wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 09:33 pm BST

PDB ID	:	8PW5 / pdb_00008pw5
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 (i) symbol.

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

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

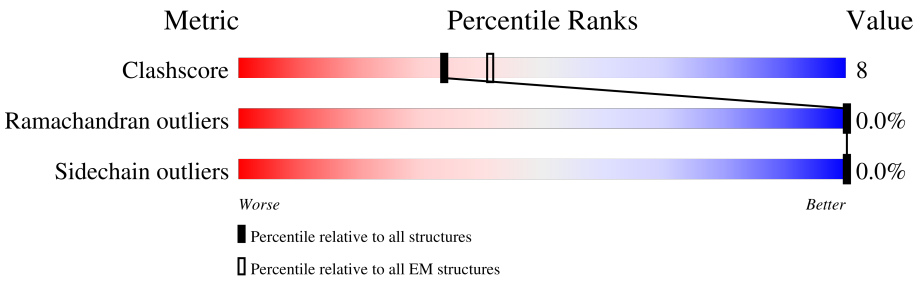
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

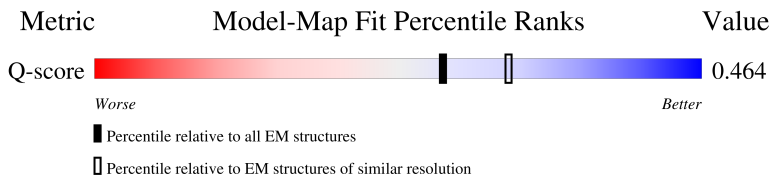
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	g	111	• 43% 25% 32%
1	t	111	12% 51% 17% 32%
2	m	69	• 35% 29% 36%
2	z	69	12% 39% 23% • 36%

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Mol	Chain	Length	Quality of chain
3	A	480	78% 15% 7%
3	L	480	79% 14% 7%
4	B	453	74% 19% 7%
4	M	453	78% 14% 7%
5	C	381	88% 12%
5	N	381	86% 13%
6	D	325	66% 8% 26%
6	O	325	66% 8% 26%
7	E	274	32% 67% 28%
7	P	274	35% 65% 6% 28%
7	T	274	24% 5% 72%
8	F	111	77% 11% 12%
8	Q	111	84% 8% 8%
9	G	82	77% 17% 6%
9	R	82	85% 9% 6%
10	H	89	70% 26%
10	S	89	62% 15% 24%
11	J	64	78% 16% 6%
11	U	64	5% 78% 16% 6%
12	K	56	18% 73% 20% 7%
12	V	56	11% 71% 23% 5%
13	I	113	23% 82% 16%
14	a	514	67% 32%
14	n	514	70% 30%
15	b	227	67% 33%

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Mol	Chain	Length	Quality of chain
15	o	227	71% 29%
16	c	261	74% 25%
16	p	261	75% 25%
17	d	169	63% 20% 18%
17	q	169	64% 18% 18%
18	e	146	54% 16% 29%
18	r	146	52% 19% 29%
19	f	128	45% 27% 27%
19	s	128	5% 55% 19% 27%
20	h	86	73% 19% 8%
20	u	86	73% 19% 8%
21	i	76	68% 24% 5%
21	v	76	5% 71% 22% 7%
22	k	80	49% 11% 40%
22	x	80	48% 14% 39%
23	l	63	56% 17% 27%
23	y	63	54% 21% 25%
24	w	83	57% 12% 31%
25	6	224	54% 16% 30%
26	C1	263	68% 11% 21%
27	D1	463	6% 72% 21% 7%
28	2	248	73% 13% 14%
29	1	464	76% 16% 7%
30	3	727	81% 14% 5%
31	9	212	66% 18% 16%

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Mol	Chain	Length	Quality of chain
32	P1	377	72% 19% 9%
33	Q1	175	64% 8% 28%
34	7	116	73% 9% 17%
35	S1	99	68% 17% 15%
36	T1	156	42% 8% 49%
36	U1	156	40% 17% 44%
37	V1	116	91% 7%
38	W1	131	79% 8% 13%
39	q1	145	92% 8%
40	r1	113	78% 10% 12%
41	s1	104	34% 7% 60%
42	A1	115	6% 84% 16%
43	H1	318	73% 27%
44	J1	172	19% 77% 23%
45	K1	98	74% 26%
46	L1	607	78% 22%
47	M1	459	74% 26%
48	N1	345	70% 29%
49	O1	355	74% 16% 10%
50	X1	172	83% 17%
51	Y1	141	86% 13%
52	Z1	144	79% 19%
53	a1	70	84% 16%
54	b1	84	88% 10%
55	c1	76	58% 5% 37%

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Mol	Chain	Length	Quality of chain
56	d1	120	87% 13%
57	e1	106	82% 17%
58	f1	57	11% 86% 7% 7%
59	g1	151	5% 52% 15% 33%
60	h1	189	65% 9% 26%
61	i1	128	10% 70% 13% 17%
62	j1	105	53% 9% 38%
63	k1	104	59% 15% 26%
64	l1	186	68% 16% 16%
65	m1	129	5% 78% 20%
66	n1	179	86% 13%
67	o1	137	78% 8% 14%
68	p1	176	82% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
73	HEC	D	301	X	-	-	-
73	HEC	O	303	X	-	-	-
74	FES	P	201	-	-	X	-

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 130610 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	t	76	620	404	112	102	2	0	0
1	g	76	620	404	112	102	2	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	m	44	343	220	59	61	3	0	0
2	z	44	343	220	59	61	3	0	0

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

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

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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

- Molecule 5 is a protein called Cytochrome b.

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

- Molecule 6 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

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

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

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 8.

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

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

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

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 9.

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

- Molecule 12 is a protein called Cytochrome b-c1 complex subunit 10.

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

- Molecule 13 is a protein called Cox7a2l protein.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 16 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 17 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6C.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	w	57	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
			Total	C	N	O	S		
25	6	157	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
			Total	C	N	O	S		
26	C1	208	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
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
			Total	C	N	O	S		
53	a1	70	572	370	101	97	4	0	0

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

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

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

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

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

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

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

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

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

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

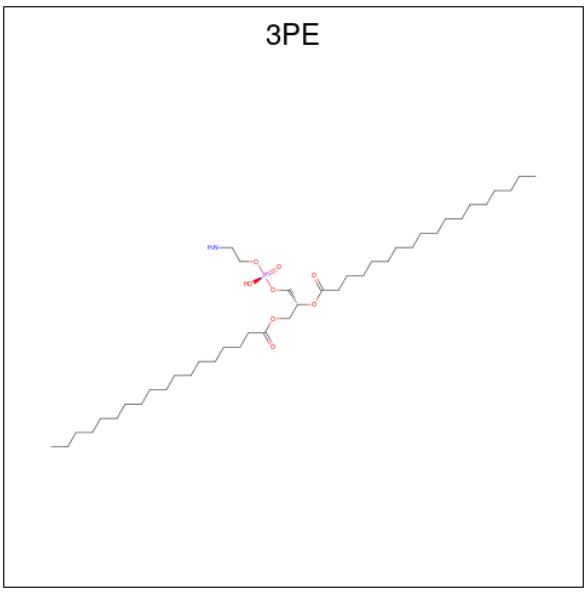
- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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 (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



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

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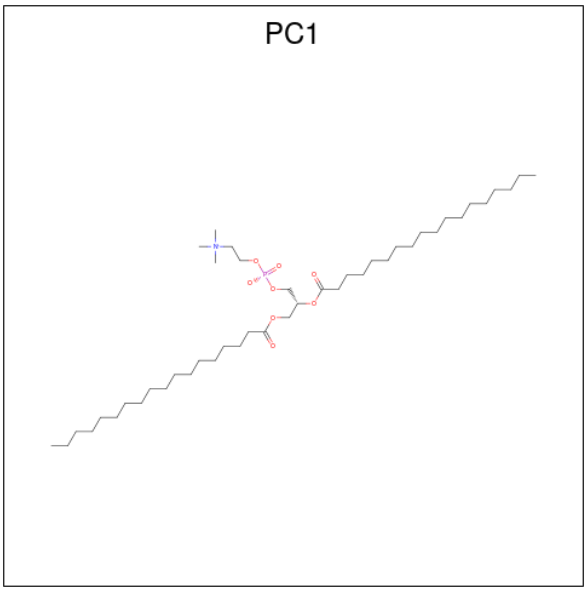
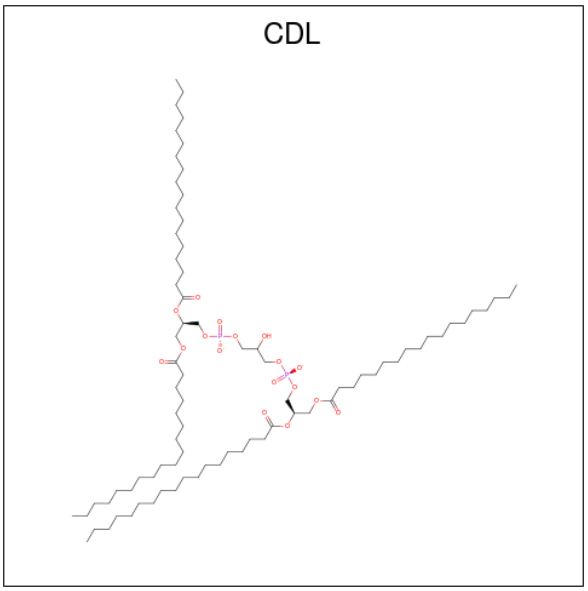
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	L1	1	51	41	1	8	1	0
			Total	C	N	O	P	
69	L1	1	51	41	1	8	1	0
			Total	C	N	O	P	
69	M1	1	51	41	1	8	1	0
			Total	C	N	O	P	
69	M1	1	51	41	1	8	1	0
			Total	C	N	O	P	
69	N1	1	38	28	1	8	1	0
			Total	C	N	O	P	
69	Y1	1	28	18	1	8	1	0
			Total	C	N	O	P	
69	Y1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

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
70	z	1	28	18	1	8	1	0
70	J	1	35	25	1	8	1	0
70	K	1	28	18	1	8	1	0
70	L	1	24	14	1	8	1	0
70	V	1	28	18	1	8	1	0
70	I	1	50	40	1	8	1	0
70	p	1	35	25	1	8	1	0
70	6	1	43	33	1	8	1	0
70	9	1	54	44	1	8	1	0
70	9	1	47	37	1	8	1	0
70	P1	1	31	21	1	8	1	0
70	M1	1	54	44	1	8	1	0
70	g	1	50	40	1	8	1	0

- Molecule 71 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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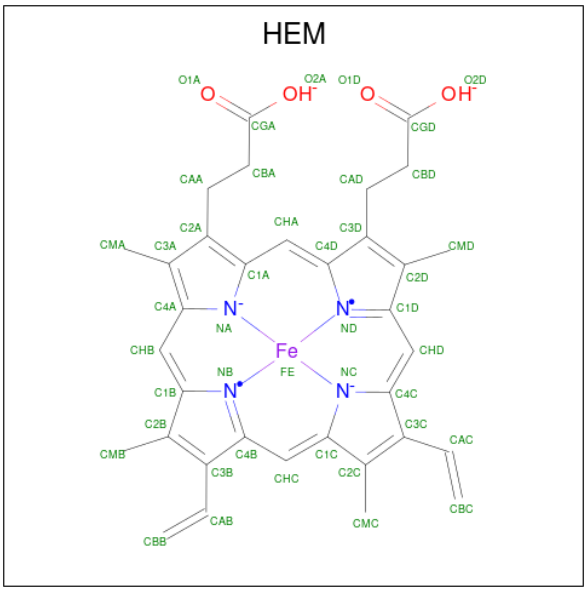
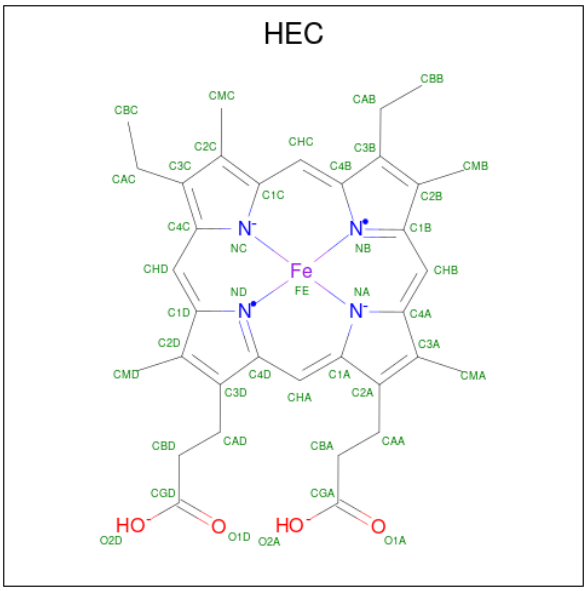
Mol	Chain	Residues	Atoms				AltConf
71	Y1	1	Total	C	O	P	0
			94	75	17	2	
71	d1	1	Total	C	O	P	0
			67	48	17	2	
71	h1	1	Total	C	O	P	0
			70	51	17	2	
71	g	1	Total	C	O	P	0
			38	20	16	2	

- Molecule 72 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



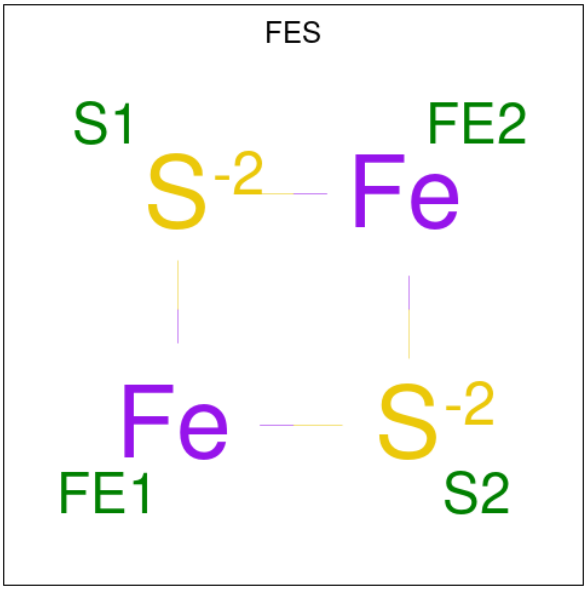
Mol	Chain	Residues	Atoms					AltConf
72	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 73 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
74	2	1	4	2	2	0
74	3	1	4	2	2	0

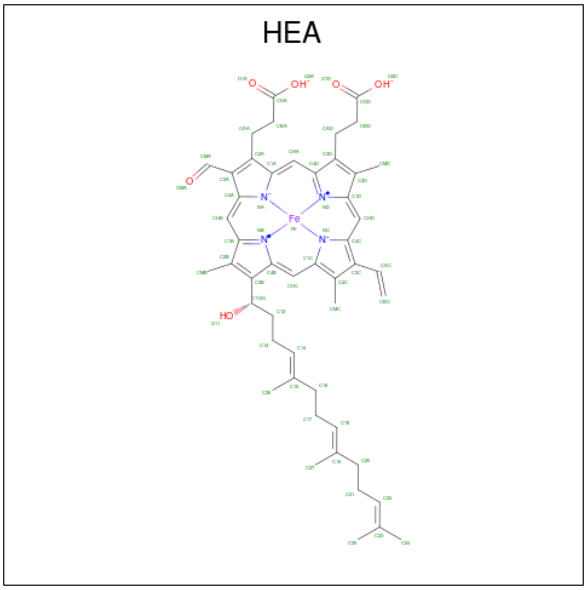
- Molecule 75 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 76 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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



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

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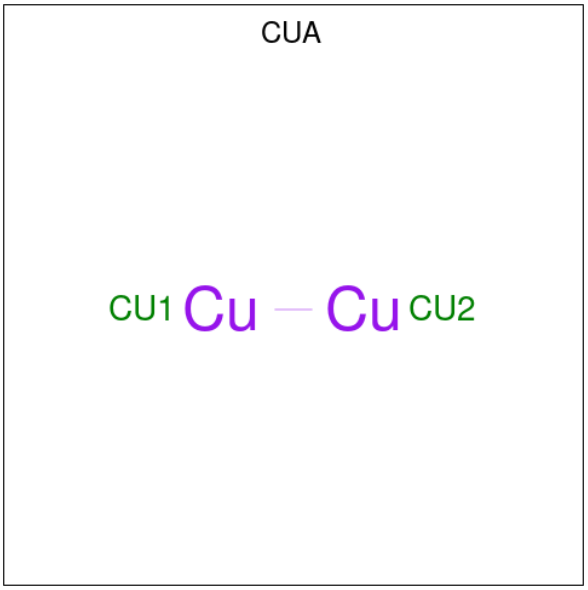
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
77	n	1	60	49	1	4	6	0
77	a	1	60	49	1	4	6	0
77	a	1	60	49	1	4	6	0

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 79 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).

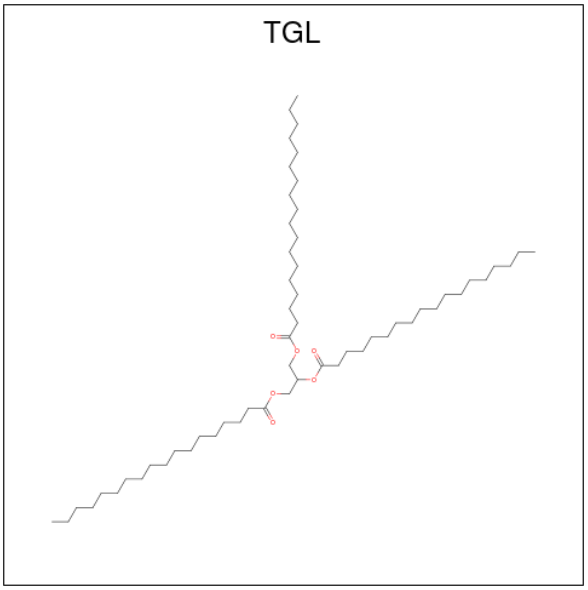


Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
79	o	1	2	2	0
79	b	1	2	2	0

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

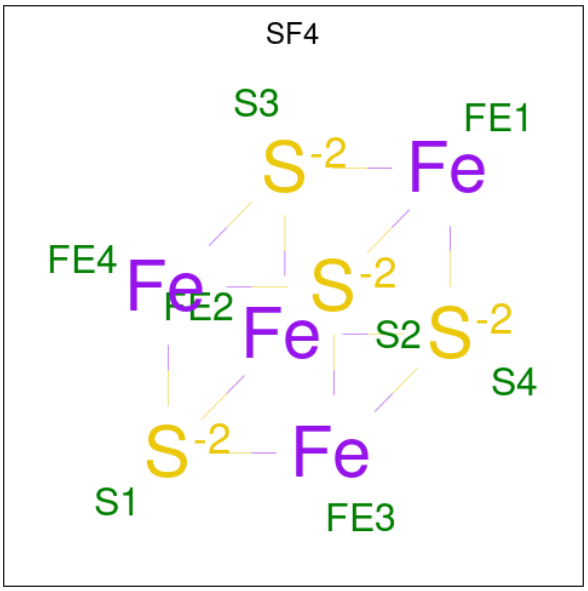
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	s	1	1	1	0
			Total	Zn	
80	7	1	1	1	0
			Total	Zn	
80	f	1	1	1	0

- Molecule 81 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



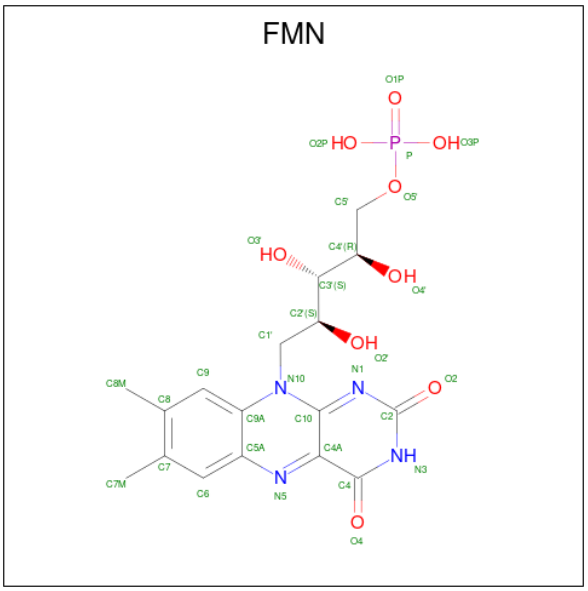
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
81	y	1	37	31	6	0
			Total	C	O	
81	l	1	37	31	6	0

- Molecule 82 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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

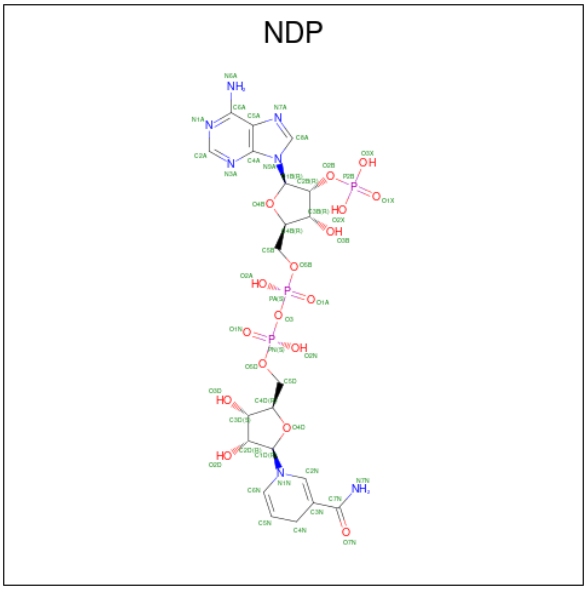


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
83	1	1	31	17	4	9	1	0

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

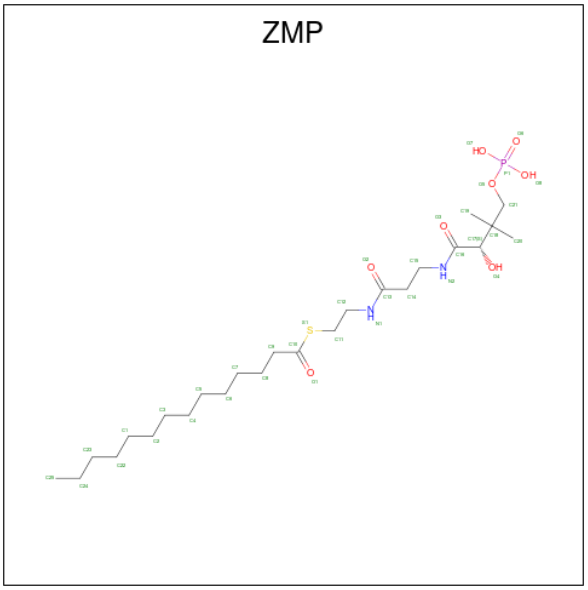
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
84	3	1	1	1	0

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



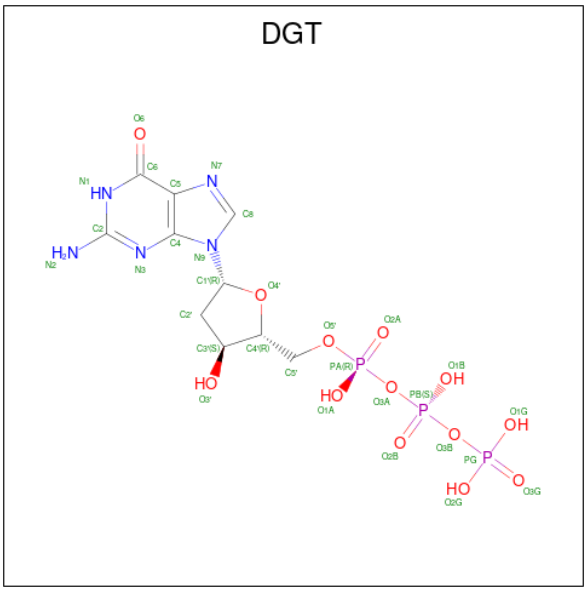
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	P1	1	48	21	7	17	3	0

- Molecule 86 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: 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 (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



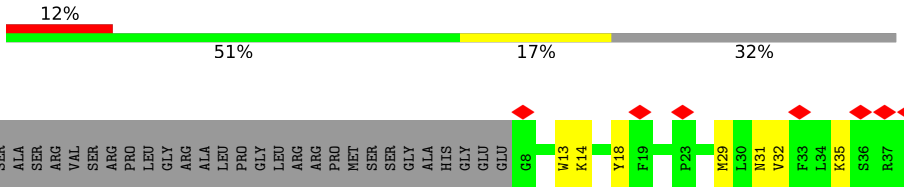
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	O1	1	31	10	5	13	3	0

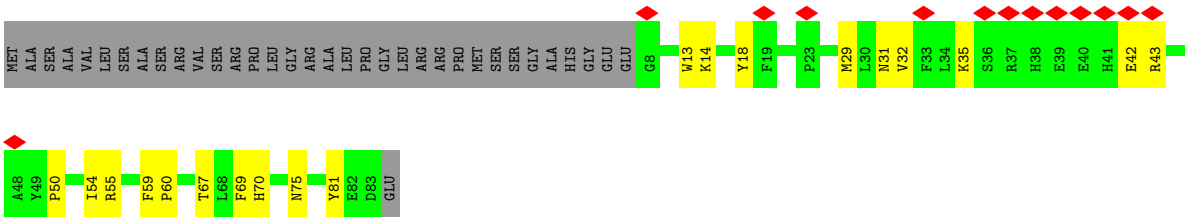
3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 6A1, mitochondrial

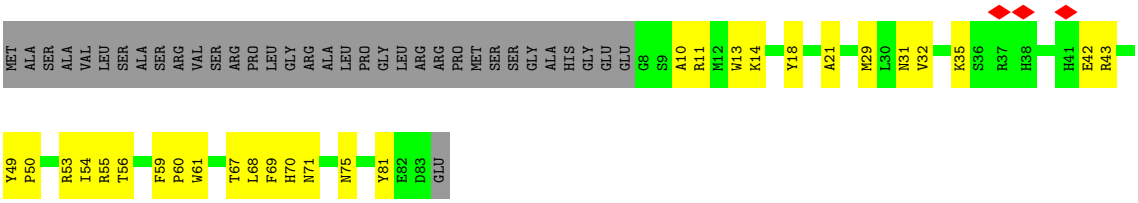
Chain t:





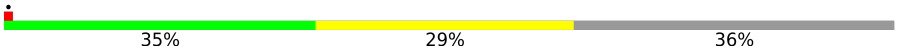
• Molecule 1: Cytochrome c oxidase subunit 6A1, mitochondrial

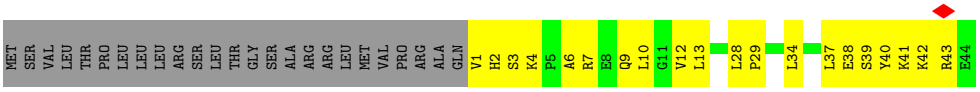
Chain g:



• Molecule 2: Cytochrome c oxidase subunit 8A, mitochondrial

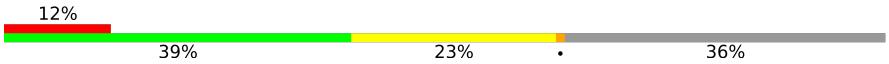
Chain m:

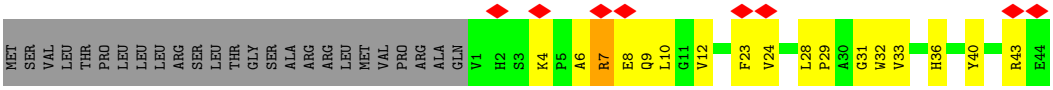




• Molecule 2: Cytochrome c oxidase subunit 8A, mitochondrial

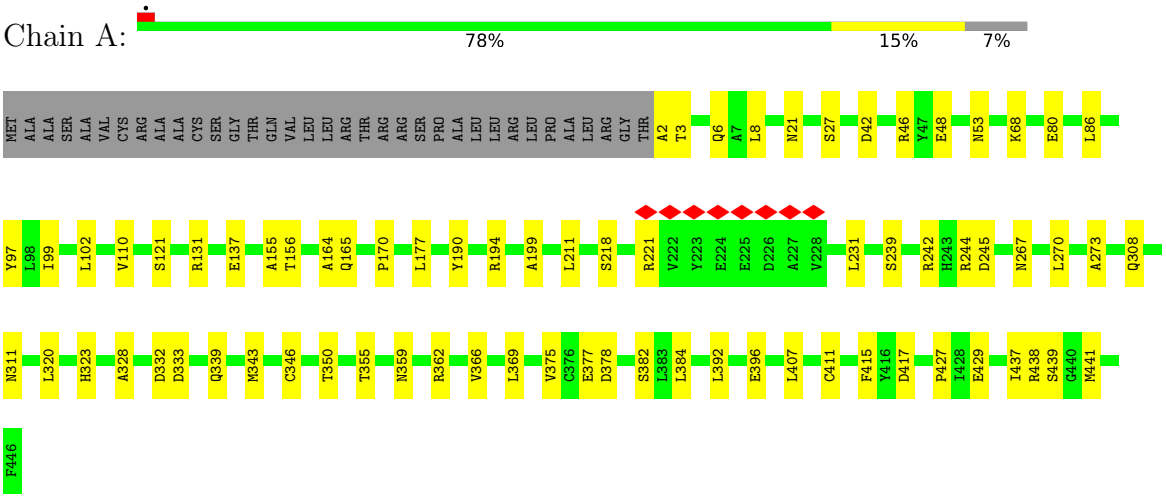
Chain z:





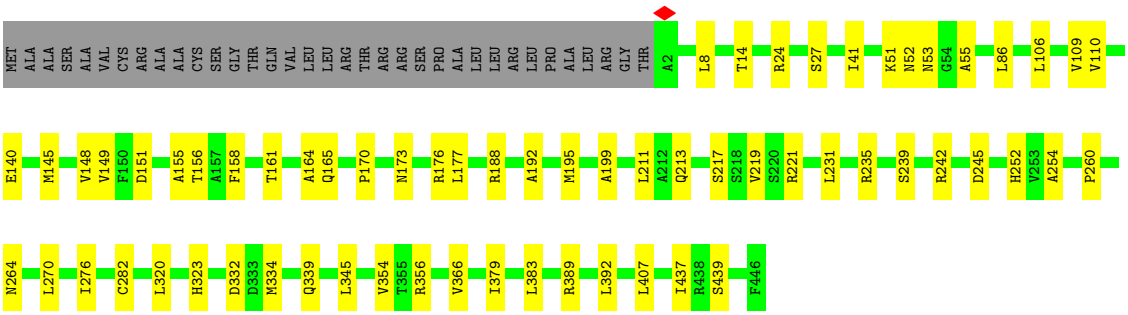
• Molecule 3: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



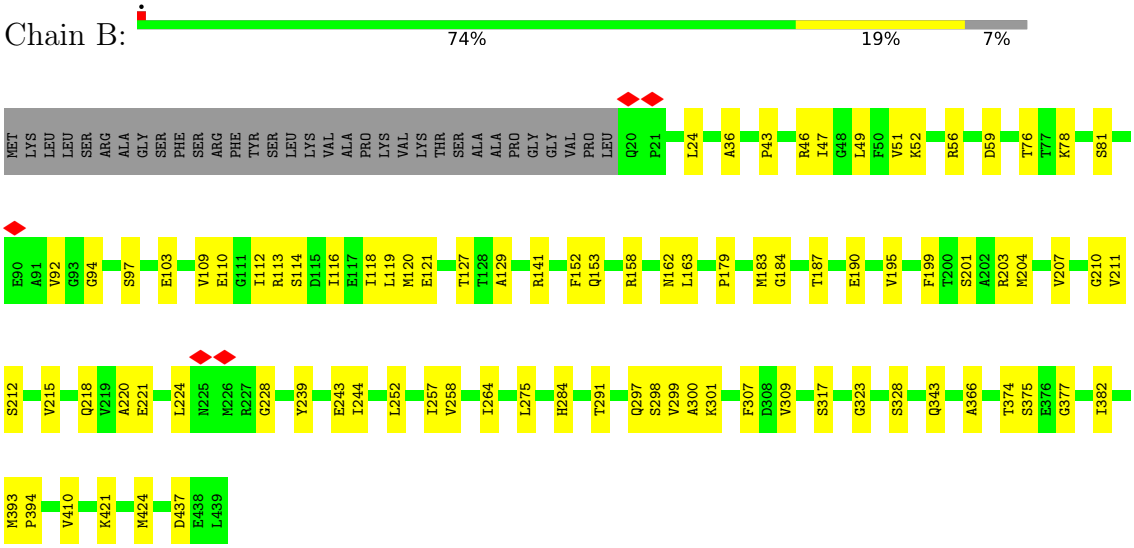
• Molecule 3: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



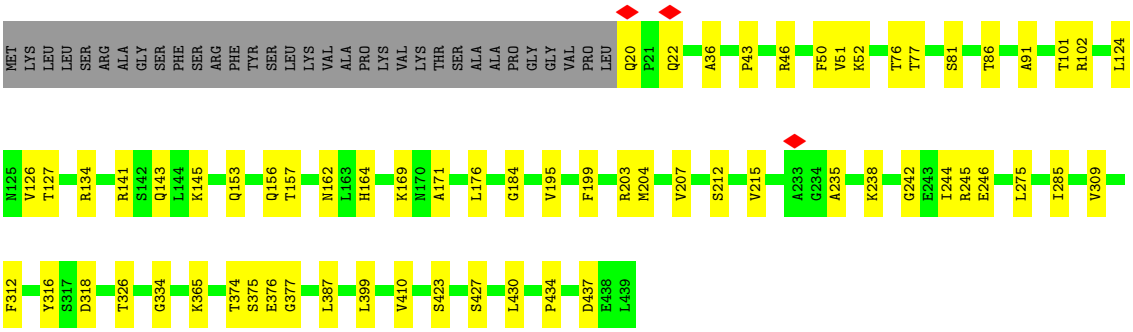
• Molecule 4: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



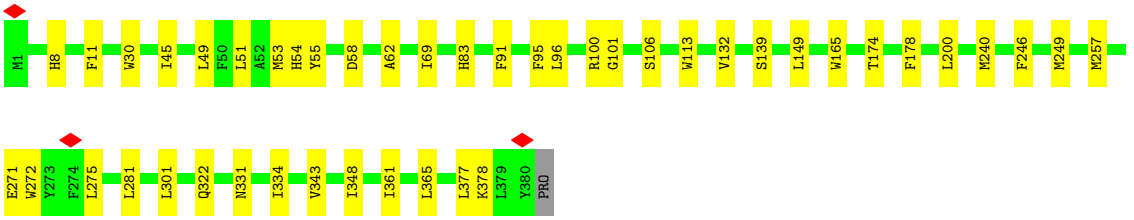
• Molecule 4: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



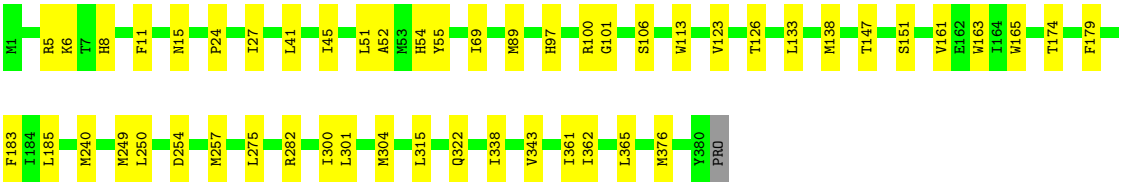
- Molecule 5: Cytochrome b

Chain C:



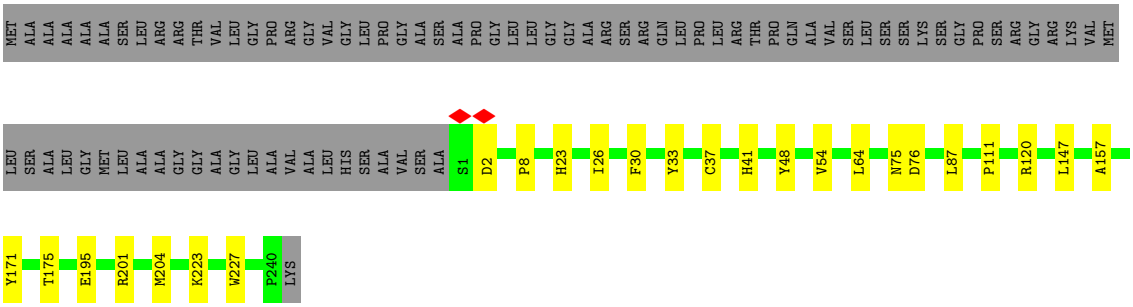
- Molecule 5: Cytochrome b

Chain N:



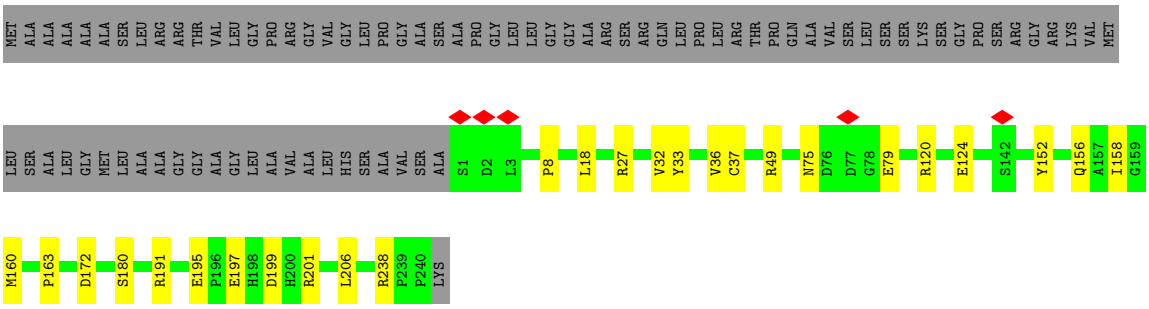
- Molecule 6: Cytochrome c1, heme protein, mitochondrial

Chain D:



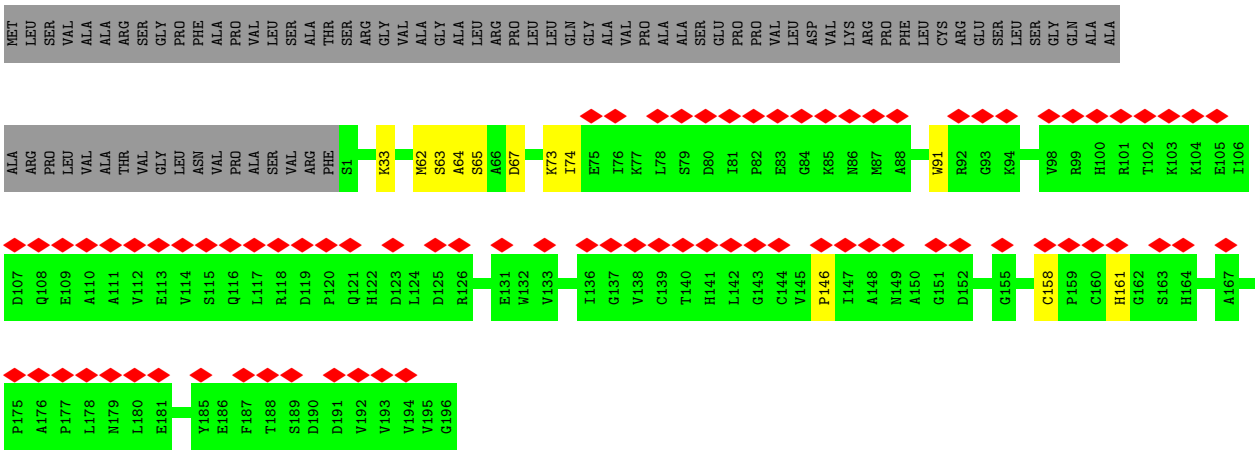
- Molecule 6: Cytochrome c1, heme protein, mitochondrial

Chain O:



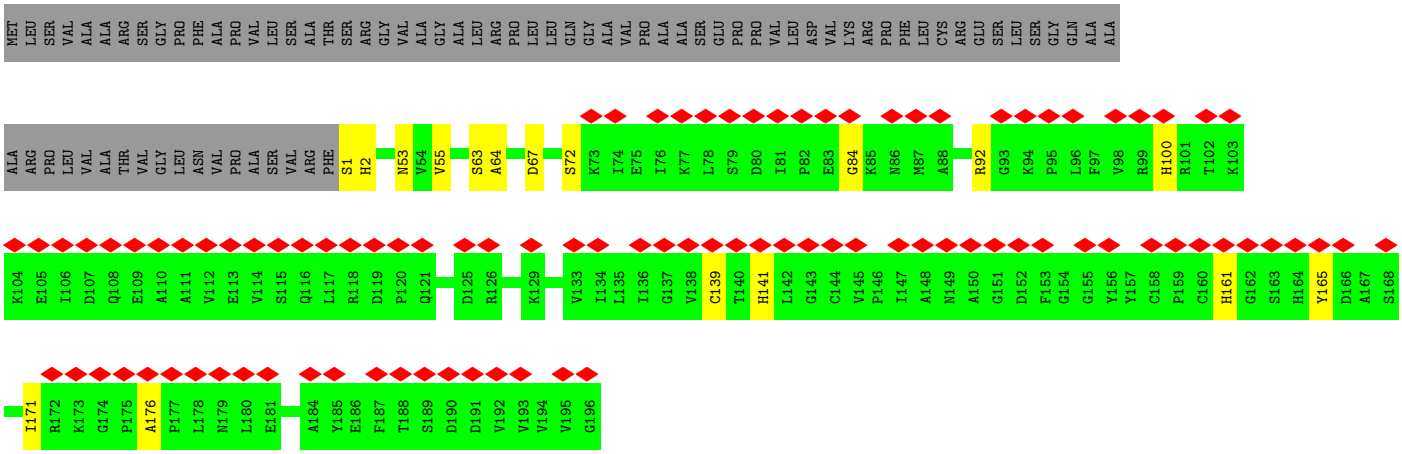
• Molecule 7: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



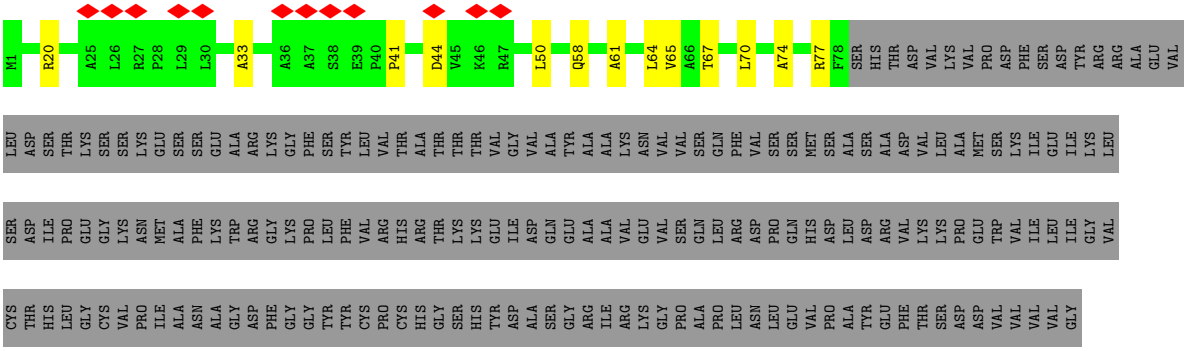
• Molecule 7: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



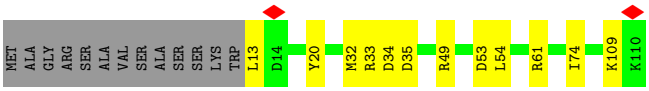
• Molecule 7: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain T:



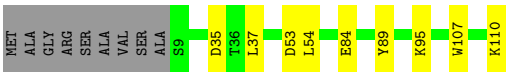
- Molecule 8: Cytochrome b-c1 complex subunit 7

Chain F:



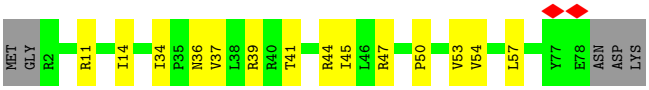
- Molecule 8: Cytochrome b-c1 complex subunit 7

Chain Q:



- Molecule 9: Cytochrome b-c1 complex subunit 8

Chain G:

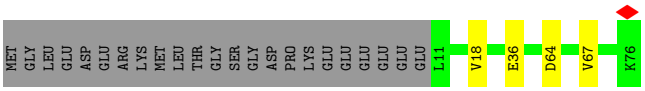


- Molecule 9: Cytochrome b-c1 complex subunit 8

Chain R:

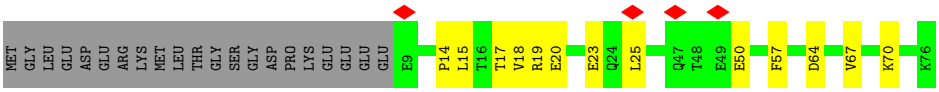
- Molecule 10: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



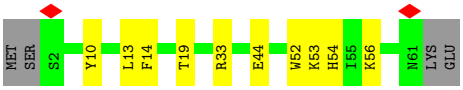
- Molecule 10: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain S:



• Molecule 11: Cytochrome b-c1 complex subunit 9

Chain J:

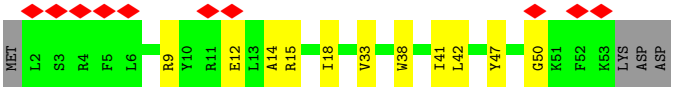


• Molecule 11: Cytochrome b-c1 complex subunit 9

Chain U:

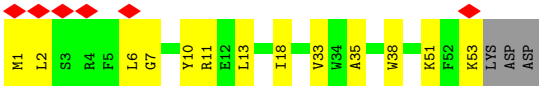
• Molecule 12: Cytochrome b-c1 complex subunit 10

Chain K:



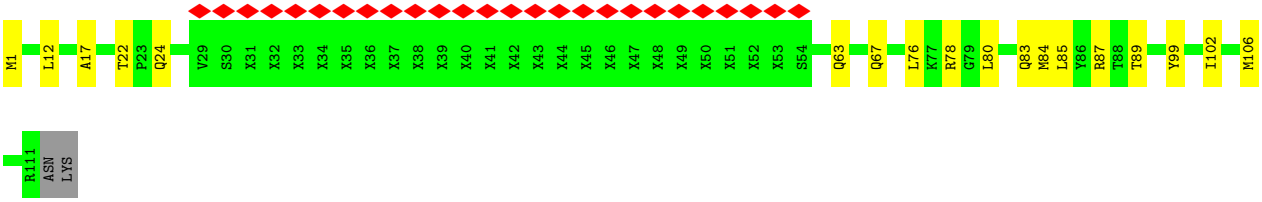
• Molecule 12: Cytochrome b-c1 complex subunit 10

Chain V:



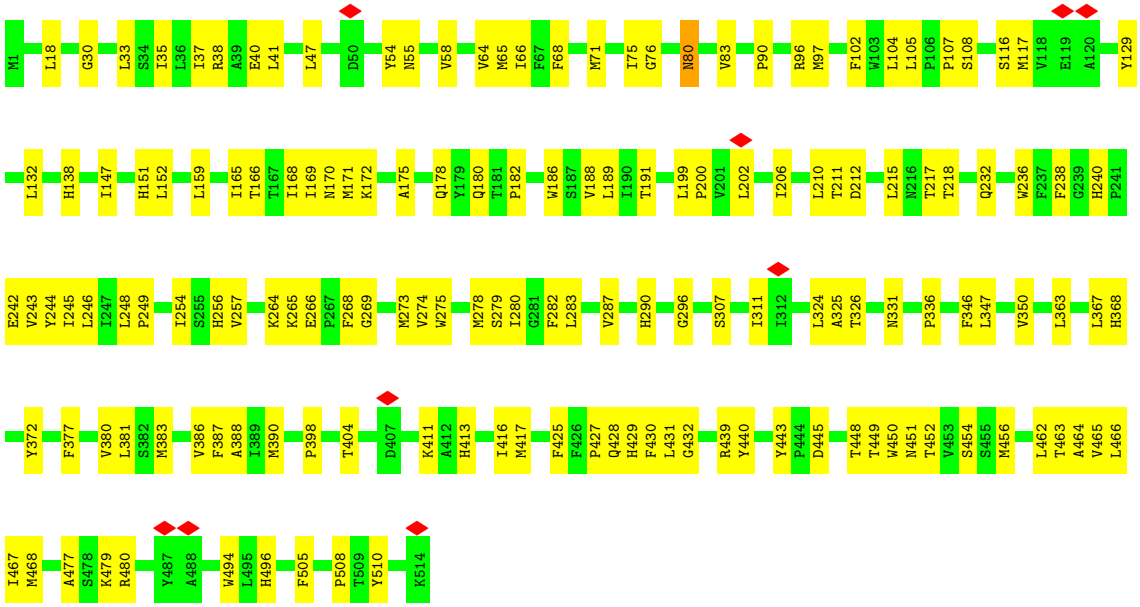
• Molecule 13: Cox7a2l protein

Chain I:



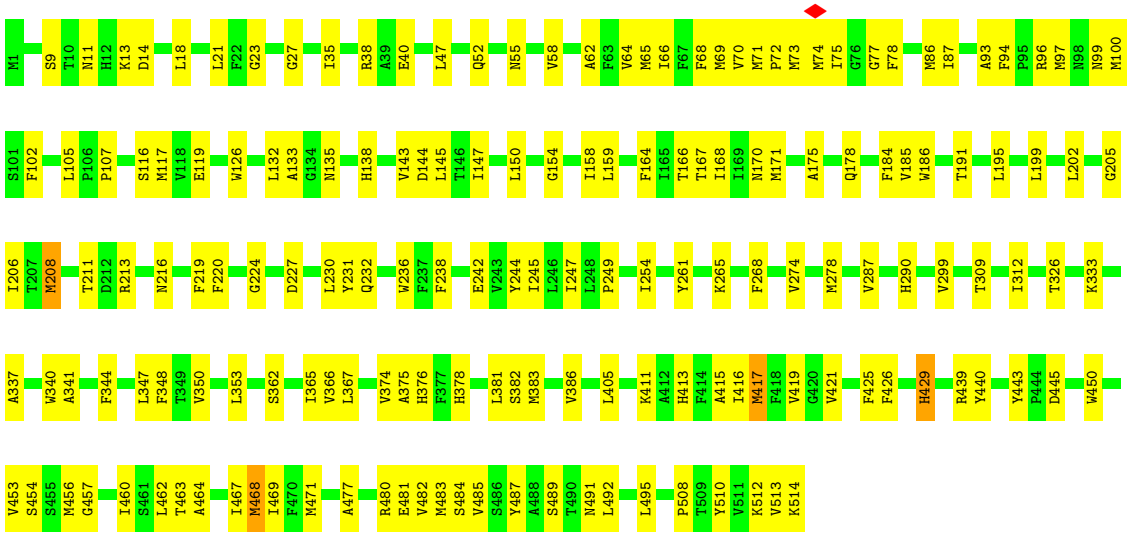
• Molecule 14: Cytochrome c oxidase subunit 1

Chain n:



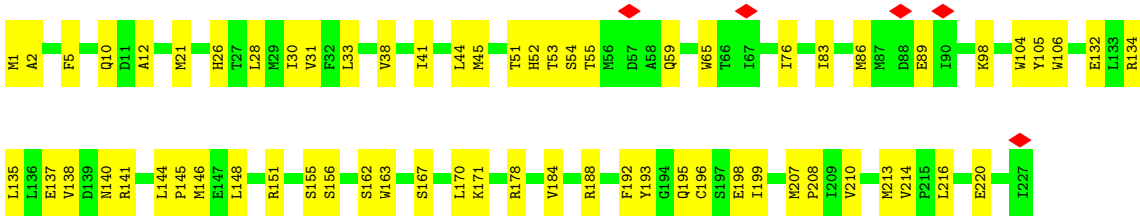
- Molecule 14: Cytochrome c oxidase subunit 1

Chain a:



- Molecule 15: Cytochrome c oxidase subunit 2

Chain o:



- Molecule 15: Cytochrome c oxidase subunit 2

Chain b: 67% 33%

M1 Q10 T13 S14 P15 E18 H26 T27 L28 M29 I30 V31 I41 M45 T51 H52 T53 S54 V61 I64 W65 T66 I67 I68 P69 I72 I76 R82 I83 M86 M87 D88 V94 L95 K98 G101 H102 Q103 W104 M122 I123 P124

