wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 01:29 pm GMT

PDB ID	:	6YNZ
EMDB ID	:	EMD-10861
Title	:	Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase - F1Fo composite tetramer model
Authors	:	Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on	:	2020-04-14
Resolution	:	3.10 Å(reported)

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

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

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

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

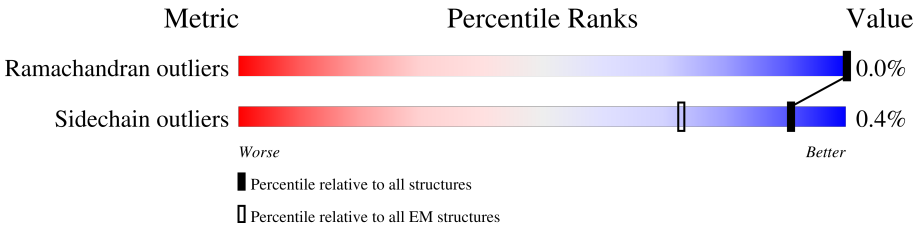
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	446	97% .
1	A3	446	97% .
1	a	446	97% .
1	a3	446	97% .
2	B	381	42% 93% 7%
2	B3	381	50% 93% 7%
2	b	381	50% 93% 7%
2	b3	381	42% 93% 7%
3	D	234	23% 88% 12%

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Mol	Chain	Length	Quality of chain
3	D3	234	30% 88% 12%
3	d	234	29% 88% 12%
3	d3	234	23% 88% 12%
4	F	204	98%
4	F3	204	98%
4	f	204	12% 97%
4	f3	204	8% 97%
5	I	209	99%
5	I3	209	99%
5	i	209	99%
5	i3	209	100%
6	K	179	100%
6	K3	179	100%
6	k	179	99%
6	k3	179	99%
7	C	100	95%
7	C3	100	95%
7	c	100	95%
7	c3	100	95%
8	G	286	89% 10%
8	G3	286	89% 10%
8	g	286	89% 10%
8	g3	286	89% 10%
9	H	268	86% 14%
9	H3	268	12% 86% 14%

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Mol	Chain	Length	Quality of chain
9	h	268	13% 86% 14%
9	h3	268	7% 86% 14%
10	J	273	98%
10	J3	273	98%
10	j	273	99%
10	j3	273	99%
11	L	247	99%
11	L3	247	99%
11	l	247	99%
11	l3	247	99%
12	M	221	100%
12	M3	221	100%
12	m	221	100%
12	m3	221	100%
13	N	179	66% 34%
13	N3	179	66% 34%
13	n	179	66% 34%
13	n3	179	66% 34%
14	O	154	64% 36%
14	O3	154	64% 36%
14	o	154	64% 36%
14	o3	154	64% 36%
15	P	152	9% 99%
15	P3	152	99%
15	p	152	99%

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Mol	Chain	Length	Quality of chain
15	p3	152	8% 99%
16	Q	152	71% 29%
16	Q3	152	9% 71% 29%
16	q	152	8% 71% 29%
16	q3	152	71% 29%
17	R	149	93% 6%
17	R3	149	7% 93% 6%
17	r	149	8% 97%
17	r3	149	97%
18	S	145	15% 86% 14%
18	S3	145	19% 86% 14%
18	s	145	31% 84% 14%
18	s3	145	17% 84% 14%
19	E	480	10% 86% 13%
19	E3	480	19% 86% 13%
19	e	480	20% 87% 13%
19	e3	480	10% 87% 13%
20	i1	108	60% 63% 37%
20	i2	108	56% 59% 41%
20	i4	108	56% 63% 37%
20	i5	108	57% 59% 41%
21	t	460	27% 79% 21%
21	t3	460	19% 79% 21%
22	G1	219	86% 86% 14%
22	G2	219	86% 86% 14%

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Mol	Chain	Length	Quality of chain
22	G4	219	86% 86% 14%
22	G5	219	86% 86% 14%
23	g1	299	75% 91% 8%
23	g2	299	71% 91% 8%
23	g4	299	70% 91% 8%
23	g5	299	74% 91% 8%
24	A1	546	80% 93% 6%
24	A2	546	90% 93% 6%
24	A4	546	89% 93% 6%
24	A5	546	79% 93% 6%
24	B1	546	86% 93% 6%
24	B2	546	91% 93% 6%
24	B4	546	91% 93% 6%
24	B5	546	85% 93% 6%
24	C1	546	93% 94% 6%
24	C2	546	93% 94% 6%
24	C4	546	93% 94% 6%
24	C5	546	93% 94% 6%
25	D1	497	94% 94% 5%
25	D2	497	93% 94% 5%
25	D4	497	93% 94% 5%
25	D5	497	94% 94% 5%
25	E1	497	85% 94% 5%
25	E2	497	94% 94% 5%
25	E4	497	94% 94% 5%

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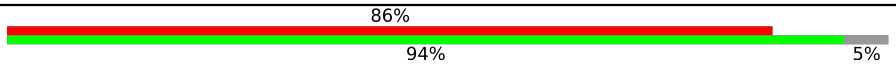
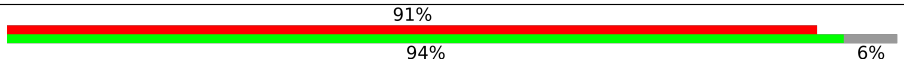
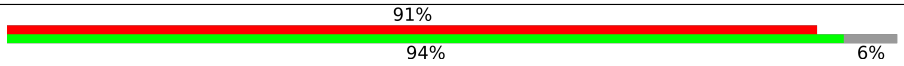
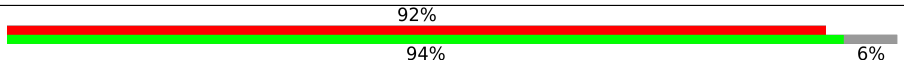
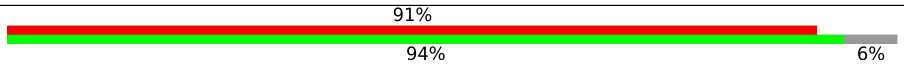
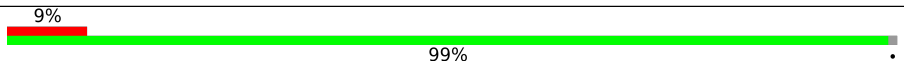
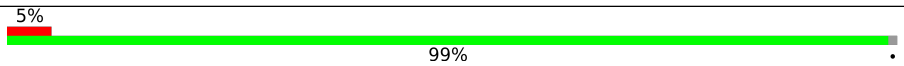
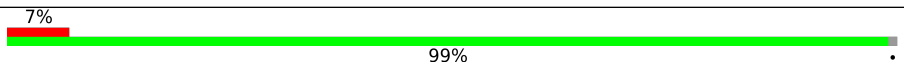
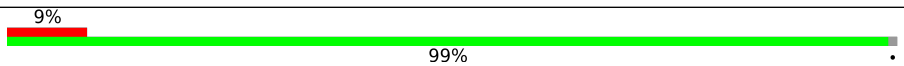
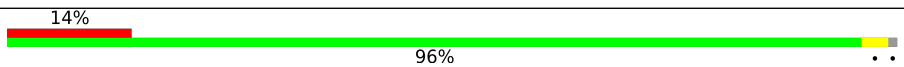
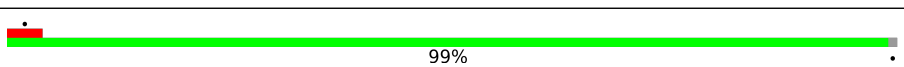
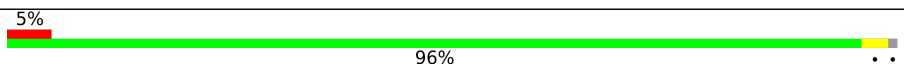
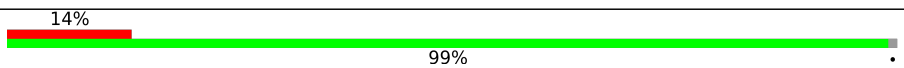
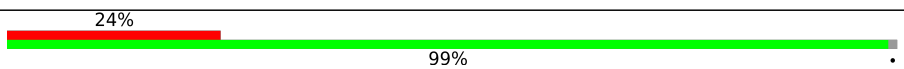
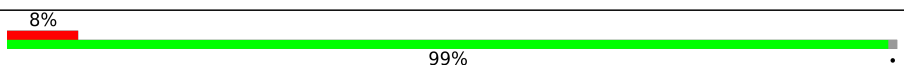
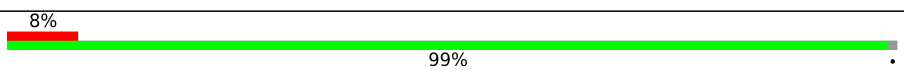
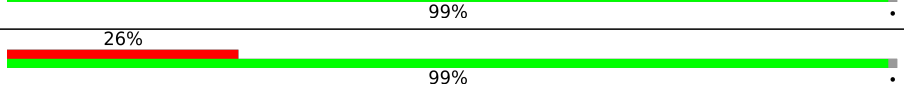
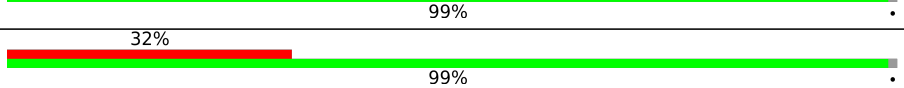
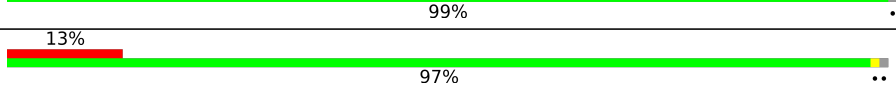
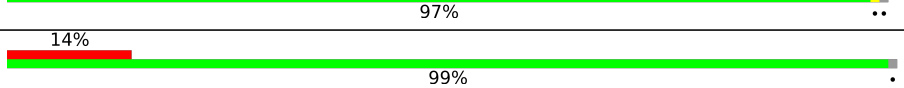
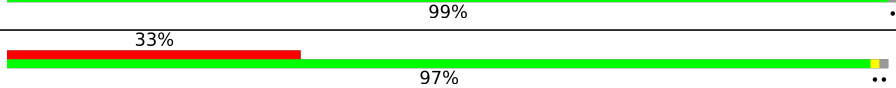
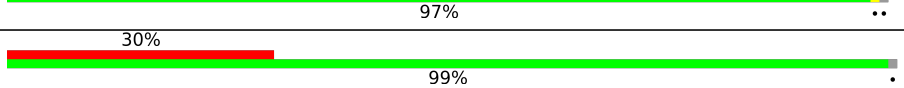
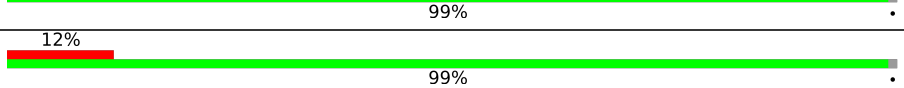
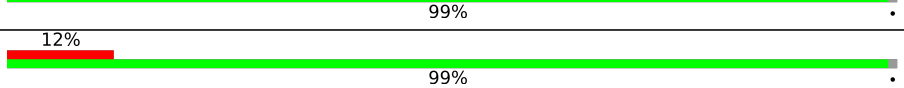
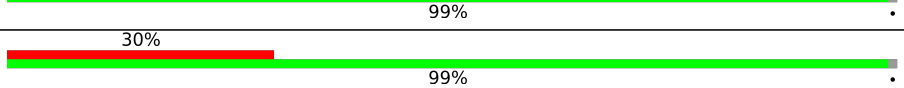
Mol	Chain	Length	Quality of chain
25	E5	497	
25	F1	497	
25	F2	497	
25	F4	497	
25	F5	497	
26	H1	76	
26	H2	76	
26	H4	76	
26	H5	76	
26	I1	76	
26	I2	76	
26	I4	76	
26	I5	76	
26	J1	76	
26	J2	76	
26	J4	76	
26	J5	76	
26	K1	76	
26	K2	76	
26	K4	76	
26	K5	76	
26	L1	76	
26	L2	76	
26	L4	76	
26	L5	76	

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Mol	Chain	Length	Quality of chain
26	M1	76	24% 99%
26	M2	76	9% 99%
26	M4	76	9% 99%
26	M5	76	24% 99%
26	N1	76	21% 99%
26	N2	76	11% 99%
26	N4	76	11% 99%
26	N5	76	20% 99%
26	O1	76	28% 99%
26	O2	76	12% 99%
26	O4	76	11% 99%
26	O5	76	22% 99%
26	P1	76	11% 99%
26	P2	76	12% 99%
26	P4	76	13% 99%
26	P5	76	12% 99%
26	Q1	76	9% 99%
26	Q2	76	5% 99%
26	Q4	76	7% 99%
26	Q5	76	12% 99%
27	d1	158	51% 84% 15%
27	d2	158	45% 84% 15%
27	d4	158	47% 84% 15%
27	d5	158	51% 84% 15%
28	e1	71	73% 96%

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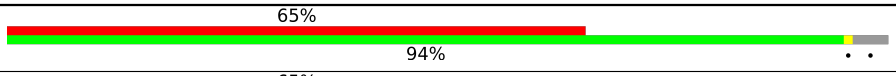
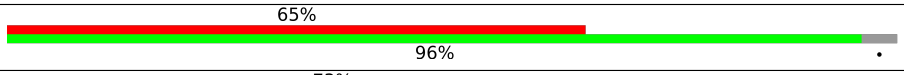
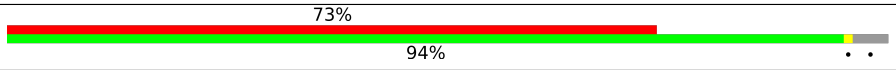
Mol	Chain	Length	Quality of chain
28	e2	71	
28	e4	71	
28	e5	71	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 571866 atoms, of which 287810 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 Ymf66.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		
1	a3	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A3	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B	354	Total	C	H	N	O	S	0	0
			5724	1845	2849	487	531	12		
2	b3	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B3	354	Total	C	H	N	O	S	0	0
			5724	1845	2849	487	531	12		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	d3	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D3	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		
4	f3	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F3	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3460	1121	1740	304	285	10		
5	i3	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I3	209	Total	C	H	N	O	S	0	0
			3460	1121	1740	304	285	10		

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		
6	k3	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K3	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called Ymf56.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	c	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	C	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	c3	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	C3	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	g3	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G3	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	h3	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H3	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	J	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	j3	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	J3	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	l	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	l3	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L3	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	m3	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M3	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	n3	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N3	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	o3	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
14	O3	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	p3	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P3	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		

- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	q3	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q3	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		
17	r3	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R3	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S	125	Total	C	H	N	O	S	0	0
			2039	652	1016	175	191	5		
18	s3	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S3	125	Total	C	H	N	O	S	0	0
			2039	652	1016	175	191	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	e3	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E3	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	i2	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i1	68	Total	C	H	N	O	S	0	0
			1167	368	582	103	113	1		
20	i5	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i4	68	Total	C	H	N	O	S	0	0
			1167	368	582	103	113	1		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	t	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		
21	t3	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		

- Molecule 22 is a protein called Oligomycin sensitivity-conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	G1	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G2	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G4	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G5	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		

- Molecule 23 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	g1	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g2	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g4	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g5	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		

- Molecule 24 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	C1	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B1	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A1	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C2	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B2	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A2	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C4	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B4	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A4	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C5	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		

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Mol	Chain	Residues	Atoms						AltConf	Trace
24	B5	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A5	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		

- Molecule 25 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F1	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F2	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D4	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F4	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E4	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D5	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F5	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E5	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		

- Molecule 26 is a protein called ATP synthase F0 subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	P1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	O1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	N1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	M1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	L1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	K1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	J1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	I1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	H1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	Q1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	P2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	O2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	N2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	M2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	L2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	K2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	J2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	I2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	H2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	Q2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	P4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	O4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	N4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	M4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	L4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	K4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	J4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	I4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	H4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	Q4	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	P5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	O5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	N5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	M5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	L5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	K5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	J5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	I5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	H5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	Q5	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

- Molecule 27 is a protein called subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d1	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		
27	d2	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		
27	d4	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

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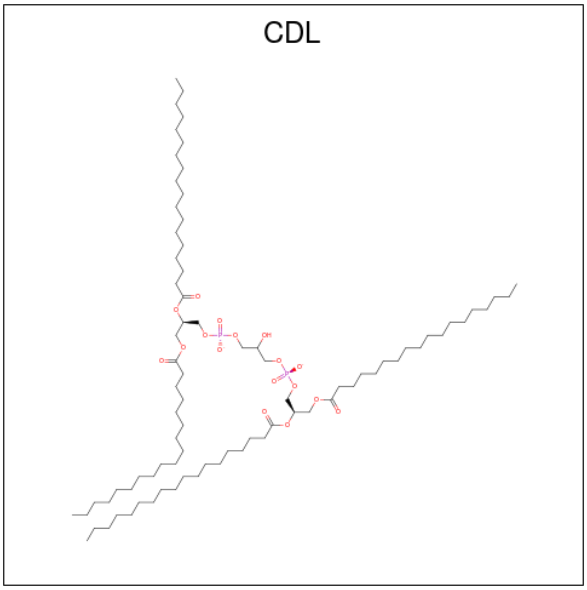
Mol	Chain	Residues	Atoms						AltConf	Trace
27	d5	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

- Molecule 28 is a protein called subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e1	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e2	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e4	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e5	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		

- Molecule 29 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	f	1	Total	C	H	O	P	0
			768	243	468	51	6	

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Mol	Chain	Residues	Atoms					AltConf
29	f	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	i	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	g	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	l	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	l	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	p	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	r	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	A	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	B	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	B	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	B	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	B	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	F	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	F	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	I	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	I	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	K	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	K	1	Total	C	H	O	P	0
			512	162	312	34	4	

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Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	J	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	L	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	L	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	P	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	a3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	a3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	b3	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f3	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	f3	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	f3	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	i3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	i3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	k3	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	g3	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	j3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	j3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	l3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	l3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	p3	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	A3	1	Total	C	H	O	P	0
			256	81	156	17	2	

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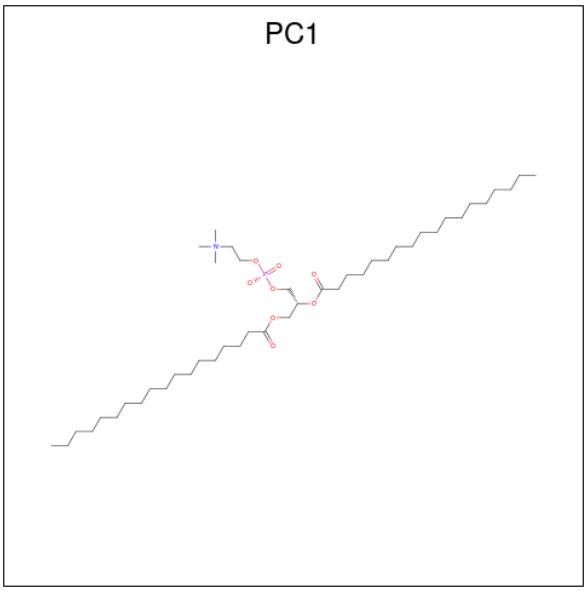
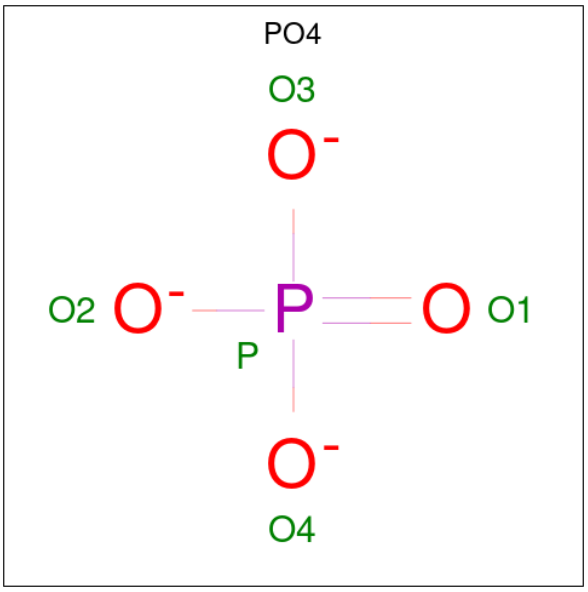
Mol	Chain	Residues	Atoms					AltConf
29	B3	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	B3	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	B3	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	B3	1	Total	C	H	O	P	0
			1024	324	624	68	8	
29	F3	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	I3	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	I3	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	I3	1	Total	C	H	O	P	0
			768	243	468	51	6	
29	K3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	K3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	J3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	J3	1	Total	C	H	O	P	0
			512	162	312	34	4	
29	L3	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	P3	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



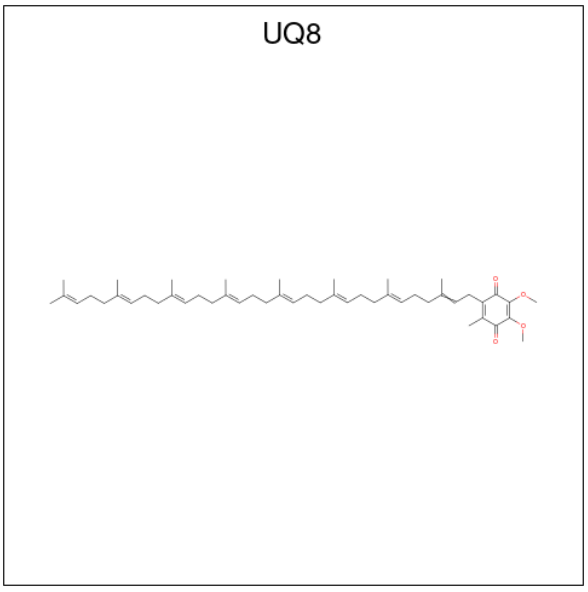
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	g	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	G	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	d3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g3	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	g3	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	D3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G3	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
30	G3	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	

- Molecule 31 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



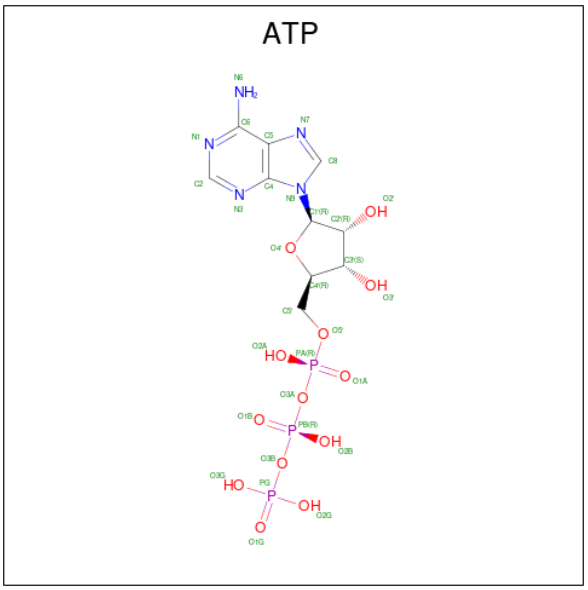
Mol	Chain	Residues	Atoms	AltConf
31	f	1	Total O P 5 4 1	0
31	F	1	Total O P 5 4 1	0
31	f3	1	Total O P 5 4 1	0
31	F3	1	Total O P 5 4 1	0

- Molecule 32 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
32	i	1	Total	C	H	O	0
			127	49	74	4	
32	I	1	Total	C	H	O	0
			127	49	74	4	
32	i3	1	Total	C	H	O	0
			127	49	74	4	
32	I3	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
33	g	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

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Mol	Chain	Residues	Atoms						AltConf
33	A2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	g3	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G3	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	
34	C1	1	Total	Mg	0
			1	1	
34	D1	1	Total	Mg	0
			1	1	
34	B1	1	Total	Mg	0
			1	1	
34	A1	1	Total	Mg	0
			1	1	
34	E1	1	Total	Mg	0
			1	1	
34	C2	1	Total	Mg	0
			1	1	
34	D2	1	Total	Mg	0
			1	1	
34	B2	1	Total	Mg	0
			1	1	

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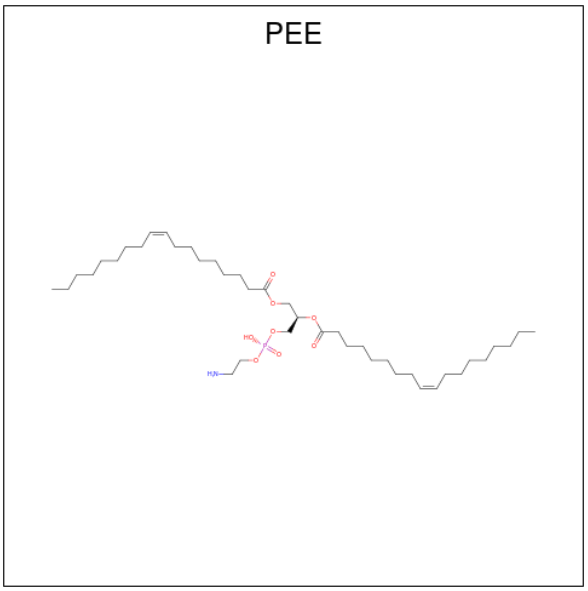
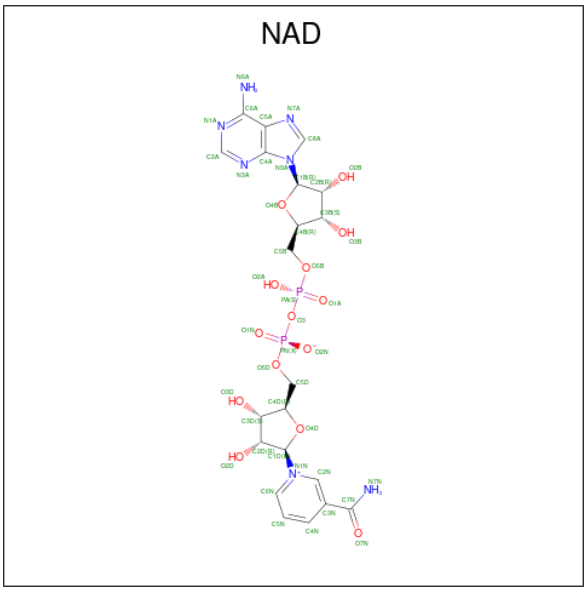
Mol	Chain	Residues	Atoms	AltConf
34	A2	1	Total Mg 1 1	0
34	E2	1	Total Mg 1 1	0
34	g3	1	Total Mg 1 1	0
34	G3	1	Total Mg 1 1	0
34	C4	1	Total Mg 1 1	0
34	D4	1	Total Mg 1 1	0
34	B4	1	Total Mg 1 1	0
34	A4	1	Total Mg 1 1	0
34	E4	1	Total Mg 1 1	0
34	C5	1	Total Mg 1 1	0
34	D5	1	Total Mg 1 1	0
34	B5	1	Total Mg 1 1	0
34	A5	1	Total Mg 1 1	0
34	E5	1	Total Mg 1 1	0

- Molecule 35 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



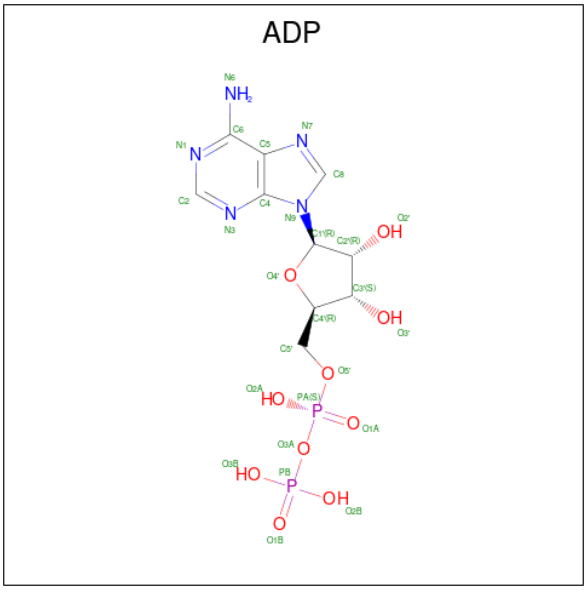
Mol	Chain	Residues	Atoms						AltConf
35	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	a3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	j3	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	l3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	L3	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
36	e	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	e3	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	E3	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



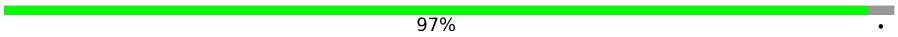
Mol	Chain	Residues	Atoms						AltConf
37	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	D4	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B4	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	D5	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B5	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

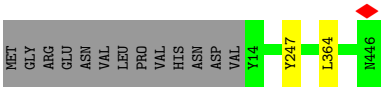
3 Residue-property plots (i)

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: Ymf66

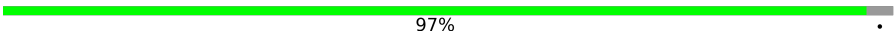
Chain a:

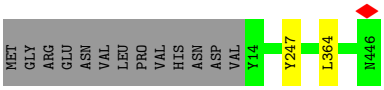




- Molecule 1: Ymf66

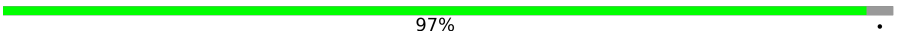
Chain A:

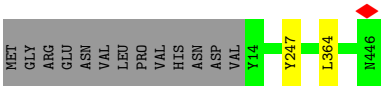




- Molecule 1: Ymf66

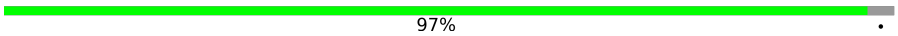
Chain a3:

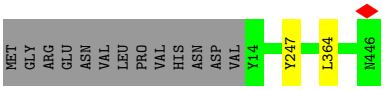




- Molecule 1: Ymf66

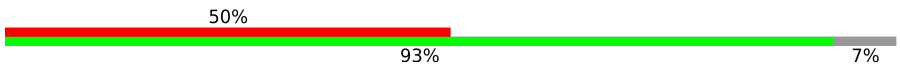
Chain A3:

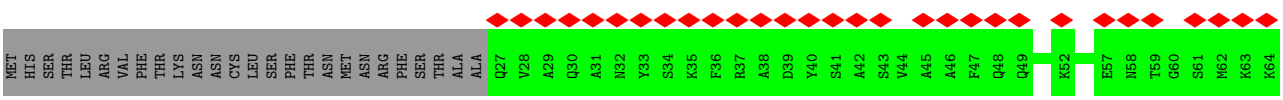


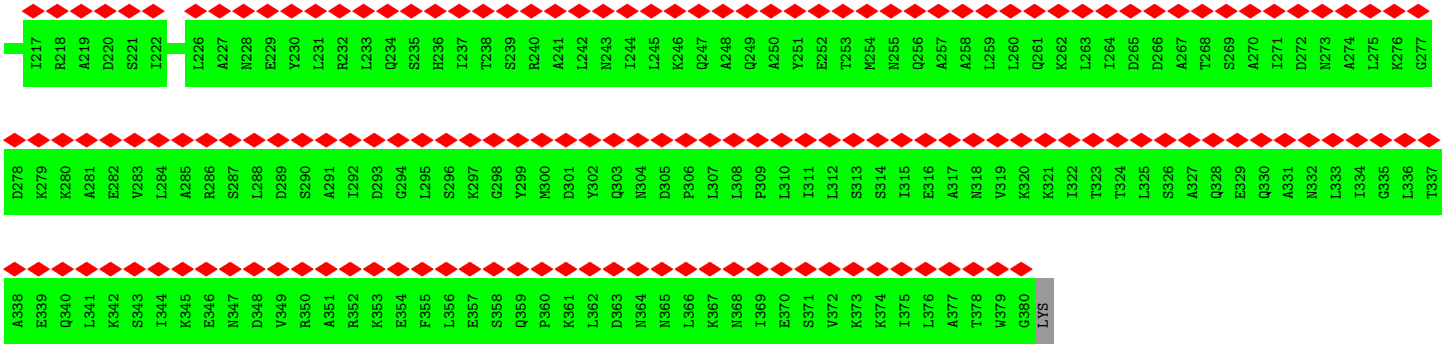


- Molecule 2: subunit b

Chain b:

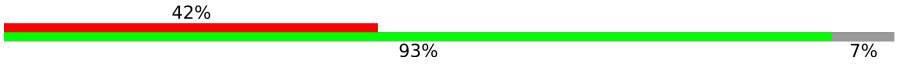


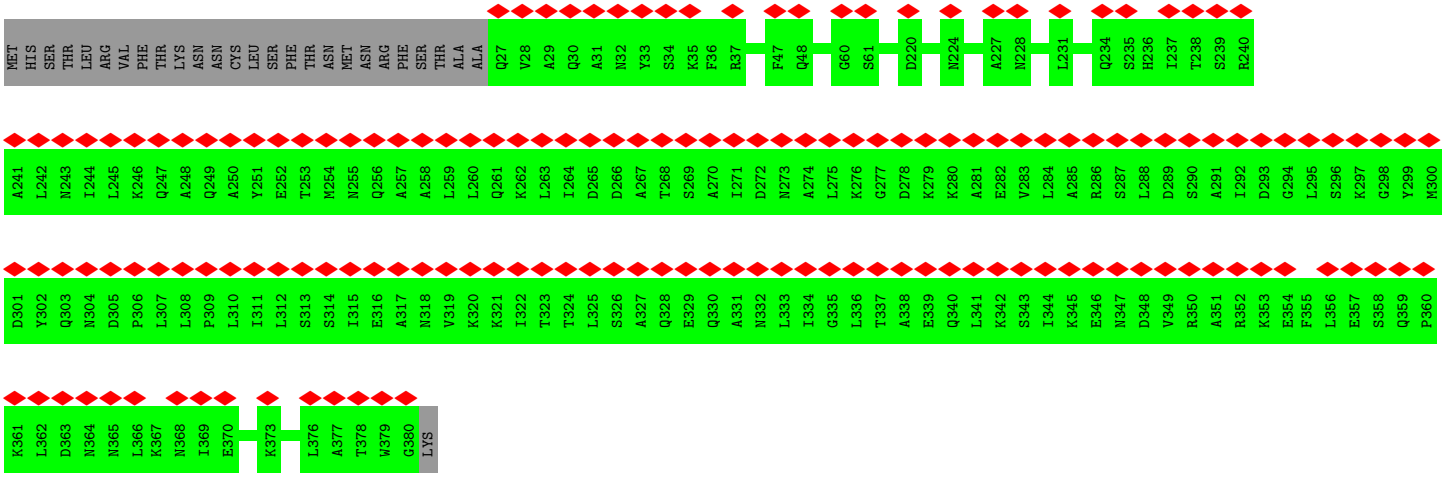




• Molecule 2: subunit b

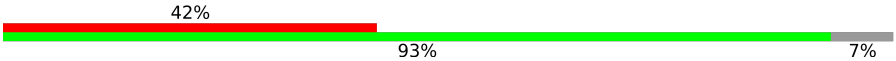
Chain B:





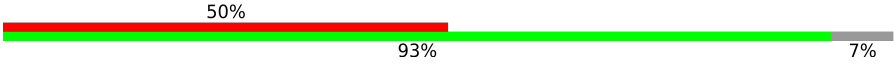
• Molecule 2: subunit b

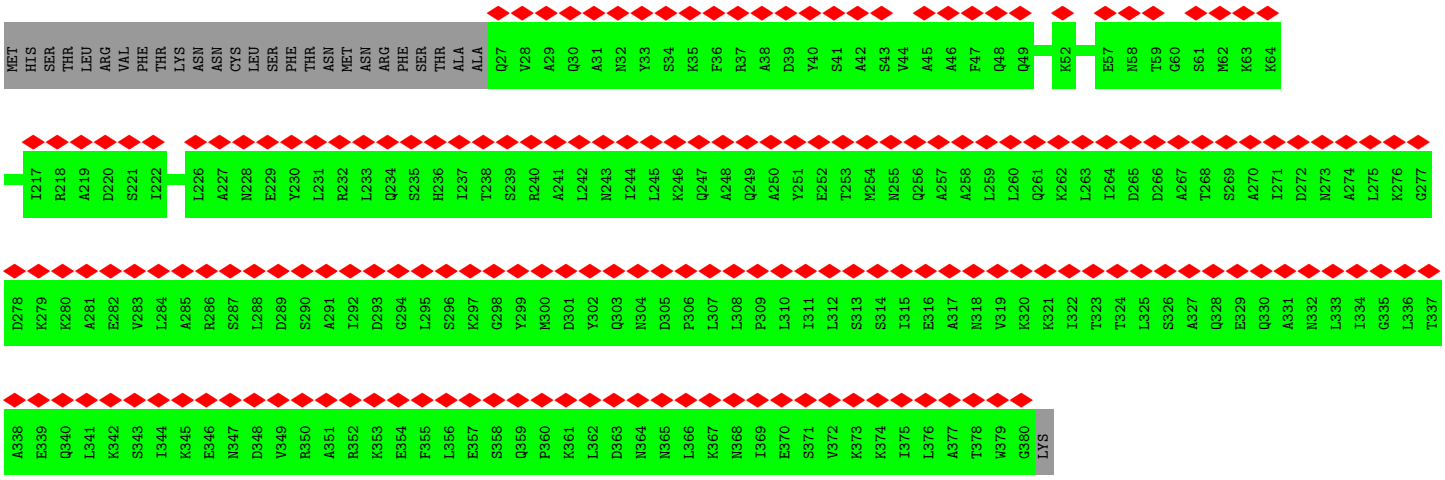
Chain b3:



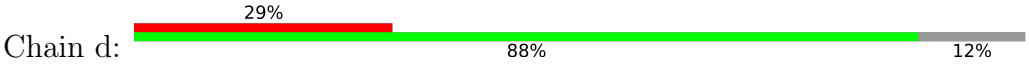
• Molecule 2: subunit b

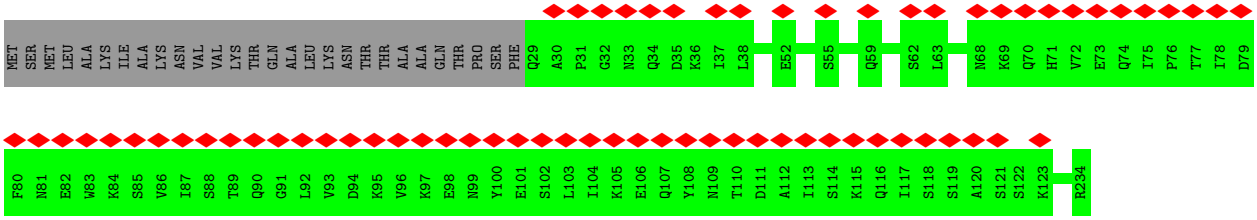
Chain B3:



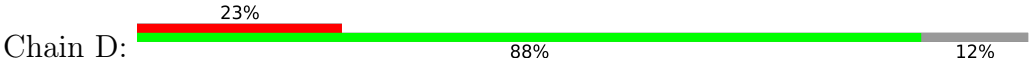


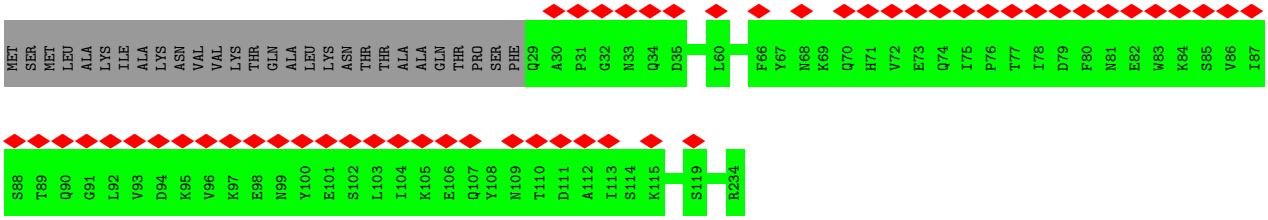
- Molecule 3: subunit d



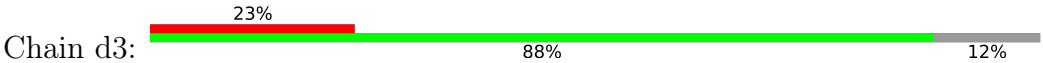


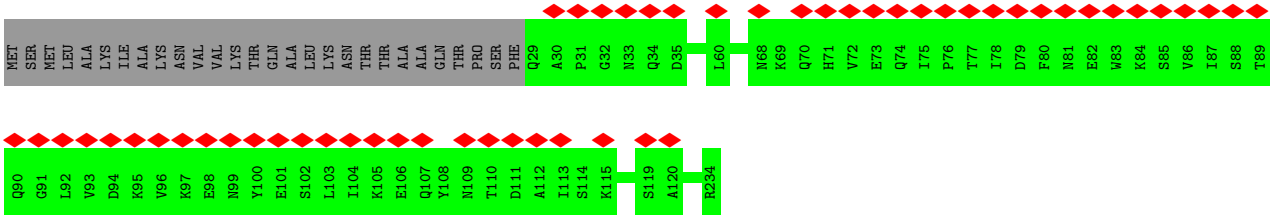
- Molecule 3: subunit d





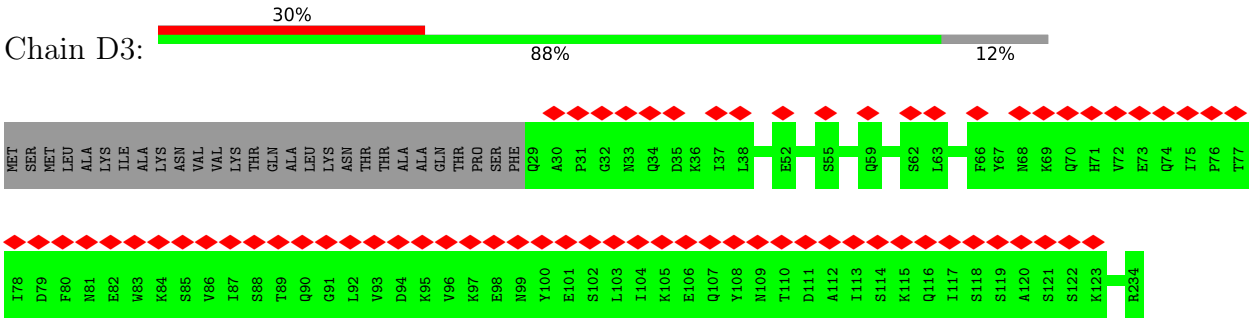
- Molecule 3: subunit d





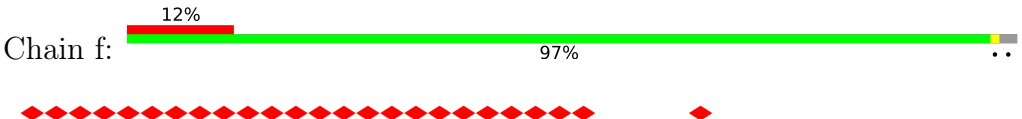
- Molecule 3: subunit d

Chain D3:



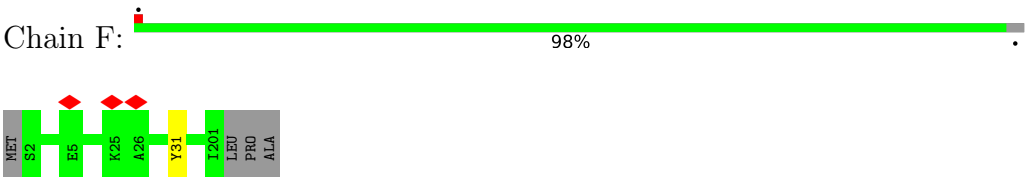
• Molecule 4: subunit f

Chain f:



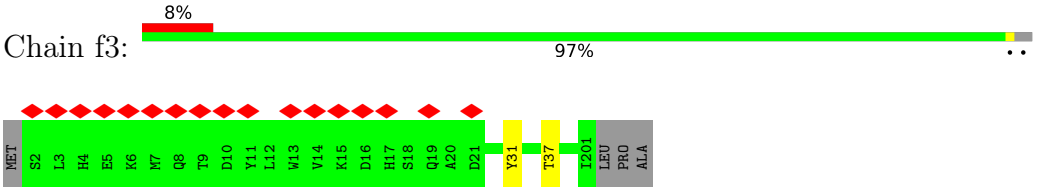
• Molecule 4: subunit f

Chain F:



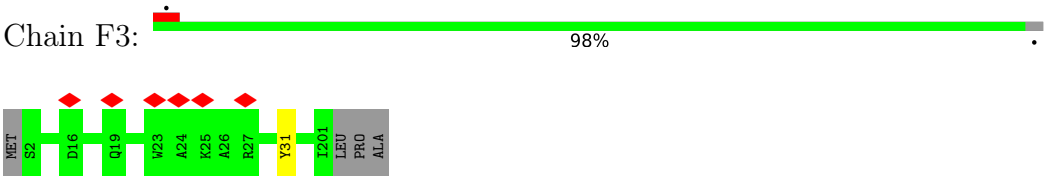
• Molecule 4: subunit f

Chain f3:



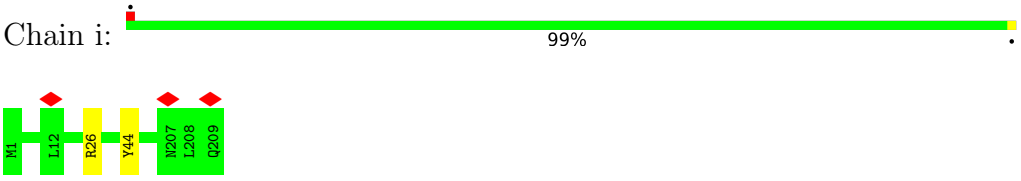
• Molecule 4: subunit f

Chain F3:



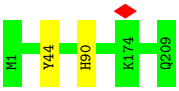
• Molecule 5: subunit i/j

Chain i:



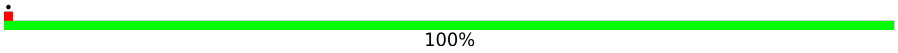
• Molecule 5: subunit i/j

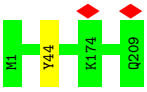
Chain I:



• Molecule 5: subunit i/j

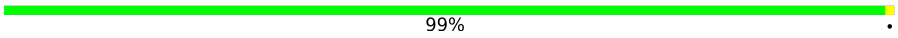
Chain i3:

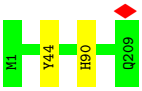




• Molecule 5: subunit i/j

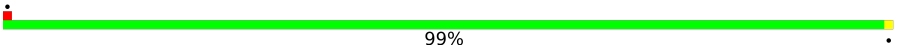
Chain I3:

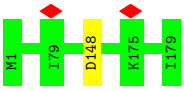




• Molecule 6: subunit k

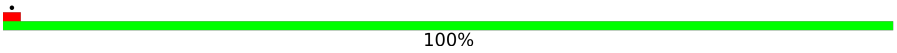
Chain k:

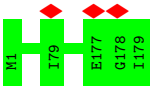




• Molecule 6: subunit k

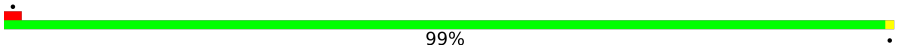
Chain K:

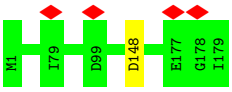




• Molecule 6: subunit k

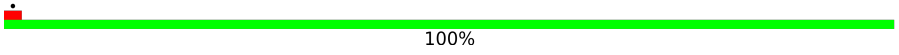
Chain k3:

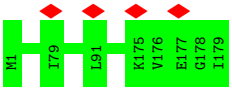




• Molecule 6: subunit k

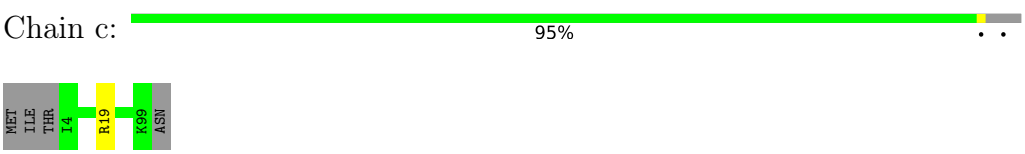
Chain K3:





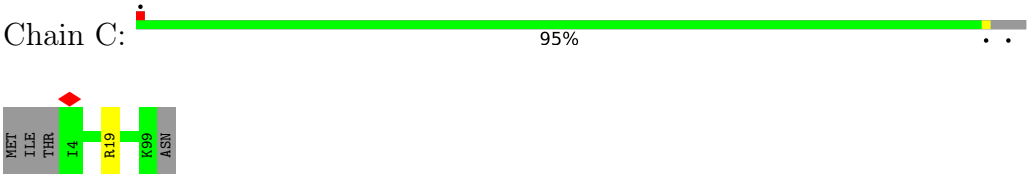
• Molecule 7: Ymf56

Chain c:



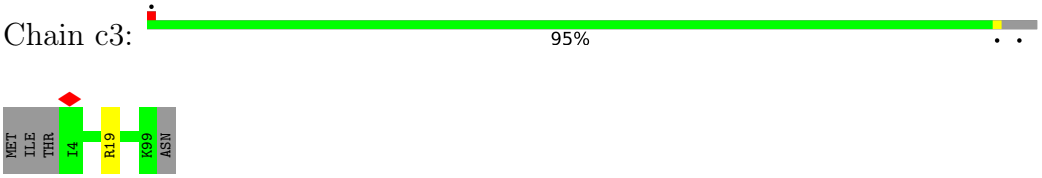
• Molecule 7: Ymf56

Chain C:



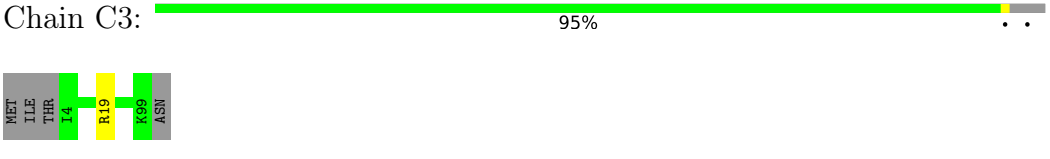
• Molecule 7: Ymf56

Chain c3:



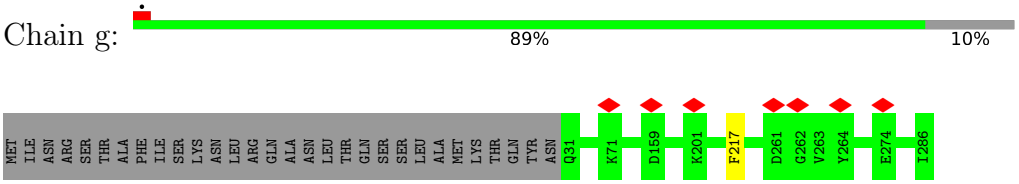
• Molecule 7: Ymf56

Chain C3:



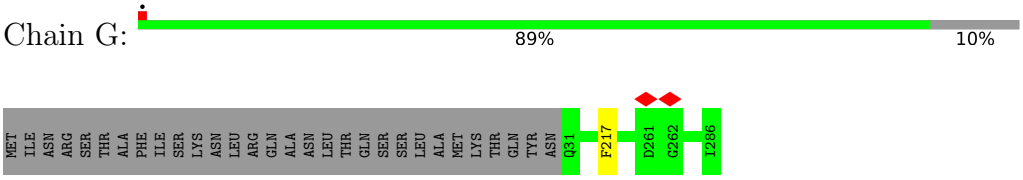
• Molecule 8: ATPTT3

Chain g:



• Molecule 8: ATPTT3

Chain G:



• Molecule 8: ATPTT3

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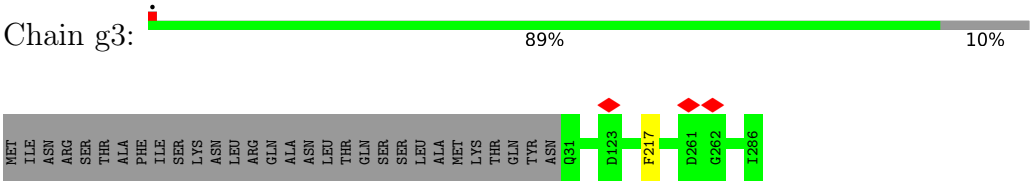
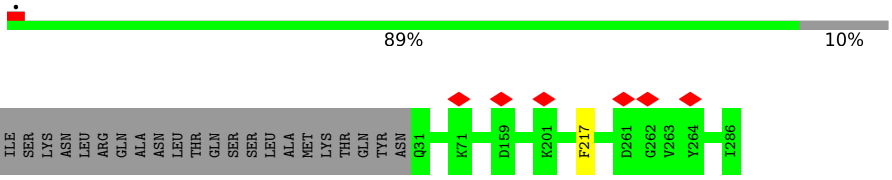


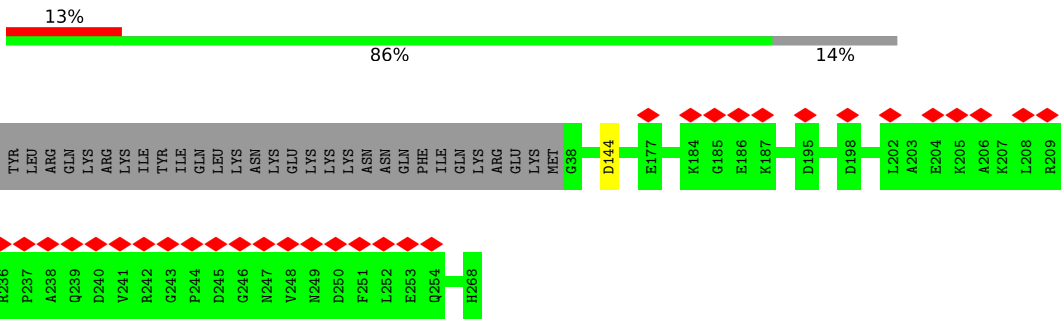
• Molecule 8: ATPTT3

Chain G3:



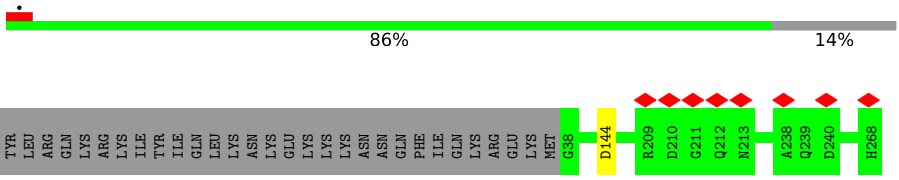
• Molecule 9: ATPTT4

Chain h:



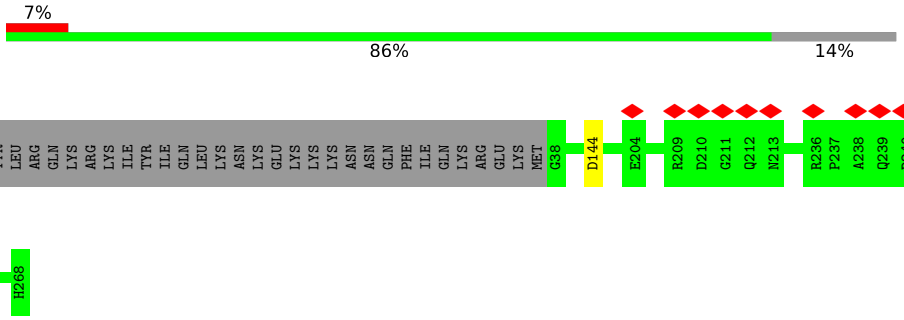
• Molecule 9: ATPTT4

Chain H:



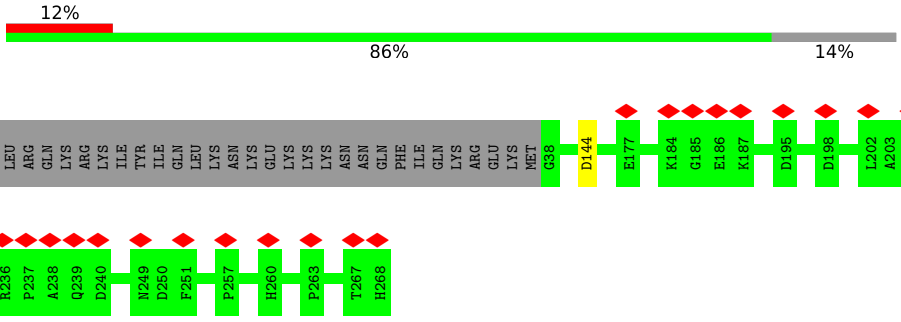
• Molecule 9: ATPTT4

Chain h3:



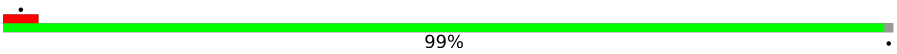
• Molecule 9: ATPTT4

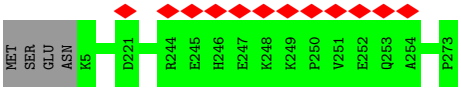
Chain H3:



• Molecule 10: ATPTT5

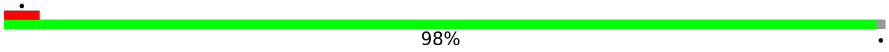
Chain j:

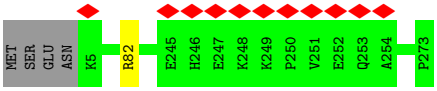




• Molecule 10: ATPTT5

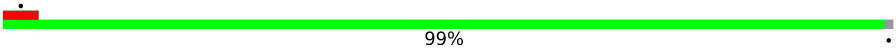
Chain J:

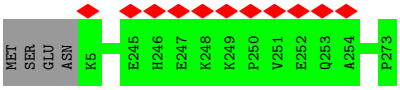




• Molecule 10: ATPTT5

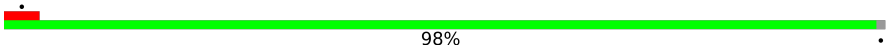
Chain j3:

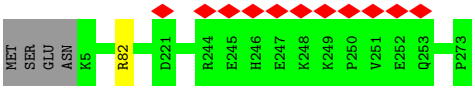




• Molecule 10: ATPTT5

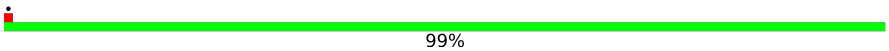
Chain J3:

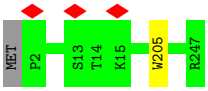




• Molecule 11: ATPTT6

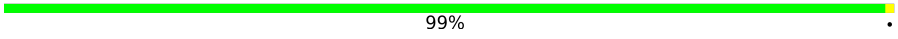
Chain l:





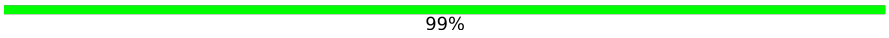
• Molecule 11: ATPTT6

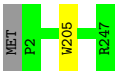
Chain L:



• Molecule 11: ATPTT6

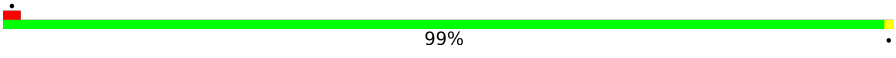
Chain l3:

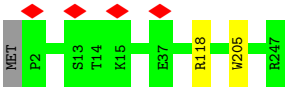




• Molecule 11: ATPTT6

Chain L3:



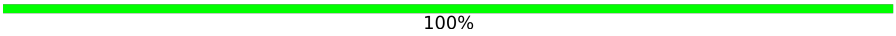


• Molecule 12: ATPTT7

Chain m:

• Molecule 12: ATPTT7

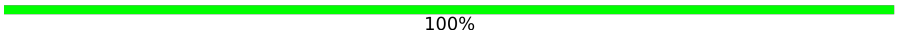
Chain M:



There are no outlier residues recorded for this chain.

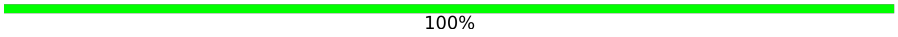
• Molecule 12: ATPTT7

Chain m3:



• Molecule 12: ATPTT7

Chain M3:



There are no outlier residues recorded for this chain.

• Molecule 13: ATPTT8

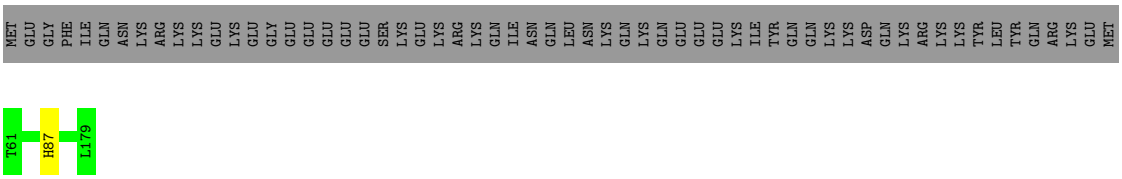
Chain n:

• Molecule 13: ATPTT8

Chain N:

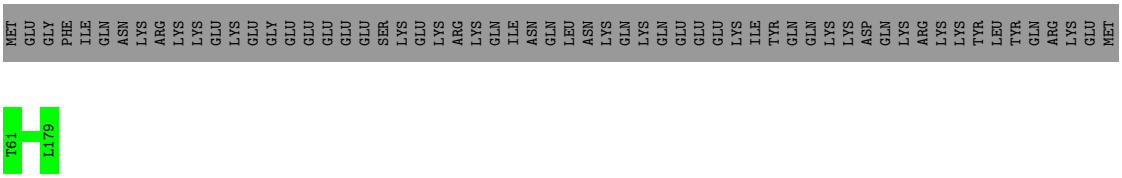
• Molecule 13: ATPTT8

Chain n3:



• Molecule 13: ATPTT8

Chain N3:

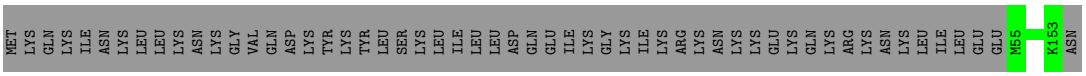


• Molecule 14: ATPTT9

Chain o:

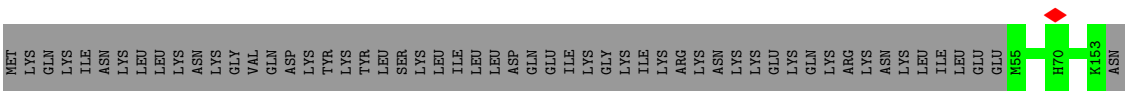
• Molecule 14: ATPTT9

Chain O:



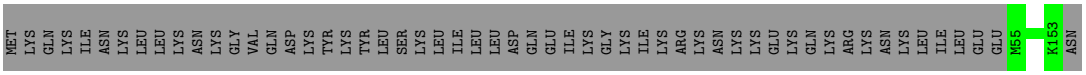
• Molecule 14: ATPTT9

Chain o3:



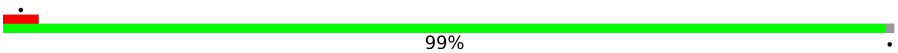
• Molecule 14: ATPTT9

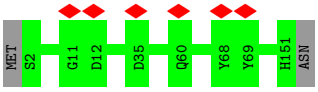
Chain O3:



• Molecule 15: ATPTT10

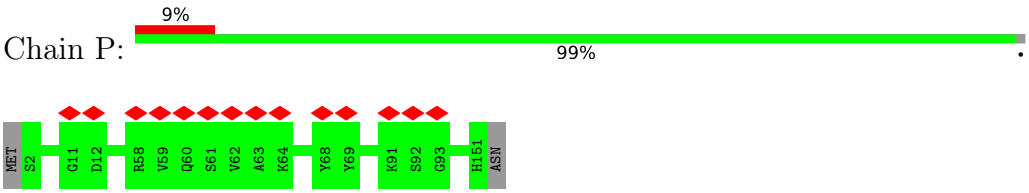
Chain p:





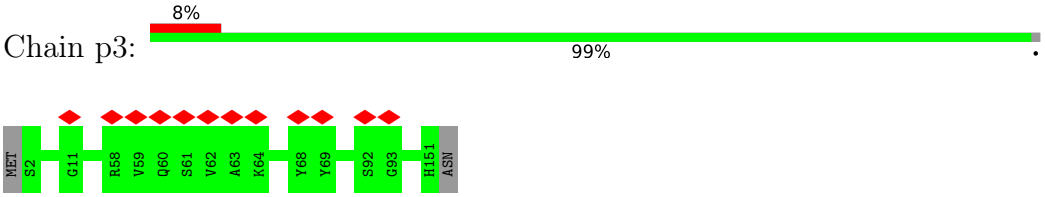
• Molecule 15: ATPTT10

Chain P:



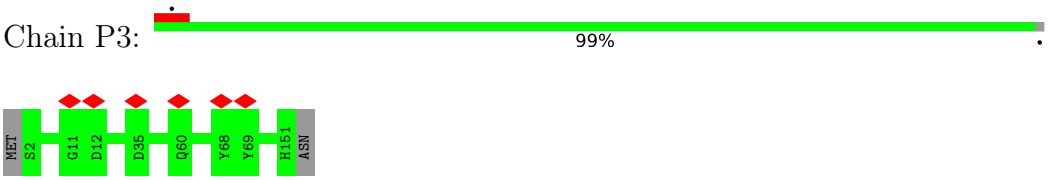
• Molecule 15: ATPTT10

Chain p3:



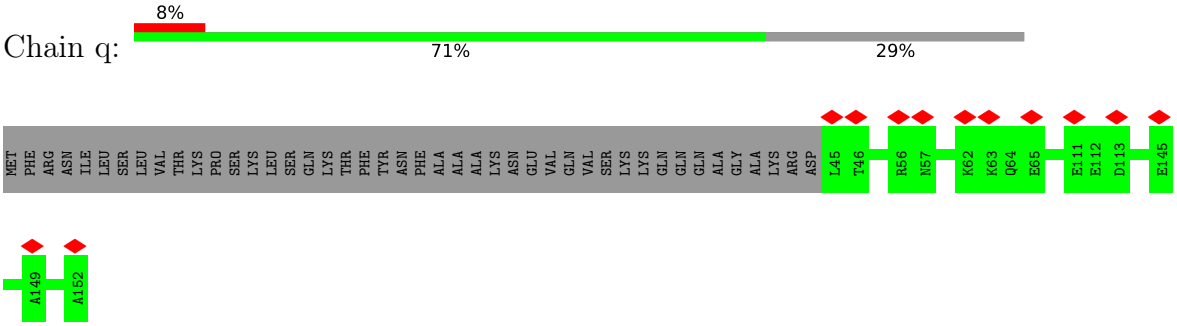
• Molecule 15: ATPTT10

Chain P3:



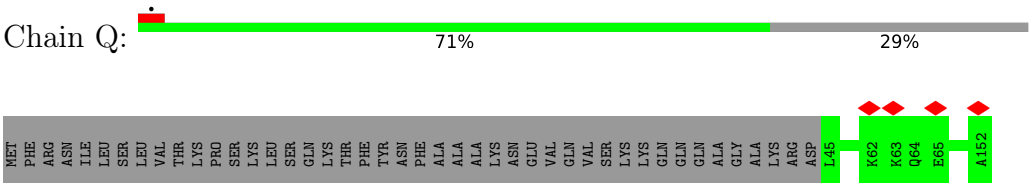
• Molecule 16: ATPTT11

Chain q:



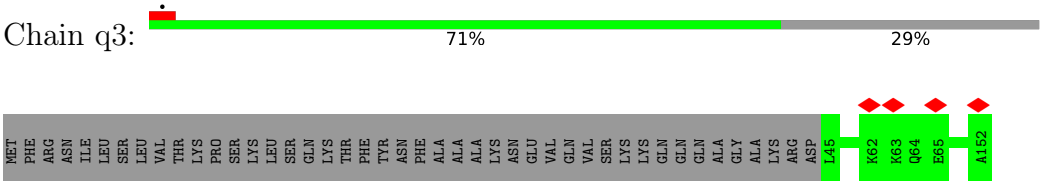
• Molecule 16: ATPTT11

Chain Q:



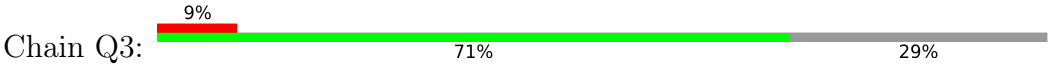
• Molecule 16: ATPTT11

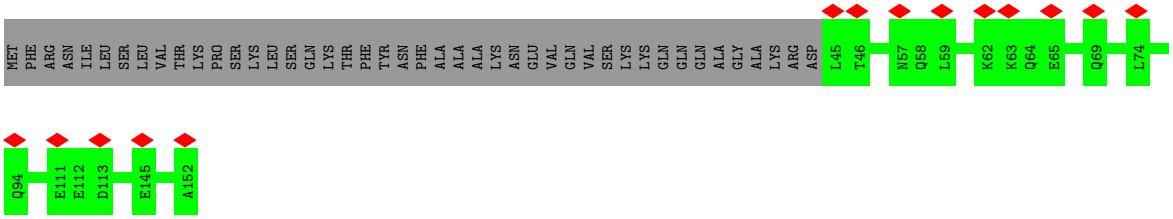
Chain q3:



• Molecule 16: ATPTT11

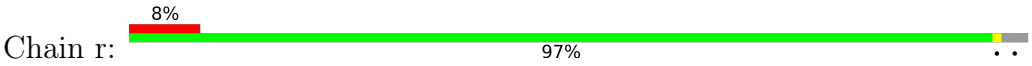
Chain Q3:

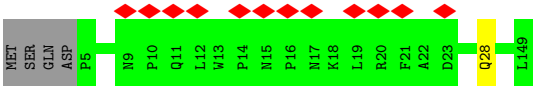




• Molecule 17: ATPTT12

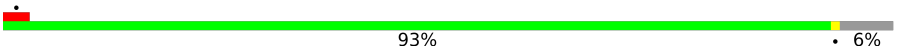
Chain r:

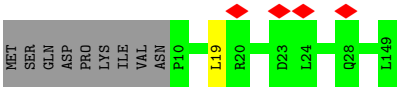




• Molecule 17: ATPTT12

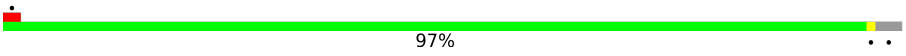
Chain R:

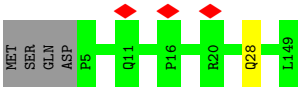




• Molecule 17: ATPTT12

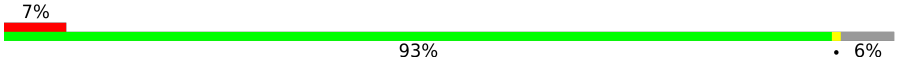
Chain r3:

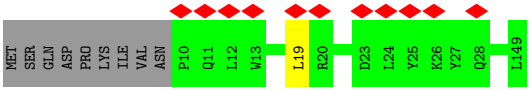




• Molecule 17: ATPTT12

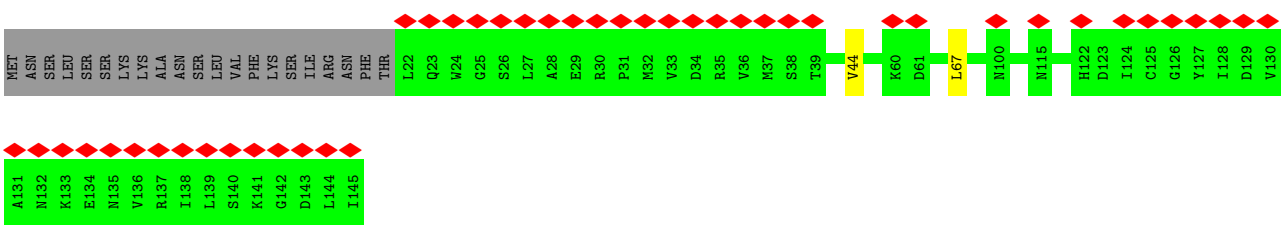
Chain R3:





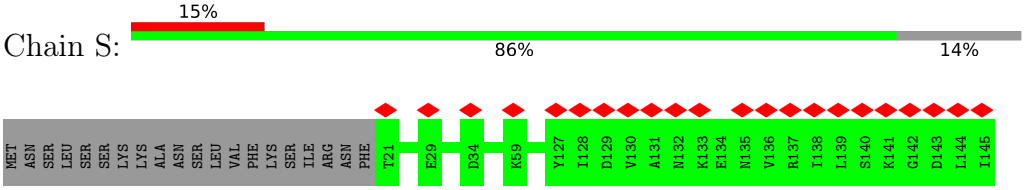
• Molecule 18: ATPTT13

Chain s:



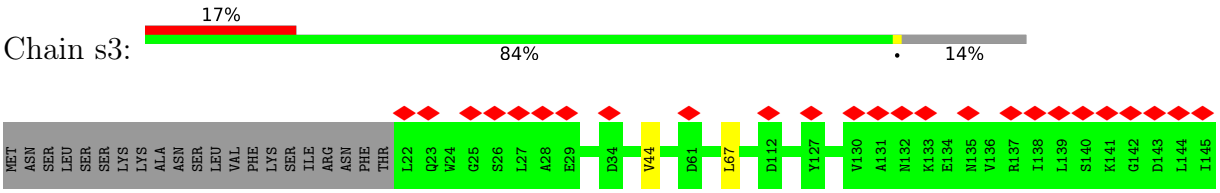
• Molecule 18: ATPTT13

Chain S:



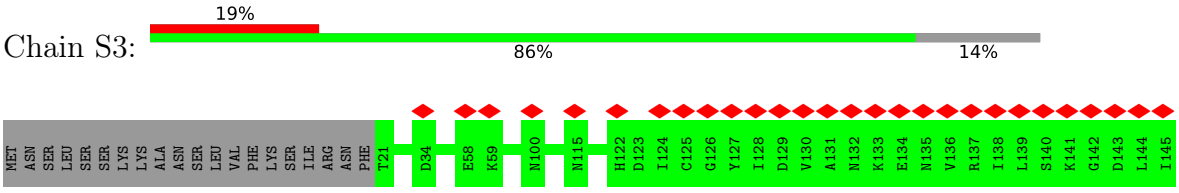
• Molecule 18: ATPTT13

Chain s3:



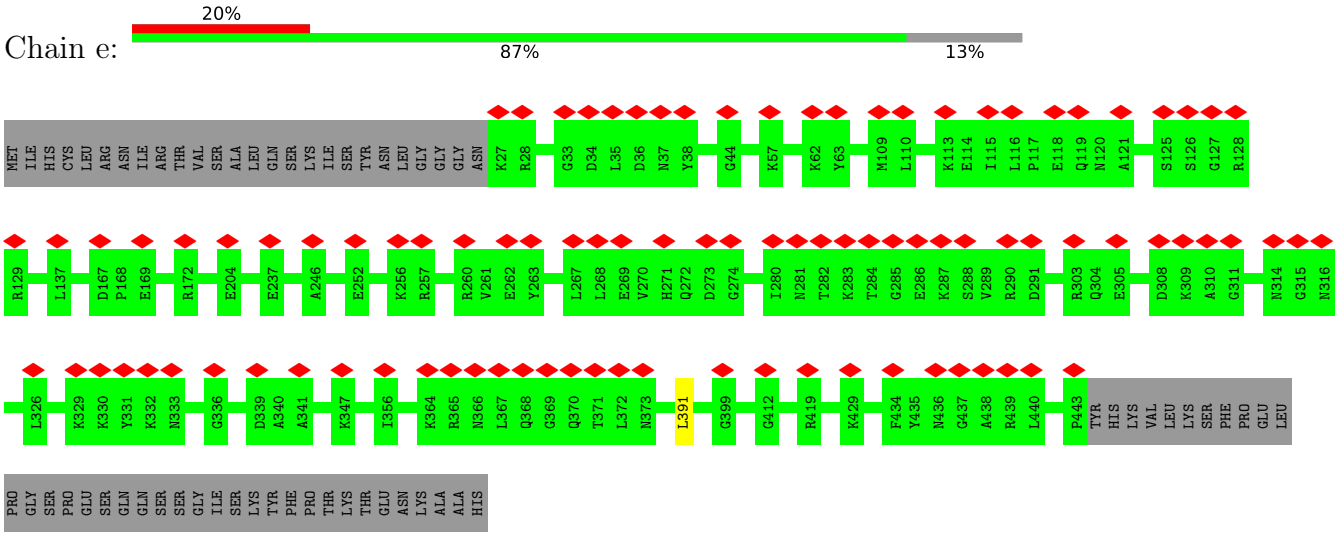
• Molecule 18: ATPTT13

Chain S3:



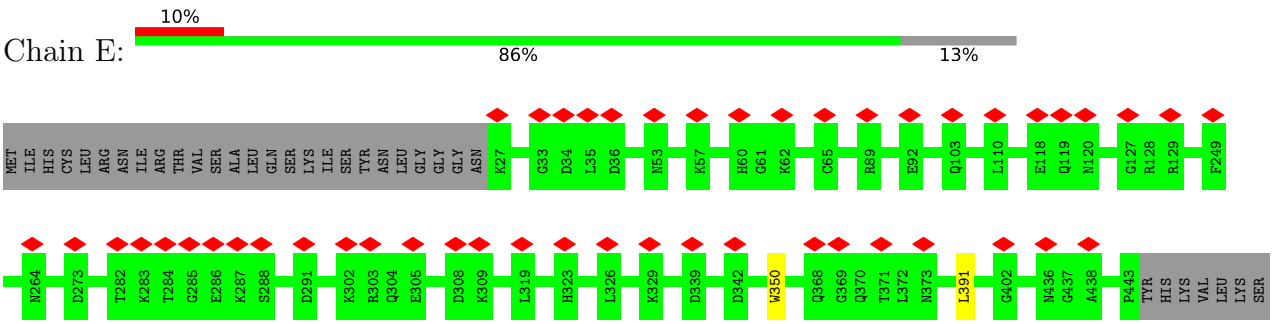
• Molecule 19: ATPTT1

Chain e:



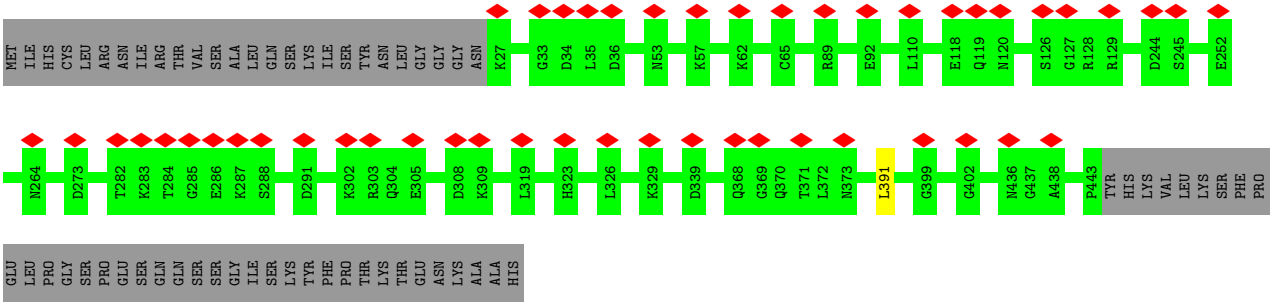
• Molecule 19: ATPTT1

Chain E:



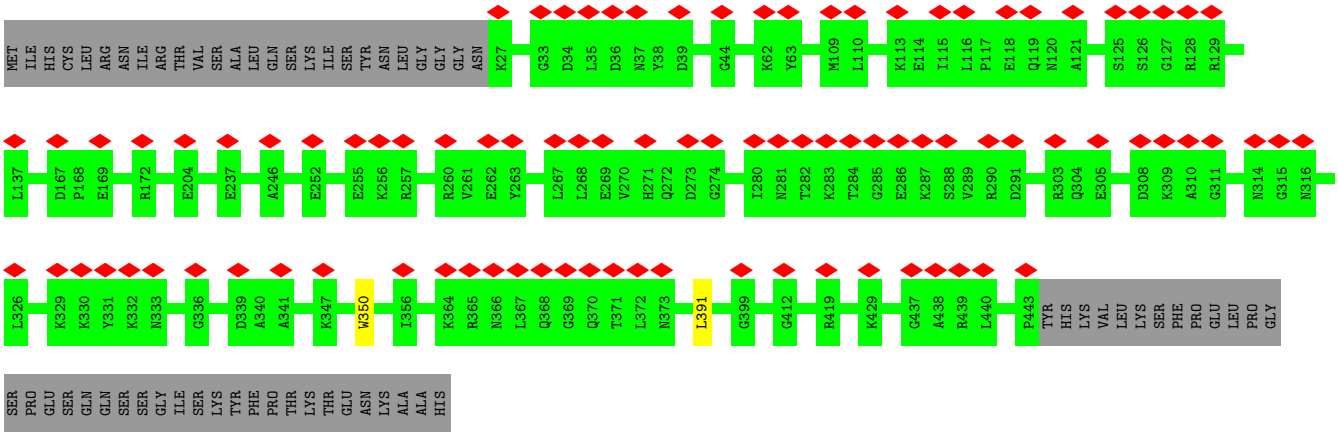
• Molecule 19: ATPTT1

Chain e3:



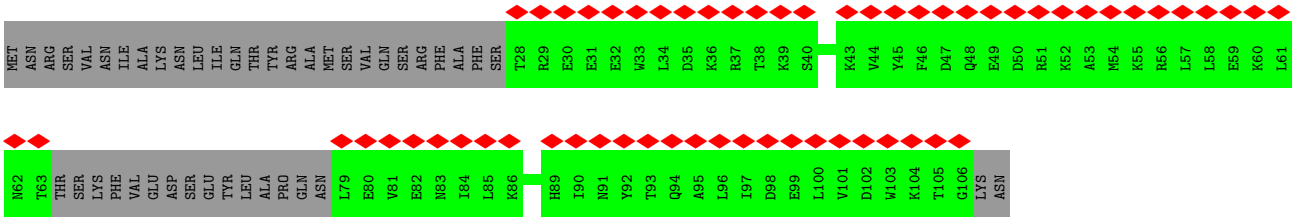
• Molecule 19: ATPTT1

Chain E3:



• Molecule 20: Inhibitor of F1 (IF1)

Chain i2:

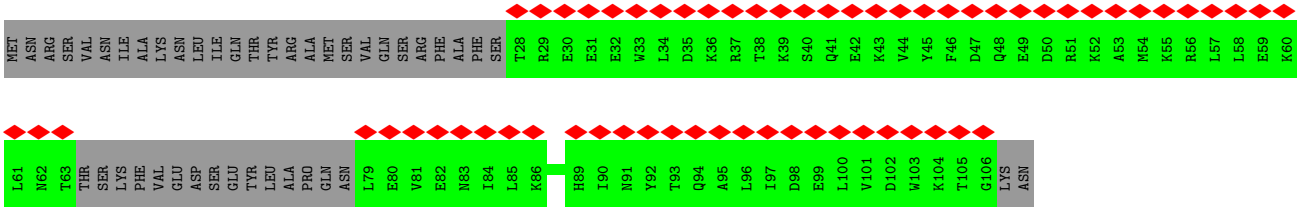


• Molecule 20: Inhibitor of F1 (IF1)

Chain i1:

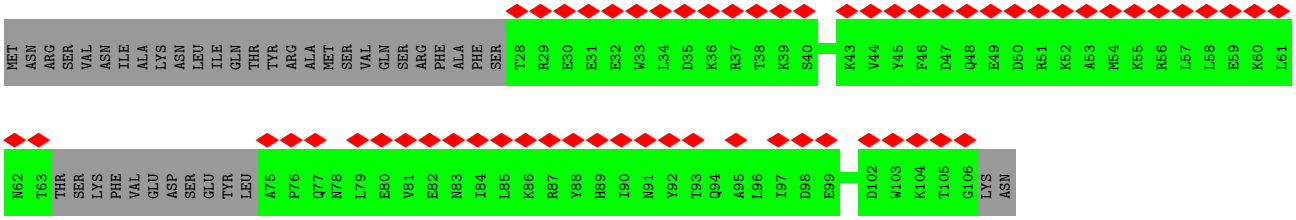
• Molecule 20: Inhibitor of F1 (IF1)

Chain i5:



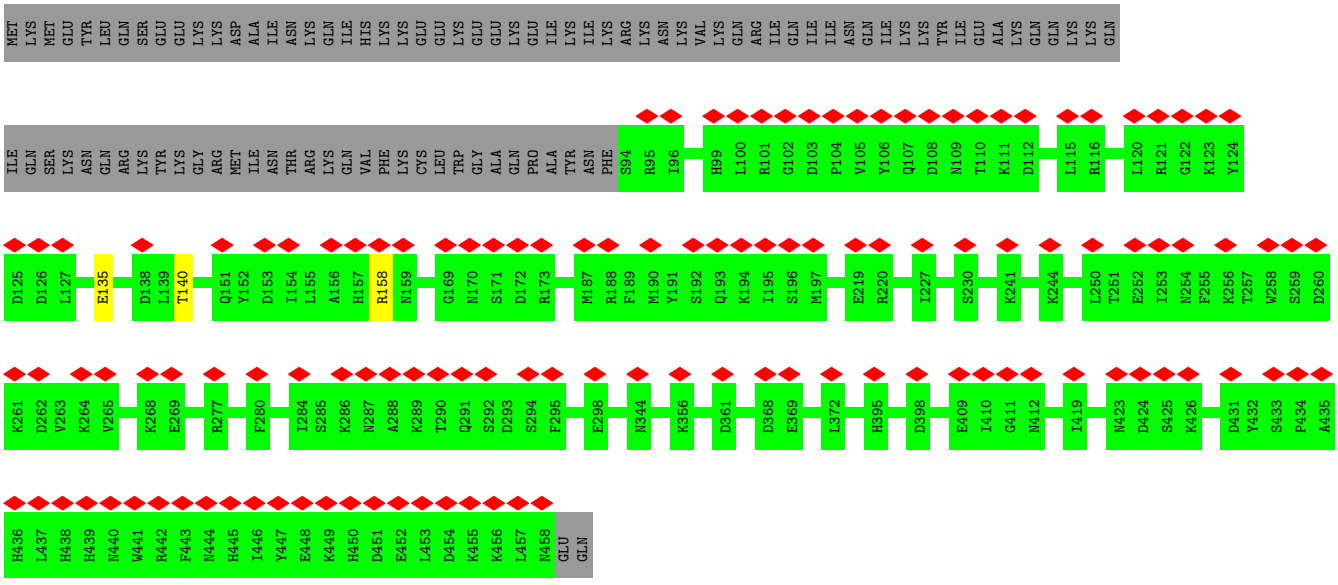
• Molecule 20: Inhibitor of F1 (IF1)

Chain i4:



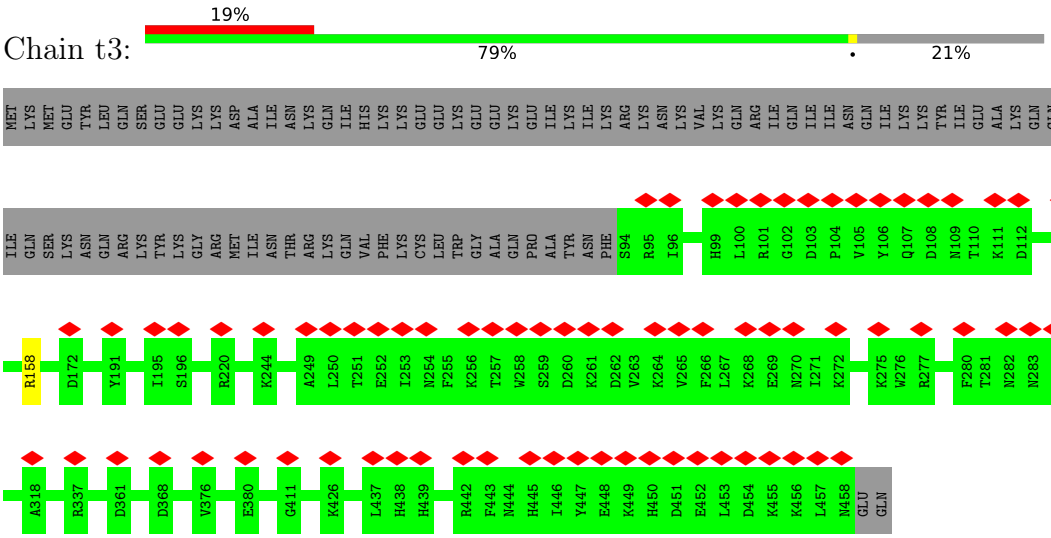
• Molecule 21: ATPTT2

Chain t:



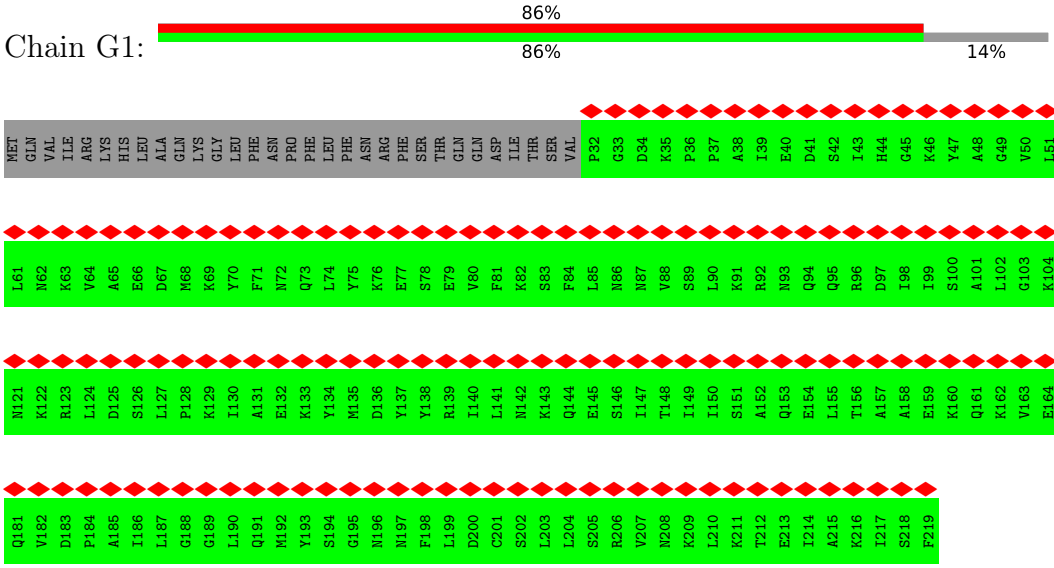
• Molecule 21: ATPTT2

Chain t3:



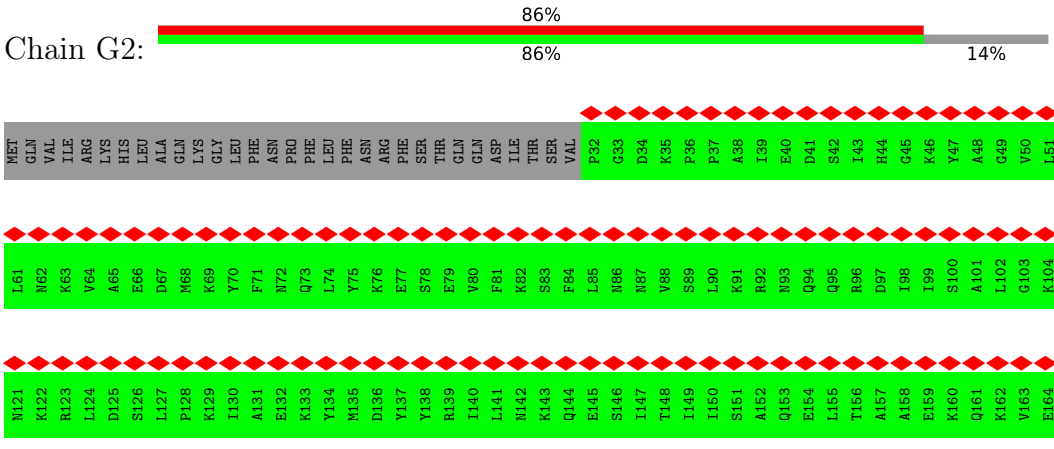
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

Chain G1:



• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

Chain G2:



Q181 V182 D183 P184 A185 I186 L187 G188 G189 L190 Q191 M192 Y193 S194 G195 N196 N197 F198 L199 D200 C201 S202 L203 L204 S205 R206 V207 N208 K209 L210 K211 T212 E213 I214 A215 K216 I217 S218 F219

• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

Chain G4:

MET GLN VAL ILE ARG LYS HIS LEU ALA GLN LYS GLY LEU PHE ASN PRO PHE LEU PHE ASN ARG PHE SER THR GLN GLN ASP ILE THR SER VAL P32 G33 D34 K35 P36 P37 A38 I39 E40 D41 S42 I43 H44 G45 K46 Y47 A48 G49 V50 L51 F52 S53 S54 A55 S56 S57 N58 K59 S60

L61 N62 K63 V64 A65 E66 D67 M68 K69 Y70 F71 N72 Q73 L74 Y75 K76 E77 S78 E79 V80 F81 K82 S83 F84 L85 N86 N87 V88 S89 L90 K91 R92 N93 Q94 Q95 R96 D97 I98 I99 S100 A101 L102 G103 K104 T105 N106 F107 N108 P109 A110 T111 N112 N113 L114 L115 E116 T117 L118 I119 E120

N121 K122 R123 L124 D125 S126 L127 P128 K129 I130 A131 E132 K133 Y134 M135 D136 Y137 Y138 R139 I140 L141 N142 K143 Q144 E145 S146 I147 T148 I149 I150 S151 A152 Q153 E154 L155 T156 A157 A158 E159 K160 Q161 K162 V163 E164 Q165 G166 L167 K168 K169 G170 N171 A172 N173 V174 Q175 F176 T177 V178 V179 Y180

Q181 V182 D183 P184 A185 I186 L187 G188 G189 L190 Q191 M192 Y193 S194 G195 N196 N197 F198 L199 D200 C201 S202 L203 L204 S205 R206 V207 N208 K209 L210 K211 T212 E213 I214 A215 K216 I217 S218 F219

• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

Chain G5:

MET GLN VAL ILE ARG LYS HIS LEU ALA GLN LYS GLY LEU PHE ASN PRO PHE LEU PHE ASN ARG PHE SER THR GLN GLN ASP ILE THR SER VAL P32 G33 D34 K35 P36 P37 A38 I39 E40 D41 S42 I43 H44 G45 K46 Y47 A48 G49 V50 L51 F52 S53 S54 A55 S56 S57 N58 K59 S60

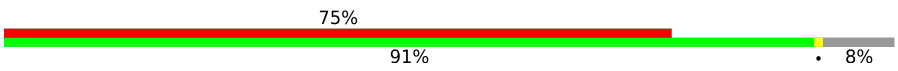
L61 N62 K63 V64 A65 E66 D67 M68 K69 Y70 F71 N72 Q73 L74 Y75 K76 E77 S78 E79 V80 F81 K82 S83 F84 L85 N86 N87 V88 S89 L90 K91 R92 N93 Q94 Q95 R96 D97 I98 I99 S100 A101 L102 G103 K104 T105 N106 F107 N108 P109 A110 T111 N112 N113 L114 L115 E116 T117 L118 I119 E120

N121 K122 R123 L124 D125 S126 L127 P128 K129 I130 A131 E132 K133 Y134 M135 D136 Y137 Y138 R139 I140 L141 N142 K143 Q144 E145 S146 I147 T148 I149 I150 S151 A152 Q153 E154 L155 T156 A157 A158 E159 K160 Q161 K162 V163 E164 Q165 G166 L167 K168 K169 G170 N171 A172 N173 V174 Q175 F176 T177 V178 V179 Y180

Q181 V182 D183 P184 A185 I186 L187 G188 G189 L190 Q191 M192 Y193 S194 G195 N196 N197 F198 L199 D200 C201 S202 L203 L204 S205 R206 V207 N208 K209 L210 K211 T212 E213 I214 A215 K216 I217 S218 F219

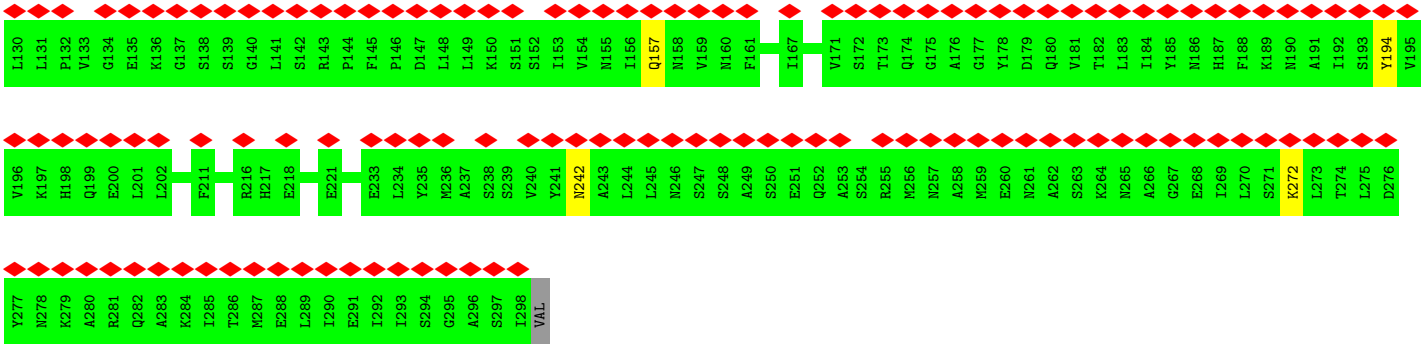
• Molecule 23: ATP synthase subunit gamma

Chain g1:



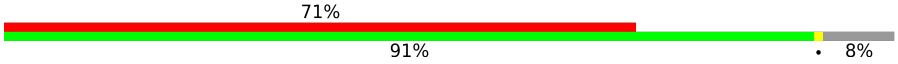
MET PHE GLY LEU ALA SER LYS GLY PHE ILE ASN THR SER LEU VAL MET VAL PRO GLN MET ASN PHE GLY A24 N25 L26 K27 Q28 L29 K30 I31 R32 M33 K34 A35 I36 G37 S38 I39 K40 K41 I42 T43 K44 A45 M46 K47 M48 V49 A50 A51 S52 K53 M54 K55 A56 E57 T58 S59 R60

L61 E62 N63 G64 R65 N66 V69 G70 Q73 Y81 K84 K85 K86 S87 T88 T89 A90 P91 K92 S93 T94 L95 L96 V97 P98 I99 T100 S101 D102 K103 G104 L105 C106 G107 S108 V109 N110 S111 S112 I113 V114 R115 E116 V117 K118 R119 L120 A121 L122 N123 N124 R125 S126 A127 F128 G129



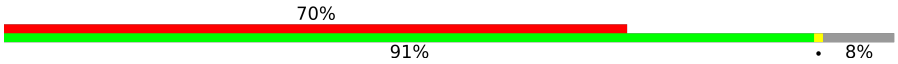
• Molecule 23: ATP synthase subunit gamma

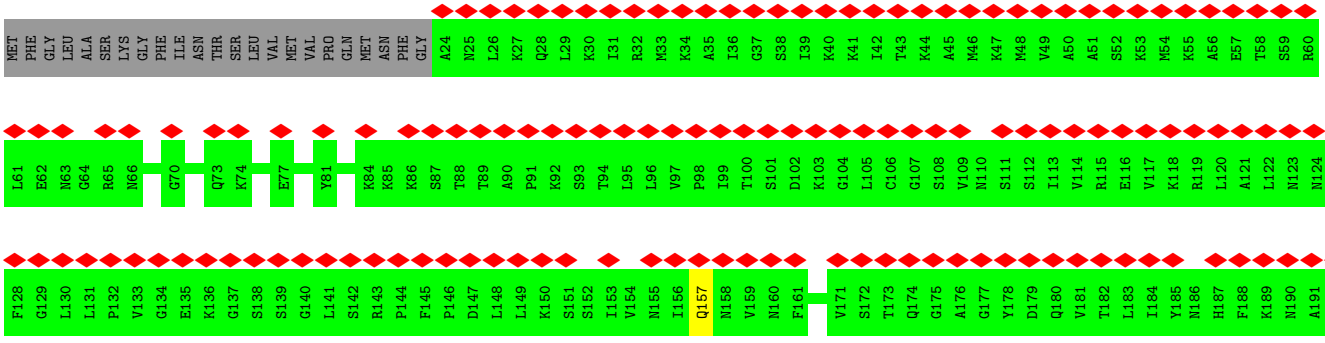
Chain g2:



• Molecule 23: ATP synthase subunit gamma

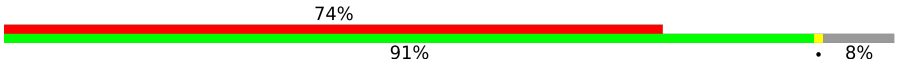
Chain g4:





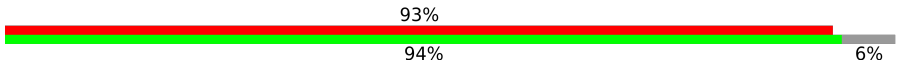
• Molecule 23: ATP synthase subunit gamma

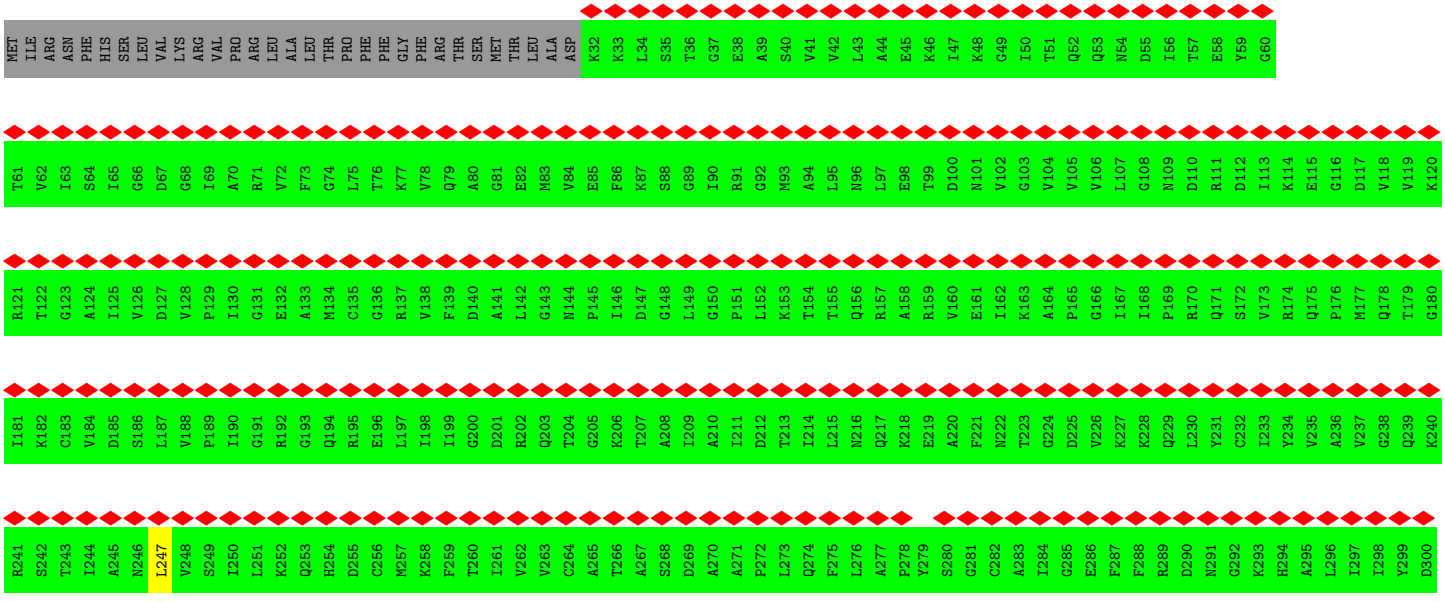
Chain g5:



• Molecule 24: ATP synthase subunit alpha

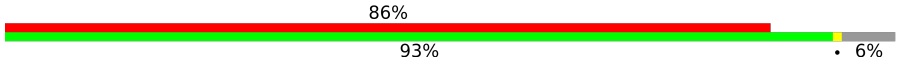
Chain C1:

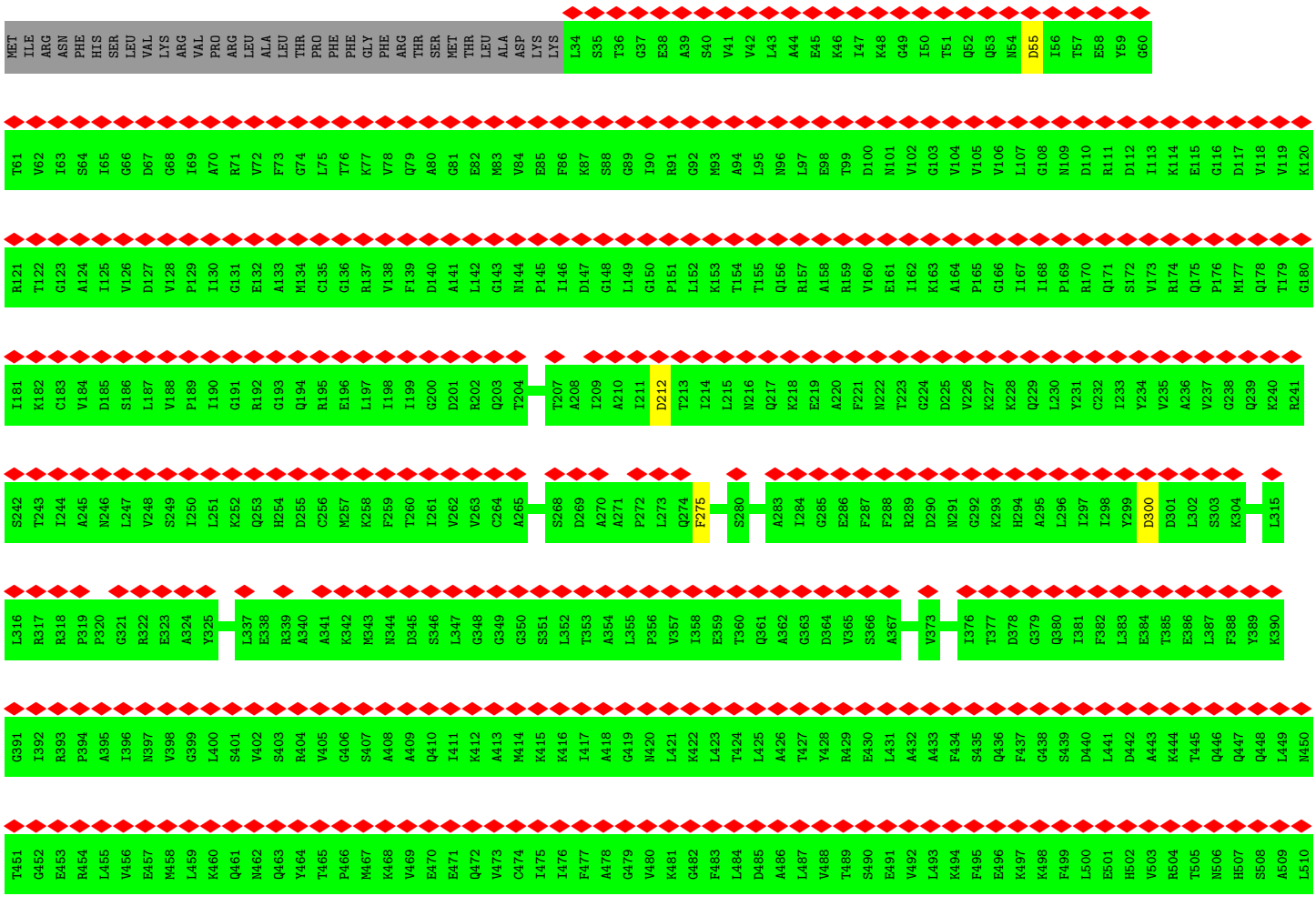


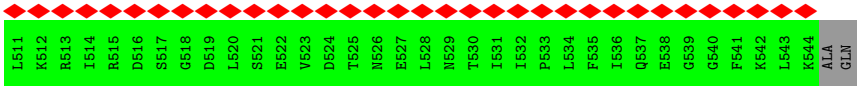


• Molecule 24: ATP synthase subunit alpha

Chain B1:

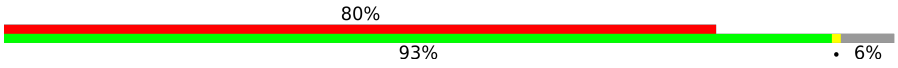


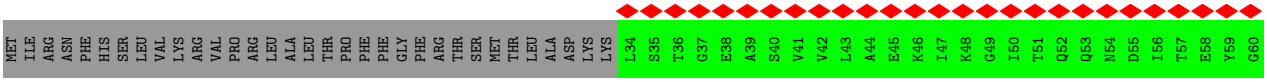


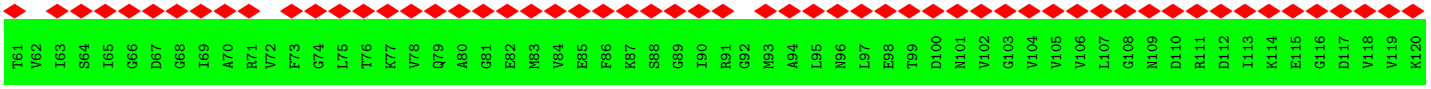


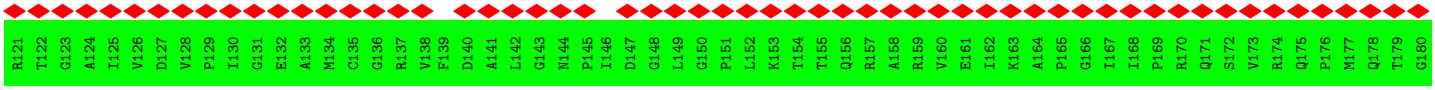
• Molecule 24: ATP synthase subunit alpha

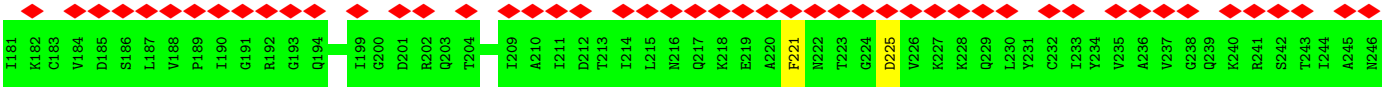
Chain A1:

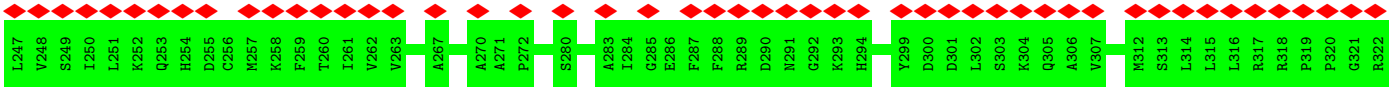


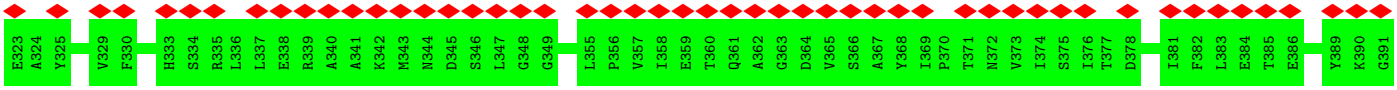


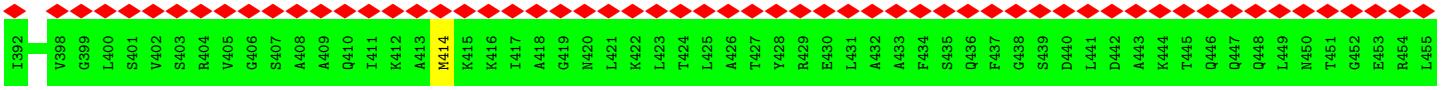


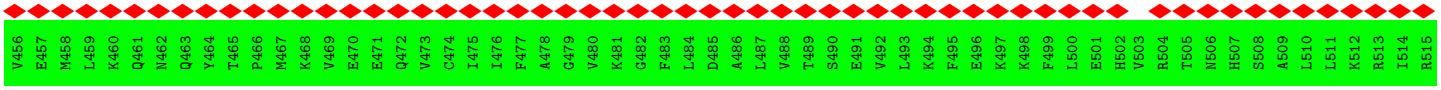


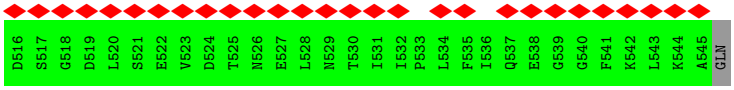






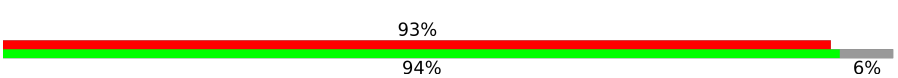


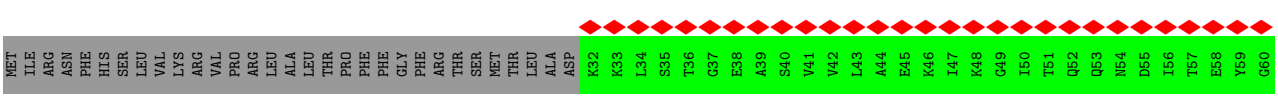


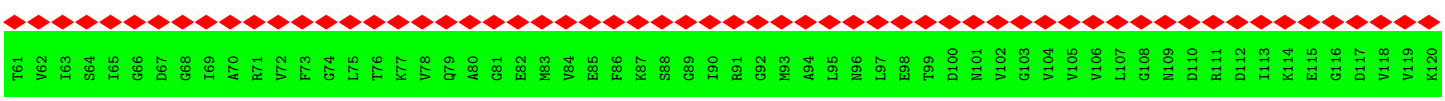


• Molecule 24: ATP synthase subunit alpha

Chain C2:

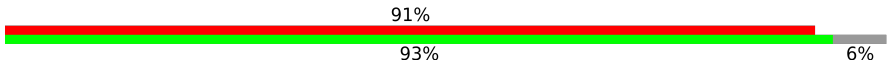


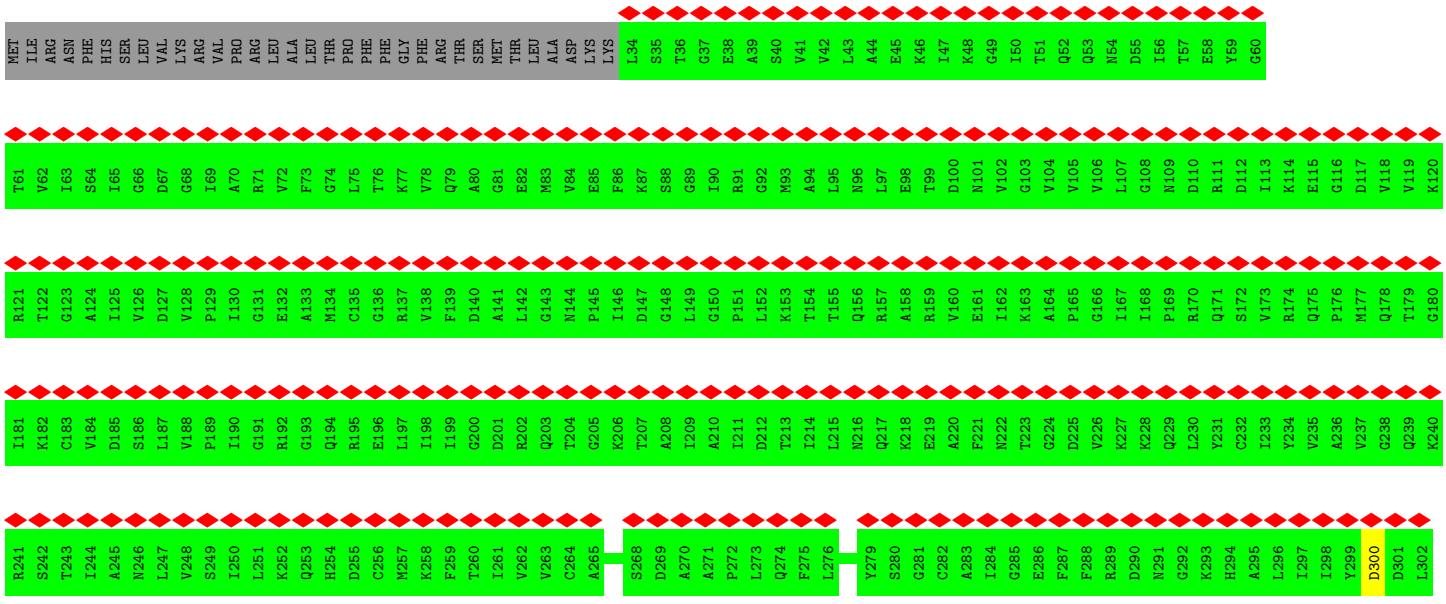




• Molecule 24: ATP synthase subunit alpha

Chain B2:





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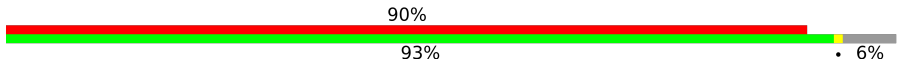
L425 A426 T427 Y428 R429 E430 L431 A432 A433 F434 S435 Q436 F437 G438 S439 D440 L441 D442 A443 K444 T445 Q446 Q447 Q448 L449 N450 T451 G452 E453 R454 L455 V456 E457 M458 L459 K460 Q461 N462 Q463 Y464 T465 P466 M467 K468 V469 E470 E471 Q472 V473 C474 I475 I476 F477 A478 G479 V480 K481 G482 F483 L484

D485 A486 L487 V488 T489 S490 E491 V492 L493 K494 F495 E496 K497 K498 F499 L500 E501 H502 V503 R504 T505 N506 H507 S508 A509 L510 L511 K512 R513 I514 R515 D516 S517 G518 D519 L520 S521 E522 V523 D524 T525 N526 E527 L528 N529 T530 I531 I532 P533 L534 F535 I536 Q537 E538 G539 G540 F541 K542 L543 K544

ALA GLN

• Molecule 24: ATP synthase subunit alpha

Chain A2:



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T61 V62 I63 S64 I65 G66 D67 G68 I69 A70 R71 V72 F73 G74 L75 T76 K77 V78 Q79 A80 G81 E82 M83 V84 E85 P86 K87 S88 G89 I90 R91 G92 M93 A94 L95 N96 L97 E98 T99 D100 N101 V102 G103 V104 V105 V106 L107 G108 N109 D110 R111 D112 I113 K114 E115 G116 D117 V118 V119 K120

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R241 S242 T243 I244 A245 N246 L247 V248 S249 I250 L251 K252 Q253 H254 D255 C256 M257 K258 F259 T260 I261 V262 V263 C264 A265 T266 A267 S268 D269 A270 A271 P272 L273 Q274 F275 L276 A277 P278 Y279 S280 G281 C282 A283 I284 G285 E286 F287 F288 R289 D290 N291 G292 K293 H294 A295 L296 Y299 D300 D301

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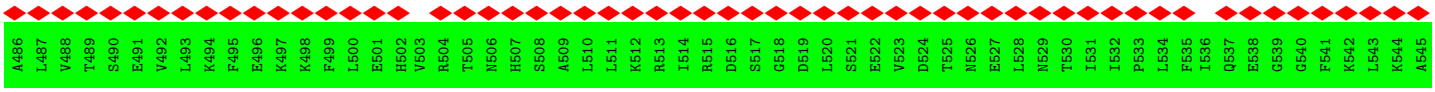
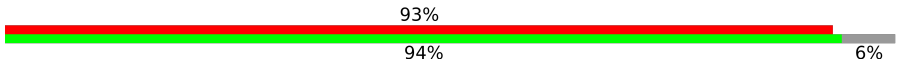
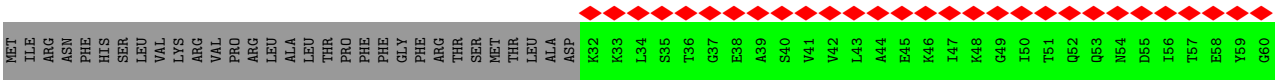
A426 T427 Y428 R429 E430 L431 A432 A433 F434 S435 Q436 F437 G438 S439 D440 L441 D442 A443 K444 T445 Q446 Q447 Q448 L449 N450 T451 G452 E453 R454 L455 V456 E457 M458 L459 K460 Q461 N462 Q463 Y464 T465 P466 M467 K468 V469 E470 E471 Q472 V473 C474 I475 I476 F477 A478 G479 V480 K481 G482 F483 L484 D485

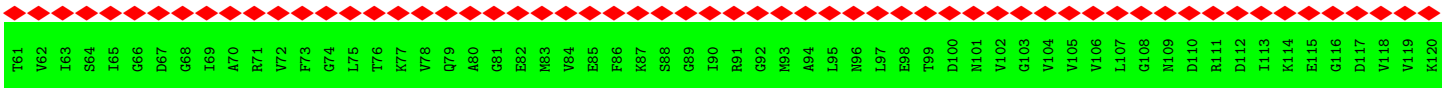


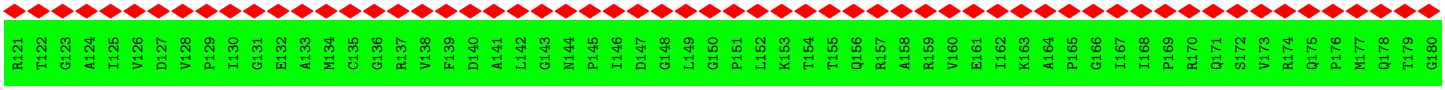
• Molecule 24: ATP synthase subunit alpha

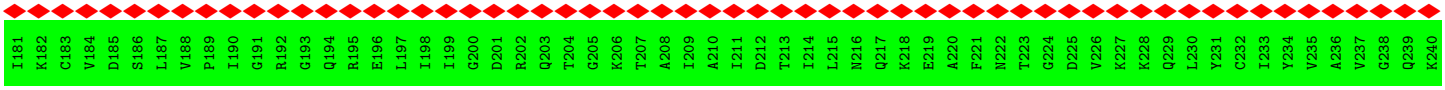
Chain C4:

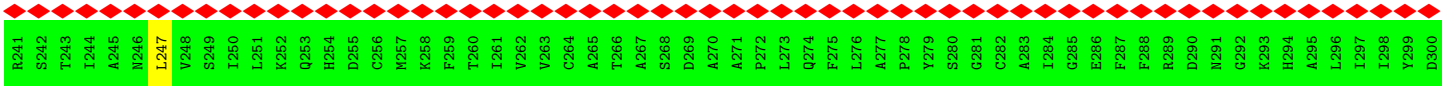


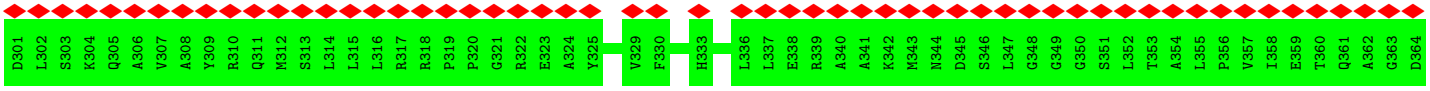


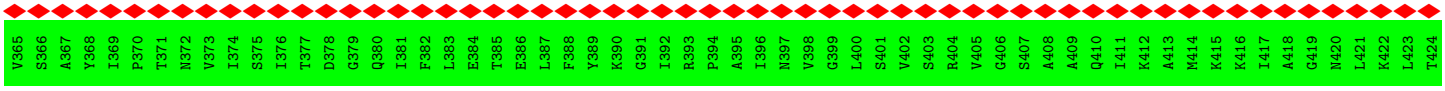


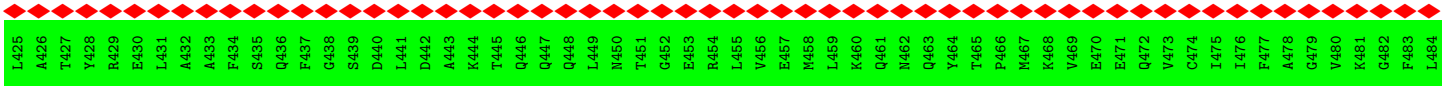


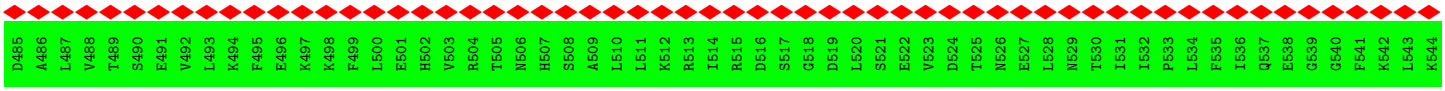






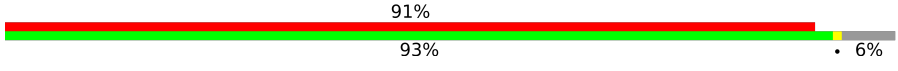


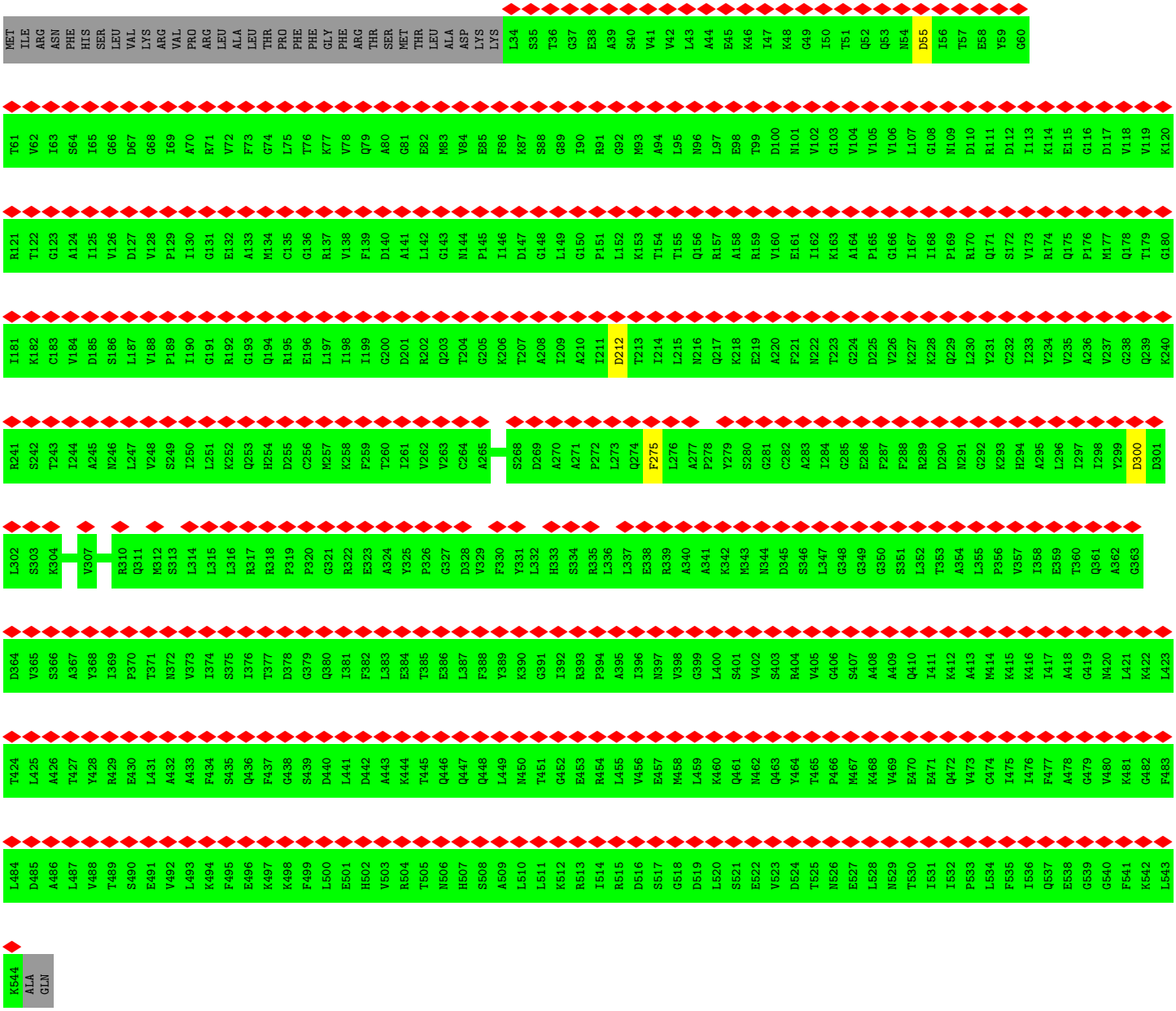




• Molecule 24: ATP synthase subunit alpha

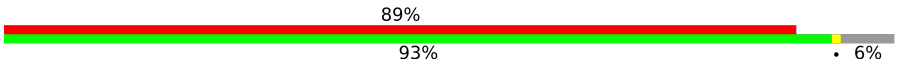
Chain B4:

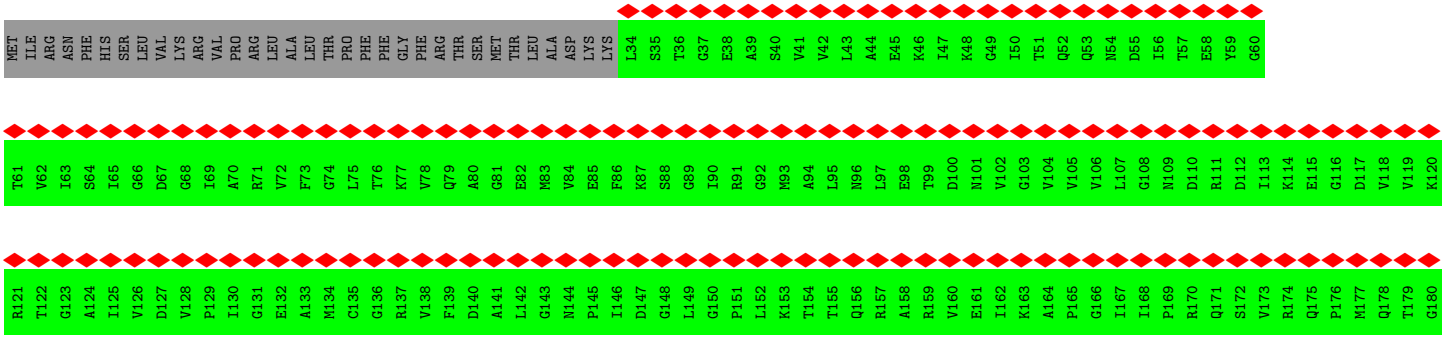


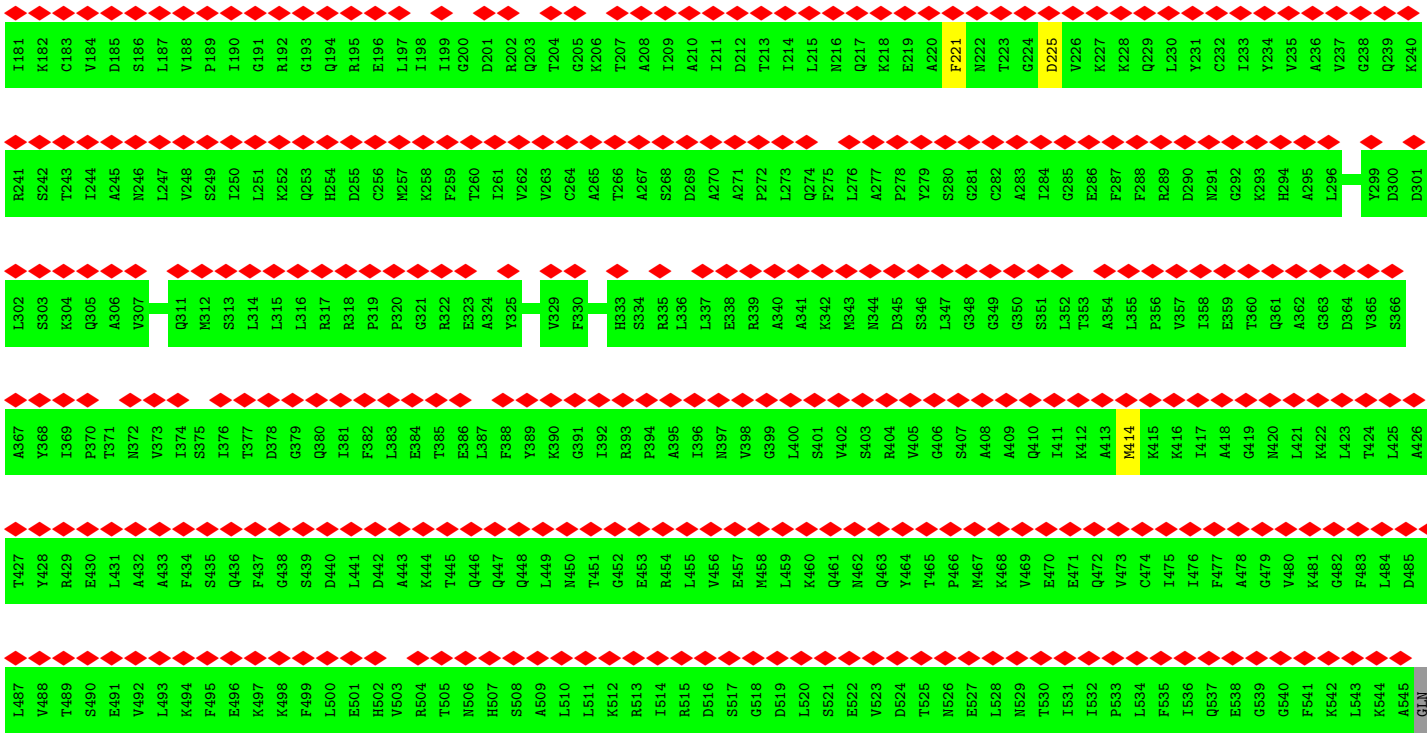


• Molecule 24: ATP synthase subunit alpha

Chain A4:

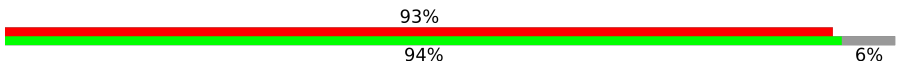


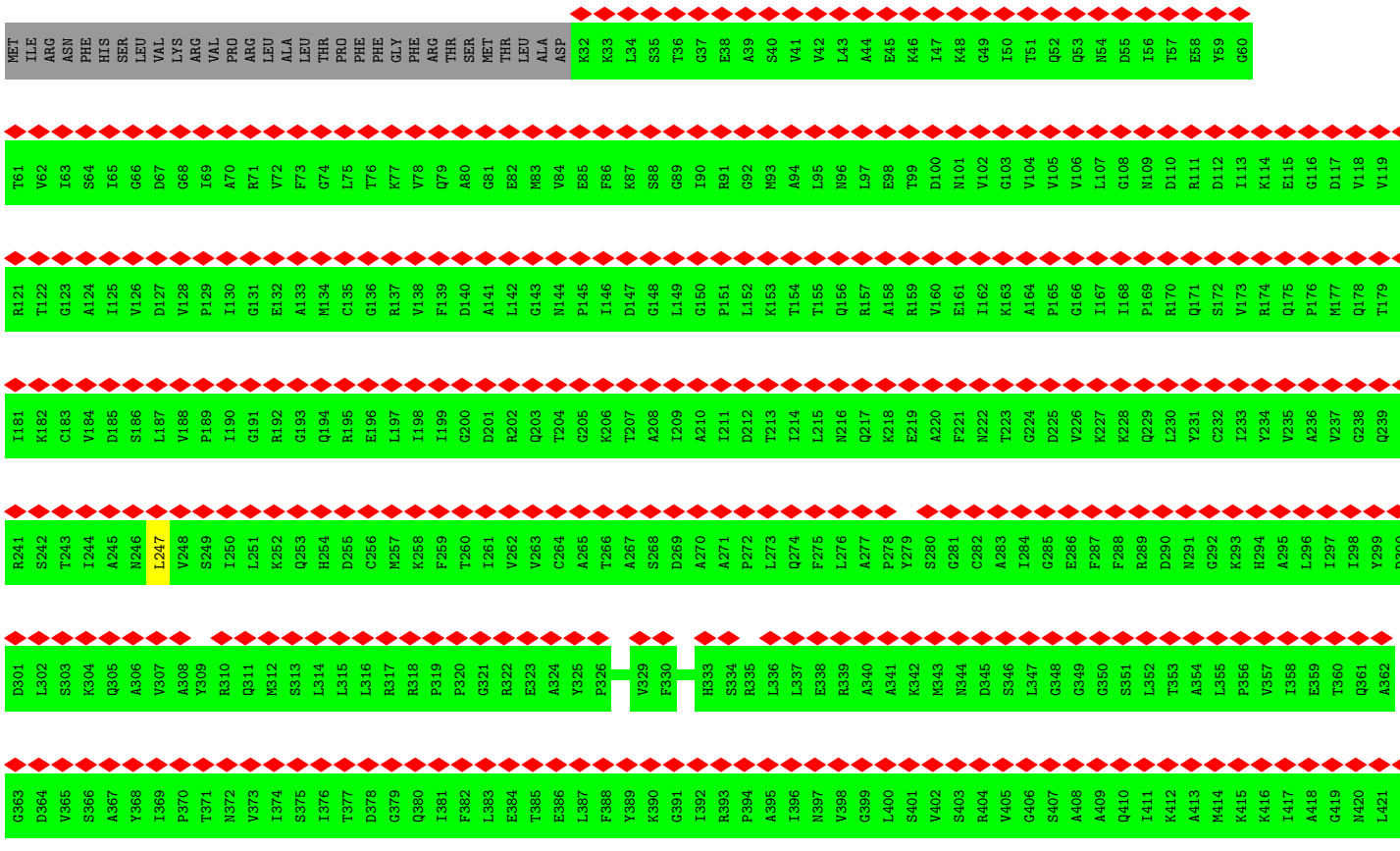


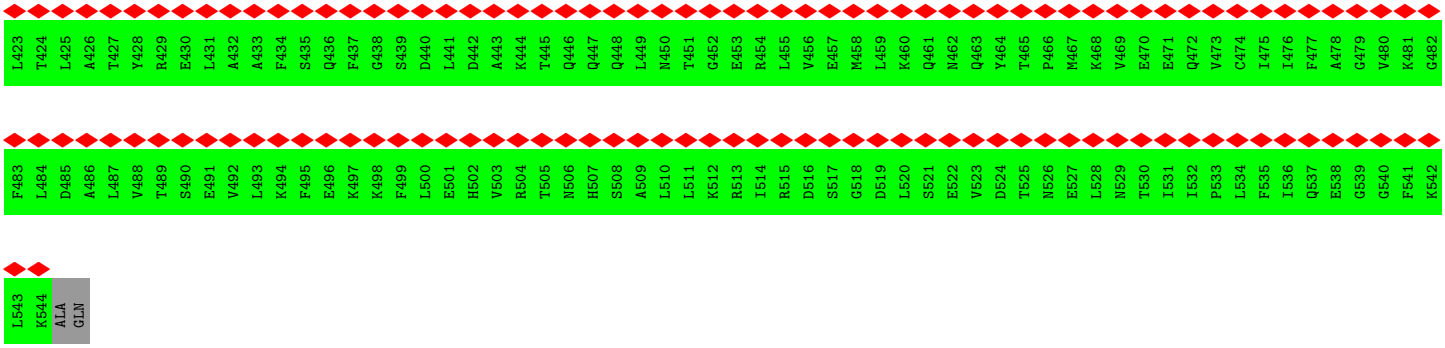


• Molecule 24: ATP synthase subunit alpha

Chain C5:

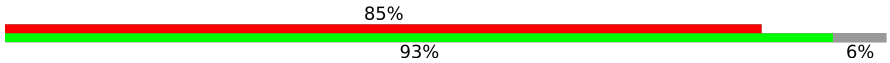






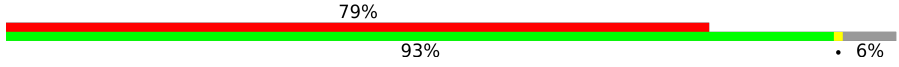
• Molecule 24: ATP synthase subunit alpha

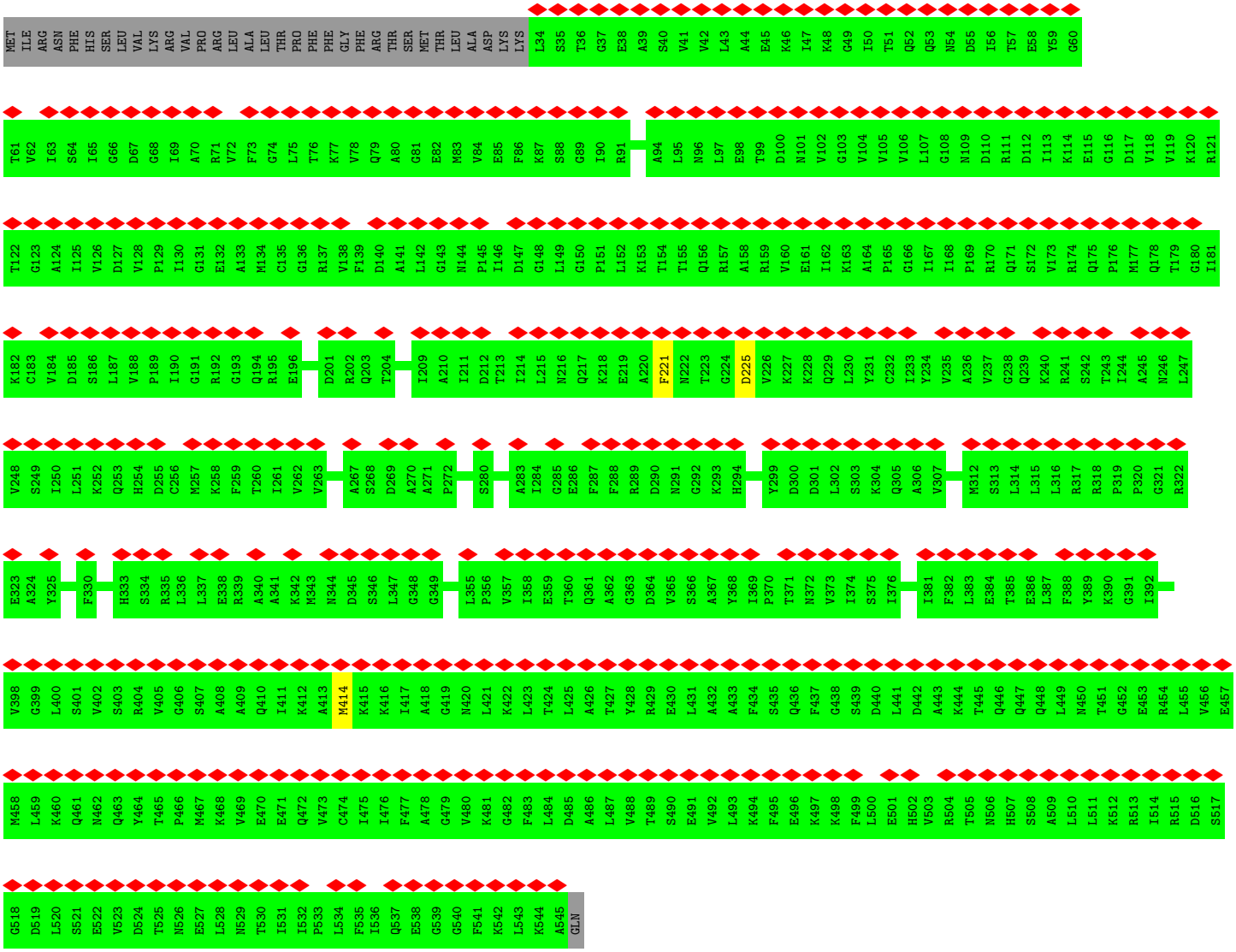
Chain B5:



• Molecule 24: ATP synthase subunit alpha

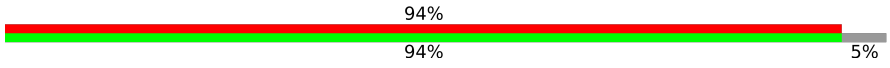
Chain A5:

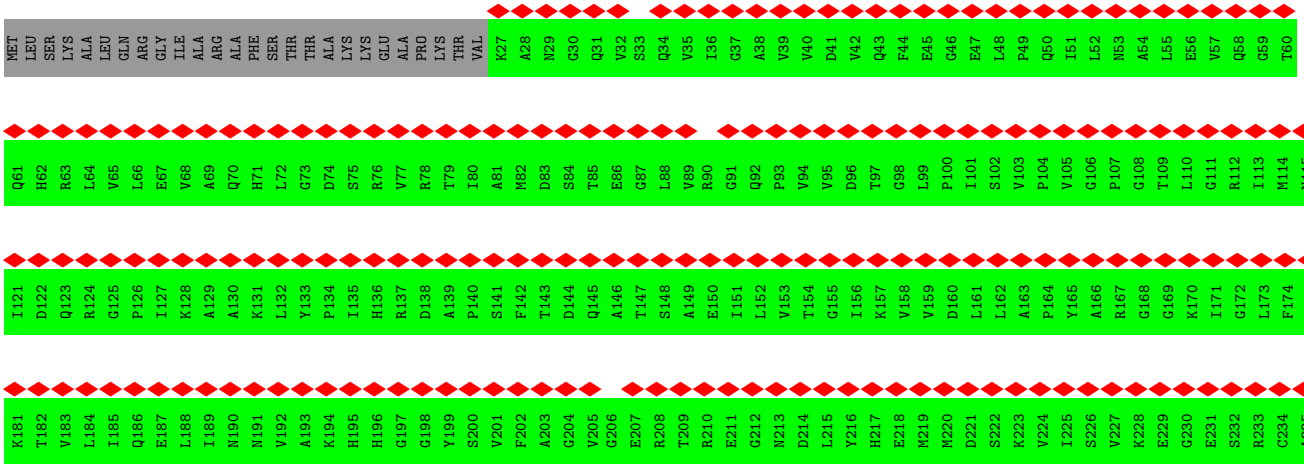


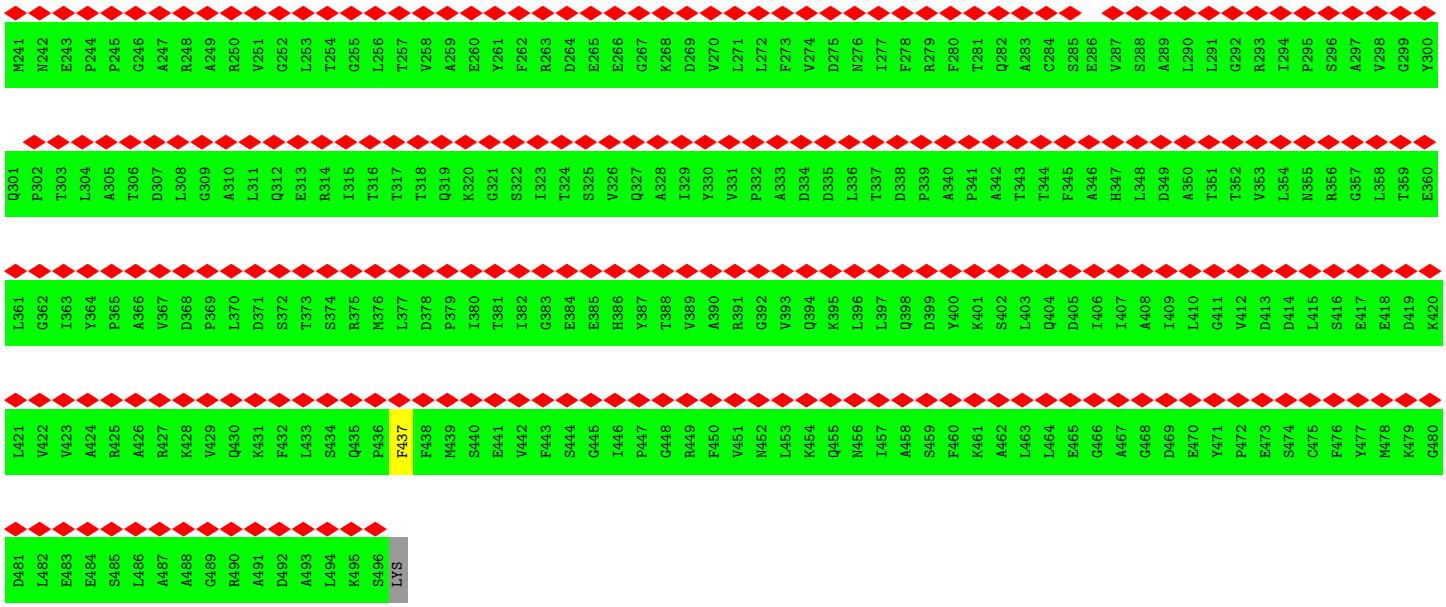


• Molecule 25: ATP synthase subunit beta

Chain D1:

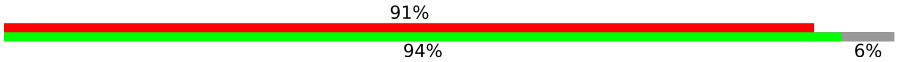


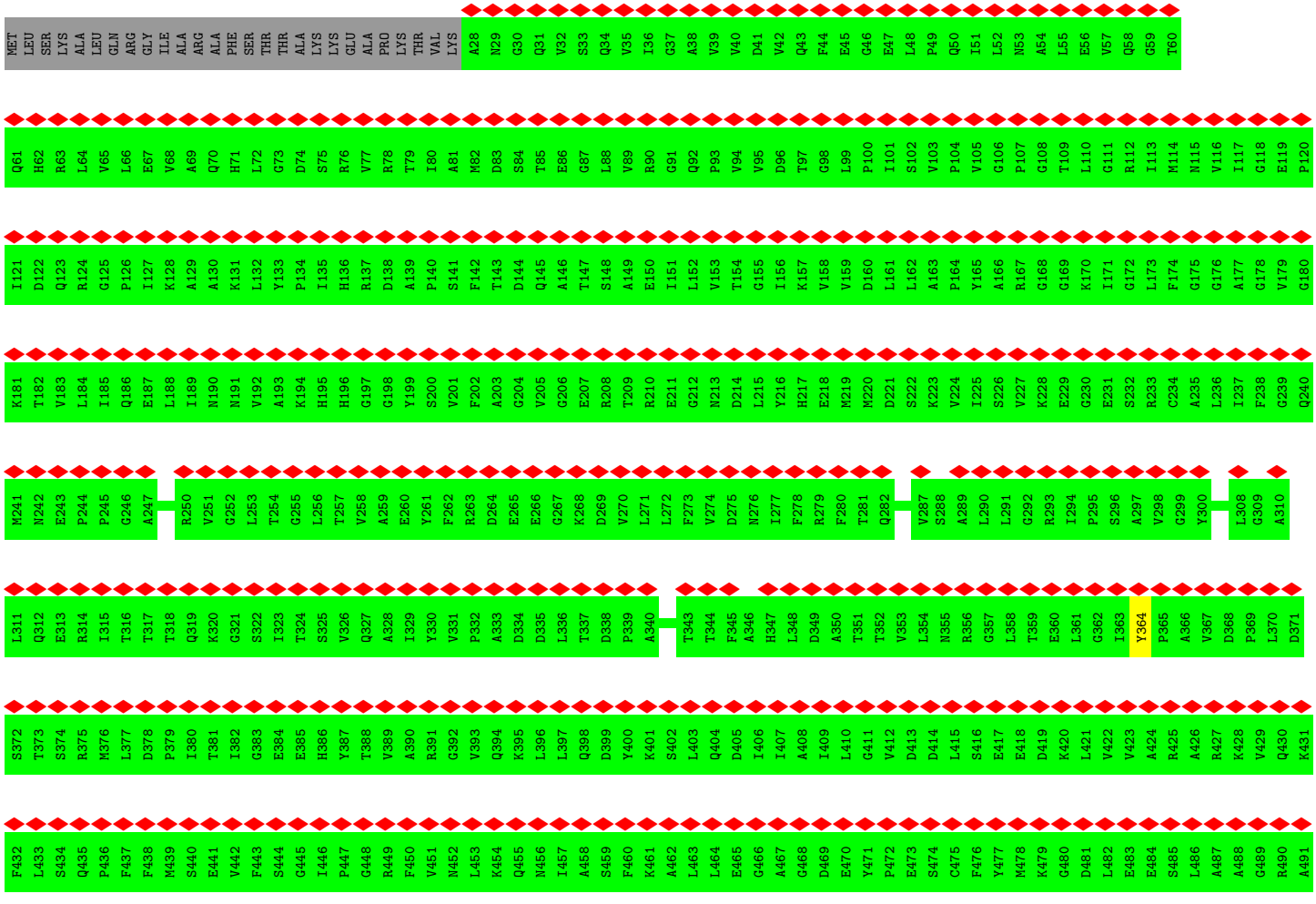


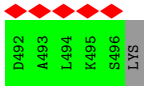


• Molecule 25: ATP synthase subunit beta

Chain F1:

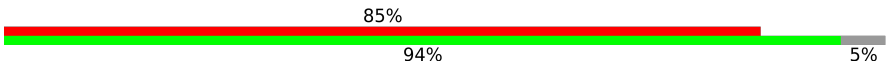


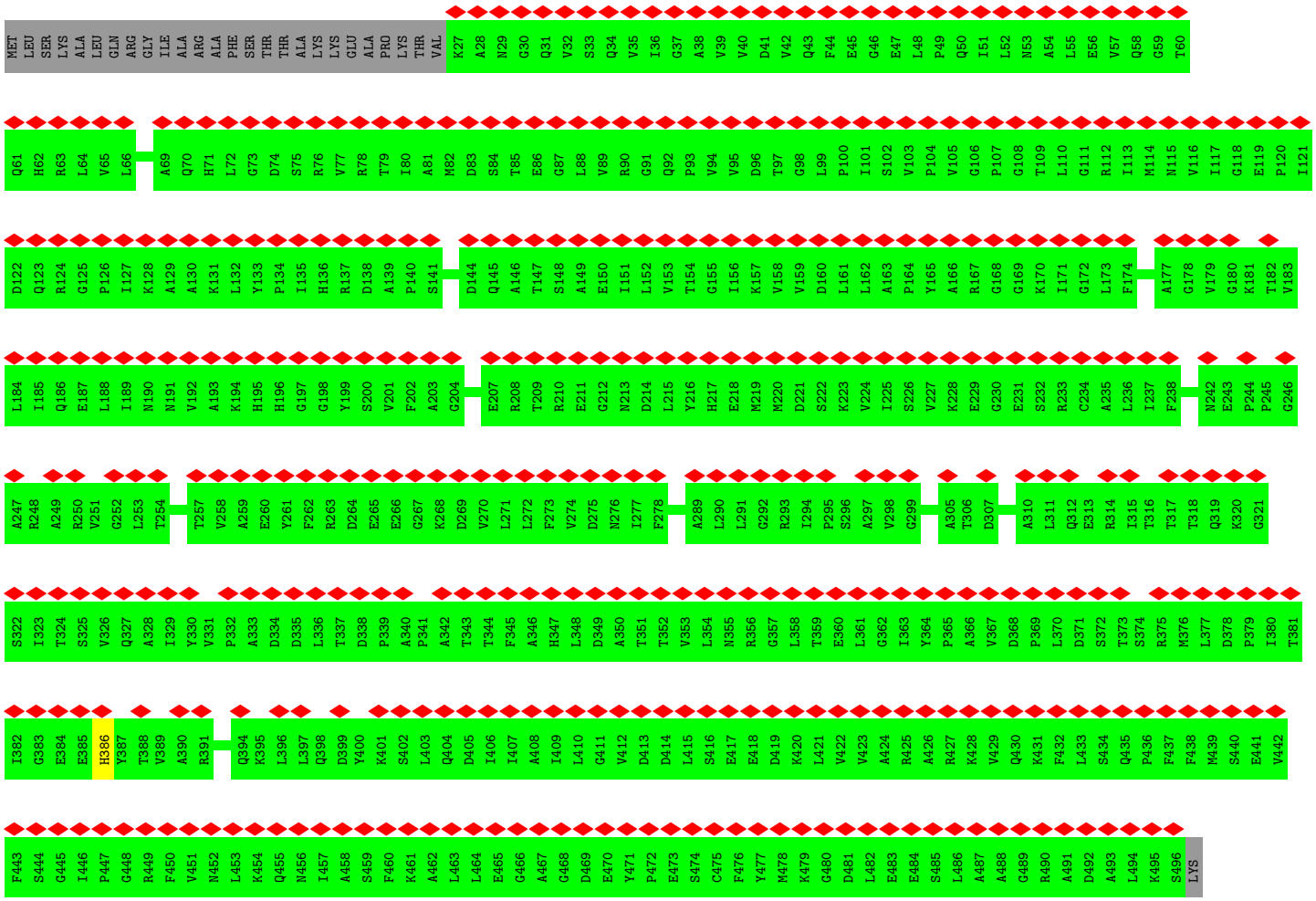




• Molecule 25: ATP synthase subunit beta

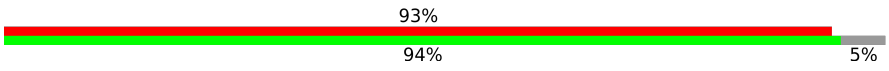
Chain E1:

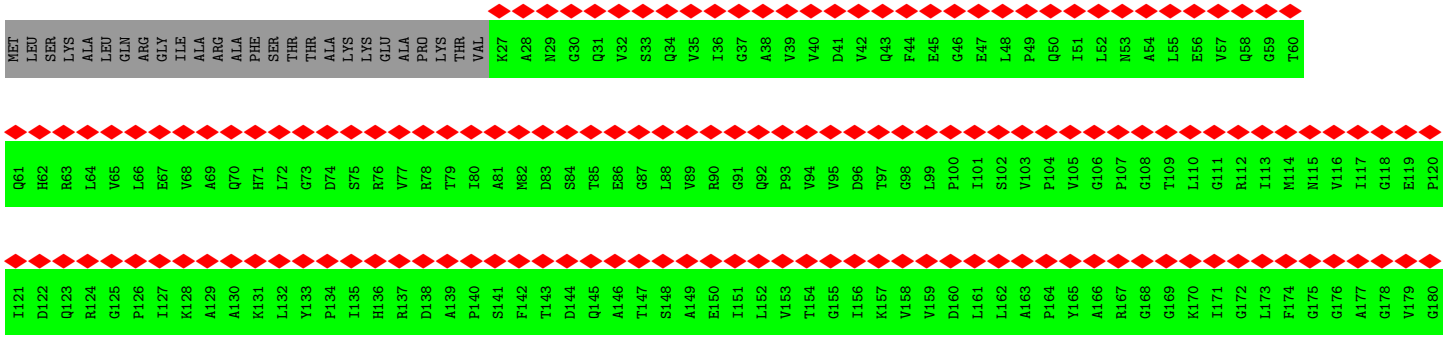




• Molecule 25: ATP synthase subunit beta

Chain D2:





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M241 N242 E243 P244 P245 G246 A247 R248 A249 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 K268 D269 V270 L271 L272 F273 V274 D275 N276 I277 F278 R279 F280 T281 Q282 A283 C284 S285 E286 V287 S288 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 Y300

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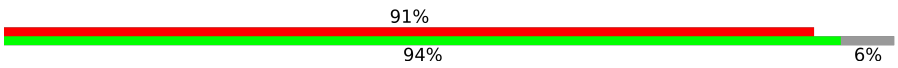
- Molecule 25: ATP synthase subunit beta

Chain F2:



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Q61 H62 R63 L64 V65 L66 E67 V68 A69 Q70 H71 L72 G73 D74 S75 R76 V77 R78 T79 I80 A81 M82 D83 S84 T85 E86 G87 L88 V89 R90 G91 Q92 P93 V94 V95 D96 T97 G98 L99 P100 I101 S102 V103 P104 V105 G106 P107 G108 T109 L110 G111 R112 I113 M114 N115 V116 I117 G118 E119 P120

I121 D122 Q123 R124 G125 P126 I127 K128 A129 A130 K131 L132 Y133 P134 I135 H136 R137 D138 A139 P140 S141 F142 T143 D144 Q145 A146 T147 S148 A149 E150 I151 L152 V153 T154 G155 I156 K157 V158 V159 D160 L161 L162 A163 P164 Y165 A166 R167 G168 G169 K170 I171 G172 L173 F174 G175 G176 A177 G178 V179 G180

K181 T182 V183 L184 I185 Q186 E187 L188 I189 N190 N191 V192 A193 K194 H195 H196 G197 G198 Y199 S200 V201 F202 A203 G204 V205 G206 E207 R208 T209 R210 E211 G212 N213 D214 L215 Y216 H217 E218 M219 M220 D221 S222 K223 V224 I225 S226 V227 K228 E229 G230 E231 S232 R233 C234 A235 L236 I237 F238 G239 Q240

M241 N242 E243 P244 P245 G246 A247 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 K268 D269 V270 L271 L272 F273 V274 D275 N276 I277 F278 R279 F280 T281 Q282 V287 S288 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 Y300 L304 L308

G309 A310 L311 Q312 E313 R314 I315 T316 T317 T318 Q319 K320 G321 S322 I323 T324 S325 V326 Q327 A328 I329 Y330 V331 P332 A333 D334 D335 L336 T337 D338 P339 A340 P341 A342 T343 T344 F345 A346 H347 L348 D349 A350 T351 T352 V353 L354 N355 R356 G357 L358 T359 E360 L361 G362 I363 Y364 P365 A366 V367 D368

P369 L370 D371 S372 T373 S374 R375 M376 L377 D378 P379 I380 T381 I382 G383 E384 E385 H386 Y387 T388 V389 A390 R391 G392 V393 Q394 K395 L396 L397 Q398 D399 Y400 K401 S402 L403 Q404 D405 I406 I407 A408 I409 L410 G411 V412 D413 D414 L415 S416 E417 E418 D419 K420 L421 V422 V423 A424 R425 A426 R427 K428

V429 Q430 K431 F432 L433 S434 Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 C475 F476 Y477 M478 K479 G480 D481 L482 E483 E484 S485 L486 A487 A488

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• Molecule 25: ATP synthase subunit beta

Chain E2: 94% 94% 5%

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Q61 H62 R63 L64 V65 L66 E67 V68 A69 Q70 H71 L72 G73 D74 S75 R76 V77 R78 T79 I80 A81 M82 D83 S84 T85 E86 G87 L88 V89 R90 G91 Q92 P93 V94 V95 D96 T97 G98 L99 P100 I101 S102 V103 P104 V105 G106 P107 G108 T109 L110 G111 R112 I113 M114 N115 V116 I117 G118 E119 P120

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K181 T182 V183 L184 I185 Q186 E187 L188 I189 N190 N191 V192 A193 K194 H195 H196 G197 G198 Y199 S200 V201 F202 A203 G204 V205 G206 E207 R208 T209 R210 E211 G212 N213 D214 L215 Y216 H217 E218 M219 M220 D221 S222 K223 V224 I225 S226 V227 K228 E229 G230 E231 S232 R233 C234 A235 L236 I237 F238 G239 Q240

M241 N242 E243 P244 P245 G246 A247 R248 A249 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 K268 D269 V270 L271 L272 P273 V274 D275 N276 I277 F278 R279 P280 T281 Q282 A283 C284 S285 E286 V287 S288 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 Y300

Q301 P302 T303 L304 A305 T306 D307 L308 G309 A310 L311 Q312 E313 R314 I315 T316 T317 T318 Q319 K320 G321 S322 I323 T324 S325 V326 Q327 A328 I329 Y330 V331 P332 A333 D334 D335 L336 T337 D338 P339 A340 P341 A342 T343 T344 F345 A346 H347 L348 D349 A350 T351 T352 V353 L354 N355 R356 G357 L358 T359 E360

L361 G362 I363 Y364 P365 A366 V367 D368 P369 L370 D371 S372 T373 S374 R375 M376 L377 D378 P379 I380 T381 I382 G383 E384 E385 H386 Y387 T388 V389 A390 R391 G392 V393 Q394 K395 L396 L397 Q398 D399 Y400 K401 S402 L403 Q404 D405 I406 I407 A408 I409 L410 G411 V412 D413 D414 L415 S416 E417 E418 D419 K420

L421 V422 V423 A424 R425 A426 R427 K428 V429 Q430 K431 F432 L433 S434 Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 C475 F476 Y477 M478 K479 G480

D481 L482 E483 E484 S485 L486 A487 A488 G489 R490 A491 D492 A493 L494 K495 S496 LYS

• Molecule 25: ATP synthase subunit beta

Chain D4: 93% 94% 5%

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Q61 H62 R63 L64 V65 L66 E67 V68 A69 Q70 H71 L72 G73 D74 S75 R76 V77 R78 T79 I80 A81 M82 D83 S84 T85 E86 G87 L88 V89 R90 G91 Q92 P93 V94 V95 D96 T97 G98 L99 P100 I101 S102 V103 P104 V105 G106 P107 G108 T109 L110 G111 R112 I113 M114 N115 V116 I117 G118 E119 P120

I121 D122 Q123 R124 G125 P126 I127 K128 A129 A130 K131 L132 Y133 P134 I135 H136 R137 D138 A139 P140 S141 F142 T143 D144 Q145 A146 T147 S148 A149 E150 I151 L152 V153 T154 G155 I156 K157 V158 V159 D160 L161 L162 A163 P164 Y165 A166 R167 G168 G169 K170 I171 G172 L173 F174 G175 G176 A177 G178 V179 G180

K181 T182 V183 L184 I185 Q186 E187 L188 I189 N190 N191 V192 A193 K194 H195 H196 G197 G198 Y199 S200 V201 F202 A203 G204 V205 G206 E207 R208 T209 R210 E211 G212 N213 D214 L215 Y216 H217 E218 M219 M220 D221 S222 K223 V224 I225 S226 V227 K228 E229 G230 E231 S232 R233 C234 A235 L236 I237 F238 G239 Q240

M241 N242 E243 P244 P245 G246 A247 R248 A249 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 K268 D269 V270 L271 L272 F273 V274 D275 N276 I277 F278 R279 F280 T281 Q282 A283 C284 S285 E286 V287 S288 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 Y300

T303 L304 A305 T306 D307 L308 G309 A310 L311 Q312 E313 R314 I315 T316 T317 T318 Q319 K320 G321 S322 I323 T324 S325 V326 Q327 A328 I329 Y330 V331 P332 A333 D334 D335 L336 T337 D338 P339 A340 P341 A342 T343 T344 F345 A346 H347 L348 D349 A350 T351 T352 V353 L354 N355 R356 G357 L358 T359 E360 L361

G362 I363 Y364 P365 A366 V367 D368 P369 L370 D371 S372 T373 S374 R375 M376 L377 D378 P379 I380 T381 I382 G383 E384 E385 H386 Y387 T388 V389 A390 R391 G392 V393 Q394 K395 L396 L397 Q398 D399 Y400 K401 S402 L403 Q404 D405 I406 I407 A408 I409 L410 G411 V412 D413 D414 L415 S416 E417 E418 D419 K420 L421

V422 V423 A424 R425 A426 R427 K428 V429 Q430 K431 F432 L433 S434 Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 C475 F476 Y477 M478 K479 G480 D481

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• Molecule 25: ATP synthase subunit beta

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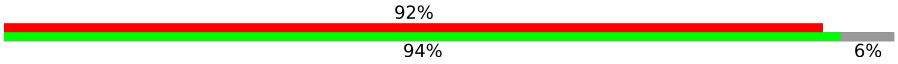

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Q61 H62 R63 L64 V65 L66 E67 V68 A69 Q70 H71 L72 G73 D74 S75 R76 V77 R78 T79 I80 A81 M82 D83 S84 T85 E86 G87 L88 V89 R90 G91 Q92 P93 V94 V95 D96 T97 G98 L99 P100 I101 S102 V103 P104 V105 G106 P107 G108 T109 L110 G111 R112 I113 M114 N115 V116 I117 G118 E119 P120

I121 D122 Q123 R124 G125 P126 I127 K128 A129 A130 K131 L132 Y133 P134 I135 H136 R137 D138 A139 P140 S141 F142 T143 D144 Q145 A146 T147 S148 A149 E150 I151 L152 V153 T154 G155 I156 K157 V158 V159 D160 L161 L162 A163 P164 Y165 A166 R167 G168 G169 K170 I171 G172 L173 F174 G175 G176 A177 G178 V179 G180

K181 T182 V183 L184 I185 Q186 E187 L188 I189 N190 N191 V192 A193 K194 H195 H196 G197 G198 Y199 S200 V201 F202 A203 G204 V205 G206 E207 R208 T209 R210 E211 G212 N213 D214 L215 Y216 H217 E218 M219 M220 D221 S222 K223 V224 I225 S226 V227 K228 E229 G230 E231 S232 R233 C234 A235 L236 I237 F238 G239 Q240

M241 N242 E243 P244 P245 G246 A247 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 K268 D269 V270 L271 L272 F273 V274 D275 N276 I277 F278 R279 F280 T281 Q282 V287 S288 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 Y300 L304 A305 T306

D307 L308 G309 A310 L311 Q312 E313 R314 I315 T316 T317 T318 Q319 K320 G321 S322 I323 T324 S325 V326 Q327 A328 I329 Y330 V331 P332 A333 D334 D335 L336 T337 D338 P339 A340 P341 A342 T343 T344 F345 A346 H347 L348 D349 A350 T351 T352 V353 L354 N355 R356 G357 L358 T359 E360 L361 G362 I363 Y364 P365 A366

V367 D368 P369 L370 D371 S372 T373 S374 R375 M376 L377 D378 P379 I380 T381 I382 G383 E384 E385 H386 Y387 T388 V389 A390 R391 G392 V393 Q394 K395 L396 L397 Q398 D399 Y400 K401 S402 L403 Q404 D405 I406 I407 A408 I409 L410 G411 V412 D413 D414 L415 S416 E417 E418 D419 K420 L421 V422 V423 A424 R425 A426

R427 K428 V429 Q430 K431 F432 L433 S434 Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 C475 F476 Y477 M478 K479 G480 D481 L482 E483 E484 S485 L486

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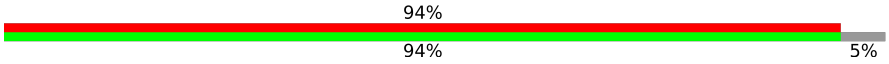
- Molecule 25: ATP synthase subunit beta

Chain E4:



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I121 D122 Q123 R124 G125 P126 I127 K128 A129 A130 K131 L132 Y133 P134 I135 H136 R137 D138 A139 P140 S141 F142 T143 D144 Q145 A146 T147 S148 A149 E150 I151 L152 V153 T154 G155 I156 K157 V158 V159 D160 L161 L162 A163 P164 Y165 A166 R167 G168 G169 K170 I171 G172 L173 F174 G175 G176 A177 G178 V179 G180

K181 T182 V183 L184 I185 Q186 E187 L188 I189 N190 N191 V192 A193 K194 H195 H196 G197 G198 Y199 S200 V201 F202 A203 G204 V205 G206 E207 R208 T209 R210 E211 G212 N213 D214 L215 Y216 H217 E218 M219 M220 D221 S222 K223 V224 I225 S226 V227 K228 E229 G230 E231 S232 R233 C234 A235 L236 I237 F238 G239 Q240

M241 N242 E243 P244 P245 G246 A247 R248 A249 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 K268 D269 V270 L271 L272 F273 V274 D275 N276 I277 F278 R279 F280 T281 Q282 A283 C284 S285 E286 V287 S288 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 Y300

Q301 P302 T303 L304 A305 T306 D307 L308 G309 A310 L311 Q312 E313 R314 I315 T316 T317 T318 Q319 K320 G321 S322 I323 T324 S325 V326 Q327 A328 I329 Y330 V331 P332 A333 D334 D335 L336 T337 D338 P339 A340 P341 A342 T343 T344 F345 A346 H347 L348 D349 A350 T351 T352 V353 L354 N355 R356 G357 L358 T359 E360

L361 G362 I363 Y364 P365 A366 V367 D368 P369 L370 D371 S372 T373 S374 R375 M376 L377 D378 P379 I380 T381 I382 G383 E384 E385 H386 Y387 T388 V389 A390 R391 G392 V393 Q394 K395 L396 L397 Q398 D399 Y400 K401 S402 L403 Q404 D405 I406 I407 A408 I409 L410 G411 V412 D413 D414 L415 S416 E417 E418 D419 K420

L421 V422 V423 A424 R425 A426 R427 K428 V429 Q430 K431 F432 L433 S434 Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 C475 F476 Y477 M478 K479 G480

D481 L482 E483 E484 S485 L486 A487 A488 G489 R490 A491 D492 A493 L494 K495 S496 LYS

• Molecule 25: ATP synthase subunit beta

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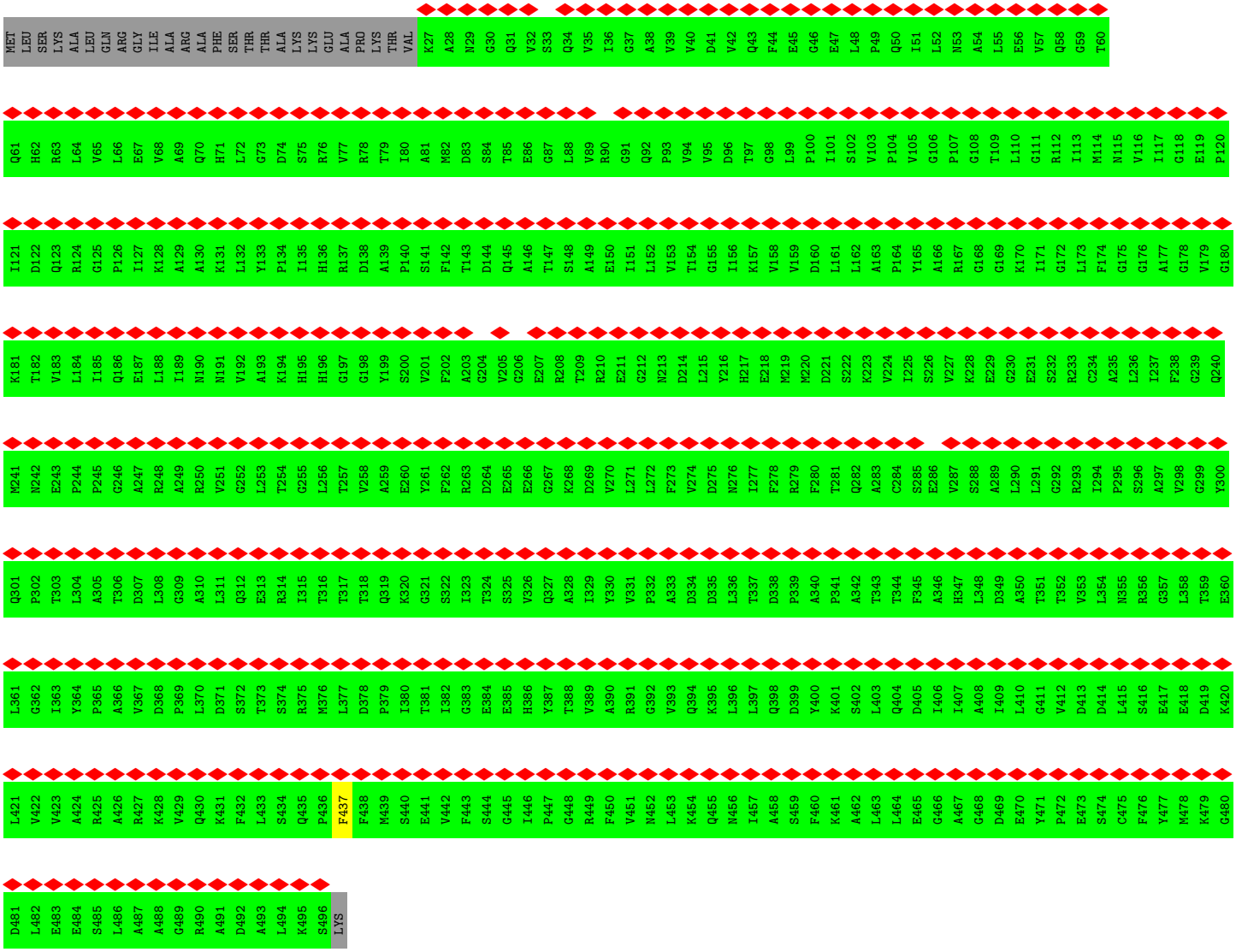

