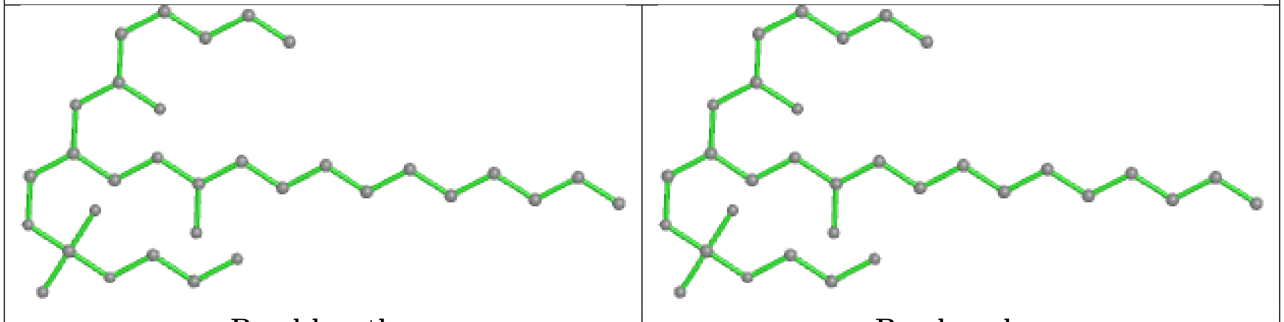
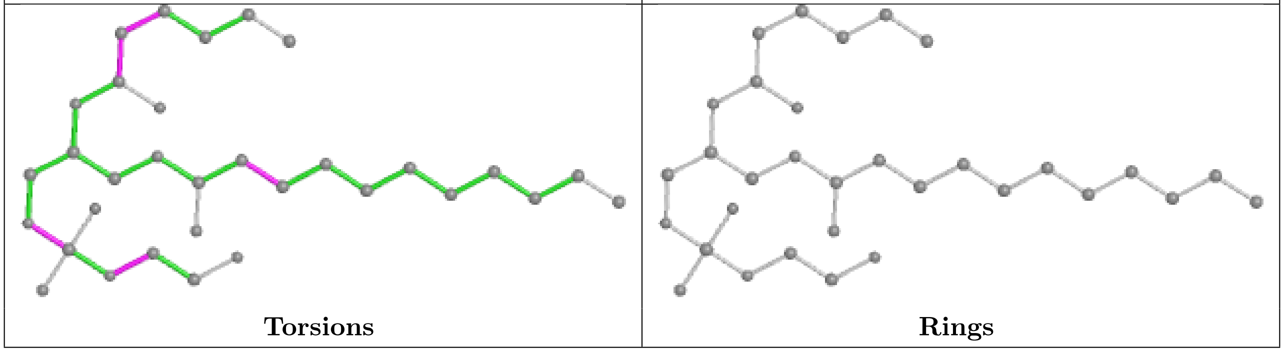


Rings

Ligand 3PE d1 203



Bond lengths **Bond angles**



Torsions **Rings**

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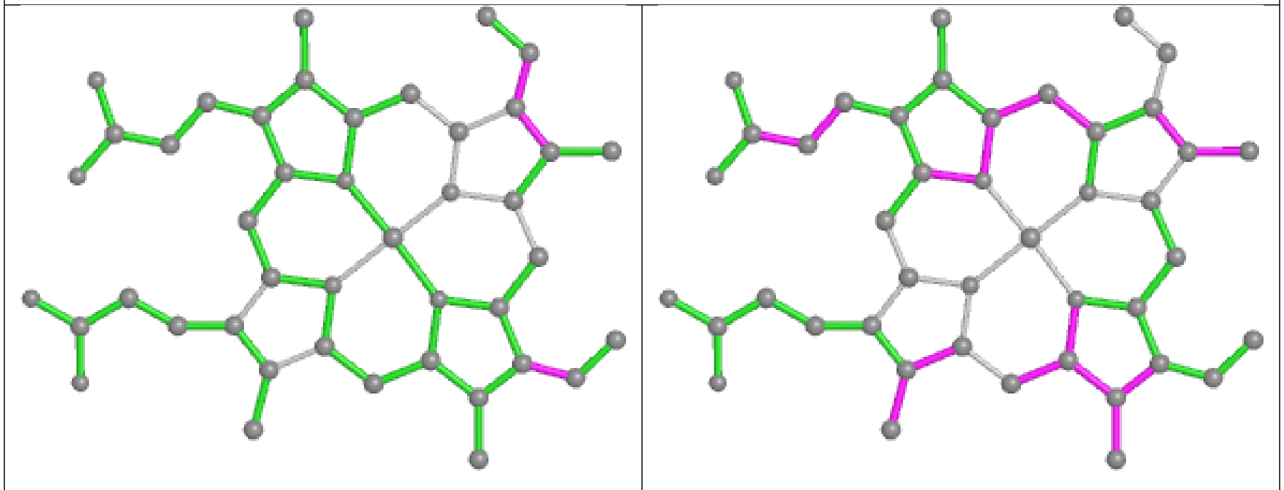
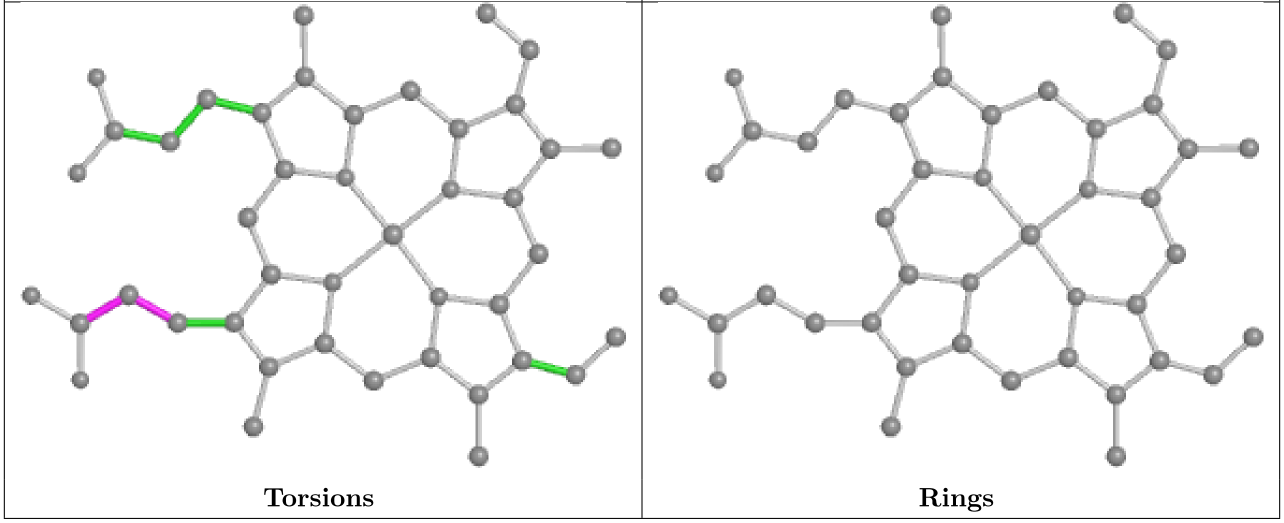
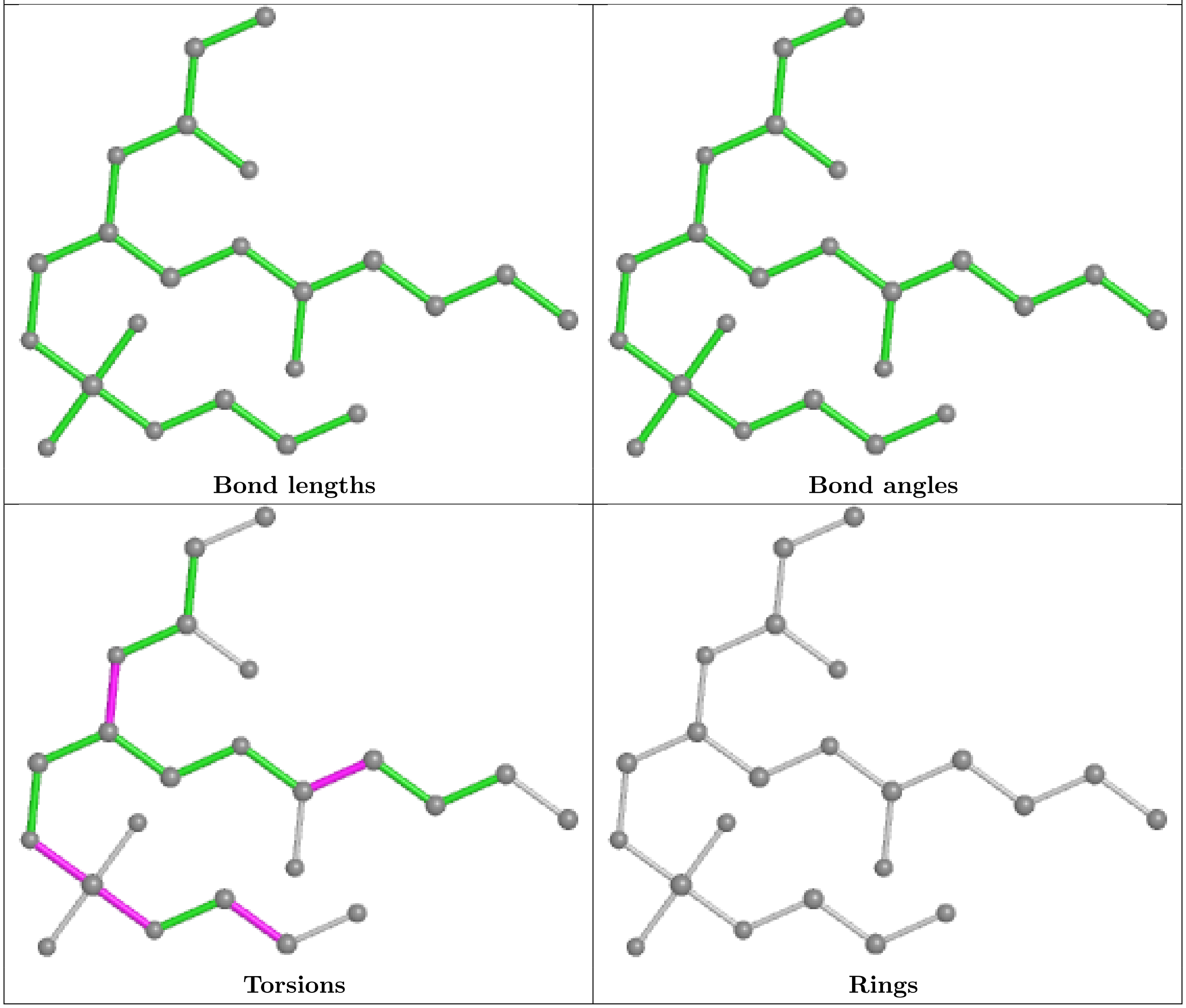


Bond lengths **Bond angles**



Torsions **Rings**

Ligand 3PE A 501



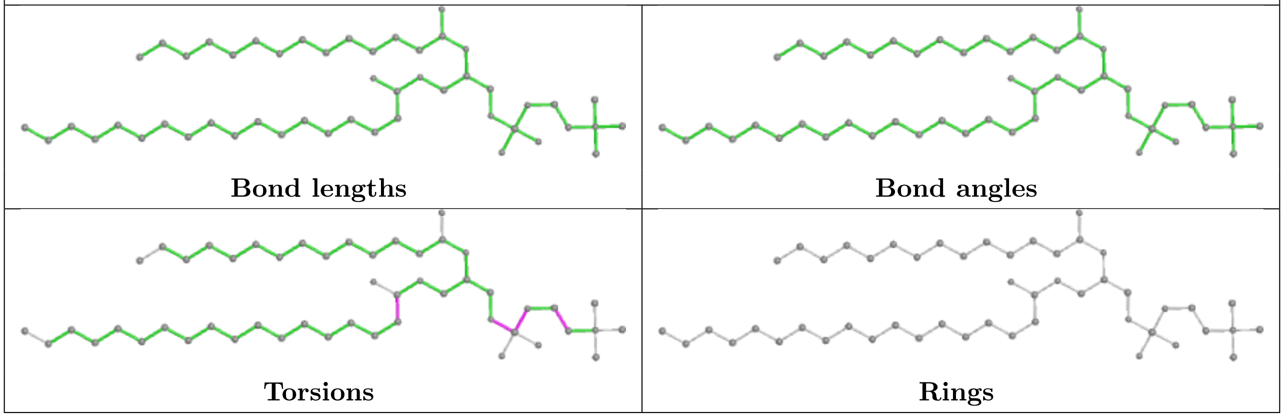
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 g 302



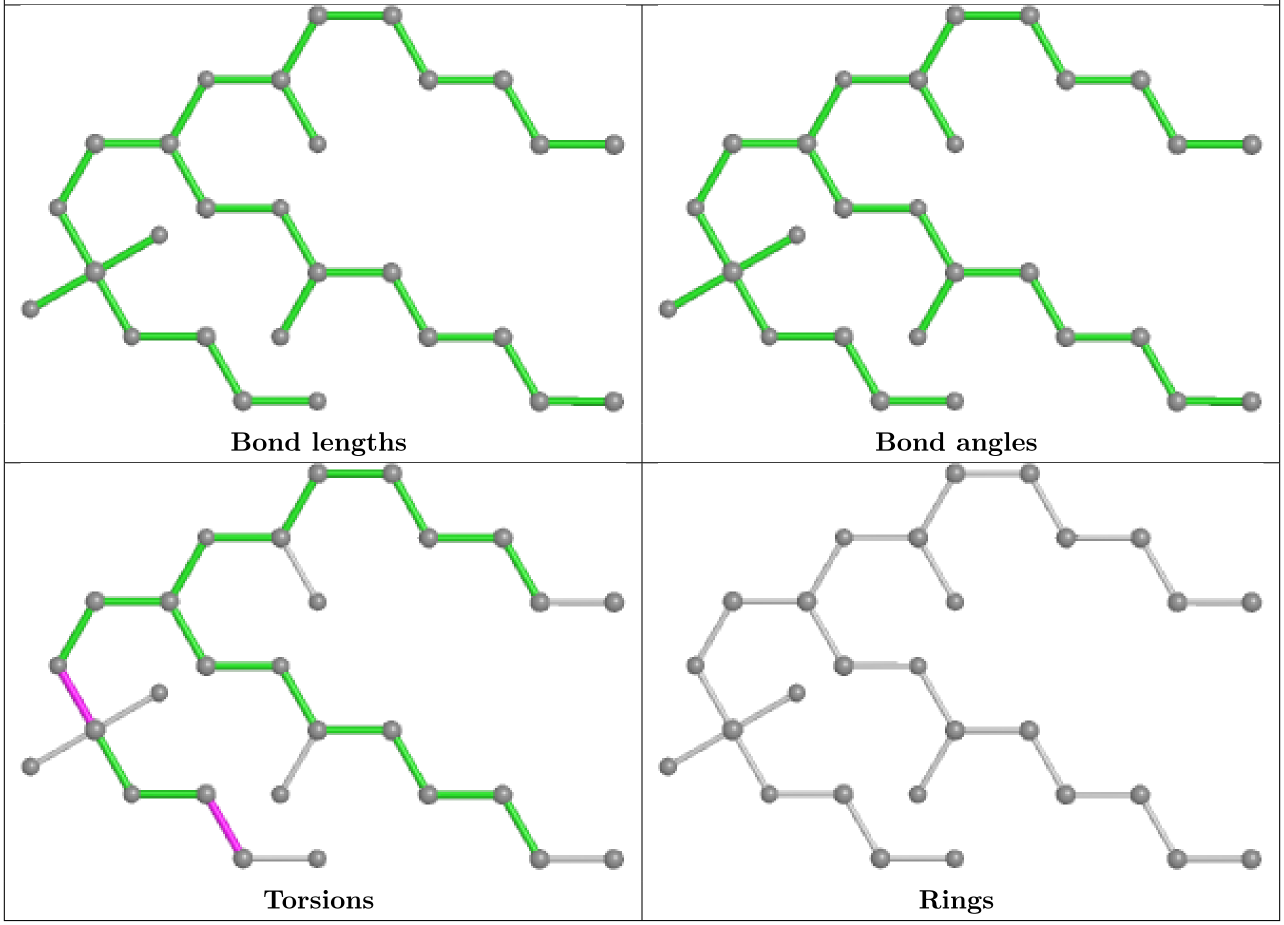
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Y1 402



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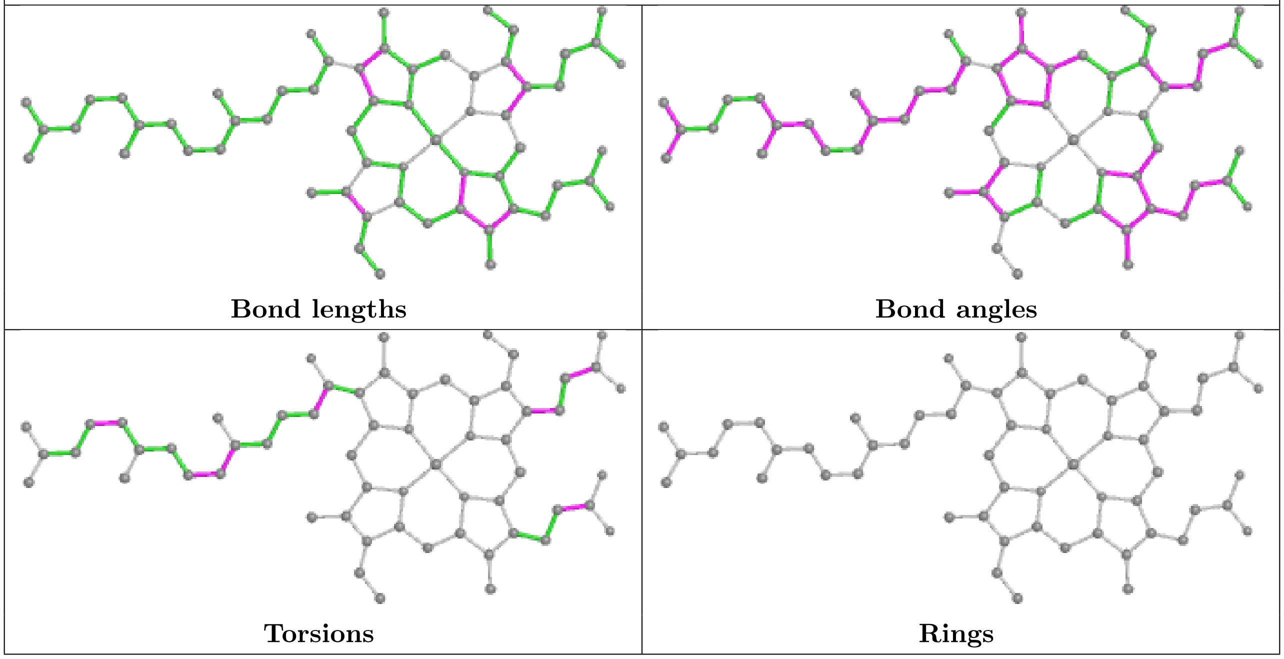
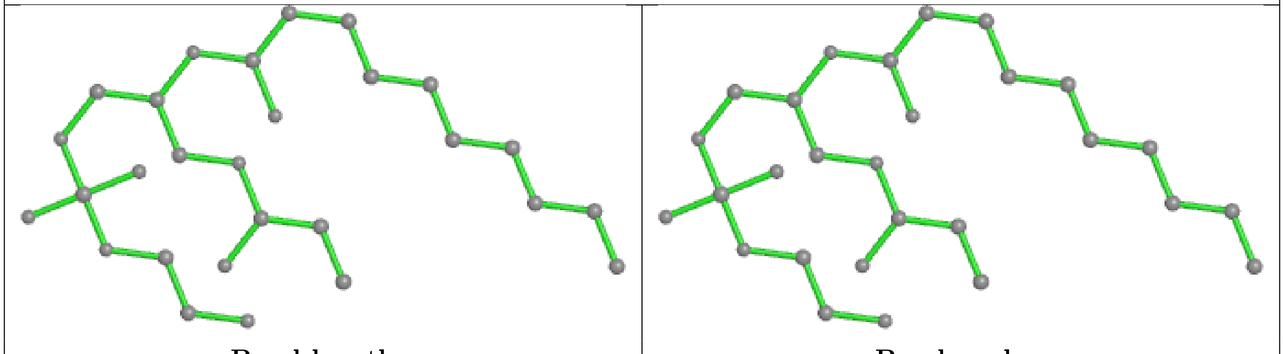
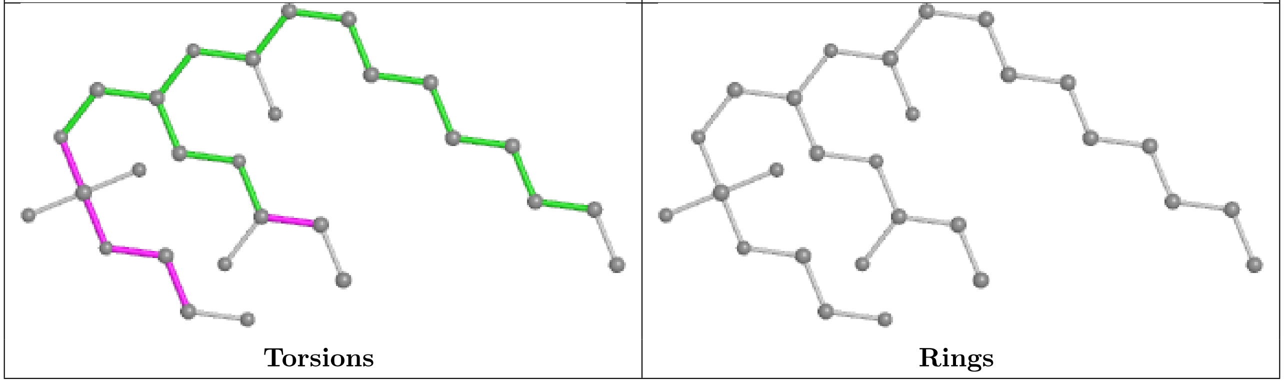