D127 L128 K129 E132 L133 R134 V138 D139 N140 R141 V142 P145 M146 E147 L148 P149 I150 I154 H161 S162 W163 A164 V165 L168 G169 L170 K171 T172 L179 T185 R188 P189 Y193 G194 Q195 C196 S197 E198 I199 C200 G201 S202 N203 H204 S205 F206 M207 P208 I209 V210

L211 V214 I227

• Molecule 16: Cytochrome c oxidase subunit 3

Chain p: 75% 25%

MET T2 H6 A7 Y8 H9 P15 W16 A21 L25 M33 W34 F35 H36 Y37 L42 N50 I51 L52 Q56 W57 W58 R59 D60 V61 I62 R63 E64 Y67 Q68 T72 P73 M83 I87 F93 L112 G113 G114 C115 P118 P126 L127 E128 V129

P130 W146 L151 K155 M159 L163 M168 Y172 E183 T184 S187 G194 F198 H204 G205 V208 I209 I210 G211 S212 T213 F214 L215 I216 V217 R221 K224 F225 T228 F235 W249 Y253 V254 S255 I256 Y257 W258 W259 G260 S261

• Molecule 16: Cytochrome c oxidase subunit 3

Chain c: 74% 25%

MET THR H3 A7 N12 W16 F22 L25 L26 V32 M33 W34 F35 H36 T40 L43 T49 N50 M54 Y55 Q56 W57 W58 R59 R63 T66 Y67 H71 T72 Q76 L79 F86 S89 F98 H103 G120 N125 P126 L127

E128 L132 S135 V142 S143 I144 T145 W146 A147 H148 H149 S150 R156 N157 H158 M159 M160 Q161 A162 L163 Y172 F182 S187 I188 S189 D190 G191 S195 T196 F197 T213 F214 L215 I216 L219 Q222 L223 T228 H231 H232 F233 A239 Y253 Y257

S261

• Molecule 17: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

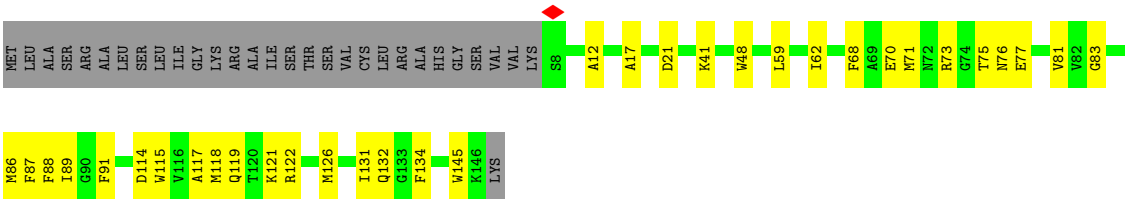
Chain q: 64% 18% 18%

MET LEU ALA SER ARG ALA LEU SER LEU ILE GLY LYS ARG ALA ILE SER THR SER VAL CYS LEU ARG ALA HIS GLY SER VAL VAL LYS S8 F13 P14 D18 R19 R20 D21 Y22 P23 L24 P25 W48 R61 F64 N65 E66 S67 M71 K79 V82 A85

I89 A93 L96 I97 W98 E99 T110 D114 W115 T120 K121 R122 M123 I131 K146 LYS

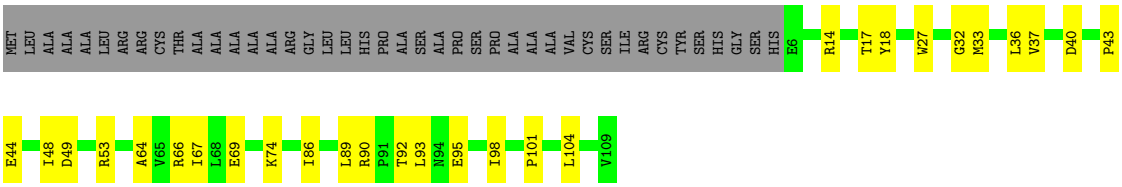
• Molecule 17: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain d:



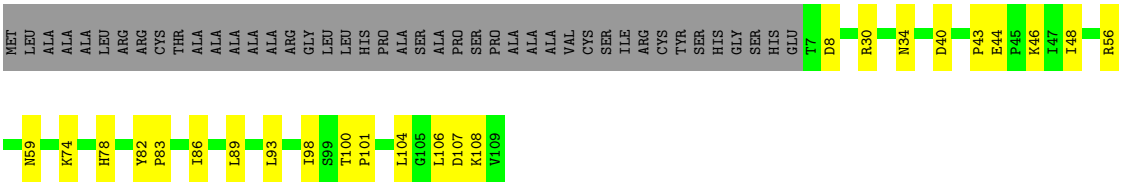
• Molecule 18: Cytochrome c oxidase subunit 5A, mitochondrial

Chain r:



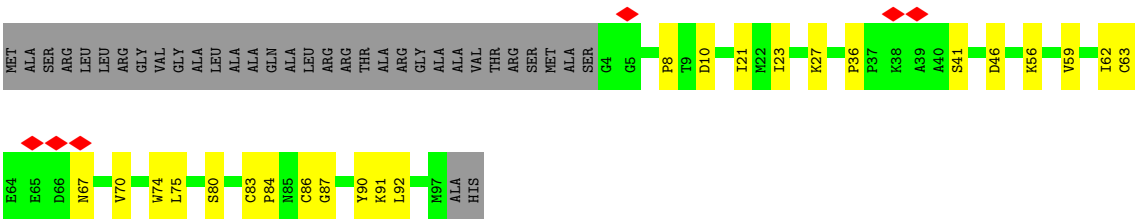
• Molecule 18: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:



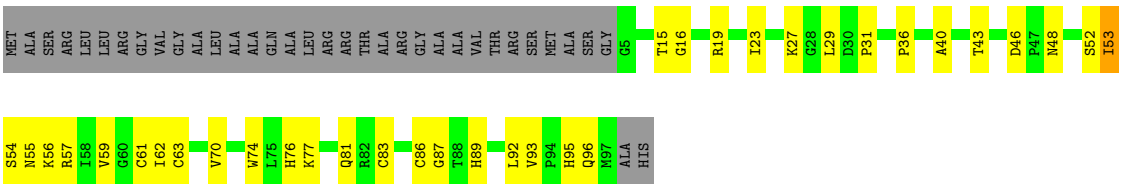
• Molecule 19: Cytochrome c oxidase subunit 5B, mitochondrial

Chain s:



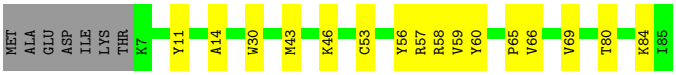
• Molecule 19: Cytochrome c oxidase subunit 5B, mitochondrial

Chain f:



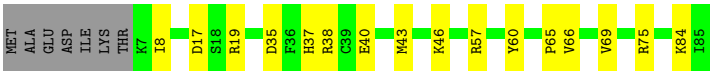
• Molecule 20: Cytochrome c oxidase subunit 6B1

Chain u:



• Molecule 20: Cytochrome c oxidase subunit 6B1

Chain h:

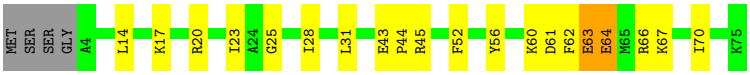


• Molecule 21: Cytochrome c oxidase subunit 6C

Chain v:

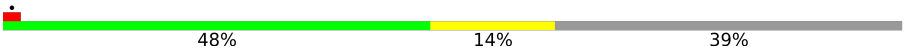
• Molecule 21: Cytochrome c oxidase subunit 6C

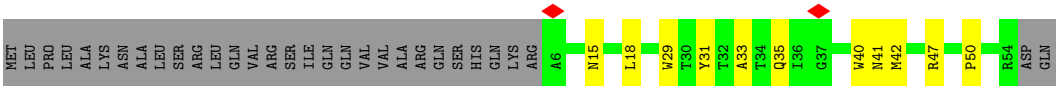
Chain i:



• Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

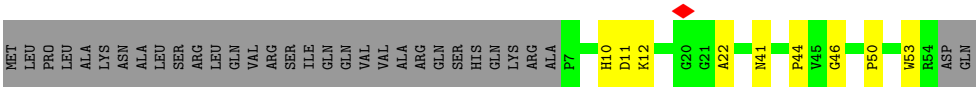
Chain x:





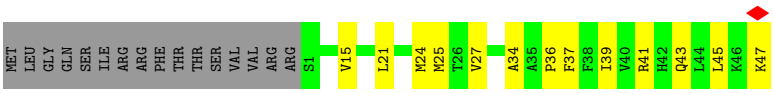
• Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k:



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

Chain y:

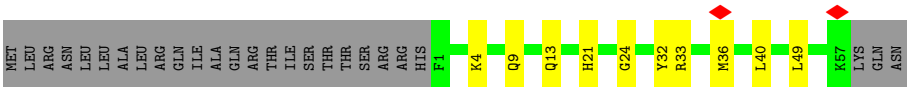


• Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial

Chain l:

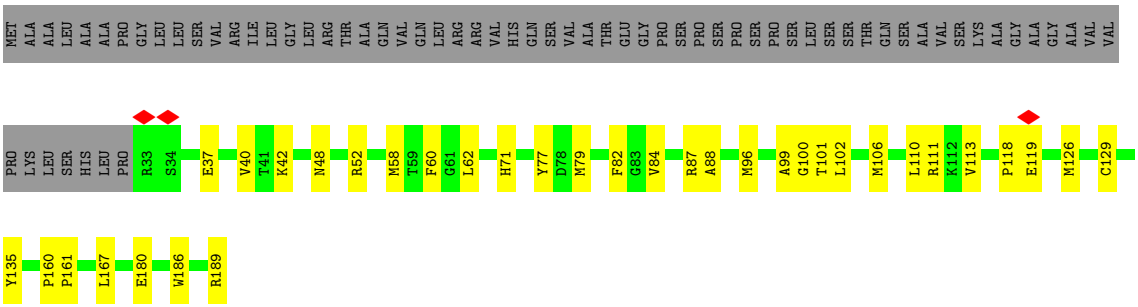
• Molecule 24: Cytochrome c oxidase subunit 7A2, mitochondrial

Chain w:



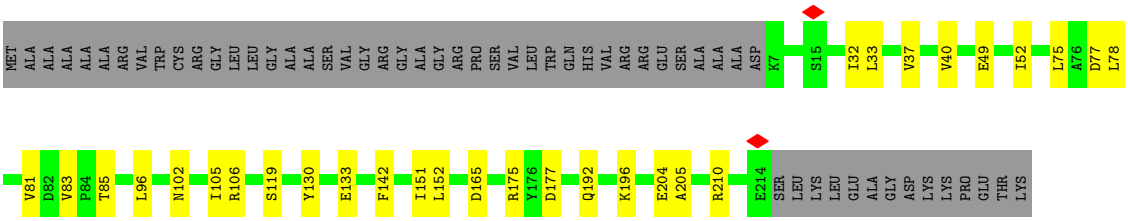
• Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:



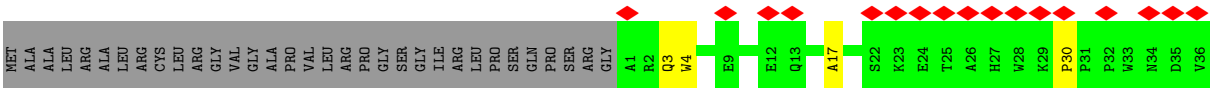
• Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C1:



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

Chain D1:



D37 I38 L39 K40 E41 K42 A43 V44 F51 G52 P53 Q54 R63 L64 V65 L66 E67 R74 K75 C76 D77 P78 H79 R85 Q98 F103 D104 R105 L106 D107 Y108 N114 E115 Q116 A117 L126 N127 I128 I137 F141 I144 T145 L148 N149 H150 I151 V154

T155 M164 T165 P166 F167 F168 W169 M170 R174 E175 K176 M177 R188 M189 H190 I194 L208 I211 F214 D223 I234 D249 G257 L260 I265 L269 Q273 P274 Y275 Y278 D279 Q280 V281 D292 D295 R296 Y297 E303 M304 R305

M318 A328 K329 V330 R335 M338 K339 M342 E343 I346 H347 K350 L351 Y352 V358 P359 P360 I367 E368 G372 Y377 L378 V379 S380 R388 C389 K390 I391 K392 K404 K407 D422 F425 I428 D429 R430

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

Chain 2:

MET PHE SER LEU ALA LEU ARG ALA ARG ALA THR GLY LEU ALA ALA GLN TRP GLY ARG HIS ALA ARG ASN LEU HIS LYS THR ALA VAL HIS ASN GLY ALA GLY G4 A5 L6 N27 R30 V35 Q43 L51 Q57 W60 L61 P76 R79 A84 Y90

N91 R92 G96 T105 T106 S115 E118 T119 G129 T138 L139 I140 N150 I156 E162 D163 L164 T165 P166 I169 I173 L176 K207 L217

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

Chain 1:

MET LEU ALA ALA ARG HIS PHE LEU GLY GLY LEU VAL PRO VAL ARG VAL SER VAL ARG PHE SER SER GLY THR THR ALA PRO LYS K9 L15 R20 N24 I48 G69 F73 P74 M82 R89 P90 K91 Y92 L93 N96 A97 D98 E99 G100 E101 P102 C105

M111 R112 H113 L118 M129 G130 A131 R132 A133 A134 R139 G140 E141 F142 E145 Q150 I153 Y171 I185 C186 G187 E188 E189 T190 A191 L192 K202 P203 R204 V215 F216 G217 C218 P219 T220 T221 N224 V225 C235 R247 T267 E271 M272 S273

L276 K277 E278 L279 K282 H283 T288 N293 V297 L306 K309 C312 L322 T327 G328 L329 D342 I343 C359 G368 M376 F379 I399 R429 R438 ALA TRP GLN ALA ALA SER

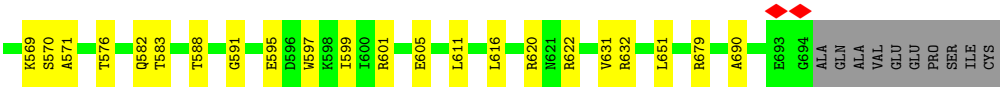
- Molecule 30: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:

MET LEU ARG ILE PRO ILE LYS ARG ALA LEU ILE GLY LEU SER ASN SER PRO LYS GLY TYR VAL ARG THR THR GLY THR ALA A5 V26 L27 Q28 Q36 E44 E60 A68 N78 H101 C108 G114 Q117 D118 M121 M122 D126 I142 L145

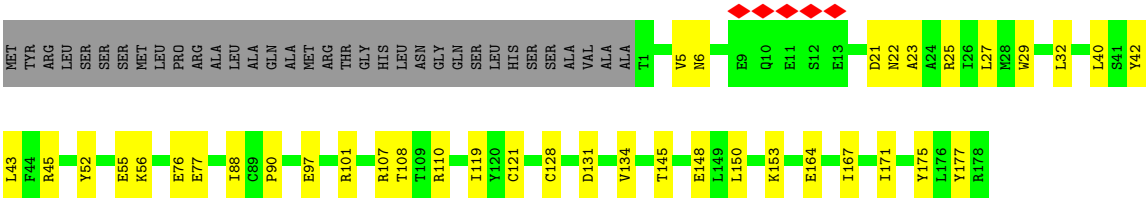
T157 I160 M190 F191 N198 D201 R218 E221 I228 R243 T244 K266 T267 R268 F269 A270 G273 R276 Q277 E281 R285 Y293 E297 E311 D324 D333 L334 L335 S340 F349 L364 N365 T366 G370 L379

P384 R396 W399 L400 T416 S438 F439 C440 E441 K444 V452 Q459 D462 V470 M473 V474 Q475 K476 I477 T480 K488 V489 M490 N491 H494 R495 P509 A513 K516 T533 L537 V544 H549 G550 D551 M556 A557 D558 V559



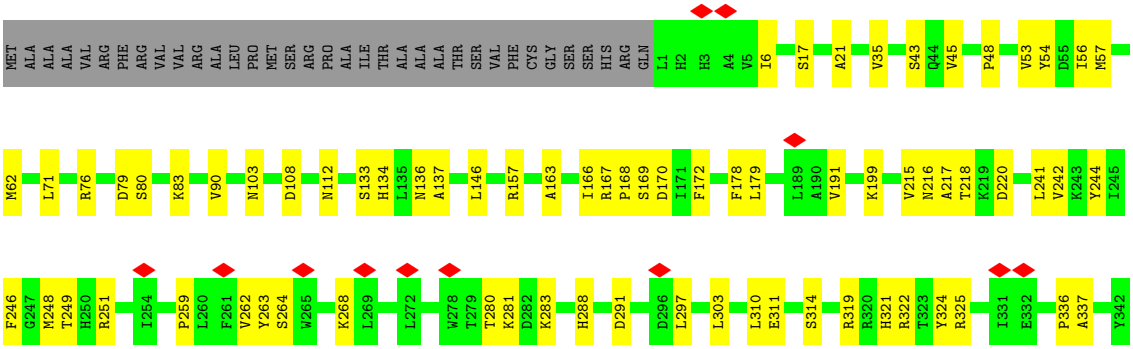
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:



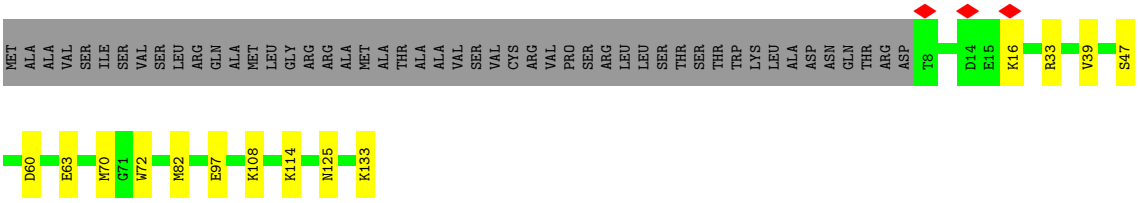
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P1:



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

Chain Q1:



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

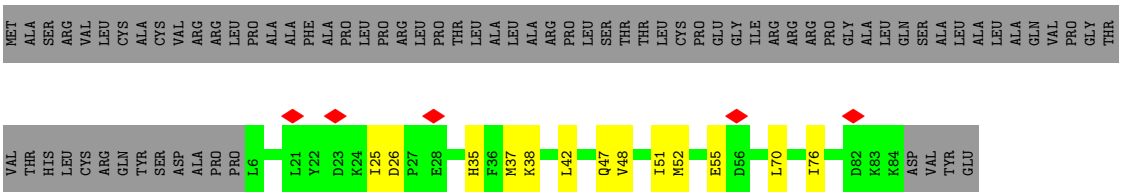
Chain 7:

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

Chain S1:

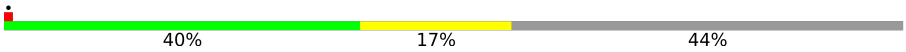
• Molecule 36: Acyl carrier protein, mitochondrial

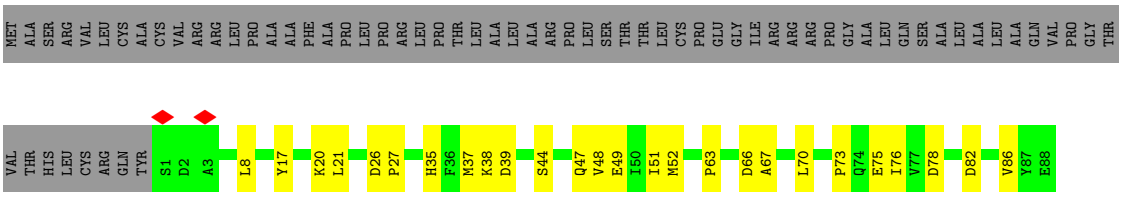
Chain T1:



• Molecule 36: Acyl carrier protein, mitochondrial

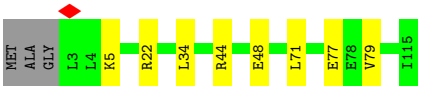
Chain U1:





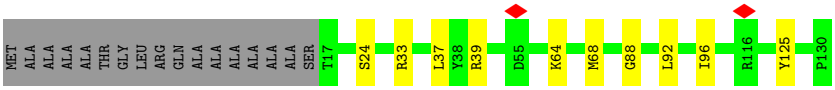
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1:



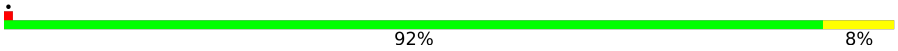
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

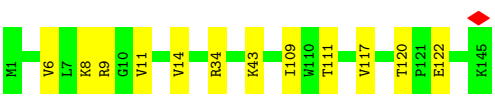
Chain W1:



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

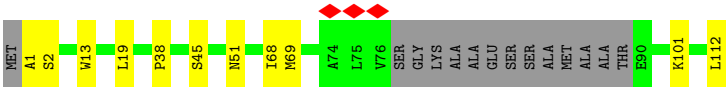
Chain q1:





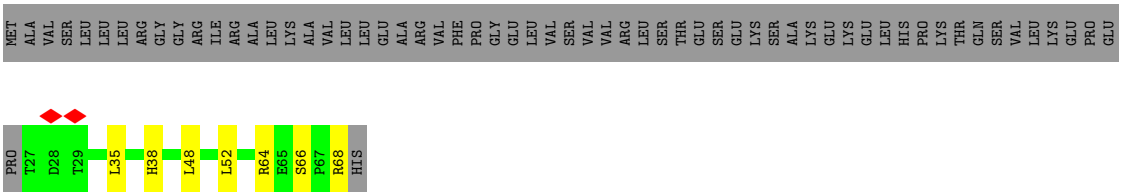
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1: 78% 10% 12%



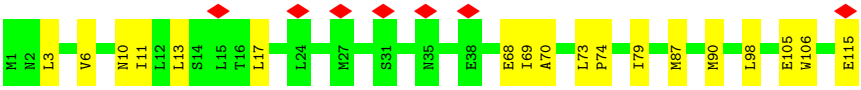
• Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s1: 34% 7% 60%



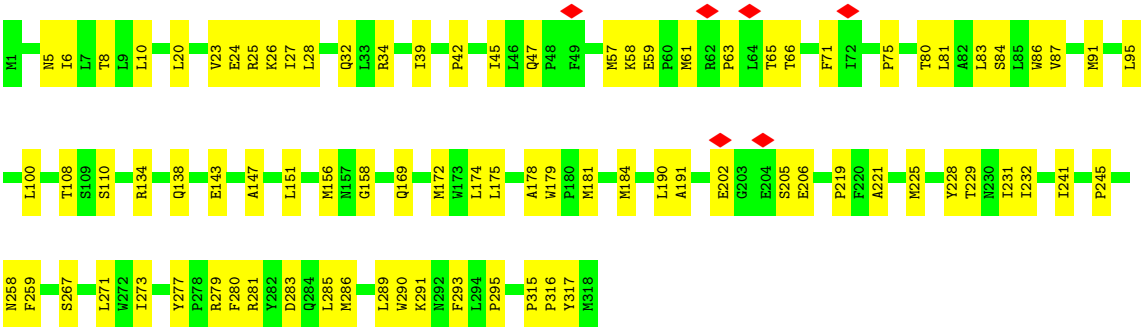
• Molecule 42: NADH-ubiquinone oxidoreductase chain 3

Chain A1: 6% 84% 16%



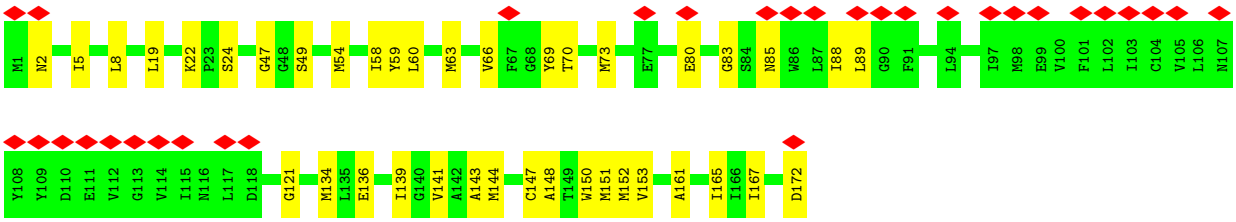
• Molecule 43: NADH-ubiquinone oxidoreductase chain 1

Chain H1: 73% 27%



• Molecule 44: NADH-ubiquinone oxidoreductase chain 6

Chain J1: 19% 77% 23%



• Molecule 45: NADH-ubiquinone oxidoreductase chain 4L

Chain K1: 74% 26%

M1 G18 M21 F22 R23 L26 M27 S28 L31 L38 S39 L40 T44 L49 M54 M57 P58 I59 P60 I63 A67 E70 L78 V79 K80 D88 Q91 N94 L95 L96 Q97 C98

• Molecule 46: NADH-ubiquinone oxidoreductase chain 5

Chain L1: 78% 22%

M1 T5 I8 I11 L15 L16 F54 N58 I63 H67 T70 S79 F80 K81 F84 T97 I100 L123 F124 L125 I126 I130 L131 T132 S133 A134 N135 N136 M137 F138 Q139 I142 V147 F152 L153 L154 Y159 G160 R161 A164

I172 L173 Y174 N175 R176 I180 L184 V187 S190 M193 N194 S195 W196 E197 L213 L217 T221 C222 K223 Q226 W232 V243 S244 A245 L246 L247 H248 S249 V253 R262 L266 M277 I290 C291 A292 L293 I298 I302 A303 F304 S305

T306 S307 L310 M313 M314 V315 G318 L324 I329 H332 K336 M341 C342 S345 I346 D352 R357 I362 I365 M366 P367 F368 T369 L378 M383 L386 D393 E397 M418 T419 A420 M421 Y422 I427 T431 I441 E445

I454 L457 P473 P474 T481 F485 T489 I493 L496 E503 L504 L507 N514 K515 A516 N517 P518 Y519 L525 P530 H534 R535 P538 L542 K547 T548 S549 L550 T551 L552 L553 D554 L555 K560 T561 S565 M573 T574 T575 L576

T577 T578 N579 I584 L606 GLU

• Molecule 47: NADH-ubiquinone oxidoreductase chain 4

Chain M1: 74% 26%

M1 L2 P7 L11 L14 L17 N26 L33 I34 S35 L36 Q44 T45 D46 E47 K50 S53 N54 S58 D59 L65 I66 I67 P74 L75 M76 L77 N82 M98 L99 I100 I104 L105 L106 I107 M108 T109 E114 Y119 L130 R135

N138 R142 L150 F151 S157 L164 I165 T173 D187 S191 N192 W196 L204 M207 P208 L209 L216 G227 I230 L231 A232 A233 I234 L235 L236 K237 L238 I244 R245 P252 M257 L264 T272 I275 R278 Q279 A287

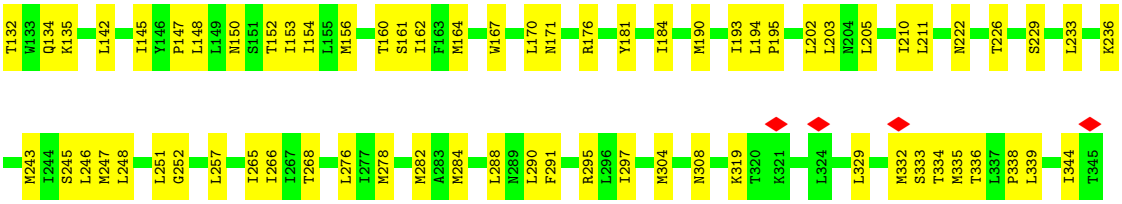
M294 A295 L296 V297 I298 A299 S300 I301 M302 T305 P306 W307 S308 F309 N310 T313 M316 H319 T322 L329 N333 Y334 E335 R336 I337 W359 P370 I373 N374 L375 L379 F380 I381 T382 M383 I393 M396 G397 I400 T403 G404 M405 Y406 R416

H422 P428 S429 H430 T431 R432 E433 L434 T435 L436 M437 H440 P443 L447 I454 T455 T458 M459

• Molecule 48: NADH-ubiquinone oxidoreductase chain 2

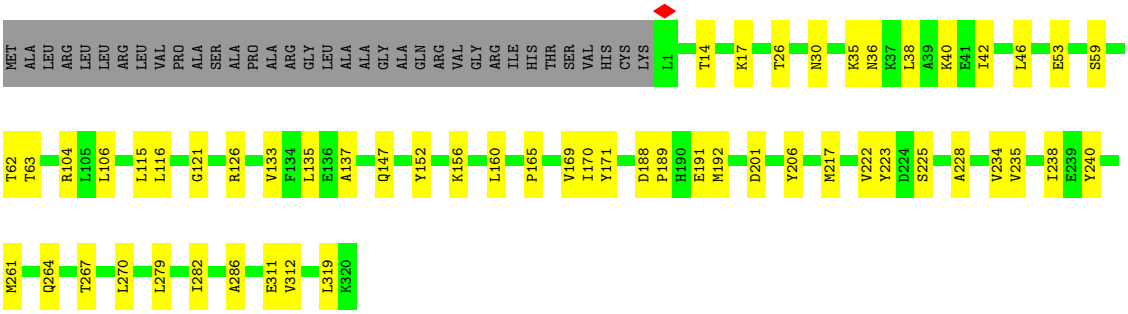
Chain N1: 70% 29%

M1 I9 I13 I19 T20 M21 S22 S23 T24 M27 V31 S36 A39 P42 M43 L44 I45 N46 N49 P50 R51 S52 K58 L71 F86 M97 M100 A109 P110 F111 H112 L115 T119 Q120 G121 I122 P123 M126 G127 L128 L131



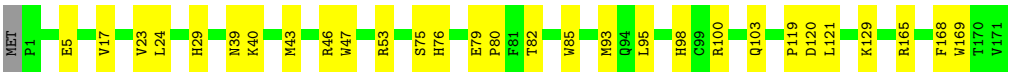
• Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1:



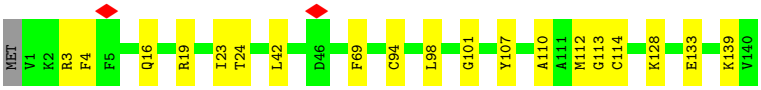
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1:



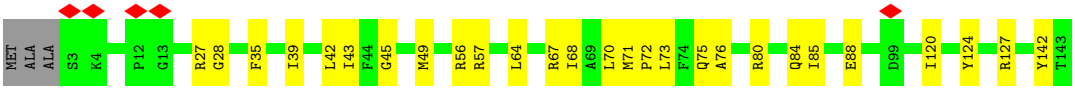
• Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y1:



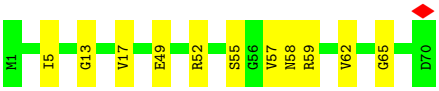
• Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z1:



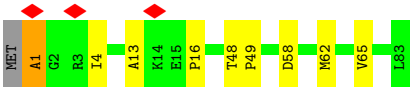
• Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a1:



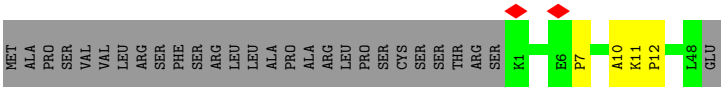
• Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b1:



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

Chain c1:



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

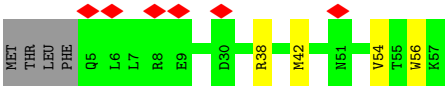
Chain d1:

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

Chain e1:

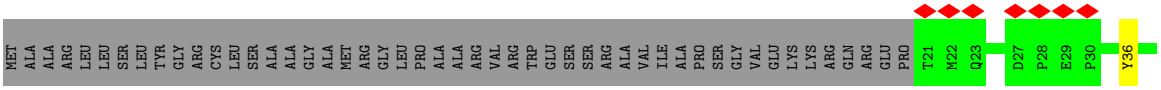
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

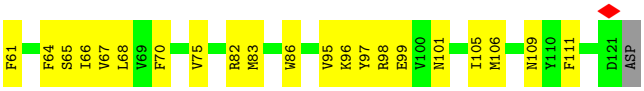
Chain f1:



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

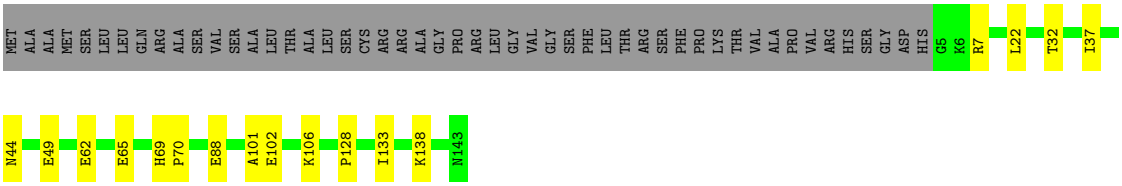
Chain g1:





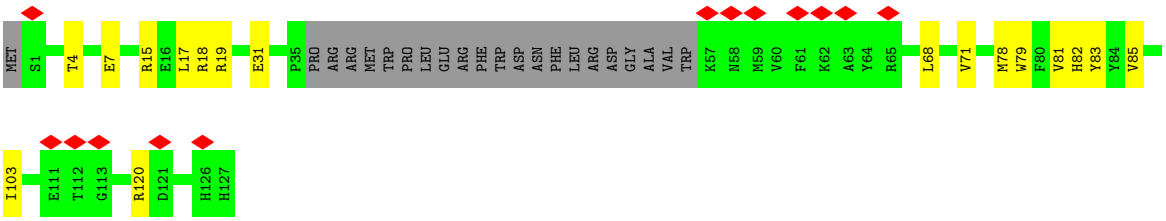
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h1:



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

Chain i1:

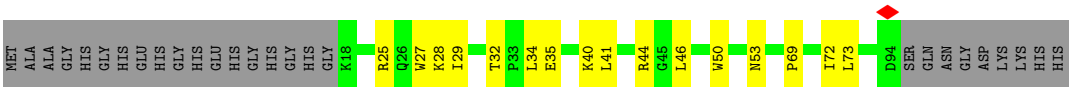


• Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j1:

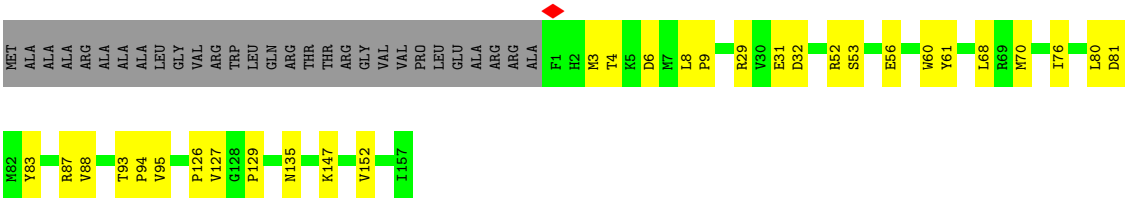
• Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k1:



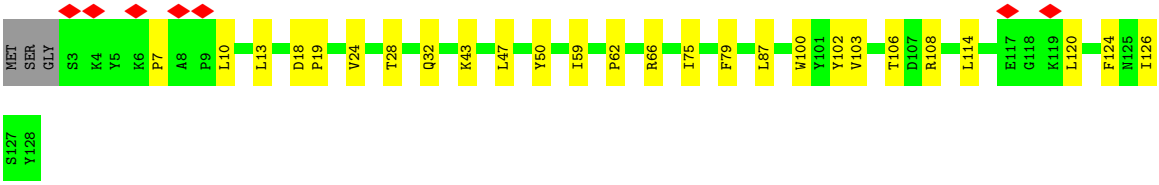
• Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l1:



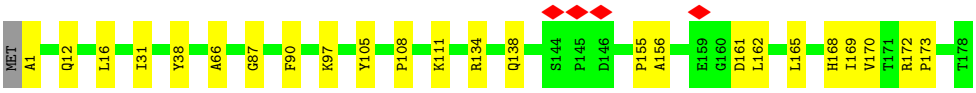
• Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m1:



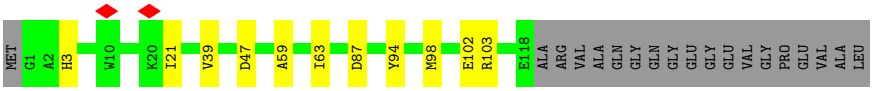
• Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

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 (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, K, MG, AYA, FES, HEM, DGT, 2MR, HEC, CUA, CU, NDP, FME, SAC, HEA, TGL, FMN, ZN, 3PE, NA, CDL, SF4, 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	g	0.83	0/646	1.20	1/882 (0.1%)
1	t	0.83	0/646	1.20	1/882 (0.1%)
2	m	0.98	0/350	1.11	0/472
2	z	0.99	0/350	1.11	0/472
3	A	0.17	0/3529	0.43	0/4793
3	L	0.17	0/3530	0.40	1/4793 (0.0%)
4	B	0.16	0/3205	0.36	0/4332
4	M	0.15	0/3205	0.35	0/4332
5	C	0.21	0/3147	0.48	0/4297
5	N	0.21	0/3147	0.47	0/4297
6	D	0.17	0/1968	0.42	0/2674
6	O	0.17	0/1968	0.39	0/2674
7	E	0.14	0/1176	0.36	0/1609
7	P	0.16	0/1173	0.37	0/1605
7	T	0.15	0/565	0.44	0/772
8	F	0.18	0/885	0.46	0/1184
8	Q	0.17	0/922	0.40	0/1234
9	G	0.22	0/673	0.51	0/909
9	R	0.22	0/673	0.50	0/909
10	H	0.25	0/552	0.70	1/739 (0.1%)
10	S	0.25	0/570	0.61	0/763
11	J	0.19	0/509	0.45	0/687
11	U	0.21	0/509	0.49	0/687
12	K	0.19	0/446	0.49	0/609
12	V	0.20	0/454	0.52	0/619
13	I	0.21	0/709	0.60	0/955
14	a	0.27	0/4162	0.66	4/5686 (0.1%)
14	n	0.26	0/4162	0.56	0/5686
15	b	0.25	0/1863	0.67	0/2542
15	o	0.23	0/1863	0.56	1/2542 (0.0%)
16	c	0.21	0/2195	0.54	0/3000

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	p	0.22	0/2202	0.54	0/3010
17	d	0.19	0/1190	0.59	0/1609
17	q	0.23	0/1190	0.57	0/1609
18	e	0.25	0/851	0.64	0/1155
18	r	0.21	0/860	0.55	0/1167
19	f	0.22	0/734	0.61	1/996 (0.1%)
19	s	0.20	0/738	0.52	0/1001
20	h	0.26	0/674	0.81	0/910
20	u	0.23	0/674	0.63	0/910
21	i	0.28	0/584	0.86	3/778 (0.4%)
21	v	0.25	0/579	0.64	0/771
22	k	0.18	0/391	0.43	0/533
22	x	0.22	0/396	0.55	0/541
23	l	0.22	0/393	0.57	0/527
23	y	0.25	0/399	0.55	0/535
24	w	0.17	0/444	0.45	0/598
25	6	0.24	0/1289	0.57	0/1744
26	C1	0.16	0/1780	0.37	0/2424
27	D1	0.22	0/3540	0.45	0/4795
28	2	0.18	0/1700	0.42	0/2316
29	1	0.19	0/3396	0.46	0/4586
30	3	0.18	0/5392	0.40	0/7305
31	9	0.22	0/1461	0.41	0/1974
32	P1	0.18	0/2823	0.45	0/3828
33	Q1	0.16	0/1045	0.34	0/1411
34	7	0.16	0/773	0.35	0/1041
35	S1	0.20	0/682	0.51	0/920
36	T1	0.19	0/646	0.51	0/869
36	U1	0.21	0/718	0.51	0/970
37	V1	0.16	0/945	0.31	0/1281
38	W1	0.19	0/993	0.42	0/1335
39	q1	0.17	0/1251	0.38	0/1702
40	r1	0.17	0/806	0.34	0/1090
41	s1	0.15	0/360	0.50	0/489
42	A1	0.25	0/948	0.53	0/1295
43	H1	0.28	0/2607	0.59	0/3564
44	J1	0.22	0/1330	0.52	0/1810
45	K1	0.25	0/738	0.51	0/1002
46	L1	0.23	0/4913	0.51	0/6686
47	M1	0.24	0/3709	0.52	0/5052
48	N1	0.23	0/2755	0.53	0/3751
49	O1	0.16	0/2674	0.39	0/3626
50	X1	0.17	0/1434	0.44	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
51	Y1	0.17	0/1061	0.43	0/1439
52	Z1	0.17	0/1198	0.37	0/1616
53	a1	0.22	0/585	0.45	0/788
54	b1	0.15	0/666	0.39	0/914
55	c1	0.14	0/409	0.37	0/555
56	d1	0.17	0/1028	0.42	0/1387
57	e1	0.18	0/900	0.41	0/1199
58	f1	0.17	0/468	0.45	0/630
59	g1	0.15	0/878	0.41	0/1196
60	h1	0.18	0/1201	0.45	0/1626
61	i1	0.15	0/917	0.35	0/1243
62	j1	0.19	0/587	0.49	0/804
63	k1	0.19	0/646	0.47	0/873
64	l1	0.16	0/1379	0.43	0/1882
65	m1	0.22	0/1079	0.52	0/1463
66	n1	0.18	0/1596	0.38	0/2162
67	o1	0.18	0/1039	0.44	0/1394
68	p1	0.16	0/1471	0.36	0/1988
All	All	0.23	0/129867	0.50	13/176249 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	m	0	2
2	z	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	468	MET	CG-SD-CE	6.78	115.81	100.90
21	i	64	GLU	CA-C-N	-6.31	112.56	122.65
21	i	64	GLU	C-N-CA	-6.31	112.56	122.65
14	a	417	MET	CB-CG-SD	-6.22	94.05	112.70
19	f	53	ILE	N-CA-C	-5.62	108.37	113.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	m	43	ARG	Sidechain
2	m	7	ARG	Sidechain
2	z	7	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	620	0	597	121	0
1	t	620	0	597	27	0
2	m	343	0	356	26	0
2	z	343	0	356	42	0
3	A	3459	0	3367	47	0
3	L	3460	0	3367	43	0
4	B	3154	0	3158	54	0
4	M	3154	0	3158	41	0
5	C	3046	0	3112	41	0
5	N	3046	0	3112	40	0
6	D	1909	0	1854	16	0
6	O	1909	0	1854	18	0
7	E	1167	0	842	14	0
7	P	1164	0	833	13	0
7	T	554	0	590	12	0
8	F	865	0	854	11	0
8	Q	900	0	887	6	0
9	G	654	0	656	12	0
9	R	654	0	656	7	0
10	H	545	0	531	2	0
10	S	563	0	541	14	0
11	J	495	0	489	8	0
11	U	495	0	489	7	0
12	K	430	0	431	9	0
12	V	438	0	443	11	0
13	I	807	0	736	21	0
14	a	4021	0	3997	149	0
14	n	4021	0	3997	131	0
15	b	1817	0	1822	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	o	1817	0	1822	50	0
16	c	2111	0	2047	104	0
16	p	2118	0	2054	61	0
17	d	1156	0	1112	27	0
17	q	1156	0	1112	23	0
18	e	833	0	832	19	0
18	r	842	0	838	19	0
19	f	717	0	695	24	0
19	s	721	0	698	19	0
20	h	654	0	622	27	0
20	u	654	0	622	11	0
21	i	572	0	596	15	0
21	v	567	0	591	13	0
22	k	378	0	363	11	0
22	x	383	0	367	9	0
23	l	380	0	378	10	0
23	y	386	0	386	14	0
24	w	435	0	446	11	0
25	6	1258	0	1268	28	0
26	C1	1730	0	1686	22	0
27	D1	3464	0	3416	69	0
28	2	1660	0	1653	18	0
29	1	3321	0	3278	55	0
30	3	5305	0	5330	70	0
31	9	1431	0	1383	31	0
32	P1	2748	0	2768	43	0
33	Q1	1022	0	1023	13	0
34	7	758	0	731	7	0
35	S1	671	0	688	11	0
36	T1	637	0	640	10	0
36	U1	706	0	699	20	0
37	V1	923	0	965	5	0
38	W1	970	0	991	6	0
39	q1	1209	0	1170	9	0
40	r1	796	0	831	9	0
41	s1	351	0	331	5	0
42	A1	932	0	967	19	0
43	H1	2540	0	2626	69	0
44	J1	1308	0	1319	36	0
45	K1	737	0	768	24	0
46	L1	4800	0	4985	105	0
47	M1	3632	0	3853	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	N1	2703	0	2902	77	0
49	O1	2607	0	2566	35	0
50	X1	1396	0	1385	22	0
51	Y1	1037	0	1025	13	0
52	Z1	1167	0	1166	24	0
53	a1	572	0	583	7	0
54	b1	651	0	653	8	0
55	c1	398	0	401	2	0
56	d1	996	0	1001	13	0
57	e1	877	0	871	15	0
58	f1	456	0	452	3	0
59	g1	850	0	783	20	0
60	h1	1166	0	1166	14	0
61	i1	897	0	902	15	0
62	j1	562	0	515	8	0
63	k1	626	0	620	11	0
64	l1	1323	0	1216	23	0
65	m1	1050	0	1061	21	0
66	n1	1541	0	1473	20	0
67	o1	1014	0	1002	10	0
68	p1	1438	0	1404	26	0
69	6	32	0	38	1	0
69	A	23	0	20	2	0
69	C	66	0	80	3	0
69	E	66	0	80	2	0
69	G	51	0	82	1	0
69	H1	51	0	82	2	0
69	K1	41	0	59	0	0
69	L	23	0	20	1	0
69	L1	102	0	164	6	0
69	M1	102	0	164	6	0
69	N	37	0	48	1	0
69	N1	38	0	50	1	0
69	O	33	0	40	1	0
69	R	30	0	34	2	0
69	Y1	70	0	88	2	0
69	a	55	0	58	3	0
69	b	29	0	32	1	0
69	b1	43	0	60	1	0
69	c	45	0	67	5	0
69	d	34	0	42	2	0
69	d1	63	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	g	25	0	24	11	0
69	i	28	0	30	0	0
69	i1	42	0	61	1	0
69	m1	36	0	46	0	0
69	n	89	0	100	3	0
69	o	29	0	32	2	0
69	p	45	0	67	6	0
69	r1	46	0	66	1	0
69	t	25	0	24	11	0
69	v	28	0	30	1	0
69	z	26	0	26	2	0
70	6	43	0	63	2	0
70	9	101	0	159	4	0
70	I	50	0	77	0	0
70	J	35	0	44	0	0
70	K	28	0	30	1	0
70	L	24	0	22	0	0
70	M1	54	0	88	4	0
70	P1	31	0	36	1	0
70	V	28	0	30	0	0
70	g	50	0	77	3	0
70	p	35	0	44	1	0
70	z	28	0	30	20	0
71	A	46	0	36	0	0
71	D	56	0	56	1	0
71	G	42	0	28	1	0
71	H1	51	0	52	1	0
71	L	46	0	36	1	0
71	L1	124	0	136	5	0
71	N1	90	0	133	5	0
71	O	57	0	58	0	0
71	R	170	0	175	5	0
71	V	46	0	36	2	0
71	Y1	94	0	141	2	0
71	d1	67	0	81	1	0
71	g	38	0	22	7	0
71	h1	70	0	87	4	0
71	r1	57	0	58	3	0
72	C	86	0	60	6	0
72	N	86	0	60	4	0
73	D	43	0	29	1	0
73	O	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	2	4	0	0	0	0
74	3	4	0	0	0	0
74	E	4	0	0	0	0
74	P	4	0	0	2	0
75	a	1	0	0	0	0
75	n	1	0	0	0	0
76	a	1	0	0	0	0
76	n	1	0	0	0	0
77	a	120	0	108	8	0
77	n	120	0	108	9	0
78	O1	1	0	0	0	0
78	a	1	0	0	0	0
78	o	1	0	0	0	0
79	b	2	0	0	0	0
79	o	2	0	0	0	0
80	7	1	0	0	0	0
80	f	1	0	0	0	0
80	s	1	0	0	0	0
81	l	37	0	49	1	0
81	y	37	0	49	1	0
82	1	8	0	0	0	0
82	3	16	0	0	0	0
82	6	8	0	0	0	0
82	9	16	0	0	1	0
83	1	31	0	19	2	0
84	3	1	0	0	0	0
85	P1	48	0	26	1	0
86	W1	34	0	40	0	0
86	n1	32	0	36	2	0
87	O1	31	0	12	1	0
All	All	130610	0	130128	2135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2135 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:240:HIS:NE2	14:n:244:TYR:CE2	1.69	1.60
1:g:50:PRO:CG	20:h:75:ARG:CZ	1.80	1.59
1:g:50:PRO:HG2	20:h:75:ARG:NH1	1.13	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:91:PHE:HB3	5:C:272:TRP:CH2	1.54	1.41
1:g:11:ARG:HH21	71:g:301:CDL:CA6	1.28	1.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
1	t	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
2	m	42/69 (61%)	41 (98%)	1 (2%)	0	100	100
2	z	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
3	A	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
3	L	443/480 (92%)	429 (97%)	14 (3%)	0	100	100
4	B	418/453 (92%)	409 (98%)	9 (2%)	0	100	100
4	M	418/453 (92%)	403 (96%)	15 (4%)	0	100	100
5	C	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
5	N	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
6	D	238/325 (73%)	233 (98%)	5 (2%)	0	100	100
6	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
7	E	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
7	P	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
7	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
8	F	96/111 (86%)	96 (100%)	0	0	100	100
8	Q	100/111 (90%)	100 (100%)	0	0	100	100
9	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
10	H	64/89 (72%)	64 (100%)	0	0	100	100
10	S	66/89 (74%)	63 (96%)	3 (4%)	0	100	100
11	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
11	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
12	K	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
12	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
13	I	86/113 (76%)	82 (95%)	4 (5%)	0	100	100
14	a	512/514 (100%)	491 (96%)	20 (4%)	1 (0%)	43	72
14	n	512/514 (100%)	489 (96%)	23 (4%)	0	100	100
15	b	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
15	o	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
16	c	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
16	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
17	d	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
17	q	137/169 (81%)	127 (93%)	10 (7%)	0	100	100
18	e	101/146 (69%)	100 (99%)	1 (1%)	0	100	100
18	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
19	f	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
19	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
20	h	77/86 (90%)	73 (95%)	3 (4%)	1 (1%)	9	39
20	u	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
21	i	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
21	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
22	k	46/80 (58%)	44 (96%)	2 (4%)	0	100	100
22	x	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
23	l	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
23	y	45/63 (71%)	45 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	15749/18172 (87%)	15149 (96%)	598 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	h	8	ILE
14	a	376	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	66/92 (72%)	66 (100%)	0	100	100
1	t	66/92 (72%)	66 (100%)	0	100	100
2	m	39/61 (64%)	39 (100%)	0	100	100
2	z	39/61 (64%)	39 (100%)	0	100	100
3	A	372/398 (94%)	372 (100%)	0	100	100
3	L	372/398 (94%)	372 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	330/356 (93%)	330 (100%)	0	100	100
4	M	330/356 (93%)	330 (100%)	0	100	100
5	C	332/333 (100%)	331 (100%)	1 (0%)	86	83
5	N	332/333 (100%)	332 (100%)	0	100	100
6	D	205/260 (79%)	205 (100%)	0	100	100
6	O	205/260 (79%)	205 (100%)	0	100	100
7	E	69/224 (31%)	69 (100%)	0	100	100
7	P	68/224 (30%)	67 (98%)	1 (2%)	57	70
7	T	58/224 (26%)	58 (100%)	0	100	100
8	F	90/99 (91%)	90 (100%)	0	100	100
8	Q	94/99 (95%)	94 (100%)	0	100	100
9	G	70/74 (95%)	70 (100%)	0	100	100
9	R	70/74 (95%)	70 (100%)	0	100	100
10	H	63/83 (76%)	63 (100%)	0	100	100
10	S	65/83 (78%)	65 (100%)	0	100	100
11	J	51/55 (93%)	51 (100%)	0	100	100
11	U	51/55 (93%)	51 (100%)	0	100	100
12	K	42/46 (91%)	42 (100%)	0	100	100
12	V	43/46 (94%)	43 (100%)	0	100	100
13	I	73/75 (97%)	73 (100%)	0	100	100
14	a	425/425 (100%)	425 (100%)	0	100	100
14	n	425/425 (100%)	424 (100%)	1 (0%)	87	85
15	b	210/210 (100%)	210 (100%)	0	100	100
15	o	210/210 (100%)	210 (100%)	0	100	100
16	c	225/227 (99%)	225 (100%)	0	100	100
16	p	226/227 (100%)	226 (100%)	0	100	100
17	d	122/146 (84%)	122 (100%)	0	100	100
17	q	122/146 (84%)	122 (100%)	0	100	100
18	e	90/118 (76%)	90 (100%)	0	100	100
18	r	91/118 (77%)	91 (100%)	0	100	100
19	f	80/101 (79%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	s	80/101 (79%)	80 (100%)	0	100	100
20	h	70/76 (92%)	70 (100%)	0	100	100
20	u	70/76 (92%)	70 (100%)	0	100	100
21	i	54/57 (95%)	54 (100%)	0	100	100
21	v	54/57 (95%)	54 (100%)	0	100	100
22	k	39/67 (58%)	39 (100%)	0	100	100
22	x	39/67 (58%)	39 (100%)	0	100	100
23	l	39/55 (71%)	39 (100%)	0	100	100
23	y	40/55 (73%)	40 (100%)	0	100	100
24	w	43/67 (64%)	43 (100%)	0	100	100
25	6	133/185 (72%)	133 (100%)	0	100	100
26	C1	190/227 (84%)	190 (100%)	0	100	100
27	D1	370/394 (94%)	370 (100%)	0	100	100
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%)	580 (100%)	0	100	100
31	9	152/178 (85%)	152 (100%)	0	100	100
32	P1	299/325 (92%)	299 (100%)	0	100	100
33	Q1	113/153 (74%)	113 (100%)	0	100	100
34	7	81/96 (84%)	80 (99%)	1 (1%)	63	73
35	S1	74/80 (92%)	74 (100%)	0	100	100
36	T1	73/135 (54%)	73 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	284 (100%)	0	100	100
50	X1	153/154 (99%)	153 (100%)	0	100	100
51	Y1	105/106 (99%)	105 (100%)	0	100	100
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%)	92 (100%)	0	100	100
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	13571/15439 (88%)	13567 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	271	GLU
7	P	53	ASN
14	n	80	ASN
34	7	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
15	b	161	HIS
16	c	160	ASN
27	D1	50	ASN
26	C1	124	HIS
16	c	222	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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
47	FME	M1	1	47	8,9,10	0.96	0	7,9,11	0.76	0
48	FME	N1	1	48	8,9,10	0.96	0	7,9,11	1.04	1 (14%)
45	FME	K1	1	45	8,9,10	0.94	0	7,9,11	1.66	2 (28%)
44	FME	J1	1	44	8,9,10	0.95	0	7,9,11	0.85	0
42	FME	A1	1	42	8,9,10	0.94	0	7,9,11	0.79	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
46	FME	L1	1	46	8,9,10	0.92	0	7,9,11	0.91	0
27	2MR	D1	85	27	10,12,13	2.58	2 (20%)	5,13,15	2.84	2 (40%)
40	AYA	r1	1	40	6,7,8	1.28	1 (16%)	5,8,10	1.28	1 (20%)