• Molecule 25: ATP synthase subunit beta

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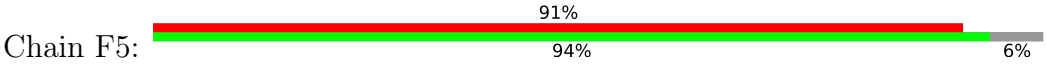

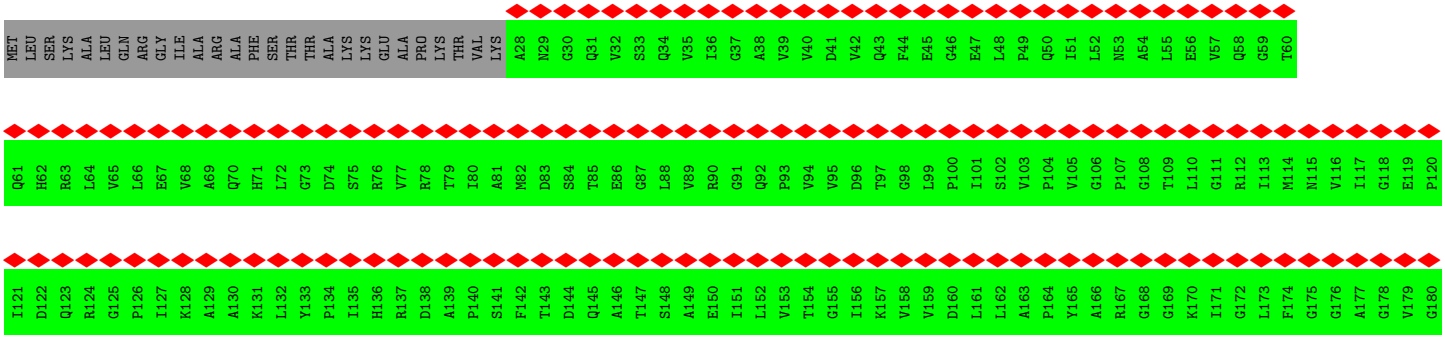

• Molecule 25: ATP synthase subunit beta

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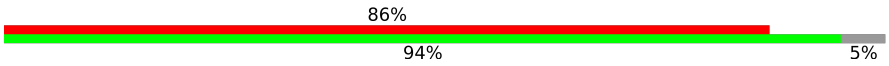
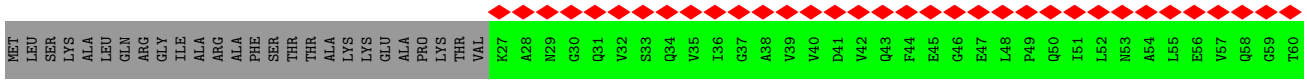
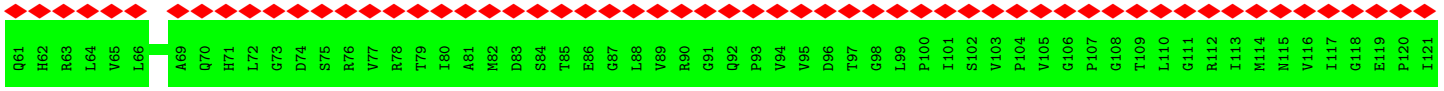
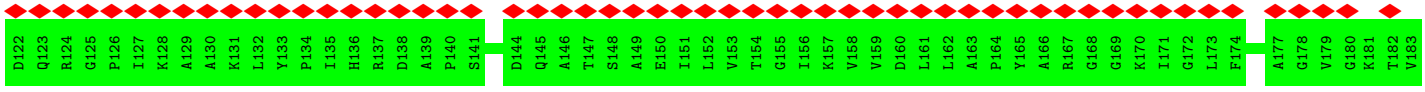
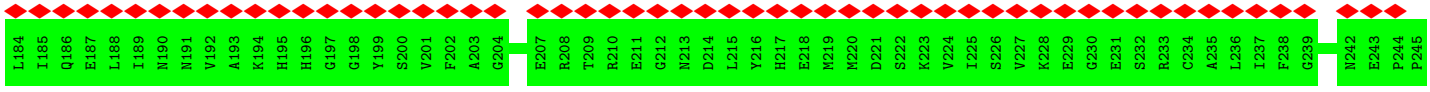
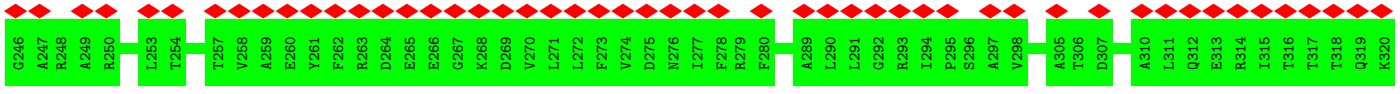


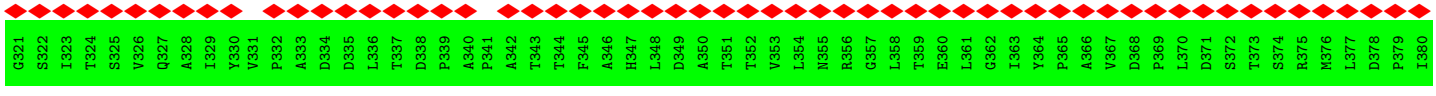


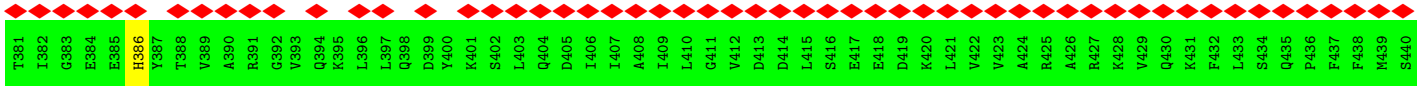


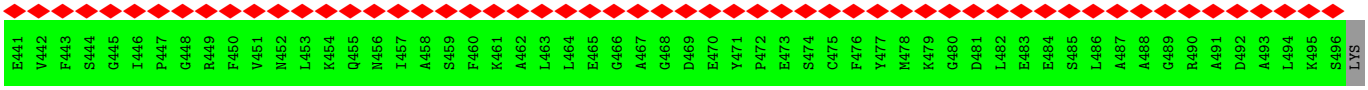






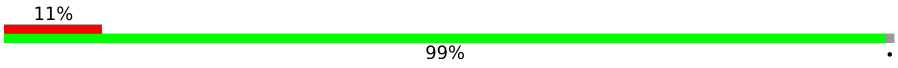


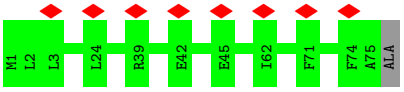




• Molecule 26: ATP synthase F0 subunit 9

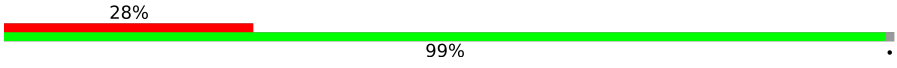
Chain P1:

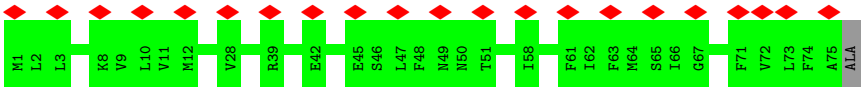




• Molecule 26: ATP synthase F0 subunit 9

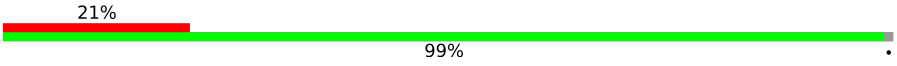
Chain O1:

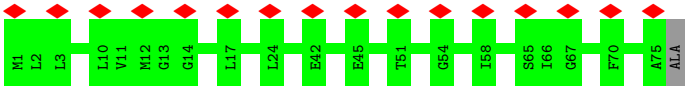




• Molecule 26: ATP synthase F0 subunit 9

Chain N1:





• Molecule 26: ATP synthase F0 subunit 9

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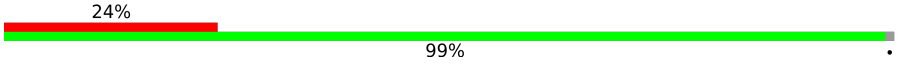
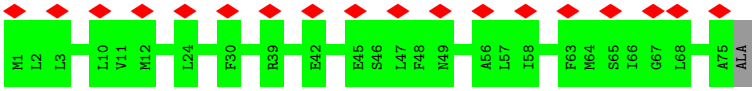
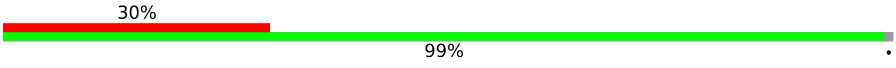
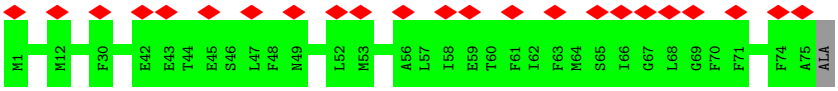




• Molecule 26: ATP synthase F0 subunit 9

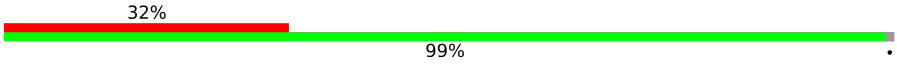
Chain L1:

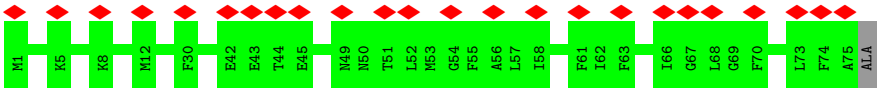




• Molecule 26: ATP synthase F0 subunit 9

Chain K1:





• Molecule 26: ATP synthase F0 subunit 9

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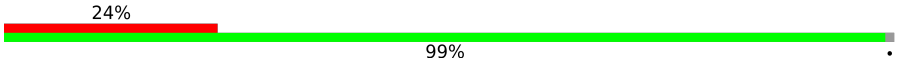

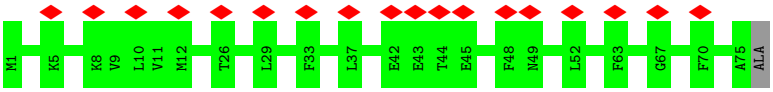

• Molecule 26: ATP synthase F0 subunit 9

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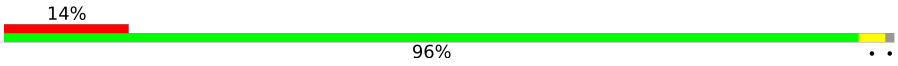
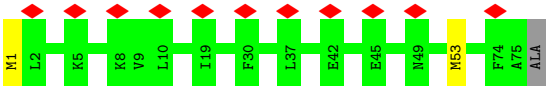
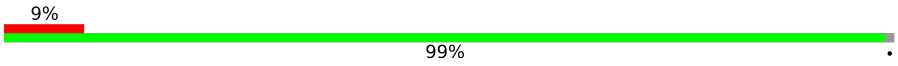
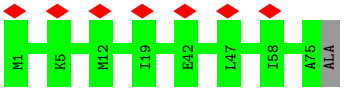




• Molecule 26: ATP synthase F0 subunit 9

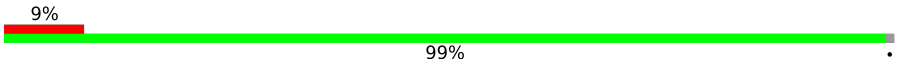
Chain H1:

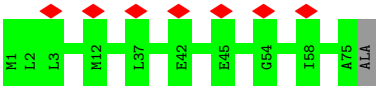




• Molecule 26: ATP synthase F0 subunit 9

Chain Q1:





• Molecule 26: ATP synthase F0 subunit 9

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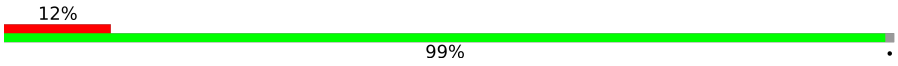
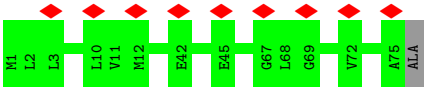
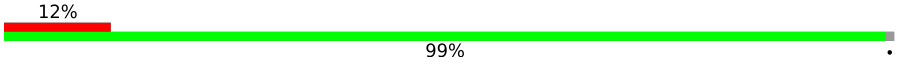
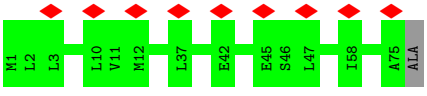




• Molecule 26: ATP synthase F0 subunit 9

Chain O2:





• Molecule 26: ATP synthase F0 subunit 9

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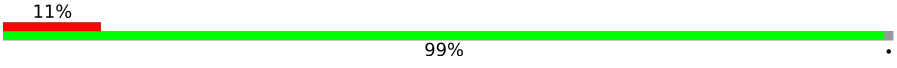

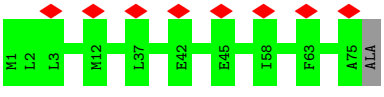

• Molecule 26: ATP synthase F0 subunit 9

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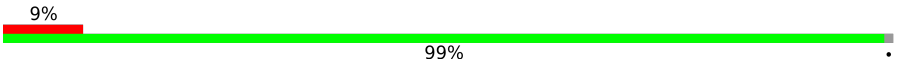
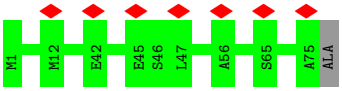
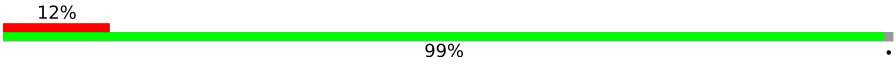
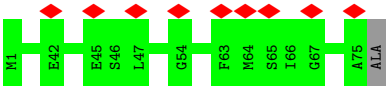




• Molecule 26: ATP synthase F0 subunit 9

Chain L2:





• Molecule 26: ATP synthase F0 subunit 9

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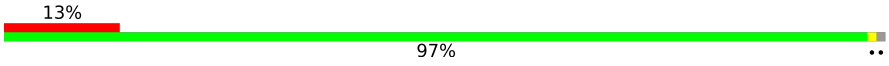

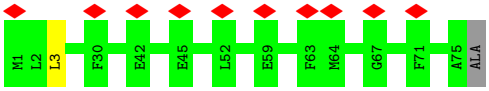

• Molecule 26: ATP synthase F0 subunit 9

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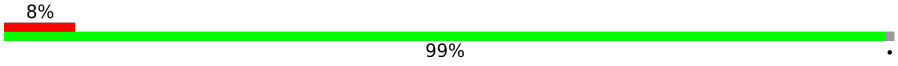

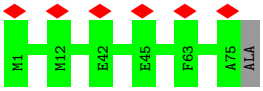

• Molecule 26: ATP synthase F0 subunit 9

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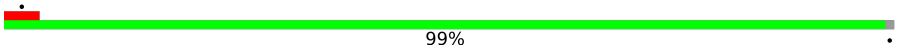

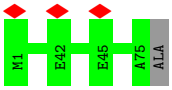

• Molecule 26: ATP synthase F0 subunit 9

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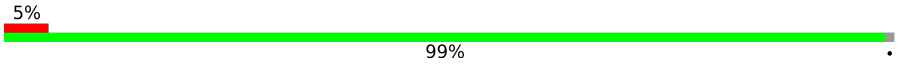

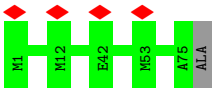

• Molecule 26: ATP synthase F0 subunit 9

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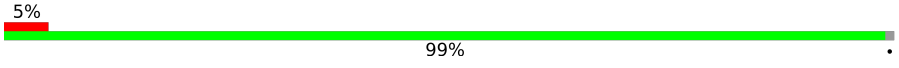

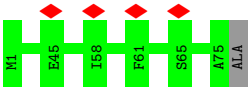

• Molecule 26: ATP synthase F0 subunit 9

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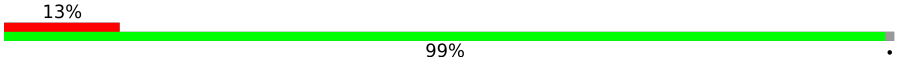

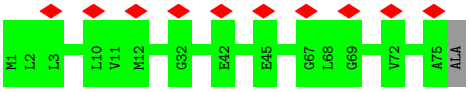

• Molecule 26: ATP synthase F0 subunit 9

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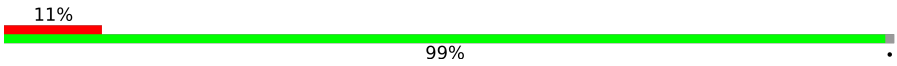

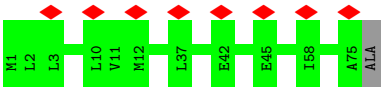

• Molecule 26: ATP synthase F0 subunit 9

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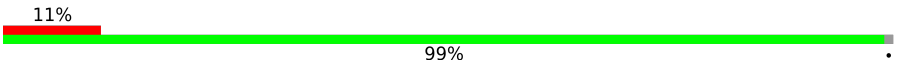

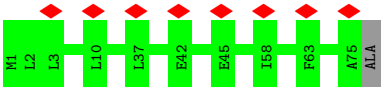

• Molecule 26: ATP synthase F0 subunit 9

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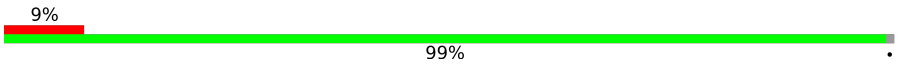

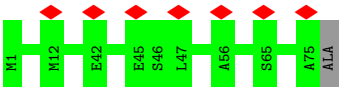

• Molecule 26: ATP synthase F0 subunit 9

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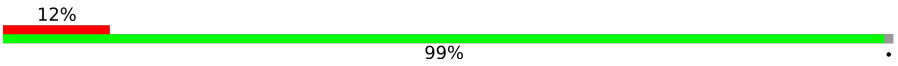

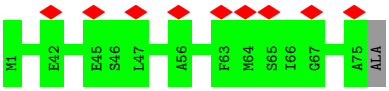

• Molecule 26: ATP synthase F0 subunit 9

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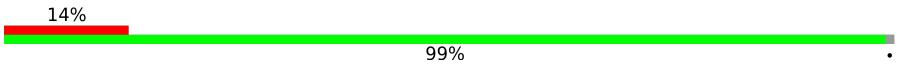

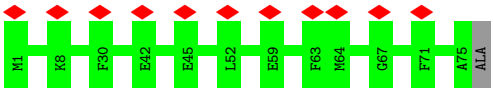

• Molecule 26: ATP synthase F0 subunit 9

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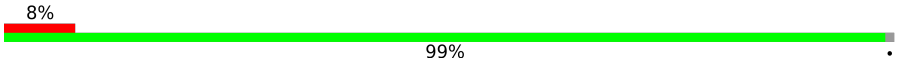
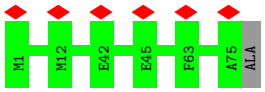
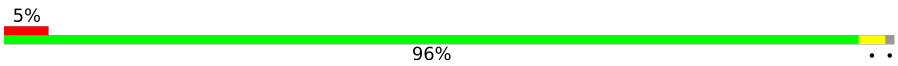
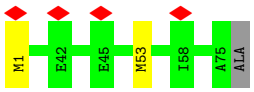




• Molecule 26: ATP synthase F0 subunit 9

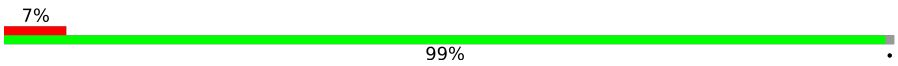
Chain I4:

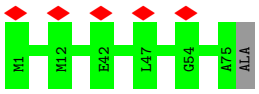




• Molecule 26: ATP synthase F0 subunit 9

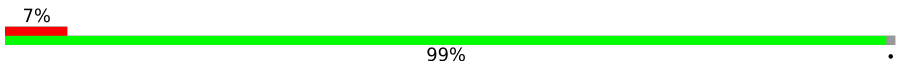
Chain H4:

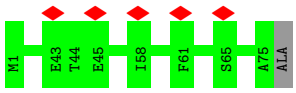




• Molecule 26: ATP synthase F0 subunit 9

Chain Q4:





• Molecule 26: ATP synthase F0 subunit 9

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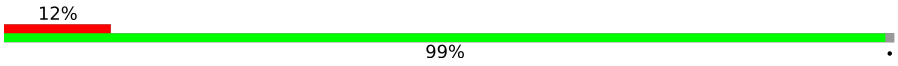
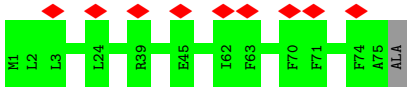
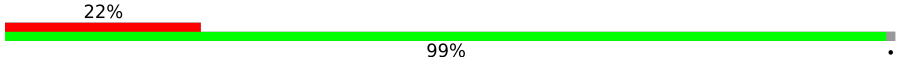
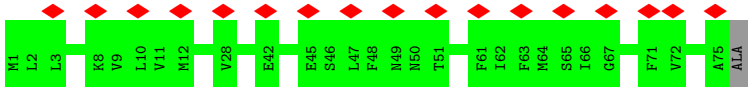




• Molecule 26: ATP synthase F0 subunit 9

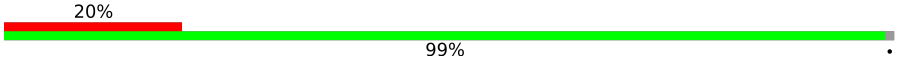
Chain O5:

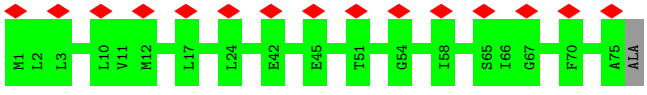




• Molecule 26: ATP synthase F0 subunit 9

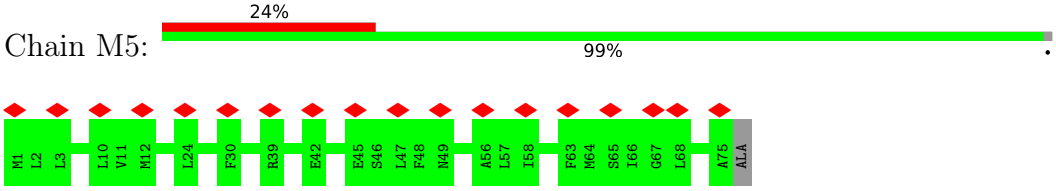
Chain N5:





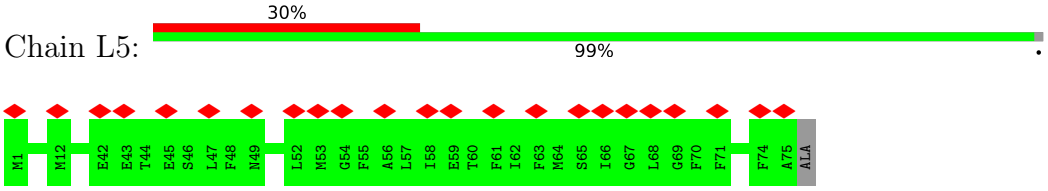
• Molecule 26: ATP synthase F0 subunit 9

Chain M5:



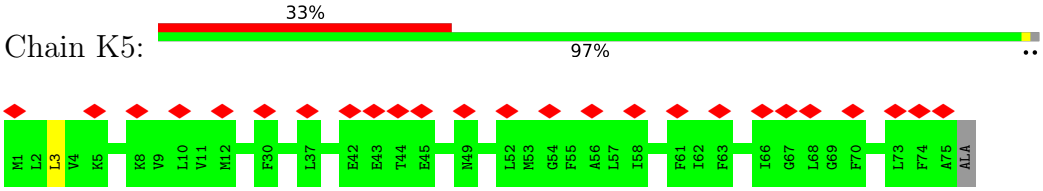
• Molecule 26: ATP synthase F0 subunit 9

Chain L5:



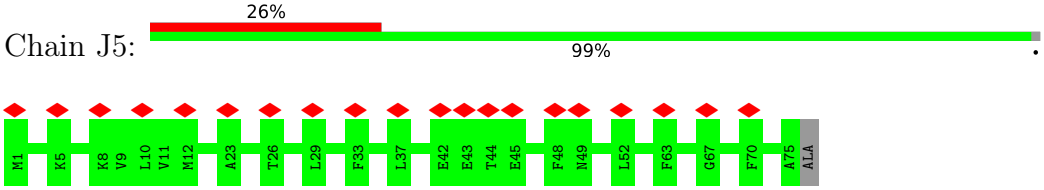
• Molecule 26: ATP synthase F0 subunit 9

Chain K5:



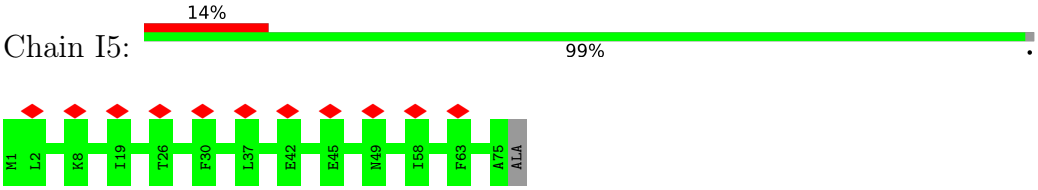
• Molecule 26: ATP synthase F0 subunit 9

Chain J5:



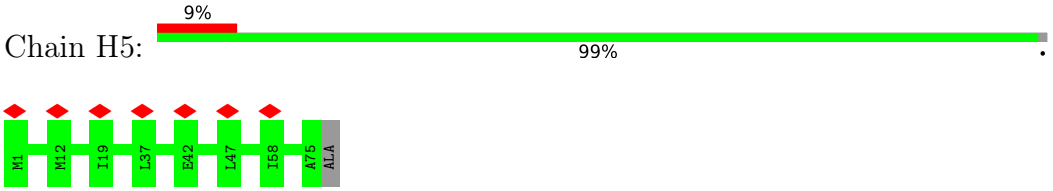
• Molecule 26: ATP synthase F0 subunit 9

Chain I5:



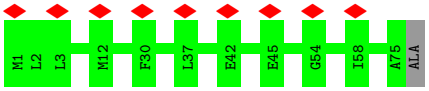
• Molecule 26: ATP synthase F0 subunit 9

Chain H5:



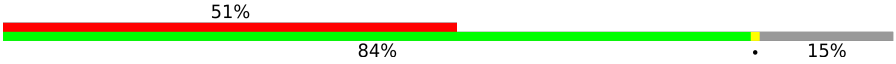
• Molecule 26: ATP synthase F0 subunit 9

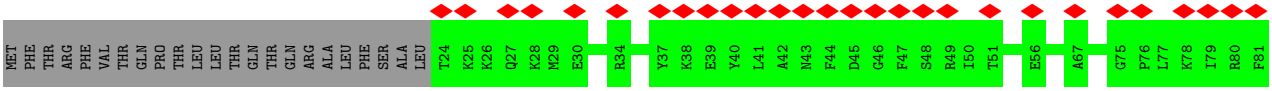
Chain Q5:



• Molecule 27: subunit delta

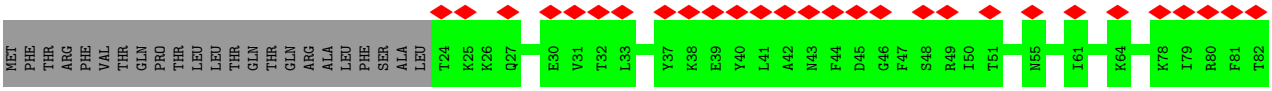
Chain d1:

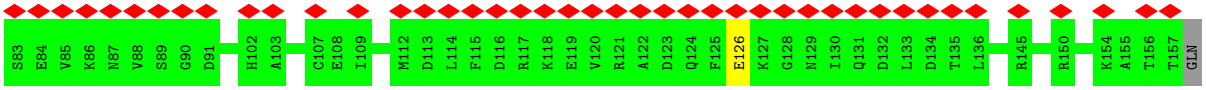




• Molecule 27: subunit delta

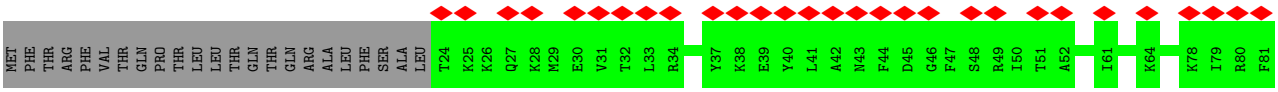
Chain d2:

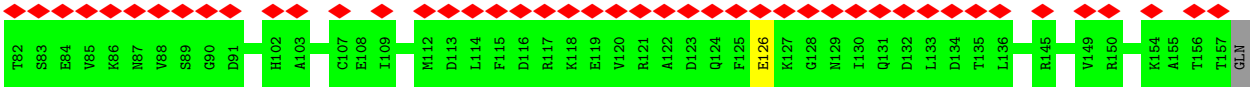




• Molecule 27: subunit delta

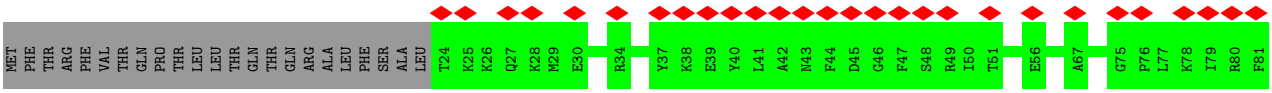
Chain d4:

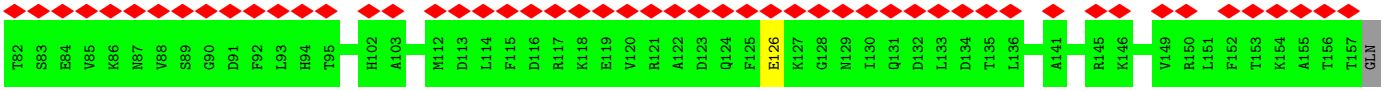




• Molecule 27: subunit delta

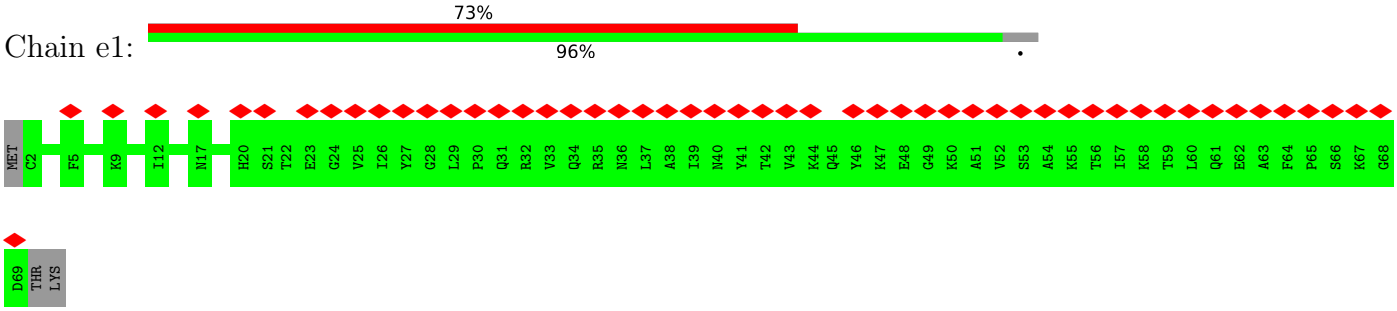
Chain d5:





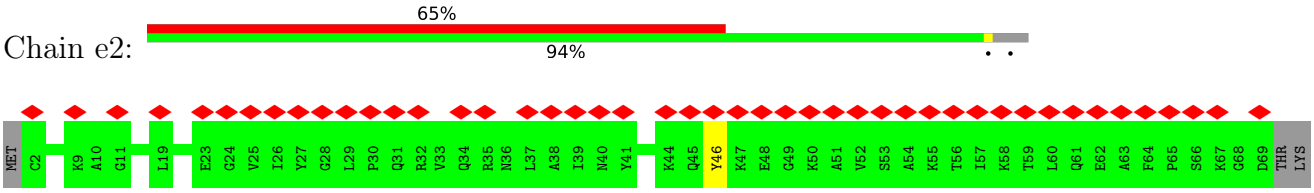
• Molecule 28: subunit epsilon

Chain e1:



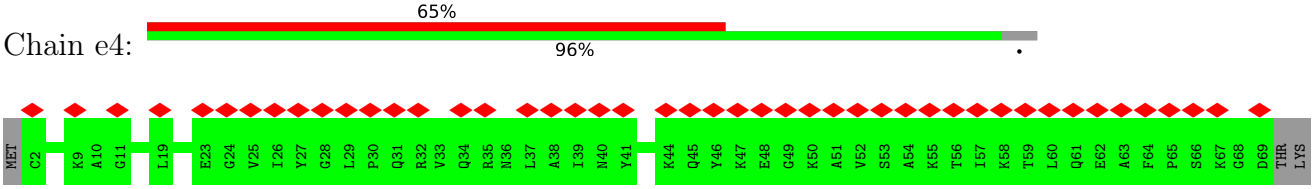
• Molecule 28: subunit epsilon

Chain e2:



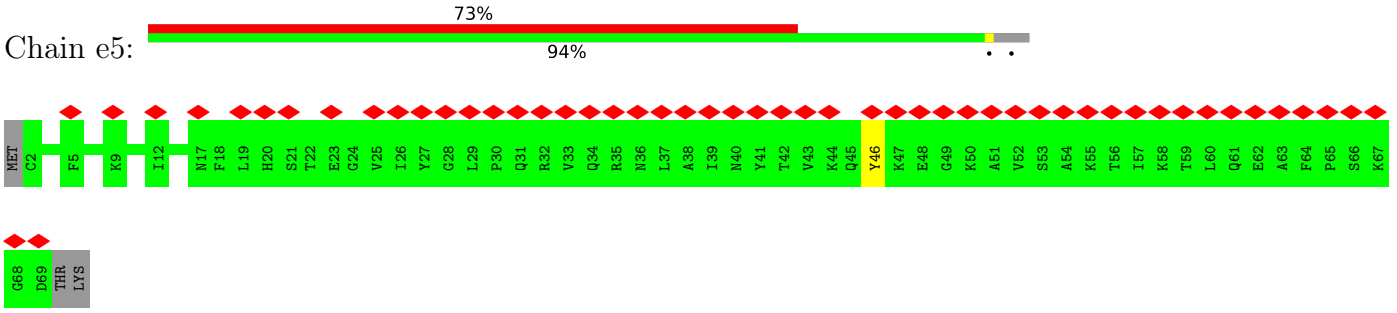
• Molecule 28: subunit epsilon

Chain e4:



• Molecule 28: subunit epsilon

Chain e5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	40691	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 ($e^-/Å^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAD, CDL, ADP, PEE, PC1, ATP, PO4, UQ8

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.29	0/3752	0.38	0/5109
1	A3	0.29	0/3752	0.38	0/5109
1	a	0.29	0/3752	0.38	0/5109
1	a3	0.30	0/3752	0.38	0/5109
2	B	0.26	0/2940	0.36	0/3969
2	B3	0.26	0/2940	0.36	0/3969
2	b	0.26	0/2940	0.36	0/3969
2	b3	0.26	0/2940	0.36	0/3969
3	D	0.26	0/1715	0.37	0/2321
3	D3	0.26	0/1715	0.37	0/2321
3	d	0.26	0/1715	0.37	0/2321
3	d3	0.26	0/1715	0.37	0/2321
4	F	0.29	0/1733	0.40	0/2327
4	F3	0.29	0/1733	0.39	0/2327
4	f	0.29	0/1733	0.39	0/2327
4	f3	0.29	0/1733	0.39	0/2327
5	I	0.29	0/1771	0.38	0/2394
5	I3	0.28	0/1771	0.38	0/2394
5	i	0.28	0/1771	0.39	0/2394
5	i3	0.29	0/1771	0.38	0/2394
6	K	0.26	0/1508	0.37	0/2024
6	K3	0.26	0/1508	0.37	0/2024
6	k	0.26	0/1508	0.38	0/2024
6	k3	0.26	0/1508	0.38	0/2024
7	C	0.28	0/866	0.39	0/1176
7	C3	0.27	0/866	0.39	0/1176
7	c	0.27	0/866	0.39	0/1176
7	c3	0.28	0/866	0.38	0/1176
8	G	0.28	0/2302	0.40	0/3115
8	G3	0.27	0/2302	0.40	0/3115
8	g	0.27	0/2302	0.40	0/3115
8	g3	0.28	0/2302	0.40	0/3115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
9	H	0.26	0/2006	0.39	0/2704
9	H3	0.26	0/2006	0.39	0/2704
9	h	0.25	0/2006	0.39	0/2704
9	h3	0.26	0/2006	0.38	0/2704
10	J	0.28	0/2256	0.40	0/3069
10	J3	0.27	0/2256	0.40	0/3069
10	j	0.27	0/2256	0.40	0/3069
10	j3	0.28	0/2256	0.40	0/3069
11	L	0.29	0/2140	0.39	0/2903
11	L3	0.29	0/2140	0.39	0/2903
11	l	0.29	0/2140	0.39	0/2903
11	l3	0.29	0/2140	0.38	0/2903
12	M	0.28	0/1912	0.37	0/2598
12	M3	0.27	0/1912	0.37	0/2598
12	m	0.27	0/1912	0.37	0/2598
12	m3	0.28	0/1912	0.37	0/2598
13	N	0.30	0/1030	0.39	0/1393
13	N3	0.29	0/1030	0.39	0/1393
13	n	0.29	0/1030	0.40	0/1393
13	n3	0.30	0/1030	0.40	0/1393
14	O	0.26	0/821	0.39	0/1104
14	O3	0.26	0/821	0.40	0/1104
14	o	0.27	0/821	0.40	0/1104
14	o3	0.26	0/821	0.40	0/1104
15	P	0.25	0/1249	0.37	0/1695
15	P3	0.24	0/1249	0.37	0/1695
15	p	0.24	0/1249	0.38	0/1695
15	p3	0.25	0/1249	0.38	0/1695
16	Q	0.26	0/888	0.39	0/1200
16	Q3	0.25	0/888	0.39	0/1200
16	q	0.25	0/888	0.39	0/1200
16	q3	0.26	0/888	0.39	0/1200
17	R	0.28	0/1185	0.38	0/1594
17	R3	0.28	0/1185	0.38	0/1594
17	r	0.28	0/1225	0.38	0/1649
17	r3	0.29	0/1225	0.38	0/1649
18	S	0.26	0/1044	0.41	0/1414
18	S3	0.26	0/1044	0.41	0/1414
18	s	0.25	0/1037	0.41	0/1404
18	s3	0.26	0/1037	0.41	0/1404
19	E	0.25	0/3492	0.40	0/4720
19	E3	0.25	0/3492	0.40	0/4720
19	e	0.24	0/3492	0.40	0/4720

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
19	e3	0.25	0/3492	0.40	0/4720
20	i1	0.22	0/593	0.34	0/795
20	i2	0.22	0/563	0.34	0/753
20	i4	0.22	0/593	0.34	0/795
20	i5	0.22	0/563	0.34	0/753
21	t	0.25	0/3103	0.39	0/4200
21	t3	0.25	0/3103	0.39	0/4200
22	G1	0.24	0/1507	0.37	0/2027
22	G2	0.24	0/1507	0.37	0/2027
22	G4	0.24	0/1507	0.37	0/2027
22	G5	0.24	0/1507	0.37	0/2027
23	g1	0.24	0/2156	0.38	0/2900
23	g2	0.24	0/2156	0.38	0/2900
23	g4	0.24	0/2156	0.38	0/2900
23	g5	0.24	0/2156	0.38	0/2900
24	A1	0.24	0/3961	0.40	0/5346
24	A2	0.24	0/3961	0.40	0/5346
24	A4	0.24	0/3961	0.40	0/5346
24	A5	0.24	0/3961	0.40	0/5346
24	B1	0.24	0/3956	0.40	0/5339
24	B2	0.24	0/3956	0.40	0/5339
24	B4	0.23	0/3956	0.40	0/5339
24	B5	0.24	0/3956	0.40	0/5339
24	C1	0.24	0/3974	0.40	0/5361
24	C2	0.24	0/3974	0.40	0/5361
24	C4	0.24	0/3974	0.40	0/5361
24	C5	0.24	0/3974	0.40	0/5361
25	D1	0.24	0/3613	0.39	0/4900
25	D2	0.24	0/3613	0.40	0/4900
25	D4	0.24	0/3613	0.39	0/4900
25	D5	0.24	0/3613	0.39	0/4900
25	E1	0.24	0/3613	0.40	0/4900
25	E2	0.24	0/3613	0.40	0/4900
25	E4	0.24	0/3613	0.40	0/4900
25	E5	0.24	0/3613	0.40	0/4900
25	F1	0.24	0/3604	0.40	0/4889
25	F2	0.24	0/3604	0.40	0/4889
25	F4	0.24	0/3604	0.40	0/4889
25	F5	0.24	0/3604	0.40	0/4889
26	H1	0.27	0/572	0.35	0/771
26	H2	0.27	0/572	0.37	0/771
26	H4	0.27	0/572	0.35	0/771
26	H5	0.27	0/572	0.36	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
26	I1	0.27	0/572	0.36	0/771
26	I2	0.27	0/572	0.37	0/771
26	I4	0.27	0/572	0.36	0/771
26	I5	0.27	0/572	0.37	0/771
26	J1	0.27	0/572	0.35	0/771
26	J2	0.26	0/572	0.35	0/771
26	J4	0.27	0/572	0.35	0/771
26	J5	0.27	0/572	0.35	0/771
26	K1	0.27	0/572	0.35	0/771
26	K2	0.26	0/572	0.36	0/771
26	K4	0.26	0/572	0.35	0/771
26	K5	0.26	0/572	0.36	0/771
26	L1	0.26	0/572	0.35	0/771
26	L2	0.26	0/572	0.35	0/771
26	L4	0.26	0/572	0.35	0/771
26	L5	0.26	0/572	0.35	0/771
26	M1	0.26	0/572	0.35	0/771
26	M2	0.26	0/572	0.35	0/771
26	M4	0.26	0/572	0.35	0/771
26	M5	0.26	0/572	0.35	0/771
26	N1	0.26	0/572	0.35	0/771
26	N2	0.26	0/572	0.35	0/771
26	N4	0.26	0/572	0.35	0/771
26	N5	0.26	0/572	0.35	0/771
26	O1	0.26	0/572	0.35	0/771
26	O2	0.27	0/572	0.35	0/771
26	O4	0.26	0/572	0.35	0/771
26	O5	0.26	0/572	0.35	0/771
26	P1	0.26	0/572	0.36	0/771
26	P2	0.26	0/572	0.35	0/771
26	P4	0.26	0/572	0.36	0/771
26	P5	0.26	0/572	0.35	0/771
26	Q1	0.27	0/572	0.35	0/771
26	Q2	0.26	0/572	0.34	0/771
26	Q4	0.27	0/572	0.35	0/771
26	Q5	0.26	0/572	0.35	0/771
27	d1	0.25	0/1081	0.45	0/1459
27	d2	0.25	0/1081	0.45	0/1459
27	d4	0.25	0/1081	0.44	0/1459
27	d5	0.25	0/1081	0.45	0/1459
28	e1	0.24	0/547	0.41	0/735
28	e2	0.24	0/547	0.42	0/735
28	e4	0.24	0/547	0.41	0/735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
28	e5	0.24	0/547	0.41	0/735
All	All	0.26	0/281952	0.39	0/381166