Ligand 3PE i 101

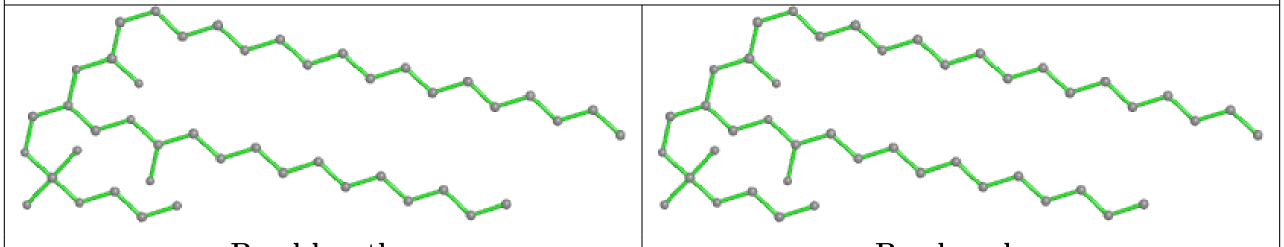


Bond lengths Bond angles

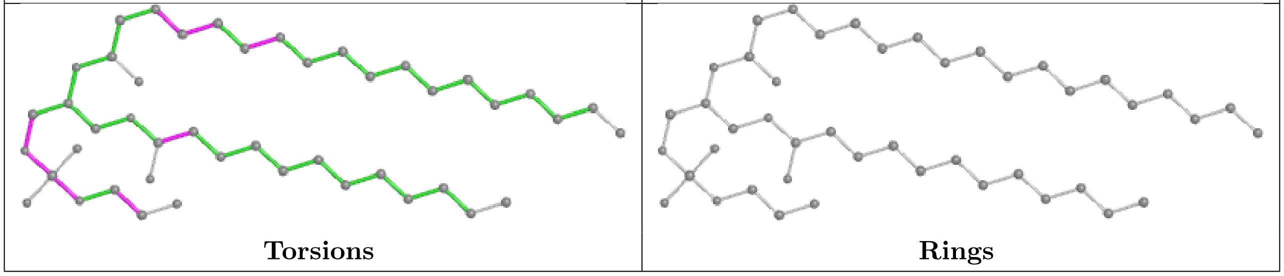


Torsions Rings

Ligand 3PE p 301



Bond lengths Bond angles



Torsions Rings

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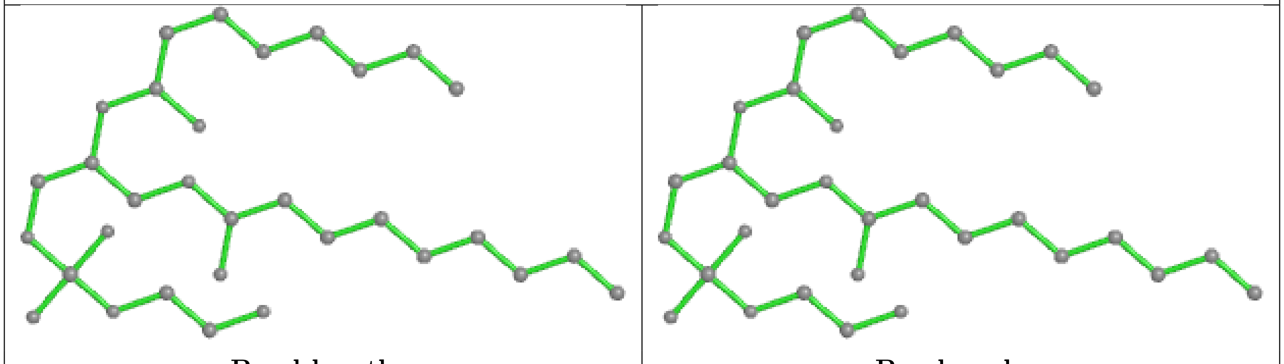
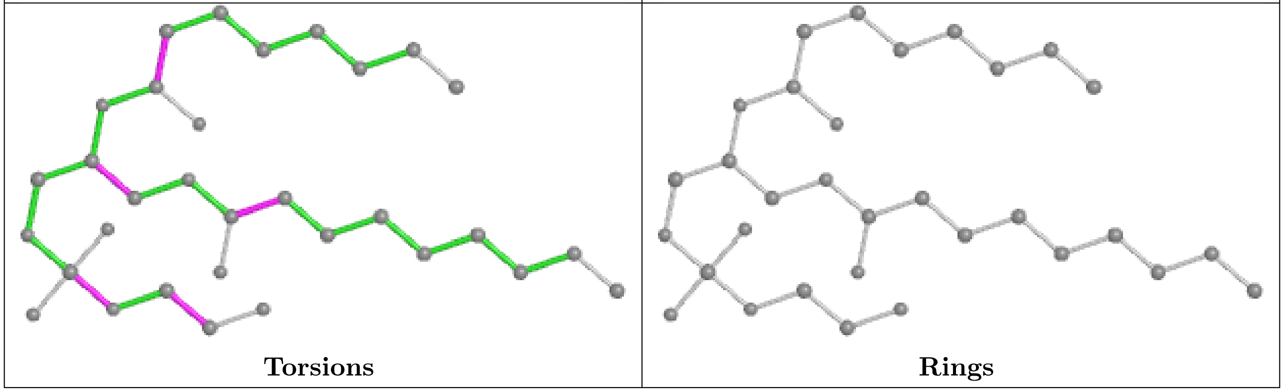
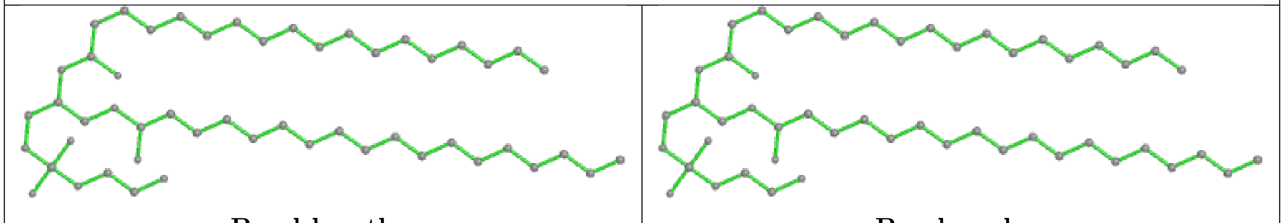


Bond lengths **Bond angles**

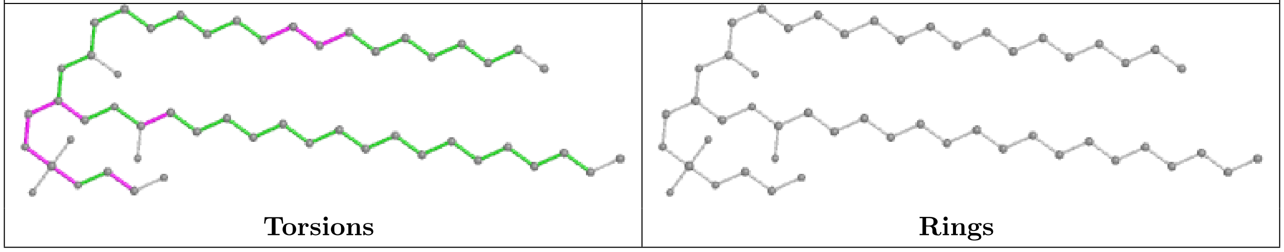


Torsions **Rings**

Ligand 3PE M1 503

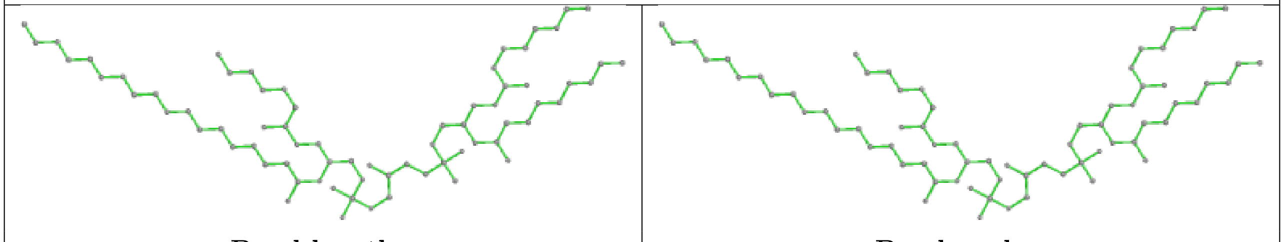


Bond lengths **Bond angles**



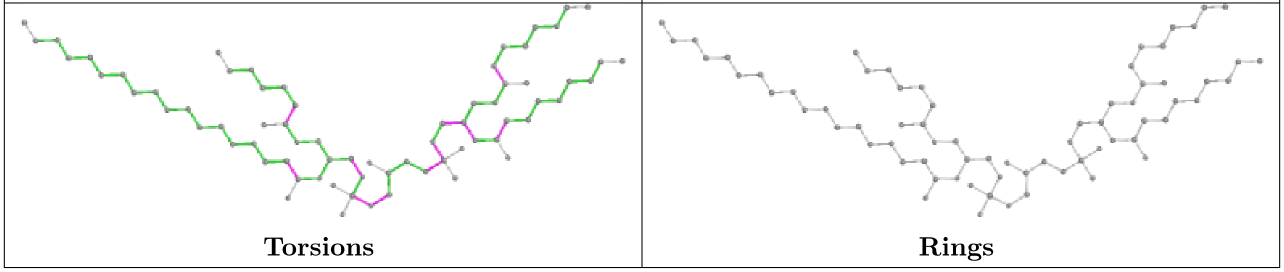
Torsions **Rings**

Ligand CDL h1 201



Bond lengths

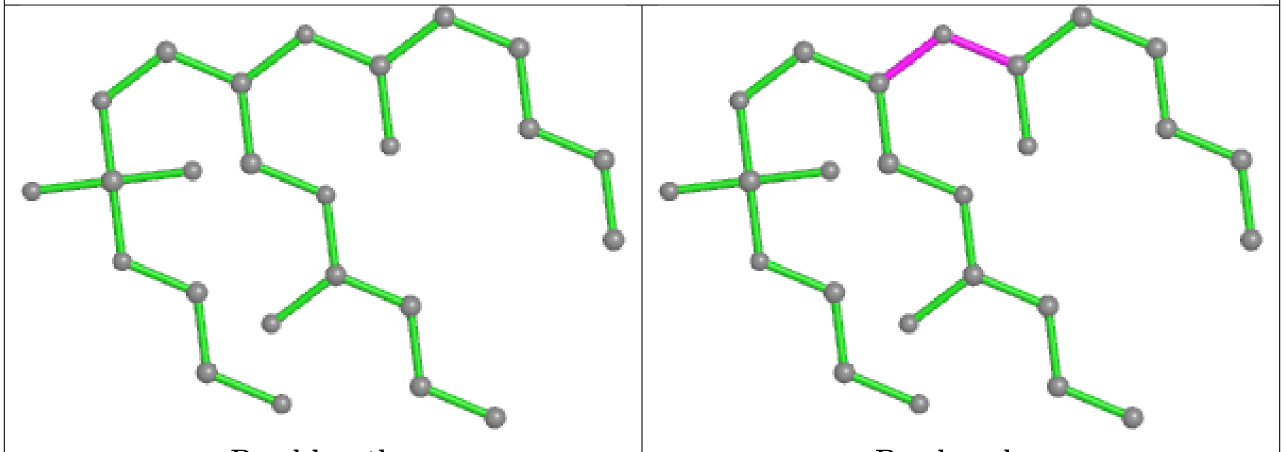
Bond angles



Torsions

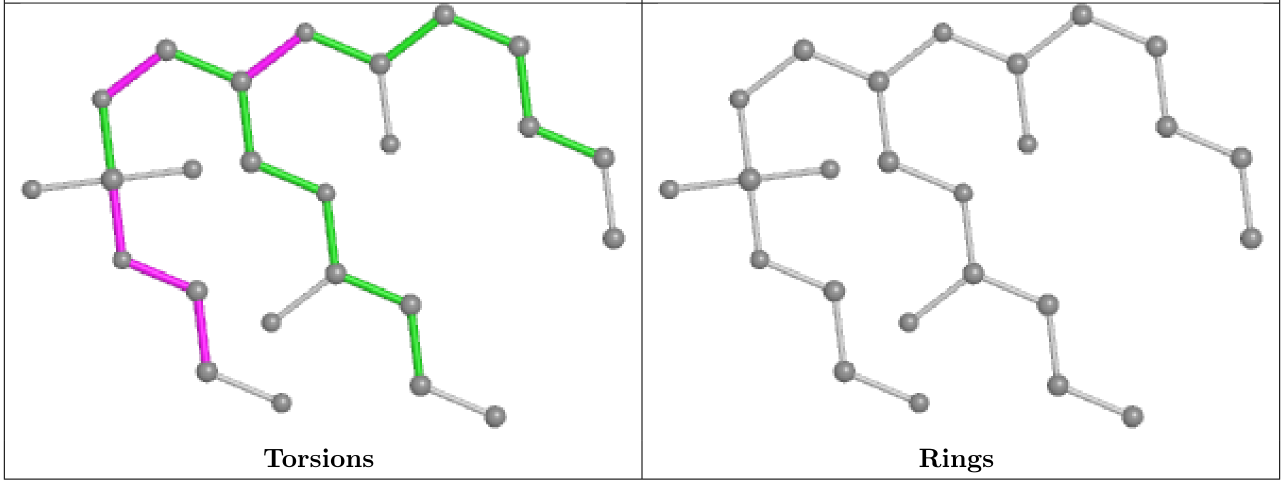
Rings

Ligand 3PE t 101



Bond lengths

Bond angles



Torsions

Rings

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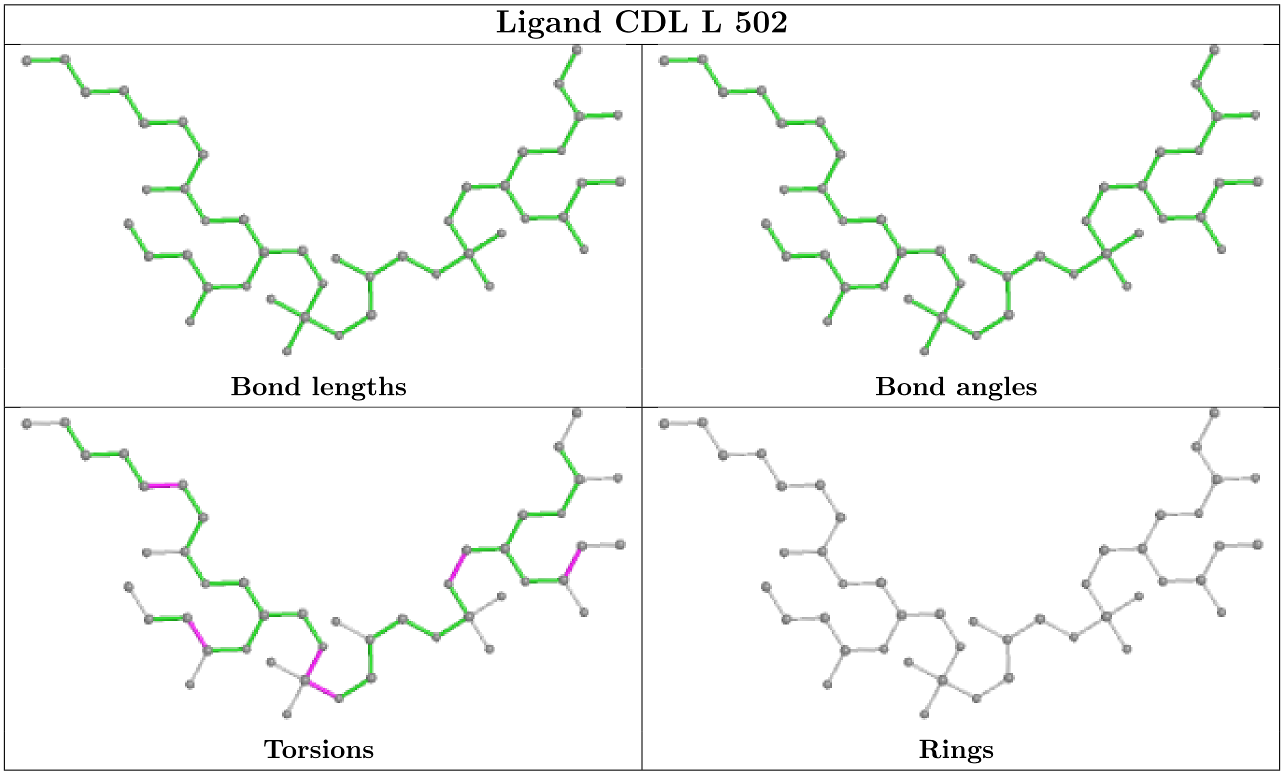
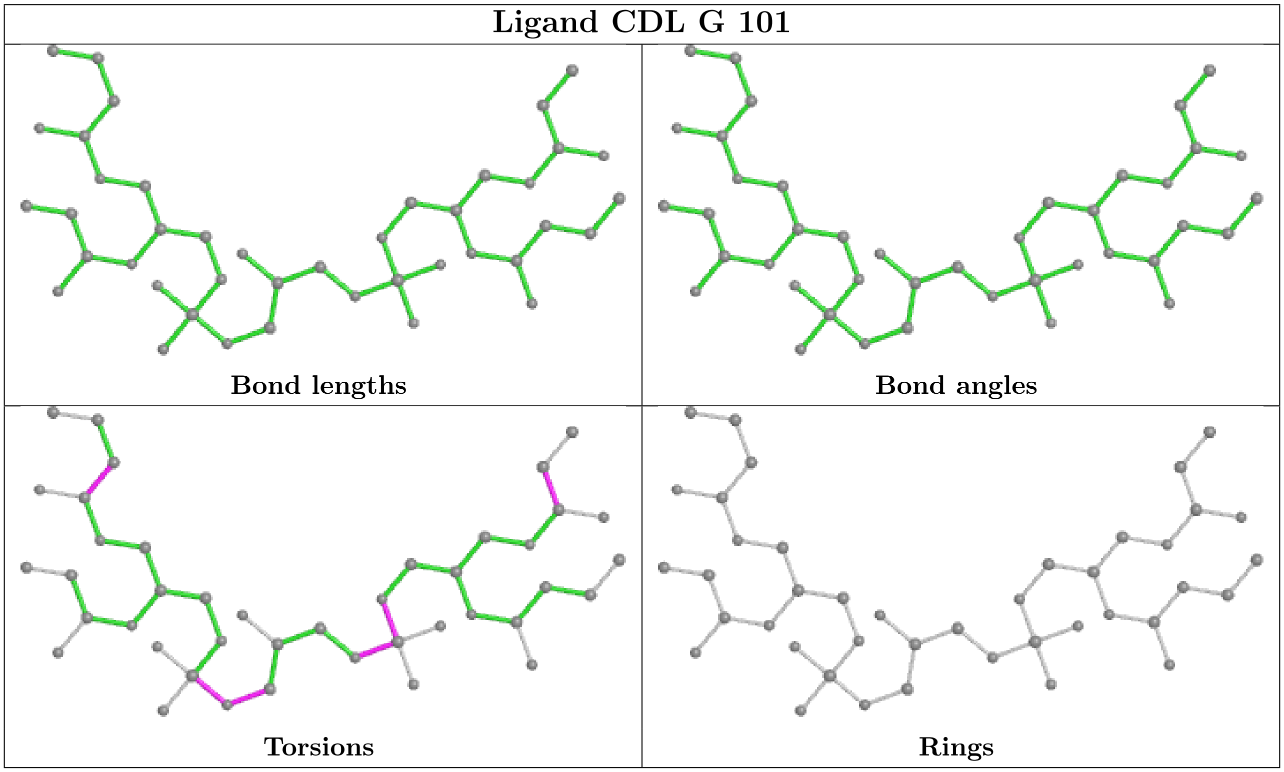