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

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	N1	1	FME	1	0
54	b1	1	AYA	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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 $|Z| > 2$ 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	$\#\|Z\| > 2$
70	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
71	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.33	0
69	3PE	G	102	-	50,50,50	0.31	0	53,55,55	0.28	0
86	ZMP	n1	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.93	1 (3%)
79	CUA	b	302	15	0,1,1	-	-	-		
69	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.55	1 (2%)
71	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.43	1 (1%)
72	HEM	N	401	5	50,50,50	1.36	5 (10%)	66,82,82	1.38	6 (9%)
83	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.47	1 (2%)
69	3PE	d	201	-	33,33,50	0.37	0	36,38,55	0.53	0
71	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
81	TGL	l	601	-	36,36,62	0.23	0	39,39,65	0.17	0
69	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.32	0
69	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.36	0
69	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.33	0
73	HEC	D	301	6	50,50,50	1.79	5 (10%)	68,82,82	1.37	5 (7%)
69	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.34	0
69	3PE	a	605	-	27,27,50	0.40	0	30,32,55	0.46	0
71	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
72	HEM	C	402	5	50,50,50	1.34	7 (14%)	66,82,82	1.24	7 (10%)
70	PC1	g	302	-	49,49,53	0.30	0	55,57,61	0.28	0
69	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.29	0
69	3PE	Y1	402	-	27,27,50	0.39	0	30,32,55	0.37	0
82	SF4	6	201	25	0,12,12	-	-	-		
82	SF4	3	802	30	0,12,12	-	-	-		
82	SF4	3	801	30	0,12,12	-	-	-		
79	CUA	o	303	15	0,1,1	-	-	-		
71	CDL	V	101	-	45,45,99	0.34	0	51,57,111	0.45	0
69	3PE	a	606	-	26,26,50	0.40	0	29,31,55	0.36	0
69	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.30	0
86	ZMP	W1	201	-	27,33,36	0.68	1 (3%)	32,40,45	0.93	1 (3%)
71	CDL	Y1	401	-	93,93,99	0.31	0	99,105,111	0.28	0
87	DGT	O1	401	78	29,33,33	0.31	0	44,52,52	0.29	0
71	CDL	r1	202	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
69	3PE	b1	101	-	42,42,50	0.33	0	45,47,55	0.35	0
69	3PE	i	101	-	27,27,50	0.39	0	30,32,55	0.33	0
69	3PE	m1	601	-	35,35,50	0.36	0	38,40,55	0.30	0
70	PC1	I	201	-	49,49,53	0.32	0	55,57,61	0.52	1 (1%)
70	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.33	0
81	TGL	y	601	-	36,36,62	0.24	0	39,39,65	0.18	0
82	SF4	9	202	31	0,12,12	-	-	-		
69	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.37	0
70	PC1	V	102	-	27,27,53	0.40	0	33,35,61	0.35	0
70	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.47	0
69	3PE	M1	503	-	50,50,50	0.30	0	53,55,55	0.27	0
69	3PE	g	303	-	24,24,50	0.43	0	27,29,55	0.63	0
71	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
69	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.32	0
69	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
70	PC1	z	101	-	27,27,53	0.40	0	33,35,61	0.35	0
73	HEC	O	303	6	50,50,50	1.78	5 (10%)	68,82,82	1.35	5 (7%)
70	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.58	0
74	FES	E	201	7	0,4,4	-	-	-		
77	HEA	n	604	14	66,67,67	1.41	6 (9%)	78,103,103	2.41	29 (37%)
69	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.60	1 (3%)
71	CDL	g	301	-	34,37,99	0.37	0	37,47,111	0.53	0
77	HEA	a	603	14	66,67,67	1.45	7 (10%)	78,103,103	2.35	28 (35%)
69	3PE	L1	704	-	50,50,50	0.31	0	53,55,55	0.28	0
69	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.30	0
82	SF4	9	201	31	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
70	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.44	0
71	CDL	L1	703	-	45,45,99	0.43	0	51,57,111	0.34	0
69	3PE	b	301	-	28,28,50	0.40	0	31,33,55	0.37	0
74	FES	P	201	7	0,4,4	-	-	-		
70	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.47	0
69	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
71	CDL	R	101	-	40,40,99	0.45	0	46,52,111	0.53	0
82	SF4	1	502	29	0,12,12	-	-	-		
69	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.34	0
69	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
69	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
71	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.42	0
85	NDP	P1	501	-	49,52,52	0.34	0	66,80,80	0.42	0
69	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.31	0
69	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.33	0
71	CDL	G	101	-	41,41,99	0.44	0	47,53,111	0.36	0
69	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.34	0
70	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.34	0
69	3PE	z	102	-	25,25,50	0.41	0	28,30,55	0.39	0
74	FES	3	803	30	0,4,4	-	-	-		
74	FES	2	301	28	0,4,4	-	-	-		
72	HEM	N	402	5	50,50,50	1.38	7 (14%)	66,82,82	1.32	10 (15%)
71	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
69	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.66	0
77	HEA	a	604	14	66,67,67	1.39	7 (10%)	78,103,103	2.32	28 (35%)
70	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.61	0
69	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.30	0
69	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.39	0
69	3PE	E	203	-	33,33,50	0.36	0	36,38,55	0.33	0
71	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
69	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
69	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.32	0
71	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.38	0
72	HEM	C	401	5	50,50,50	1.31	5 (10%)	66,82,82	1.32	6 (9%)
77	HEA	n	603	14	66,67,67	1.38	6 (9%)	78,103,103	2.37	26 (33%)
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
69	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.41	0
71	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.51	0
71	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.28	0
70	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	9	204	-	-	10/50/50/57	-
71	CDL	D	302	-	-	19/66/66/110	-
69	3PE	G	102	-	-	11/54/54/54	-
86	ZMP	n1	201	-	-	20/36/38/43	-
69	3PE	n	605	-	-	10/37/37/54	-
71	CDL	R	103	-	-	19/82/82/110	-
72	HEM	N	401	5	-	3/14/54/54	-
83	FMN	1	501	-	-	5/18/18/18	0/3/3/3
69	3PE	d	201	-	-	6/37/37/54	-
71	CDL	O	301	-	-	15/67/67/110	-
81	TGL	l	601	-	-	0/39/39/65	-
69	3PE	E	202	-	-	9/35/35/54	-
69	3PE	n	607	-	-	8/30/30/54	-
73	HEC	D	301	6	1/1/3/7	2/14/54/54	-
69	3PE	v	101	-	-	7/31/31/54	-
69	3PE	d1	202	-	-	7/34/34/54	-
69	3PE	a	605	-	-	6/31/31/54	-
71	CDL	R	102	-	-	17/67/67/110	-
72	HEM	C	402	5	-	1/14/54/54	-
70	PC1	g	302	-	-	8/53/53/57	-
69	3PE	r1	201	-	-	8/49/49/54	-
69	3PE	Y1	402	-	-	4/31/31/54	-
82	SF4	6	201	25	-	-	0/6/5/5
82	SF4	3	802	30	-	-	0/6/5/5
82	SF4	3	801	30	-	-	0/6/5/5
71	CDL	V	101	-	-	18/55/55/110	-
69	3PE	a	606	-	-	9/30/30/54	-
69	3PE	i1	201	-	-	6/45/45/54	-
86	ZMP	W1	201	-	-	5/38/40/43	-
71	CDL	Y1	401	-	-	11/104/104/110	-
87	DGT	O1	401	78	-	1/22/34/34	0/3/3/3
71	CDL	r1	202	-	-	13/67/67/110	-
69	3PE	b1	101	-	-	10/46/46/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	i	101	-	-	8/31/31/54	-
69	3PE	m1	601	-	-	13/39/39/54	-
70	PC1	I	201	-	-	9/53/53/57	-
70	PC1	p	302	-	-	10/38/38/57	-
81	TGL	y	601	-	-	3/39/39/65	-
82	SF4	9	202	31	-	-	0/6/5/5
69	3PE	d1	203	-	-	7/35/35/54	-
70	PC1	V	102	-	-	4/31/31/57	-
70	PC1	6	203	-	-	12/46/46/57	-
69	3PE	M1	503	-	-	14/54/54/54	-
69	3PE	g	303	-	-	9/28/28/54	-
71	CDL	d1	201	-	-	16/77/77/110	-
73	HEC	O	303	6	1/1/3/7	4/14/54/54	-
69	3PE	N1	402	-	-	6/41/41/54	-
69	3PE	c	301	-	-	10/48/48/54	-
70	PC1	z	101	-	-	6/31/31/57	-
70	PC1	P1	502	-	-	15/34/34/57	-
74	FES	E	201	7	-	-	0/1/1/1
77	HEA	n	604	14	-	9/36/76/76	-
69	3PE	t	101	-	-	7/28/28/54	-
71	CDL	g	301	-	-	9/41/45/110	-
77	HEA	a	603	14	-	15/36/76/76	-
69	3PE	L1	704	-	-	7/54/54/54	-
69	3PE	p	301	-	-	12/48/48/54	-
82	SF4	9	201	31	-	-	0/6/5/5
70	PC1	9	203	-	-	12/57/57/57	-
71	CDL	L1	703	-	-	15/56/56/110	-
69	3PE	b	301	-	-	9/32/32/54	-
74	FES	P	201	7	-	-	0/1/1/1
70	PC1	K	101	-	-	4/31/31/57	-
69	3PE	L1	701	-	-	9/54/54/54	-
71	CDL	R	101	-	-	15/51/51/110	-
82	SF4	1	502	29	-	-	0/6/5/5
69	3PE	R	104	-	-	5/33/33/54	-
69	3PE	H1	401	-	-	9/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	C	403	-	-	9/38/38/54	-
71	CDL	h1	201	-	-	20/80/80/110	-
85	NDP	P1	501	-	-	5/34/77/77	0/5/5/5
69	3PE	6	202	-	-	4/35/35/54	-
69	3PE	N	403	-	-	7/40/40/54	-
71	CDL	G	101	-	-	13/52/52/110	-
69	3PE	O	302	-	-	9/36/36/54	-
70	PC1	J	101	-	-	7/38/38/57	-
69	3PE	z	102	-	-	1/29/29/54	-
74	FES	3	803	30	-	-	0/1/1/1
74	FES	2	301	28	-	-	0/1/1/1
72	HEM	N	402	5	-	4/14/54/54	-
71	CDL	H1	402	-	-	12/59/59/110	-
69	3PE	A	501	-	-	9/26/26/54	-
77	HEA	a	604	14	-	14/36/76/76	-
70	PC1	L	503	-	-	9/27/27/57	-
69	3PE	K1	201	-	-	12/44/44/54	-
69	3PE	L	501	-	-	6/26/26/54	-
69	3PE	E	203	-	-	9/37/37/54	-
71	CDL	A	502	-	-	13/56/56/110	-
69	3PE	o	302	-	-	10/32/32/54	-
69	3PE	Y1	403	-	-	7/45/45/54	-
71	CDL	N1	401	-	-	21/100/100/110	-
72	HEM	C	401	5	-	1/14/54/54	-
77	HEA	n	603	14	-	12/36/76/76	-
69	3PE	C	404	-	-	4/34/34/54	-
69	3PE	M1	502	-	-	17/54/54/54	-
69	3PE	n	606	-	-	9/31/31/54	-
71	CDL	L	502	-	-	9/56/56/110	-
71	CDL	L1	702	-	-	15/88/88/110	-
70	PC1	M1	501	-	-	9/57/57/57	-

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	D	301	HEC	C3D-C2D	8.03	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	O	303	HEC	C3D-C2D	7.89	1.53	1.36
73	D	301	HEC	FE-NC	4.69	2.11	1.95
77	a	603	HEA	C3B-C2B	4.57	1.45	1.34
77	n	604	HEA	C3D-C2D	4.46	1.46	1.36

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	a	603	HEA	C3A-C2A-C1A	-7.00	100.39	107.08
77	a	604	HEA	C3A-C2A-C1A	-6.68	100.70	107.08
77	n	604	HEA	C3A-C2A-C1A	-6.61	100.76	107.08
73	D	301	HEC	C1D-ND-C4D	6.40	111.69	105.07
77	n	603	HEA	C3A-C2A-C1A	-6.10	101.25	107.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
73	D	301	HEC	NA
73	O	303	HEC	NA

5 of 828 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	t	101	3PE	C11-O13-P-O12
69	t	101	3PE	C11-O13-P-O14
69	t	101	3PE	O13-C11-C12-N
69	z	102	3PE	O13-C11-C12-N
69	A	501	3PE	C1-O11-P-O12

There are no ring outliers.

76 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	9	204	PC1	3	0
71	D	302	CDL	1	0
69	G	102	3PE	1	0
86	n1	201	ZMP	2	0
71	R	103	CDL	4	0
72	N	401	HEM	2	0
83	1	501	FMN	2	0
69	d	201	3PE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	l	601	TGL	1	0
69	E	202	3PE	2	0
69	n	607	3PE	1	0
69	v	101	3PE	1	0
73	D	301	HEC	1	0
69	d1	202	3PE	1	0
69	a	605	3PE	1	0
71	R	102	CDL	1	0
72	C	402	HEM	3	0
70	g	302	PC1	3	0
69	r1	201	3PE	1	0
69	Y1	402	3PE	1	0
71	V	101	CDL	2	0
69	a	606	3PE	2	0
69	i1	201	3PE	1	0
71	Y1	401	CDL	2	0
87	O1	401	DGT	1	0
71	r1	202	CDL	3	0
69	b1	101	3PE	1	0
70	p	302	PC1	1	0
81	y	601	TGL	1	0
70	6	203	PC1	2	0
69	M1	503	3PE	2	0
69	g	303	3PE	11	0
71	d1	201	CDL	1	0
69	c	301	3PE	5	0
69	N1	402	3PE	1	0
70	z	101	PC1	20	0
70	P1	502	PC1	1	0
77	n	604	HEA	5	0
69	t	101	3PE	11	0
71	g	301	CDL	7	0
77	a	603	HEA	3	0
69	L1	704	3PE	3	0
69	p	301	3PE	6	0
82	9	201	SF4	1	0
70	9	203	PC1	1	0
71	L1	703	CDL	3	0
69	b	301	3PE	1	0
74	P	201	FES	2	0
70	K	101	PC1	1	0
69	L1	701	3PE	3	0

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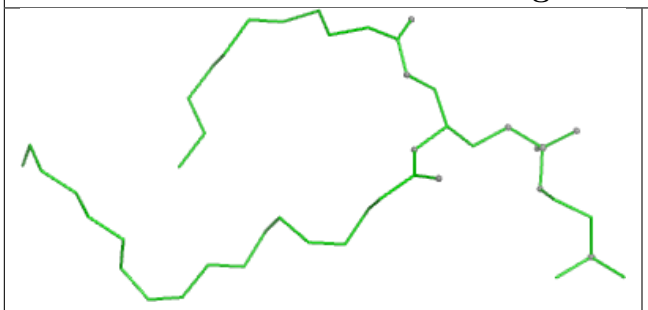
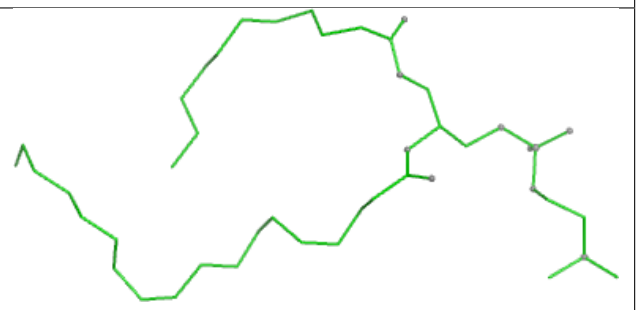
Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	R	104	3PE	2	0
69	H1	401	3PE	2	0
69	C	403	3PE	1	0
71	h1	201	CDL	4	0
85	P1	501	NDP	1	0
69	N	403	3PE	1	0
69	6	202	3PE	1	0
71	G	101	CDL	1	0
69	O	302	3PE	1	0
69	z	102	3PE	2	0
72	N	402	HEM	2	0
71	H1	402	CDL	1	0
69	A	501	3PE	2	0
77	a	604	HEA	5	0
69	L	501	3PE	1	0
69	o	302	3PE	2	0
69	Y1	403	3PE	1	0
71	N1	401	CDL	5	0
72	C	401	HEM	3	0
77	n	603	HEA	4	0
69	C	404	3PE	2	0
69	M1	502	3PE	4	0
69	n	606	3PE	2	0
71	L	502	CDL	1	0
71	L1	702	CDL	2	0
70	M1	501	PC1	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

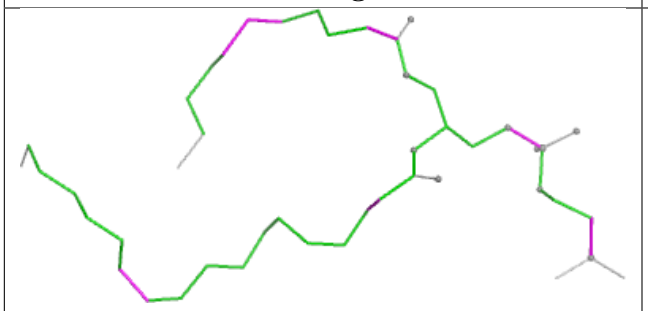
Ligand PC1 9 204



Bond lengths



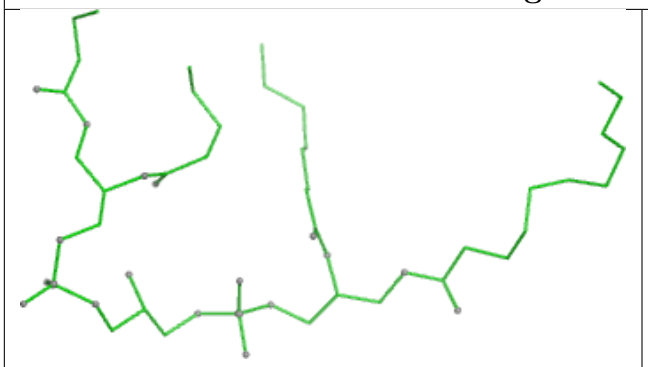
Bond angles



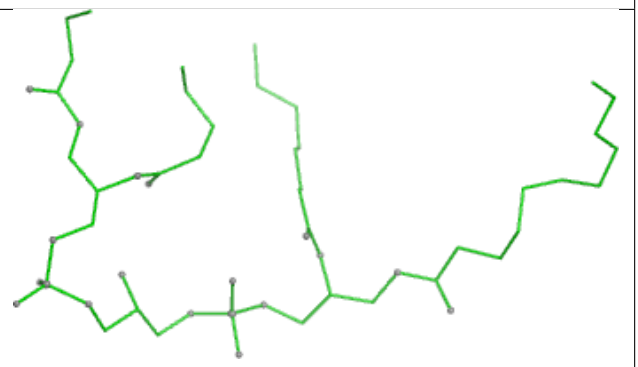
Torsions

Rings

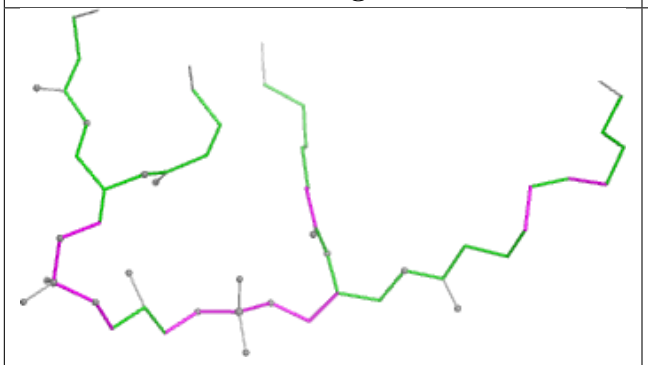
Ligand CDL D 302



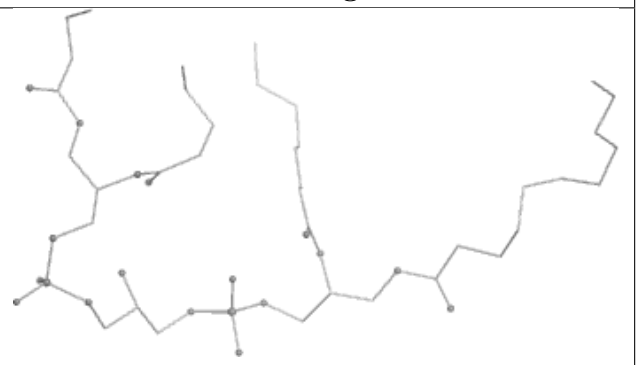
Bond lengths



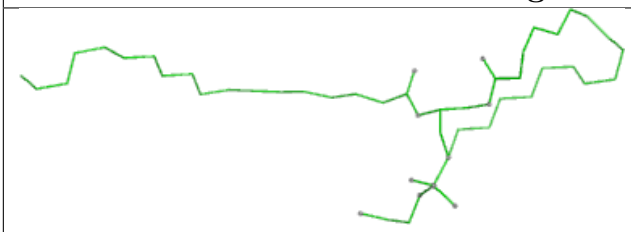
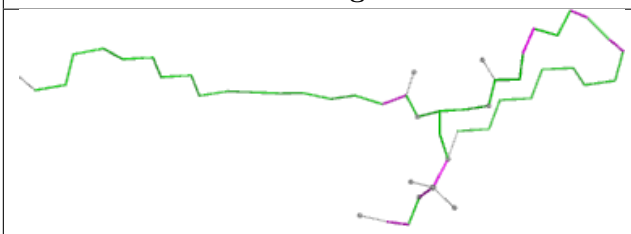
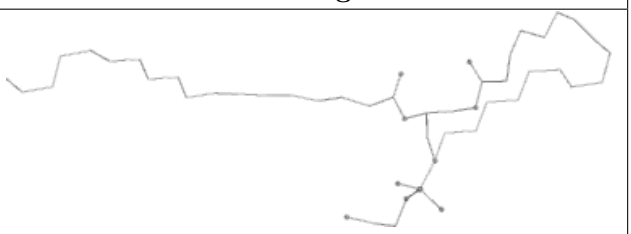
Bond angles

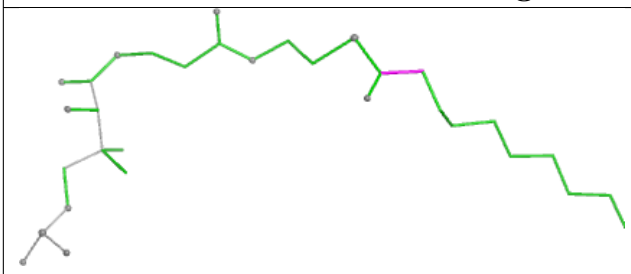
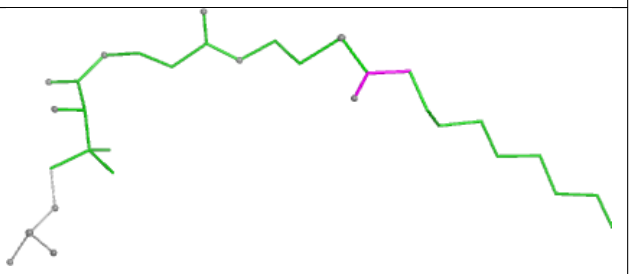
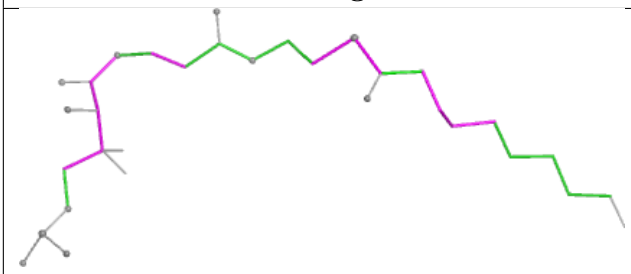
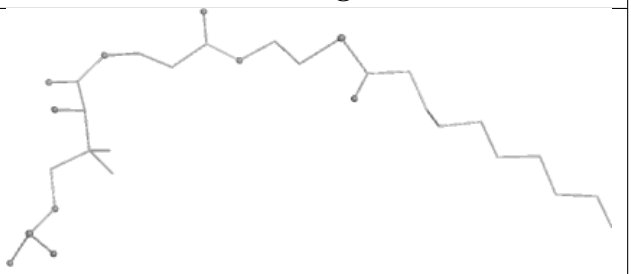


Torsions

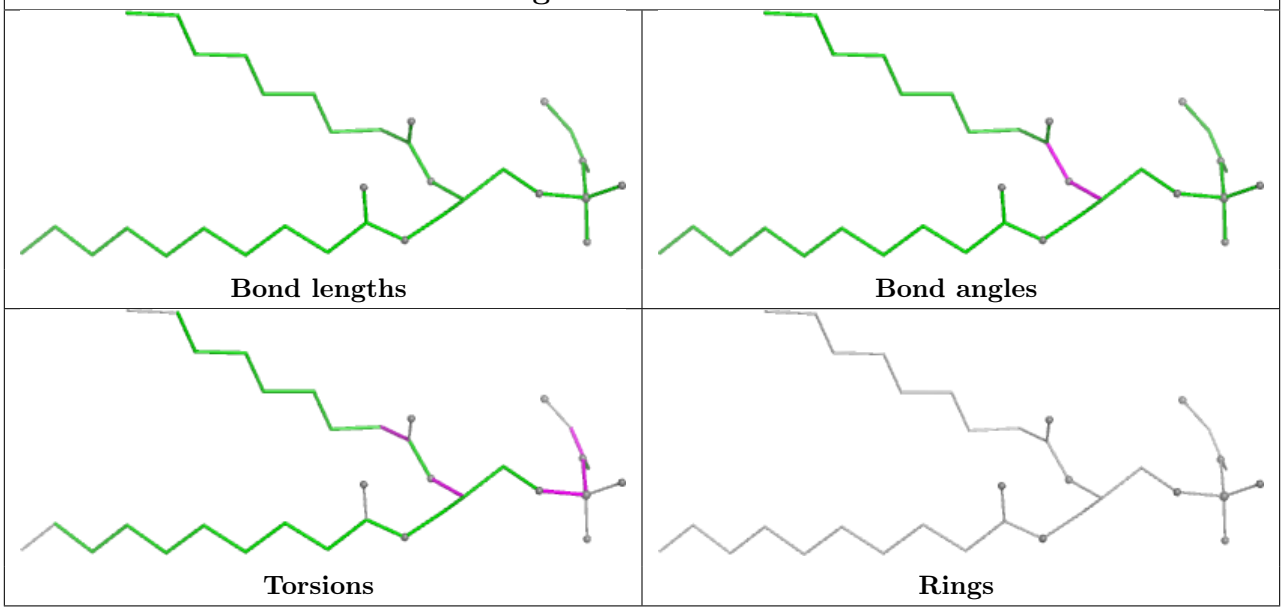


Rings

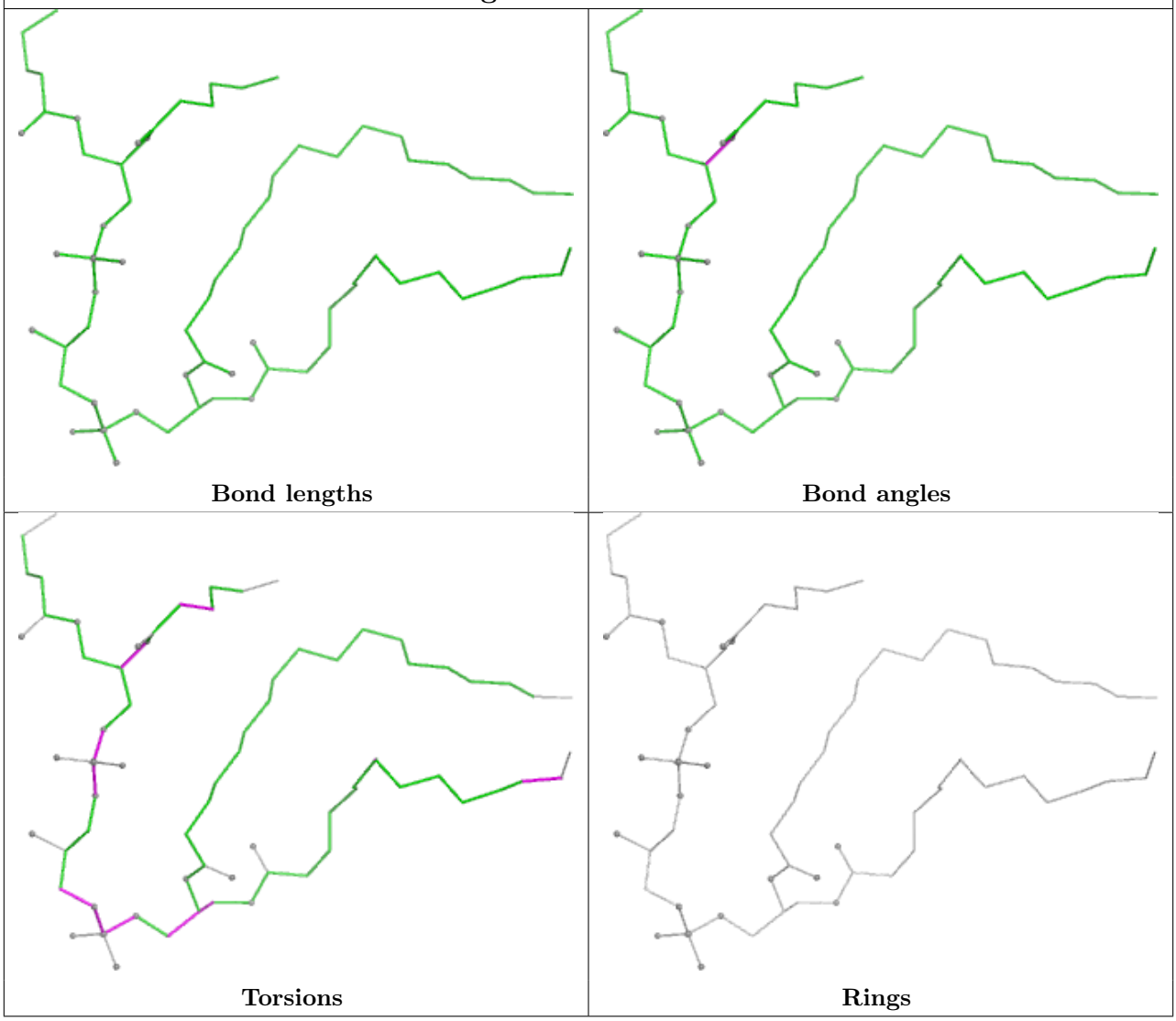
Ligand 3PE G 102	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand ZMP n1 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

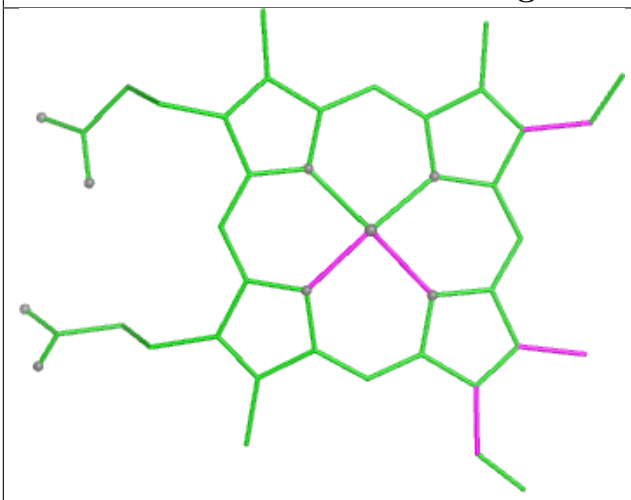
Ligand 3PE n 605



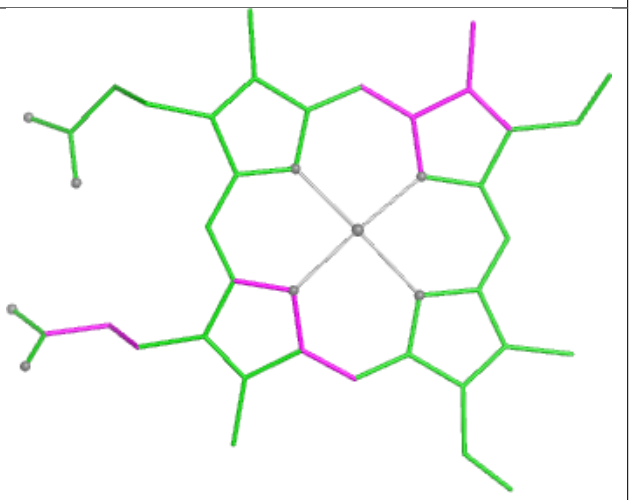
Ligand CDL R 103



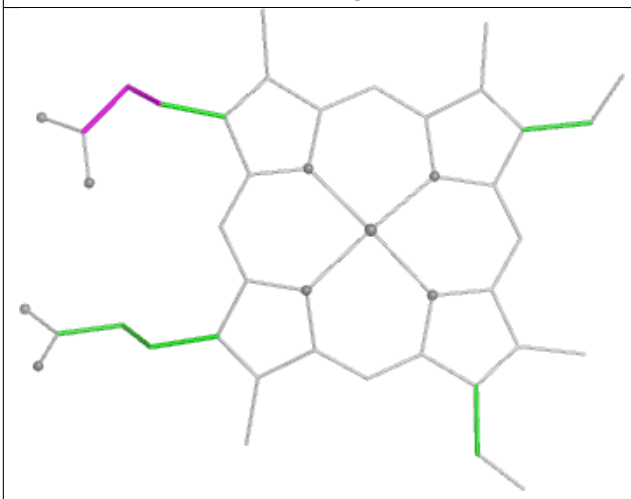
Ligand HEM N 401



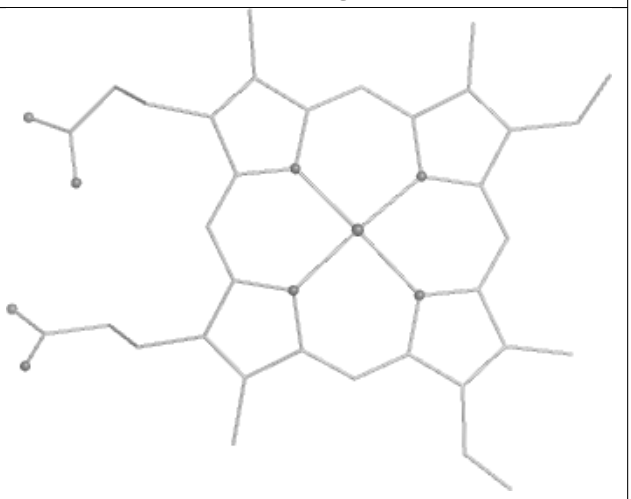
Bond lengths



Bond angles

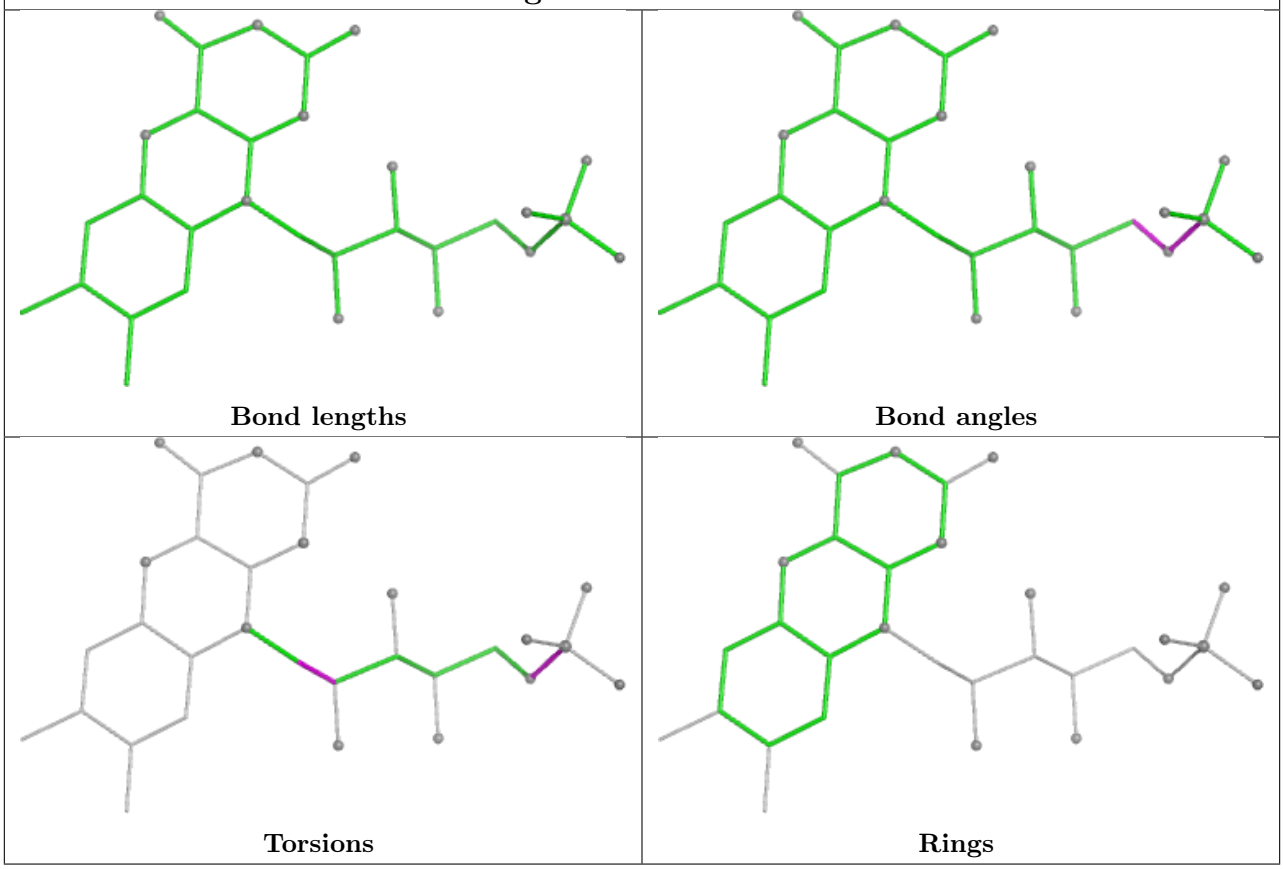


Torsions

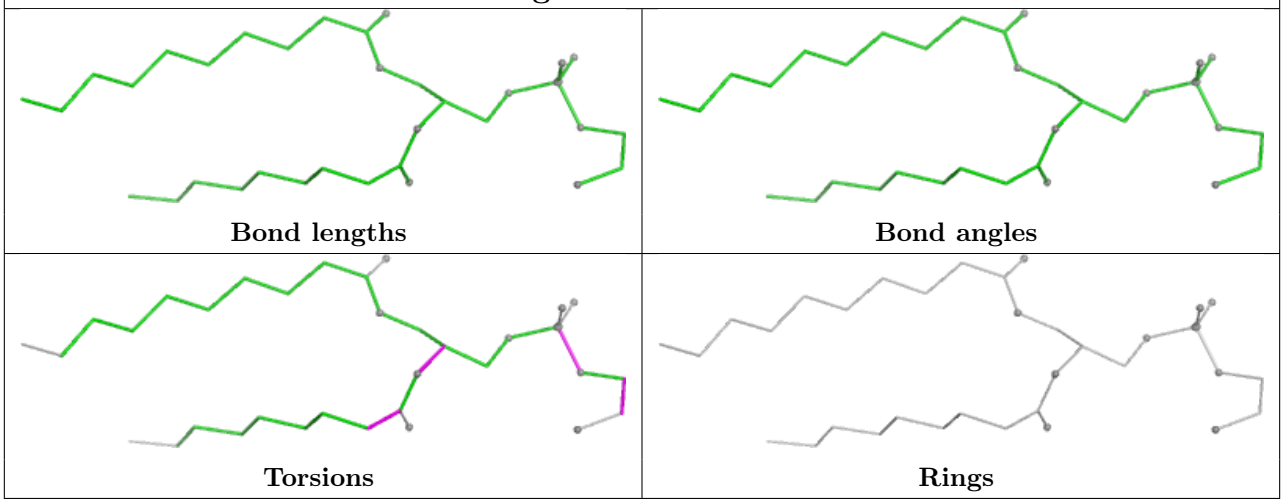


Rings

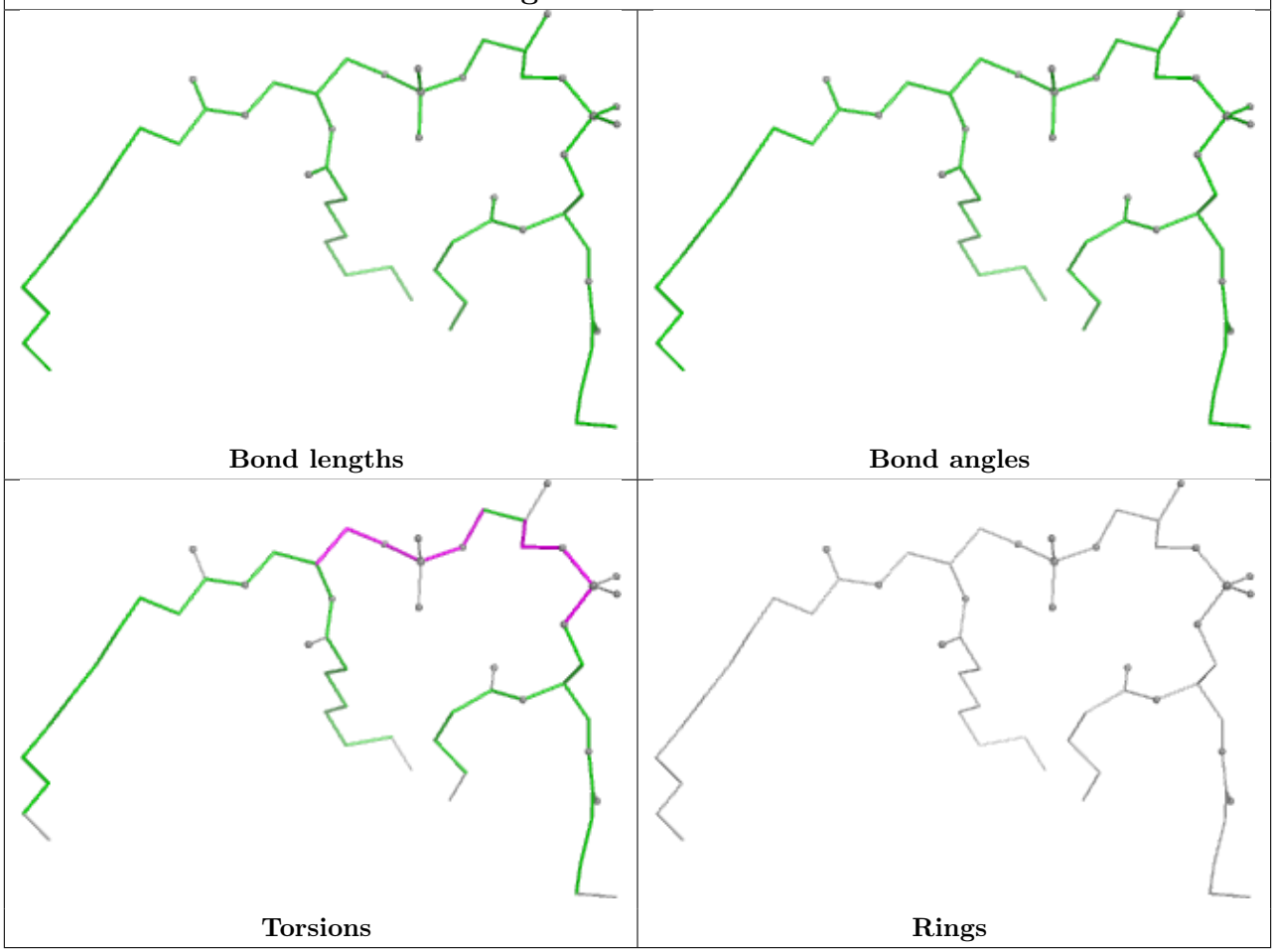
Ligand FMN 1 501



Ligand 3PE d 201



Ligand CDL O 301



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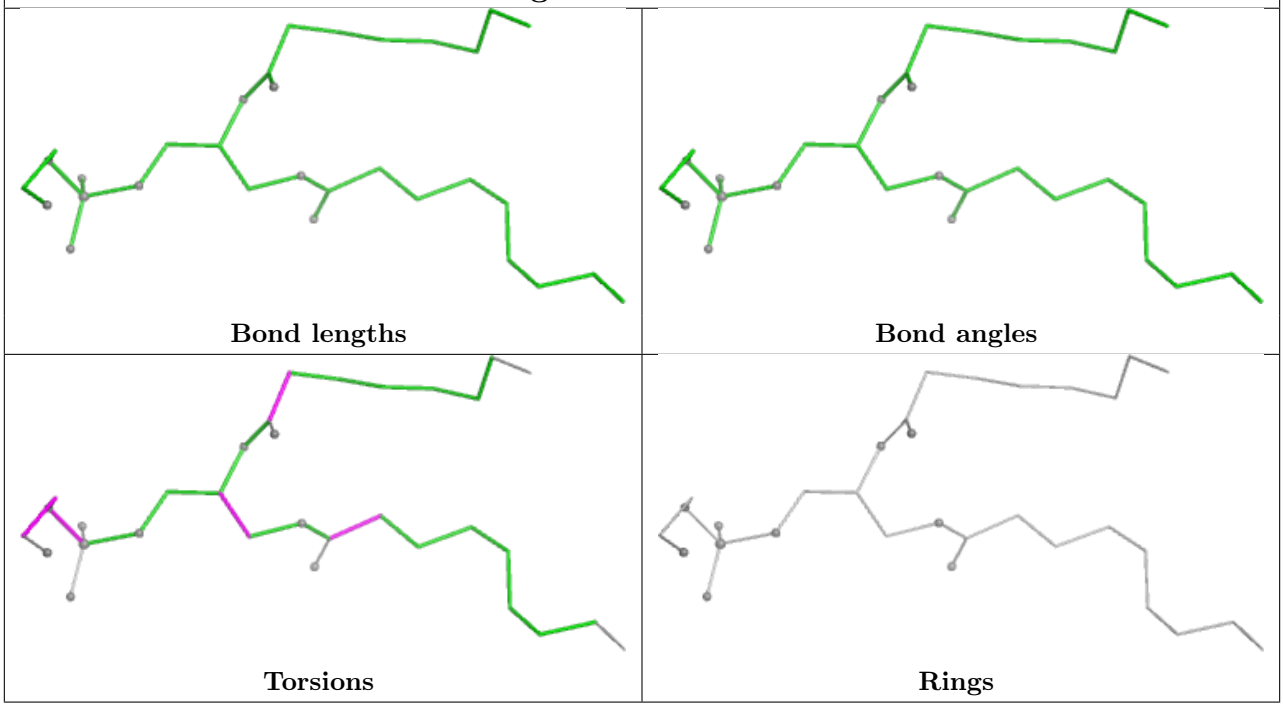