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
25	F1	0	1
25	F2	0	1
25	F4	0	1
25	F5	0	1
28	e2	0	1
28	e5	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	F1	364	TYR	Peptide
25	F2	364	TYR	Peptide
25	F4	364	TYR	Peptide
25	F5	364	TYR	Peptide
28	e2	46	TYR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	A3	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	a	431/446 (97%)	423 (98%)	8 (2%)	0	100	100
1	a3	431/446 (97%)	421 (98%)	10 (2%)	0	100	100
2	B	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	B3	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	b	352/381 (92%)	340 (97%)	12 (3%)	0	100	100
2	b3	352/381 (92%)	339 (96%)	13 (4%)	0	100	100
3	D	204/234 (87%)	199 (98%)	5 (2%)	0	100	100
3	D3	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
3	d	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
3	d3	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	F3	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f3	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	I3	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	i	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
5	i3	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
6	K	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	K3	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	k	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k3	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	C3	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c3	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
8	G	254/286 (89%)	245 (96%)	9 (4%)	0	100	100
8	G3	254/286 (89%)	246 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
8	g3	254/286 (89%)	244 (96%)	10 (4%)	0	100	100
9	H	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
9	H3	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h3	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
10	J	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	J3	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	j	267/273 (98%)	263 (98%)	4 (2%)	0	100	100
10	j3	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	L3	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
11	l3	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
12	M	219/221 (99%)	219 (100%)	0	0	100	100
12	M3	219/221 (99%)	219 (100%)	0	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
12	m3	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
13	N	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	N3	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	n	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
13	n3	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	O3	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
14	o3	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	P3	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	p	148/152 (97%)	139 (94%)	9 (6%)	0	100	100
15	p3	148/152 (97%)	138 (93%)	10 (7%)	0	100	100
16	Q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q3	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q3	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
17	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	R3	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	r	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
17	r3	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
18	S	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
18	S3	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
18	s	122/145 (84%)	122 (100%)	0	0	100	100
18	s3	122/145 (84%)	122 (100%)	0	0	100	100
19	E	415/480 (86%)	407 (98%)	8 (2%)	0	100	100
19	E3	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
19	e	415/480 (86%)	405 (98%)	10 (2%)	0	100	100
19	e3	415/480 (86%)	403 (97%)	12 (3%)	0	100	100
20	i1	64/108 (59%)	64 (100%)	0	0	100	100
20	i2	60/108 (56%)	60 (100%)	0	0	100	100
20	i4	64/108 (59%)	64 (100%)	0	0	100	100
20	i5	60/108 (56%)	60 (100%)	0	0	100	100
21	t	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
21	t3	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
22	G1	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G2	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G4	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G5	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
23	g1	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g2	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g4	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g5	273/299 (91%)	264 (97%)	9 (3%)	0	100	100
24	A1	510/546 (93%)	504 (99%)	6 (1%)	0	100	100
24	A2	510/546 (93%)	502 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	A4	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	A5	510/546 (93%)	502 (98%)	8 (2%)	0	100	100
24	B1	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	47	79
24	B2	509/546 (93%)	500 (98%)	9 (2%)	0	100	100
24	B4	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	47	79
24	B5	509/546 (93%)	499 (98%)	10 (2%)	0	100	100
24	C1	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C2	511/546 (94%)	508 (99%)	3 (1%)	0	100	100
24	C4	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C5	511/546 (94%)	507 (99%)	4 (1%)	0	100	100
25	D1	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D2	468/497 (94%)	463 (99%)	5 (1%)	0	100	100
25	D4	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D5	468/497 (94%)	462 (99%)	6 (1%)	0	100	100
25	E1	468/497 (94%)	458 (98%)	10 (2%)	0	100	100
25	E2	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	E4	468/497 (94%)	458 (98%)	10 (2%)	0	100	100
25	E5	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	F1	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F2	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
25	F4	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F5	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
26	H1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	I4	73/76 (96%)	73 (100%)	0	0	100	100
26	I5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	J1	73/76 (96%)	73 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	J2	73/76 (96%)	73 (100%)	0	0	100	100
26	J4	73/76 (96%)	73 (100%)	0	0	100	100
26	J5	73/76 (96%)	73 (100%)	0	0	100	100
26	K1	73/76 (96%)	73 (100%)	0	0	100	100
26	K2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	K4	73/76 (96%)	73 (100%)	0	0	100	100
26	K5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	L4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	M1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N5	73/76 (96%)	73 (100%)	0	0	100	100
26	O1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	O2	73/76 (96%)	73 (100%)	0	0	100	100
26	O4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	O5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	P1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	P4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q2	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
26	Q4	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q5	73/76 (96%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	d1	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d2	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d4	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d5	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
28	e1	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e2	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e4	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e5	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
All	All	34342/37732 (91%)	33598 (98%)	742 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	B1	55	ASP
24	B4	55	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/409 (97%)	395 (100%)	2 (0%)	88	94
1	A3	397/409 (97%)	395 (100%)	2 (0%)	88	94
1	a	397/409 (97%)	395 (100%)	2 (0%)	88	94
1	a3	397/409 (97%)	395 (100%)	2 (0%)	88	94
2	B	306/331 (92%)	306 (100%)	0	100	100
2	B3	306/331 (92%)	306 (100%)	0	100	100
2	b	306/331 (92%)	306 (100%)	0	100	100
2	b3	306/331 (92%)	306 (100%)	0	100	100
3	D	183/206 (89%)	183 (100%)	0	100	100
3	D3	183/206 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	d	183/206 (89%)	183 (100%)	0	100	100
3	d3	183/206 (89%)	183 (100%)	0	100	100
4	F	175/178 (98%)	174 (99%)	1 (1%)	86	94
4	F3	175/178 (98%)	174 (99%)	1 (1%)	86	94
4	f	175/178 (98%)	173 (99%)	2 (1%)	73	89
4	f3	175/178 (98%)	173 (99%)	2 (1%)	73	89
5	I	182/182 (100%)	180 (99%)	2 (1%)	73	89
5	I3	182/182 (100%)	180 (99%)	2 (1%)	73	89
5	i	182/182 (100%)	180 (99%)	2 (1%)	73	89
5	i3	182/182 (100%)	181 (100%)	1 (0%)	88	94
6	K	152/152 (100%)	152 (100%)	0	100	100
6	K3	152/152 (100%)	152 (100%)	0	100	100
6	k	152/152 (100%)	151 (99%)	1 (1%)	84	93
6	k3	152/152 (100%)	151 (99%)	1 (1%)	84	93
7	C	93/97 (96%)	92 (99%)	1 (1%)	73	89
7	C3	93/97 (96%)	92 (99%)	1 (1%)	73	89
7	c	93/97 (96%)	92 (99%)	1 (1%)	73	89
7	c3	93/97 (96%)	92 (99%)	1 (1%)	73	89
8	G	235/262 (90%)	234 (100%)	1 (0%)	91	96
8	G3	235/262 (90%)	234 (100%)	1 (0%)	91	96
8	g	235/262 (90%)	234 (100%)	1 (0%)	91	96
8	g3	235/262 (90%)	234 (100%)	1 (0%)	91	96
9	H	208/245 (85%)	207 (100%)	1 (0%)	88	94
9	H3	208/245 (85%)	207 (100%)	1 (0%)	88	94
9	h	208/245 (85%)	207 (100%)	1 (0%)	88	94
9	h3	208/245 (85%)	207 (100%)	1 (0%)	88	94
10	J	235/239 (98%)	234 (100%)	1 (0%)	91	96
10	J3	235/239 (98%)	234 (100%)	1 (0%)	91	96
10	j	235/239 (98%)	235 (100%)	0	100	100
10	j3	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	217 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	L3	219/220 (100%)	217 (99%)	2 (1%)	78 91
11	l	219/220 (100%)	218 (100%)	1 (0%)	88 94
11	l3	219/220 (100%)	218 (100%)	1 (0%)	88 94
12	M	202/202 (100%)	202 (100%)	0	100 100
12	M3	202/202 (100%)	202 (100%)	0	100 100
12	m	202/202 (100%)	201 (100%)	1 (0%)	88 94
12	m3	202/202 (100%)	201 (100%)	1 (0%)	88 94
13	N	104/162 (64%)	104 (100%)	0	100 100
13	N3	104/162 (64%)	104 (100%)	0	100 100
13	n	104/162 (64%)	103 (99%)	1 (1%)	76 90
13	n3	104/162 (64%)	103 (99%)	1 (1%)	76 90
14	O	89/142 (63%)	89 (100%)	0	100 100
14	O3	89/142 (63%)	89 (100%)	0	100 100
14	o	89/142 (63%)	89 (100%)	0	100 100
14	o3	89/142 (63%)	89 (100%)	0	100 100
15	P	131/133 (98%)	131 (100%)	0	100 100
15	P3	131/133 (98%)	131 (100%)	0	100 100
15	p	131/133 (98%)	131 (100%)	0	100 100
15	p3	131/133 (98%)	131 (100%)	0	100 100
16	Q	97/135 (72%)	97 (100%)	0	100 100
16	Q3	97/135 (72%)	97 (100%)	0	100 100
16	q	97/135 (72%)	97 (100%)	0	100 100
16	q3	97/135 (72%)	97 (100%)	0	100 100
17	R	120/129 (93%)	119 (99%)	1 (1%)	81 92
17	R3	120/129 (93%)	119 (99%)	1 (1%)	81 92
17	r	125/129 (97%)	124 (99%)	1 (1%)	81 92
17	r3	125/129 (97%)	124 (99%)	1 (1%)	81 92
18	S	112/131 (86%)	112 (100%)	0	100 100
18	S3	112/131 (86%)	112 (100%)	0	100 100
18	s	111/131 (85%)	109 (98%)	2 (2%)	59 82
18	s3	111/131 (85%)	109 (98%)	2 (2%)	59 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	E	359/414 (87%)	357 (99%)	2 (1%)	86	94
19	E3	359/414 (87%)	357 (99%)	2 (1%)	86	94
19	e	359/414 (87%)	358 (100%)	1 (0%)	92	96
19	e3	359/414 (87%)	358 (100%)	1 (0%)	92	96
20	i1	64/101 (63%)	64 (100%)	0	100	100
20	i2	61/101 (60%)	61 (100%)	0	100	100
20	i4	64/101 (63%)	64 (100%)	0	100	100
20	i5	61/101 (60%)	61 (100%)	0	100	100
21	t	325/414 (78%)	322 (99%)	3 (1%)	78	91
21	t3	325/414 (78%)	322 (99%)	3 (1%)	78	91
22	G1	166/195 (85%)	166 (100%)	0	100	100
22	G2	166/195 (85%)	166 (100%)	0	100	100
22	G4	166/195 (85%)	166 (100%)	0	100	100
22	G5	166/195 (85%)	166 (100%)	0	100	100
23	g1	234/254 (92%)	230 (98%)	4 (2%)	60	83
23	g2	234/254 (92%)	231 (99%)	3 (1%)	69	87
23	g4	234/254 (92%)	230 (98%)	4 (2%)	60	83
23	g5	234/254 (92%)	231 (99%)	3 (1%)	69	87
24	A1	422/453 (93%)	419 (99%)	3 (1%)	84	93
24	A2	422/453 (93%)	419 (99%)	3 (1%)	84	93
24	A4	422/453 (93%)	419 (99%)	3 (1%)	84	93
24	A5	422/453 (93%)	419 (99%)	3 (1%)	84	93
24	B1	422/453 (93%)	419 (99%)	3 (1%)	84	93
24	B2	422/453 (93%)	421 (100%)	1 (0%)	93	97
24	B4	422/453 (93%)	419 (99%)	3 (1%)	84	93
24	B5	422/453 (93%)	421 (100%)	1 (0%)	93	97
24	C1	424/453 (94%)	423 (100%)	1 (0%)	93	97
24	C2	424/453 (94%)	423 (100%)	1 (0%)	93	97
24	C4	424/453 (94%)	423 (100%)	1 (0%)	93	97
24	C5	424/453 (94%)	423 (100%)	1 (0%)	93	97
25	D1	381/402 (95%)	380 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	D2	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	D4	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	D5	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	E1	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	E2	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	E4	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	E5	381/402 (95%)	380 (100%)	1 (0%)	92 96
25	F1	380/402 (94%)	380 (100%)	0	100 100
25	F2	380/402 (94%)	380 (100%)	0	100 100
25	F4	380/402 (94%)	380 (100%)	0	100 100
25	F5	380/402 (94%)	380 (100%)	0	100 100
26	H1	59/59 (100%)	59 (100%)	0	100 100
26	H2	59/59 (100%)	59 (100%)	0	100 100
26	H4	59/59 (100%)	59 (100%)	0	100 100
26	H5	59/59 (100%)	59 (100%)	0	100 100
26	I1	59/59 (100%)	57 (97%)	2 (3%)	37 69
26	I2	59/59 (100%)	59 (100%)	0	100 100
26	I4	59/59 (100%)	57 (97%)	2 (3%)	37 69
26	I5	59/59 (100%)	59 (100%)	0	100 100
26	J1	59/59 (100%)	59 (100%)	0	100 100
26	J2	59/59 (100%)	59 (100%)	0	100 100
26	J4	59/59 (100%)	59 (100%)	0	100 100
26	J5	59/59 (100%)	59 (100%)	0	100 100
26	K1	59/59 (100%)	59 (100%)	0	100 100
26	K2	59/59 (100%)	58 (98%)	1 (2%)	60 83
26	K4	59/59 (100%)	59 (100%)	0	100 100
26	K5	59/59 (100%)	58 (98%)	1 (2%)	60 83
26	L1	59/59 (100%)	59 (100%)	0	100 100
26	L2	59/59 (100%)	59 (100%)	0	100 100
26	L4	59/59 (100%)	59 (100%)	0	100 100
26	L5	59/59 (100%)	59 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	M1	59/59 (100%)	59 (100%)	0	100	100
26	M2	59/59 (100%)	59 (100%)	0	100	100
26	M4	59/59 (100%)	59 (100%)	0	100	100
26	M5	59/59 (100%)	59 (100%)	0	100	100
26	N1	59/59 (100%)	59 (100%)	0	100	100
26	N2	59/59 (100%)	59 (100%)	0	100	100
26	N4	59/59 (100%)	59 (100%)	0	100	100
26	N5	59/59 (100%)	59 (100%)	0	100	100
26	O1	59/59 (100%)	59 (100%)	0	100	100
26	O2	59/59 (100%)	59 (100%)	0	100	100
26	O4	59/59 (100%)	59 (100%)	0	100	100
26	O5	59/59 (100%)	59 (100%)	0	100	100
26	P1	59/59 (100%)	59 (100%)	0	100	100
26	P2	59/59 (100%)	59 (100%)	0	100	100
26	P4	59/59 (100%)	59 (100%)	0	100	100
26	P5	59/59 (100%)	59 (100%)	0	100	100
26	Q1	59/59 (100%)	59 (100%)	0	100	100
26	Q2	59/59 (100%)	59 (100%)	0	100	100
26	Q4	59/59 (100%)	59 (100%)	0	100	100
26	Q5	59/59 (100%)	59 (100%)	0	100	100
27	d1	117/139 (84%)	116 (99%)	1 (1%)	78	91
27	d2	117/139 (84%)	116 (99%)	1 (1%)	78	91
27	d4	117/139 (84%)	116 (99%)	1 (1%)	78	91
27	d5	117/139 (84%)	116 (99%)	1 (1%)	78	91
28	e1	57/60 (95%)	57 (100%)	0	100	100
28	e2	57/60 (95%)	57 (100%)	0	100	100
28	e4	57/60 (95%)	57 (100%)	0	100	100
28	e5	57/60 (95%)	57 (100%)	0	100	100
All	All	29600/32320 (92%)	29477 (100%)	123 (0%)	91	96

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	A2	225	ASP
27	d4	126	GLU
11	l3	205	TRP
26	I4	53	MET
24	A5	225	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
16	Q3	69	GLN
22	G5	165	GLN
19	E3	361	ASN
24	A4	171	GLN
16	Q	69	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 140 ligands modelled in this entry, 24 are monoatomic - leaving 116 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	$\#\|Z\|>2$
29	CDL	l	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	3 (2%)
31	PO4	f3	301	-	4,4,4	0.98	0	6,6,6	0.45	0
29	CDL	i3	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
33	ATP	g	301	34	26,33,33	4.79	8 (30%)	31,52,52	2.45	7 (22%)
29	CDL	L	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.04	4 (3%)
29	CDL	P	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.02	5 (4%)
29	CDL	a3	501	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	5 (4%)
29	CDL	j3	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
29	CDL	L3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.00	4 (3%)
29	CDL	B	402	2	99,99,99	0.87	8 (8%)	105,111,111	1.12	5 (4%)
30	PC1	g3	303	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
29	CDL	I	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
30	PC1	d3	301	3	53,53,53	0.94	4 (7%)	59,61,61	1.07	2 (3%)
33	ATP	C1	601	34	26,33,33	4.80	8 (30%)	31,52,52	2.40	7 (22%)
33	ATP	C4	601	34	26,33,33	4.78	8 (30%)	31,52,52	2.41	7 (22%)
29	CDL	J	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
30	PC1	G	303	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
29	CDL	g3	305	-	99,99,99	0.88	8 (8%)	105,111,111	1.10	4 (3%)
29	CDL	j	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.04	4 (3%)
29	CDL	l	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.04	4 (3%)
33	ATP	B1	1003	34,24,25	26,33,33	4.80	8 (30%)	31,52,52	2.45	8 (25%)
33	ATP	B4	1003	34,24,25	26,33,33	4.79	8 (30%)	31,52,52	2.44	8 (25%)
31	PO4	f	301	-	4,4,4	0.96	0	6,6,6	0.41	0
29	CDL	i3	301	-	99,99,99	0.87	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	I3	303	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	4 (3%)
33	ATP	B5	1003	34,24,25	26,33,33	4.80	9 (34%)	31,52,52	2.45	8 (25%)
36	NAD	E3	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.15	7 (14%)
37	ADP	D5	501	34	24,29,29	3.69	9 (37%)	29,45,45	3.55	7 (24%)
29	CDL	p3	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	B	403	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
32	UQ8	i3	303	-	53,53,53	1.79	7 (13%)	64,67,67	1.61	16 (25%)
31	PO4	F	301	-	4,4,4	0.99	0	6,6,6	0.45	0
37	ADP	B2	1002	34,24	24,29,29	3.71	9 (37%)	29,45,45	3.57	6 (20%)
29	CDL	J	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
35	PEE	L	303	-	47,47,50	1.17	6 (12%)	50,52,55	1.17	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CDL	A	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.10	4 (3%)
30	PC1	g	304	8	53,53,53	0.95	4 (7%)	59,61,61	0.96	2 (3%)
32	UQ8	I	303	-	53,53,53	1.80	7 (13%)	64,67,67	1.67	15 (23%)
30	PC1	G3	304	8	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
29	CDL	a	501	-	99,99,99	0.88	8 (8%)	105,111,111	1.06	5 (4%)
29	CDL	K3	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	r	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
37	ADP	D1	501	34	24,29,29	3.66	9 (37%)	29,45,45	3.80	7 (24%)
37	ADP	B4	1002	34,24	24,29,29	3.71	9 (37%)	29,45,45	3.57	7 (24%)
29	CDL	L	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
29	CDL	B3	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
29	CDL	j	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	f3	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
35	PEE	L3	302	-	50,50,50	1.15	6 (12%)	53,55,55	1.15	4 (7%)
32	UQ8	I3	304	-	53,53,53	1.81	7 (13%)	64,67,67	1.65	15 (23%)
29	CDL	b	401	4,2	99,99,99	0.87	7 (7%)	105,111,111	1.10	4 (3%)
33	ATP	B2	1003	34,24,25	26,33,33	4.81	8 (30%)	31,52,52	2.44	8 (25%)
29	CDL	j3	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	f3	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
33	ATP	A1	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.41	7 (22%)
29	CDL	l3	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	F	303	-	99,99,99	0.87	6 (6%)	105,111,111	1.08	4 (3%)
30	PC1	G3	303	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
33	ATP	C2	601	34	26,33,33	4.80	8 (30%)	31,52,52	2.42	7 (22%)
30	PC1	G	304	8	53,53,53	0.95	4 (7%)	59,61,61	0.98	2 (3%)
35	PEE	l3	302	-	47,47,50	1.17	6 (12%)	50,52,55	1.21	2 (4%)
36	NAD	e	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.16	7 (14%)
29	CDL	K3	202	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
37	ADP	B5	1002	34,24	24,29,29	3.71	9 (37%)	29,45,45	3.58	6 (20%)
29	CDL	B3	402	2	99,99,99	0.87	7 (7%)	105,111,111	1.12	5 (4%)
30	PC1	g3	304	8	53,53,53	0.95	4 (7%)	59,61,61	0.93	2 (3%)
29	CDL	k	201	6	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
29	CDL	A3	501	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
35	PEE	A	501	-	47,47,50	1.18	6 (12%)	50,52,55	1.21	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CDL	F3	302	-	99,99,99	0.88	6 (6%)	105,111,111	1.08	4 (3%)
35	PEE	J	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.15	4 (7%)
30	PC1	D3	301	3	53,53,53	0.93	4 (7%)	59,61,61	1.09	2 (3%)
30	PC1	d	301	3	53,53,53	0.94	4 (7%)	59,61,61	1.07	2 (3%)
29	CDL	k3	201	6	99,99,99	0.89	6 (6%)	105,111,111	1.02	4 (3%)
29	CDL	J3	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.03	4 (3%)
32	UQ8	i	302	-	53,53,53	1.81	7 (13%)	64,67,67	1.60	16 (25%)
33	ATP	A2	601	34	26,33,33	4.81	8 (30%)	31,52,52	2.42	7 (22%)
29	CDL	B3	404	2	99,99,99	0.89	8 (8%)	105,111,111	1.11	5 (4%)
30	PC1	g	303	-	53,53,53	0.95	4 (7%)	59,61,61	0.98	2 (3%)
29	CDL	K	202	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)
35	PEE	a3	503	-	47,47,50	1.17	6 (12%)	50,52,55	1.17	4 (8%)
35	PEE	m	301	-	50,50,50	1.14	6 (12%)	53,55,55	1.10	4 (7%)
30	PC1	D	301	3	53,53,53	0.94	4 (7%)	59,61,61	1.08	2 (3%)
33	ATP	G	301	34	26,33,33	4.77	7 (26%)	31,52,52	2.48	7 (22%)
35	PEE	j3	303	-	50,50,50	1.14	6 (12%)	53,55,55	1.10	5 (9%)
36	NAD	e3	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.16	7 (14%)
36	NAD	E	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.14	7 (14%)
33	ATP	G3	301	34	26,33,33	4.77	8 (30%)	31,52,52	2.47	7 (22%)
37	ADP	D2	501	34	24,29,29	3.69	9 (37%)	29,45,45	3.54	7 (24%)
29	CDL	F	302	-	99,99,99	0.87	8 (8%)	105,111,111	1.02	5 (4%)
29	CDL	K	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	i	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.07	4 (3%)
29	CDL	a3	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	5 (4%)
29	CDL	I3	302	-	99,99,99	0.88	6 (6%)	105,111,111	1.02	4 (3%)
29	CDL	B	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.97	4 (3%)
33	ATP	C5	601	34	26,33,33	4.81	8 (30%)	31,52,52	2.42	7 (22%)
29	CDL	f	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
29	CDL	P3	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	4 (3%)
37	ADP	B1	1002	34,24	24,29,29	3.71	9 (37%)	29,45,45	3.58	7 (24%)
29	CDL	I	301	5	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
29	CDL	f3	304	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
29	CDL	B	404	2	99,99,99	0.88	8 (8%)	105,111,111	1.08	5 (4%)
33	ATP	A5	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.40	7 (22%)
31	PO4	F3	301	-	4,4,4	0.96	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CDL	J3	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	l3	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
33	ATP	g3	301	34	26,33,33	4.78	7 (26%)	31,52,52	2.46	7 (22%)
29	CDL	B3	403	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
33	ATP	A4	601	34	26,33,33	4.80	8 (30%)	31,52,52	2.42	7 (22%)
29	CDL	I3	301	5	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	b3	401	4,2	99,99,99	0.88	7 (7%)	105,111,111	1.12	4 (3%)
29	CDL	f	304	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	D4	501	34	24,29,29	3.66	9 (37%)	29,45,45	3.79	7 (24%)
29	CDL	g	305	-	99,99,99	0.88	8 (8%)	105,111,111	1.08	4 (3%)
29	CDL	f	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.08	5 (4%)

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
29	CDL	l	302	-	-	41/110/110/110	-
29	CDL	i3	302	-	-	38/110/110/110	-
33	ATP	g	301	34	-	0/18/38/38	0/3/3/3
29	CDL	L	302	-	-	45/110/110/110	-
29	CDL	P	201	-	-	35/110/110/110	-
29	CDL	a3	501	-	-	34/110/110/110	-
29	CDL	j3	301	-	-	40/110/110/110	-
29	CDL	L3	301	-	-	38/110/110/110	-
29	CDL	B	402	2	-	39/110/110/110	-
30	PC1	g3	303	-	-	21/57/57/57	-
29	CDL	I	302	-	-	38/110/110/110	-
30	PC1	d3	301	3	-	23/57/57/57	-
33	ATP	C1	601	34	-	5/18/38/38	0/3/3/3
33	ATP	C4	601	34	-	5/18/38/38	0/3/3/3
29	CDL	J	302	-	-	38/110/110/110	-
30	PC1	G	303	-	-	29/57/57/57	-
29	CDL	g3	305	-	-	36/110/110/110	-
29	CDL	j	301	-	-	40/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	l	301	-	-	38/110/110/110	-
33	ATP	B1	1003	34,24,25	-	2/18/38/38	0/3/3/3
33	ATP	B4	1003	34,24,25	-	2/18/38/38	0/3/3/3
36	NAD	E3	900	-	-	7/26/62/62	0/5/5/5
29	CDL	i3	301	-	-	36/110/110/110	-
29	CDL	I3	303	-	-	38/110/110/110	-
33	ATP	B5	1003	34,24,25	-	2/18/38/38	0/3/3/3
37	ADP	D5	501	34	-	2/12/32/32	0/3/3/3
29	CDL	p3	201	-	-	44/110/110/110	-
29	CDL	B	403	-	-	33/110/110/110	-
32	UQ8	i3	303	-	-	8/51/75/75	0/1/1/1
37	ADP	B2	1002	34,24	-	2/12/32/32	0/3/3/3
29	CDL	J	301	-	-	42/110/110/110	-
35	PEE	L	303	-	-	22/51/51/54	-
29	CDL	A	502	-	-	46/110/110/110	-
30	PC1	g	304	8	-	20/57/57/57	-
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
30	PC1	G3	304	8	-	19/57/57/57	-
29	CDL	a	501	-	-	34/110/110/110	-
29	CDL	K3	201	-	-	28/110/110/110	-
29	CDL	r	201	-	-	36/110/110/110	-
37	ADP	D1	501	34	-	2/12/32/32	0/3/3/3
37	ADP	B4	1002	34,24	-	1/12/32/32	0/3/3/3
29	CDL	L	301	-	-	37/110/110/110	-
29	CDL	B3	401	-	-	44/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
29	CDL	f3	302	-	-	54/110/110/110	-
35	PEE	L3	302	-	-	29/54/54/54	-
32	UQ8	I3	304	-	-	9/51/75/75	0/1/1/1
29	CDL	b	401	4,2	-	44/110/110/110	-
33	ATP	B2	1003	34,24,25	-	2/18/38/38	0/3/3/3
29	CDL	j3	302	-	-	40/110/110/110	-
29	CDL	f3	303	-	-	41/110/110/110	-
33	ATP	A1	601	34	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	l3	301	-	-	39/110/110/110	-
29	CDL	F	303	-	-	46/110/110/110	-
30	PC1	G3	303	-	-	28/57/57/57	-
33	ATP	C2	601	34	-	4/18/38/38	0/3/3/3
30	PC1	G	304	8	-	19/57/57/57	-
35	PEE	l3	302	-	-	21/51/51/54	-
36	NAD	e	900	-	-	6/26/62/62	0/5/5/5
29	CDL	K3	202	-	-	35/110/110/110	-
29	CDL	p	201	-	-	45/110/110/110	-
37	ADP	B5	1002	34,24	-	2/12/32/32	0/3/3/3
29	CDL	B3	402	2	-	40/110/110/110	-
30	PC1	g3	304	8	-	18/57/57/57	-
29	CDL	k	201	6	-	37/110/110/110	-
29	CDL	A3	501	-	-	46/110/110/110	-
35	PEE	A	501	-	-	21/51/51/54	-
29	CDL	F3	302	-	-	45/110/110/110	-
35	PEE	J	303	-	-	29/54/54/54	-
30	PC1	D3	301	3	-	22/57/57/57	-
30	PC1	d	301	3	-	23/57/57/57	-
29	CDL	k3	201	6	-	38/110/110/110	-
29	CDL	J3	301	-	-	42/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
33	ATP	A2	601	34	-	5/18/38/38	0/3/3/3
29	CDL	B3	404	2	-	46/110/110/110	-
30	PC1	g	303	-	-	21/57/57/57	-
29	CDL	K	202	-	-	35/110/110/110	-
35	PEE	a3	503	-	-	22/51/51/54	-
35	PEE	m	301	-	-	24/54/54/54	-
30	PC1	D	301	3	-	22/57/57/57	-
33	ATP	G	301	34	-	0/18/38/38	0/3/3/3
35	PEE	j3	303	-	-	23/54/54/54	-
36	NAD	e3	900	-	-	7/26/62/62	0/5/5/5
36	NAD	E	900	-	-	8/26/62/62	0/5/5/5
33	ATP	G3	301	34	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	D2	501	34	-	2/12/32/32	0/3/3/3
29	CDL	F	302	-	-	39/110/110/110	-
29	CDL	K	201	-	-	28/110/110/110	-
29	CDL	i	301	-	-	39/110/110/110	-
29	CDL	a3	502	-	-	39/110/110/110	-
29	CDL	I3	302	-	-	45/110/110/110	-
29	CDL	B	401	-	-	44/110/110/110	-
33	ATP	C5	601	34	-	4/18/38/38	0/3/3/3
29	CDL	f	302	-	-	54/110/110/110	-
29	CDL	P3	201	-	-	37/110/110/110	-
37	ADP	B1	1002	34,24	-	1/12/32/32	0/3/3/3
29	CDL	I	301	5	-	43/110/110/110	-
29	CDL	f3	304	-	-	48/110/110/110	-
29	CDL	B	404	2	-	46/110/110/110	-
33	ATP	A5	601	34	-	5/18/38/38	0/3/3/3
29	CDL	J3	302	-	-	40/110/110/110	-
29	CDL	l3	303	-	-	41/110/110/110	-
33	ATP	g3	301	34	-	0/18/38/38	0/3/3/3
29	CDL	B3	403	-	-	33/110/110/110	-
33	ATP	A4	601	34	-	5/18/38/38	0/3/3/3
29	CDL	I3	301	5	-	42/110/110/110	-
29	CDL	b3	401	4,2	-	44/110/110/110	-
29	CDL	f	304	-	-	49/110/110/110	-
37	ADP	D4	501	34	-	2/12/32/32	0/3/3/3
29	CDL	g	305	-	-	36/110/110/110	-
29	CDL	f	303	-	-	41/110/110/110	-

The worst 5 of 855 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C5	601	ATP	C2'-C1'	-17.26	1.27	1.53
33	B2	1003	ATP	C2'-C1'	-17.25	1.27	1.53
33	A1	601	ATP	C2'-C1'	-17.22	1.27	1.53
33	A5	601	ATP	C2'-C1'	-17.19	1.27	1.53
33	B5	1003	ATP	C2'-C1'	-17.15	1.27	1.53

The worst 5 of 562 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D4	501	ADP	C1'-N9-C4	15.99	154.74	126.64
37	D1	501	ADP	C1'-N9-C4	15.96	154.69	126.64
37	B5	1002	ADP	C1'-N9-C4	14.92	152.85	126.64
37	B1	1002	ADP	C1'-N9-C4	14.91	152.84	126.64
37	B2	1002	ADP	C1'-N9-C4	14.87	152.77	126.64

There are no chirality outliers.

5 of 2998 torsion outliers are listed below:

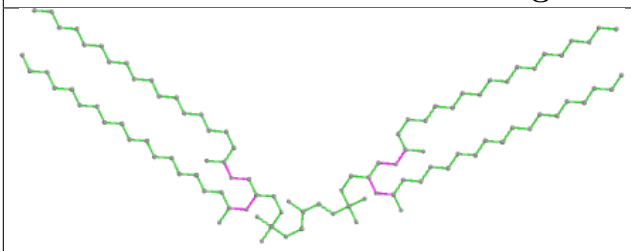
Mol	Chain	Res	Type	Atoms
29	a	501	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4
29	b	401	CDL	CB3-OB5-PB2-OB4

There are no ring outliers.

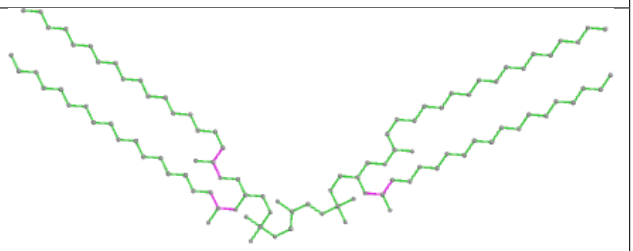
No monomer is involved in short contacts.

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

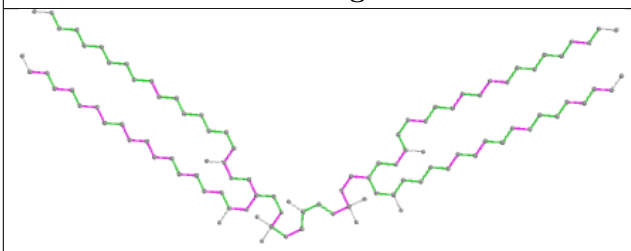
Ligand CDL l 302



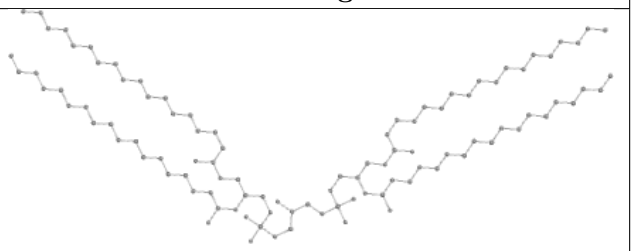
Bond lengths



Bond angles

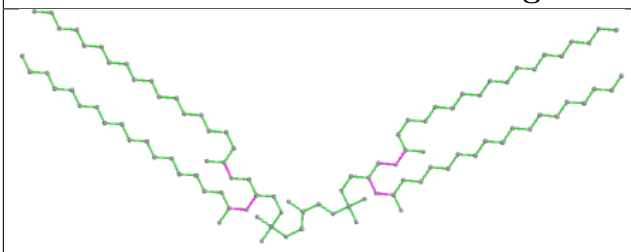


Torsions

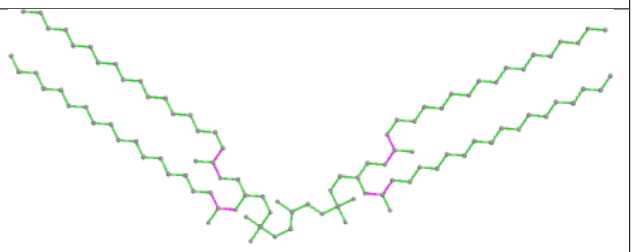


Rings

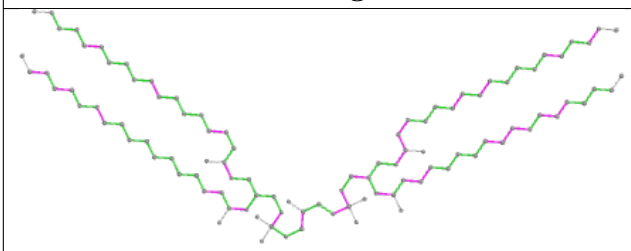
Ligand CDL i3 302



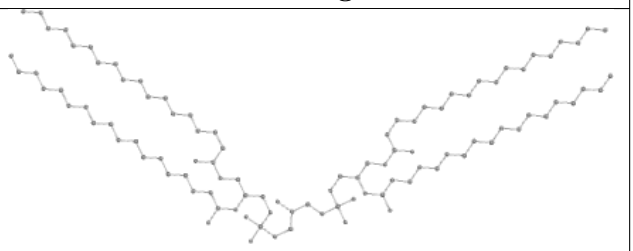
Bond lengths



Bond angles

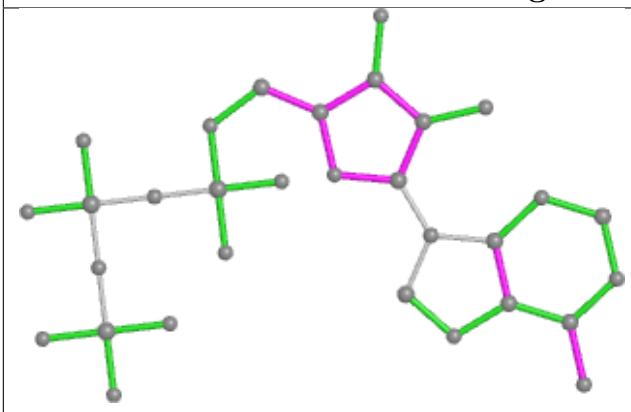


Torsions

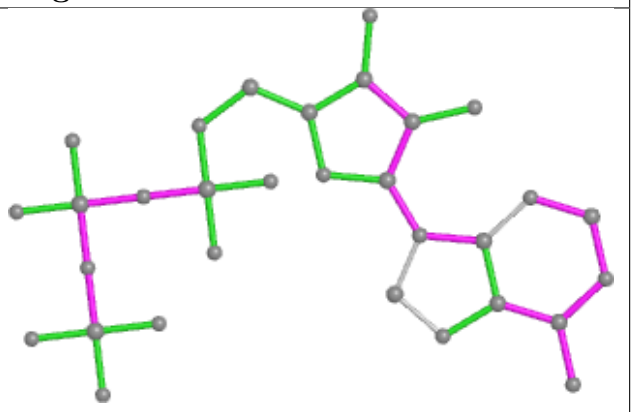


Rings

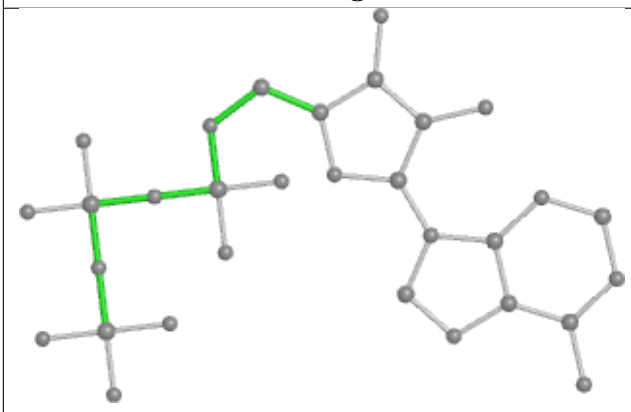
Ligand ATP g 301



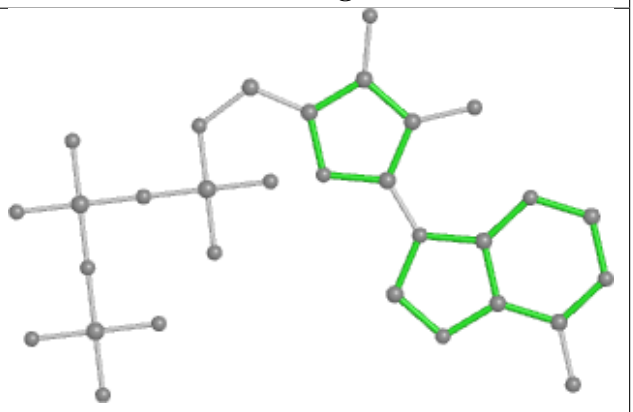
Bond lengths



Bond angles

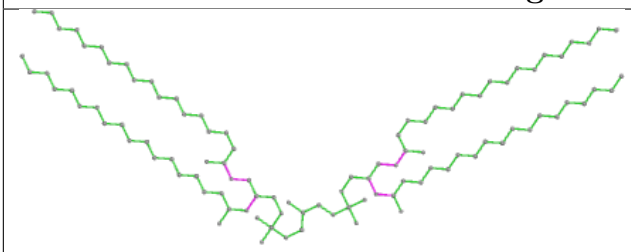


Torsions

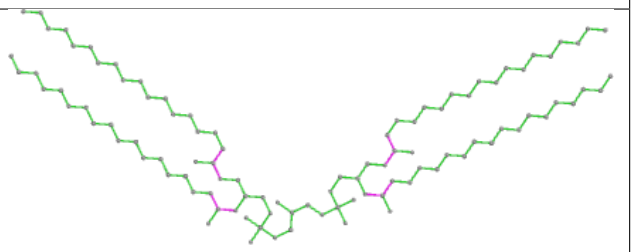


Rings

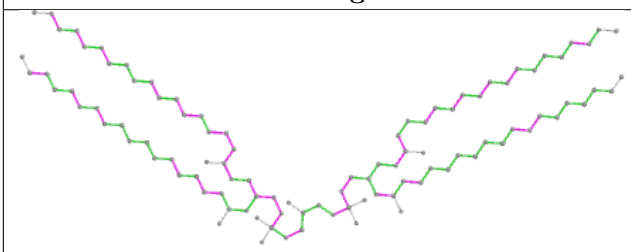
Ligand CDL L 302



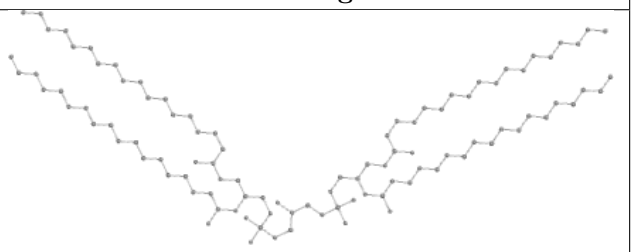
Bond lengths



Bond angles

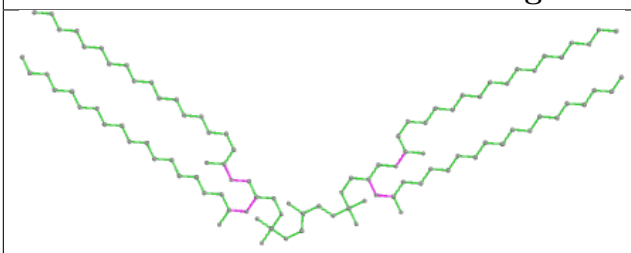


Torsions

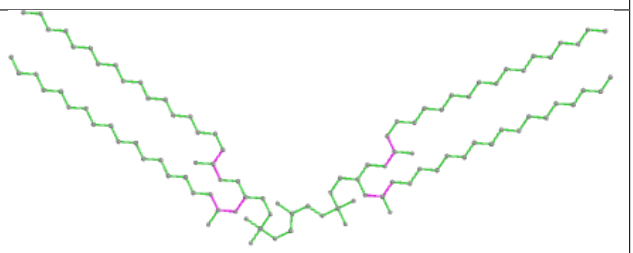


Rings

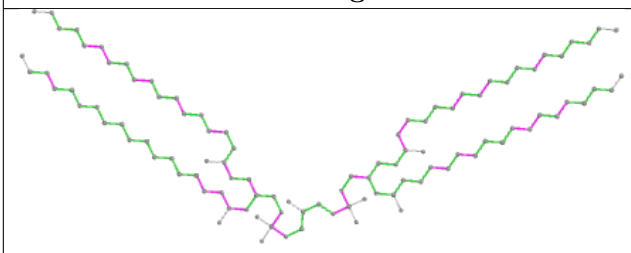
Ligand CDL P 201



Bond lengths



Bond angles



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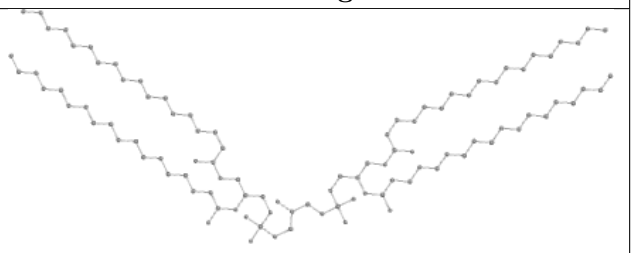
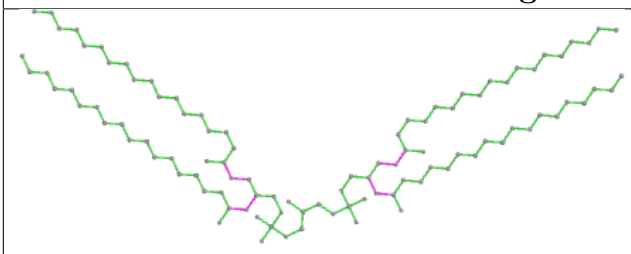
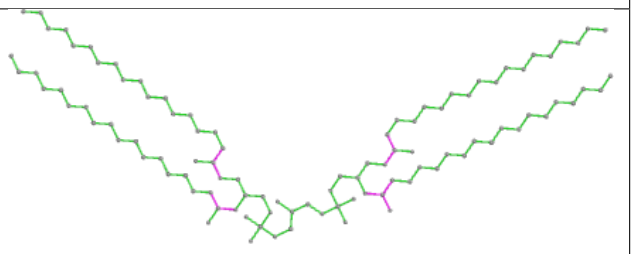