Bond lengths **Bond angles**

Torsions **Rings**

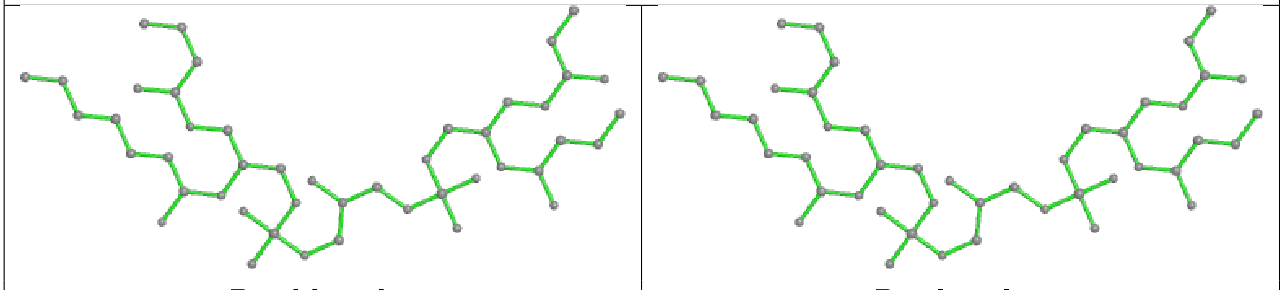
Ligand CDL G 101



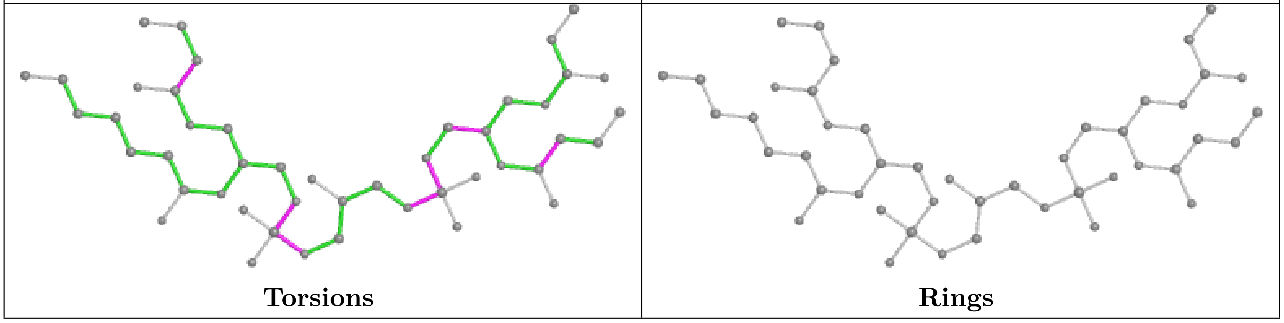
Bond lengths **Bond angles**

Torsions **Rings**

Ligand CDL L1 703



Bond lengths Bond angles



Torsions Rings

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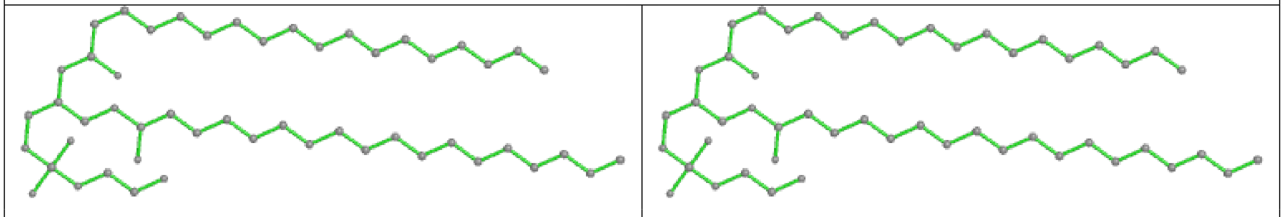
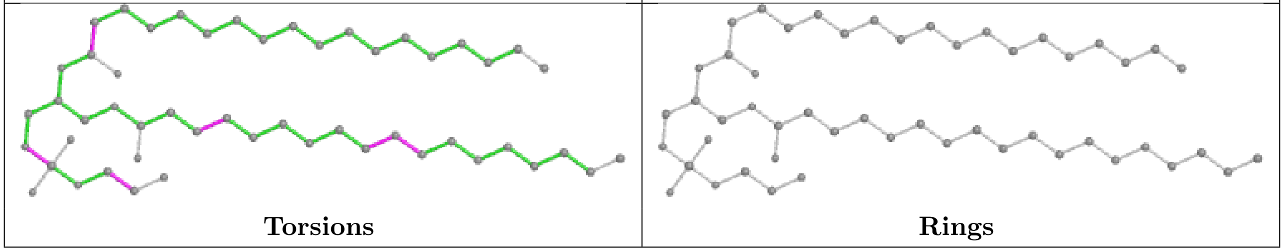
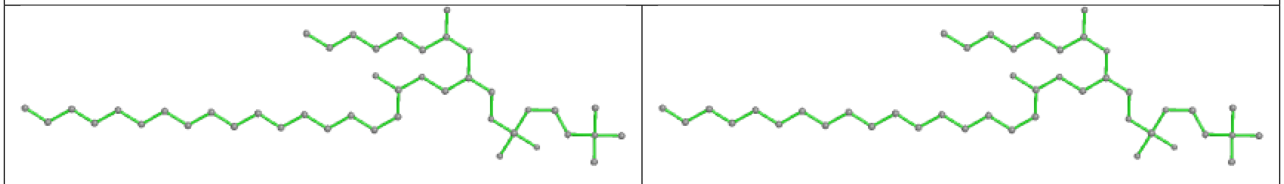


Bond lengths Bond angles



Torsions Rings

Ligand PC1 6 203



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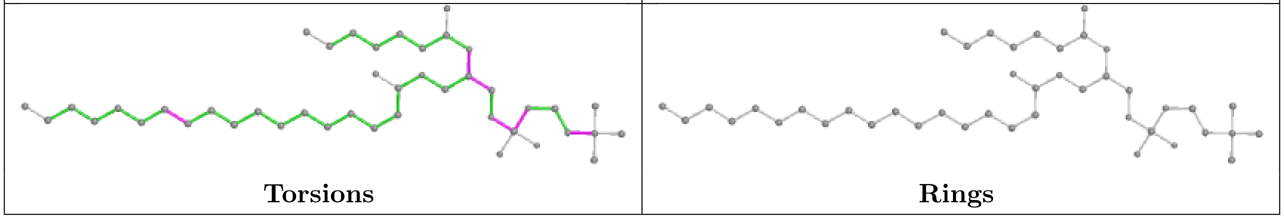

Torsions Rings

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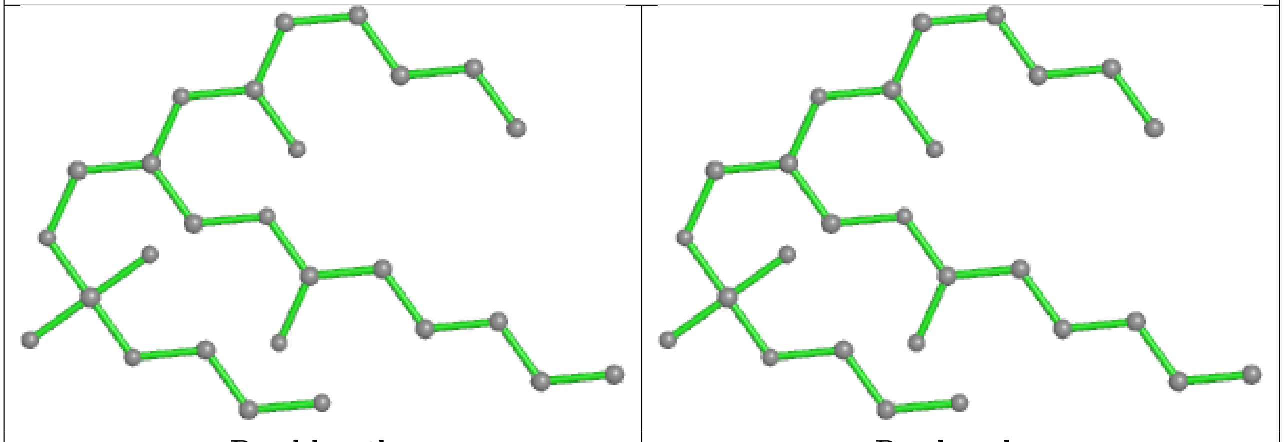
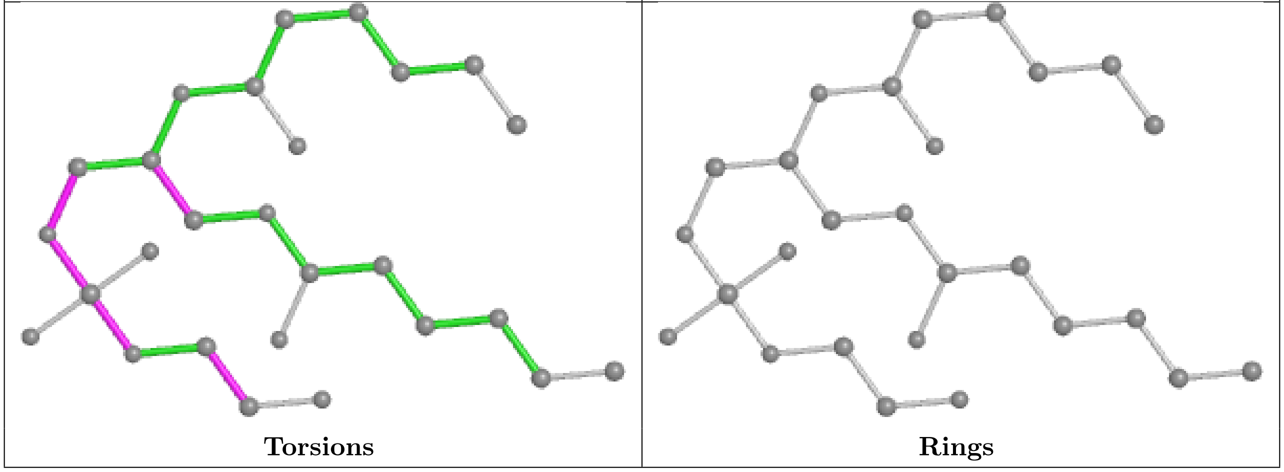
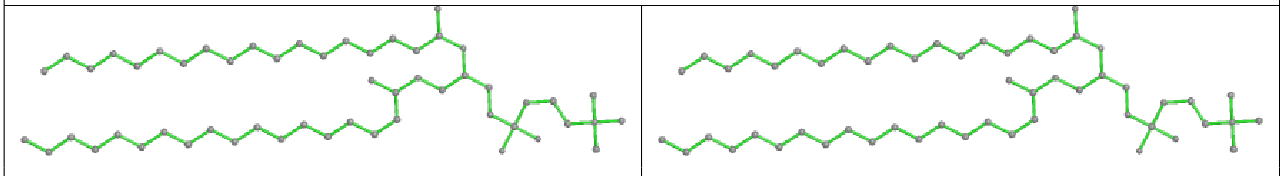


Bond lengths **Bond angles**

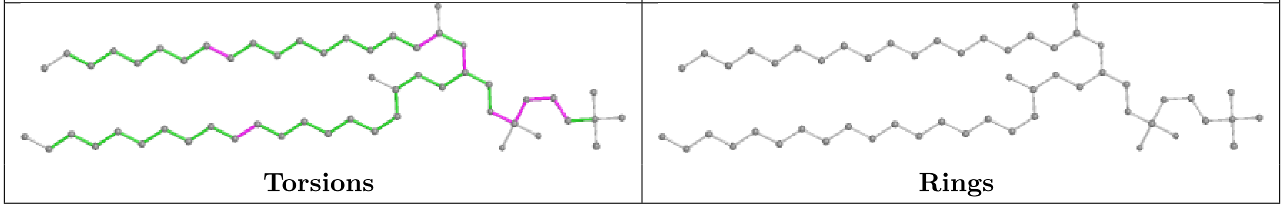


Torsions **Rings**

Ligand PC1 9 203

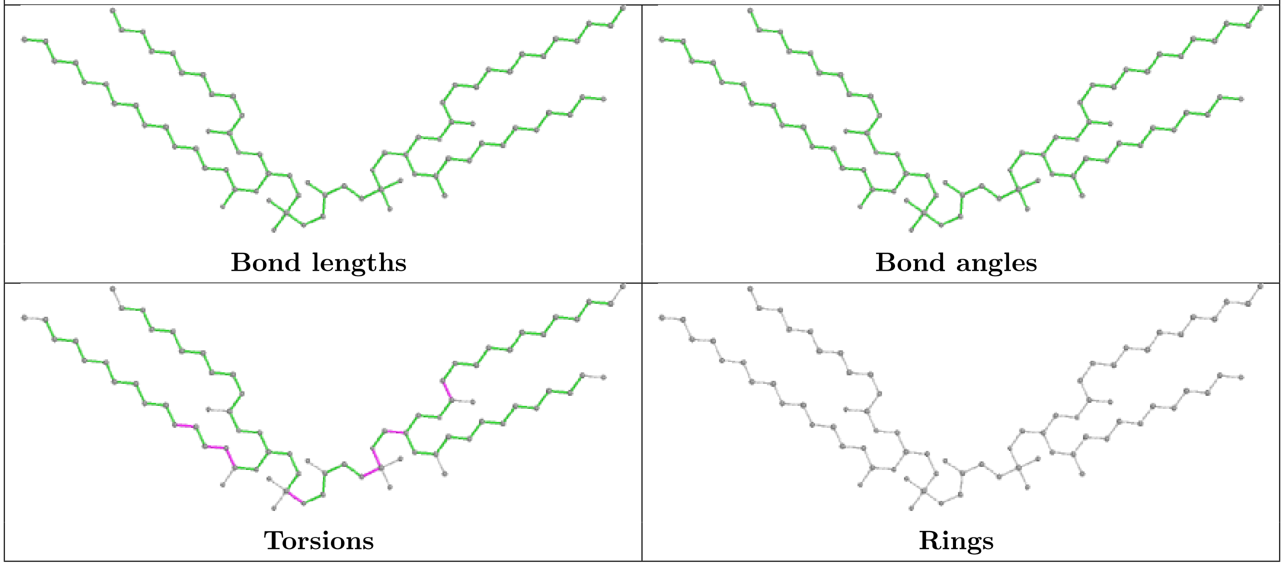


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CDL L1 702



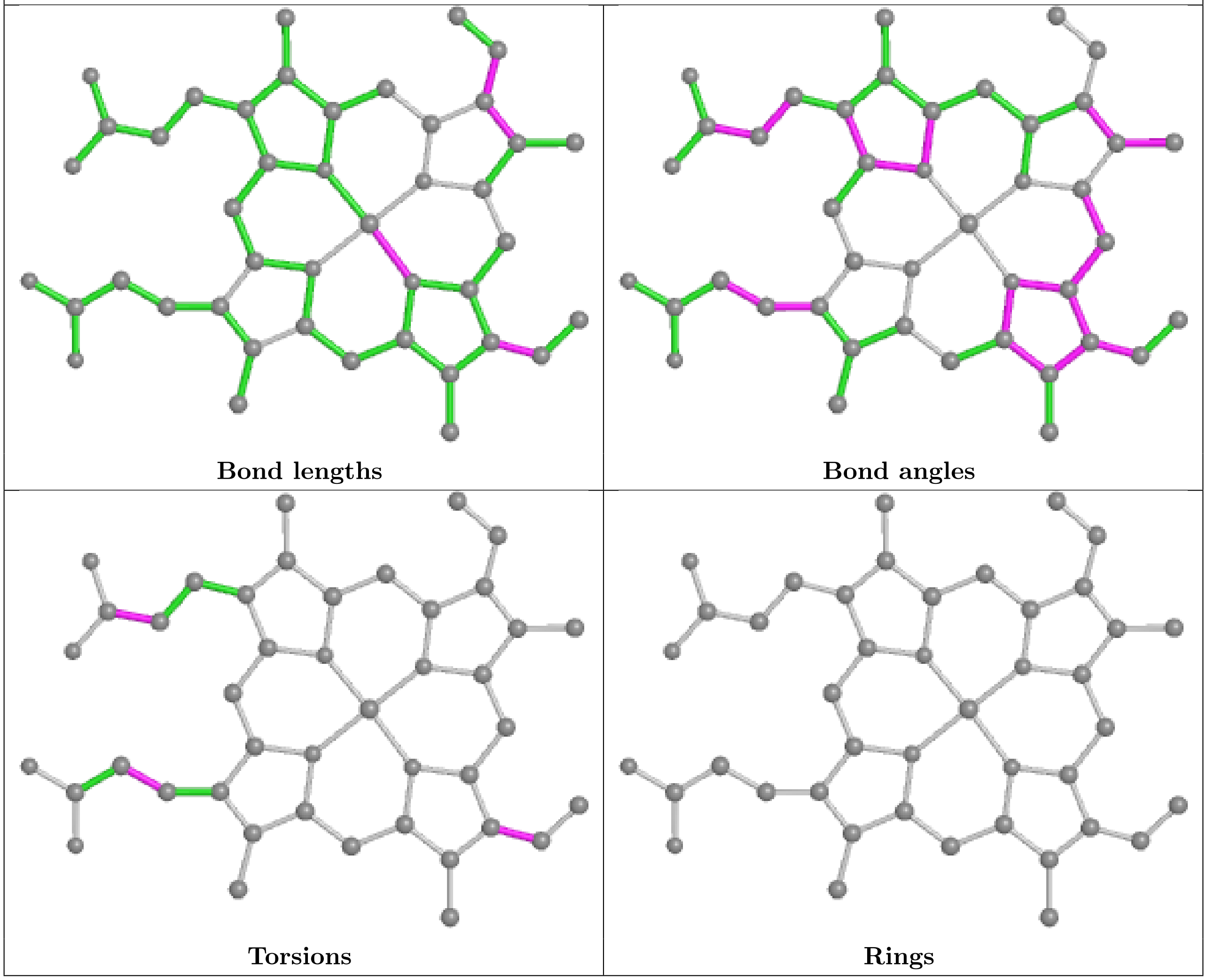
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM N 402



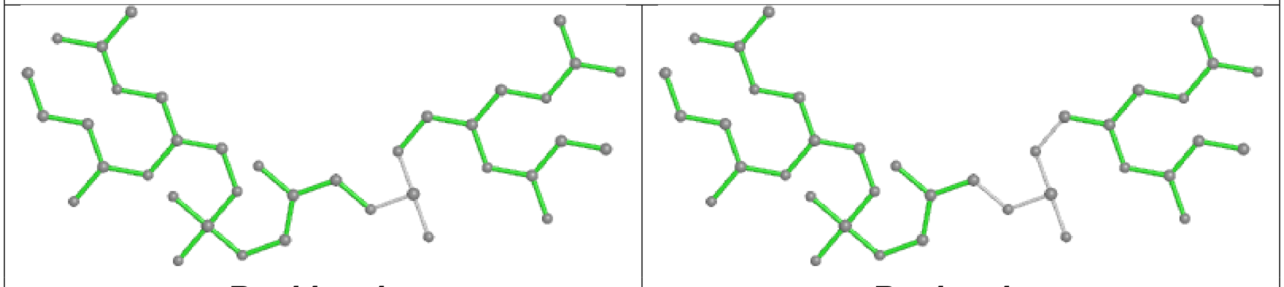
Bond lengths

Bond angles

Torsions

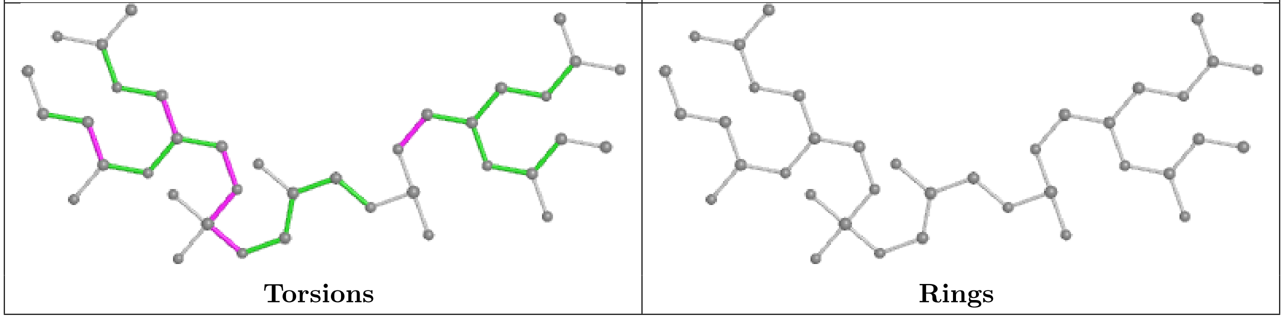
Rings

Ligand CDL g 301



Bond lengths

Bond angles



Torsions

Rings

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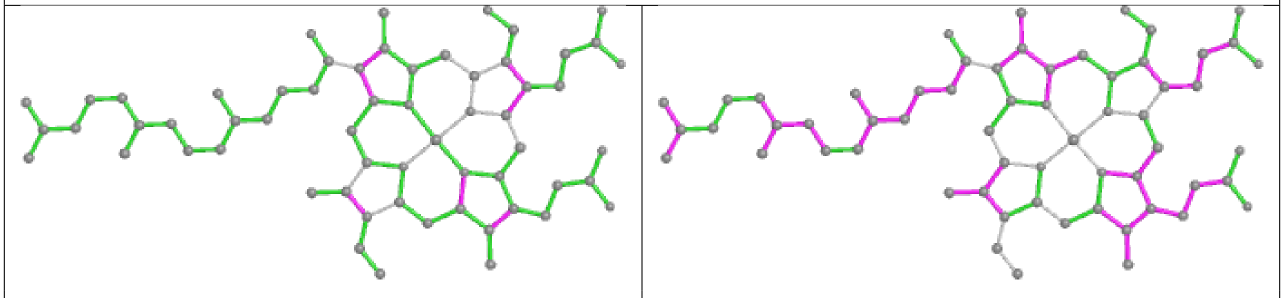
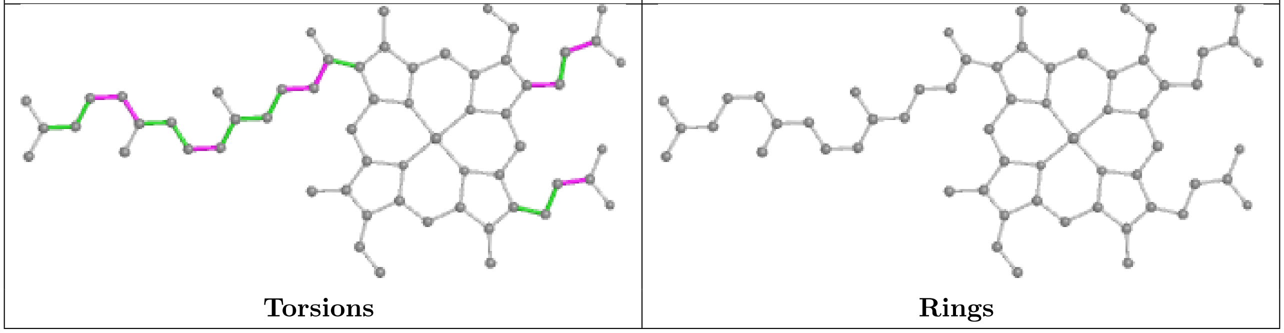