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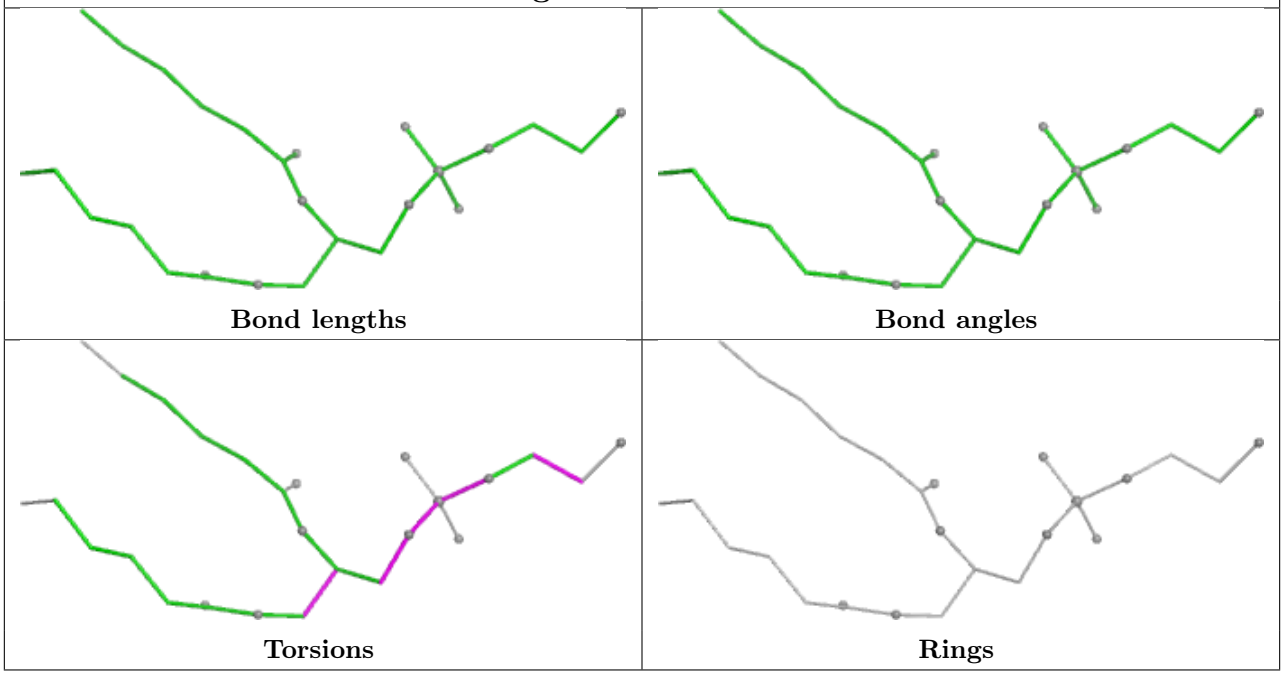
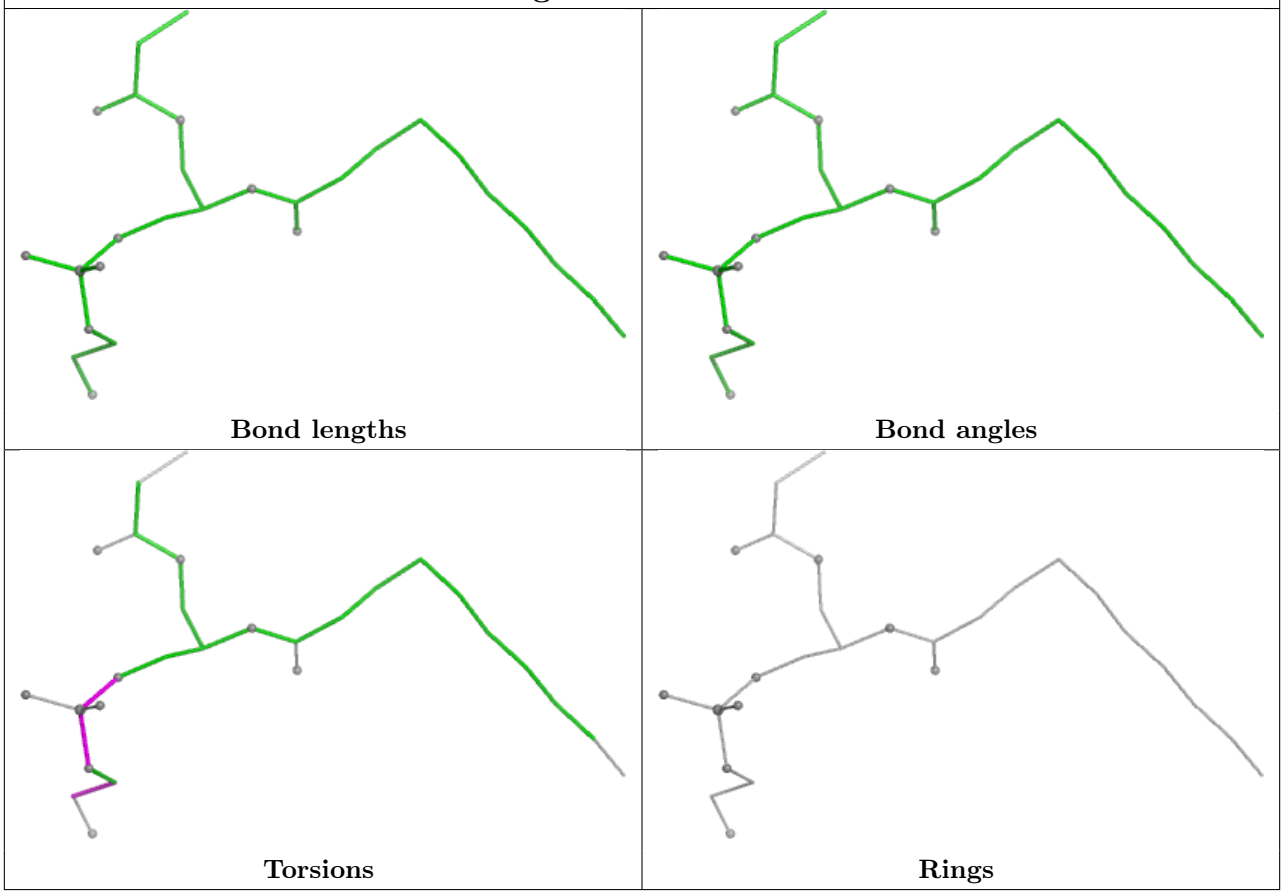
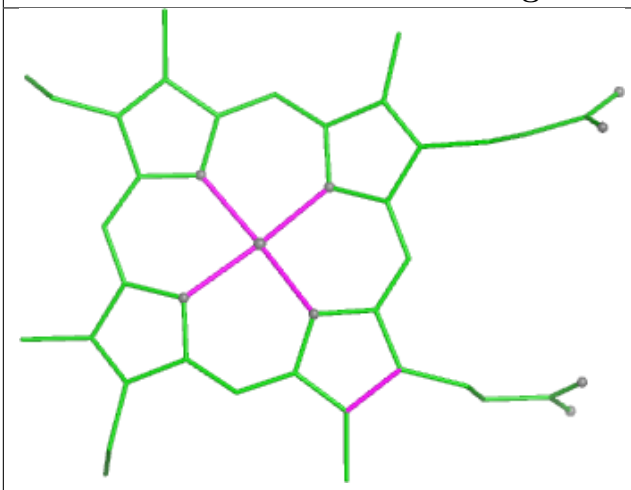


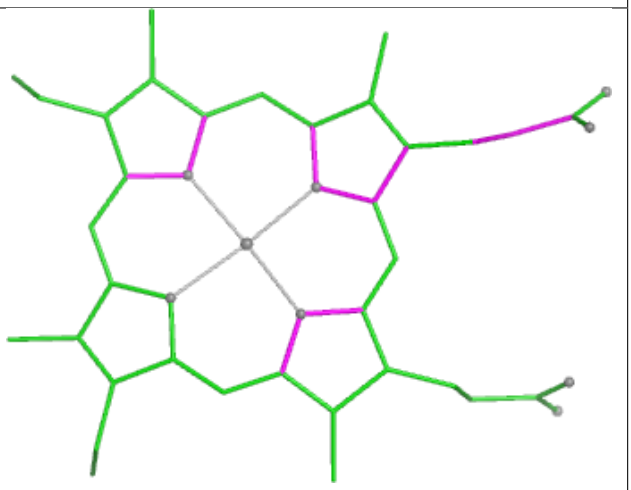
Ligand 3PE v 101



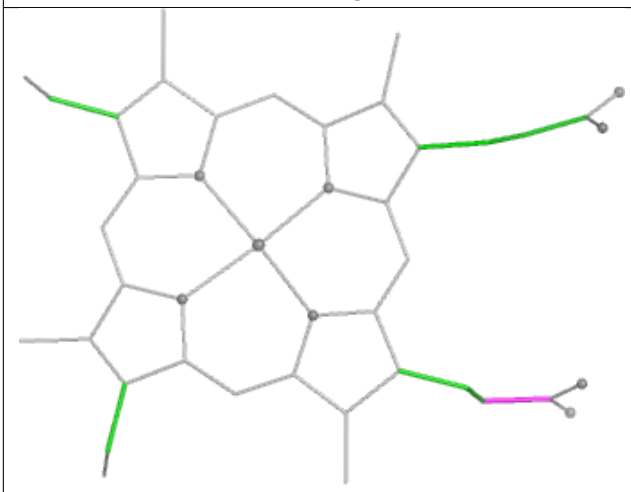
Ligand HEC D 301



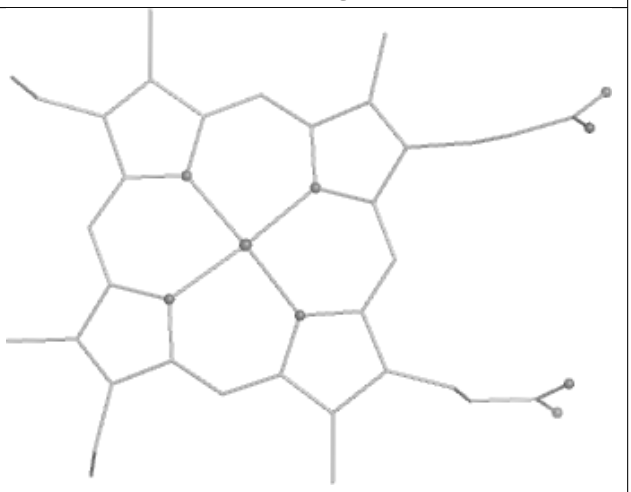
Bond lengths



Bond angles

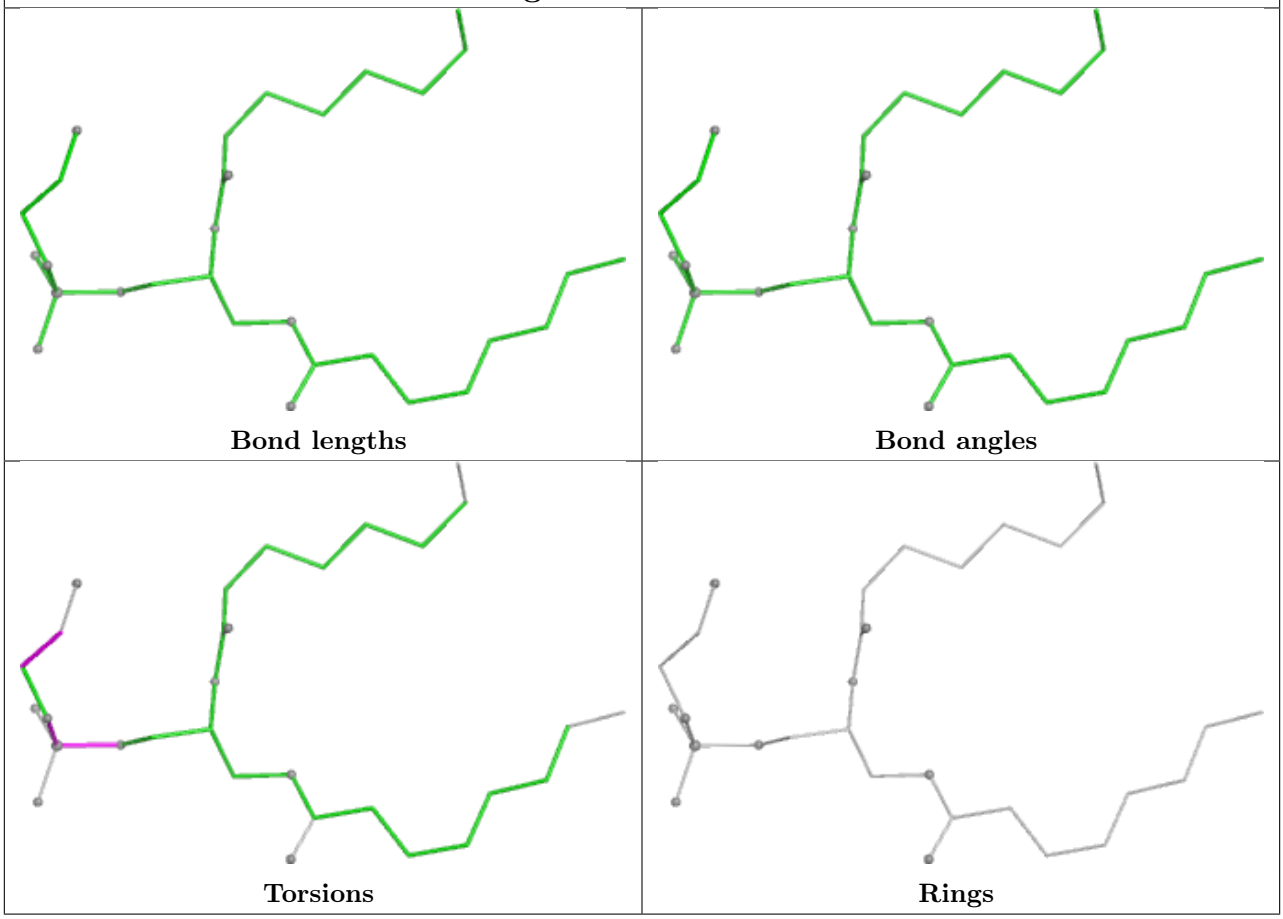


Torsions

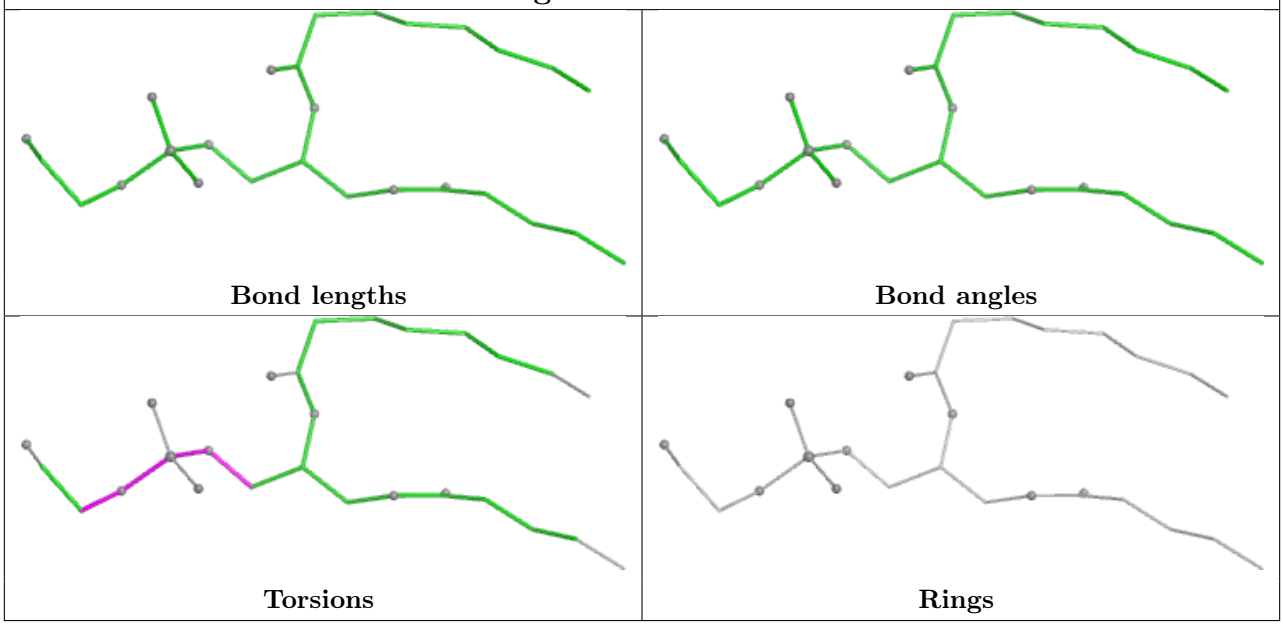


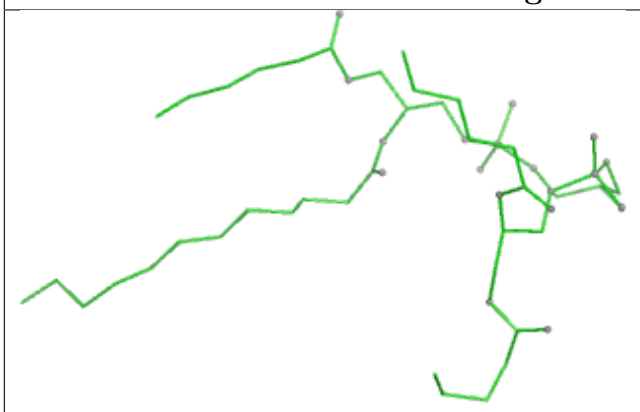
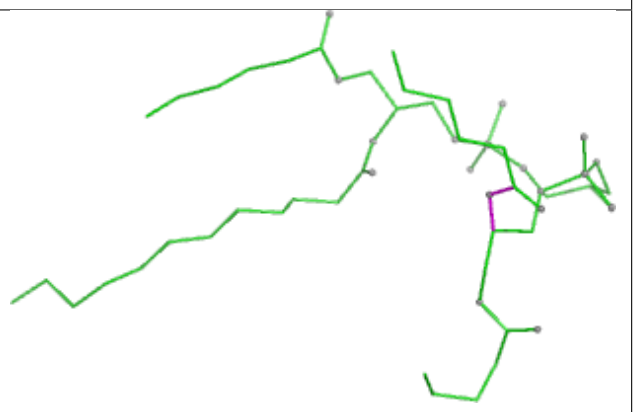
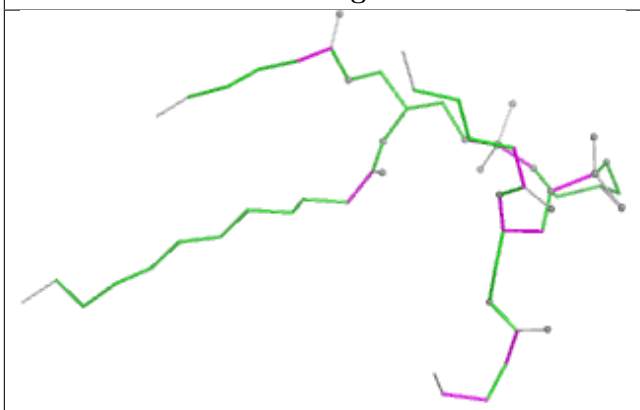
Rings

Ligand 3PE d1 202

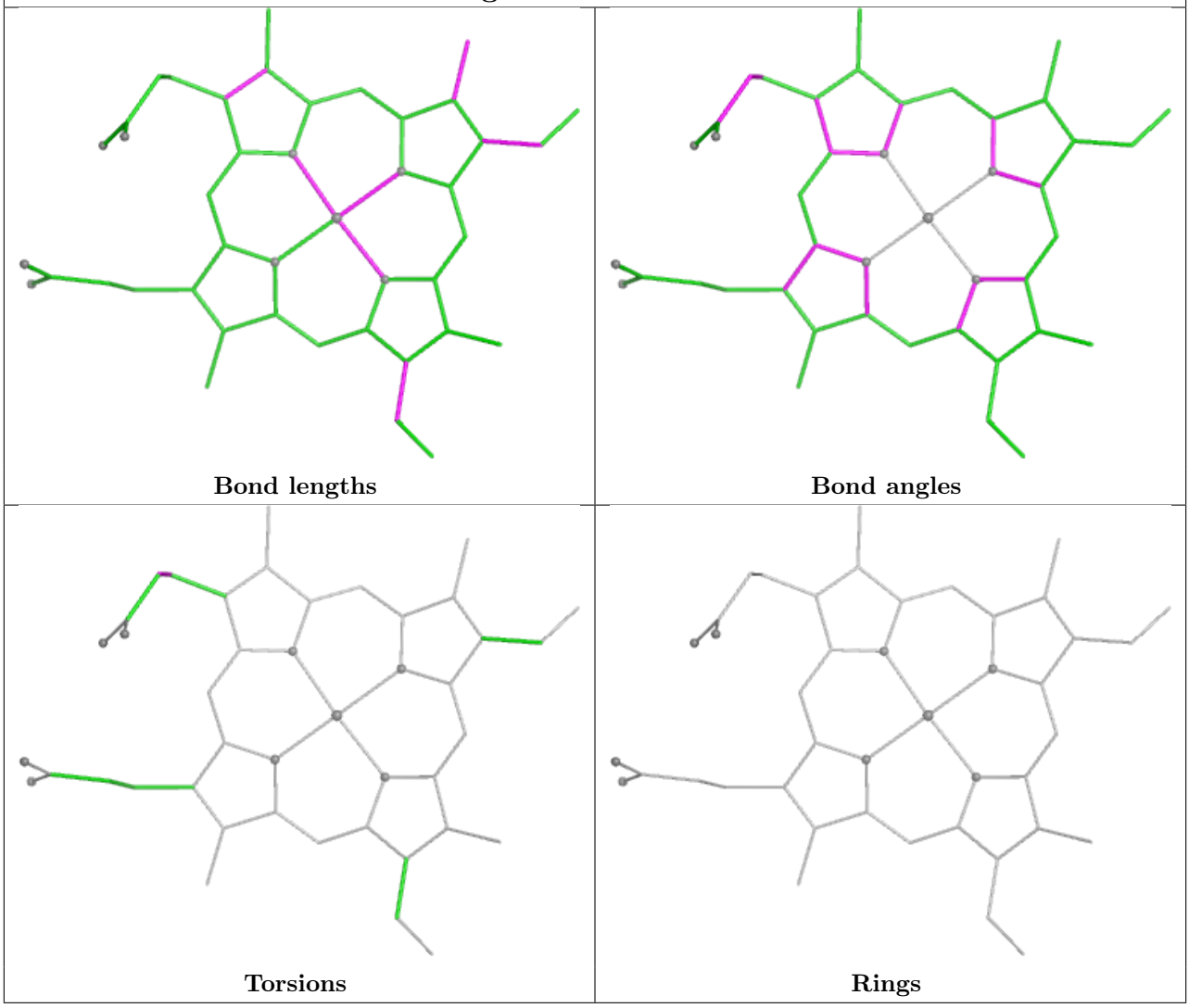


Ligand 3PE a 605

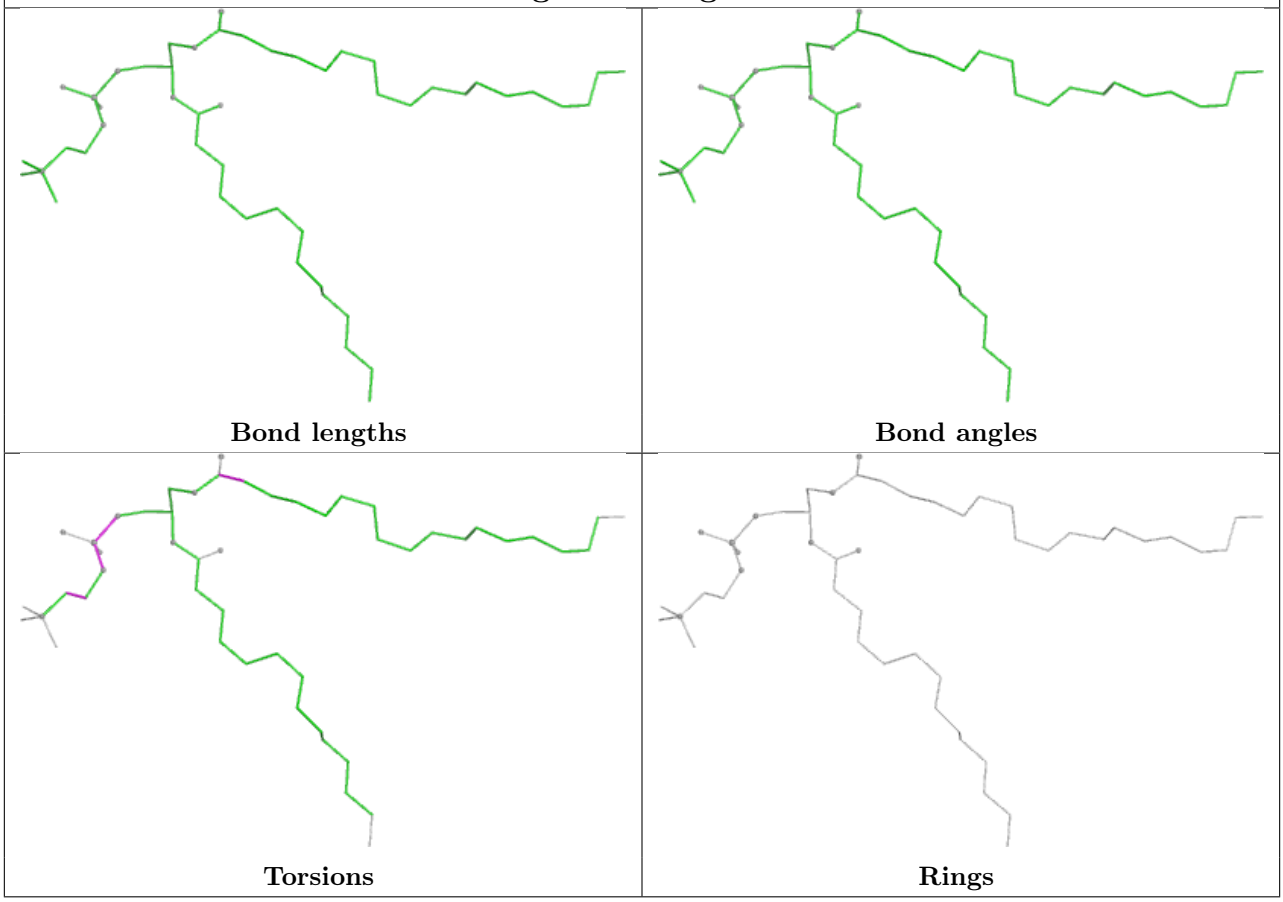


Ligand CDL R 102	
 Bond lengths	 Bond angles
 Torsions	Rings

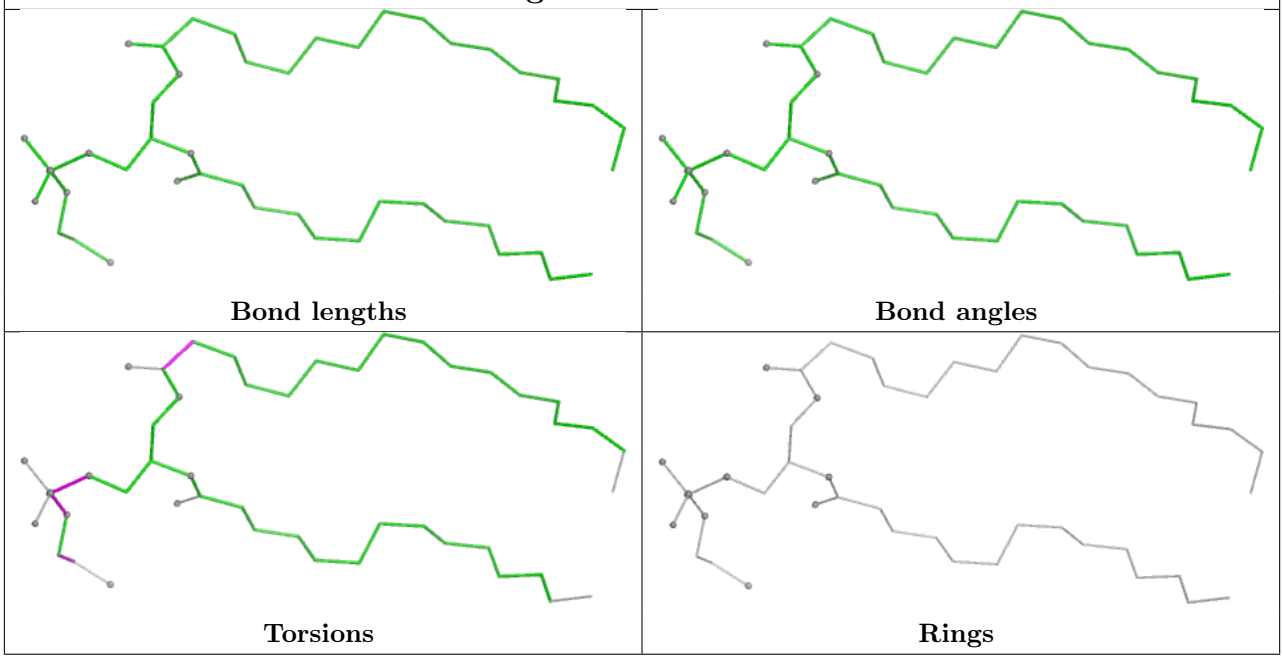
Ligand HEM C 402



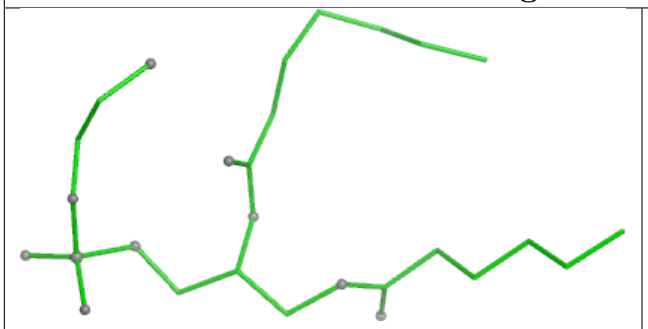
Ligand PC1 g 302



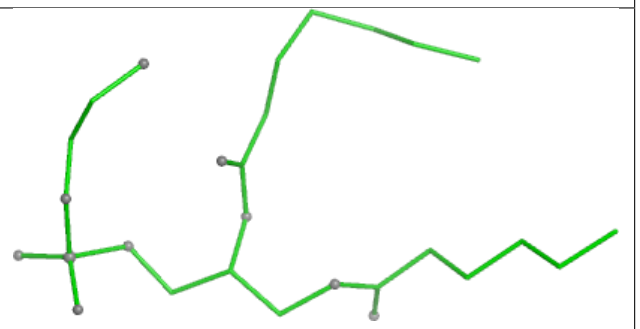
Ligand 3PE r1 201



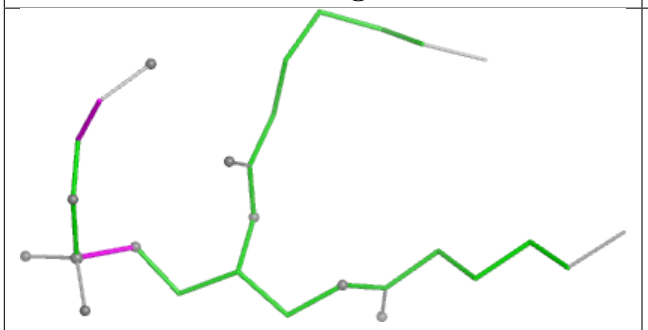
Ligand 3PE Y1 402



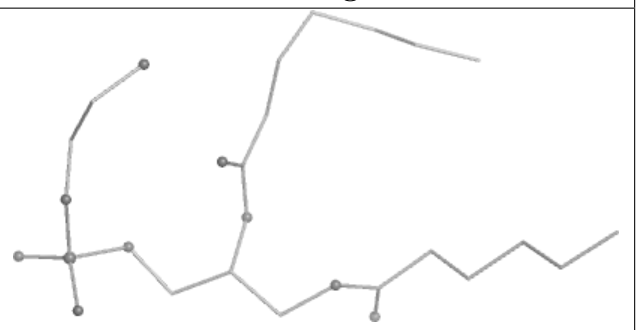
Bond lengths



Bond angles

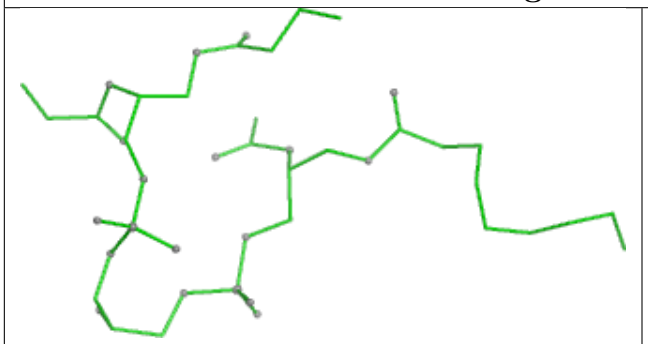


Torsions



Rings

Ligand CDL V 101



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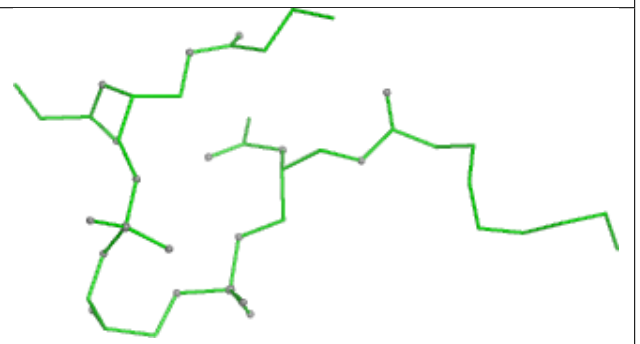
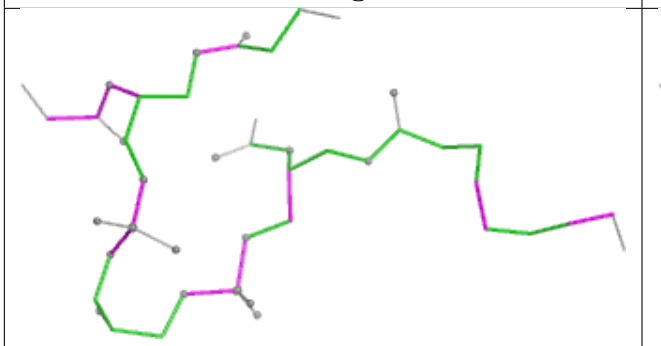
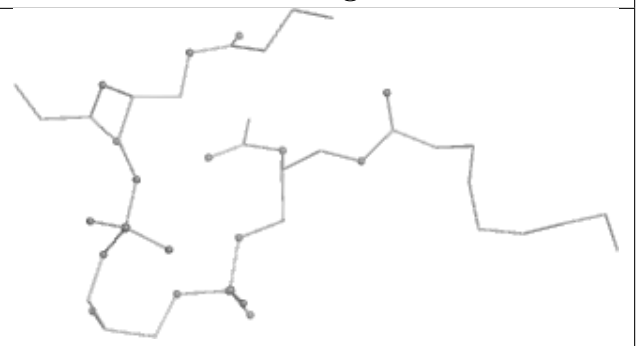


Bond angles

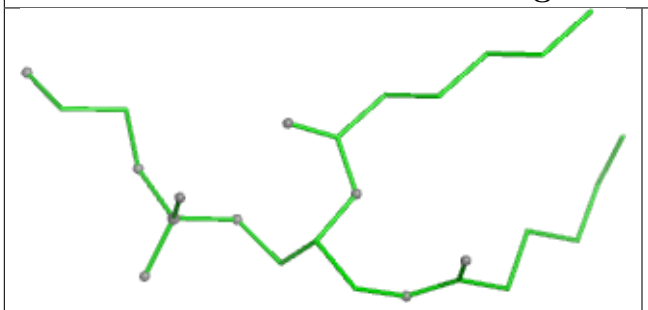


Torsions

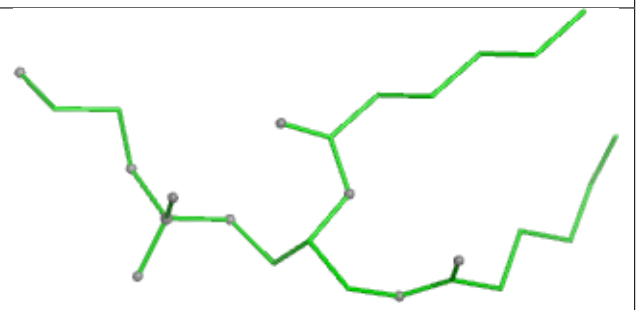


Rings

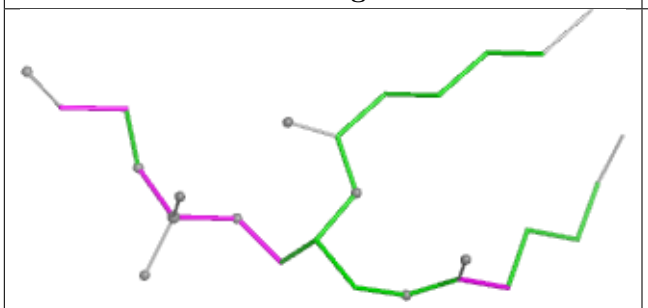
Ligand 3PE a 606



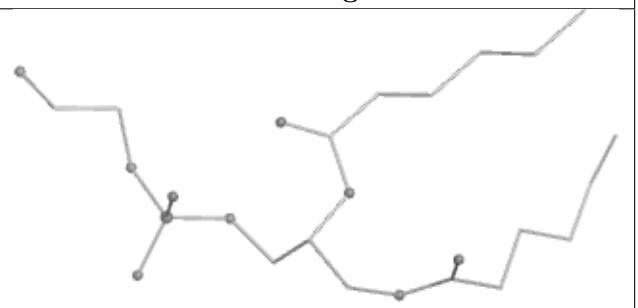
Bond lengths



Bond angles

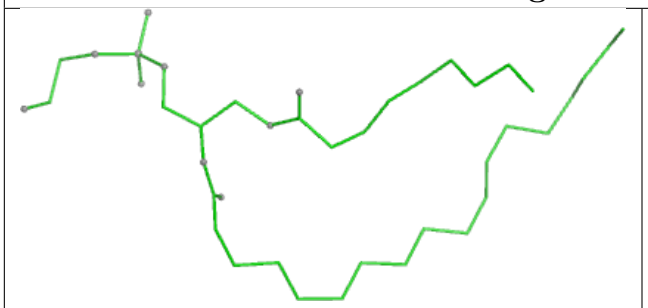


Torsions

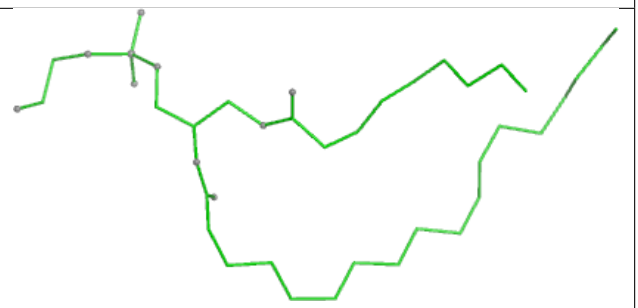


Rings

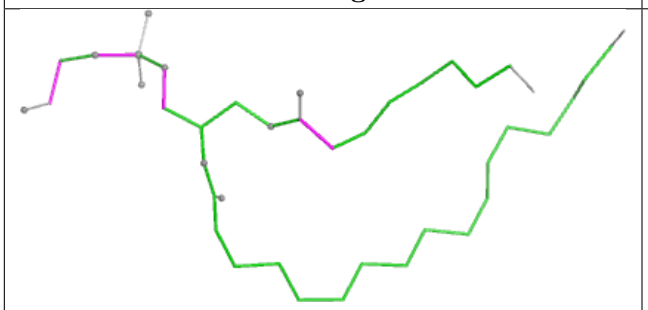
Ligand 3PE i1 201



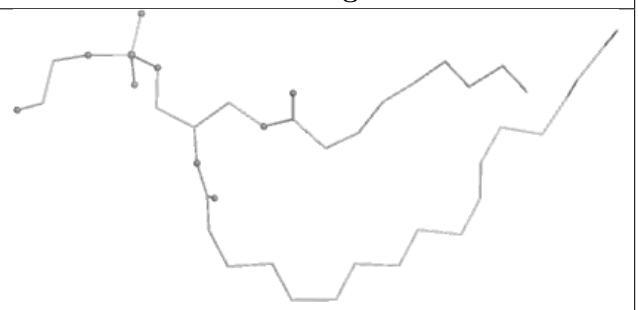
Bond lengths



Bond angles

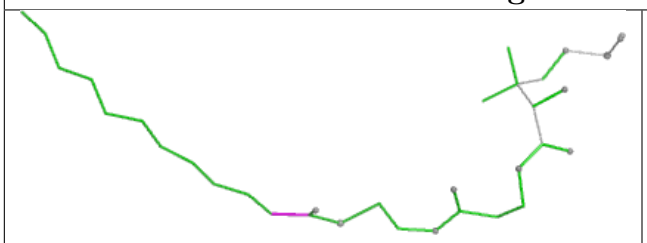


Torsions

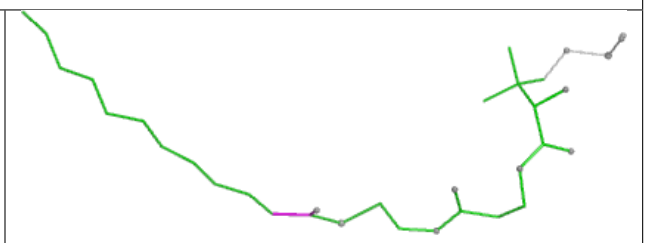


Rings

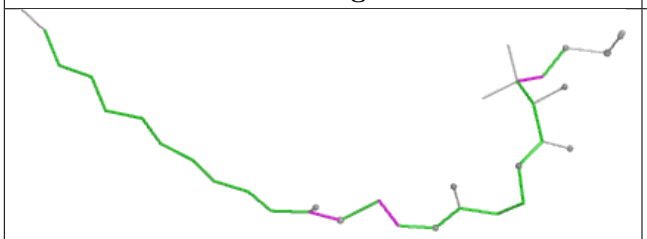
Ligand ZMP W1 201



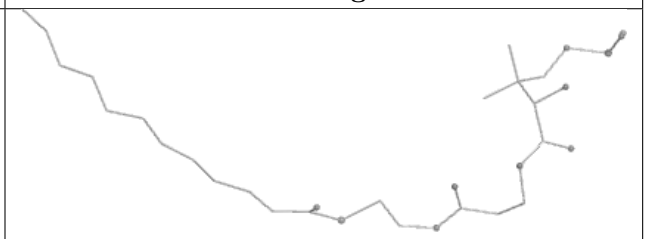
Bond lengths



Bond angles

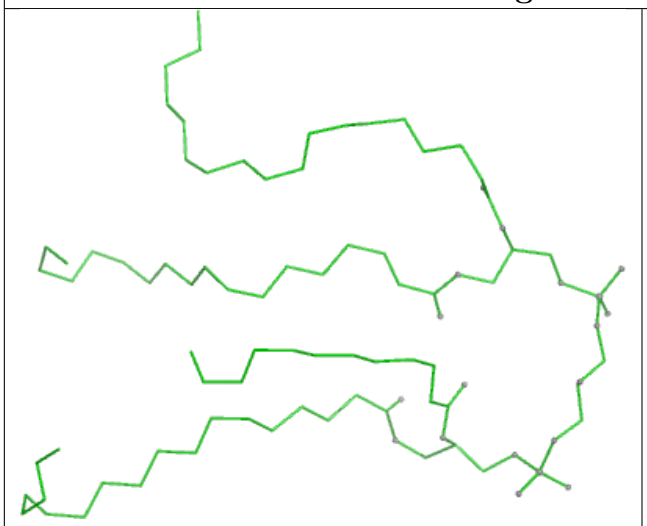


Torsions

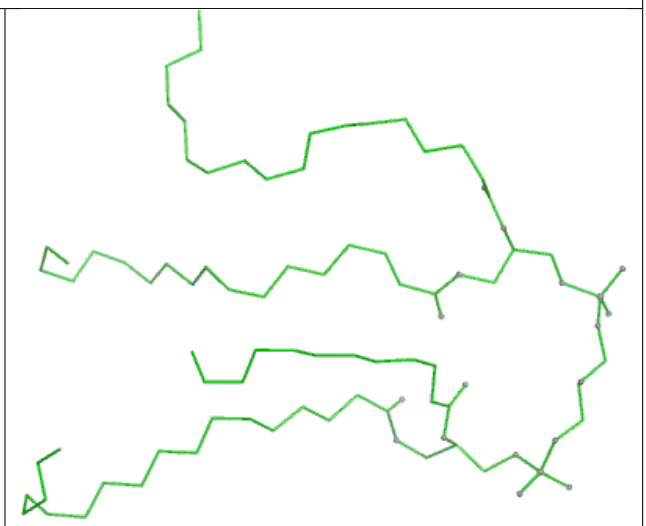


Rings

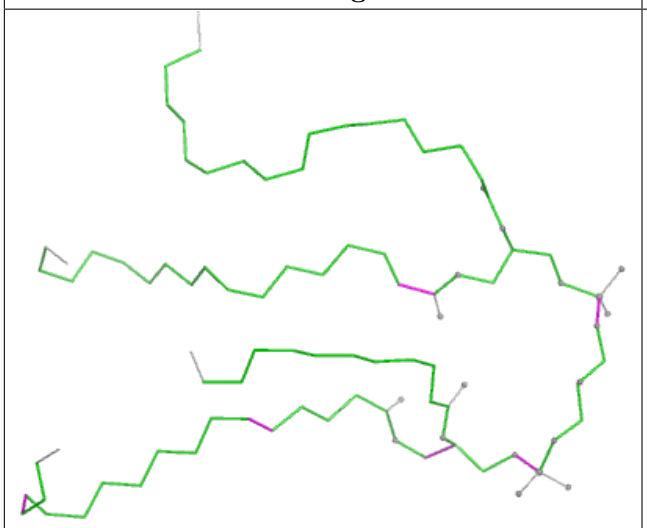
Ligand CDL Y1 401



Bond lengths

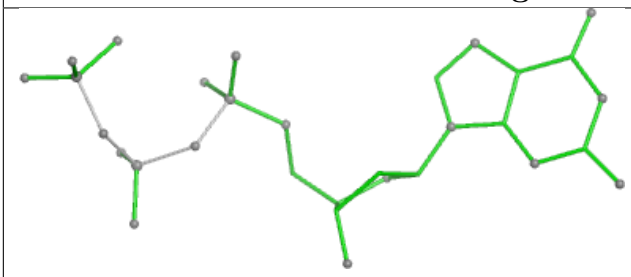
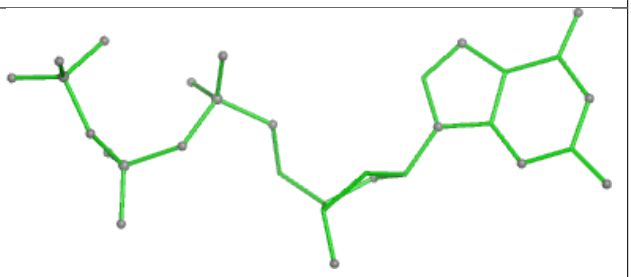
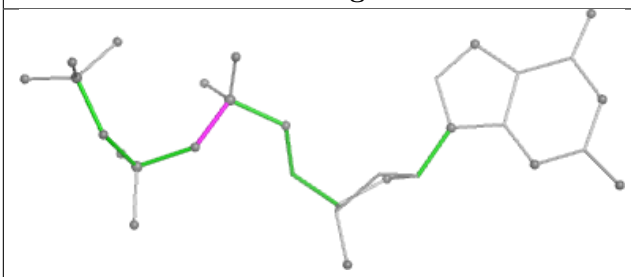
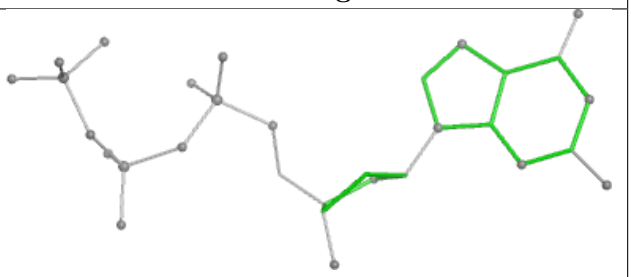