Rings

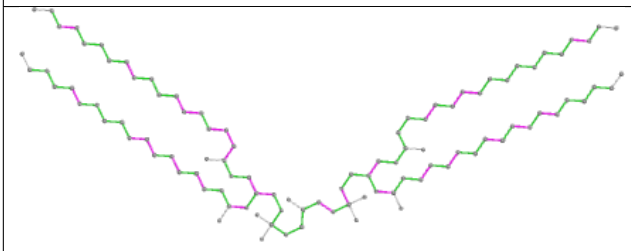
Ligand CDL a3 501



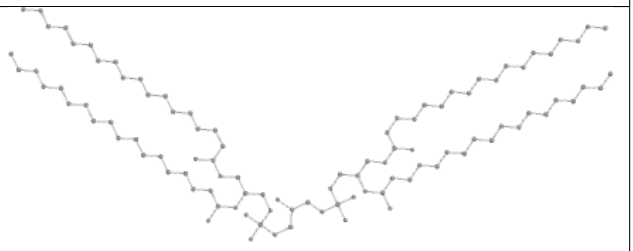
Bond lengths



Bond angles

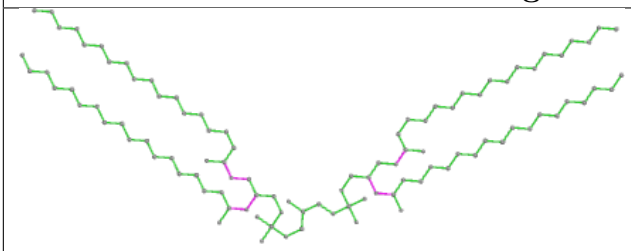


Torsions

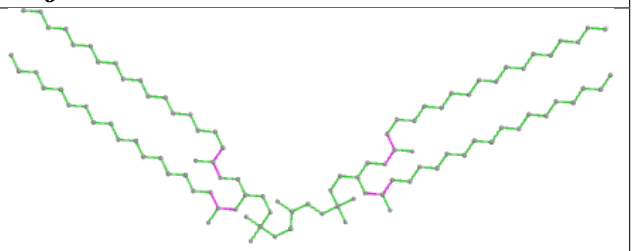


Rings

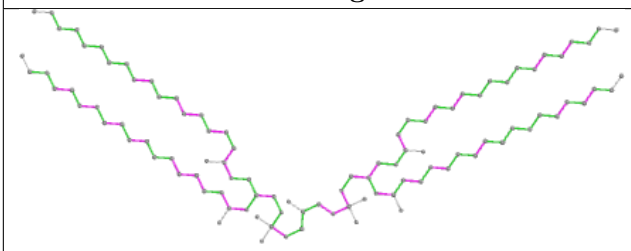
Ligand CDL j3 301



Bond lengths



Bond angles



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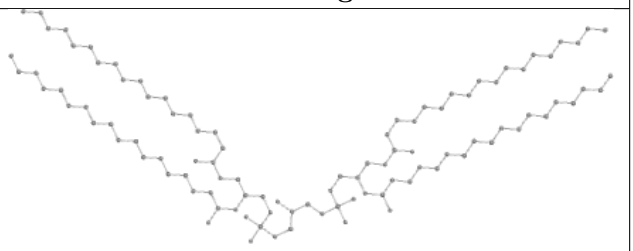
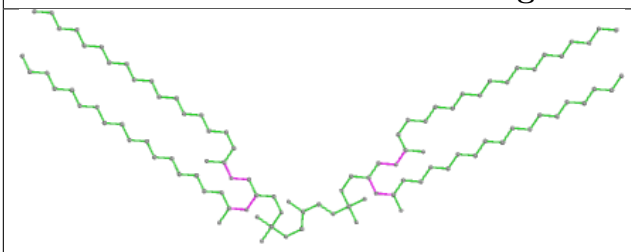


Rings

Ligand CDL L3 301



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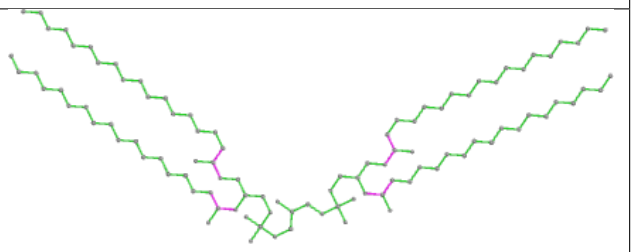
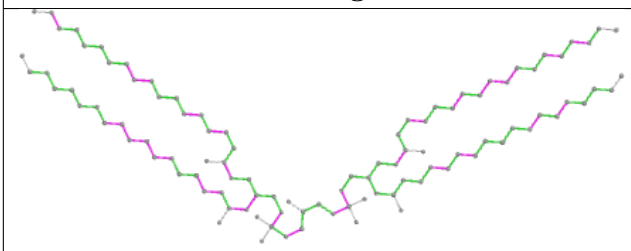
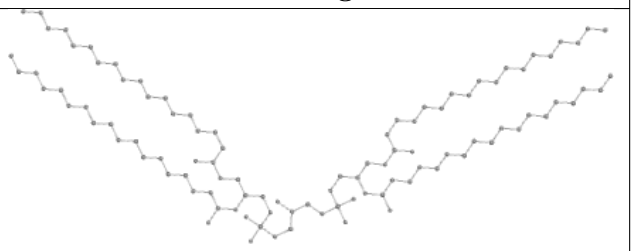


Bond angles

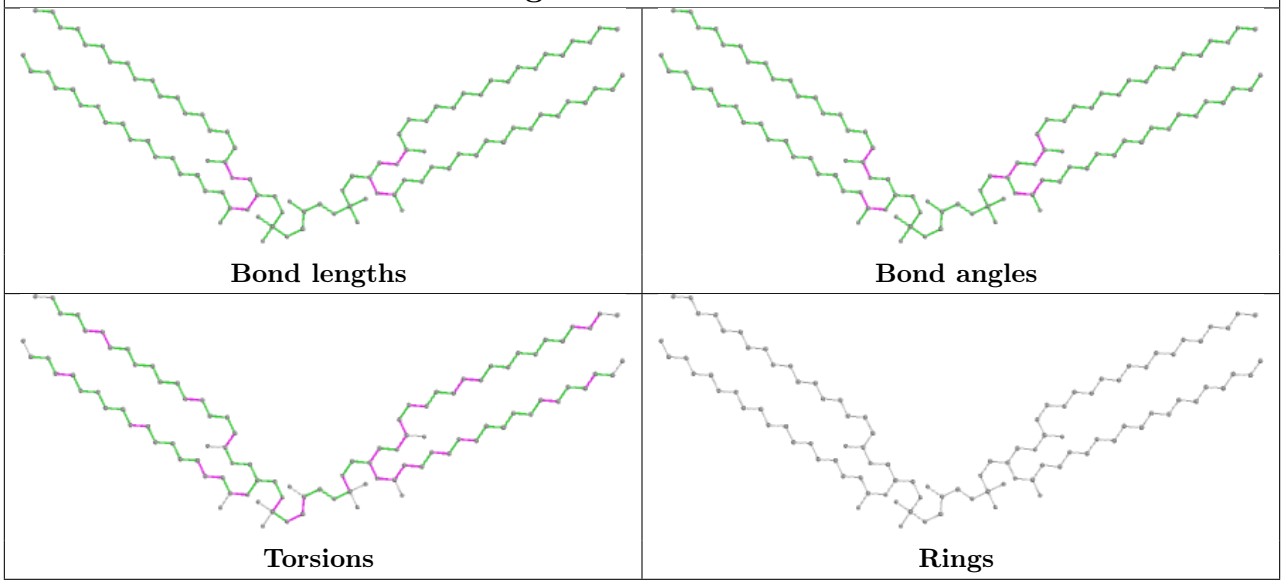


Torsions

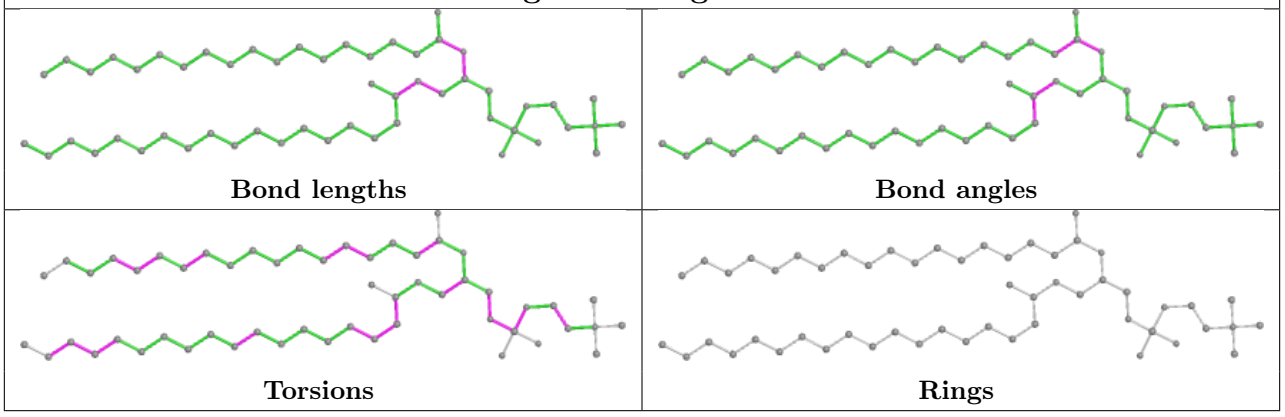


Rings

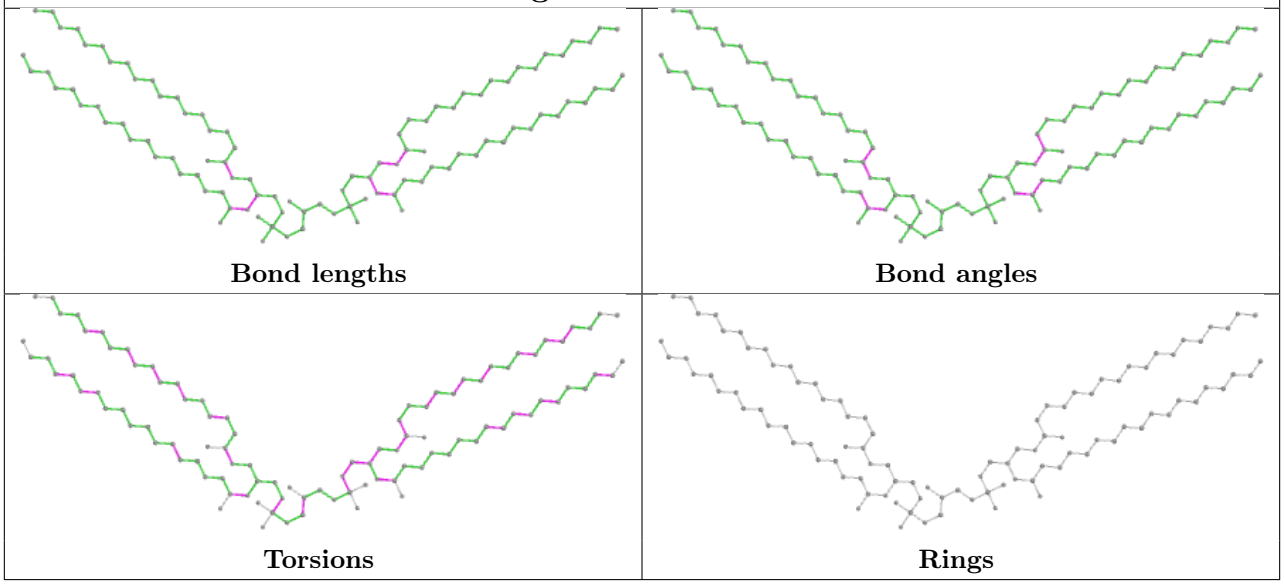
Ligand CDL B 402



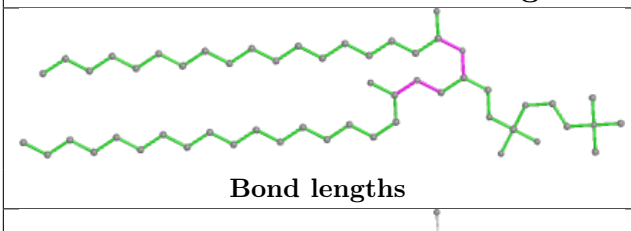
Ligand PC1 g3 303



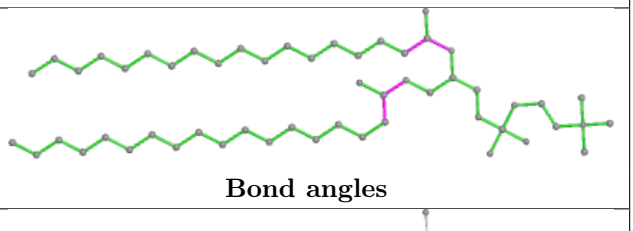
Ligand CDL I 302



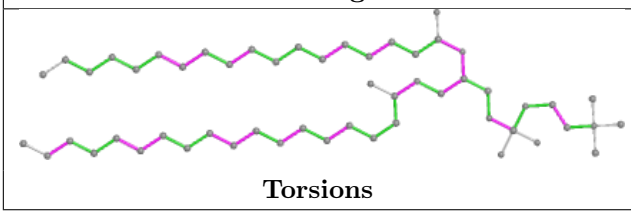
Ligand PC1 d3 301



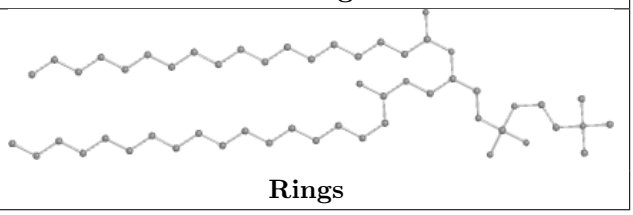
Bond lengths



Bond angles

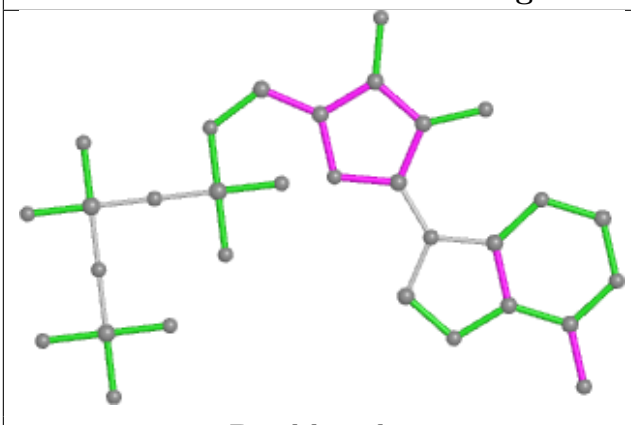


Torsions

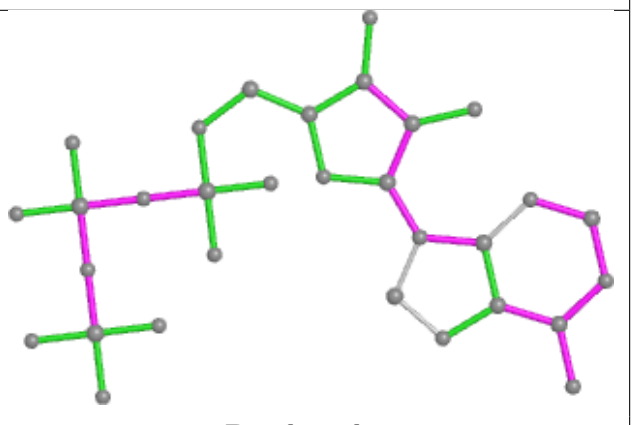


Rings

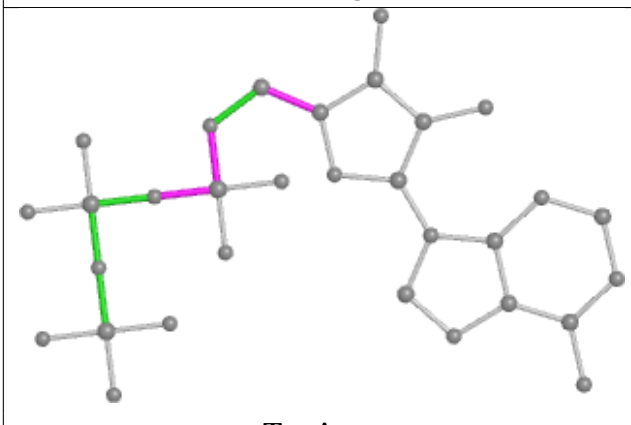
Ligand ATP C1 601



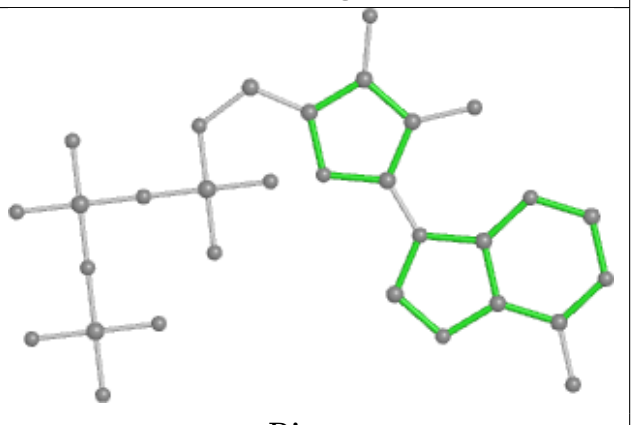
Bond lengths



Bond angles

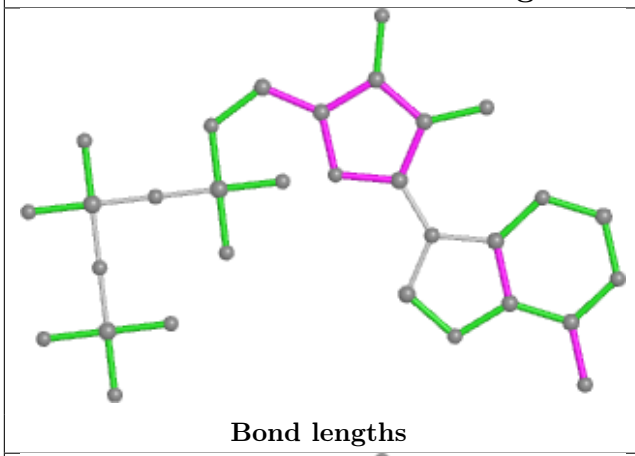


Torsions

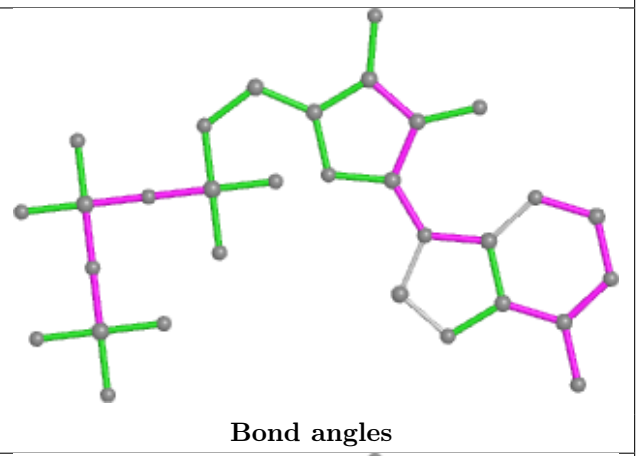


Rings

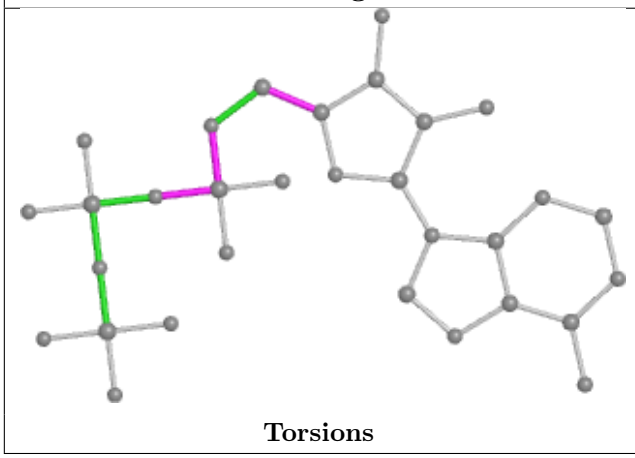
Ligand ATP C4 601



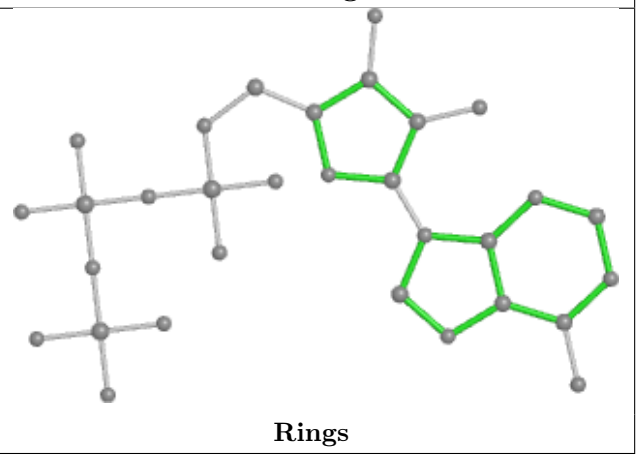
Bond lengths



Bond angles

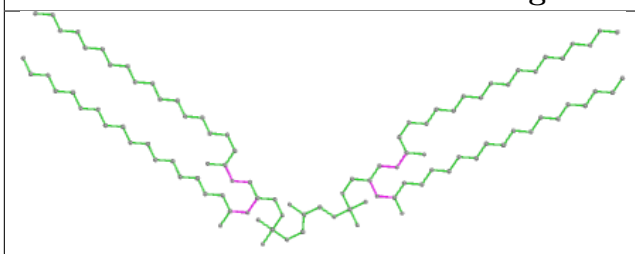


Torsions

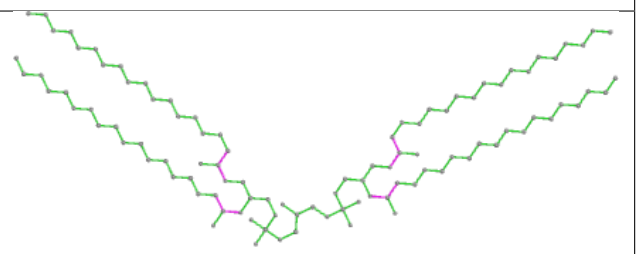


Rings

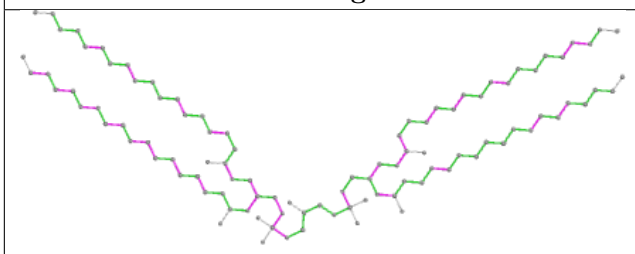
Ligand CDL J 302



Bond lengths



Bond angles



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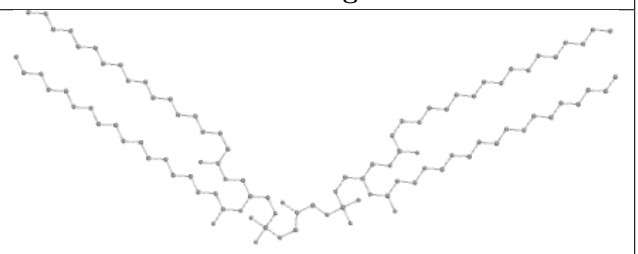
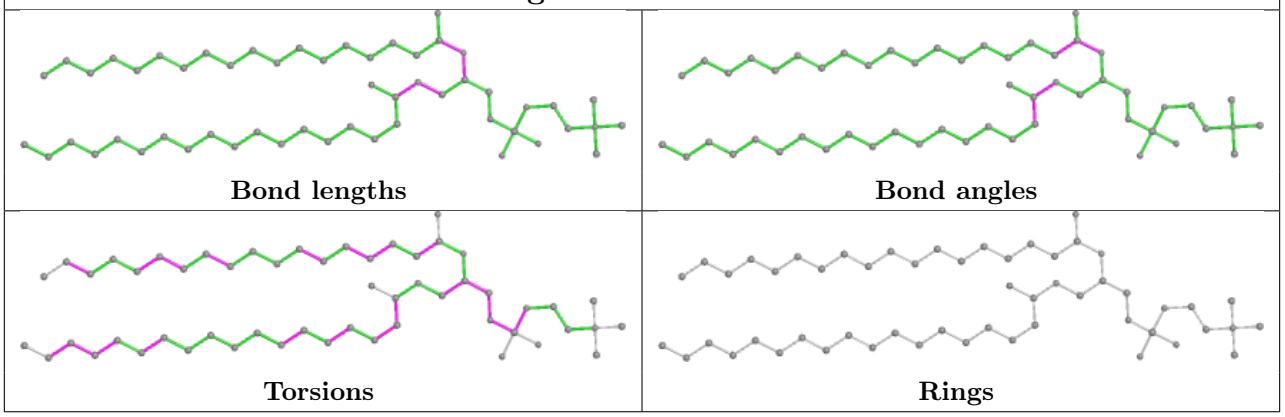
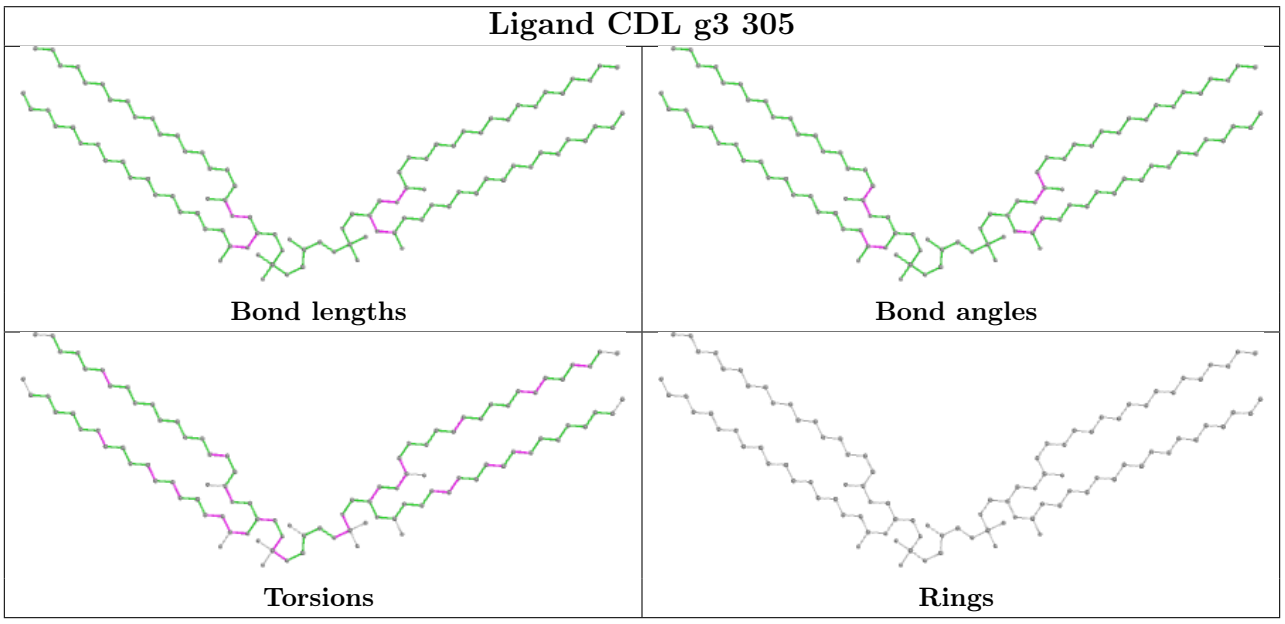


Rings

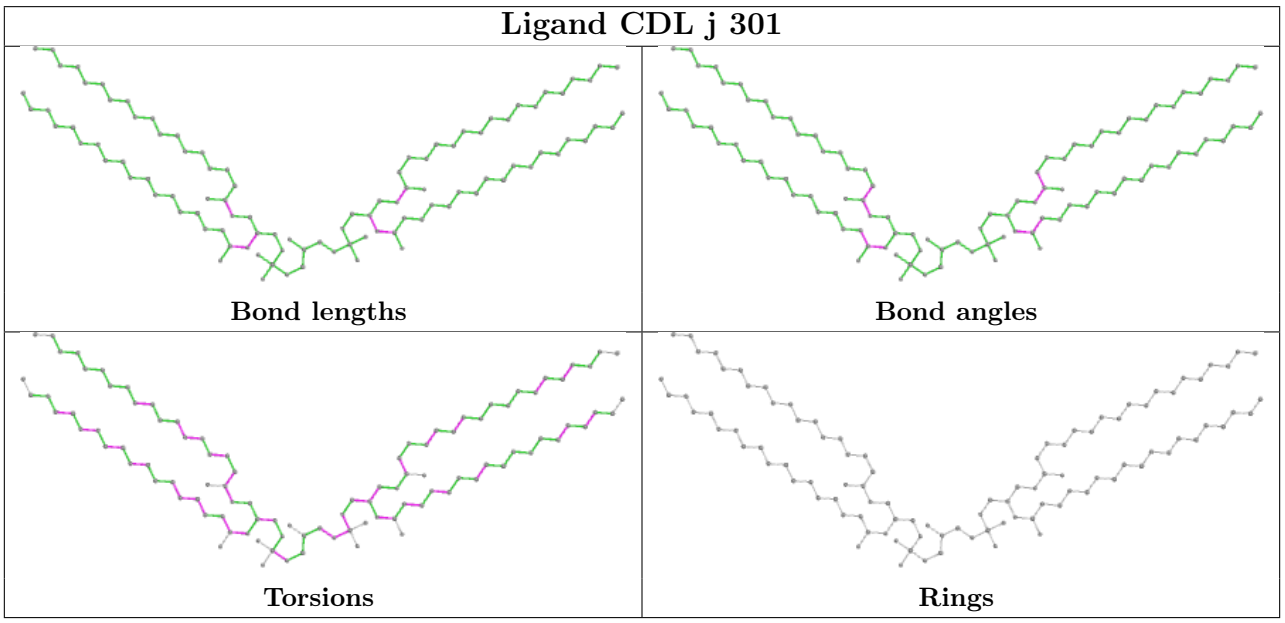
Ligand PC1 G 303



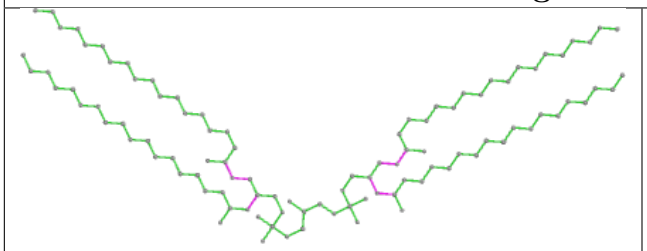
Ligand CDL g3 305



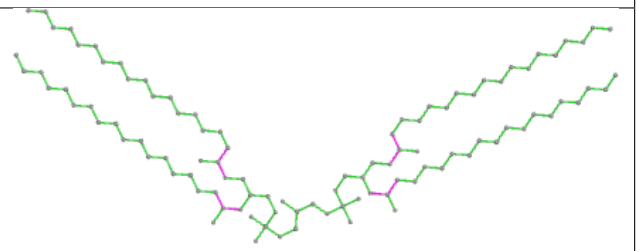
Ligand CDL j 301



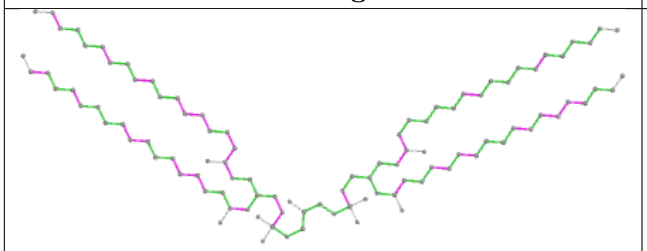
Ligand CDL l 301



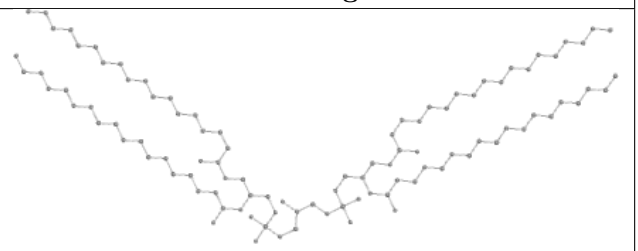
Bond lengths



Bond angles

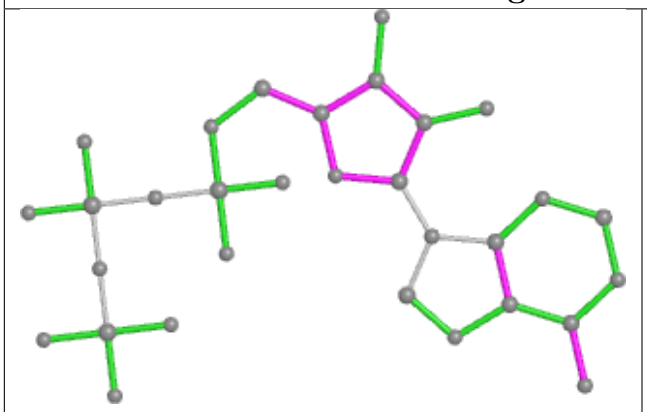


Torsions

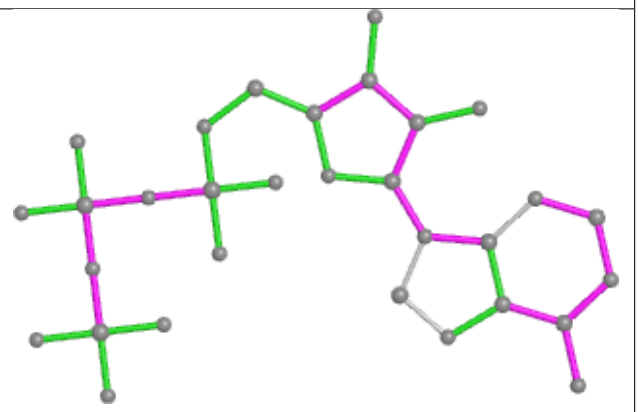


Rings

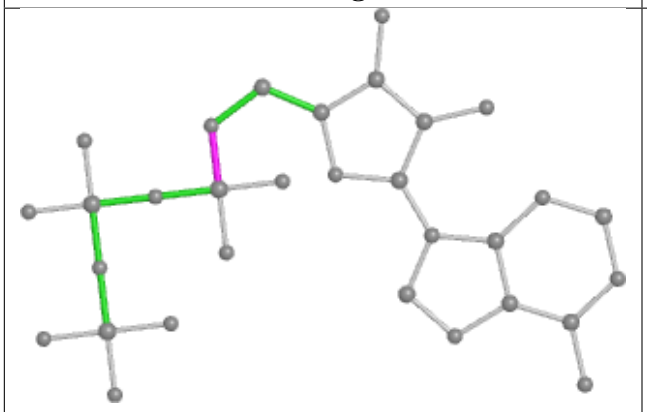
Ligand ATP B1 1003



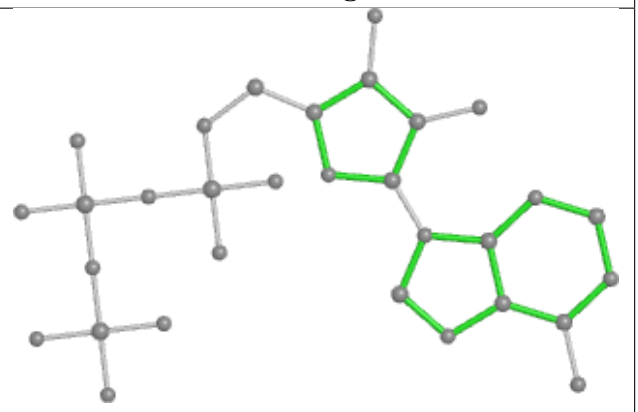
Bond lengths



Bond angles

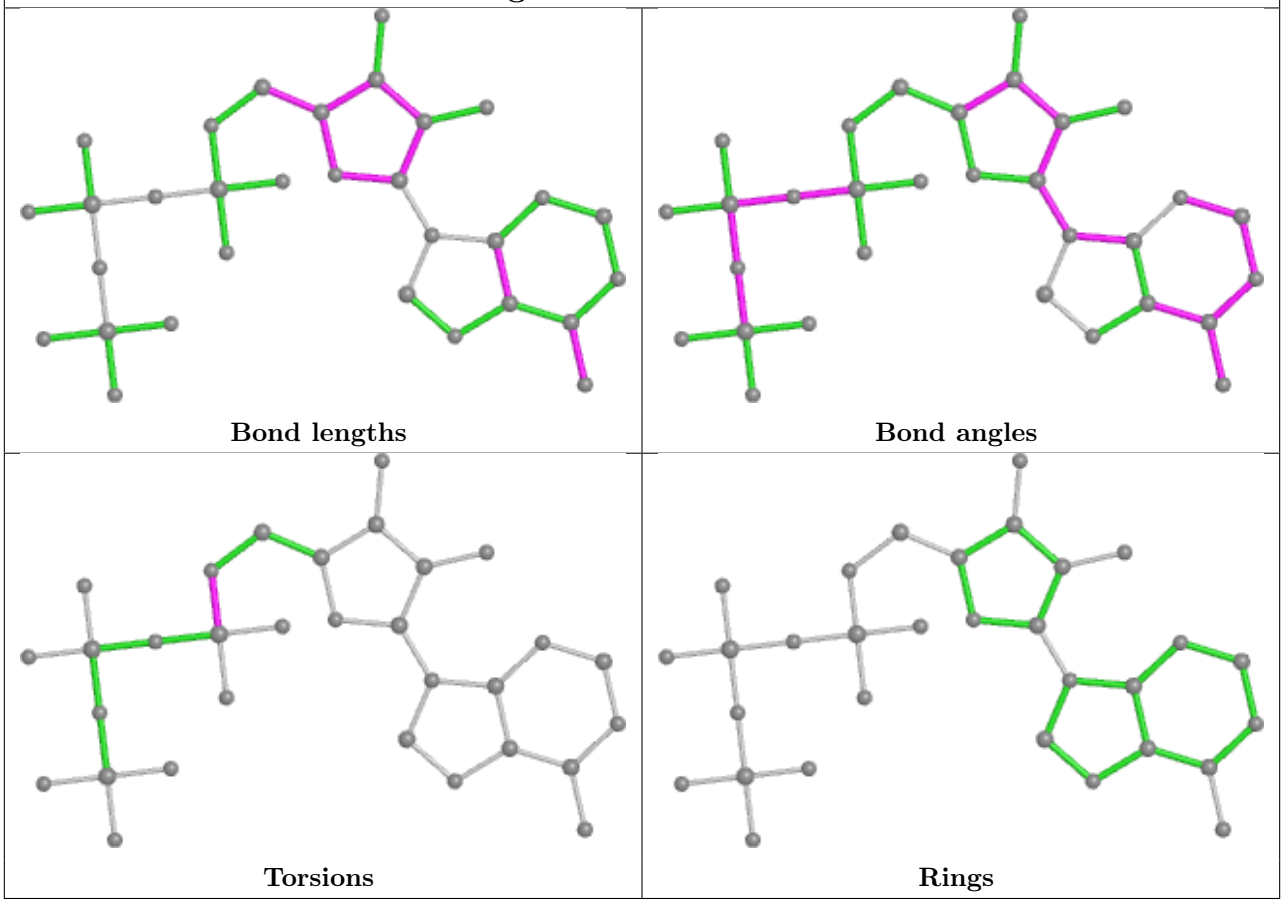


Torsions

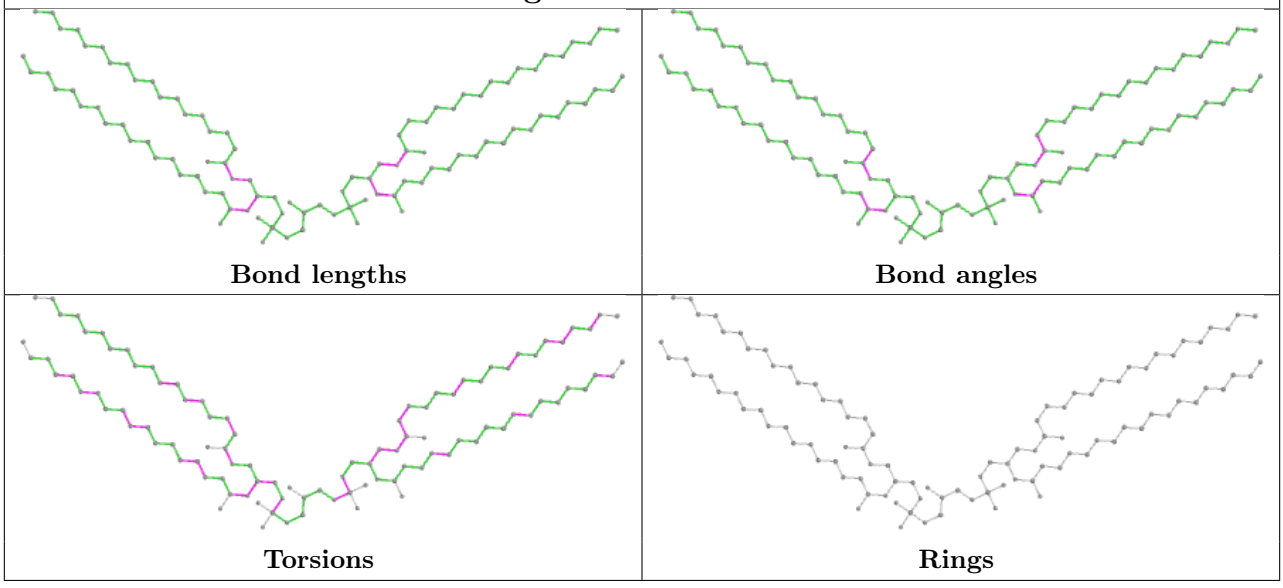


Rings

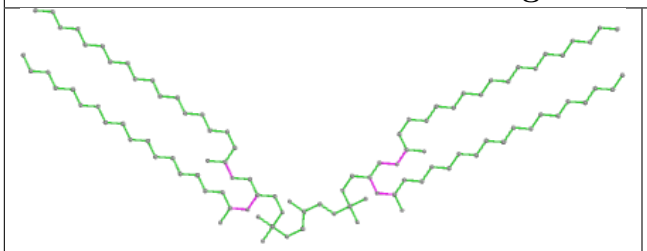
Ligand ATP B4 1003



Ligand CDL i3 301



Ligand CDL I3 303



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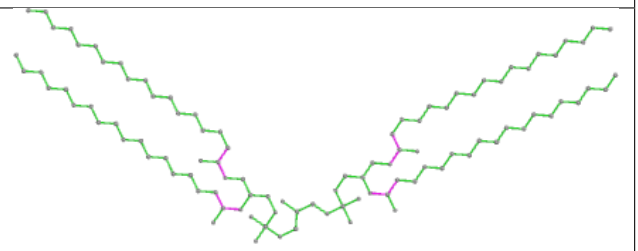
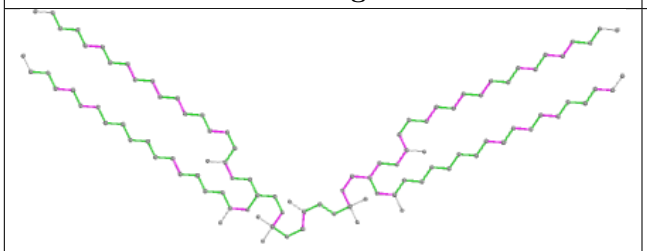
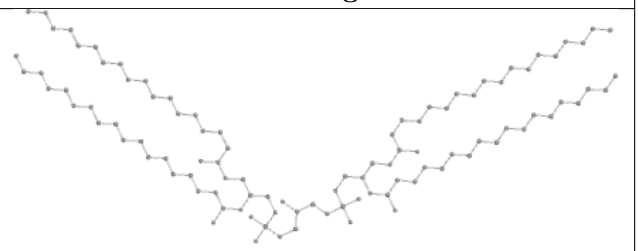