Bond lengths

Bond angles



Torsions

Rings

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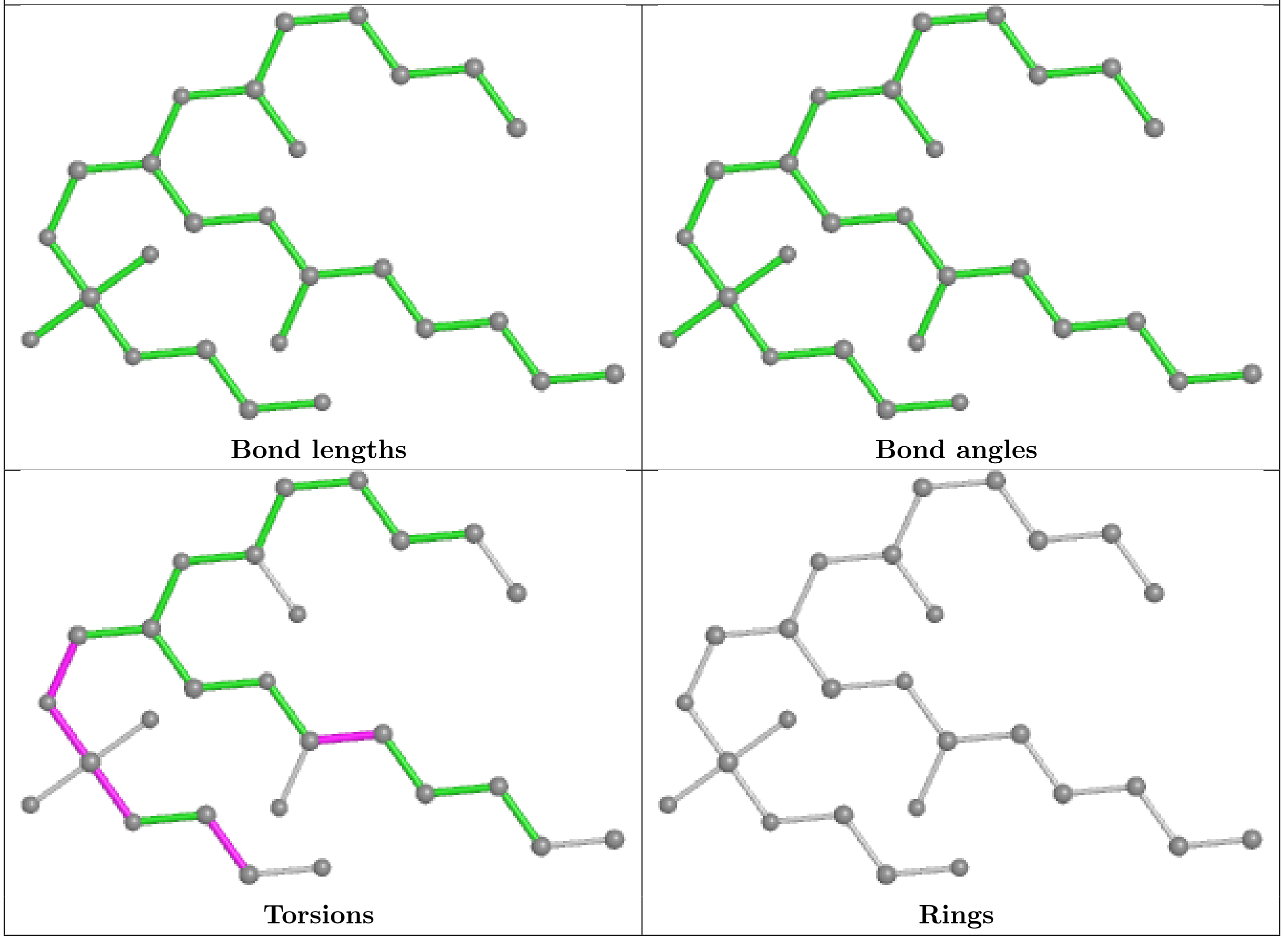


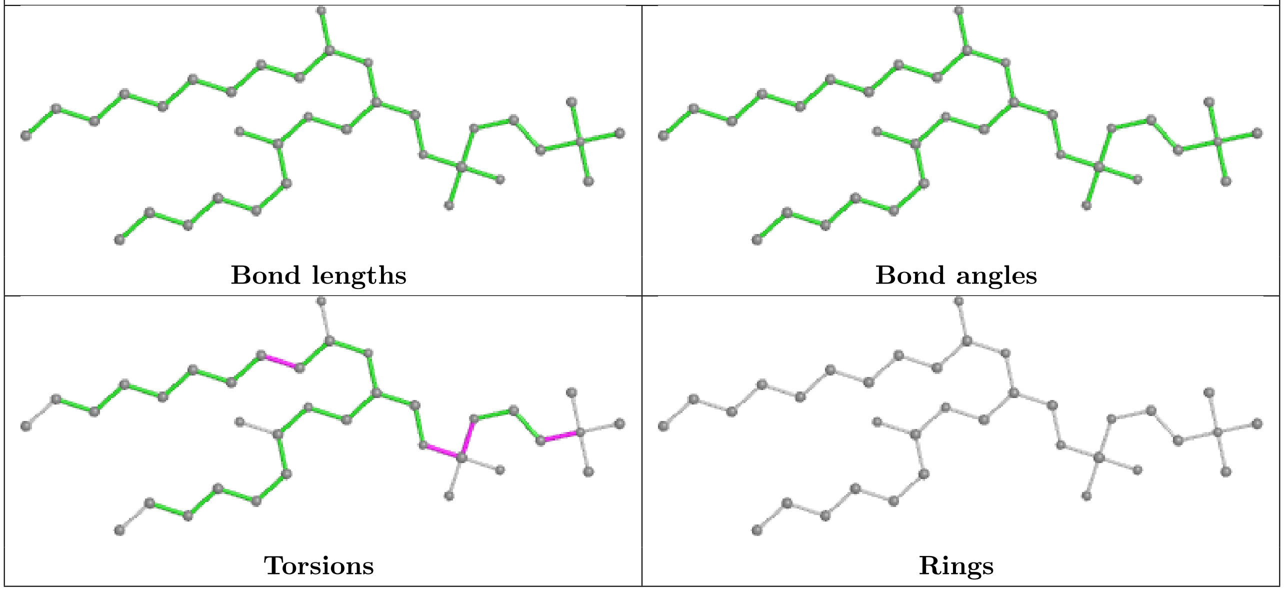
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 p 302



Bond lengths

Bond angles

Torsions

Rings

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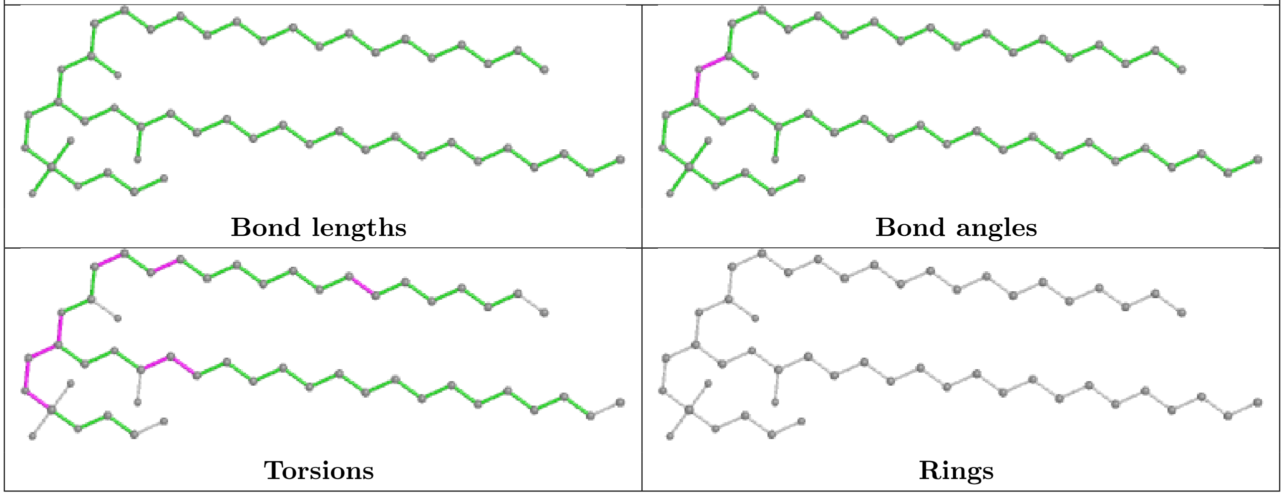

Bond lengths

Bond angles

Torsions

Rings

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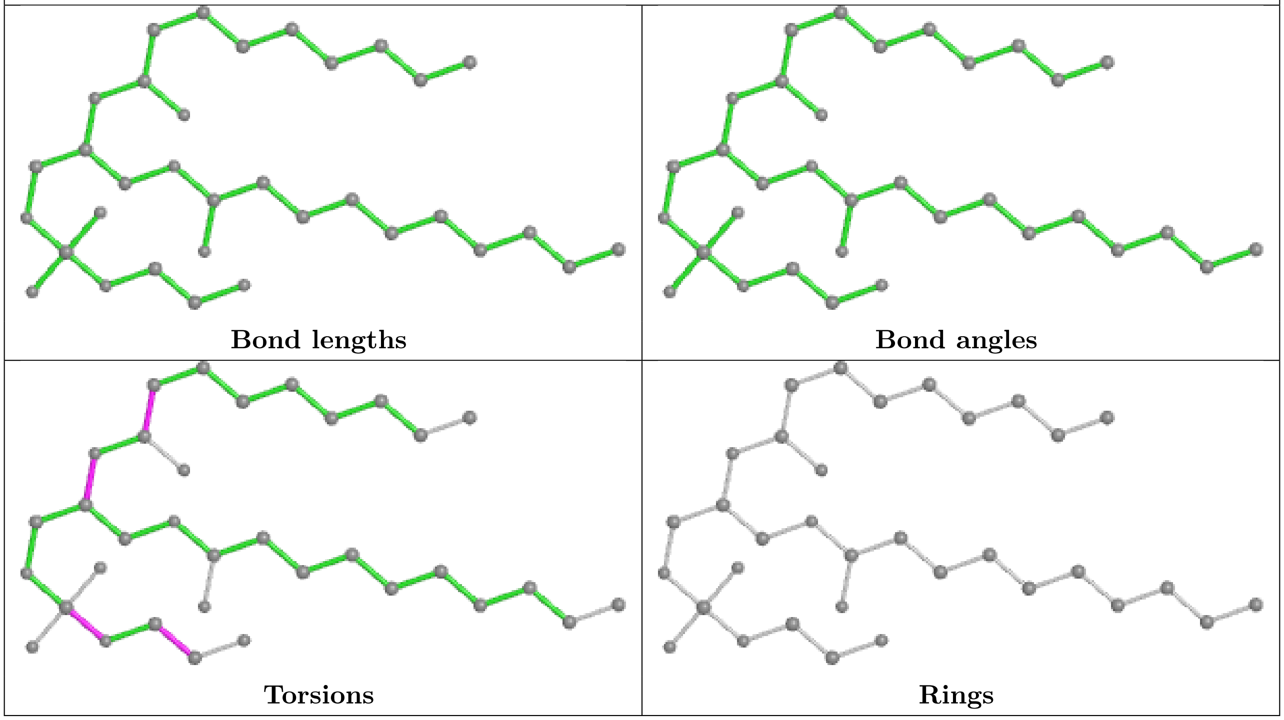

Bond lengths

Bond angles

Torsions

Rings

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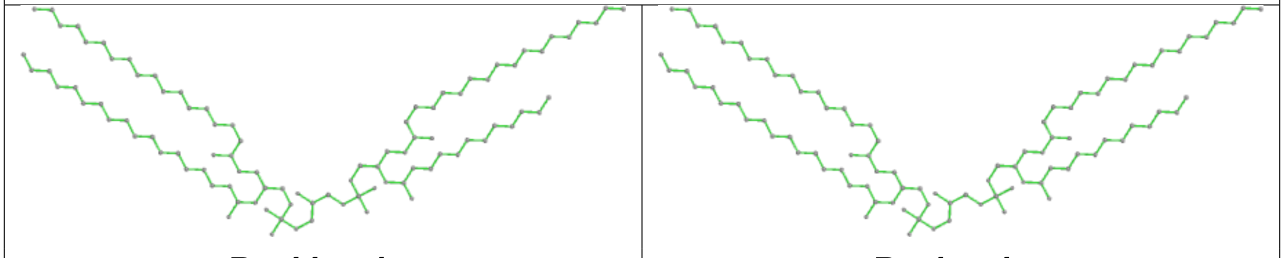
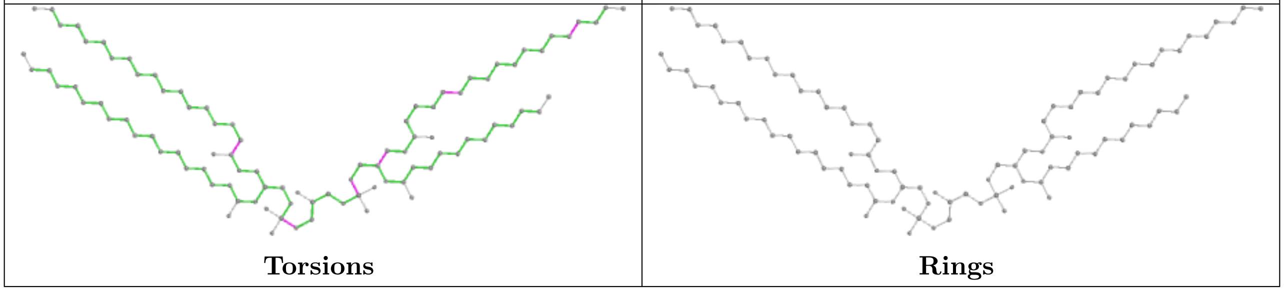


Bond lengths Bond angles



Torsions Rings

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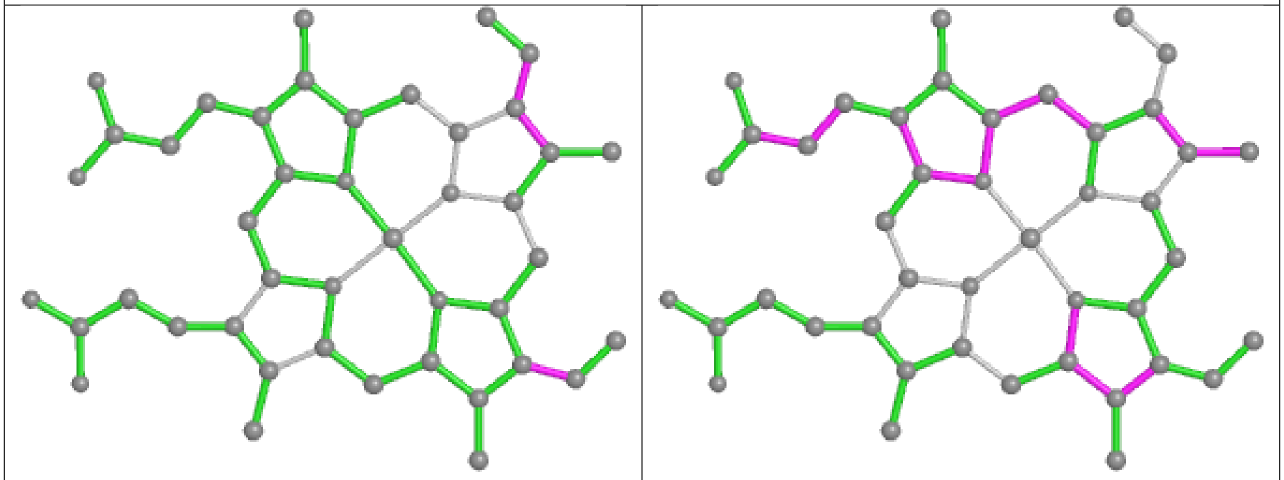
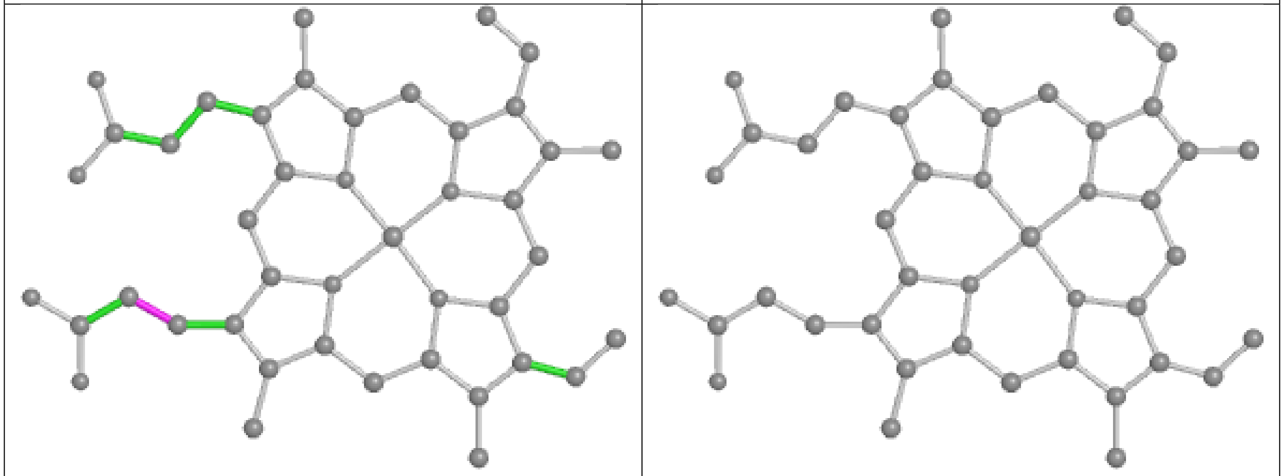
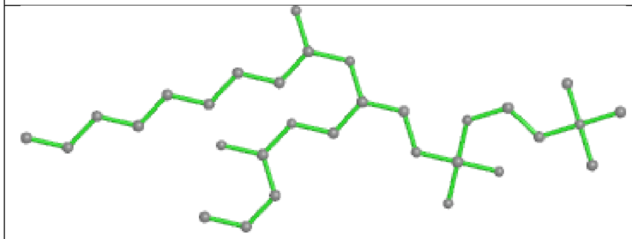


Bond lengths Bond angles

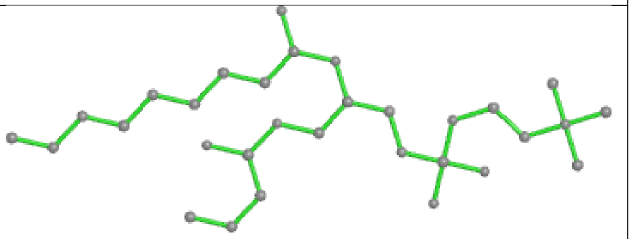


Torsions Rings

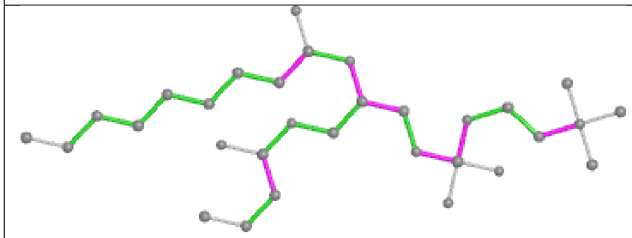
Ligand PC1 P1 502



Bond lengths



Bond angles



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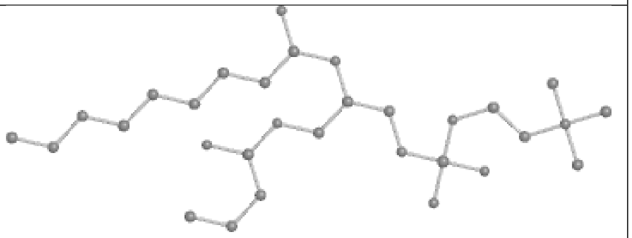
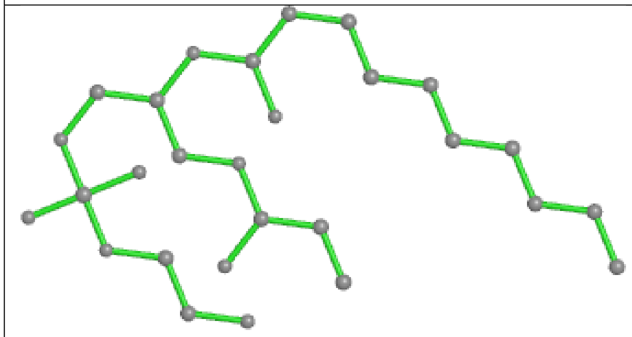


Rings

Ligand 3PE v 101



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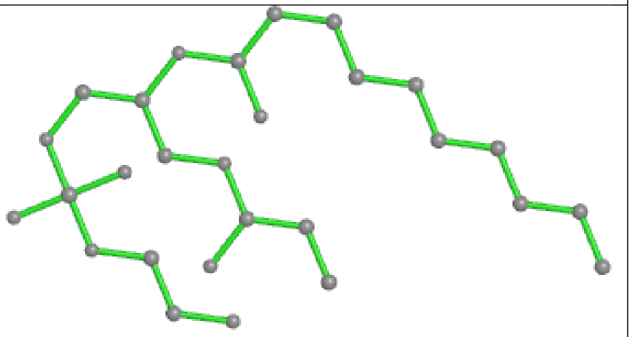
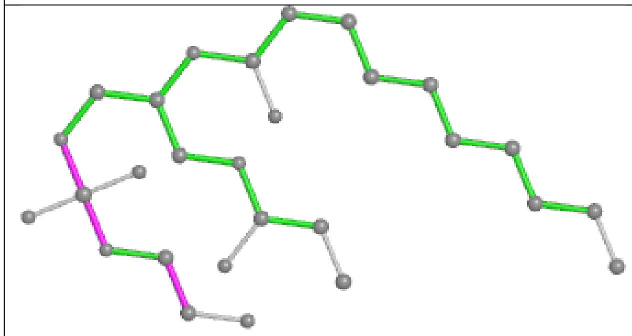