Bond angles

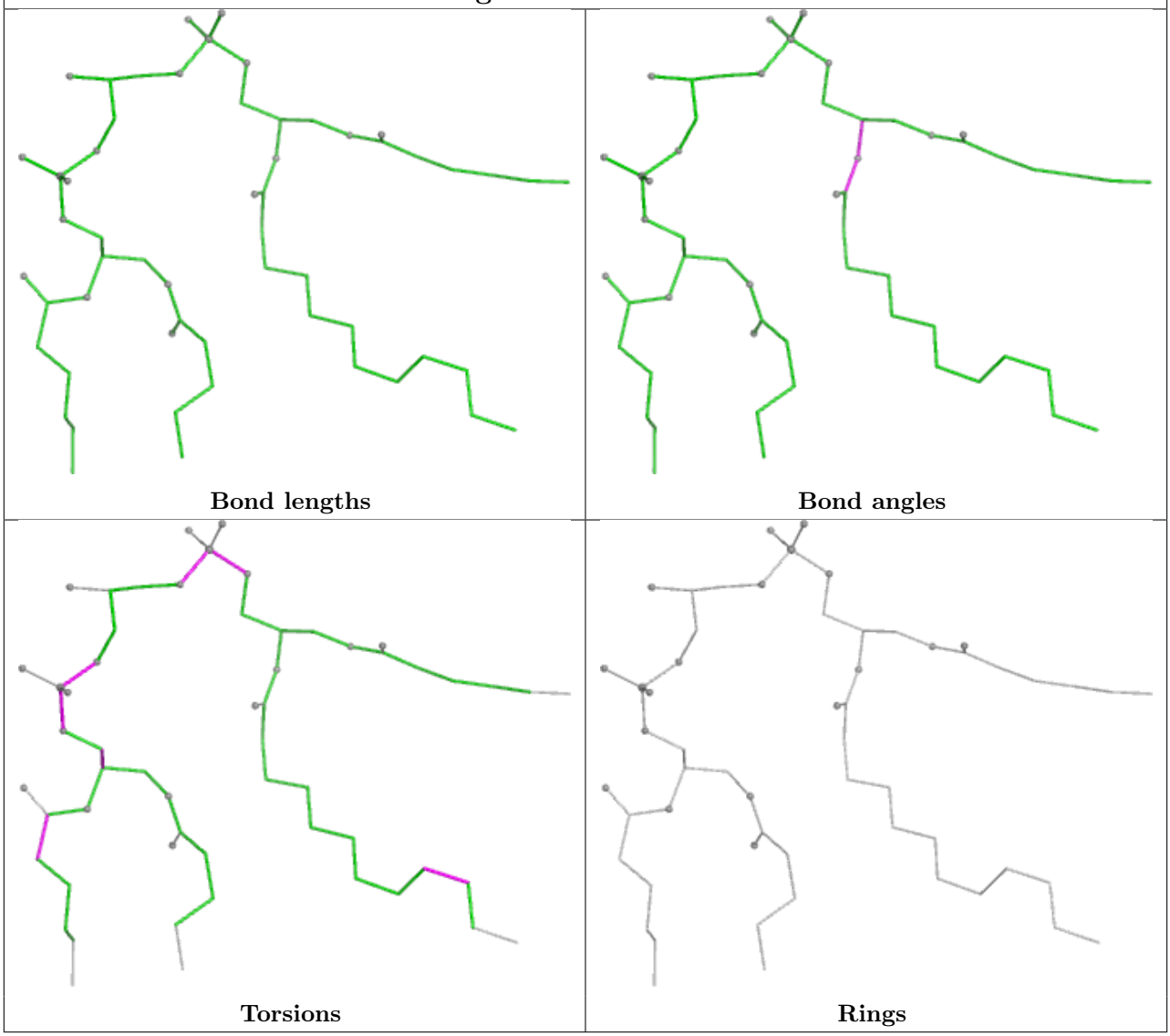


Torsions

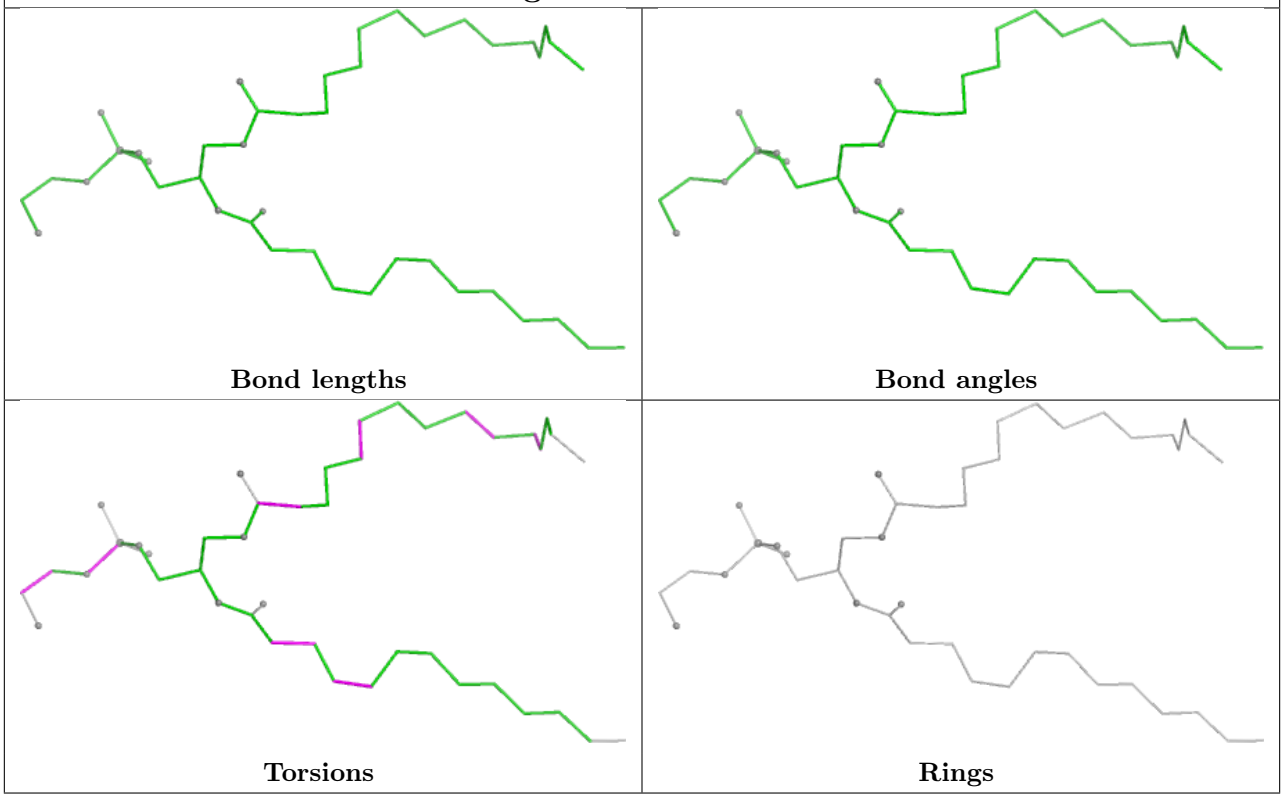
Rings

Ligand DGT O1 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

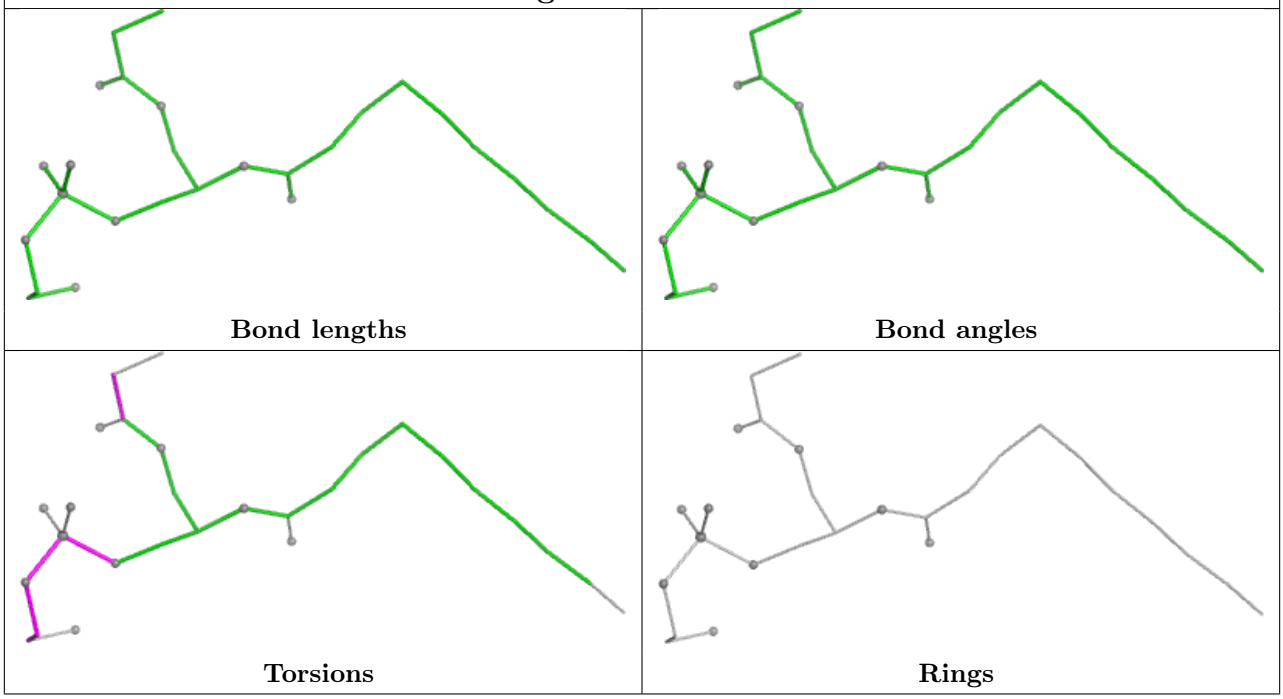
Ligand CDL r1 202



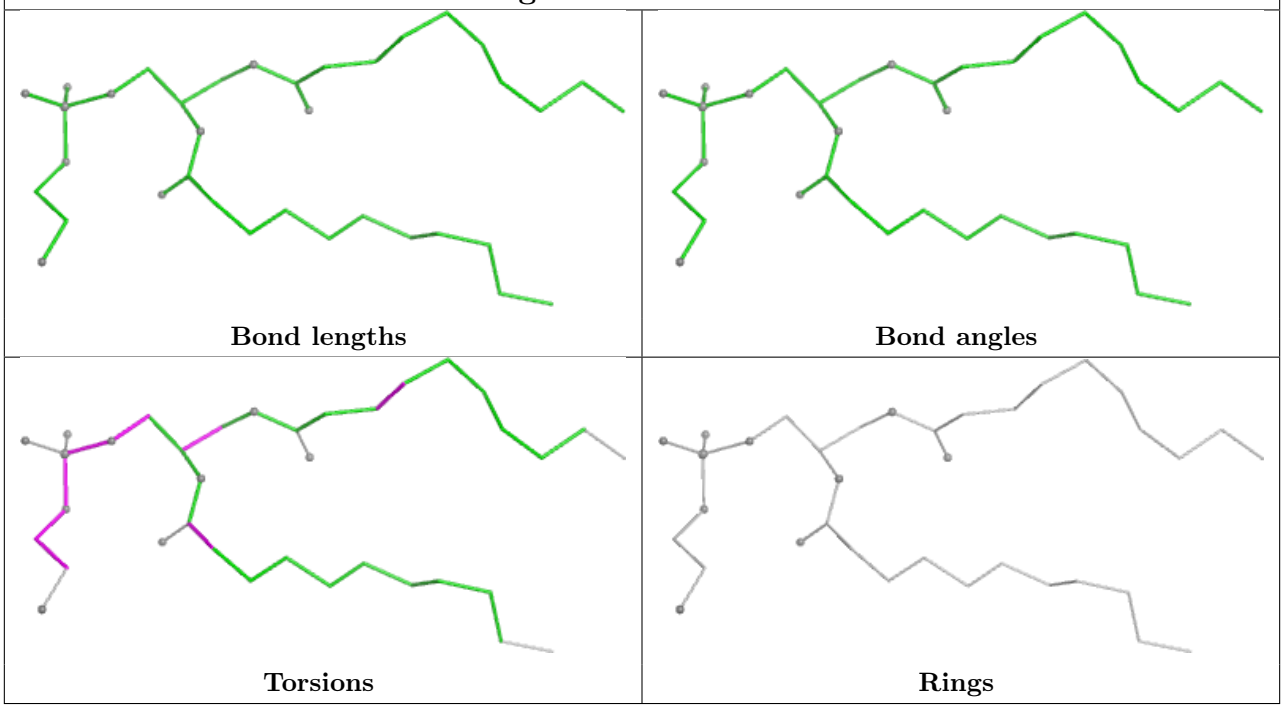
Ligand 3PE b1 101



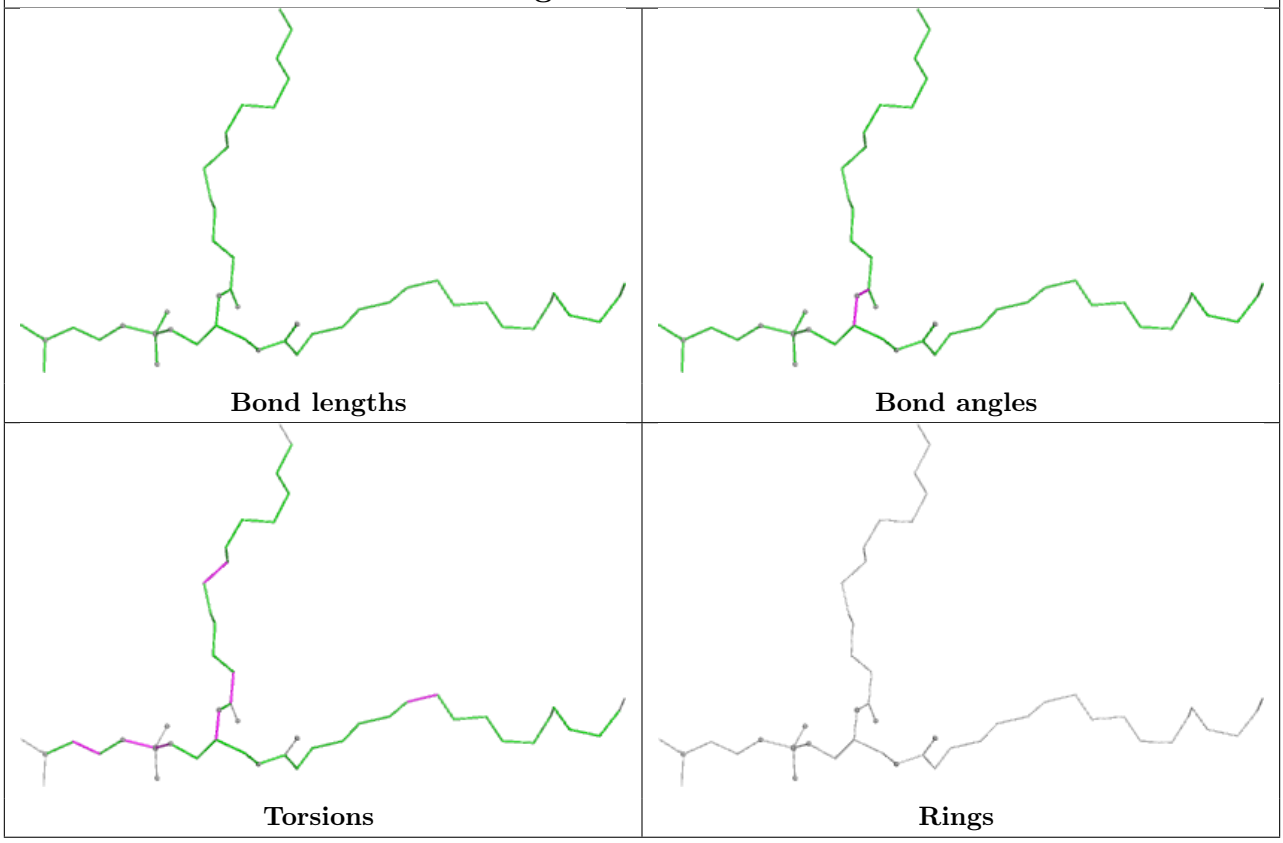
Ligand 3PE i 101

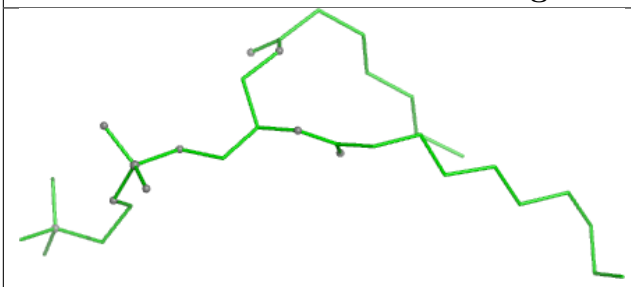
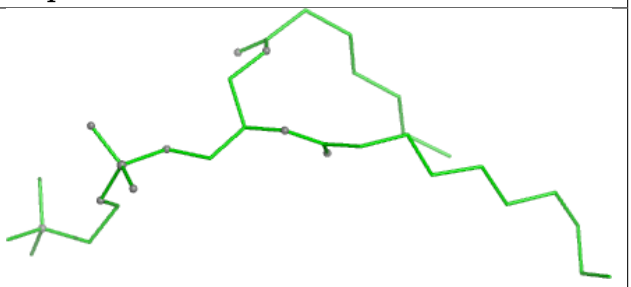
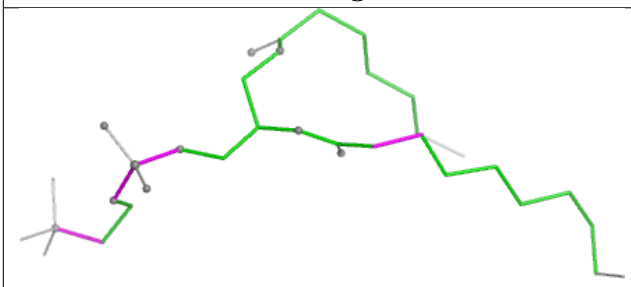
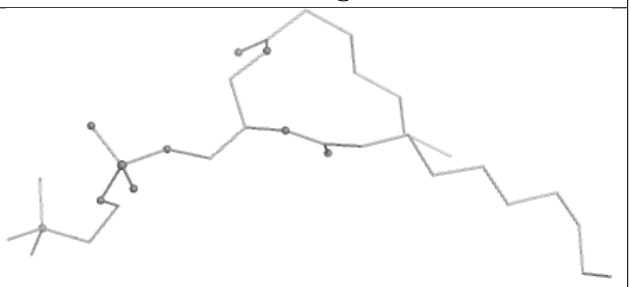


Ligand 3PE m1 601

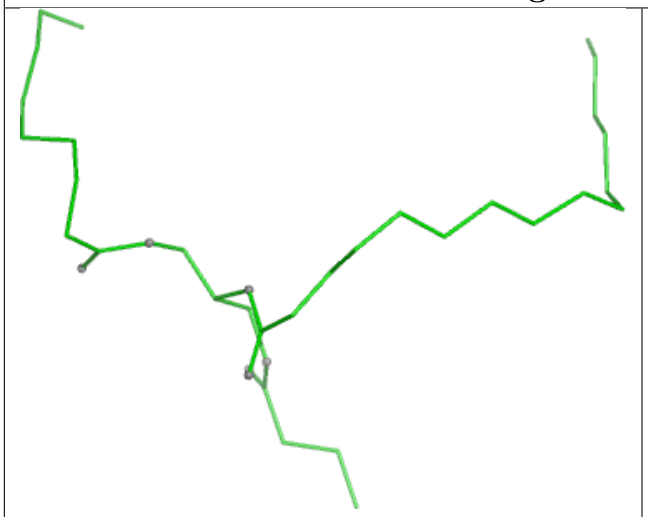


Ligand PC1 I 201



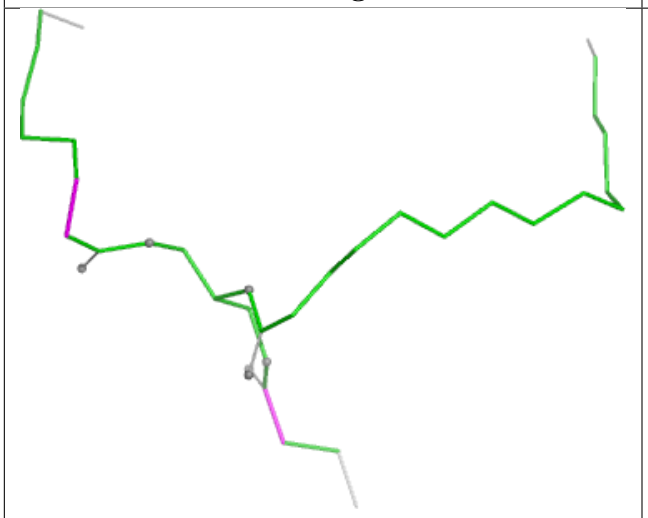
Ligand PC1 p 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TGL y 601



Bond lengths

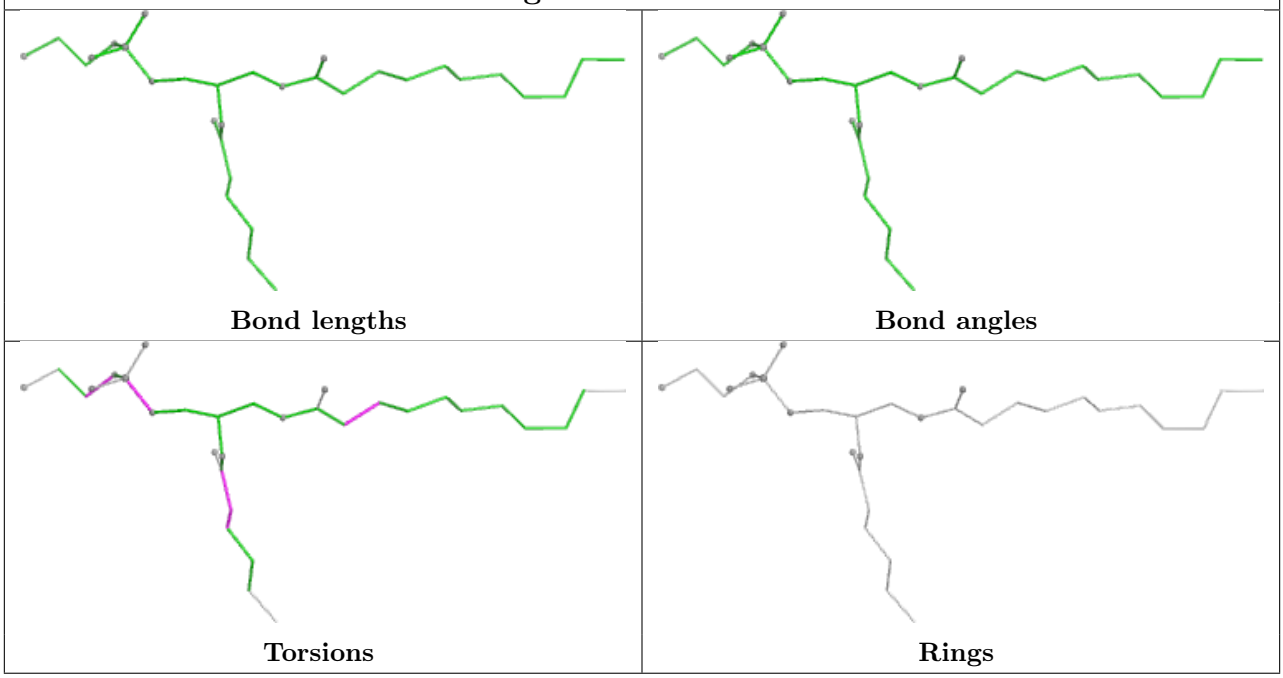
Bond angles



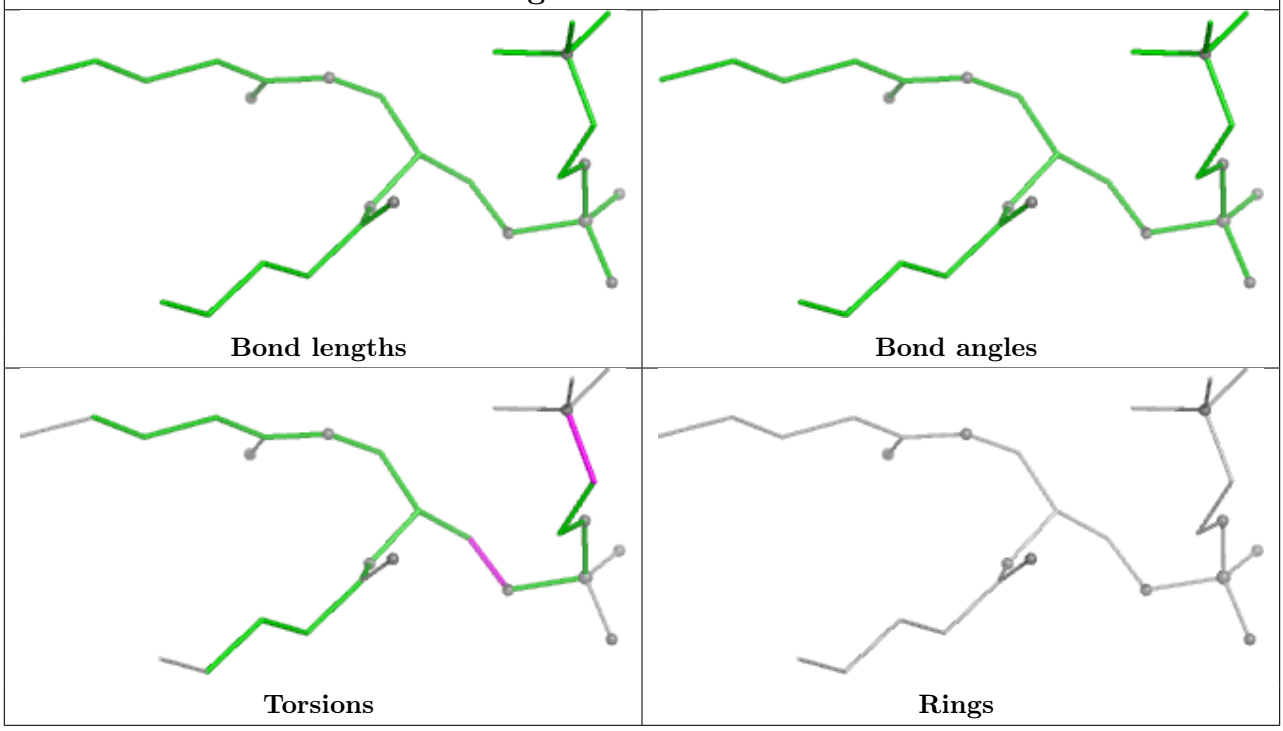
Torsions

Rings

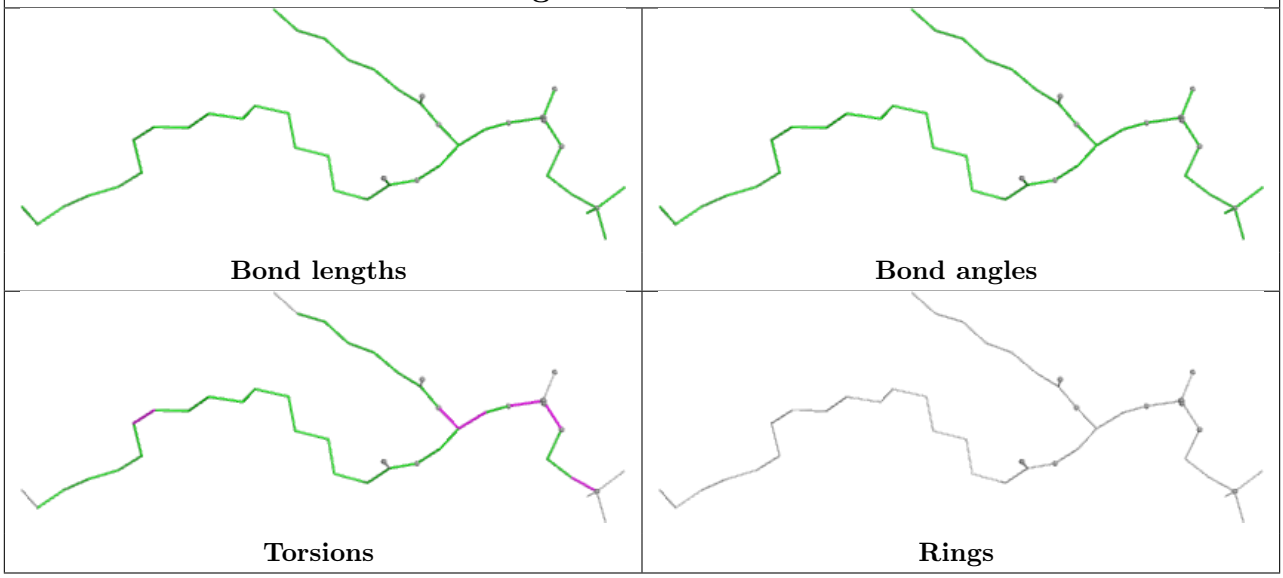
Ligand 3PE d1 203



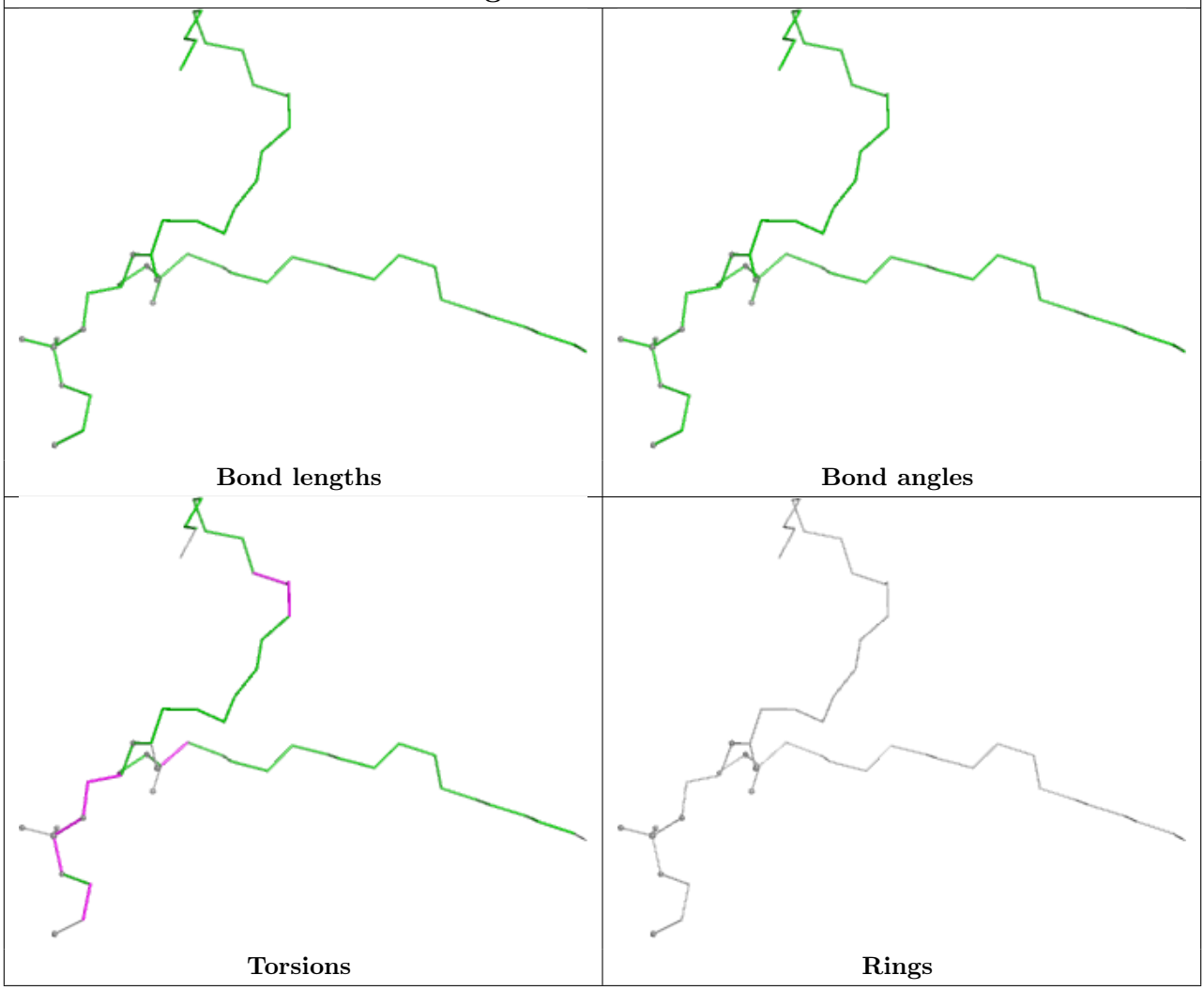
Ligand PC1 V 102



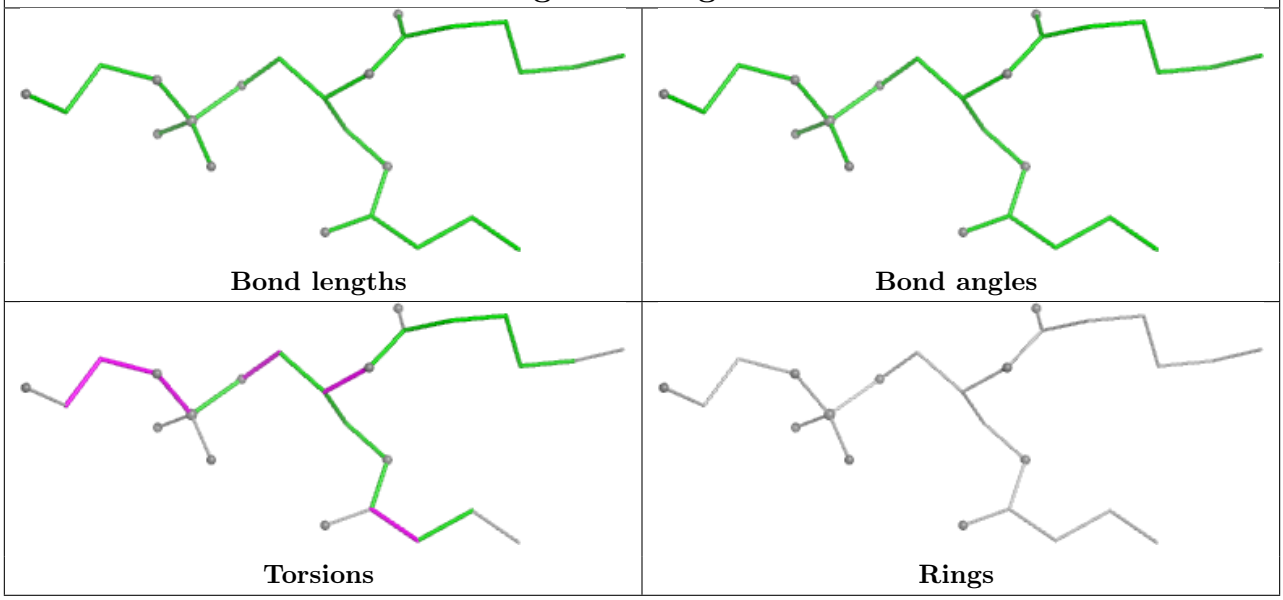
Ligand PC1 6 203



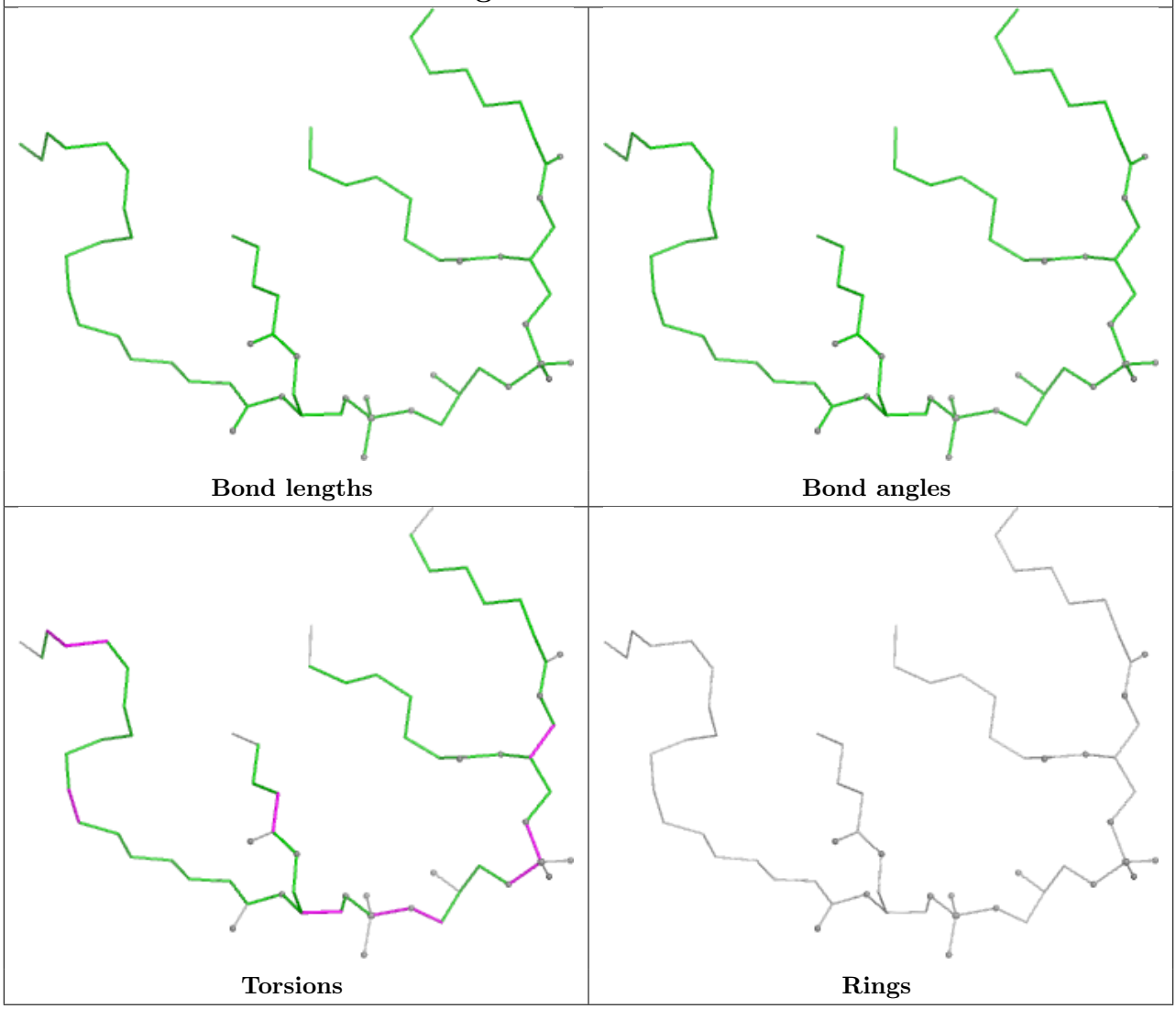
Ligand 3PE M1 503



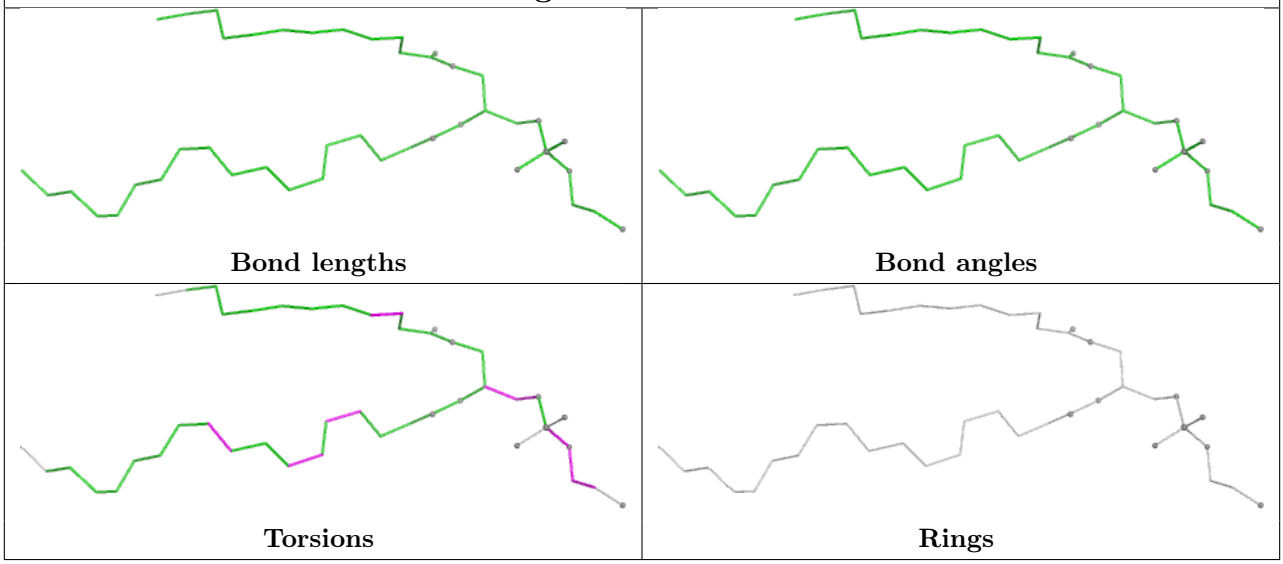
Ligand 3PE g 303



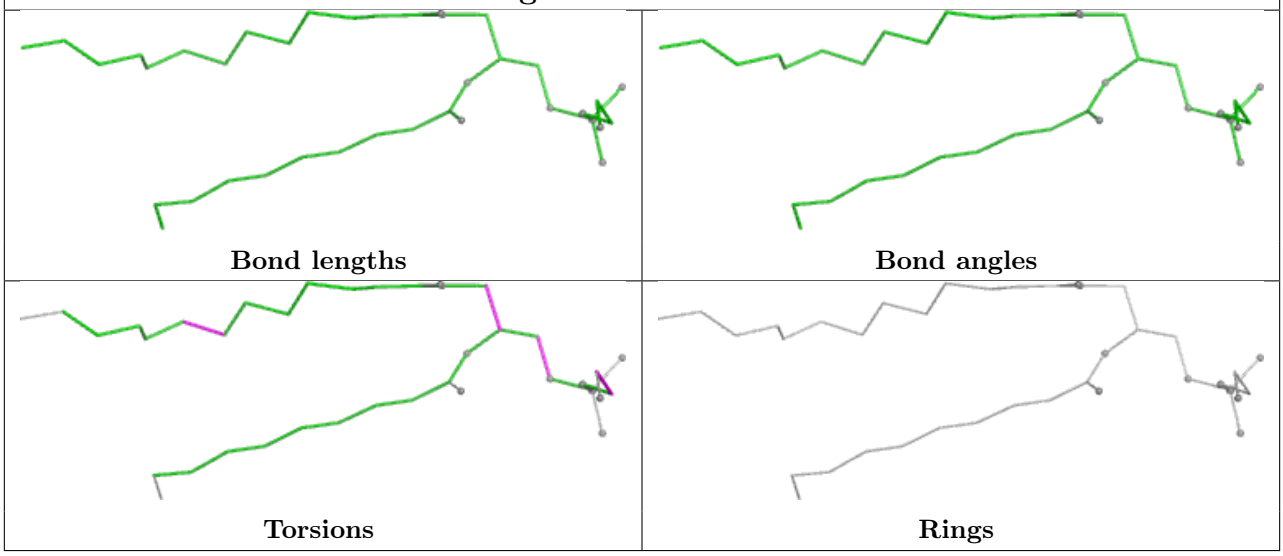
Ligand CDL d1 201

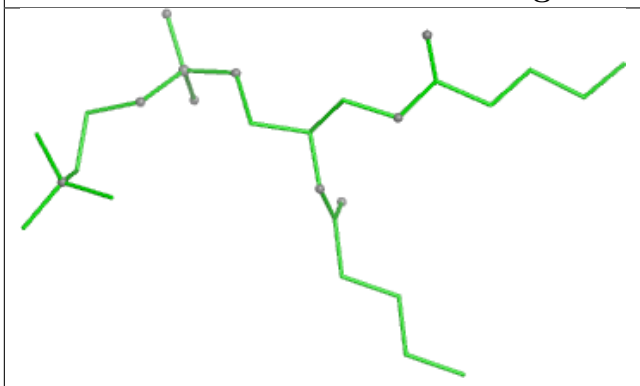
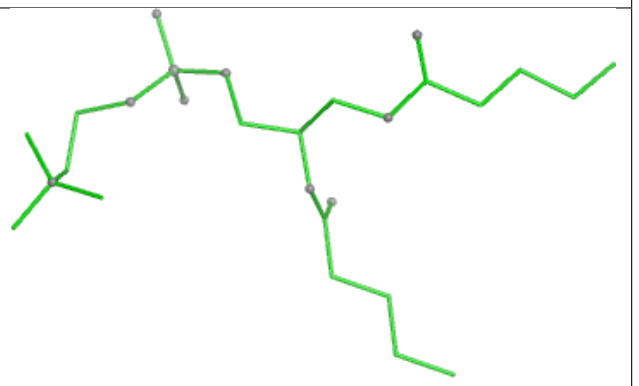
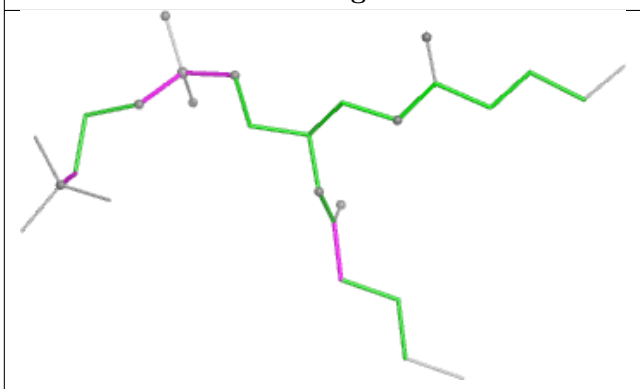
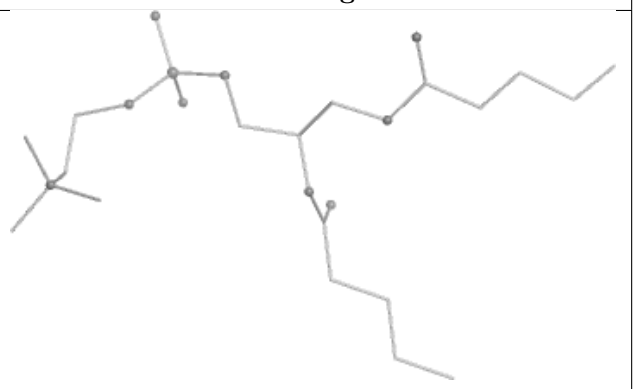


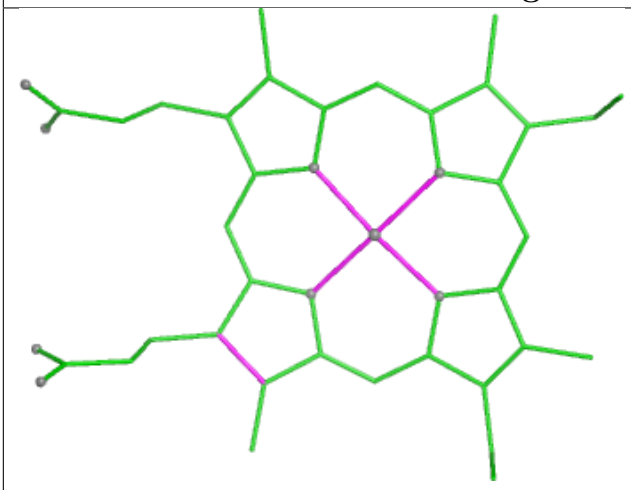
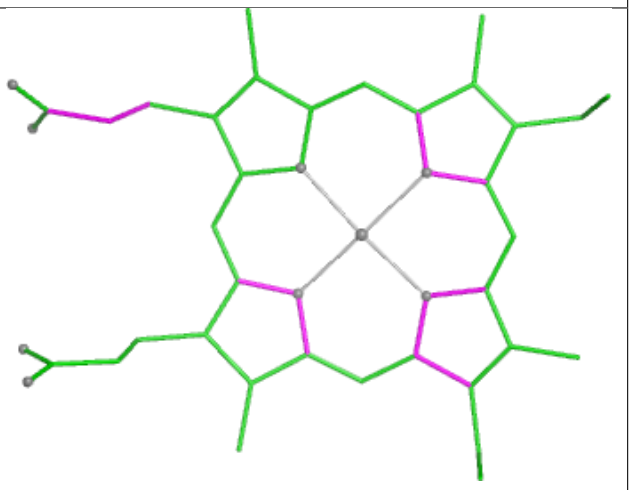
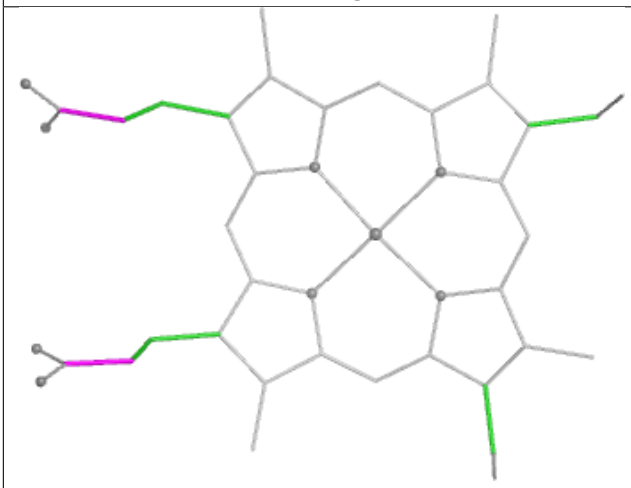
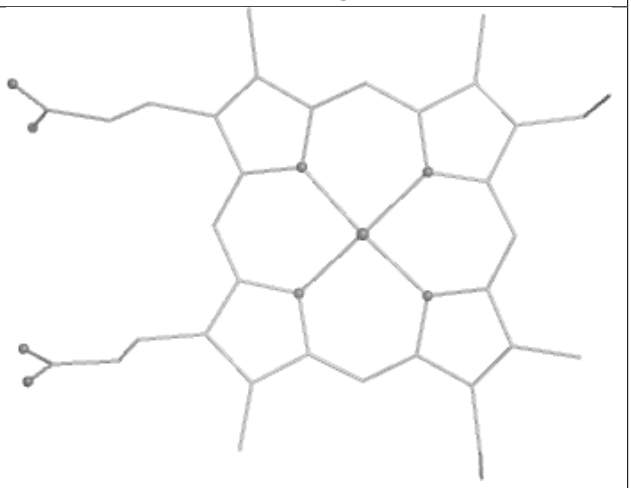
Ligand 3PE c 301



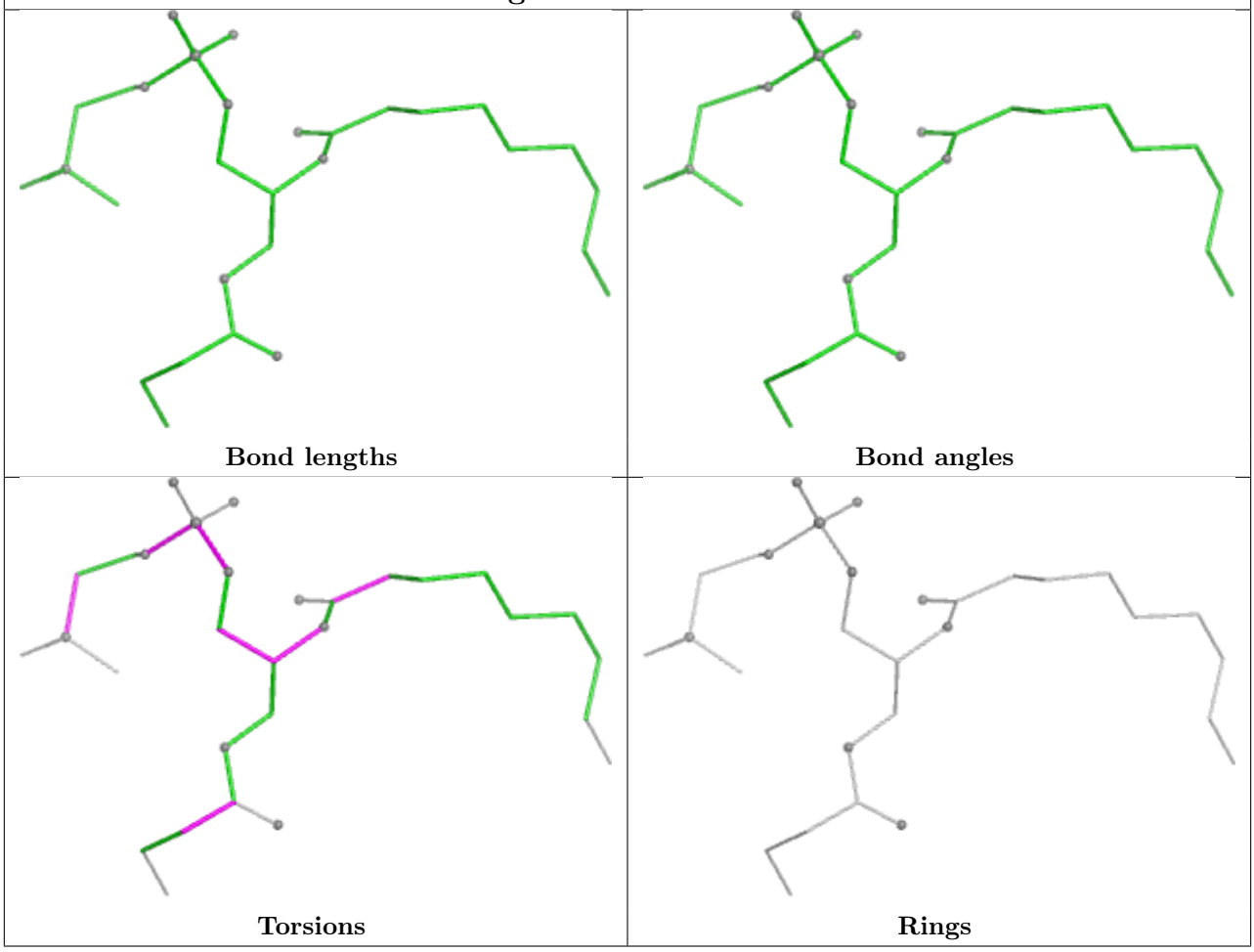
Ligand 3PE N1 402



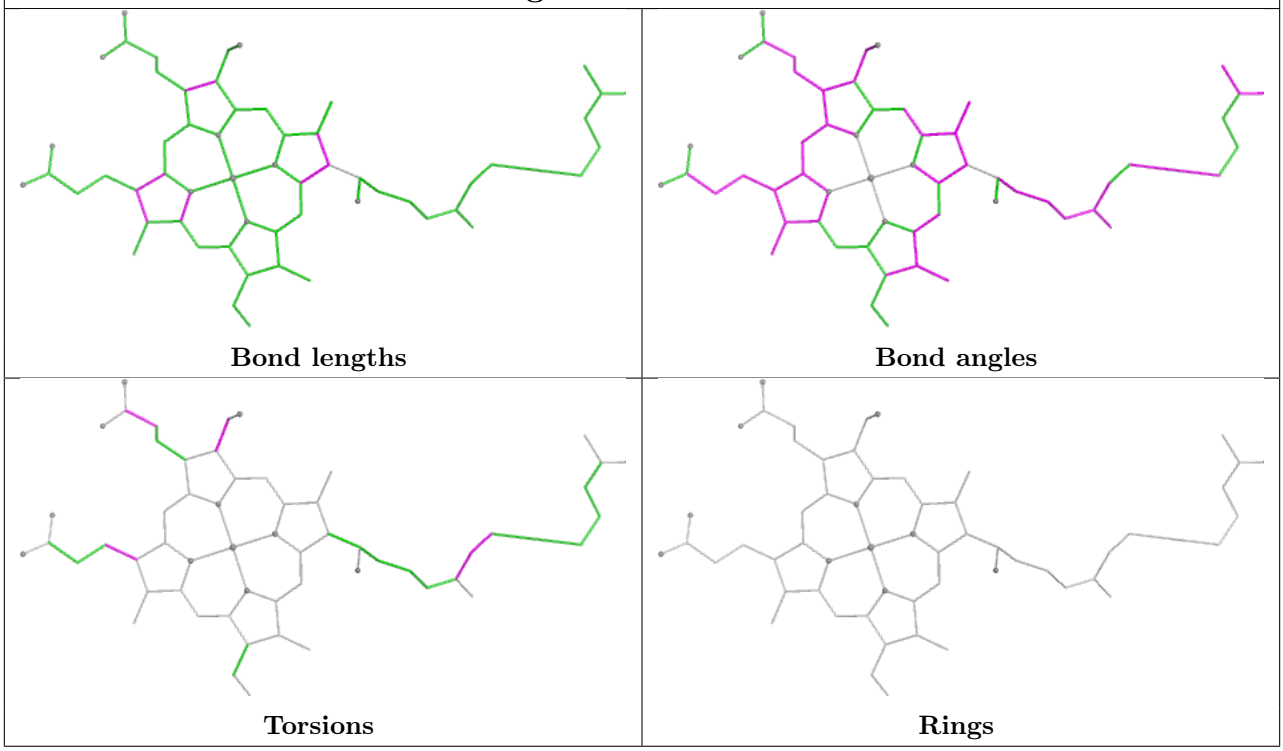
Ligand PC1 z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

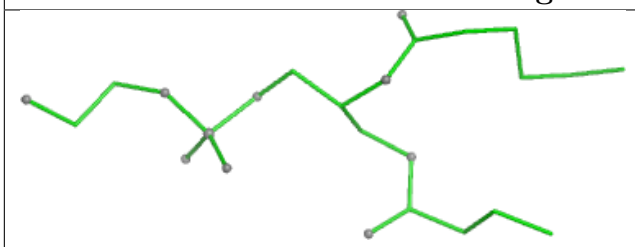
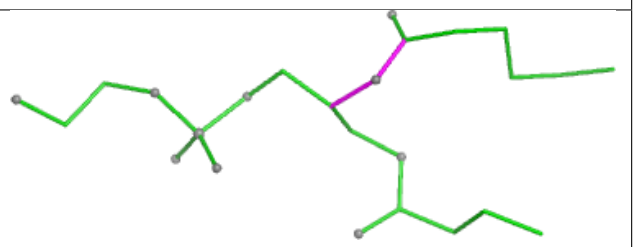
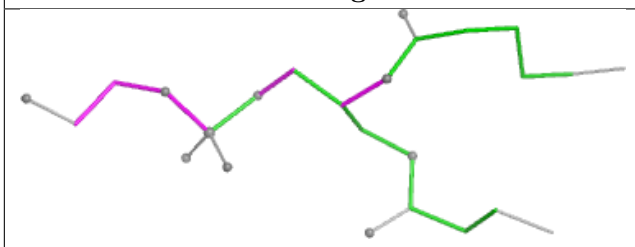
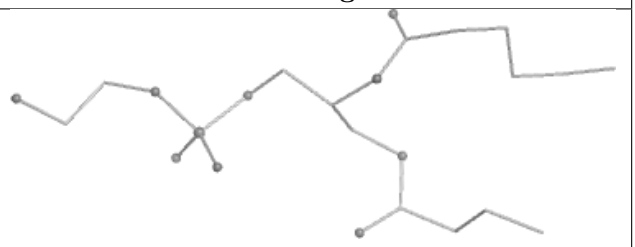
Ligand HEC O 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