Bond angles



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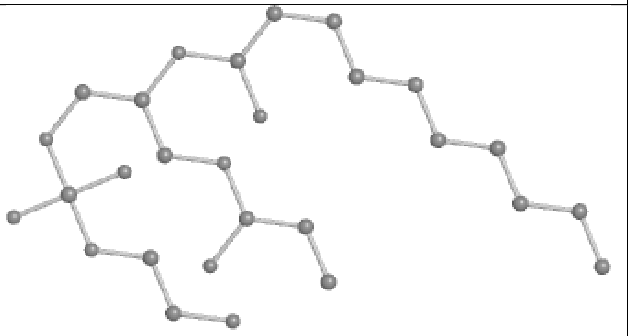
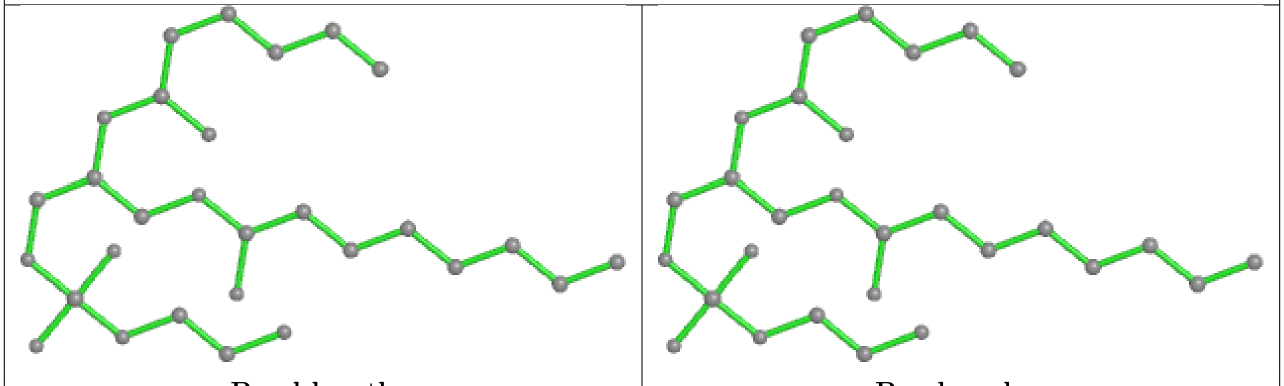
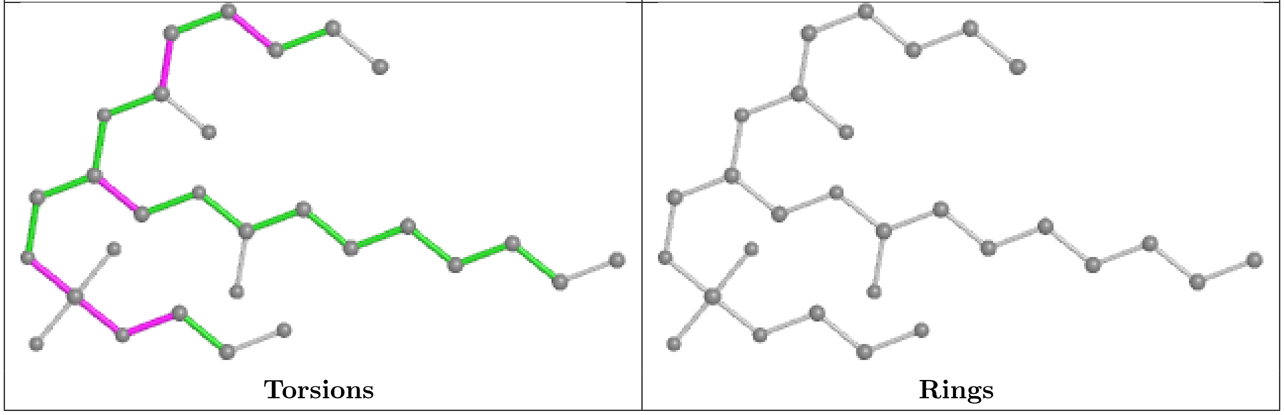


Rings

Ligand 3PE o 302

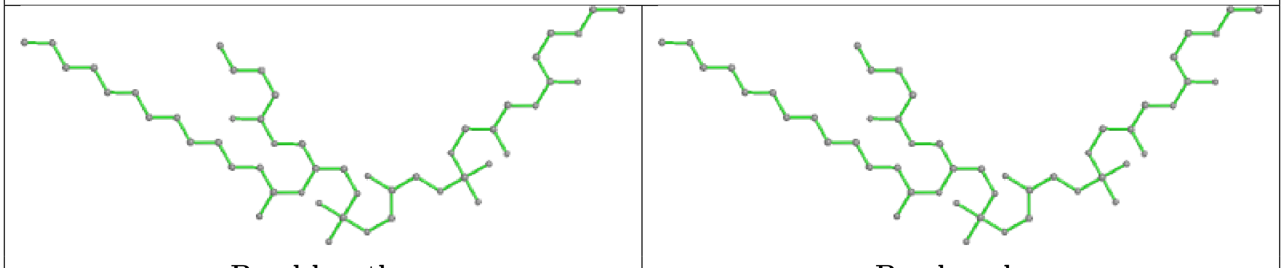


Bond lengths Bond angles

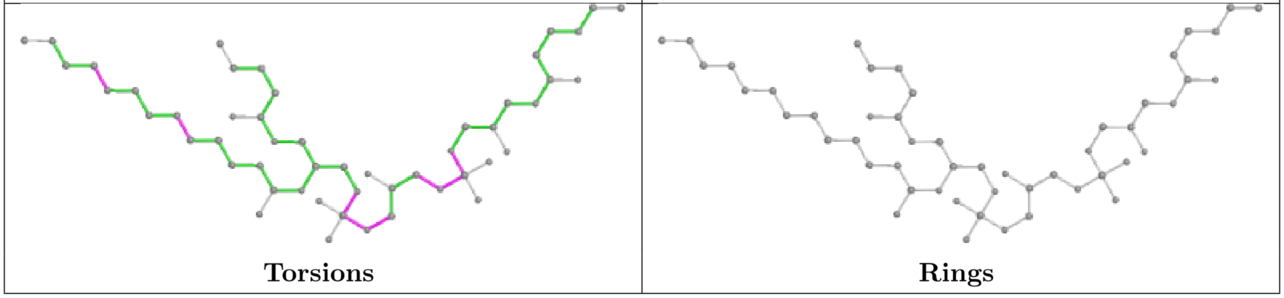


Torsions Rings

Ligand CDL H1 402

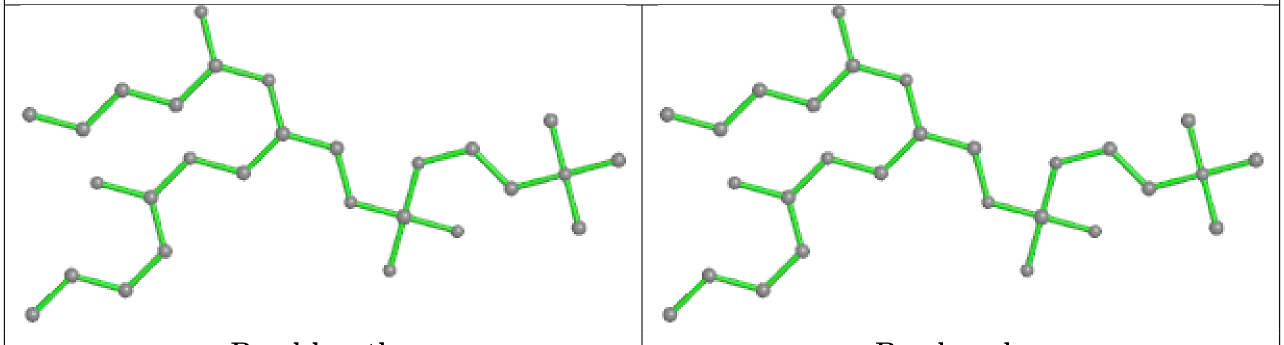


Bond lengths Bond angles



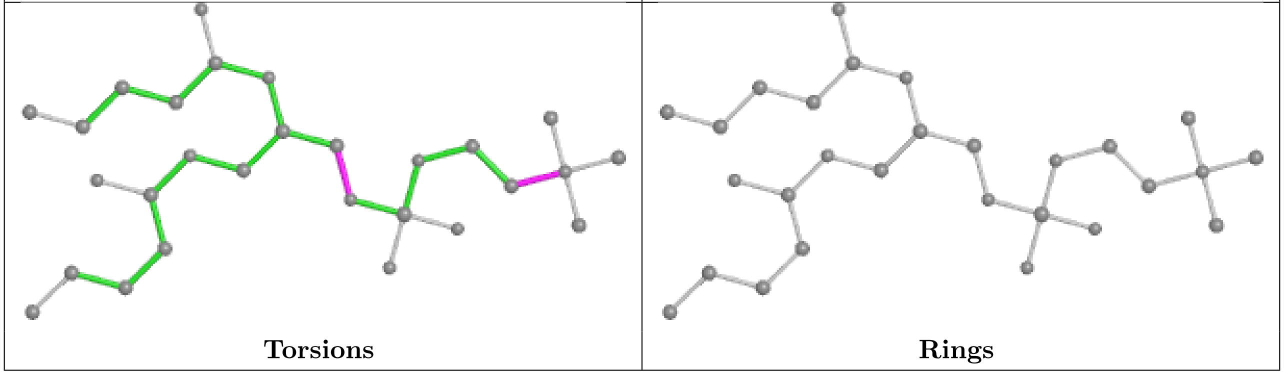
Torsions Rings

Ligand PC1 V 101



Bond lengths

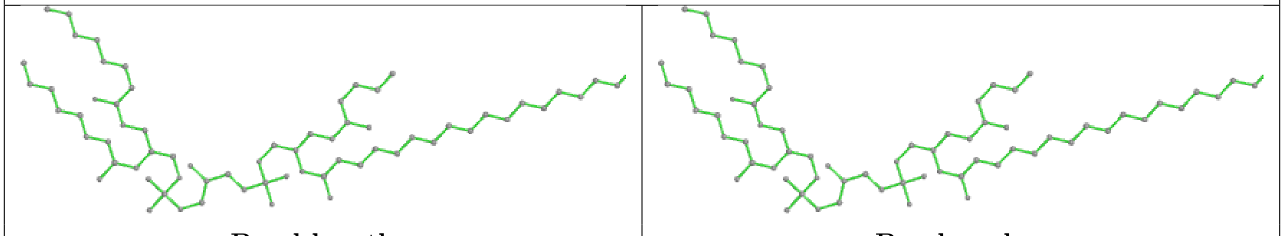
Bond angles



Torsions

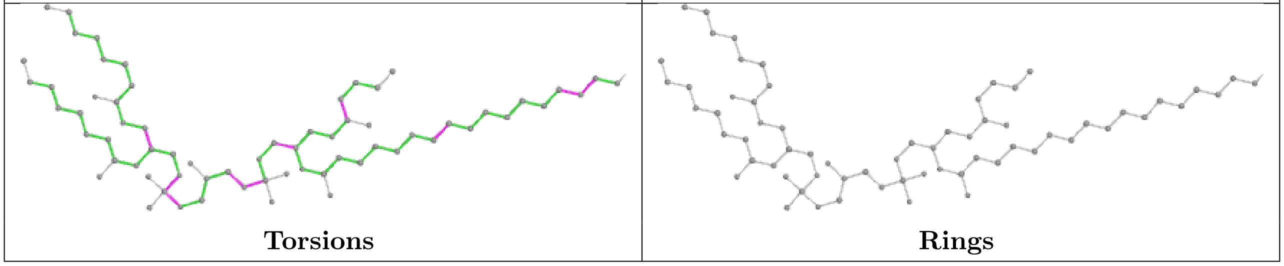
Rings

Ligand CDL d1 201



Bond lengths

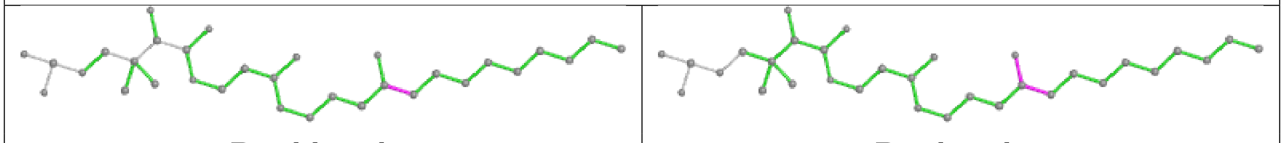
Bond angles



Torsions

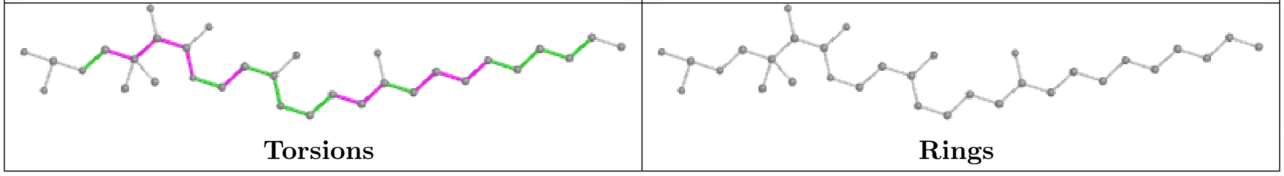
Rings

Ligand ZMP n1 201



Bond lengths

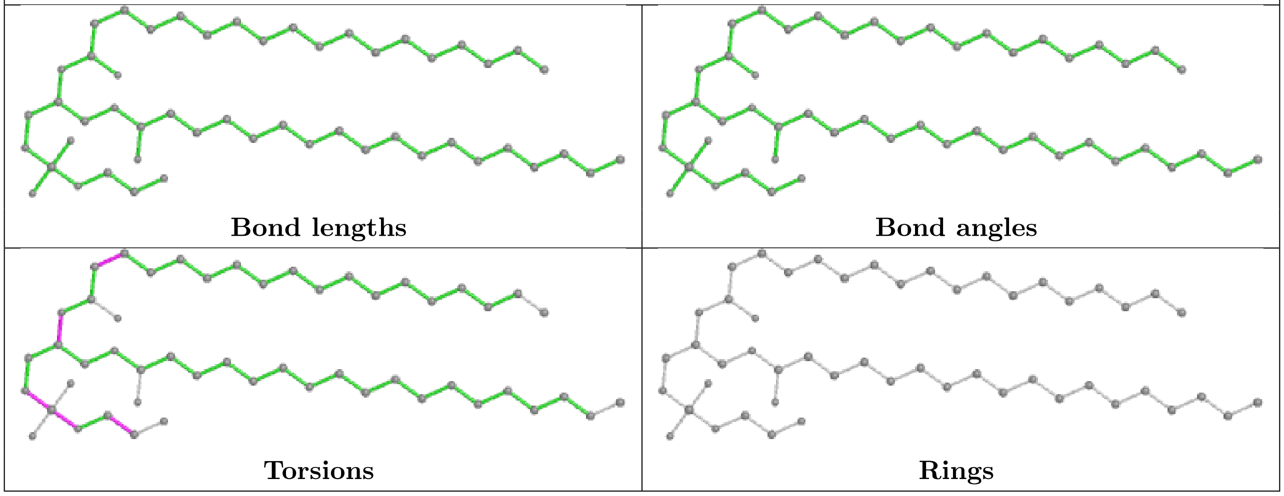
Bond angles



Torsions

Rings

Ligand 3PE L1 701



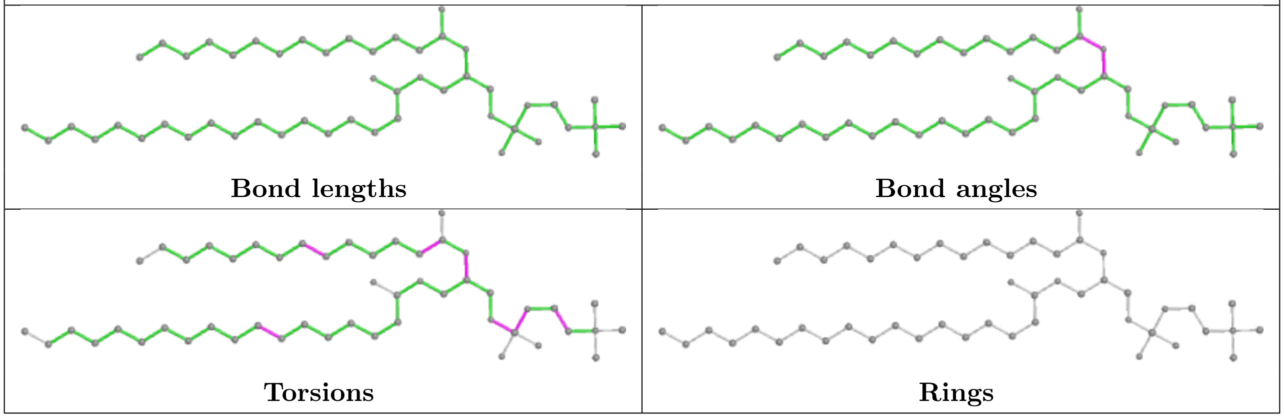
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 I 201



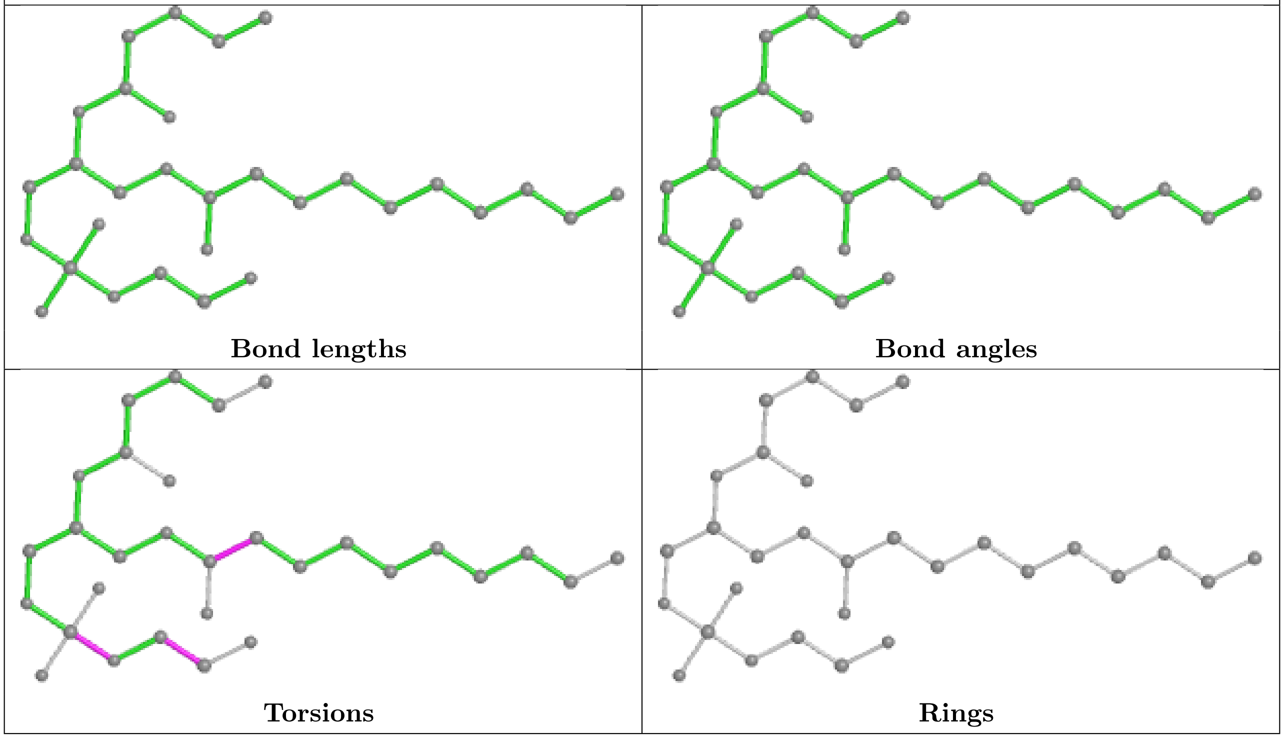
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE R 104



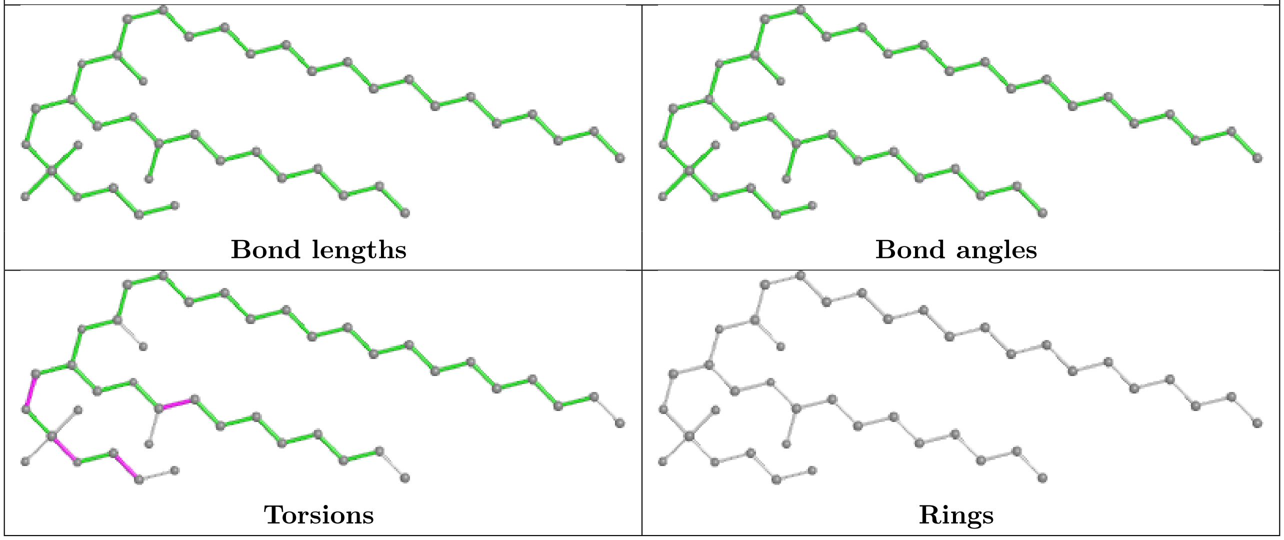
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE i1 201



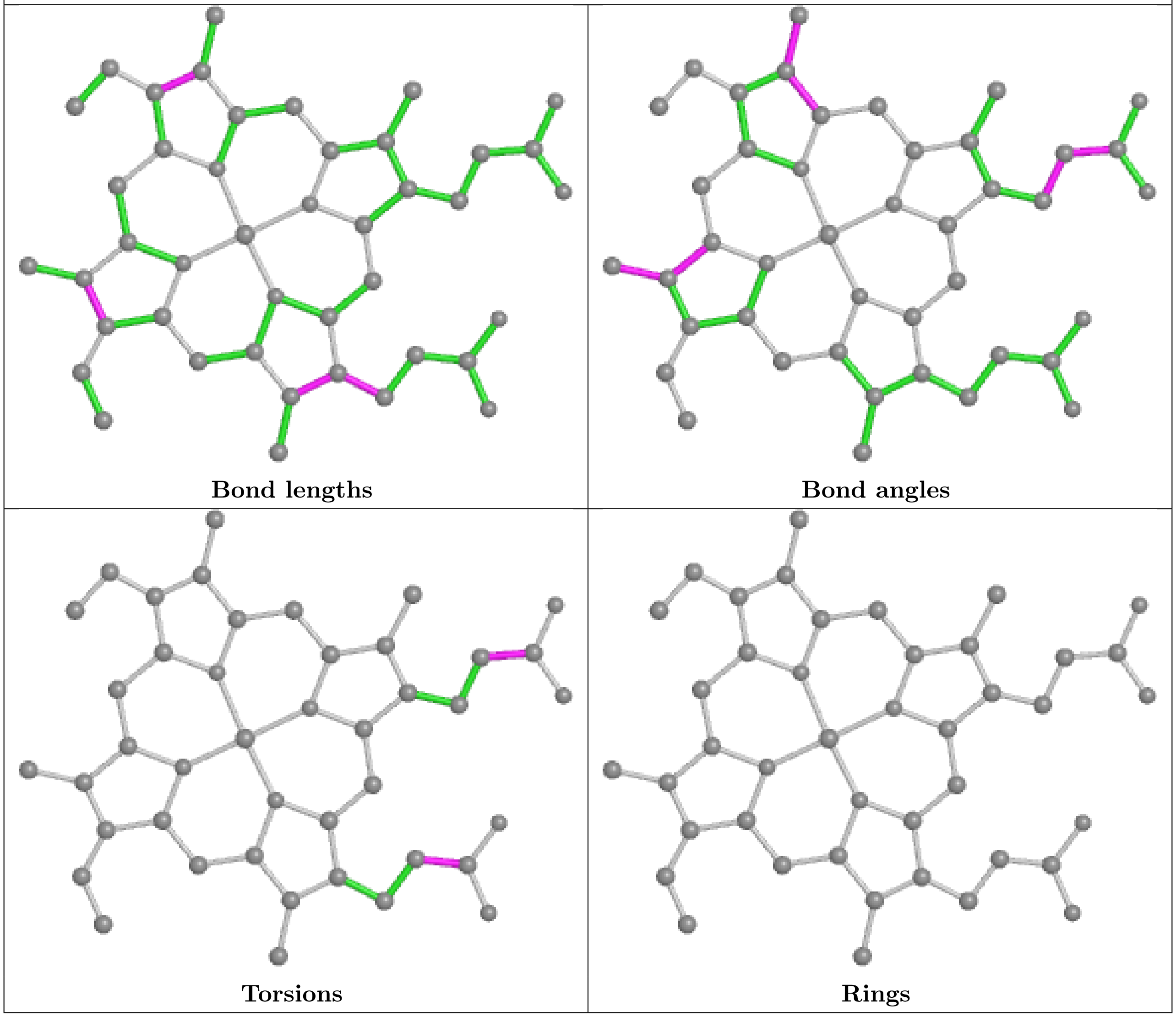
Bond lengths

Bond angles

Torsions

Rings

Ligand HEC O 303



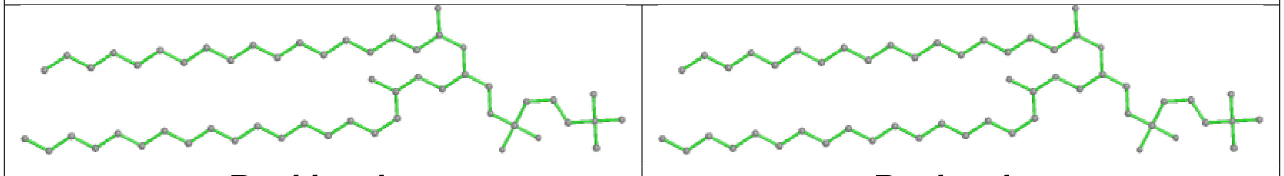
Bond lengths

Bond angles

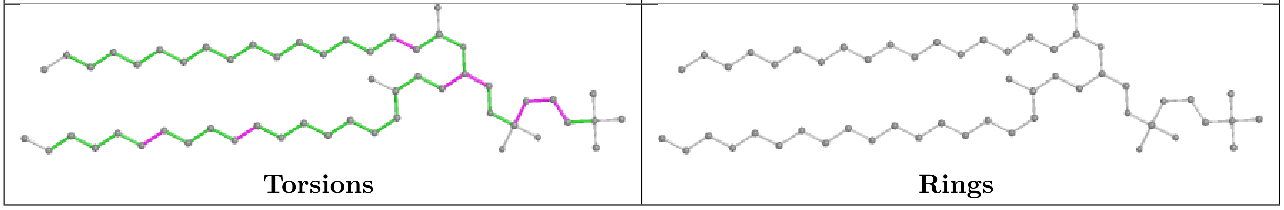
Torsions

Rings

Ligand PC1 M1 501

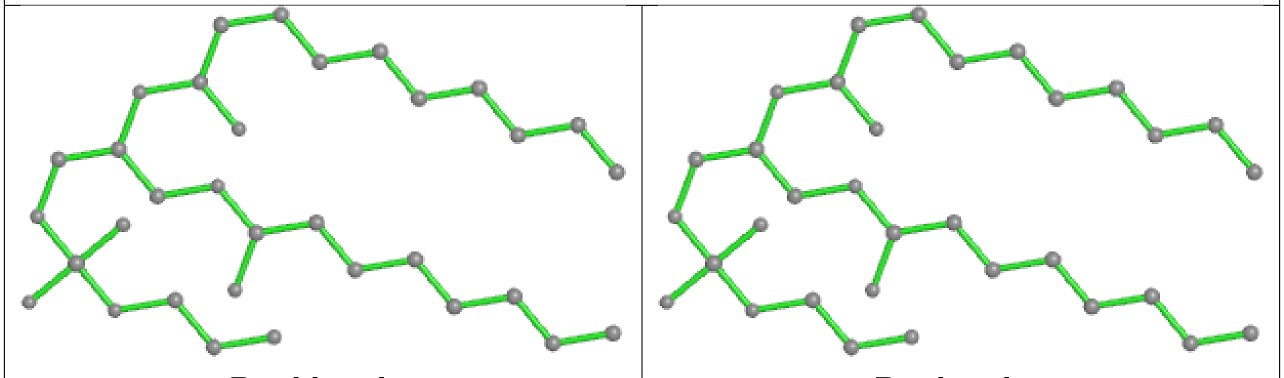


Bond lengths Bond angles

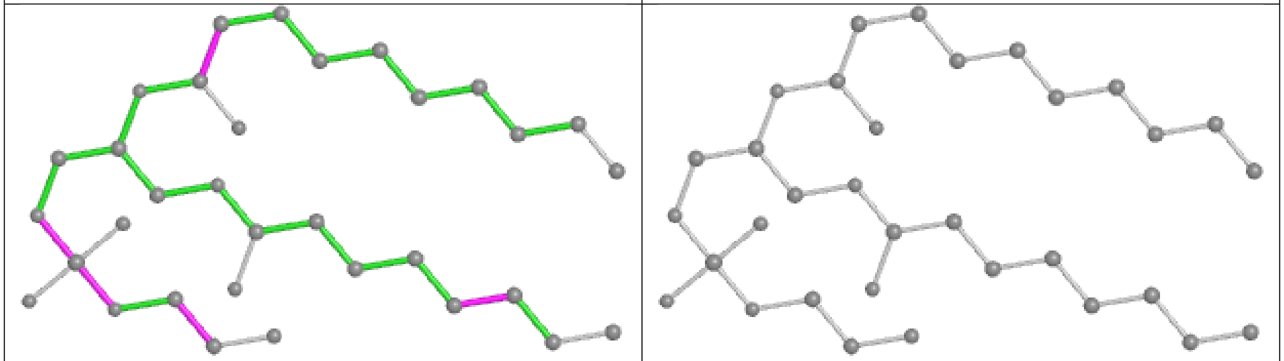


Torsions Rings

Ligand 3PE O 302

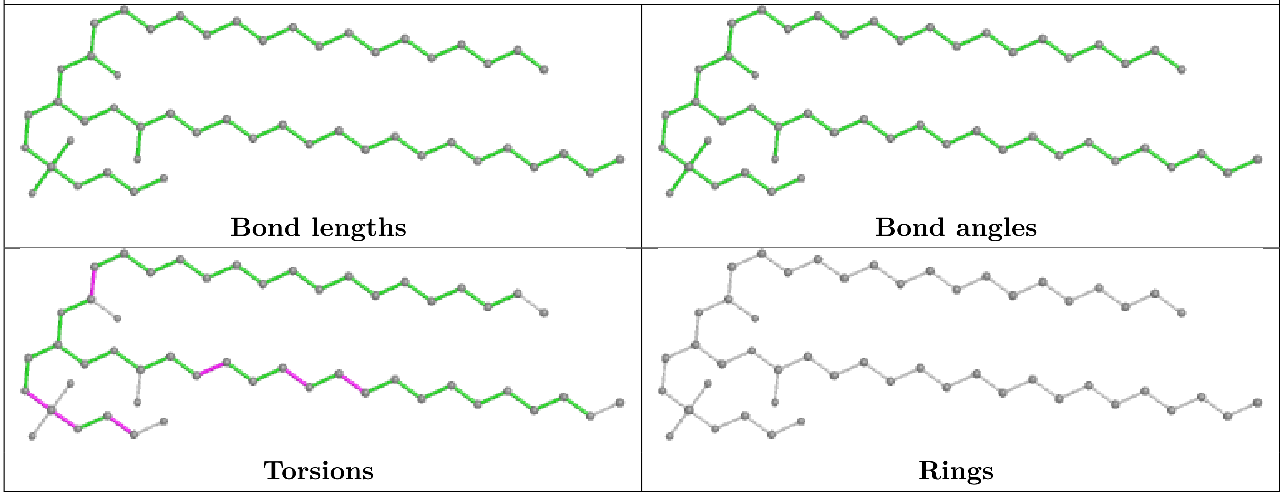


Bond lengths Bond angles



Torsions Rings

Ligand 3PE G 102



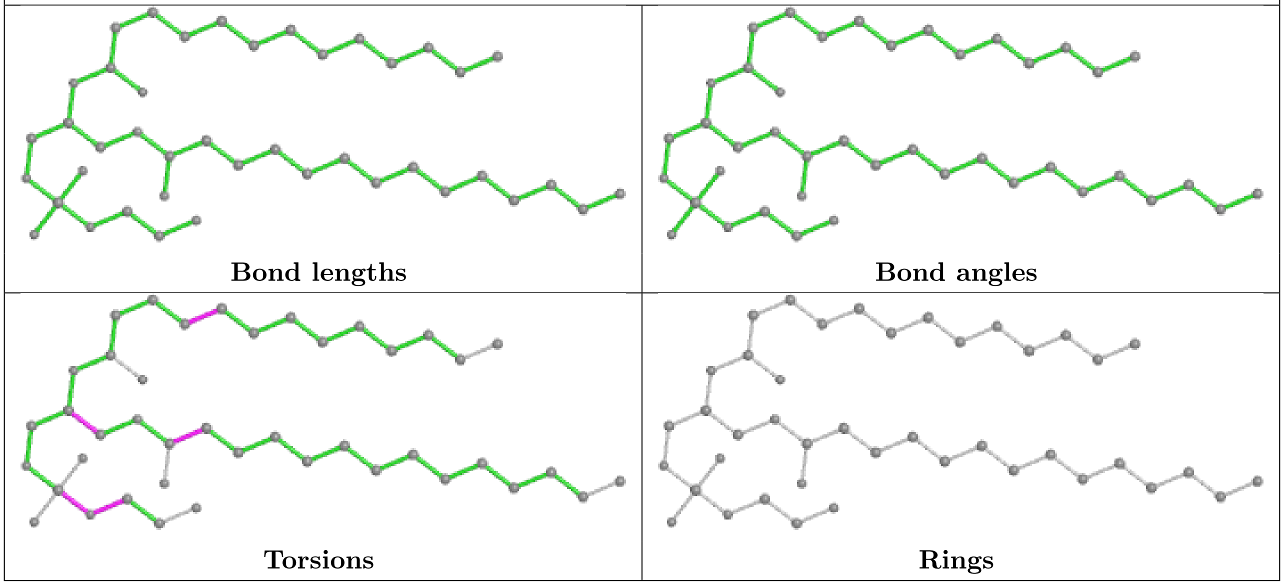
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Y1 403



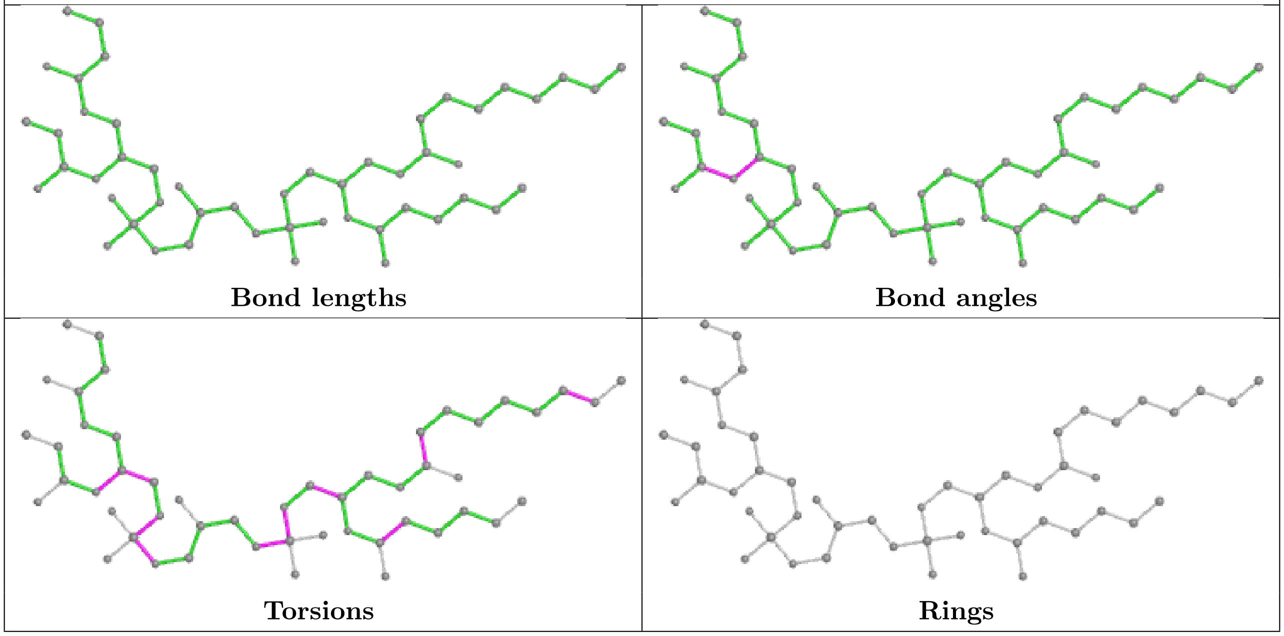
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL V 102



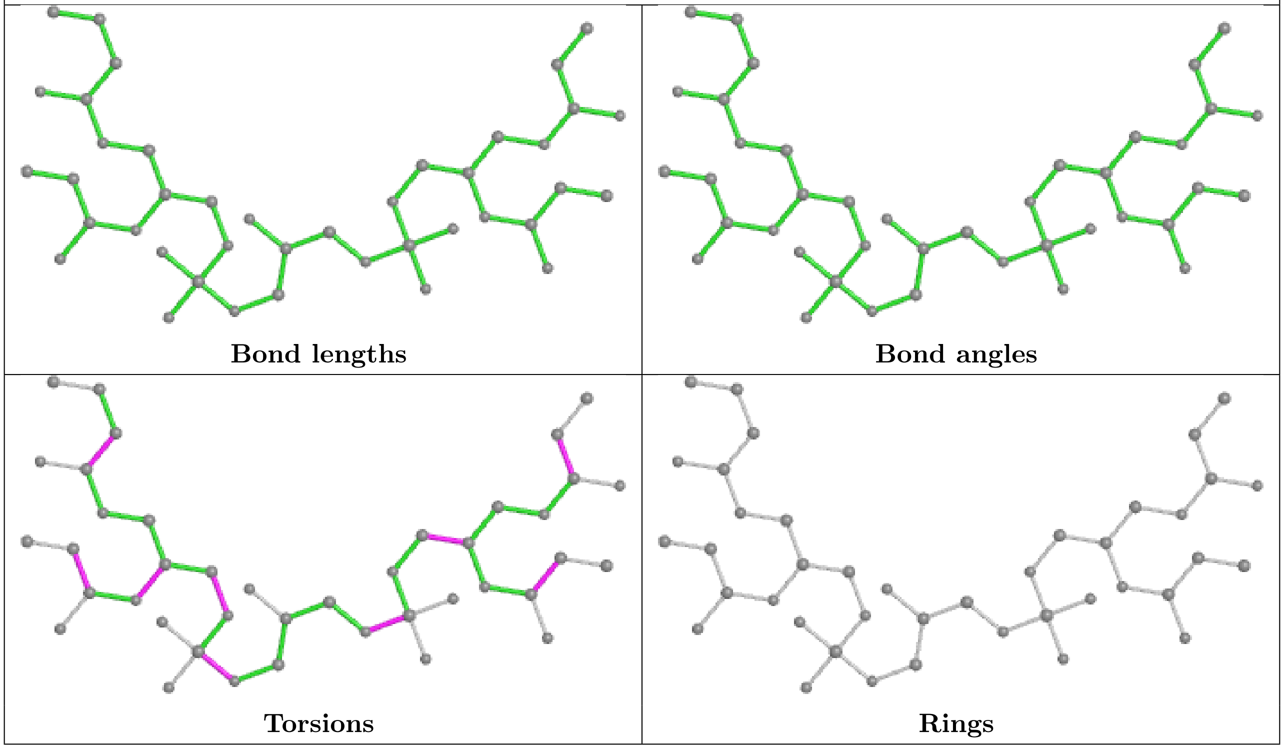
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL R 101