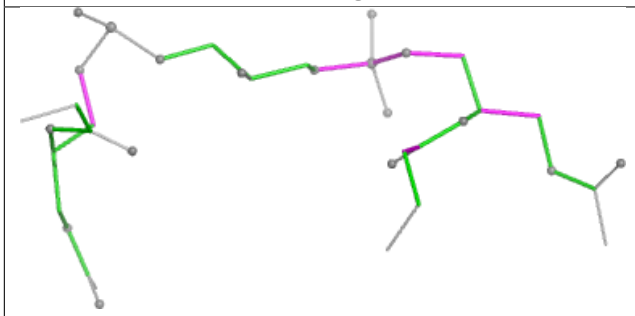
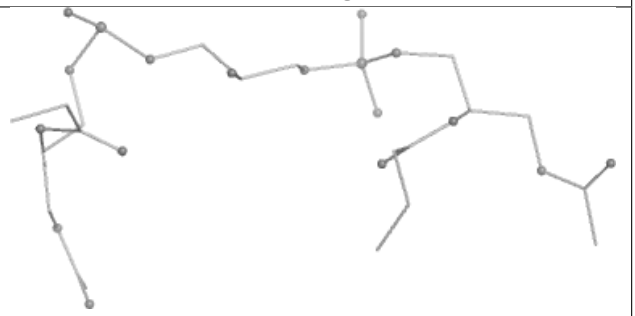
Ligand PC1 P1 502



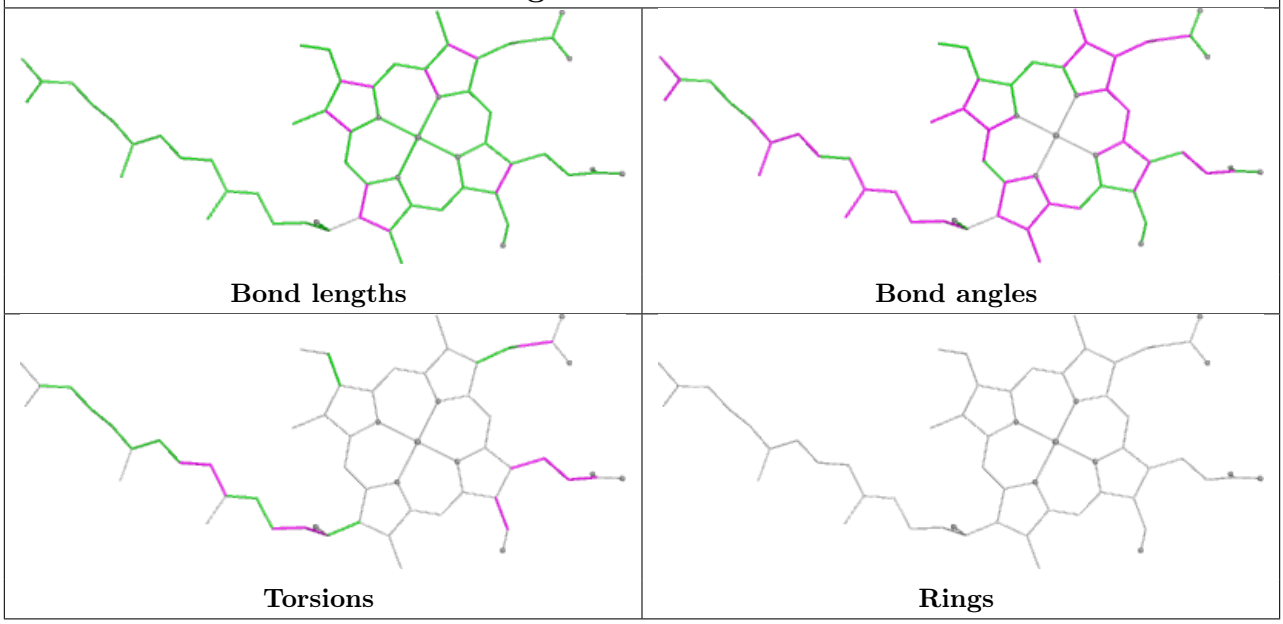
Ligand HEA n 604



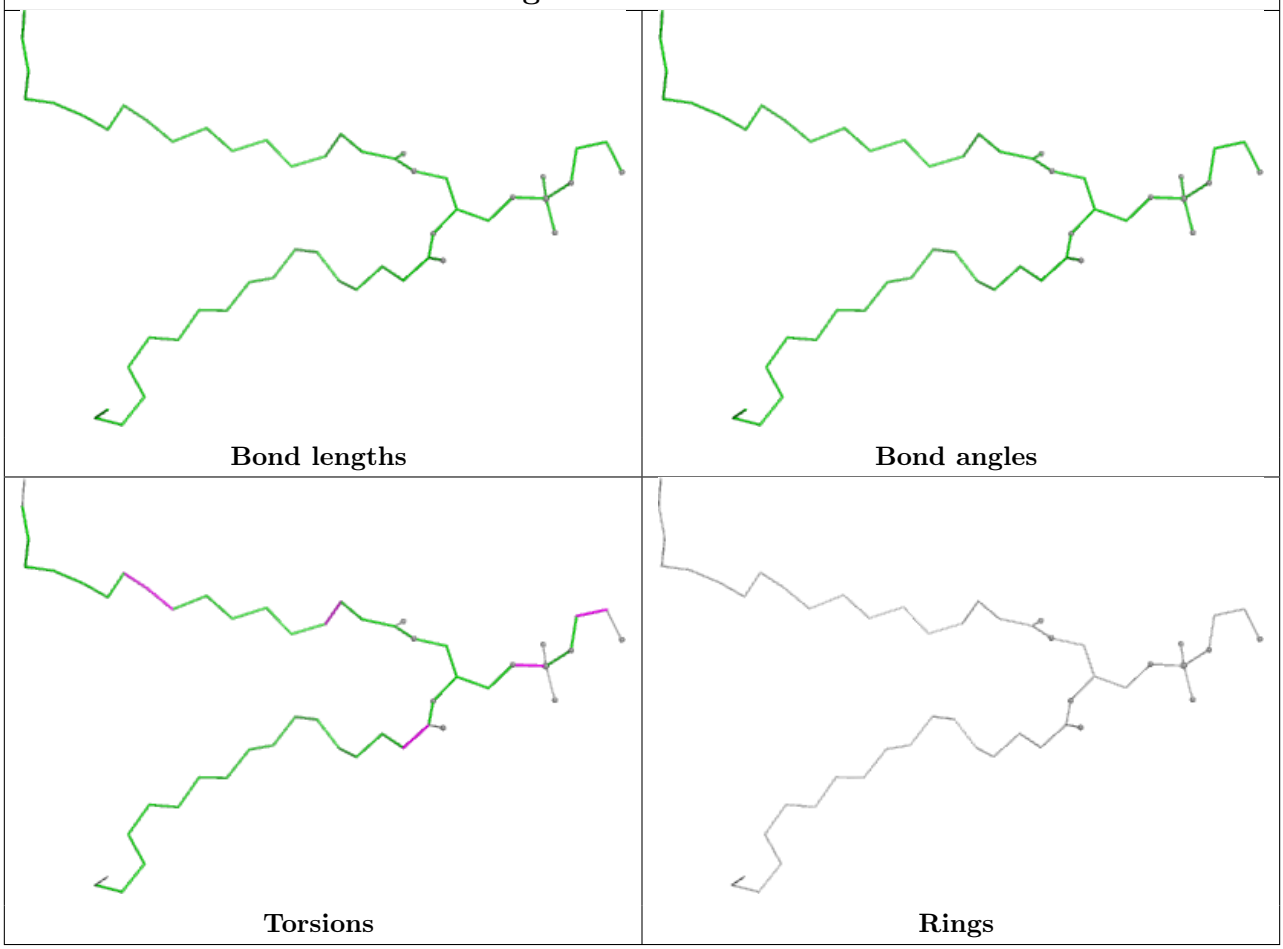
Ligand 3PE t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL g 301	
Bond lengths	Bond angles
 Torsions	 Rings

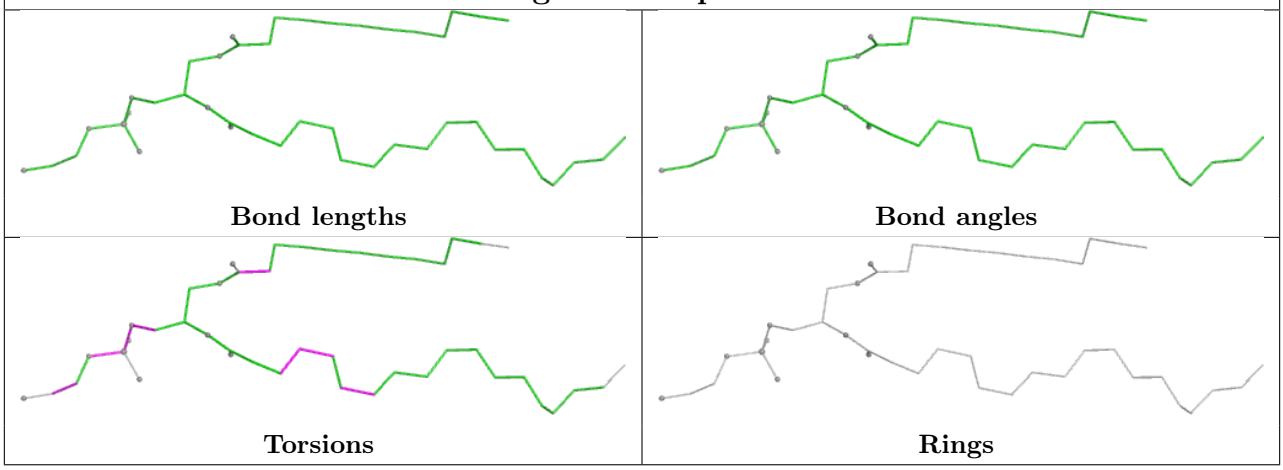
Ligand HEA a 603



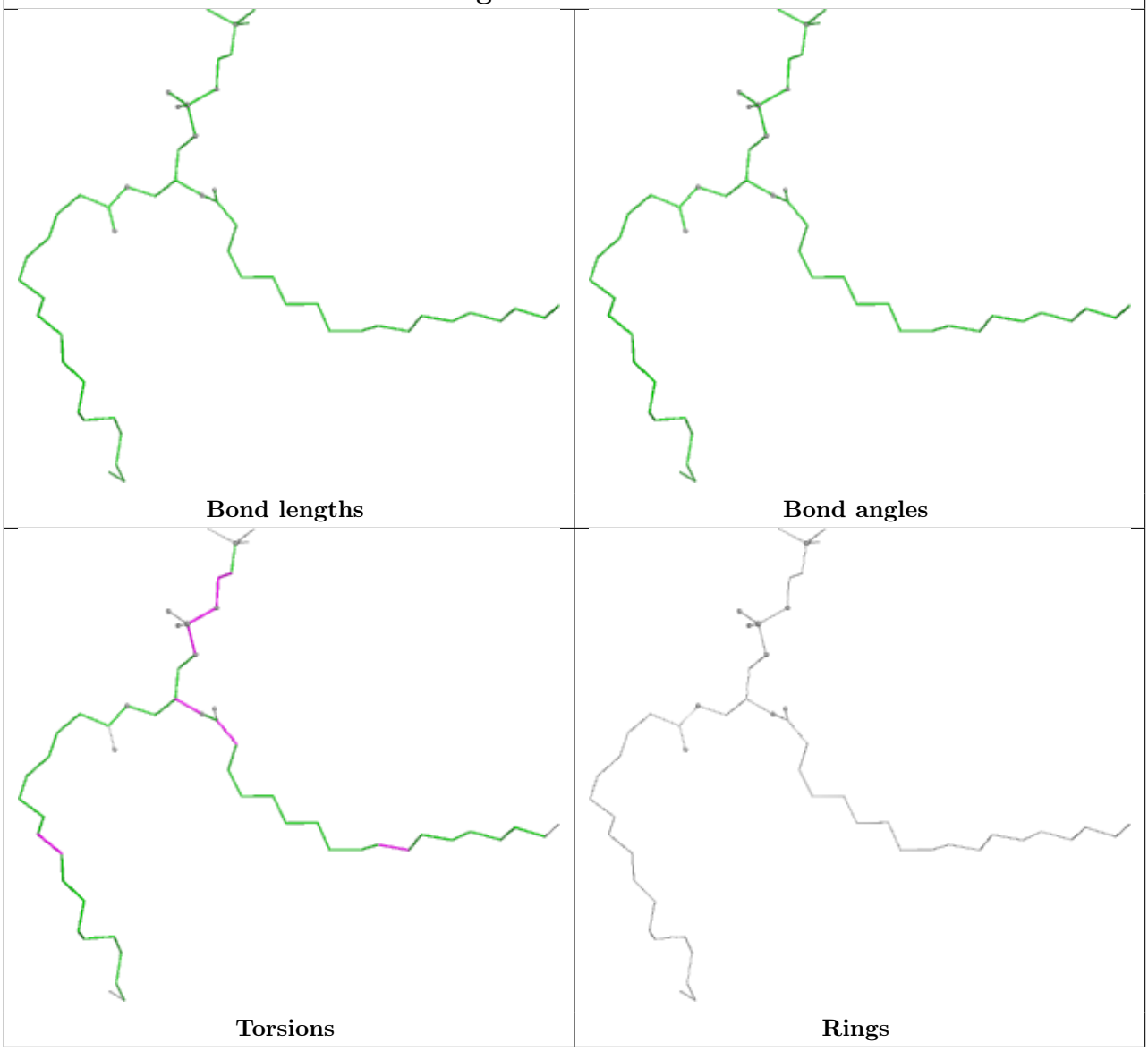
Ligand 3PE L1 704



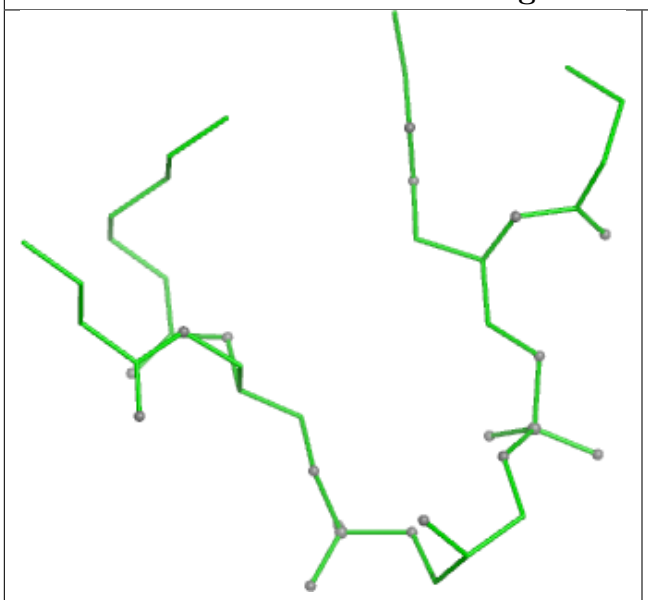
Ligand 3PE p 301



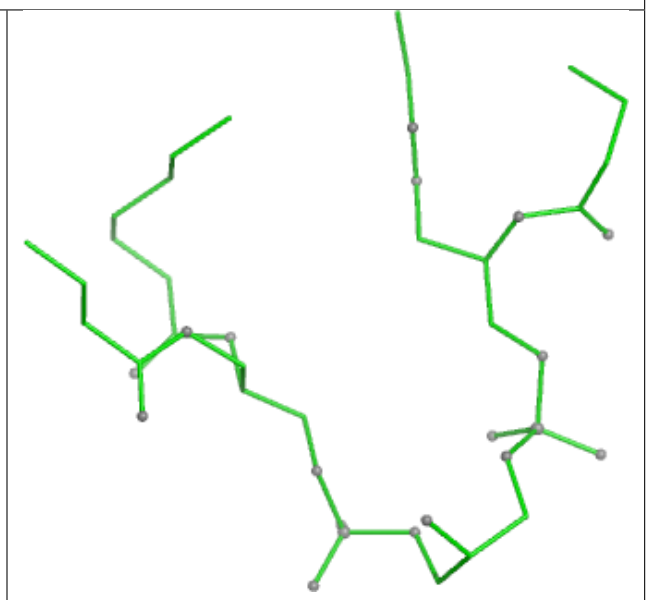
Ligand PC1 9 203



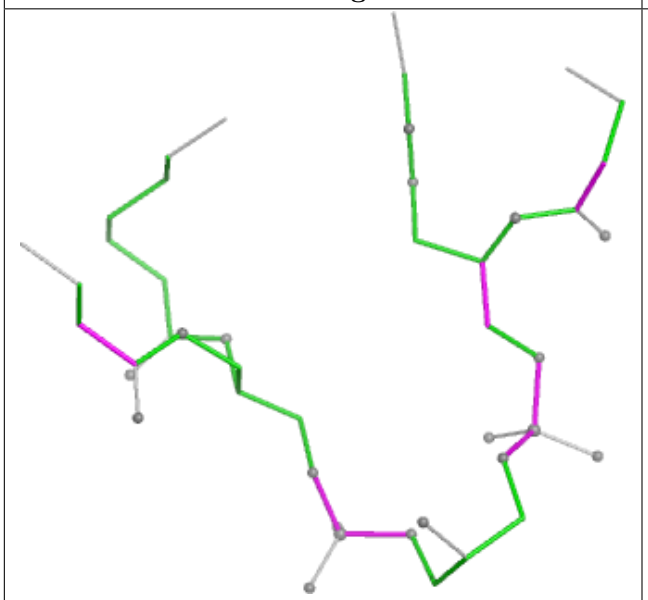
Ligand CDL L1 703



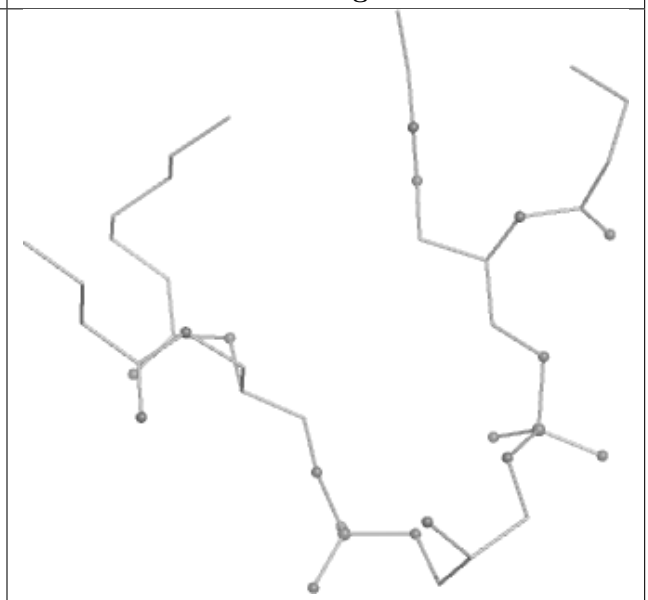
Bond lengths



Bond angles

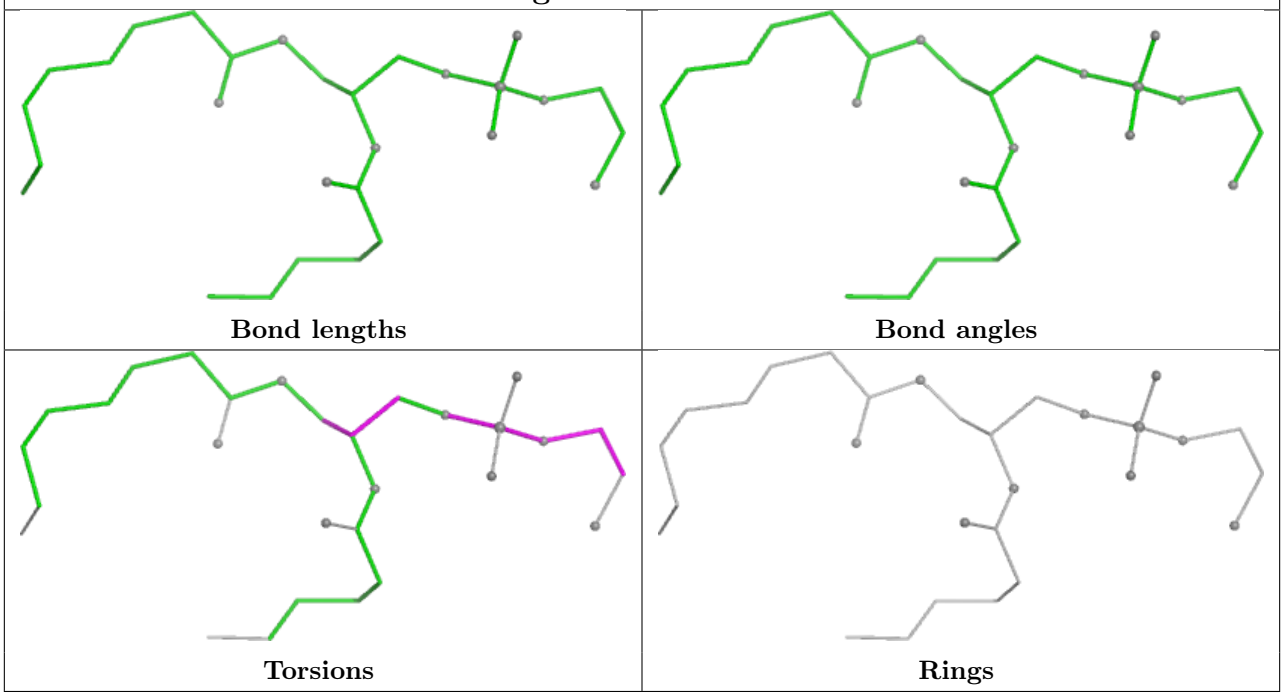


Torsions

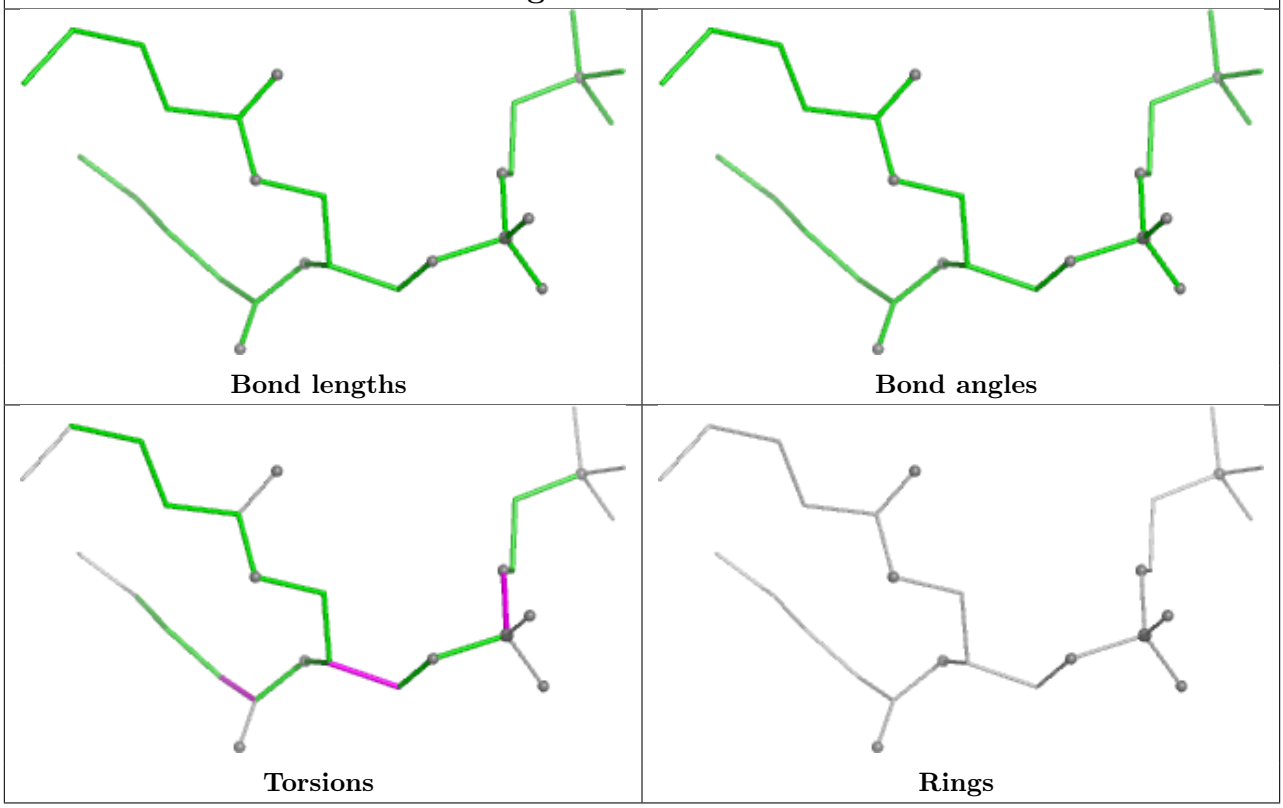


Rings

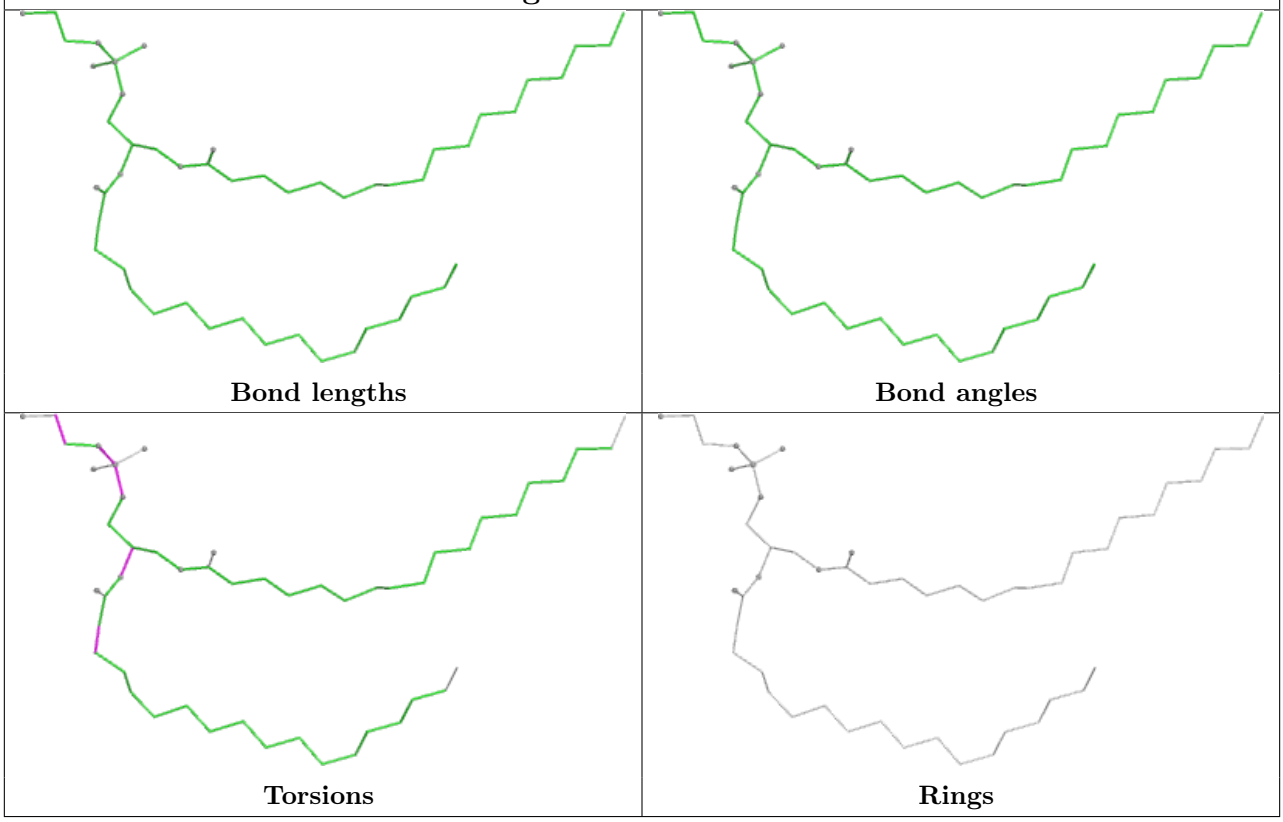
Ligand 3PE b 301



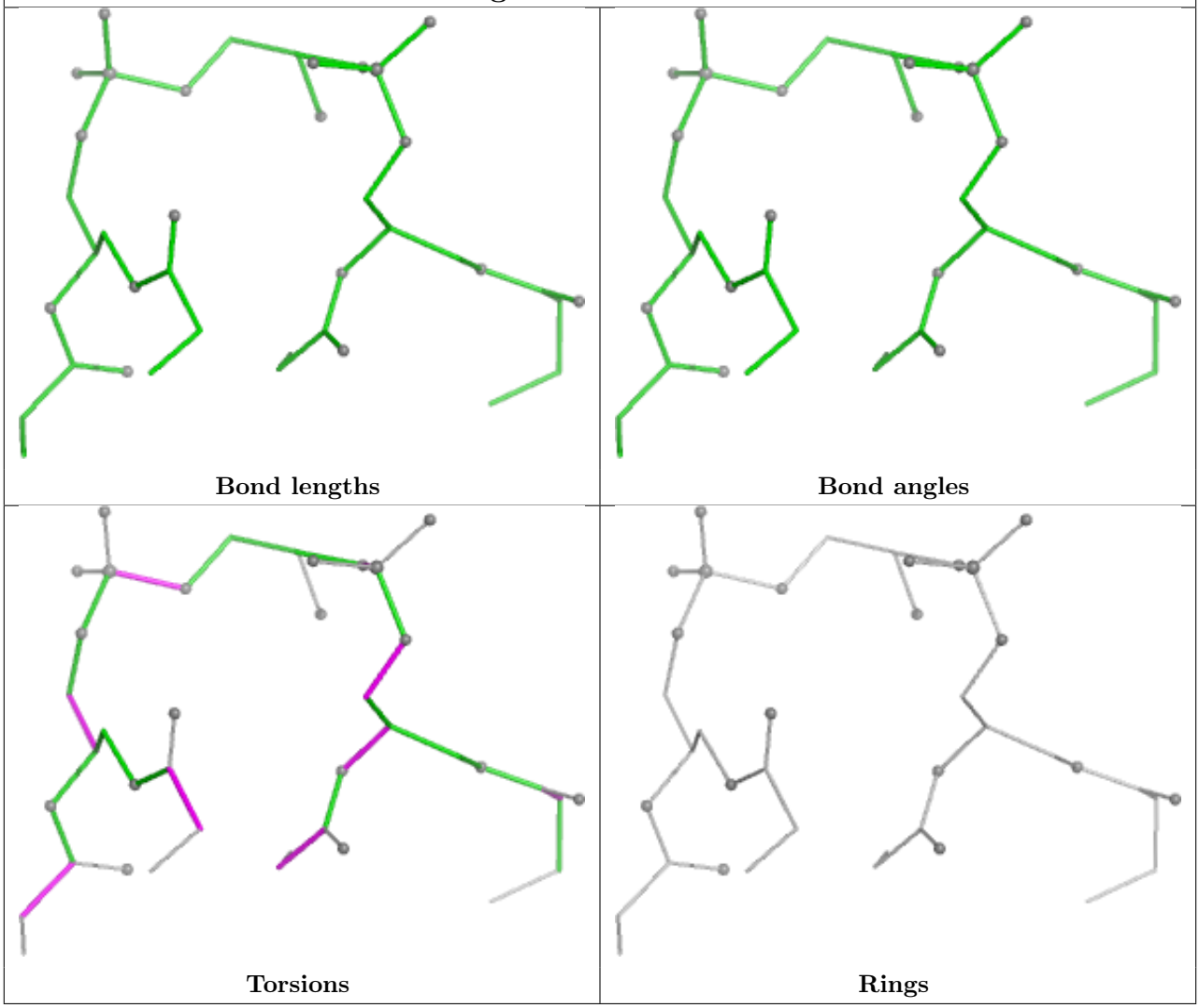
Ligand PC1 K 101



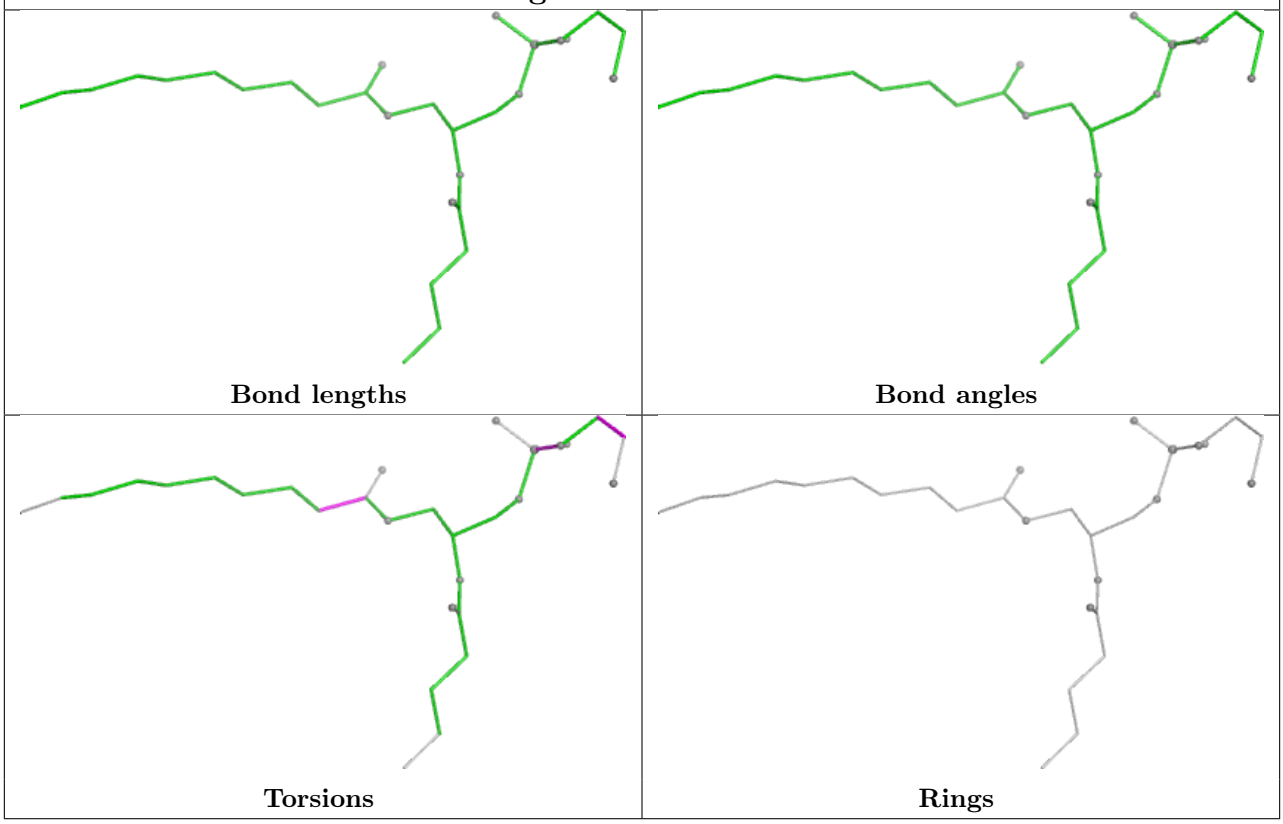
Ligand 3PE L1 701



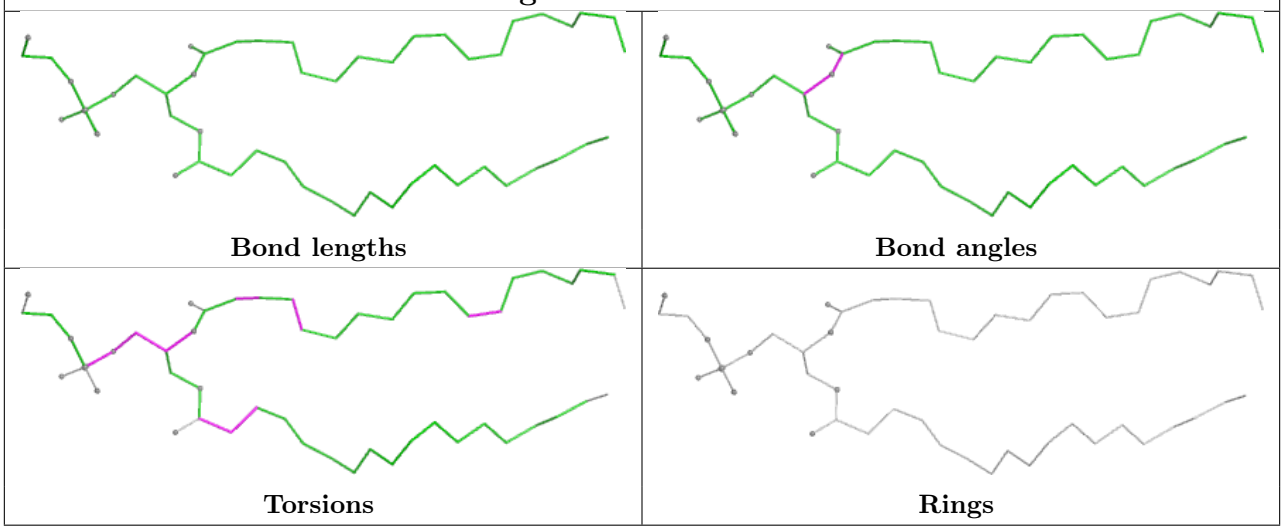
Ligand CDL R 101



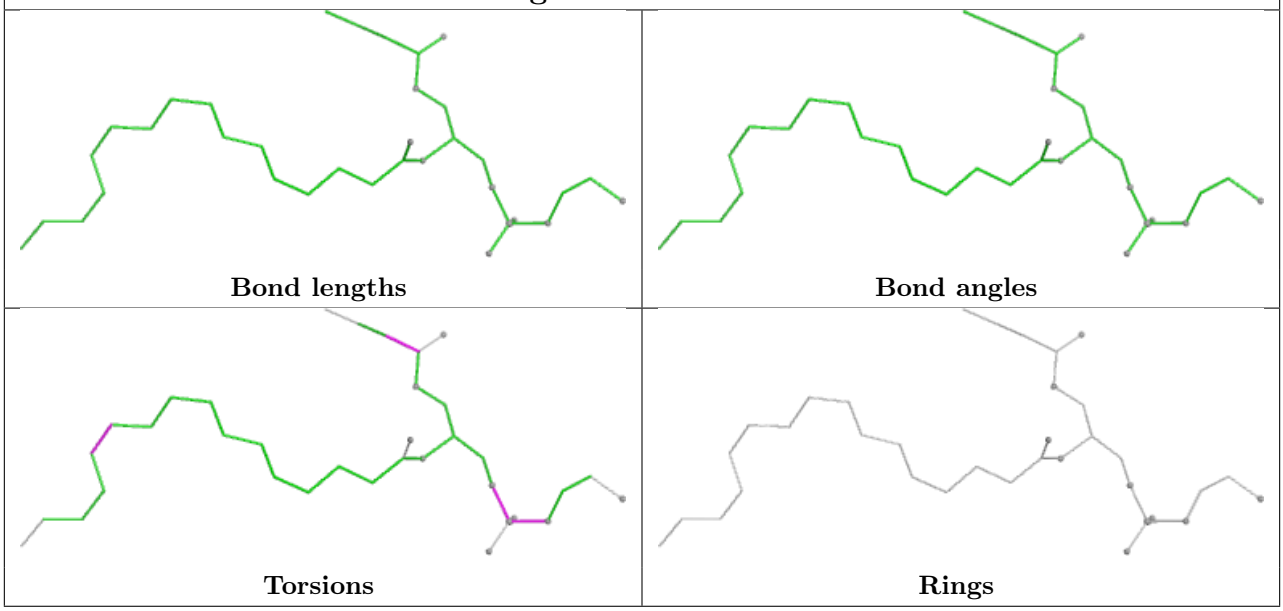
Ligand 3PE R 104



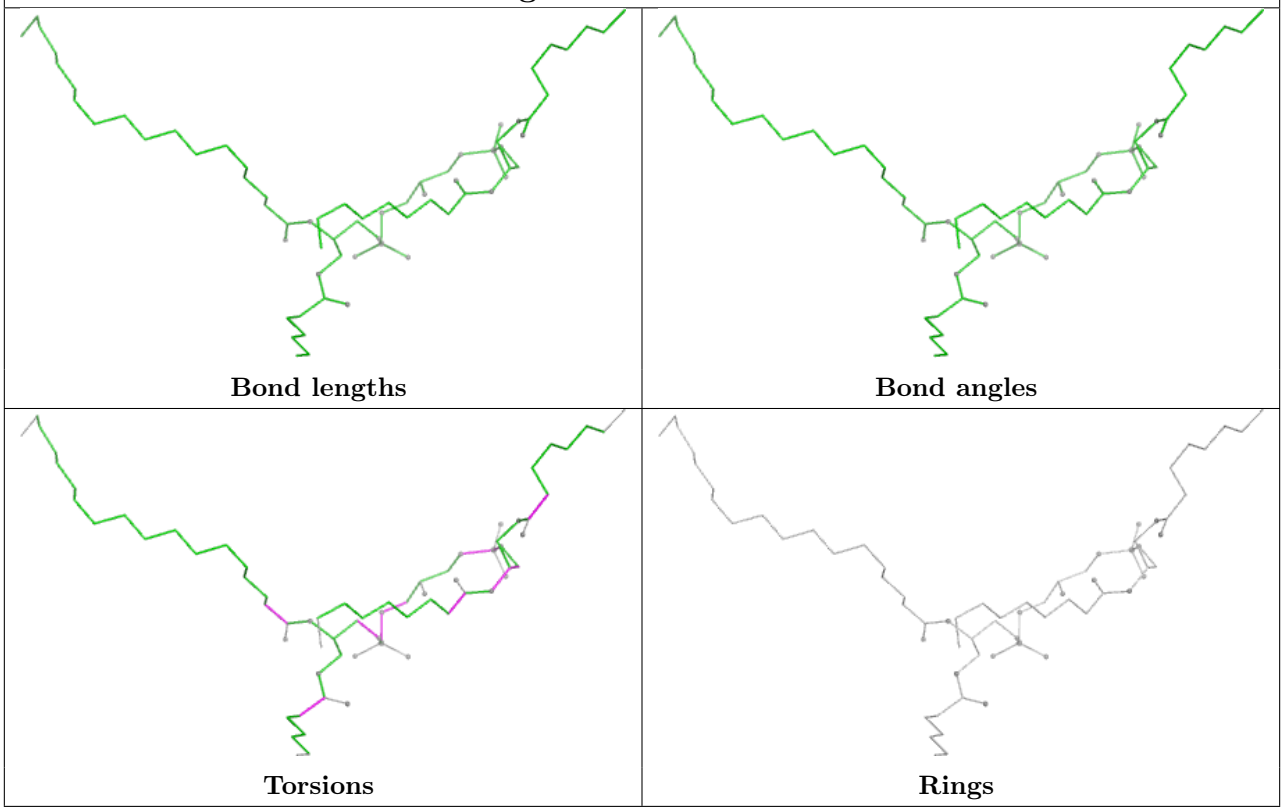
Ligand 3PE H1 401



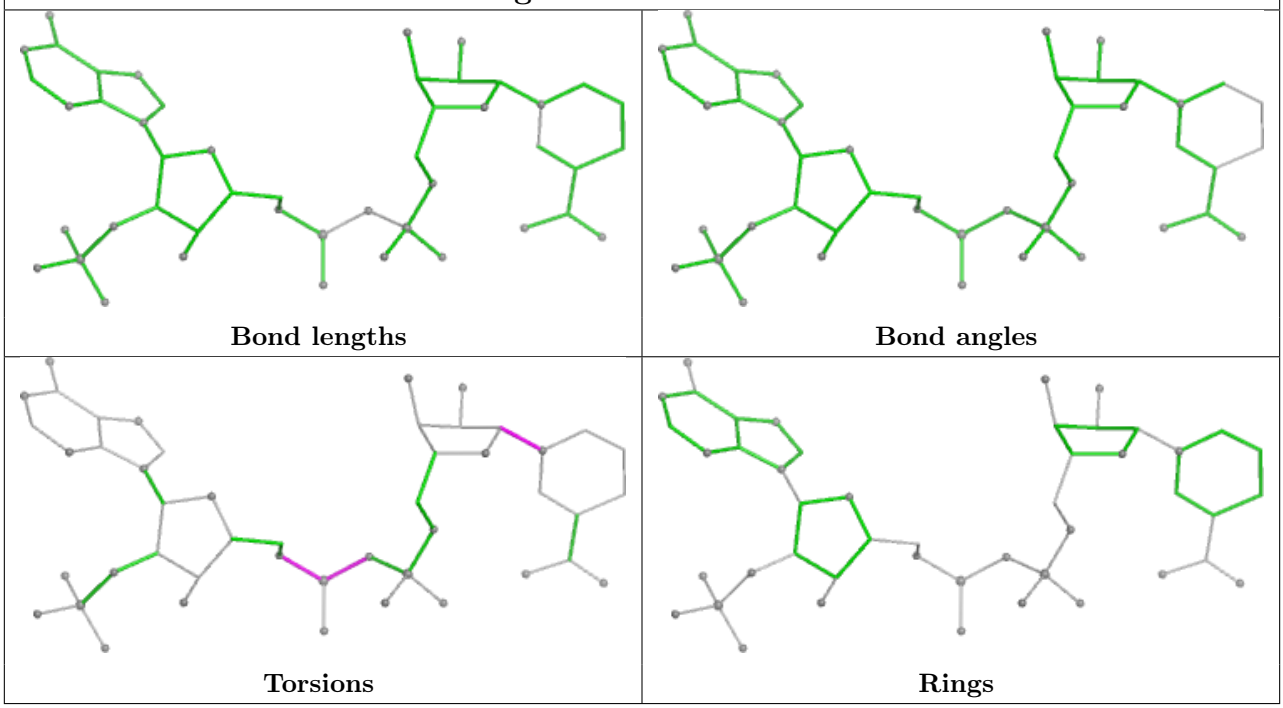
Ligand 3PE C 403



Ligand CDL h1 201



Ligand NDP P1 501



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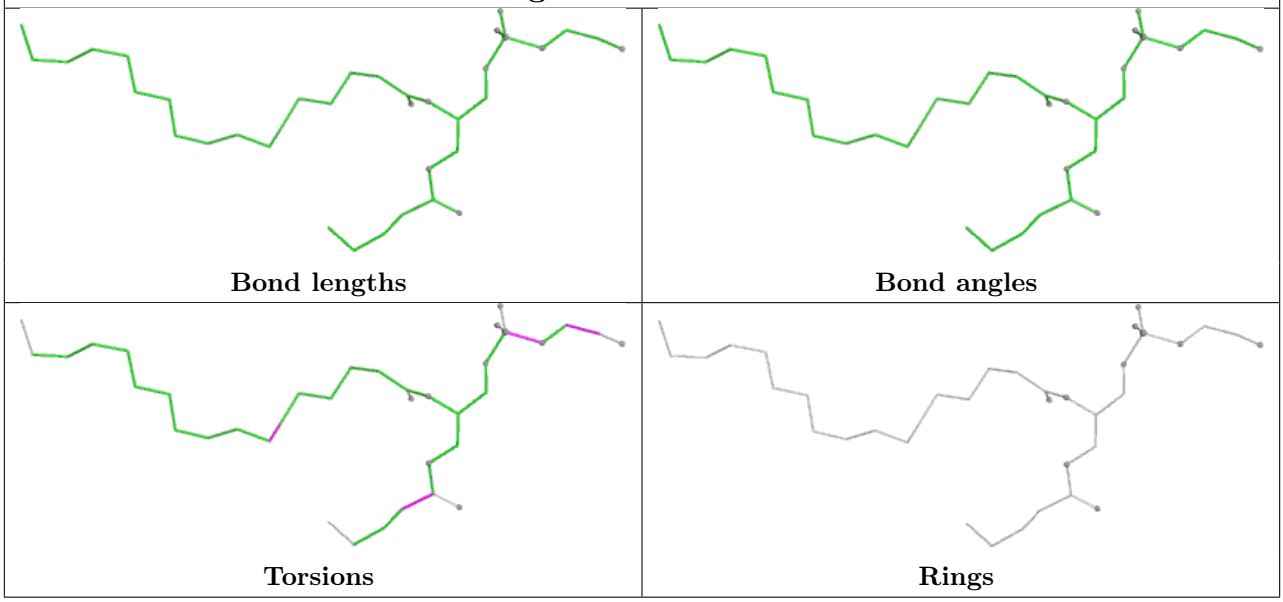