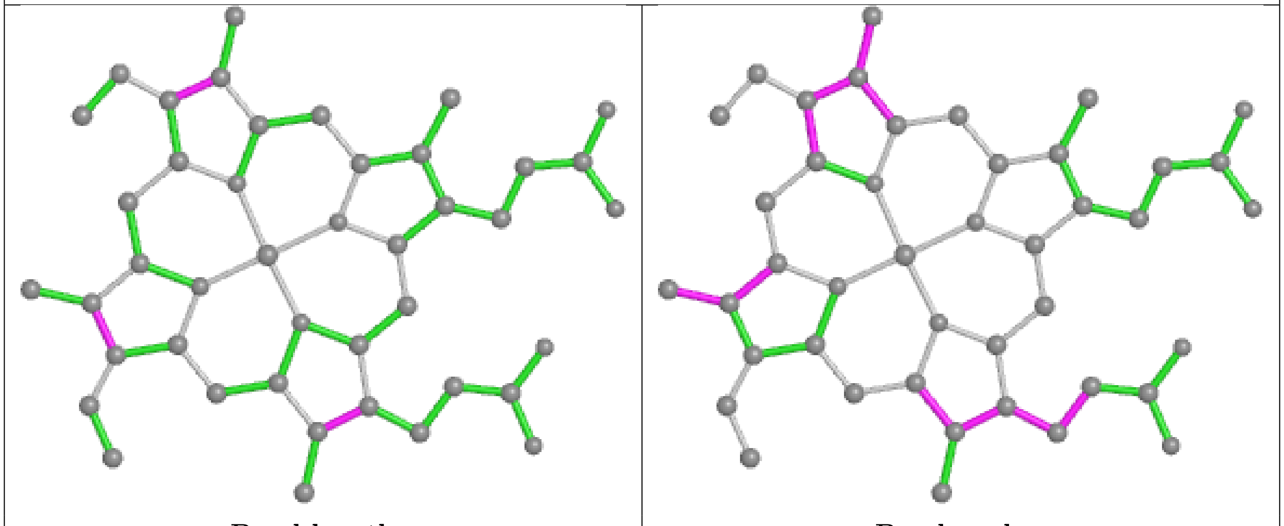
Bond lengths

Bond angles

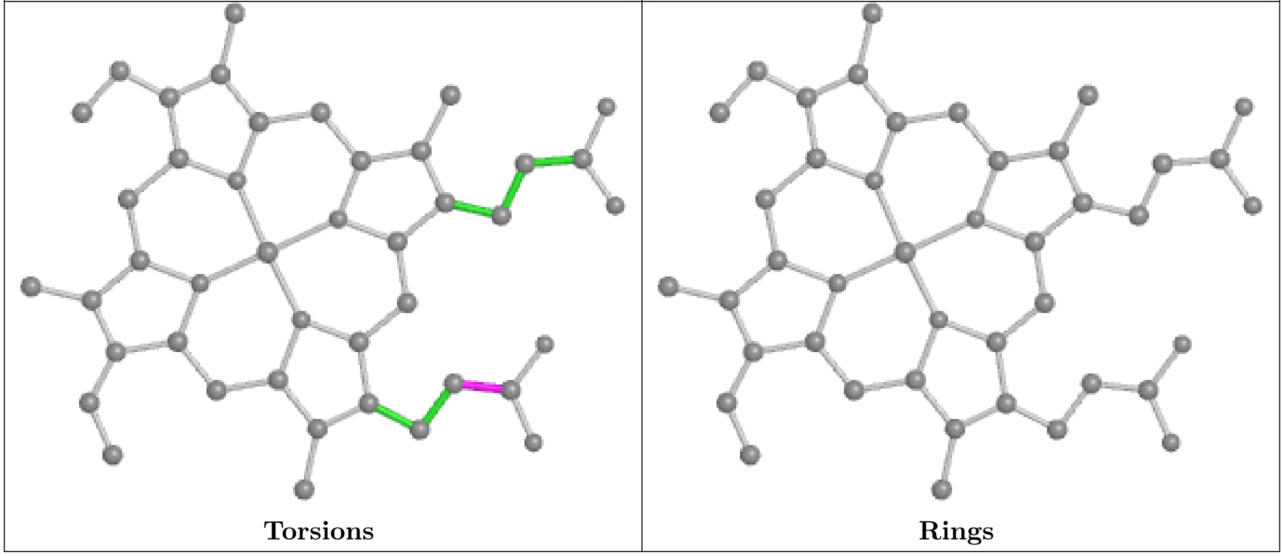
Torsions

Rings

Ligand HEC D 301

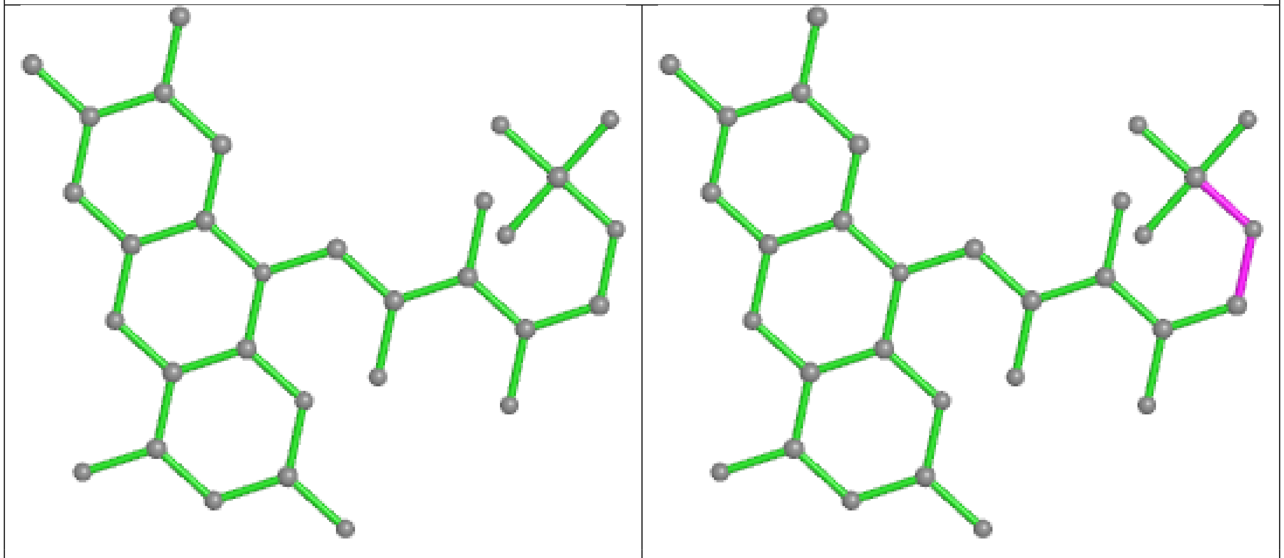


Bond lengths **Bond angles**

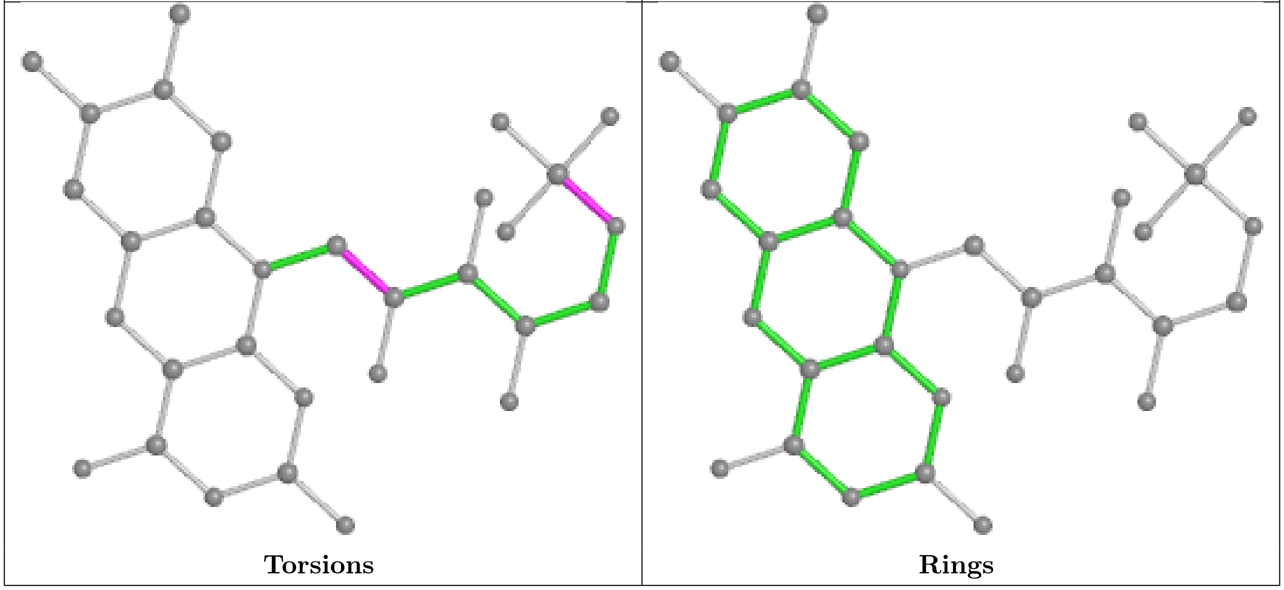


Torsions **Rings**

Ligand FMN 1 501

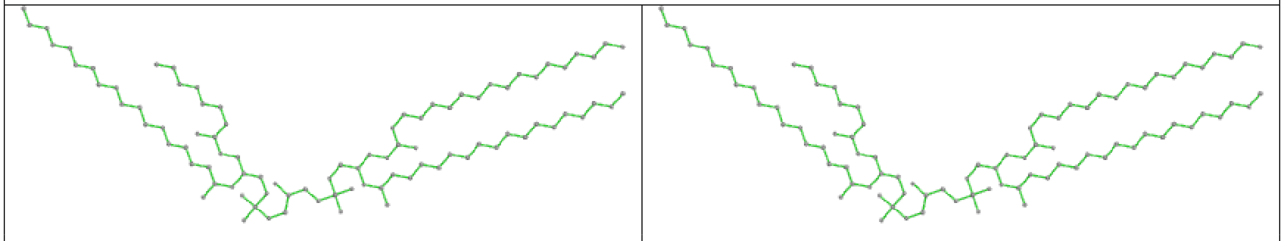


Bond lengths Bond angles

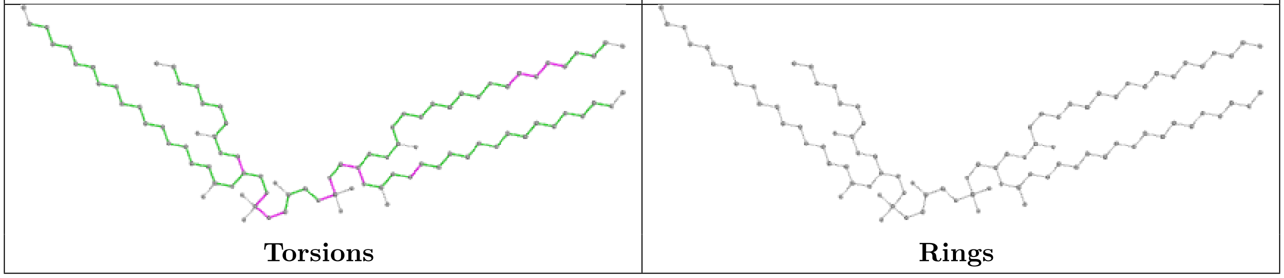


Torsions Rings

Ligand CDL N1 401

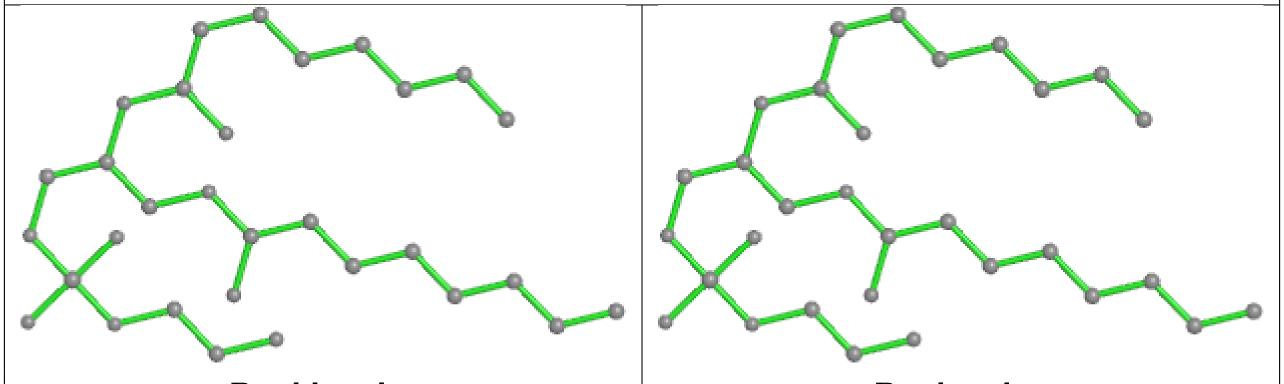


Bond lengths Bond angles

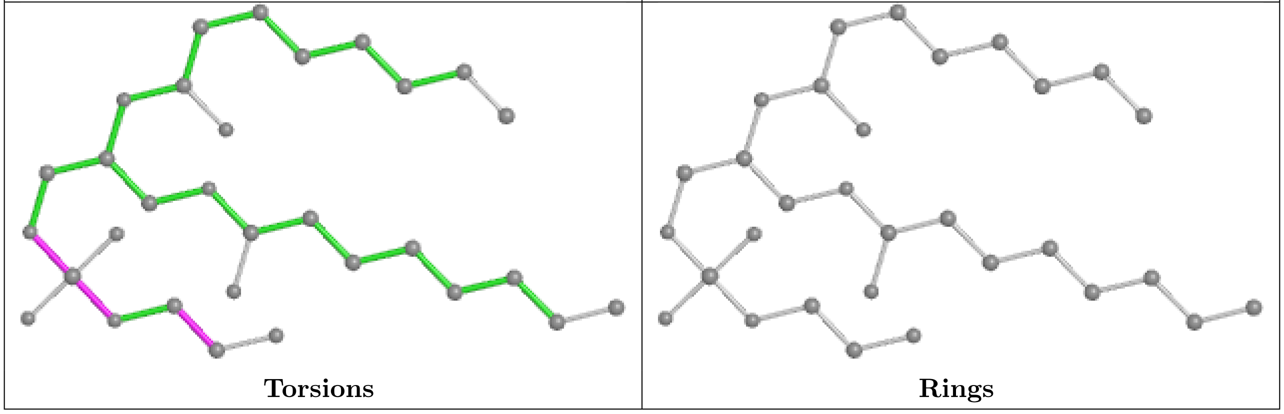


Torsions Rings

Ligand 3PE d1 202

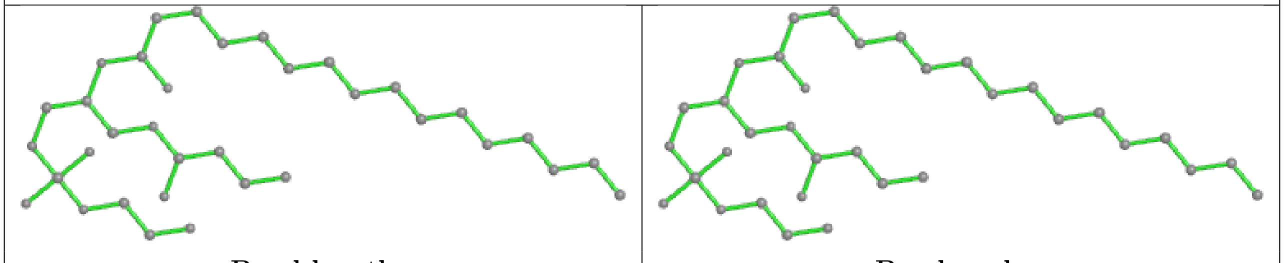


Bond lengths | Bond angles

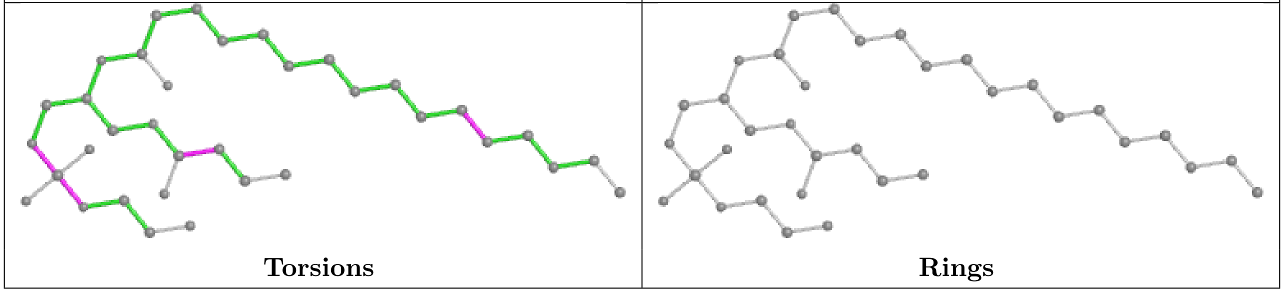


Torsions | Rings

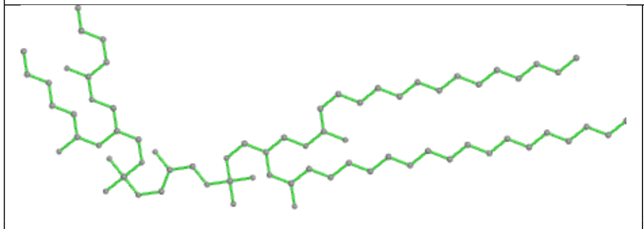
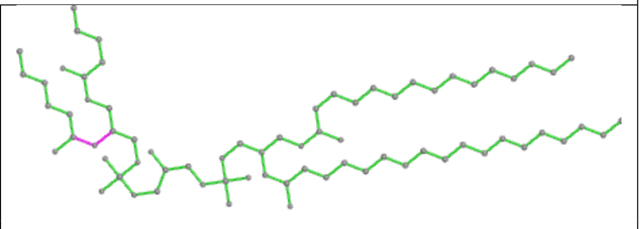
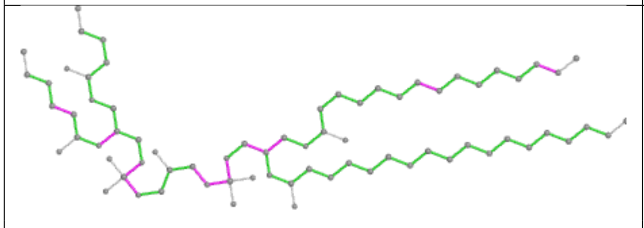
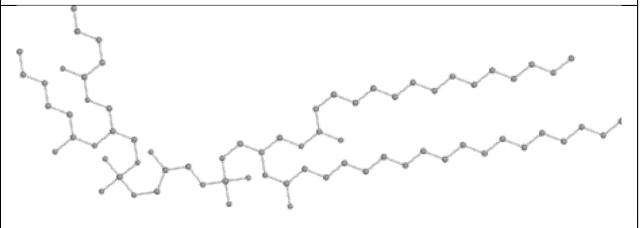
Ligand 3PE C 403



Bond lengths | Bond angles



Torsions | Rings

Ligand CDL R 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

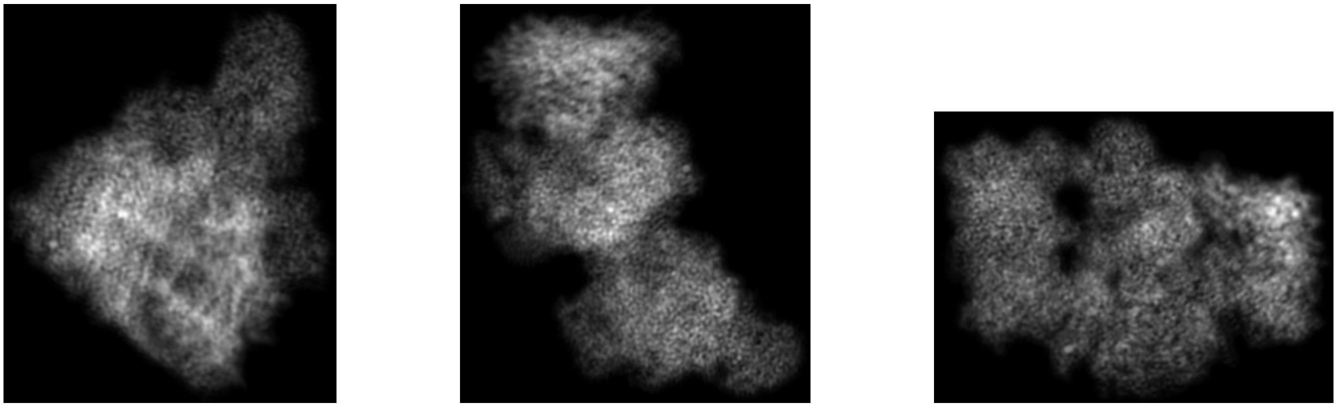
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-17989. 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



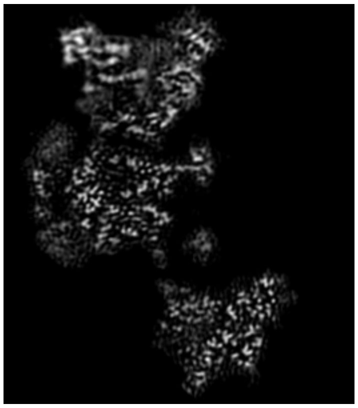
X Y Z

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

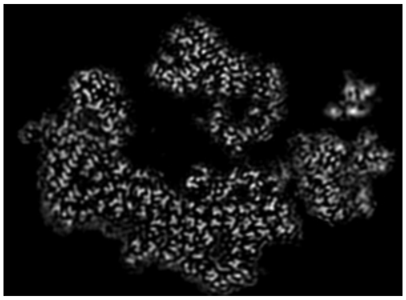
6.2 Central slices ⓘ

6.2.1 Primary map

X Index: 141



Y Index: 103

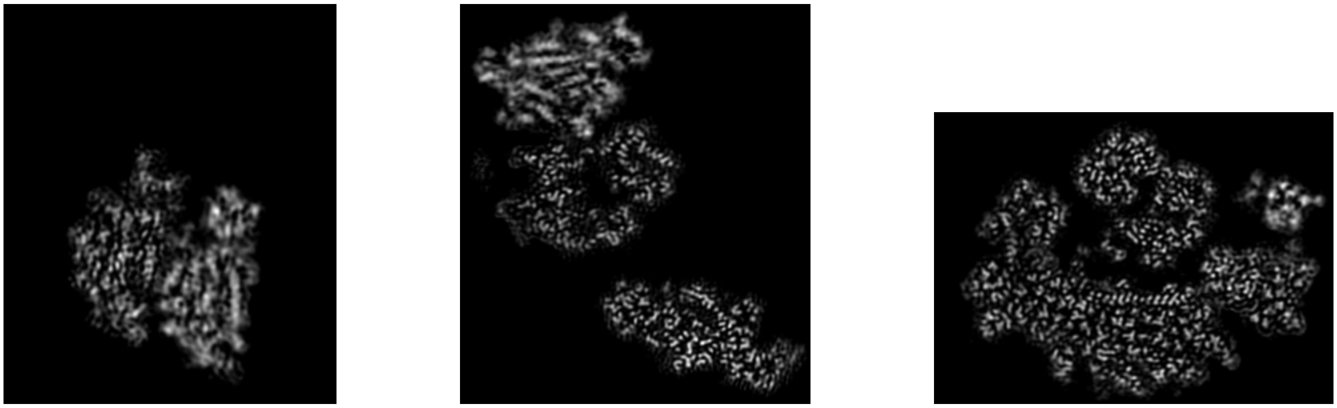


Z Index: 124

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

6.3 Largest variance slices

6.3.1 Primary map

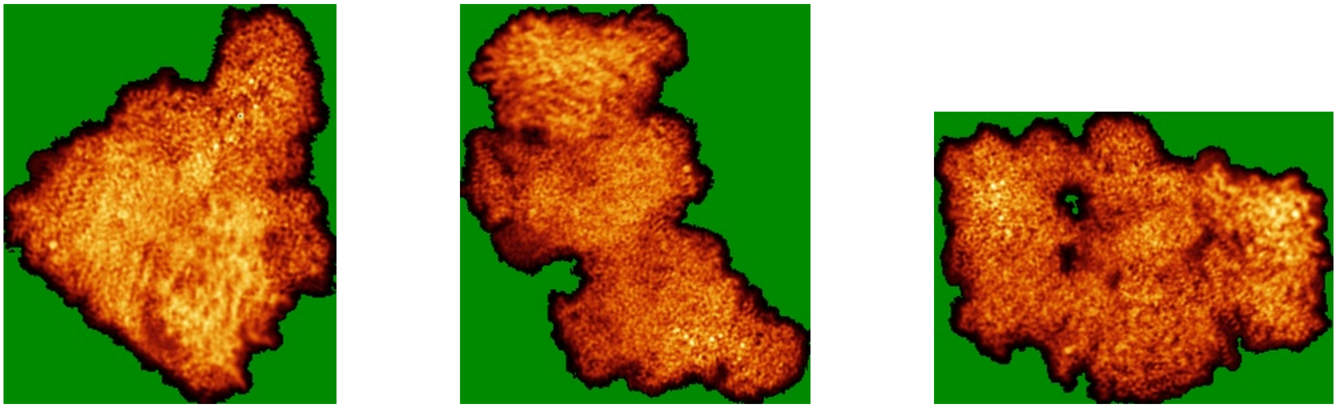


X Index: 243 Y Index: 143 Z Index: 115

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

6.4 Orthogonal standard-deviation projections (False-color)

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 ⓘ

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

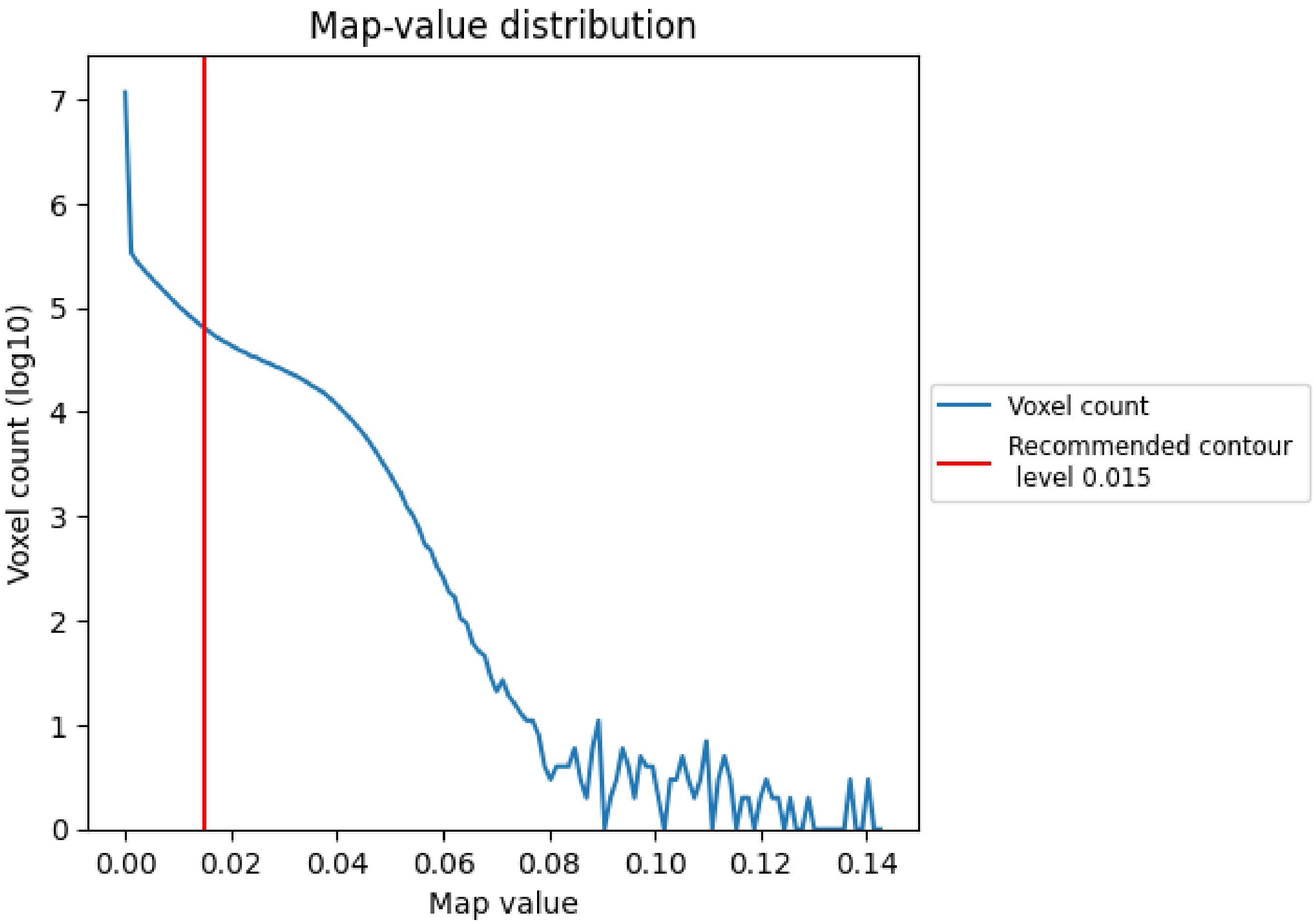
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