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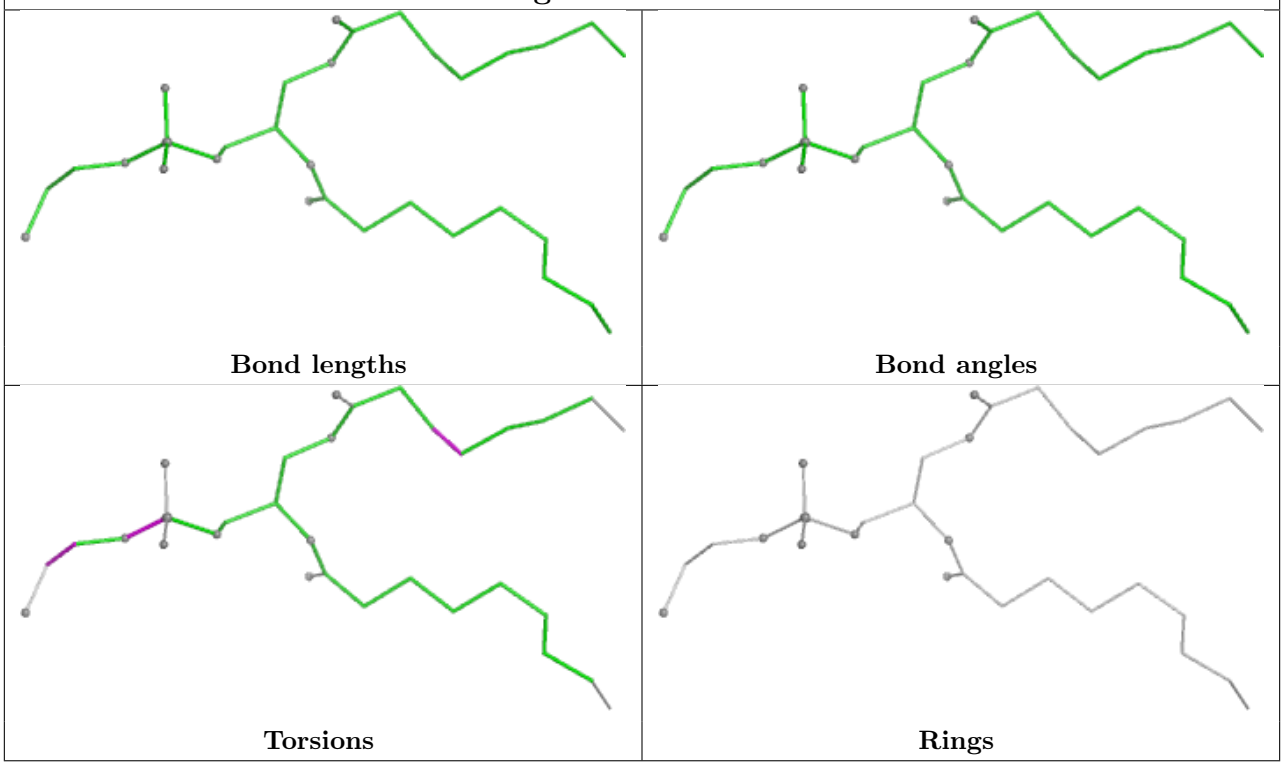
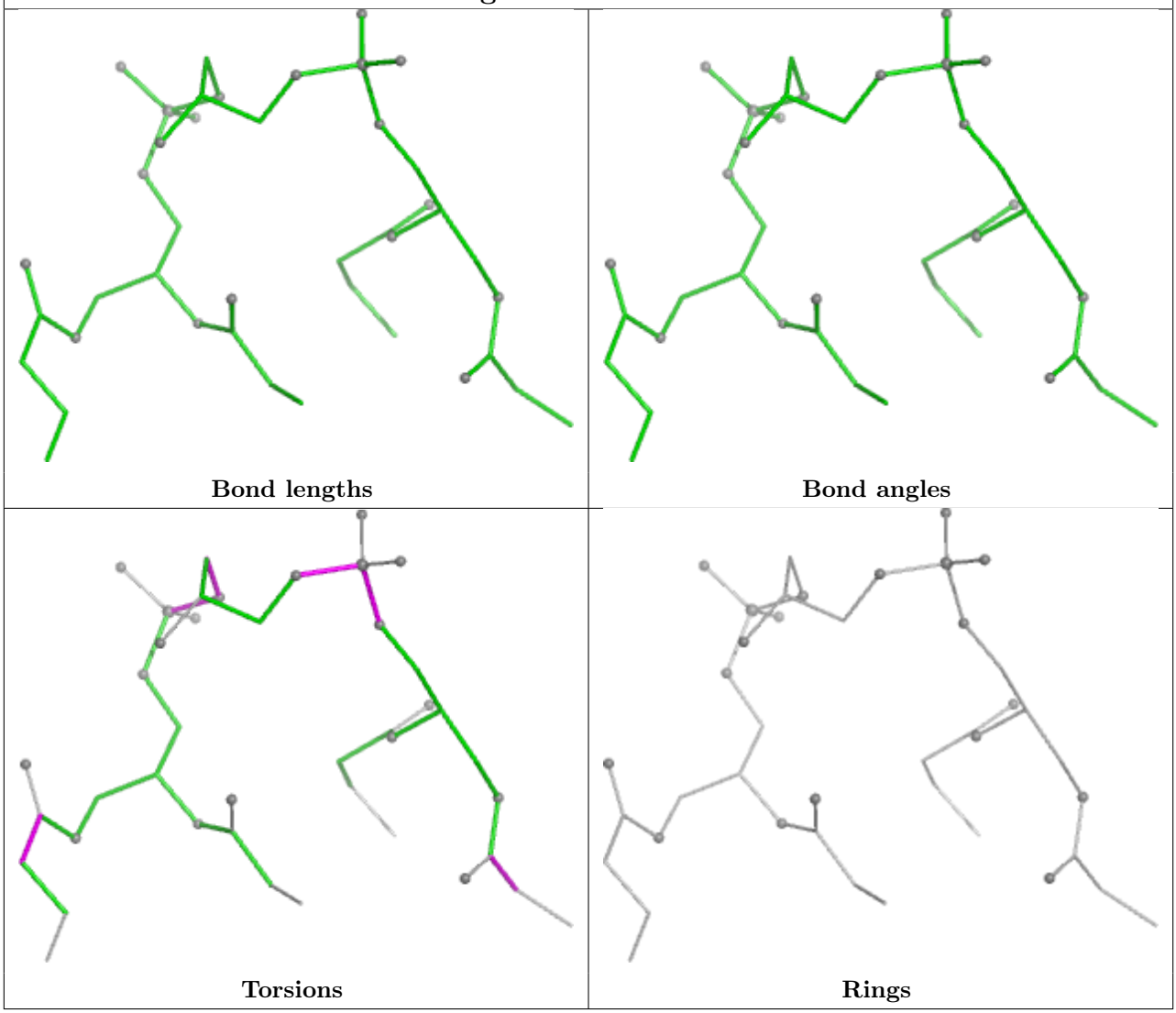
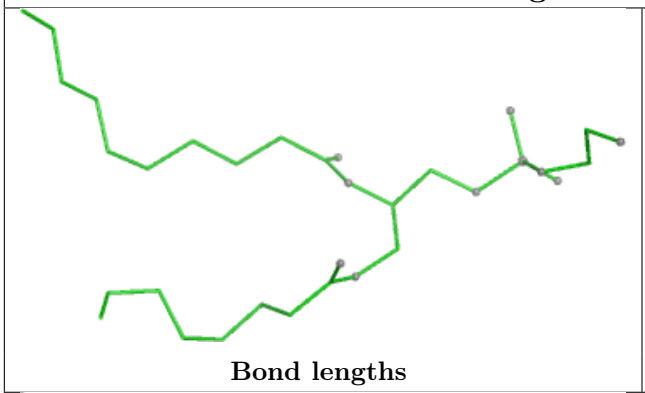


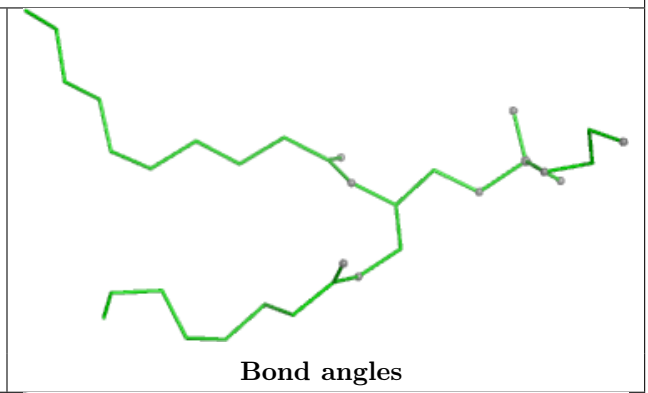
Ligand CDL G 101



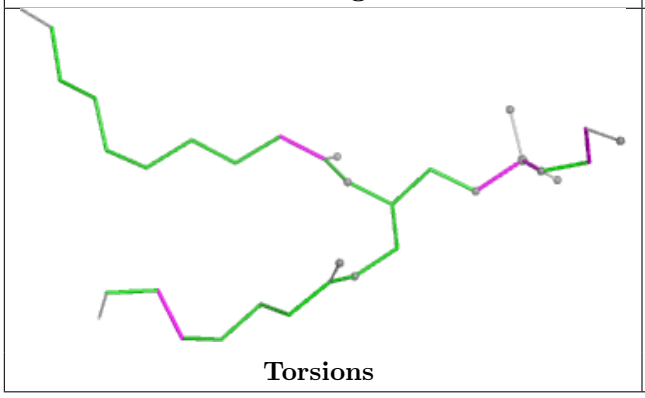
Ligand 3PE O 302



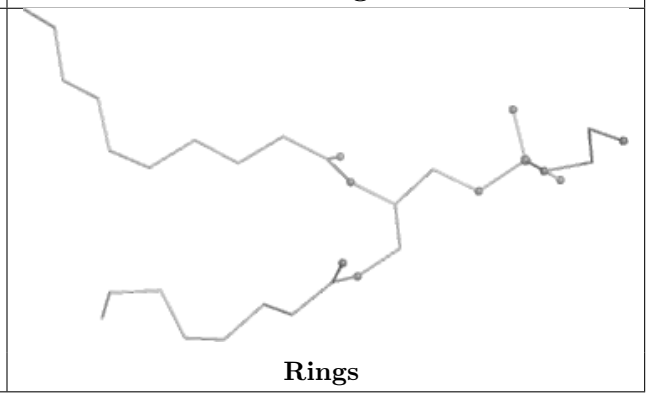
Bond lengths



Bond angles

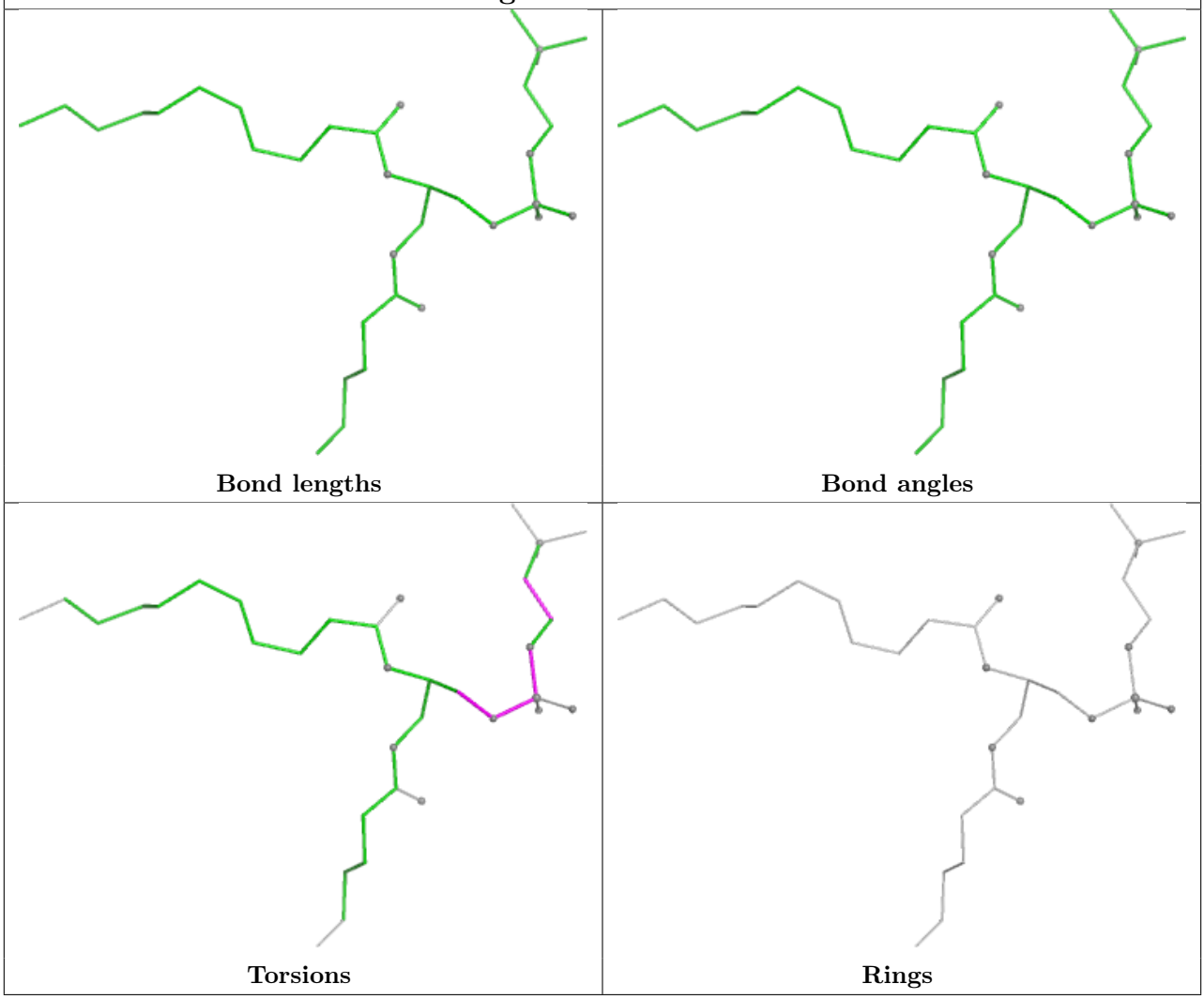


Torsions

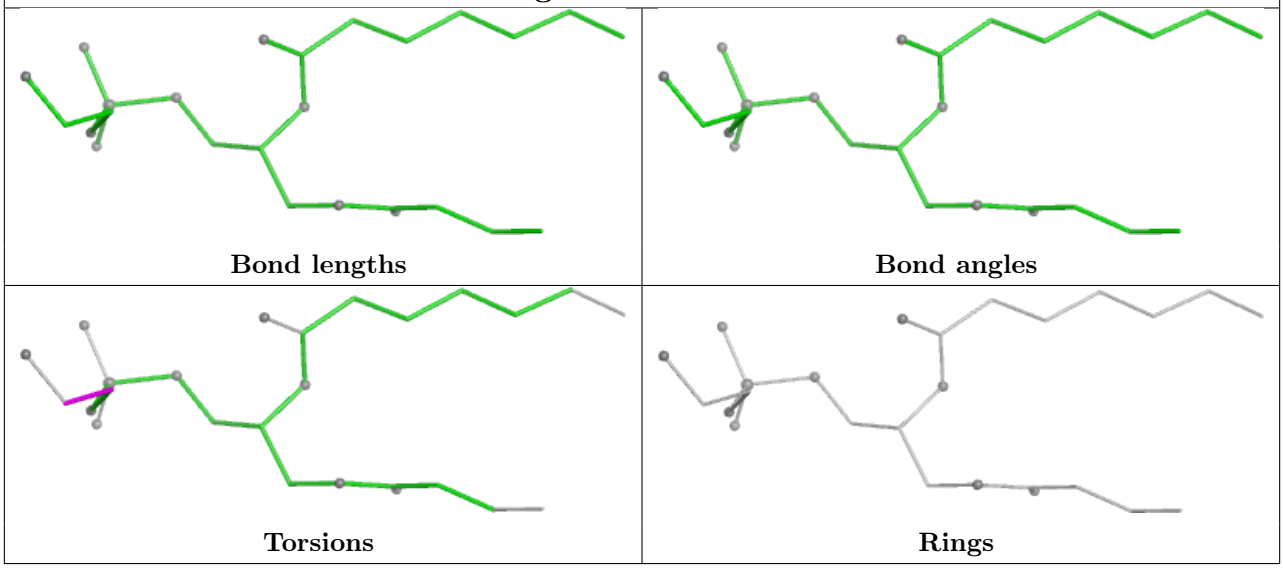


Rings

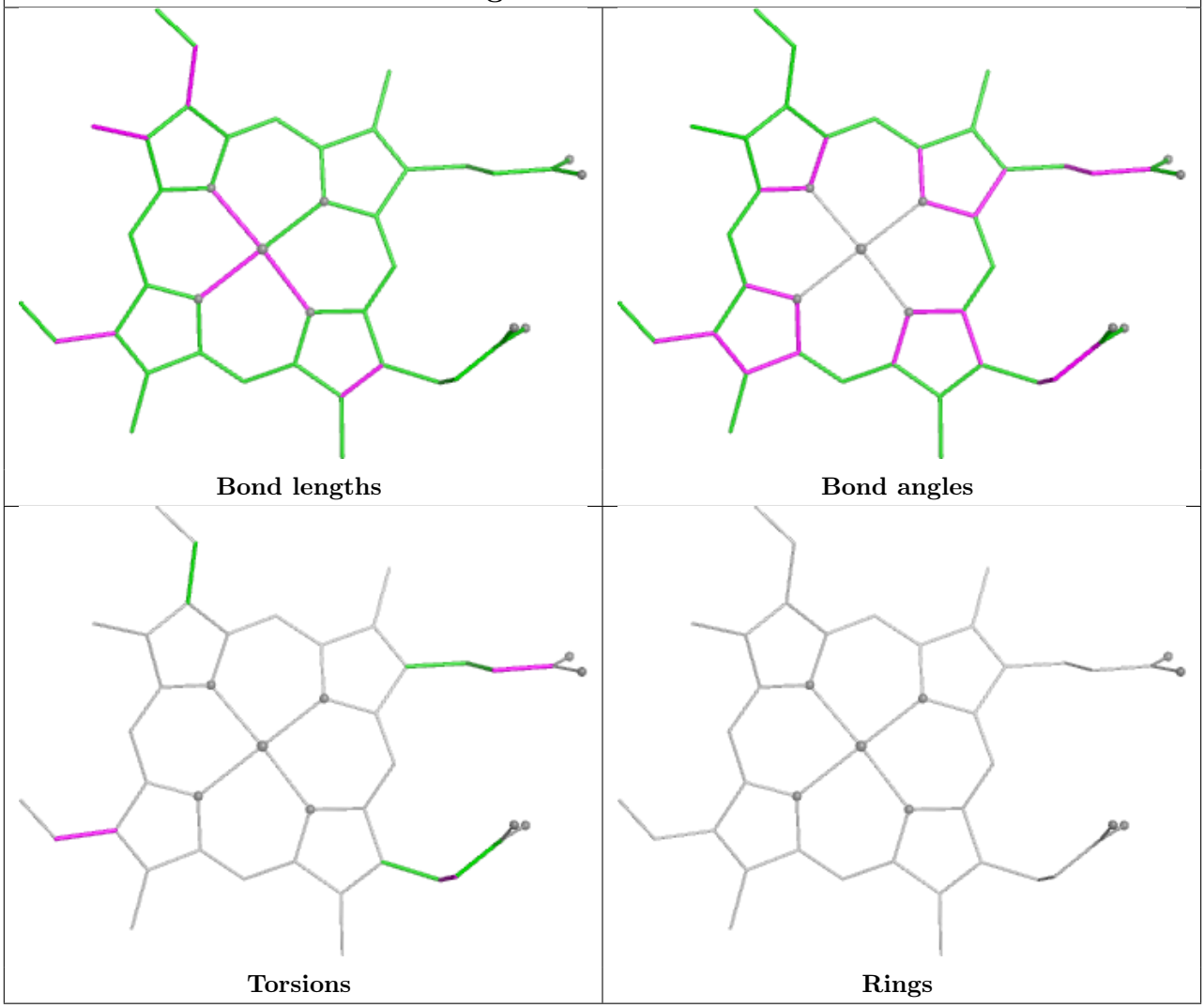
Ligand PC1 J 101



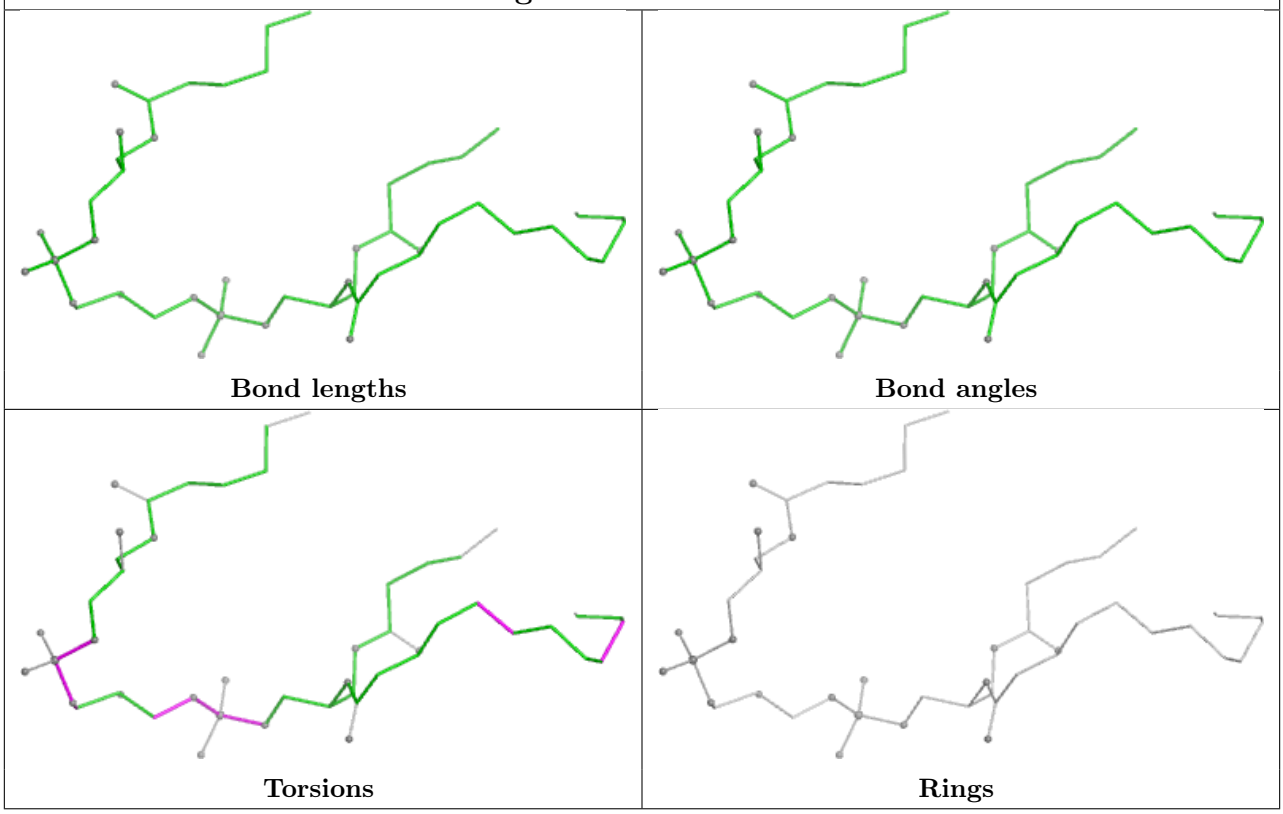
Ligand 3PE z 102



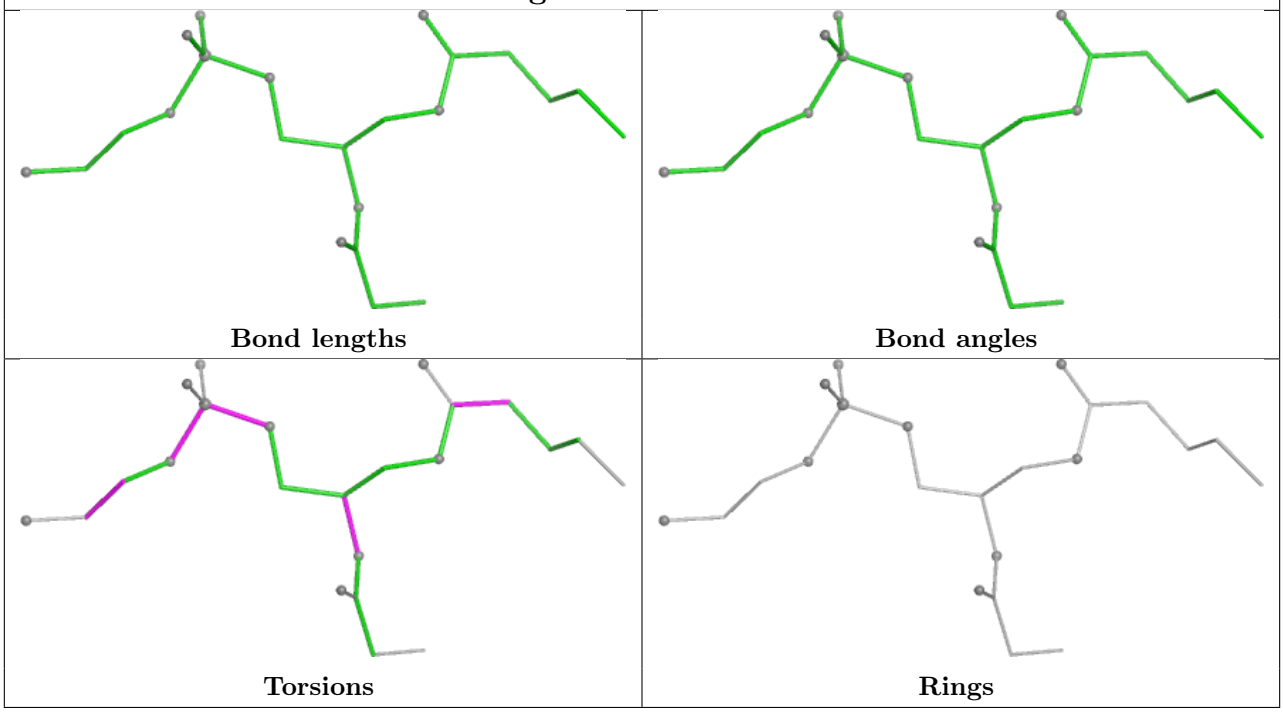
Ligand HEM N 402



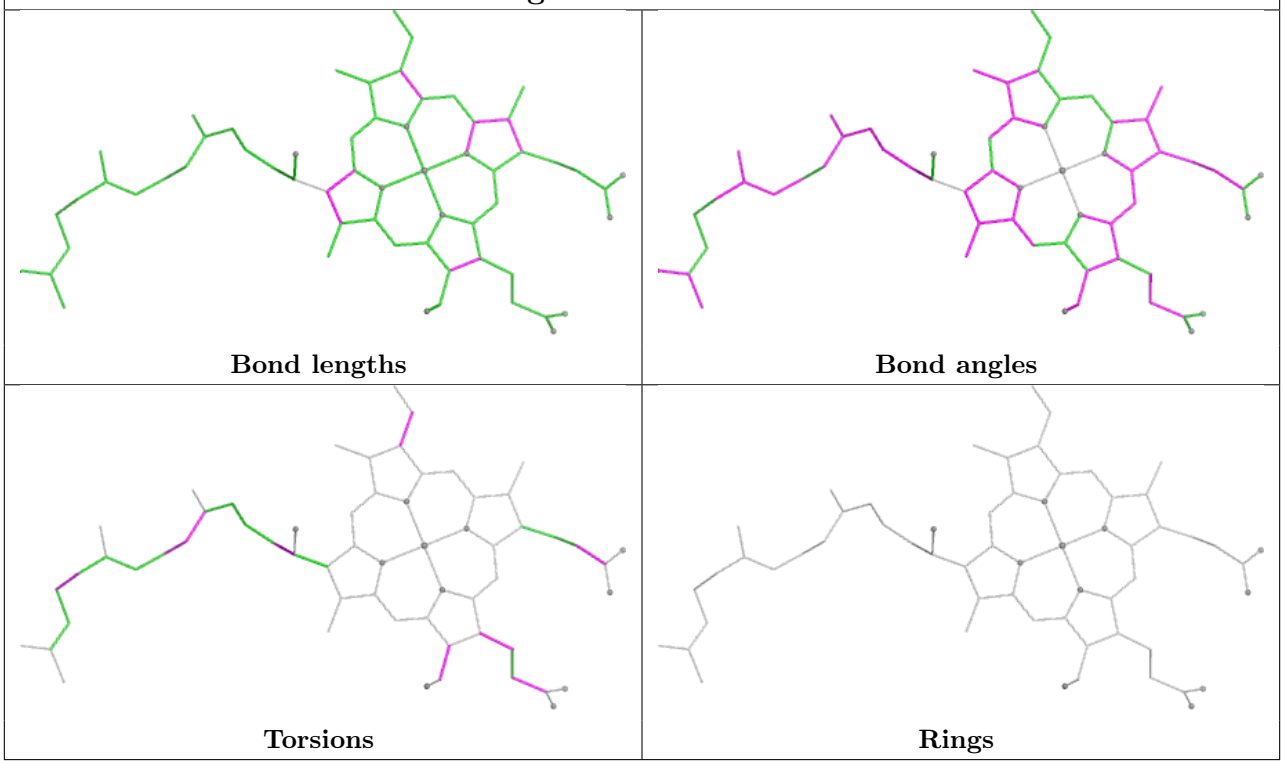
Ligand CDL H1 402



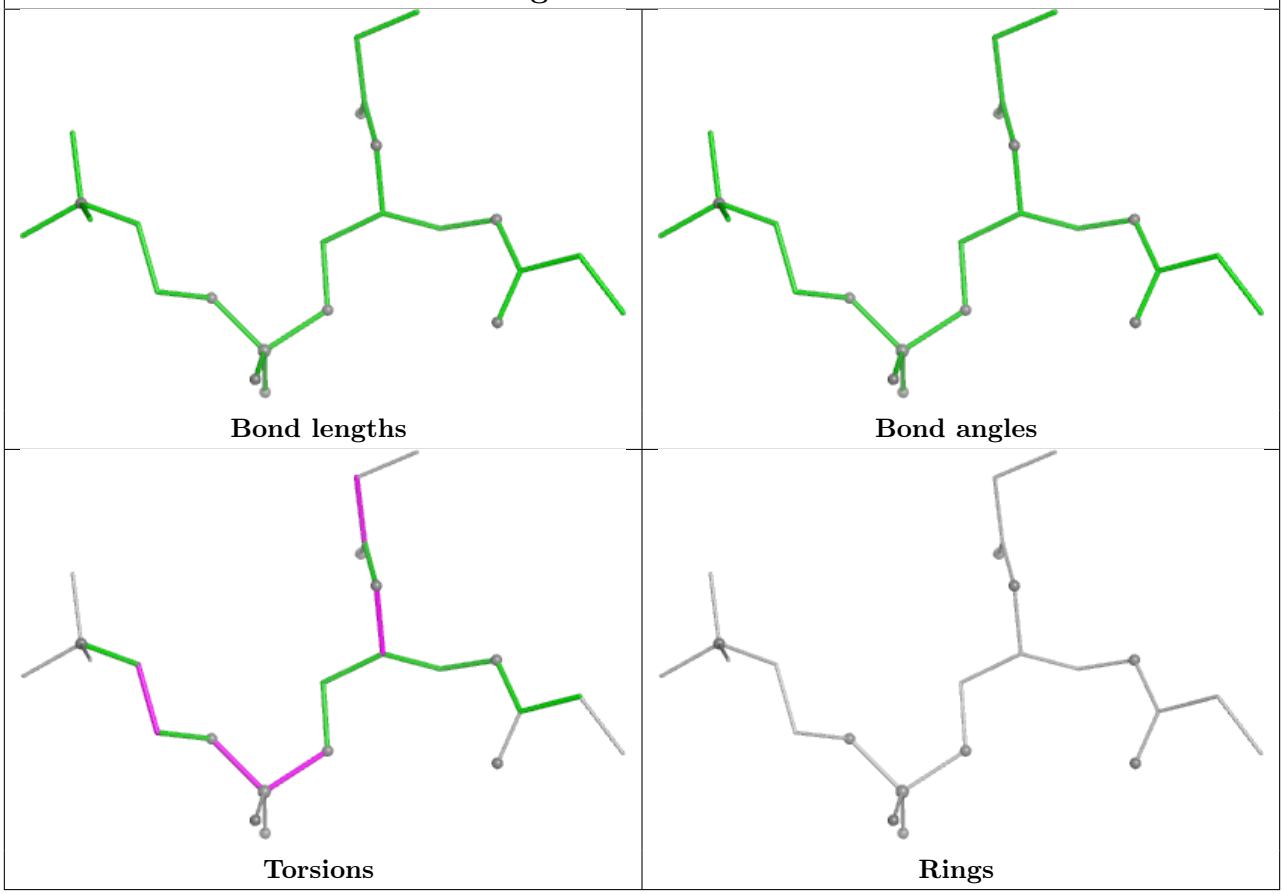
Ligand 3PE A 501



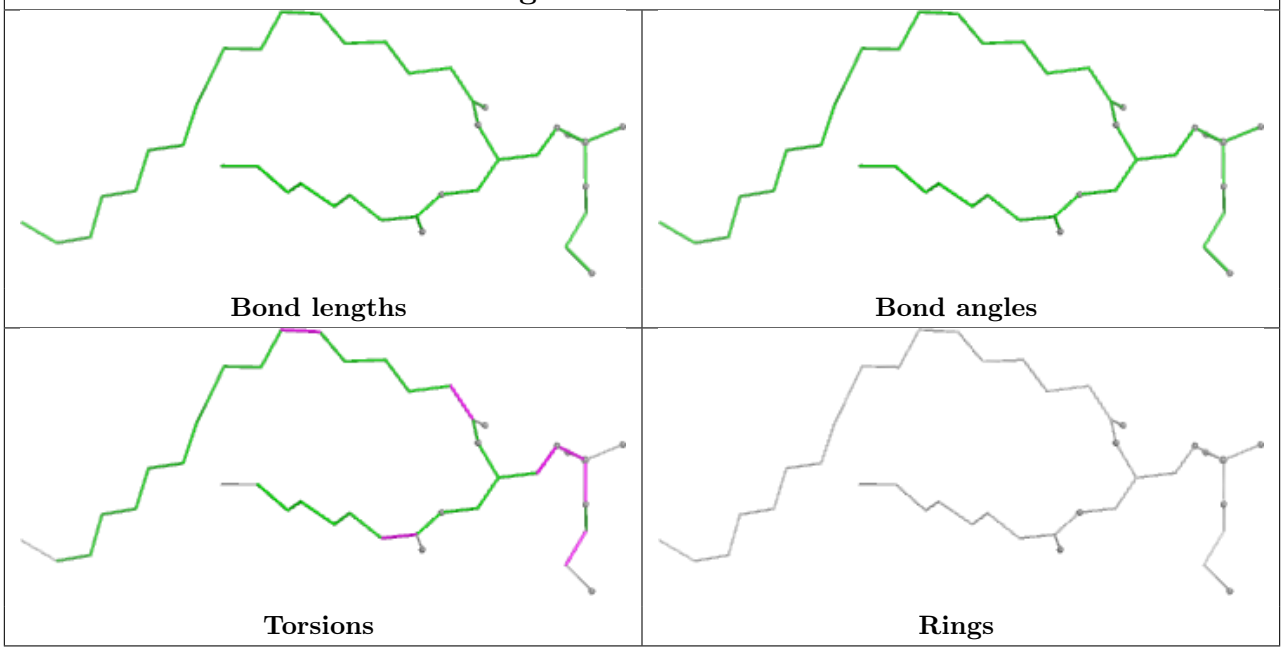
Ligand HEA a 604



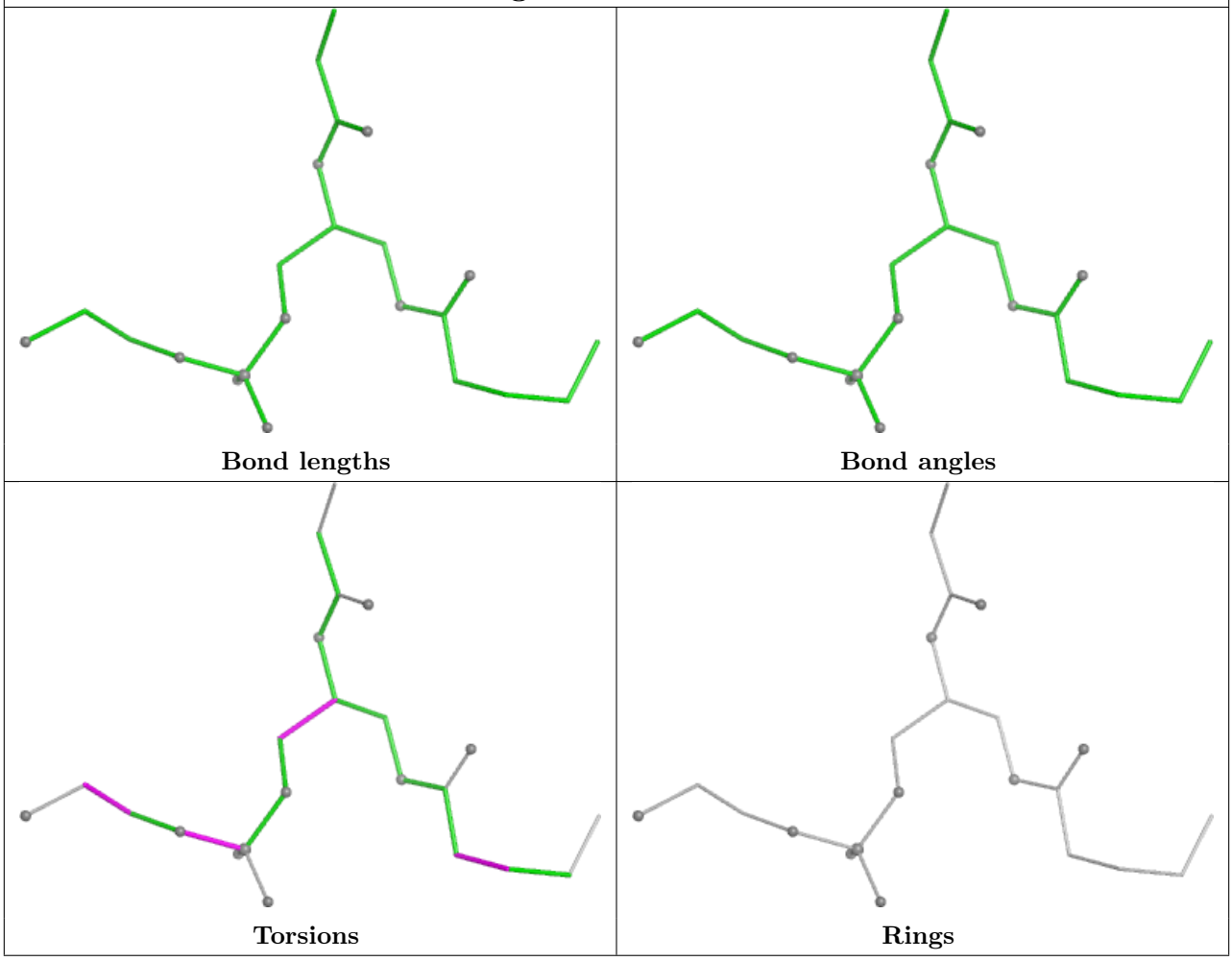
Ligand PC1 L 503



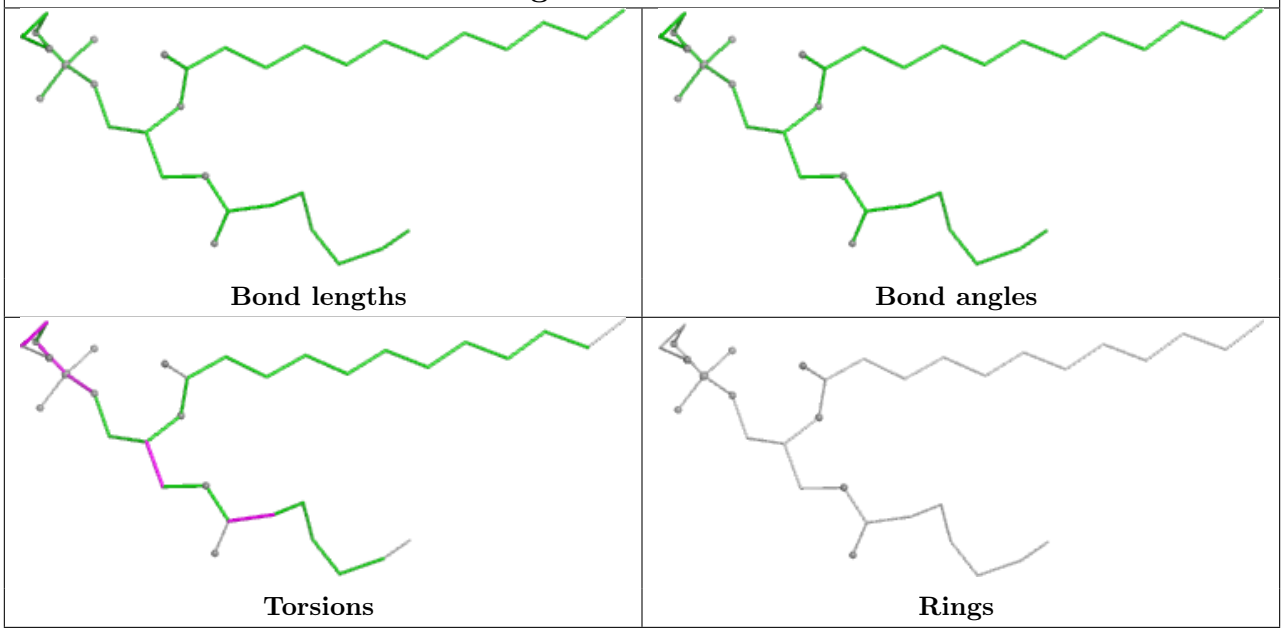
Ligand 3PE K1 201



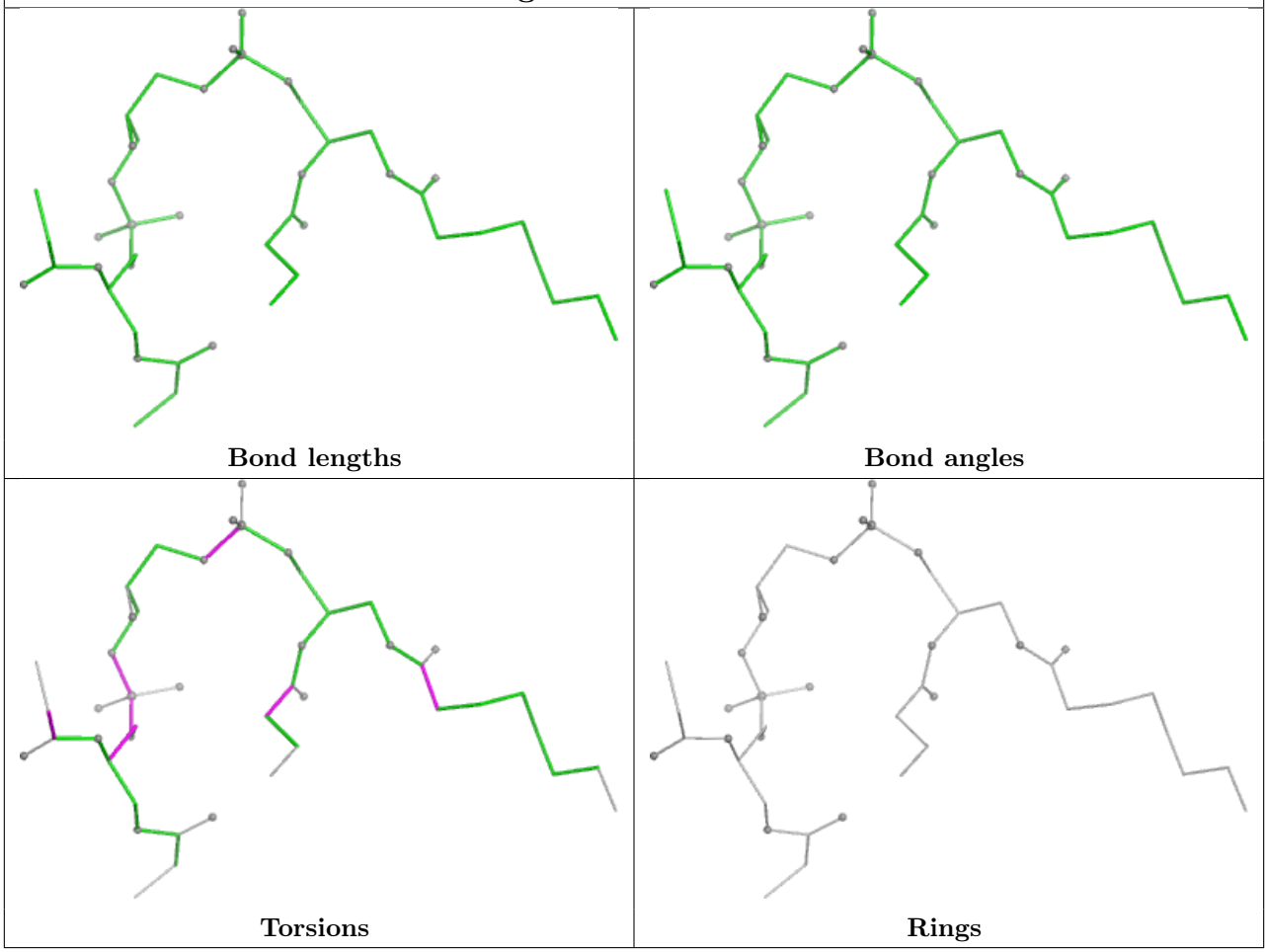
Ligand 3PE L 501



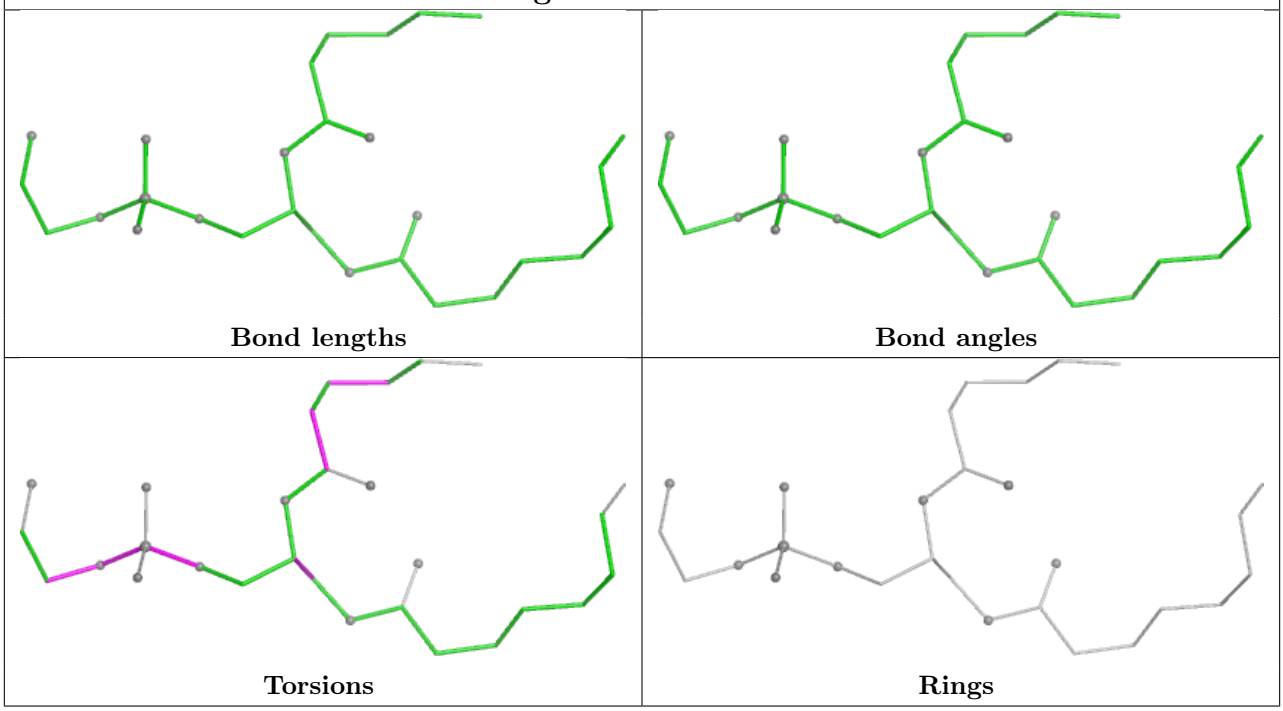
Ligand 3PE E 203



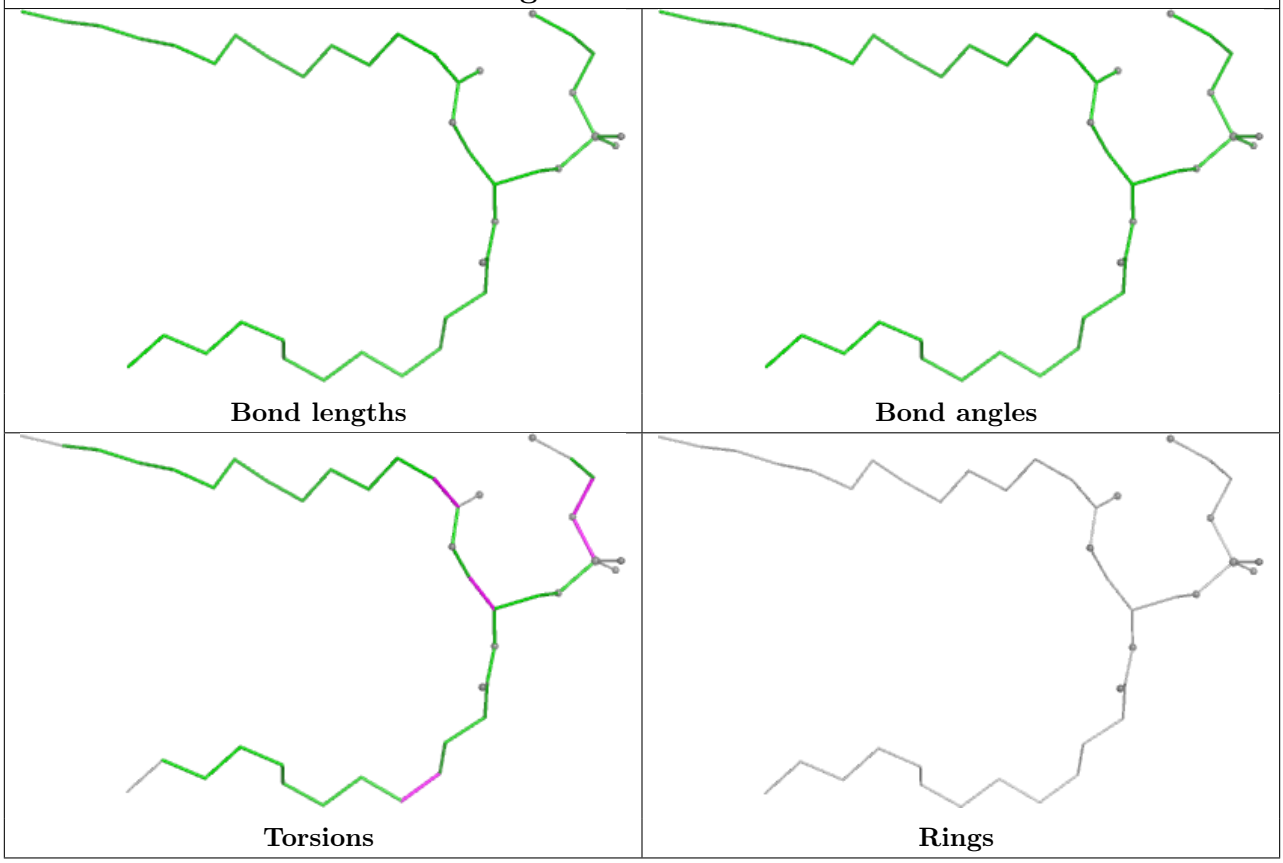
Ligand CDL A 502



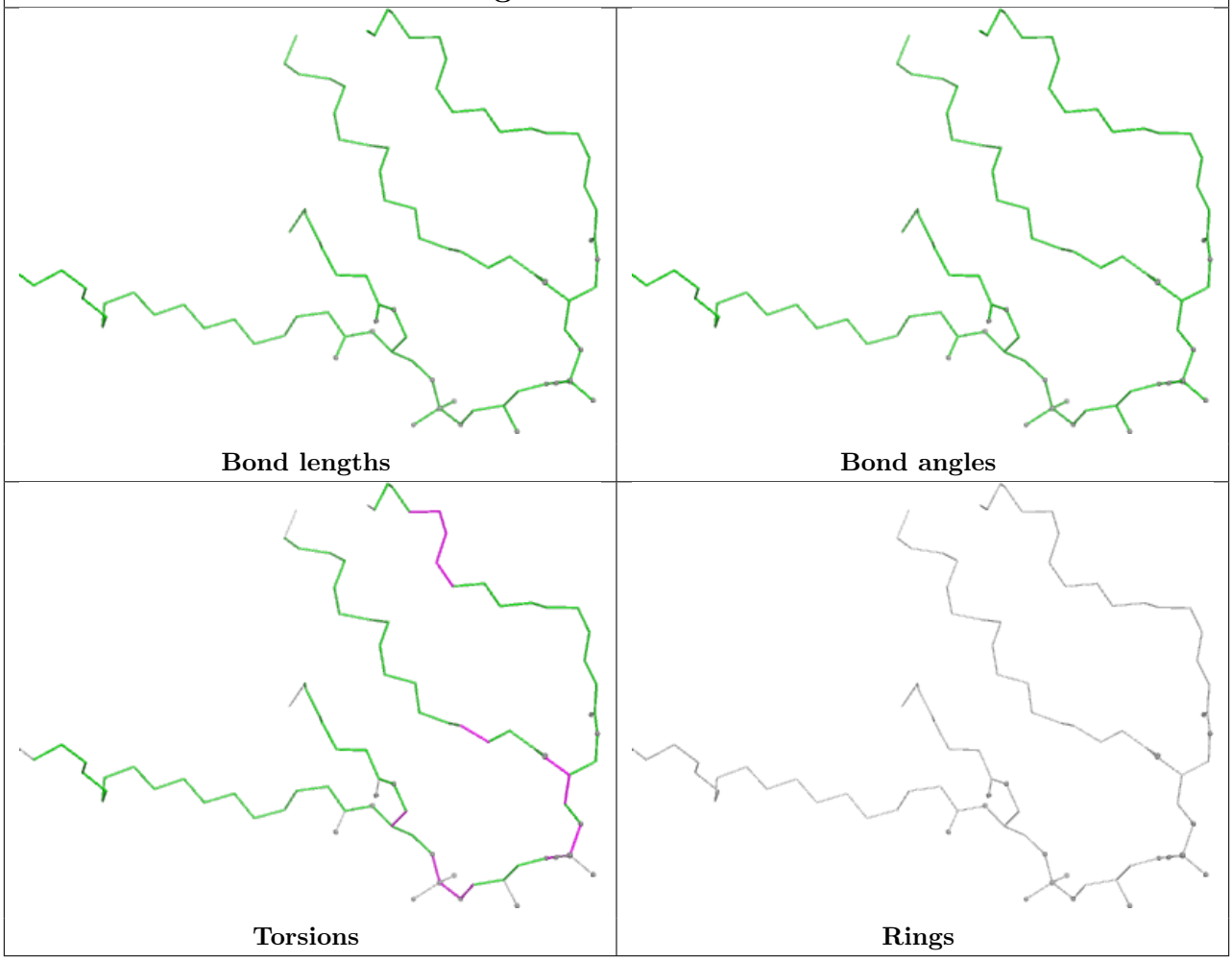
Ligand 3PE o 302



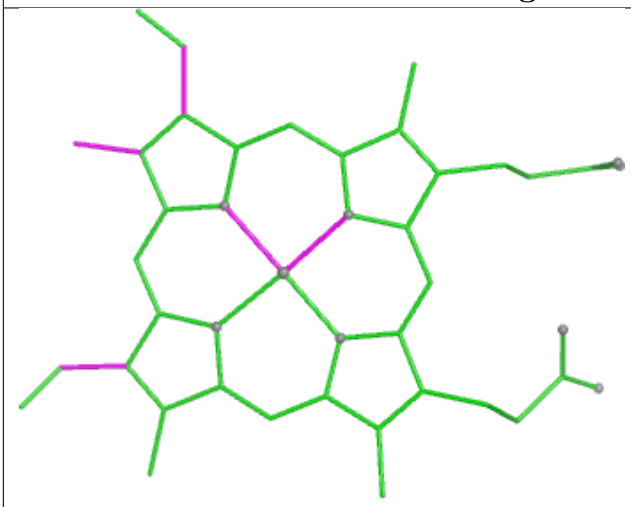
Ligand 3PE Y1 403



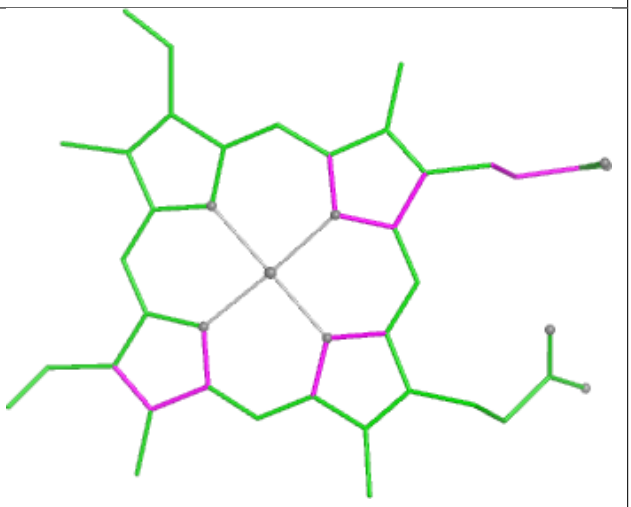
Ligand CDL N1 401



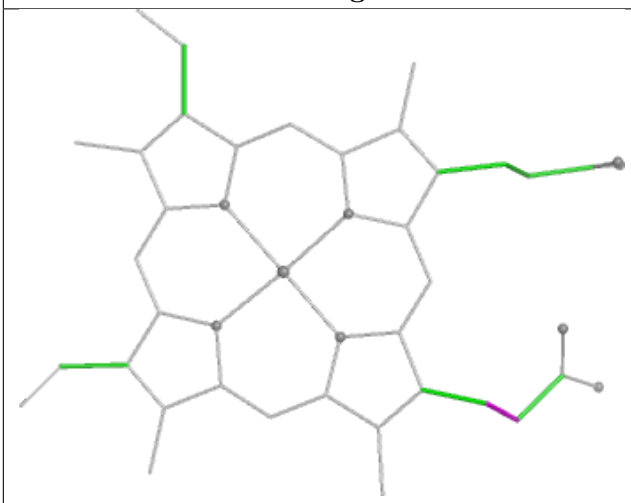
Ligand HEM C 401



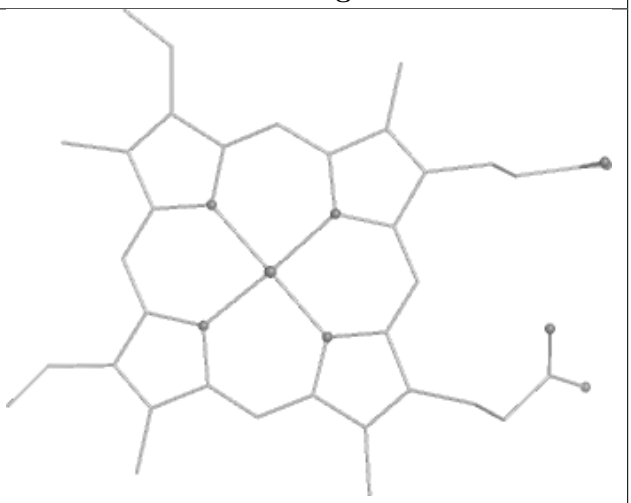
Bond lengths



Bond angles



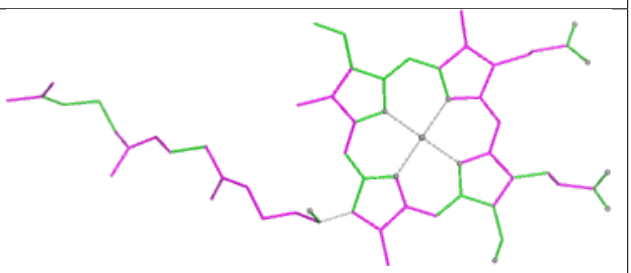
Torsions



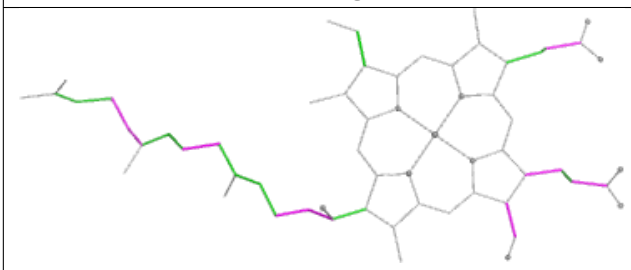
Rings

Ligand HEA n 603

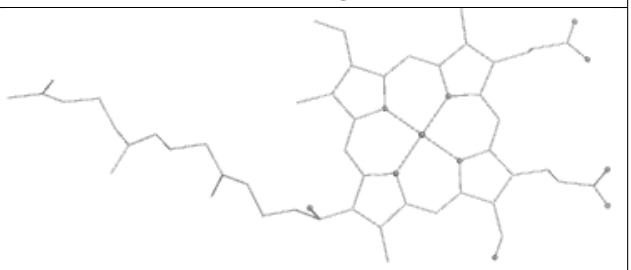
Bond lengths



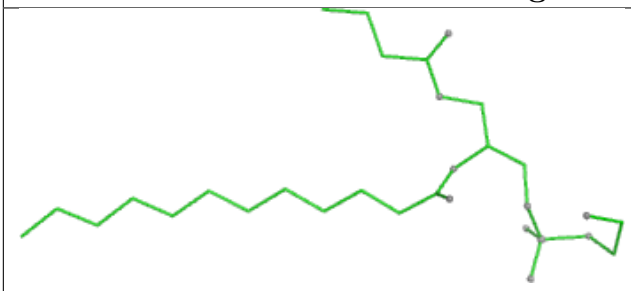
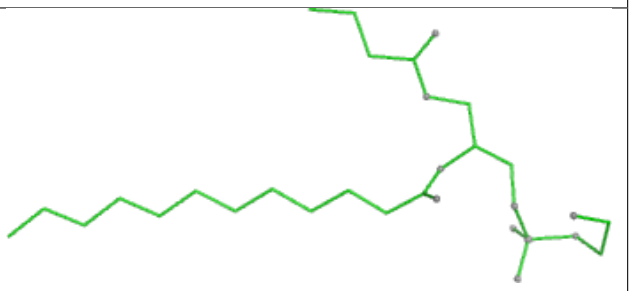
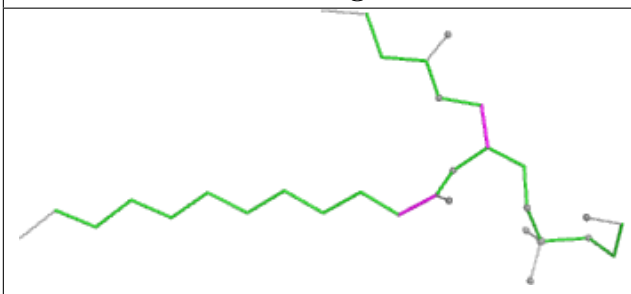
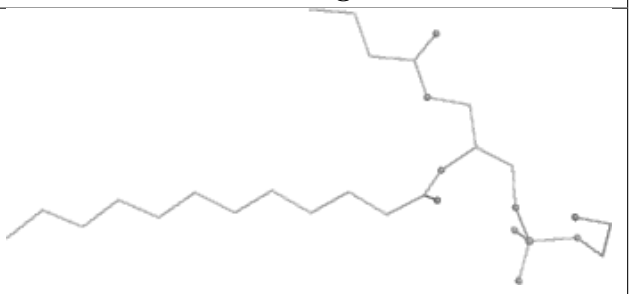
Bond angles



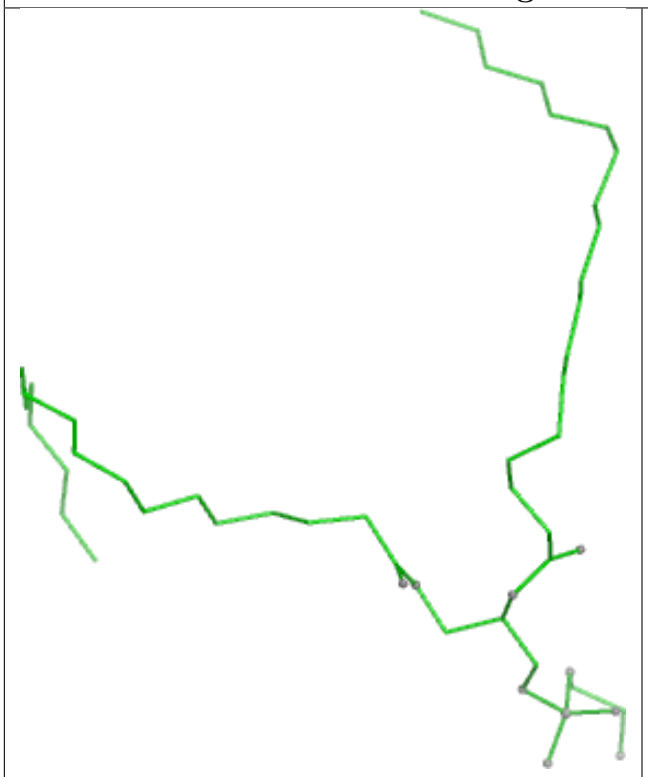
Torsions



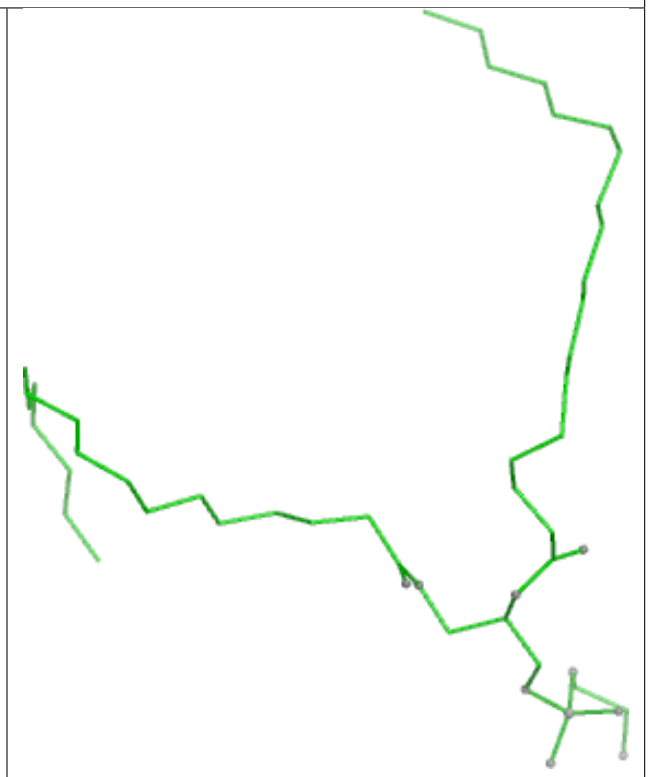
Rings

Ligand 3PE C 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE M1 502

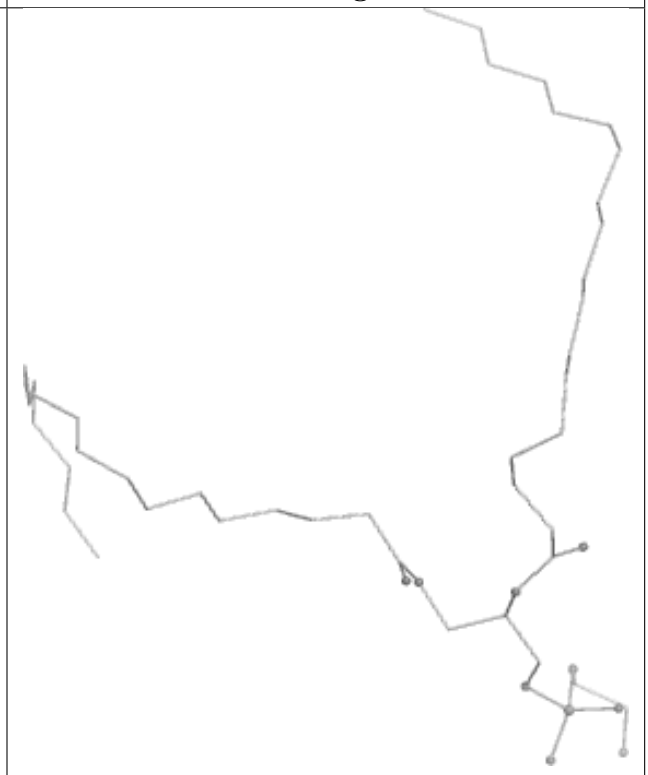


Bond lengths



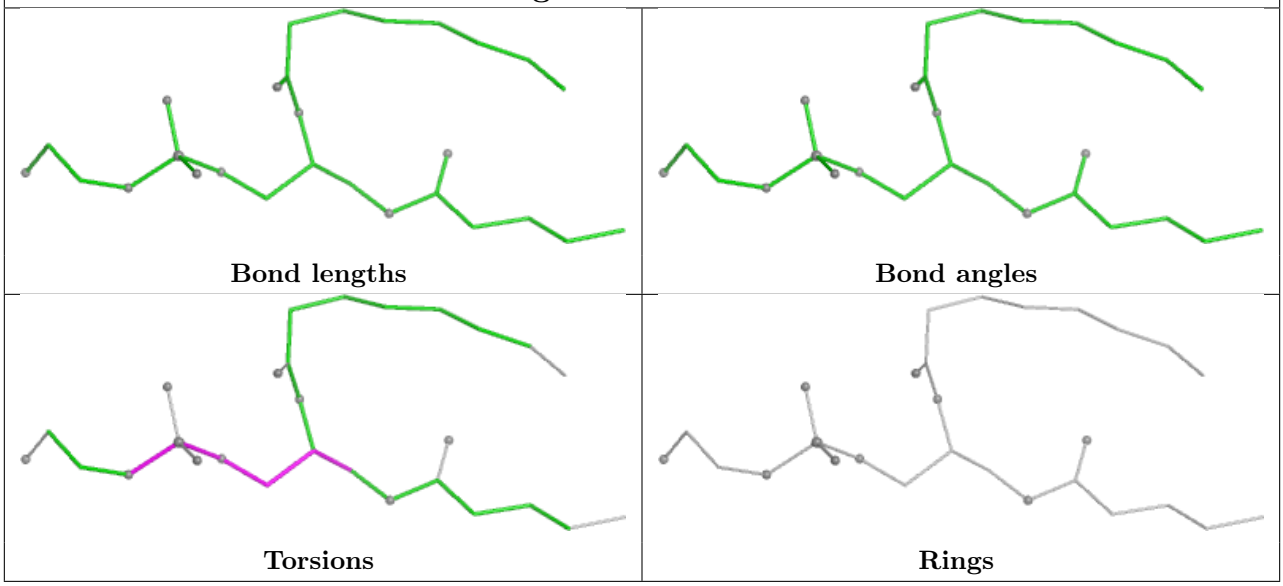
Bond angles

Torsions

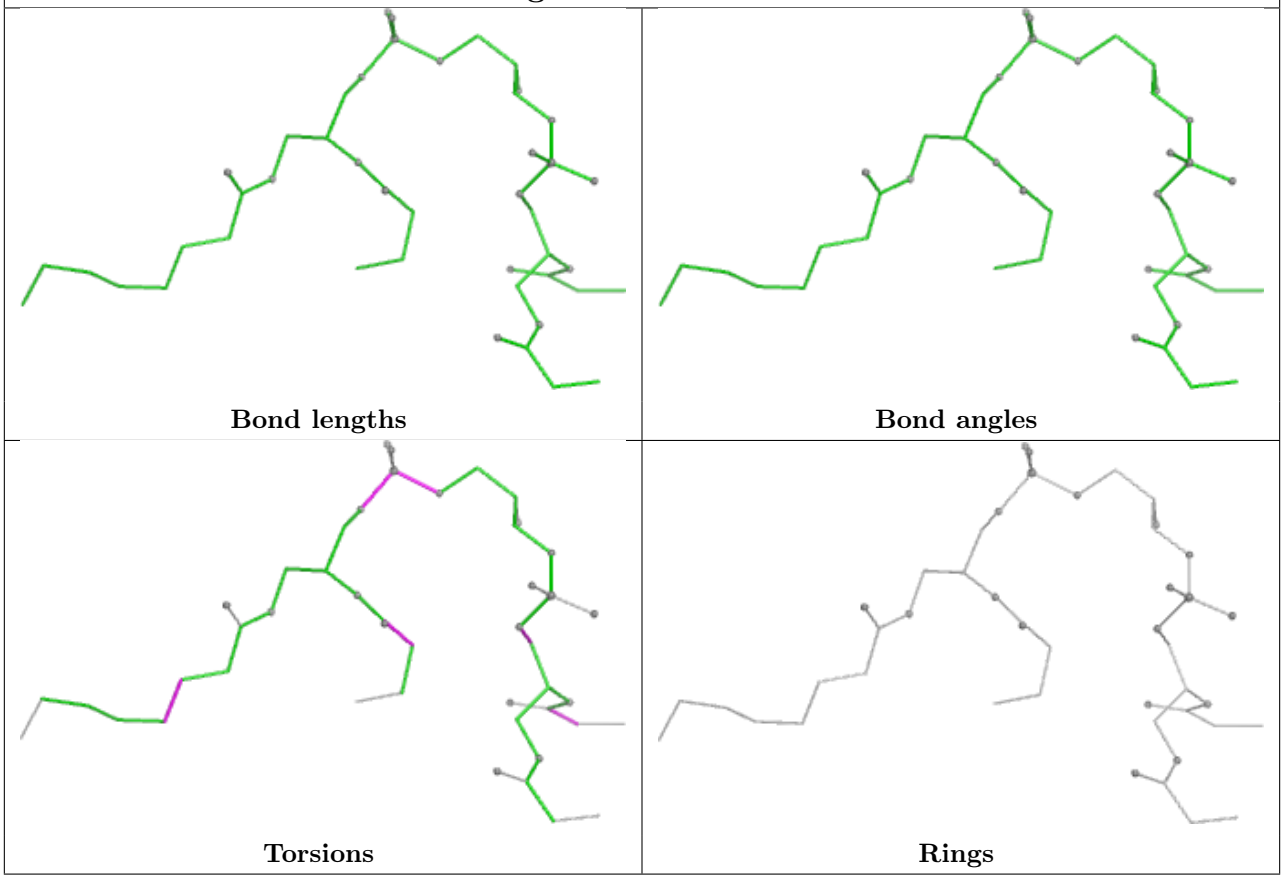


Rings

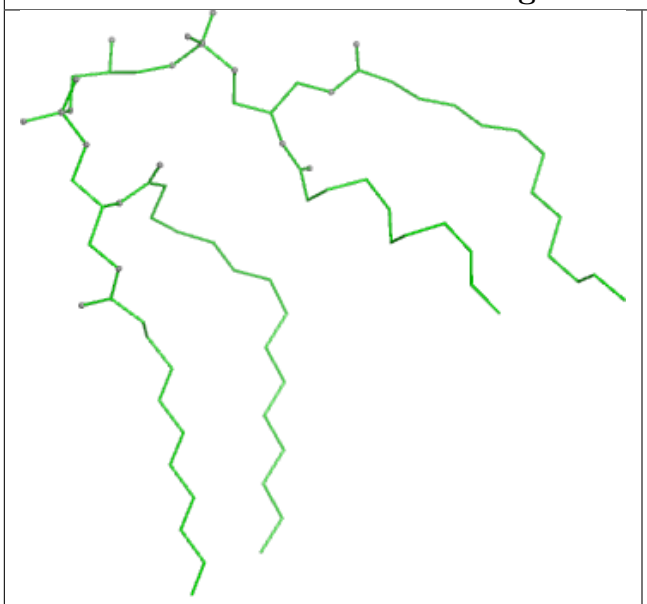
Ligand 3PE n 606



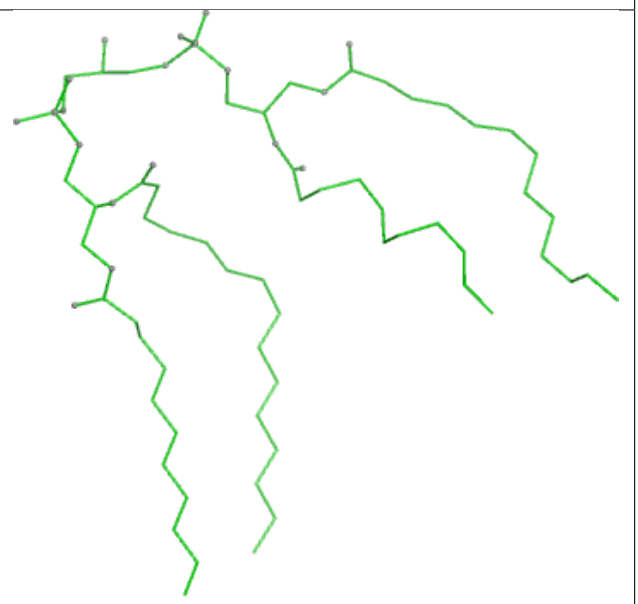
Ligand CDL L 502



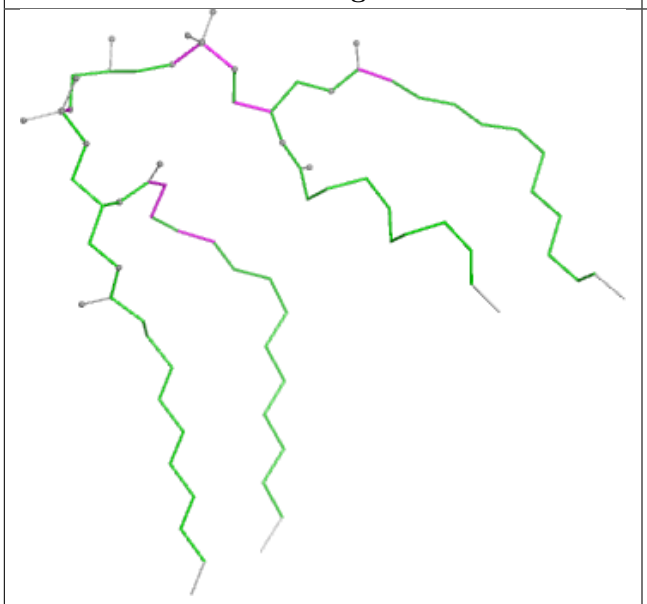
Ligand CDL L1 702



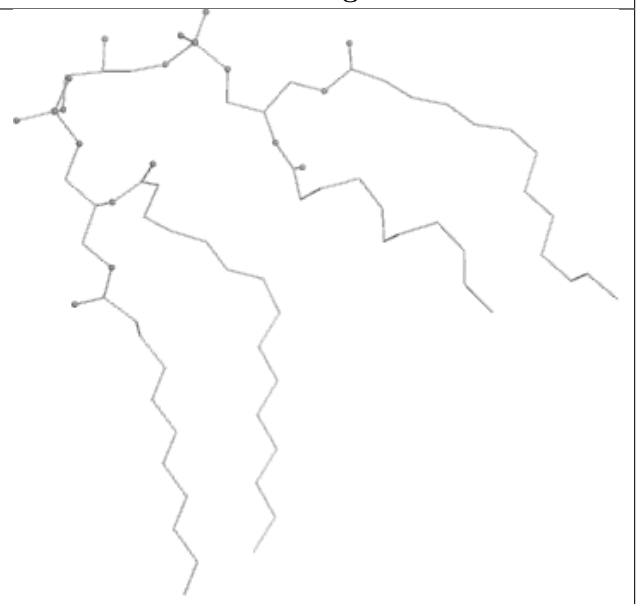
Bond lengths



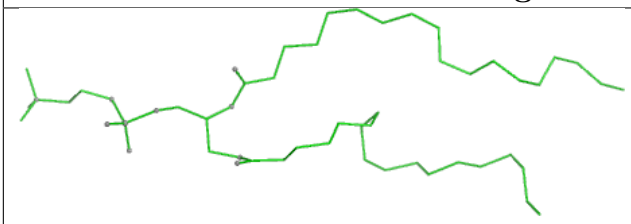
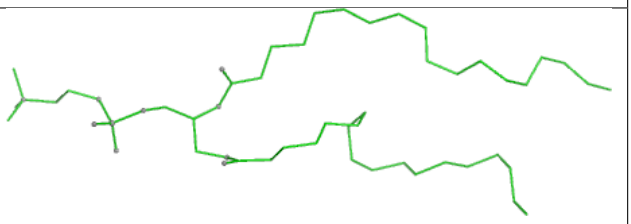
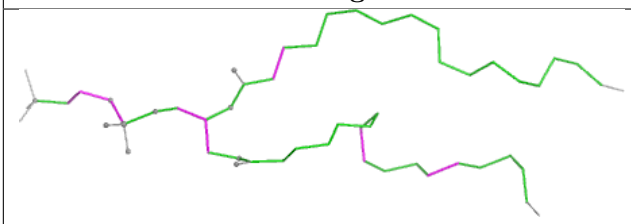
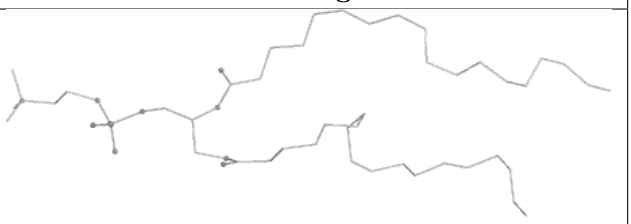
Bond angles



Torsions



Rings

Ligand PC1 M1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

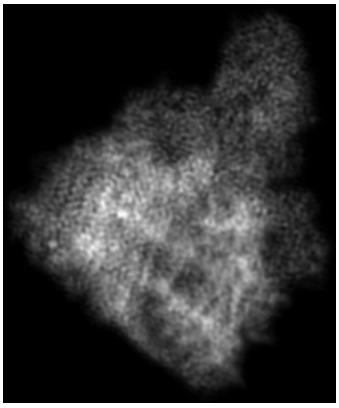
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17989. These allow visual inspection of the internal detail of the map and identification of artifacts.

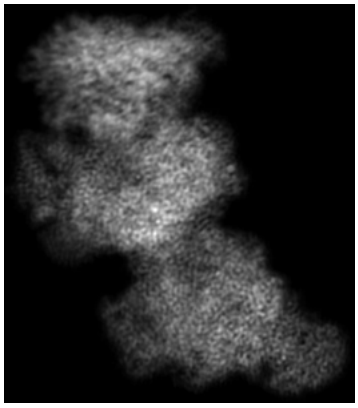
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

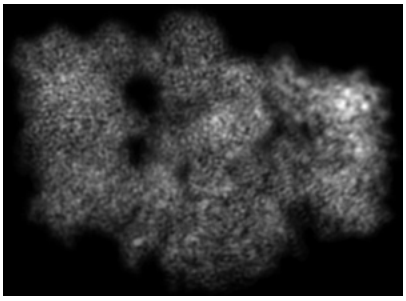
6.1.1 Primary map



X



Y



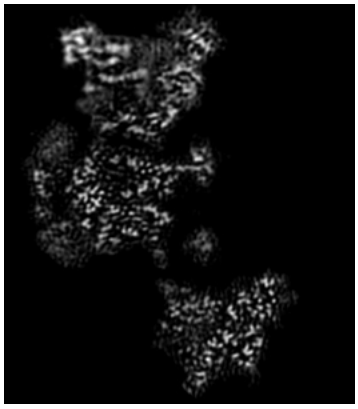
Z

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

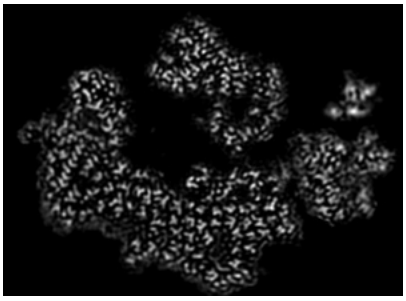
6.2 Central slices (i)

6.2.1 Primary map

X Index: 141



Y Index: 103

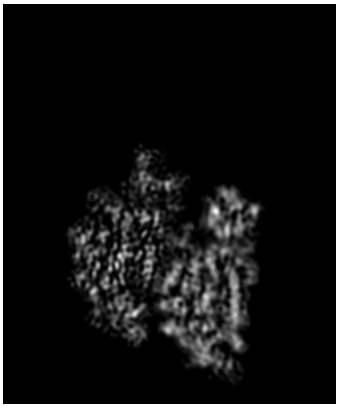


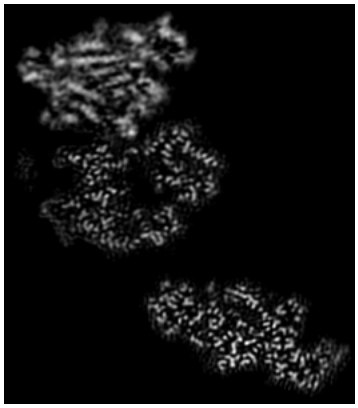
Z Index: 124

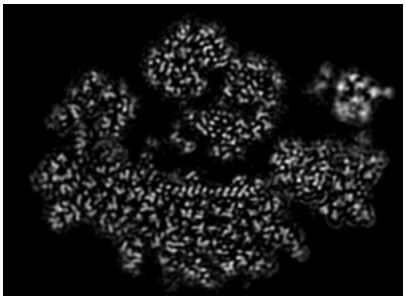
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 243

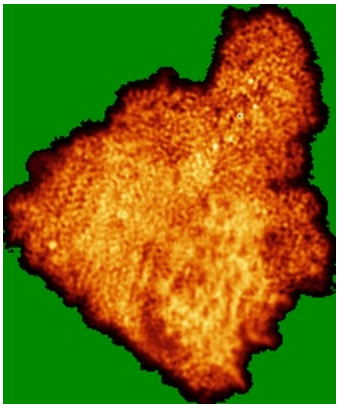

Y Index: 143

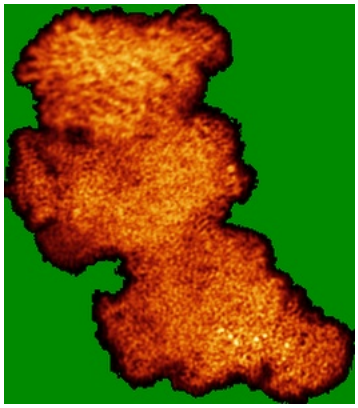

Z Index: 115

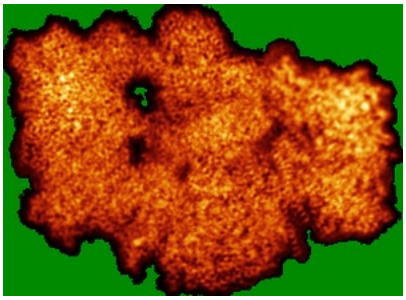
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

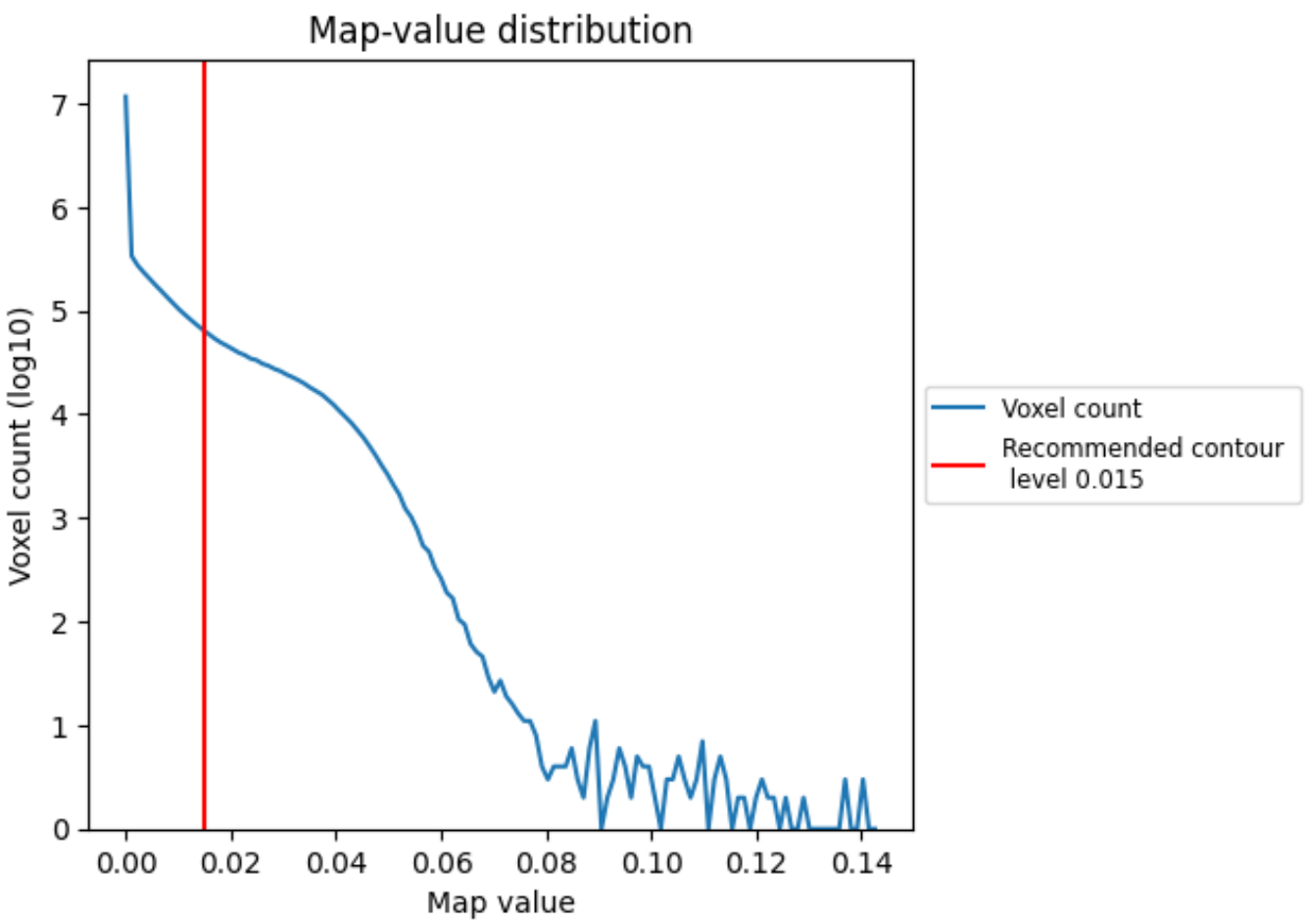
6.6 Mask visualisation (i)

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

7 Map analysis (i)

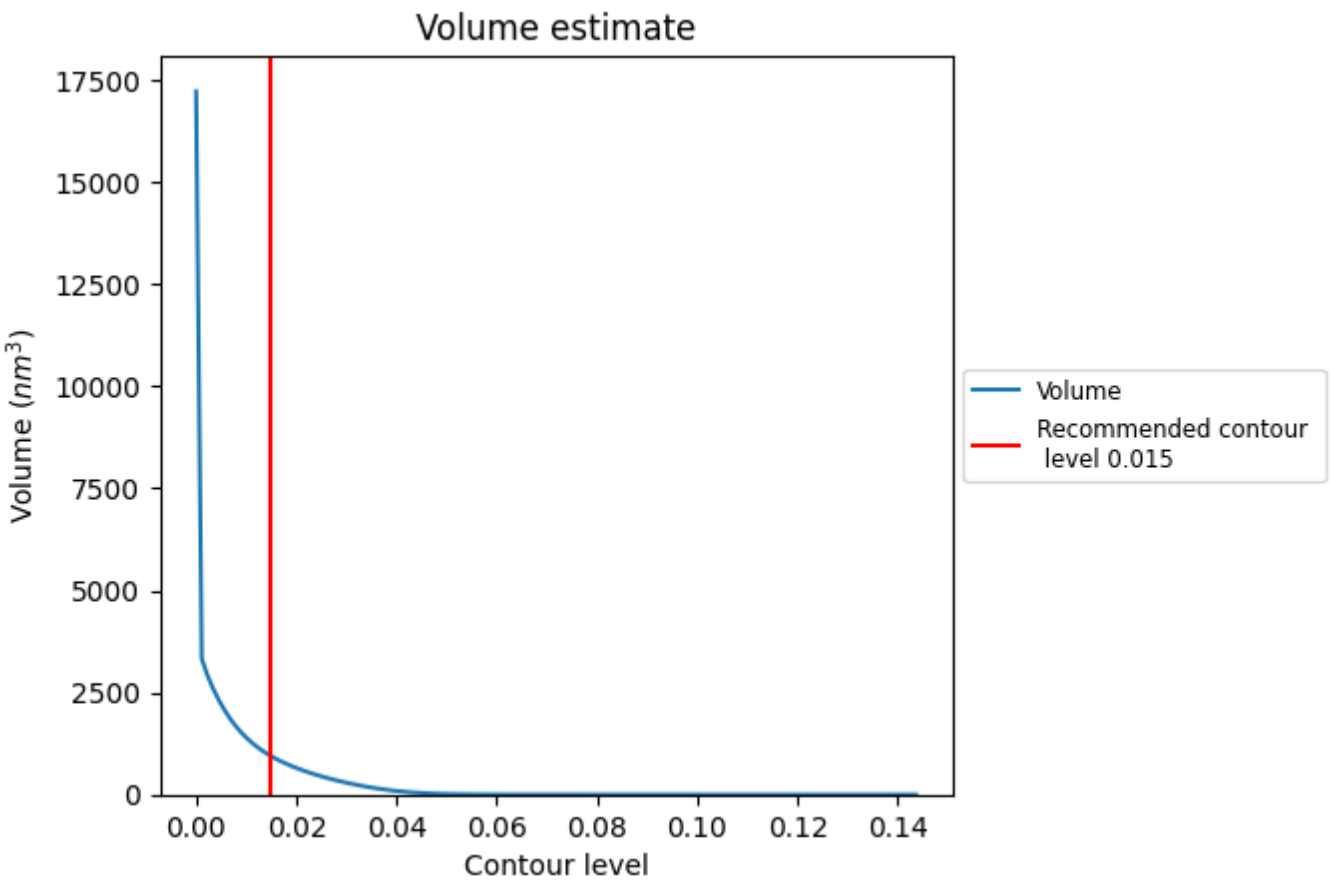
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 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.

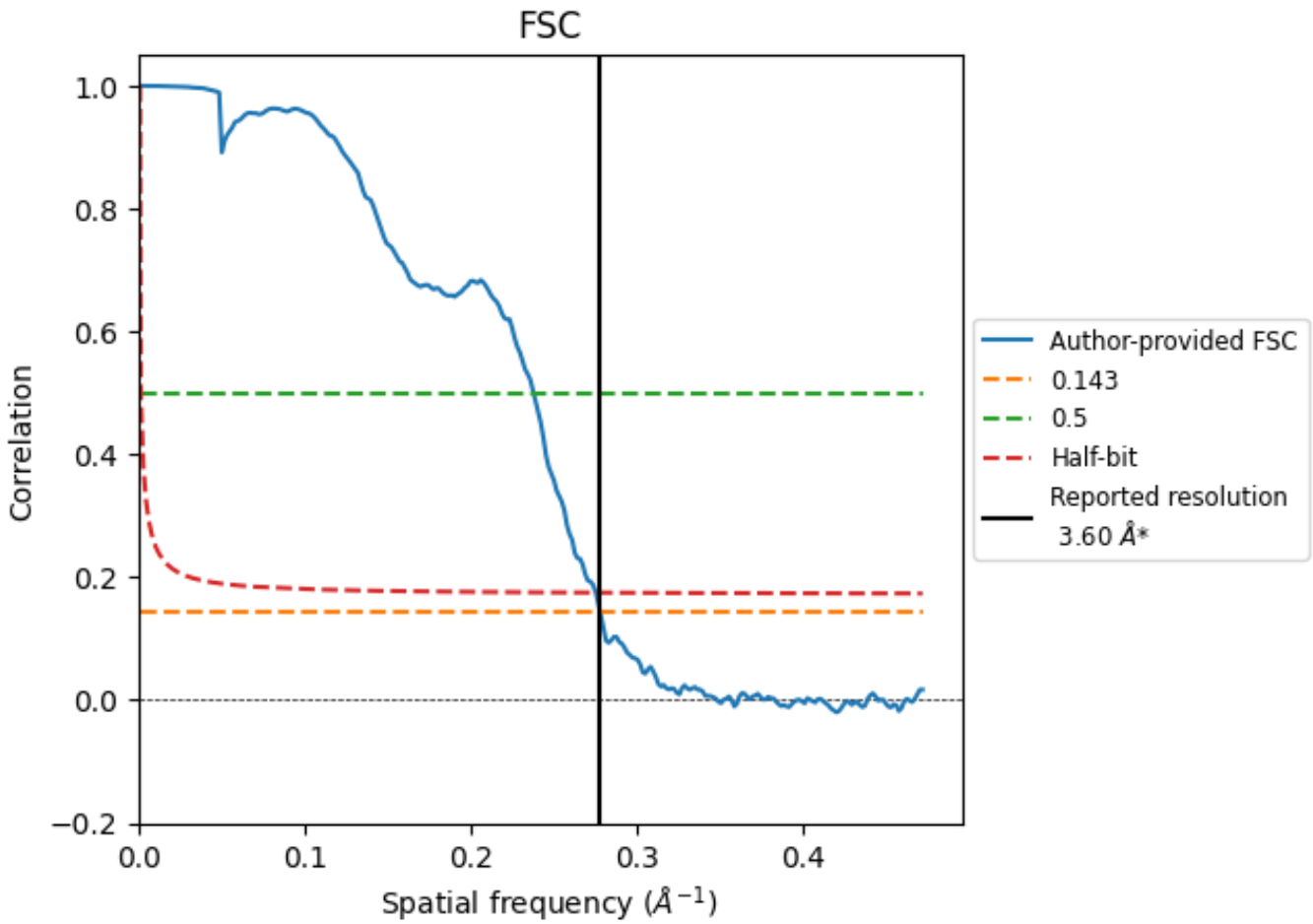
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

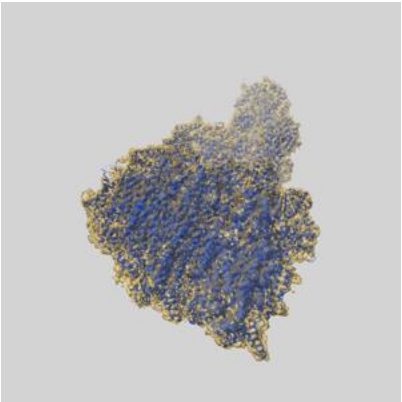
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.21	3.63
Unmasked-calculated*	-	-	-

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

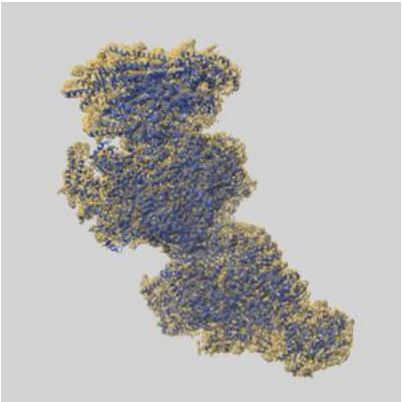
9 Map-model fit (i)

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.

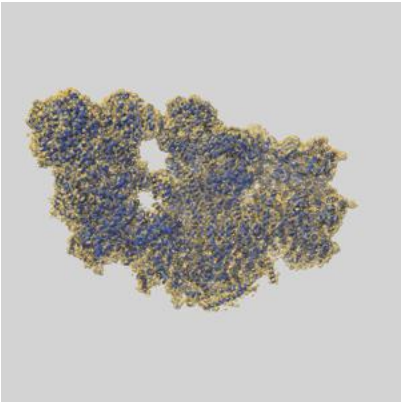
9.1 Map-model overlay (i)



X



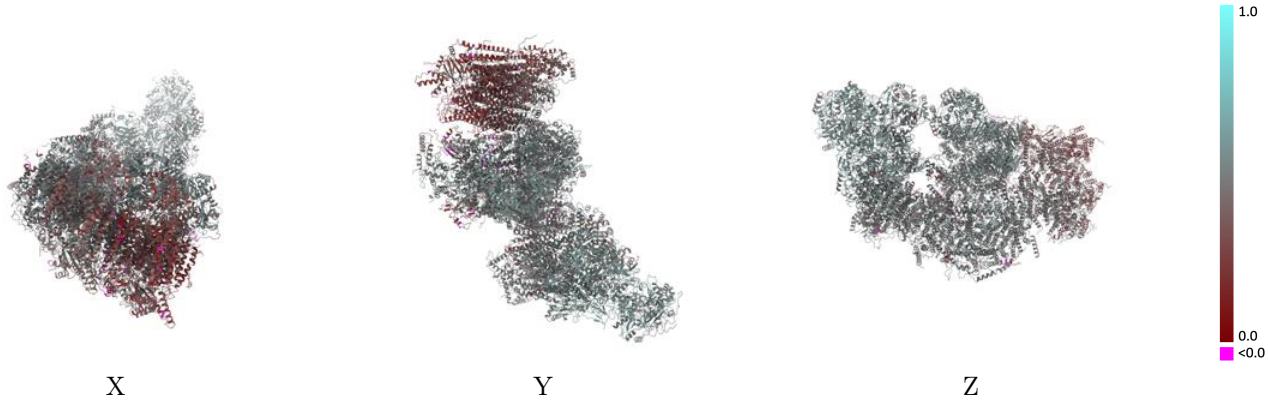
Y



Z

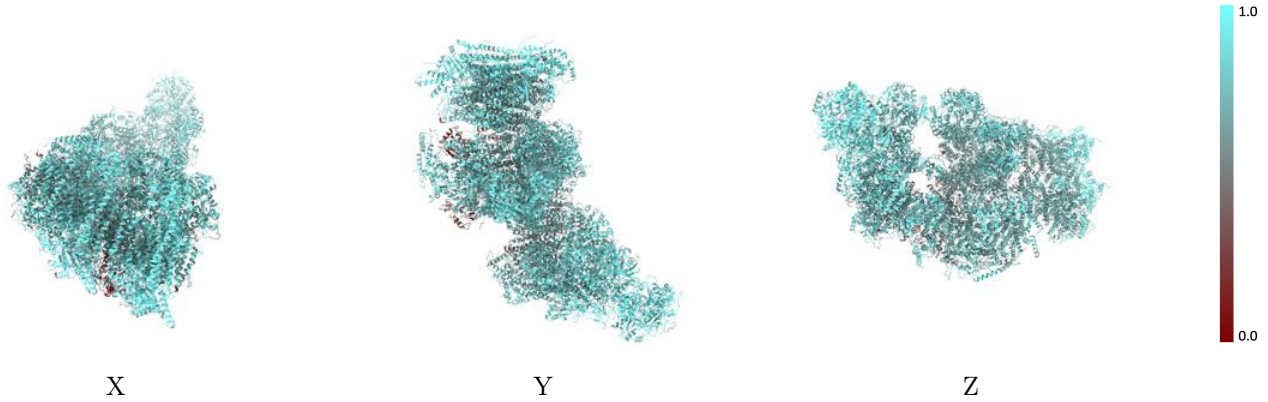
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



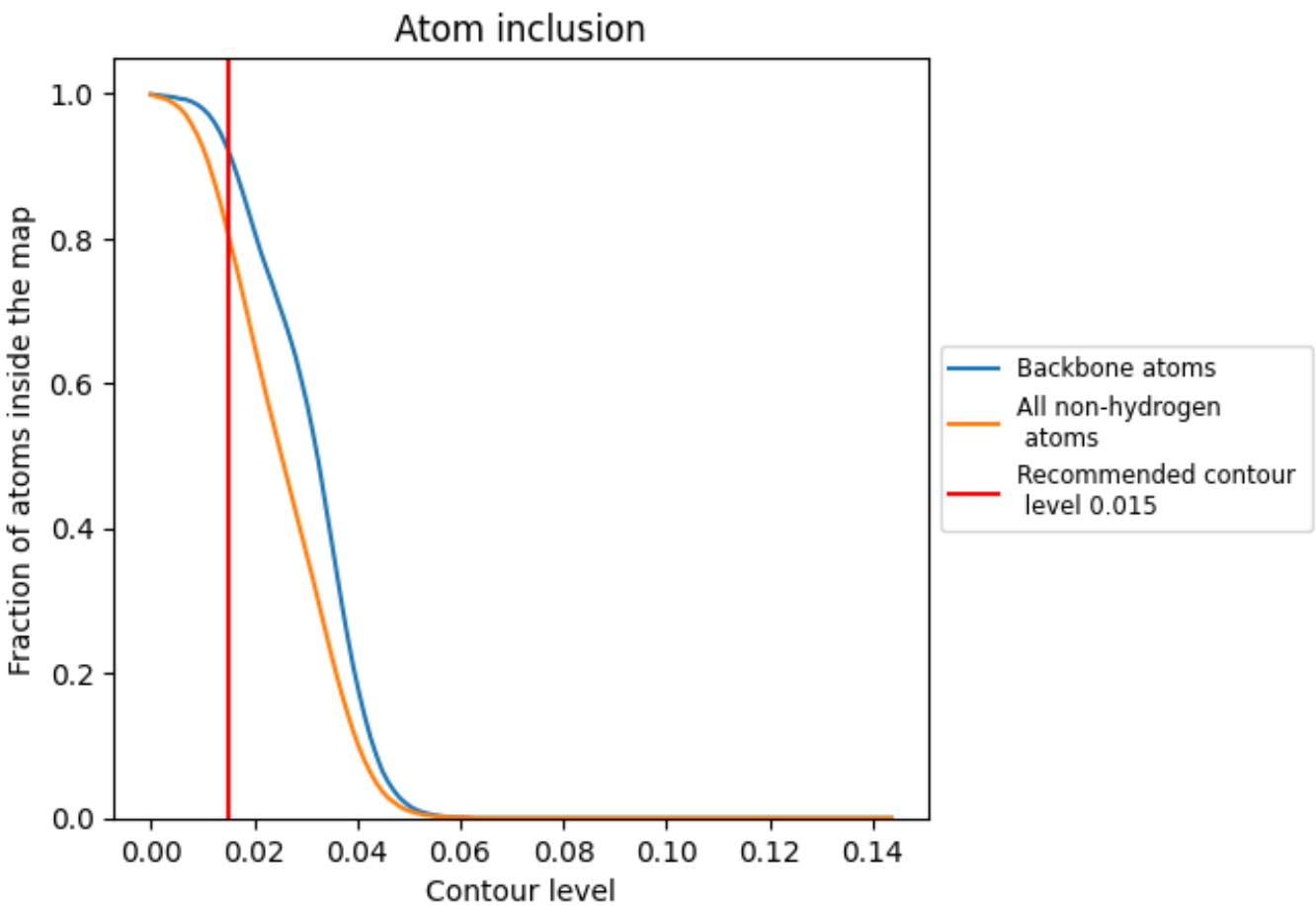
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



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 (i)

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	0.8060	0.4640
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	0.3560
F	0.8000	0.5020
G	0.7650	0.4990
H	0.7730	0.4440
H1	0.7390	0.4660
I	0.6610	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	0.6460	0.4590
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	0.7920	0.2650
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	0.7180	0.2200
m1	0.7540	0.4750
n	0.8060	0.4290
n1	0.8350	0.5020
o	0.8340	0.4160

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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	0.6790	0.3260
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	0.6440	0.2910