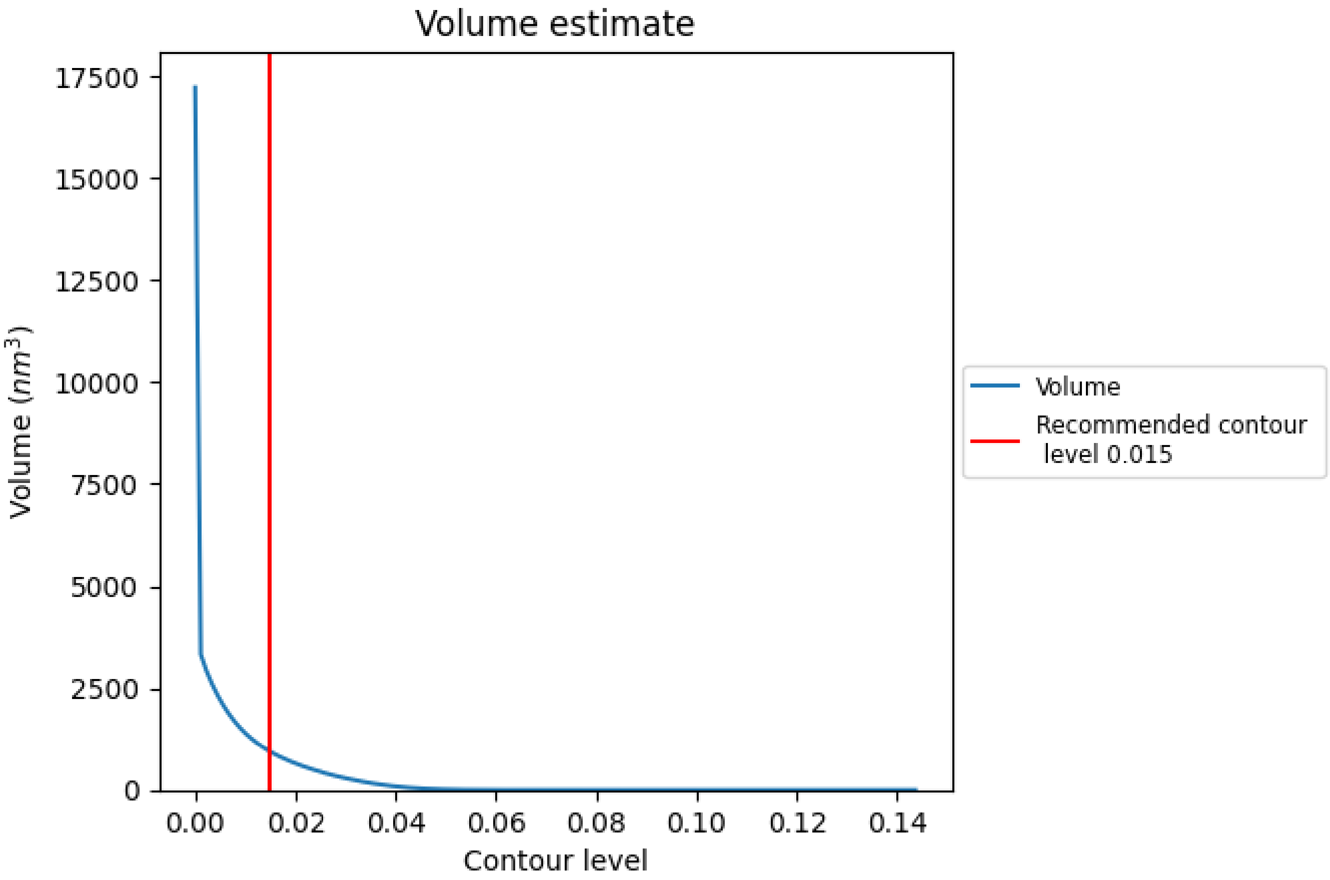
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

7.2 Volume estimate ⓘ



The volume at the recommended contour level is 940 nm^3; this corresponds to an approximate mass of 849 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.

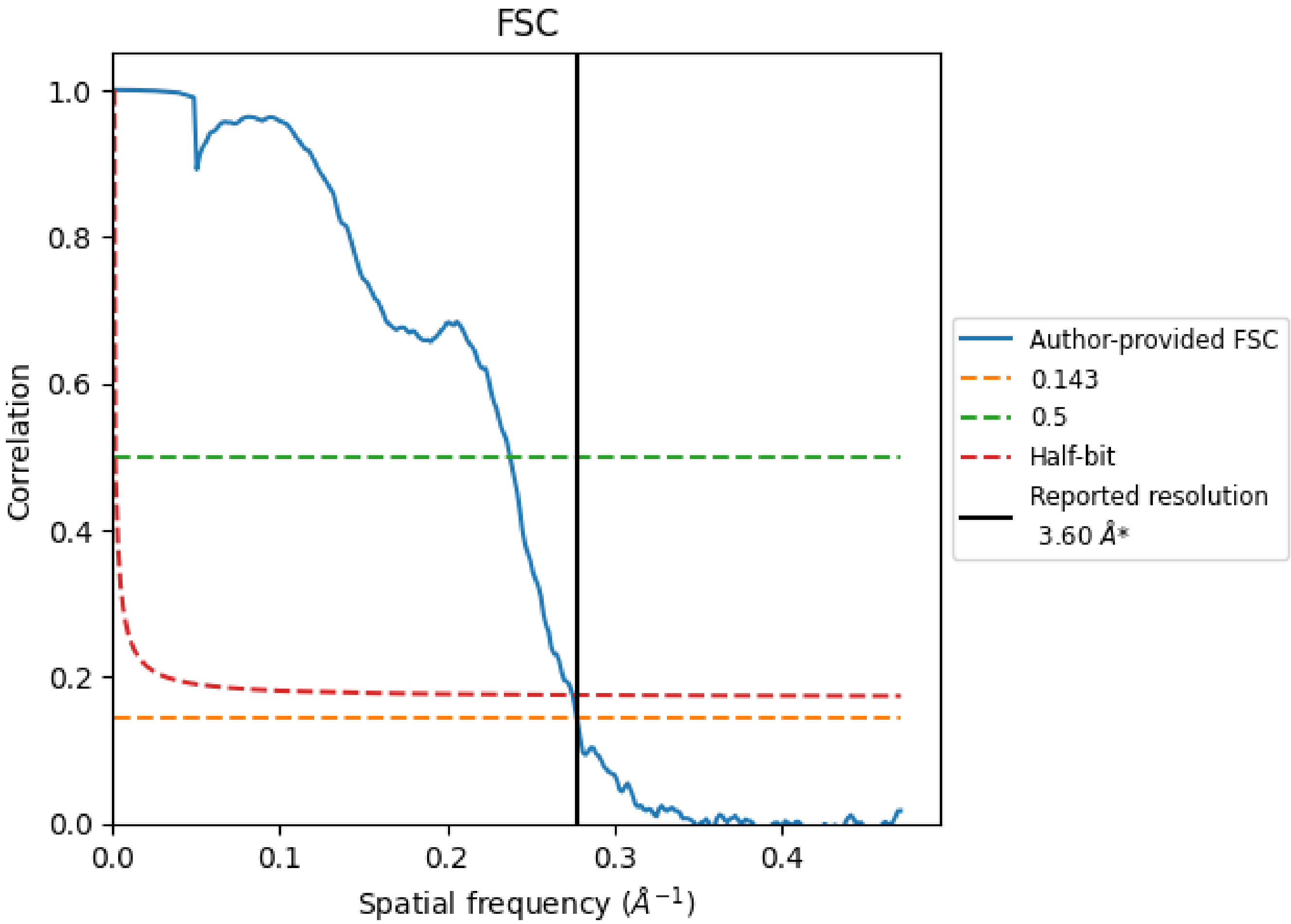
7.3 Rotationally averaged power spectrum ⓘ

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 0.278 $\AA^{-1}$

8.2 Resolution estimates ⓘ

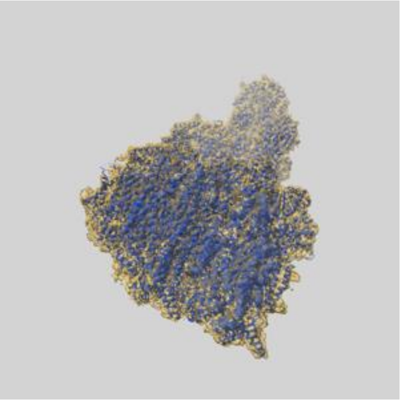
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.21	3.63
Unmasked-calculated*	-	-	-

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

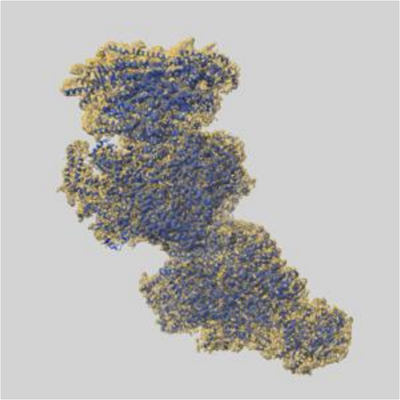
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17989 and PDB model 8PW5. Per-residue inclusion information can be found in section 3 on page 32.

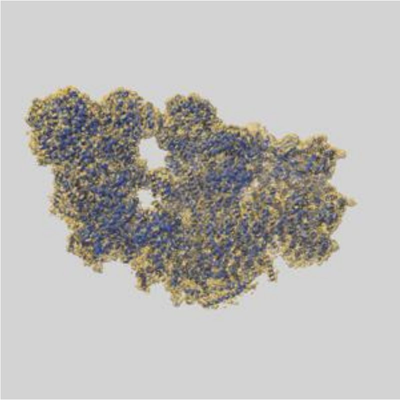
9.1 Map-model overlay ⓘ



X



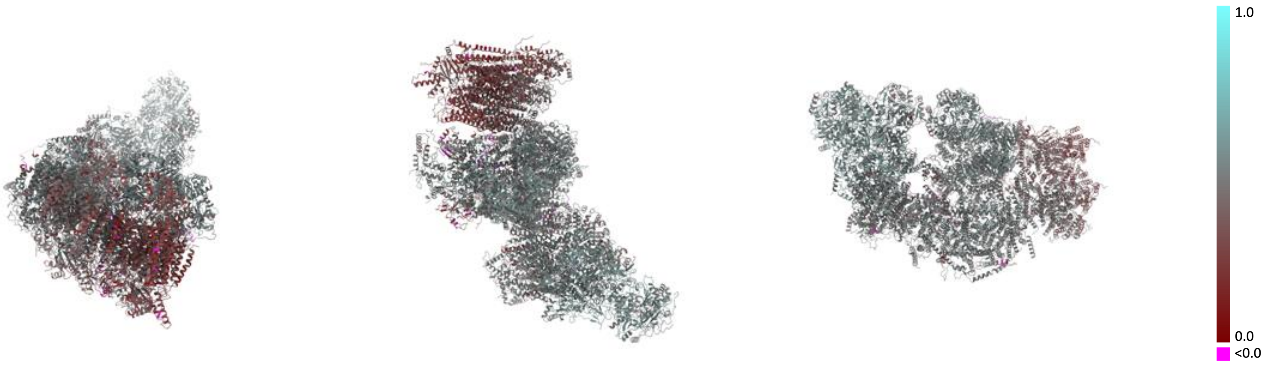
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

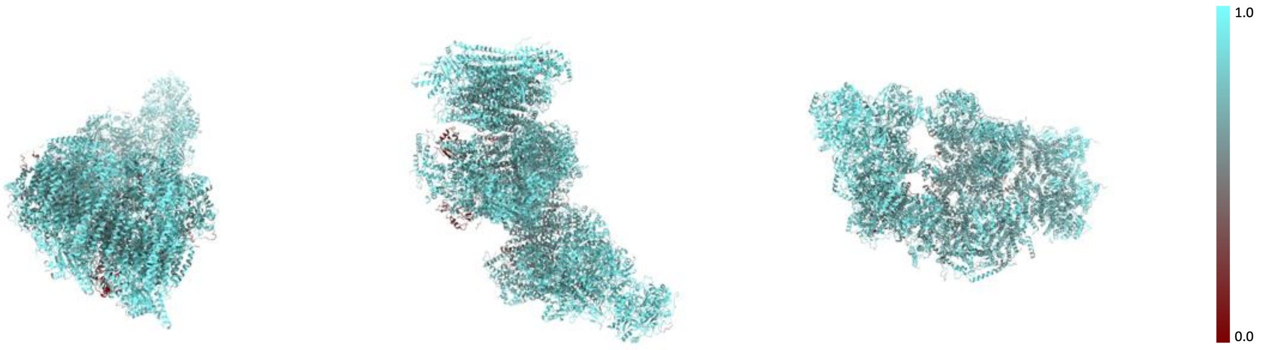
9.2 Q-score mapped to coordinate model



X Y Z

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

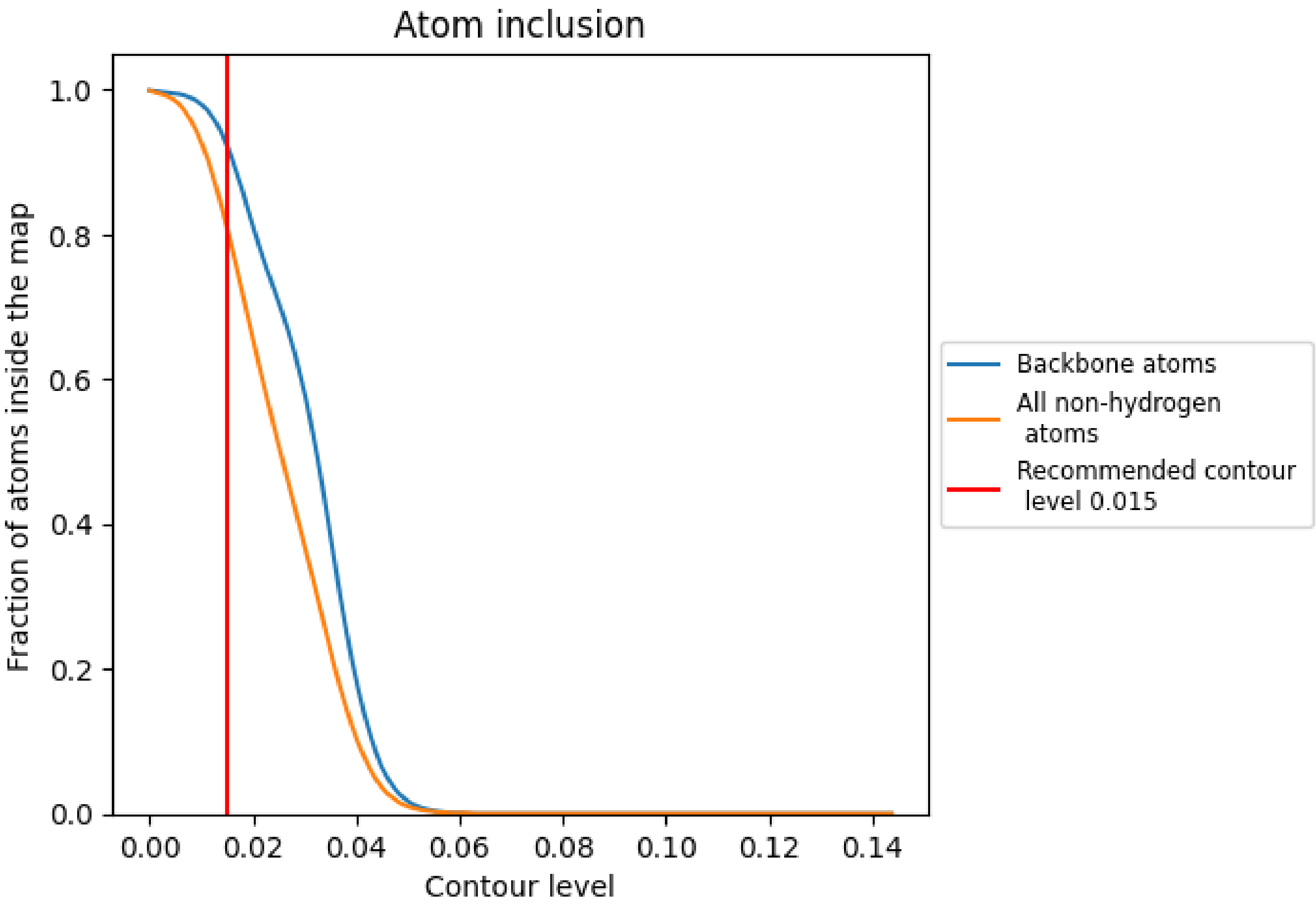
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 81% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4650
1	0.8980	0.5360
2	0.8890	0.5310
3	0.8580	0.5280
6	0.8540	0.5200
7	0.8730	0.5440
9	0.8630	0.5330
A	0.8270	0.5110
A1	0.7140	0.4720
B	0.8420	0.5200
C	0.7850	0.4980
C1	0.8800	0.5470
D	0.8520	0.5090
D1	0.8130	0.5020
E	0.5370	0.3570
F	0.8000	0.5020
G	0.7650	0.4990
H	0.7730	0.4440
H1	0.7390	0.4660
I	0.6620	0.3060
J	0.7720	0.5000
J1	0.6380	0.4250
K	0.6100	0.4630
K1	0.7170	0.4750
L	0.8180	0.5060
L1	0.7810	0.4900
M	0.8460	0.5150
M1	0.7950	0.5010
N	0.8000	0.5010
N1	0.7660	0.4930
O	0.8200	0.5070
O1	0.8260	0.4900
P	0.4970	0.3440
P1	0.7980	0.5010
Q	0.7900	0.5140

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Chain	Atom inclusion	Q-score
Q1	0.8470	0.5420
R	0.6750	0.4690
S	0.7460	0.4470
S1	0.8470	0.4820
T	0.7060	0.4930
T1	0.7500	0.4280
U	0.7500	0.5020
U1	0.8090	0.4890
V	0.6510	0.4630
V1	0.8620	0.5210
W1	0.8470	0.5290
X1	0.8360	0.4840
Y1	0.6780	0.4530
Z1	0.8260	0.4950
a	0.8350	0.3120
a1	0.8170	0.4920
b	0.9150	0.3000
b1	0.7670	0.4650
c	0.8060	0.2880
c1	0.7670	0.4680
d	0.9240	0.3070
d1	0.7590	0.4940
e	0.9290	0.3000
e1	0.7840	0.4850
f	0.8860	0.3030
f1	0.7310	0.4540
g	0.8440	0.2980
g1	0.7600	0.4690
h	0.9070	0.2810
h1	0.8220	0.4900
i	0.8940	0.2620
i1	0.7470	0.4570
j1	0.7900	0.4620
k	0.9290	0.2960
k1	0.7960	0.4800
l	0.7370	0.2750
l1	0.8240	0.5090
m	0.7830	0.2450
m1	0.7540	0.4750
n	0.8070	0.4290
n1	0.8350	0.5020
o	0.8340	0.4170

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Continued from previous page...

Chain	Atom inclusion	Q-score
o1	0.7940	0.4630
p	0.7830	0.4190
p1	0.8270	0.4910
q	0.8680	0.4120
q1	0.8950	0.5450
r	0.8580	0.3740
r1	0.8280	0.5340
s	0.8090	0.4010
s1	0.8040	0.4860
t	0.7470	0.3770
u	0.8840	0.3990
v	0.7940	0.3500
w	0.7670	0.4310
x	0.8420	0.3890
y	0.8030	0.4430
z	0.7580	0.3910