Bond angles

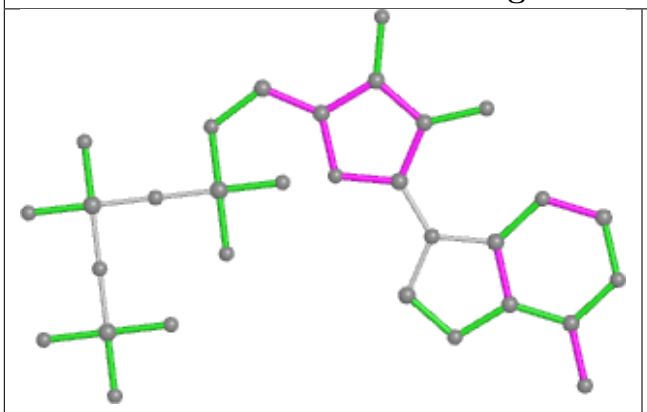


Torsions

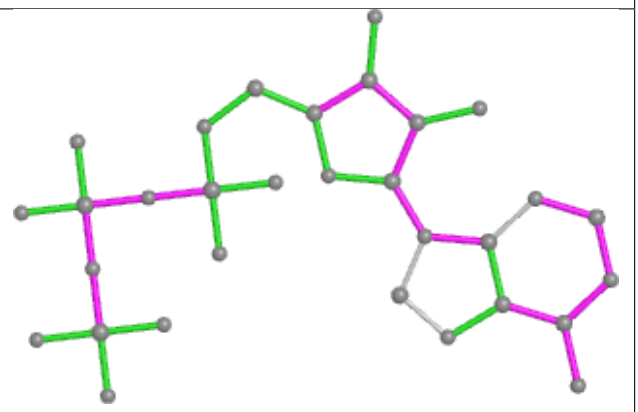


Rings

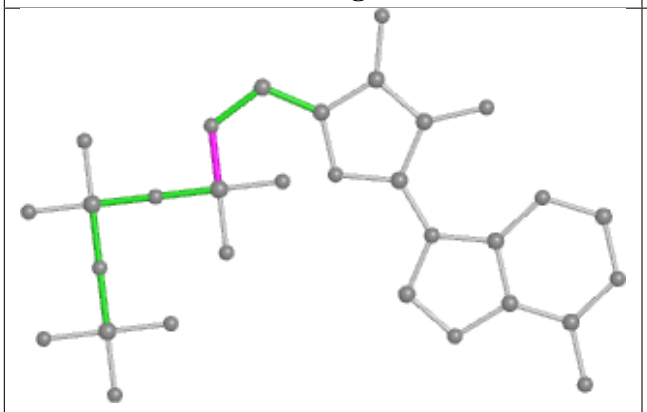
Ligand ATP B5 1003



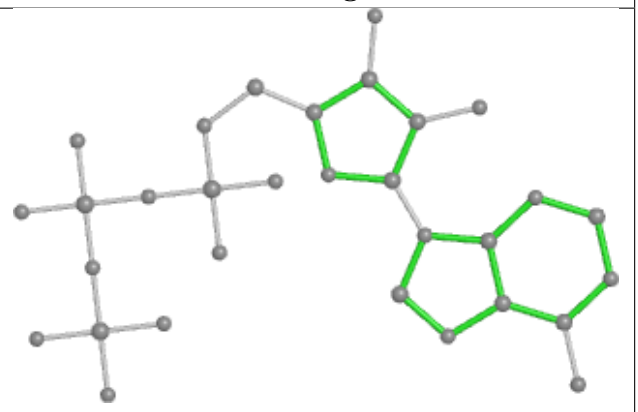
Bond lengths



Bond angles

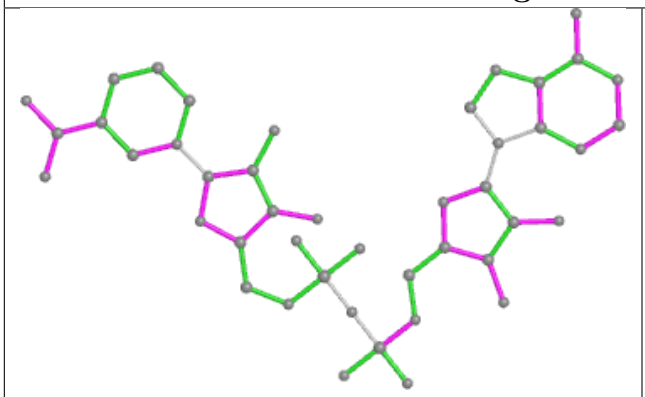


Torsions

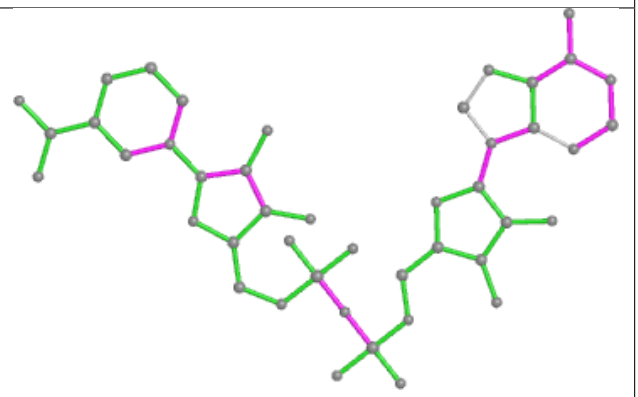


Rings

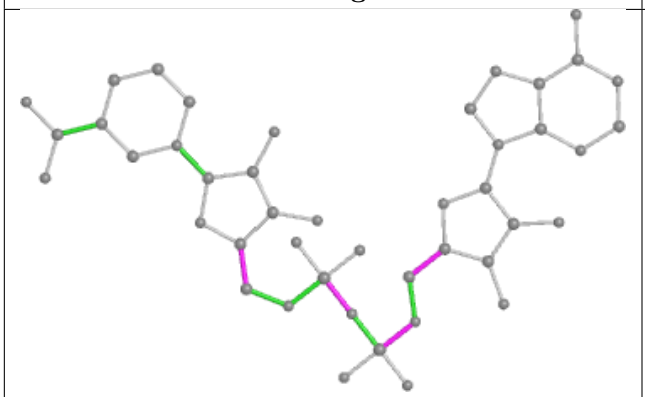
Ligand NAD E3 900



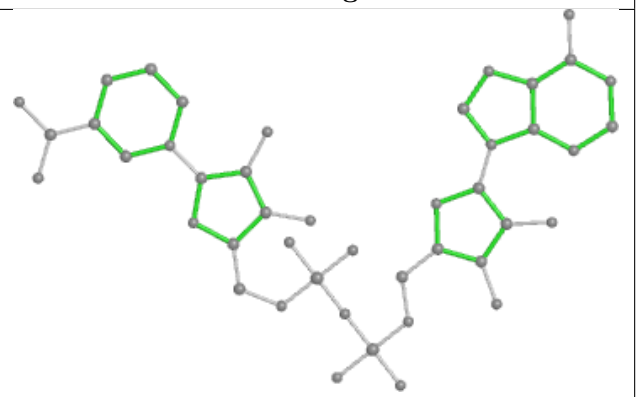
Bond lengths



Bond angles

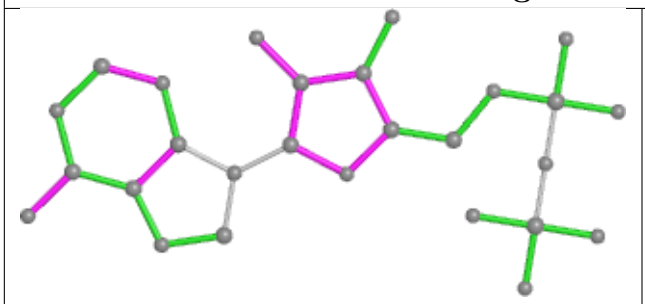


Torsions

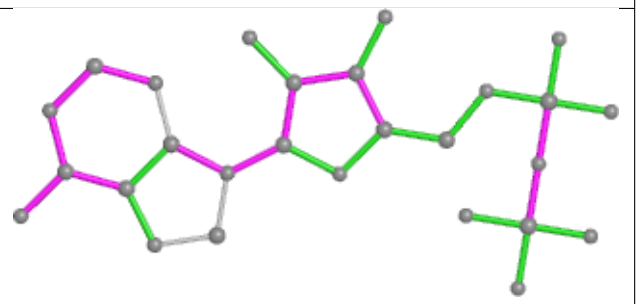


Rings

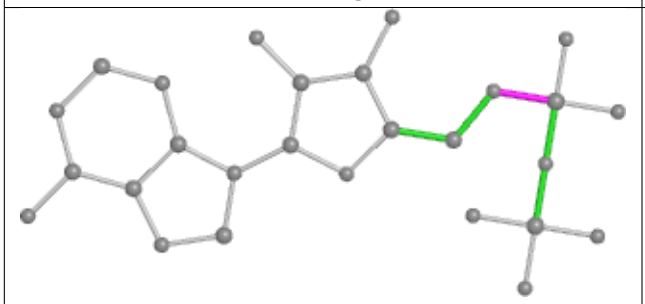
Ligand ADP D5 501



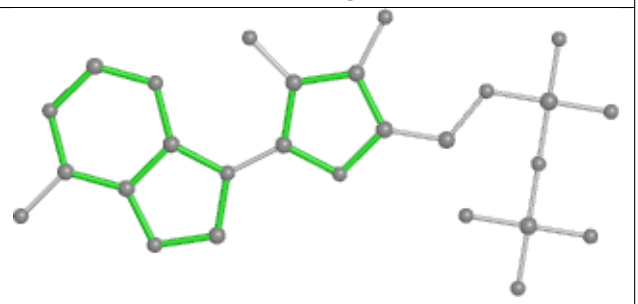
Bond lengths



Bond angles

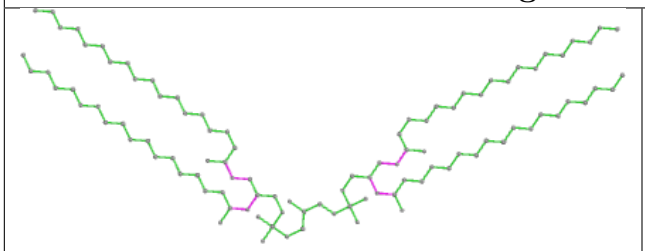


Torsions

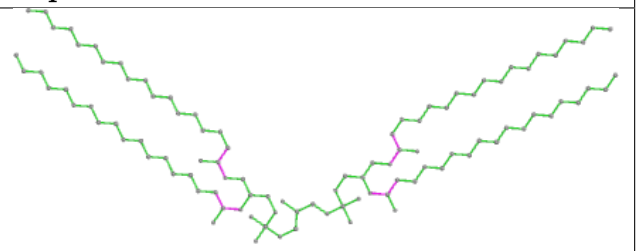


Rings

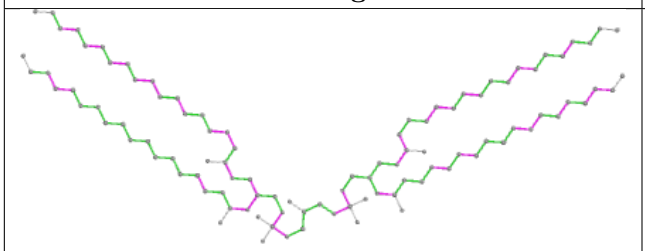
Ligand CDL p3 201



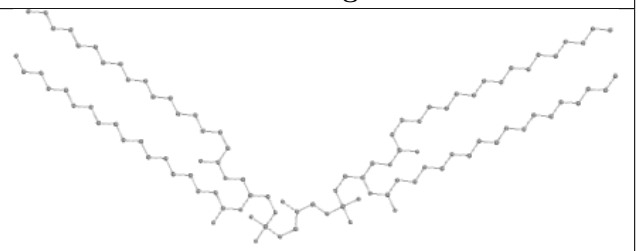
Bond lengths



Bond angles

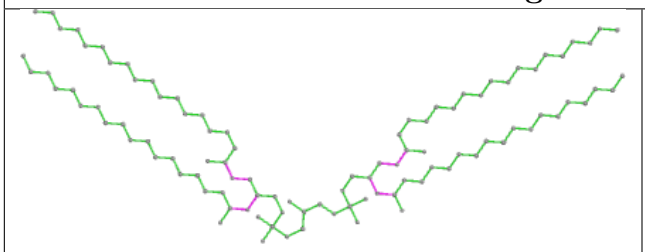


Torsions

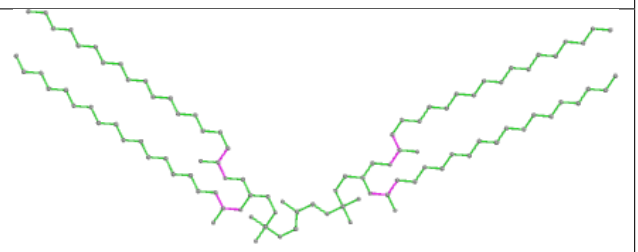


Rings

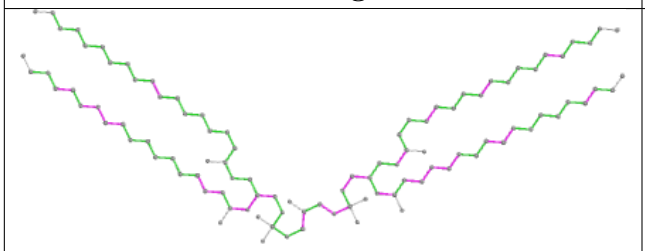
Ligand CDL B 403



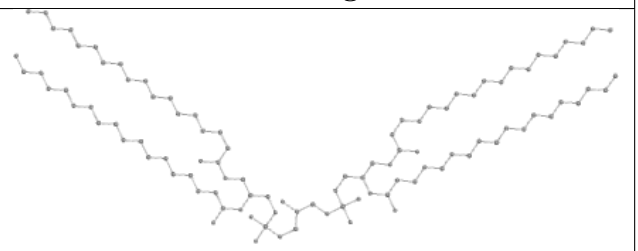
Bond lengths



Bond angles

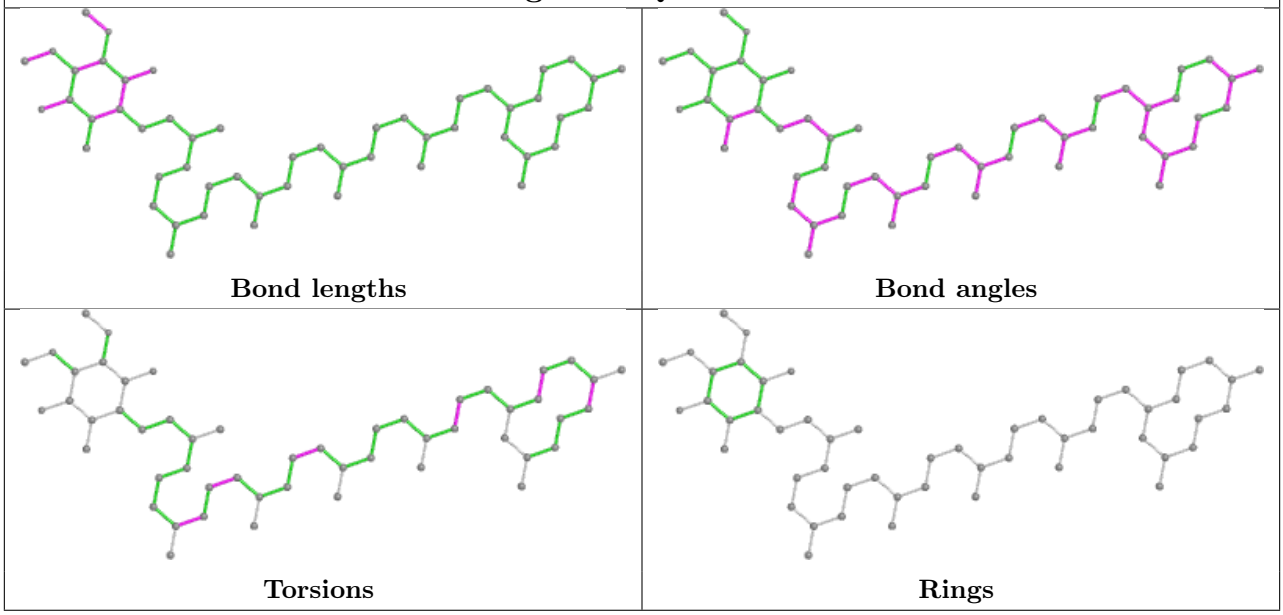


Torsions

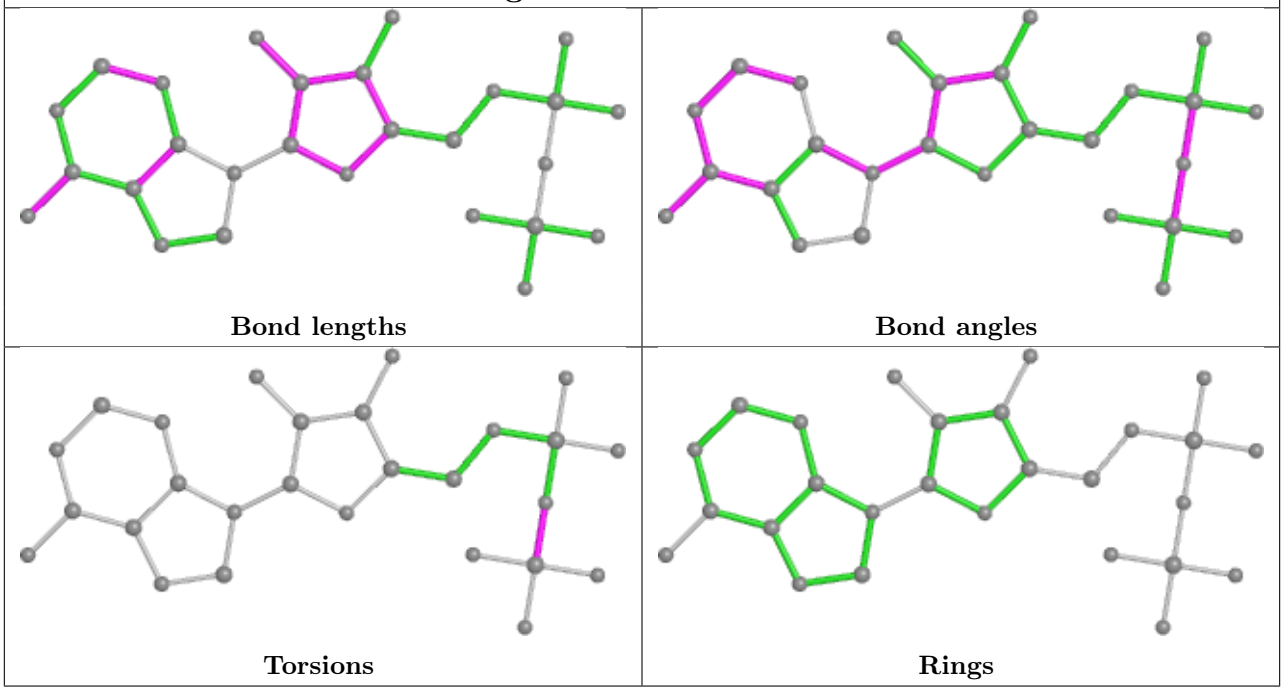


Rings

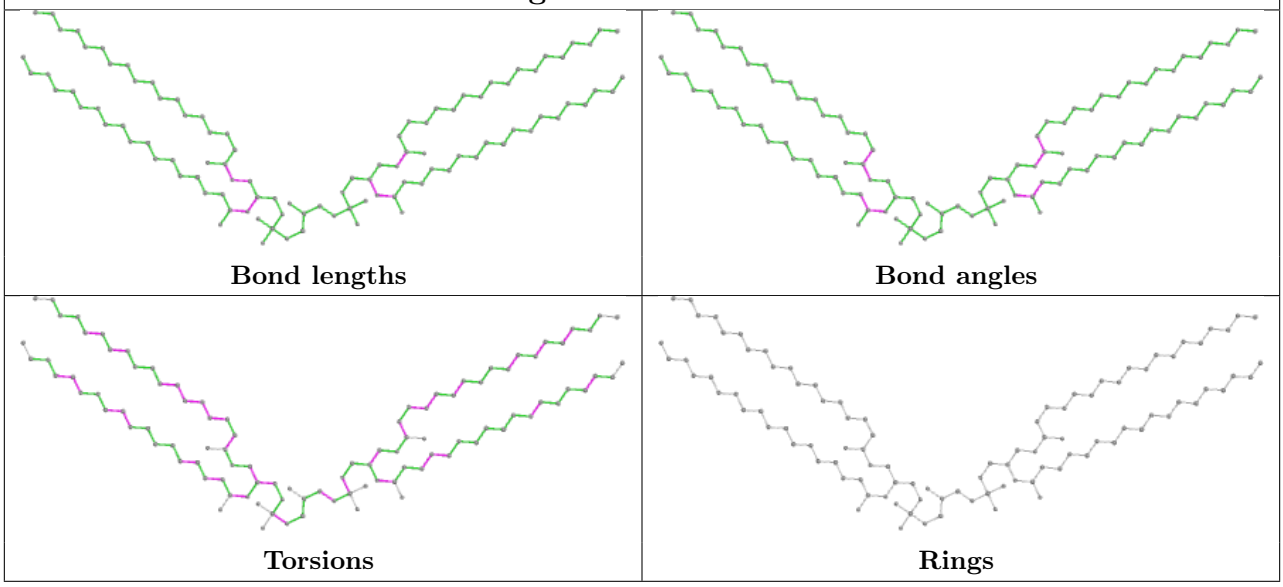
Ligand UQ8 i3 303



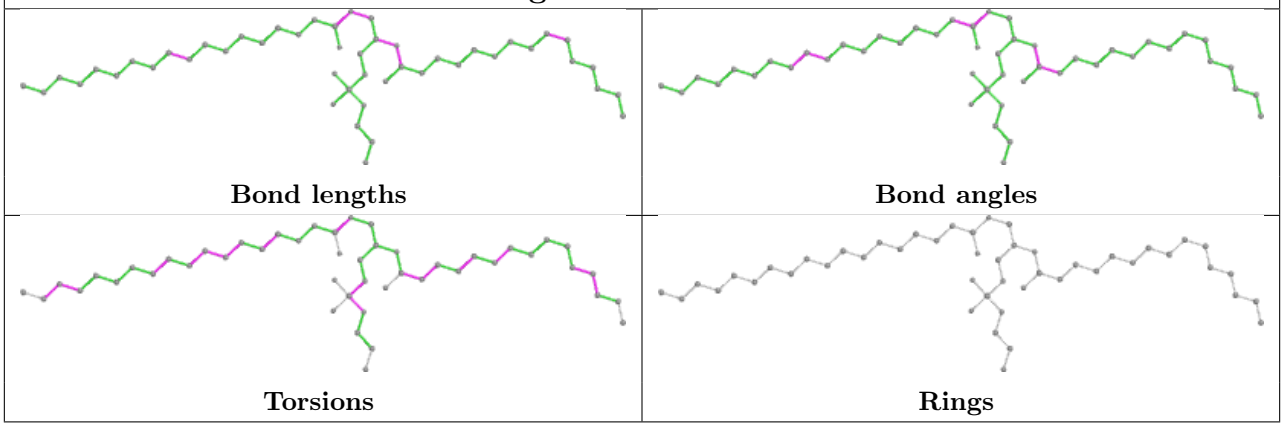
Ligand ADP B2 1002



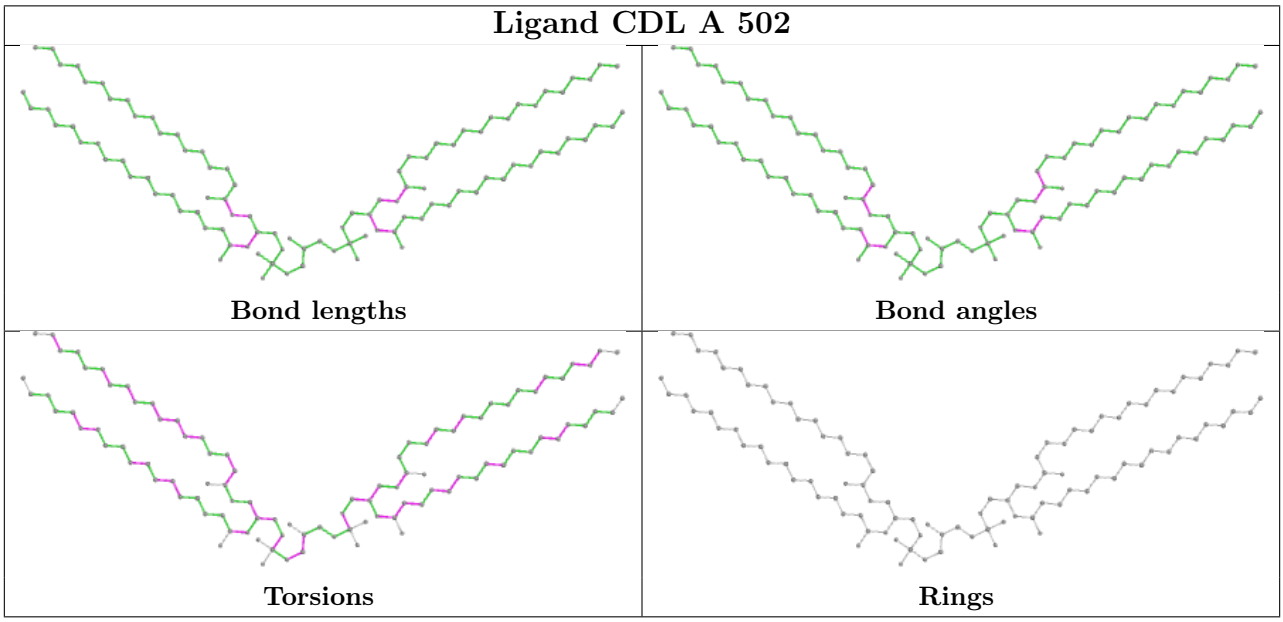
Ligand CDL J 301



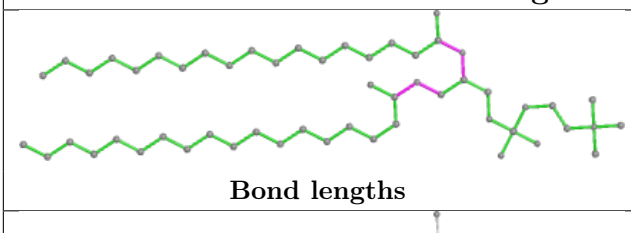
Ligand PEE L 303



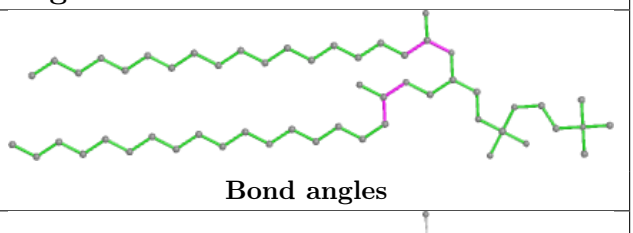
Ligand CDL A 502



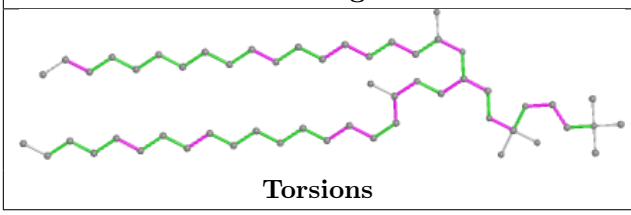
Ligand PC1 g 304



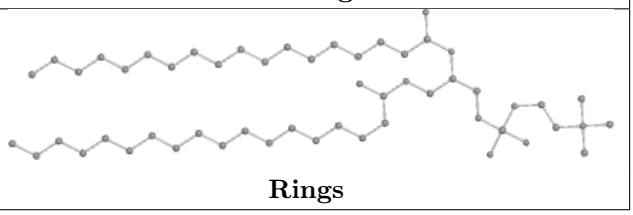
Bond lengths



Bond angles

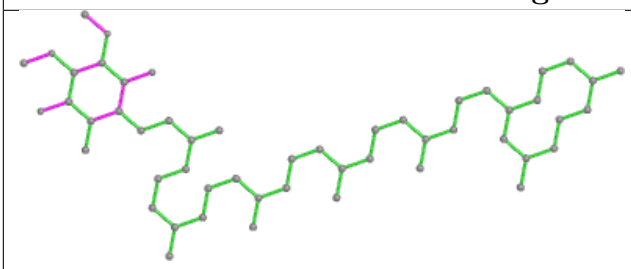


Torsions

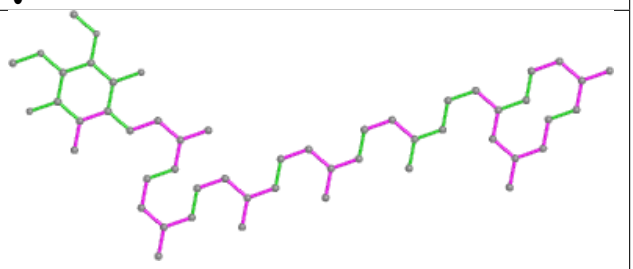


Rings

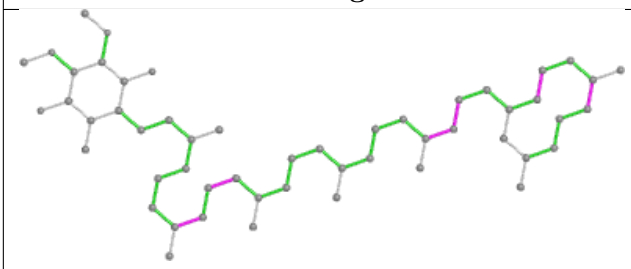
Ligand UQ8 I 303



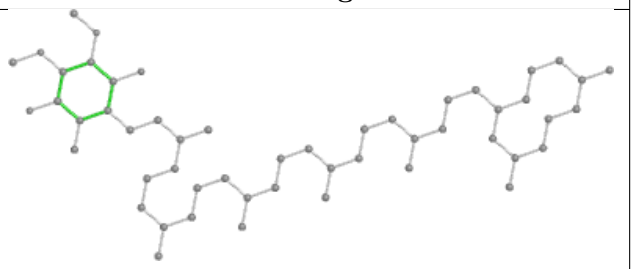
Bond lengths



Bond angles

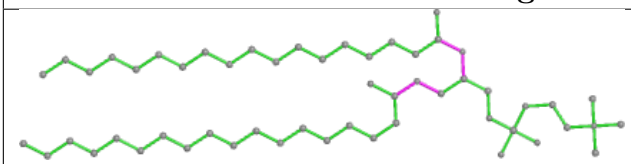


Torsions



Rings

Ligand PC1 G3 304



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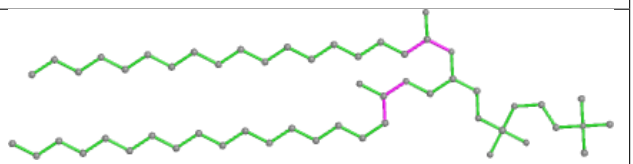

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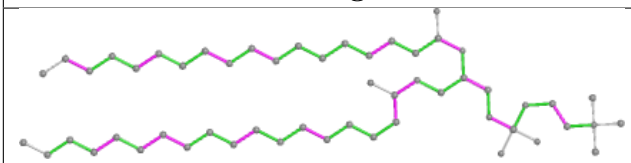

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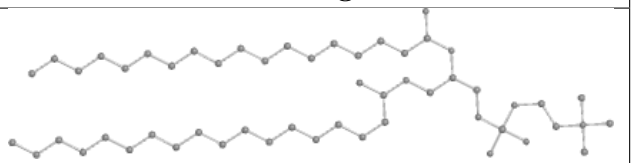
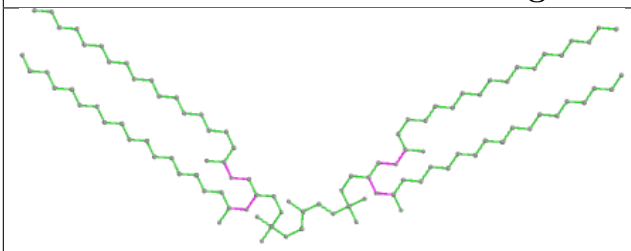


Rings

Ligand CDL a 501



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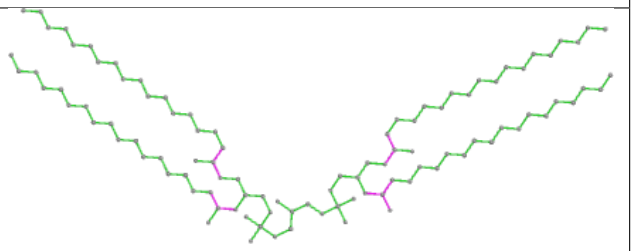
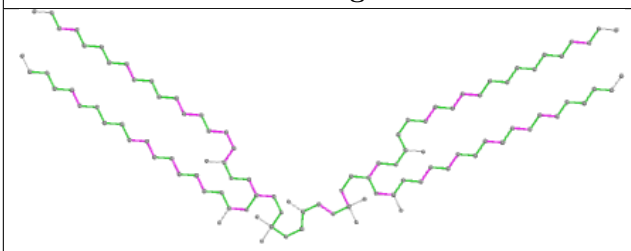


Bond angles



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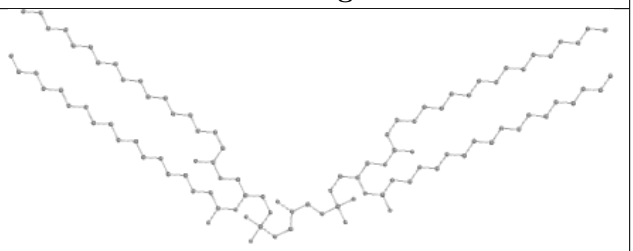
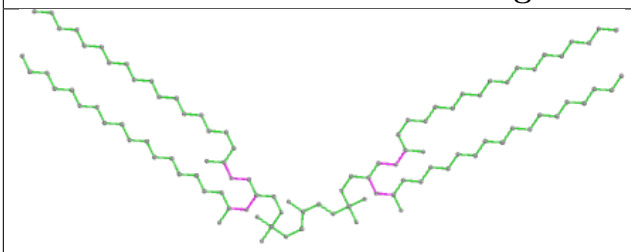


Rings

Ligand CDL K3 201



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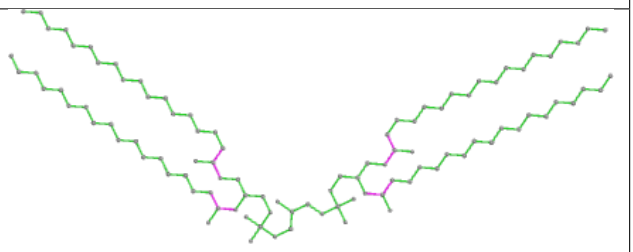
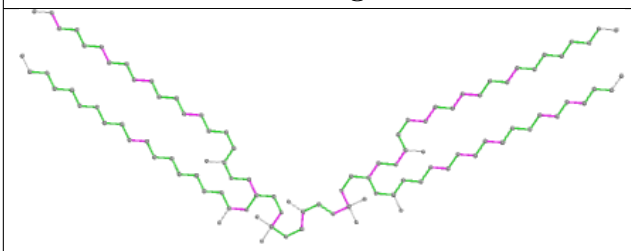


Bond angles



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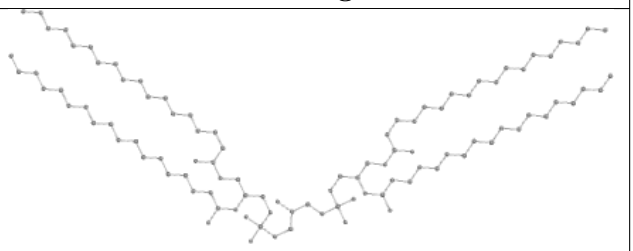
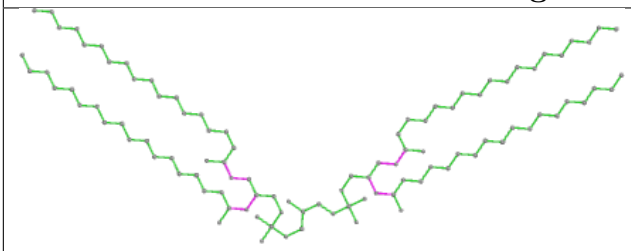


Rings

Ligand CDL r 201



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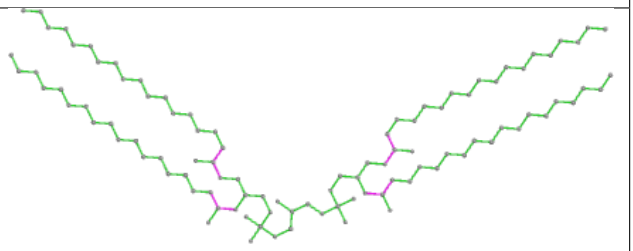
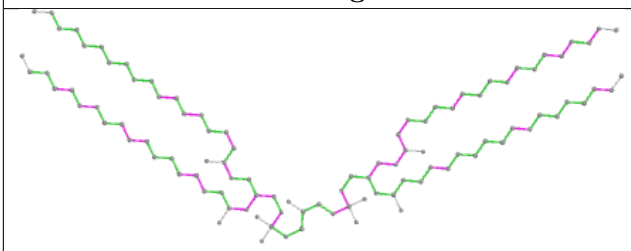


Bond angles



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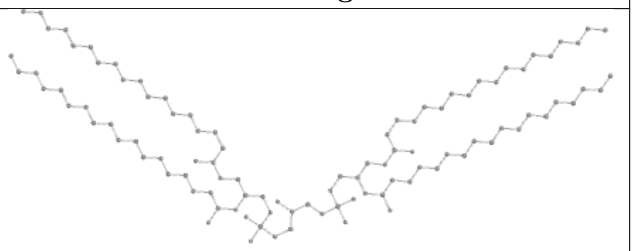
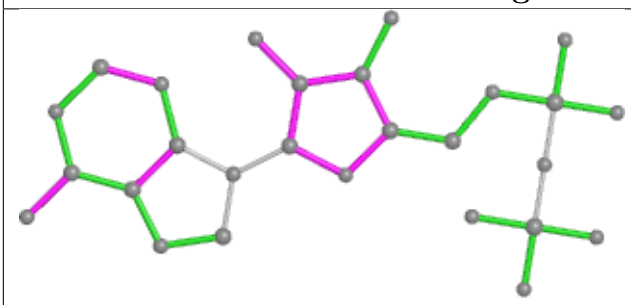


Rings

Ligand ADP D1 501



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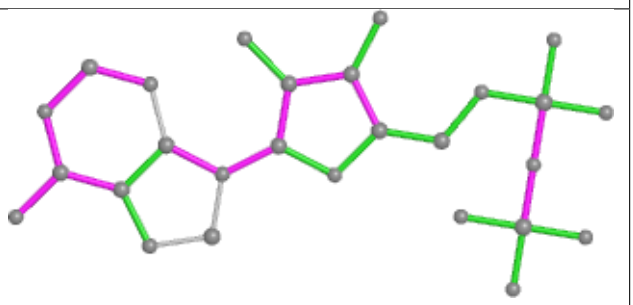
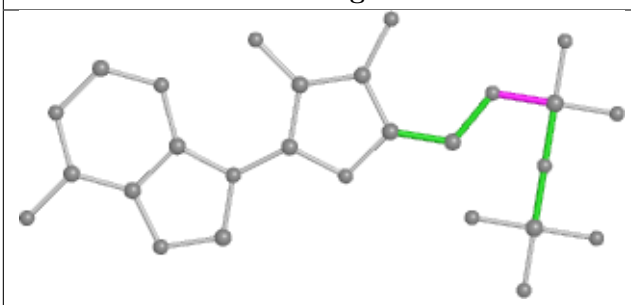
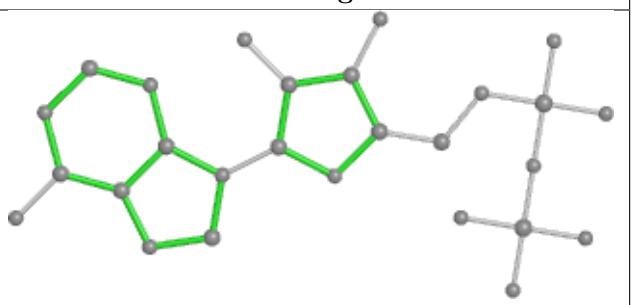


Bond angles

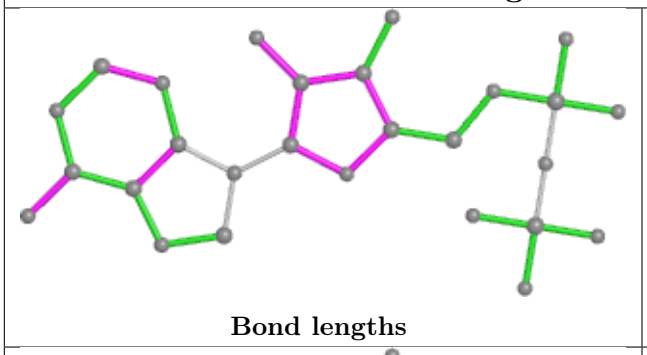


Torsions



Rings

Ligand ADP B4 1002



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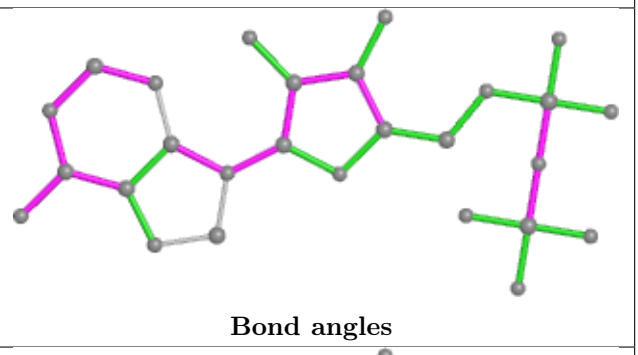

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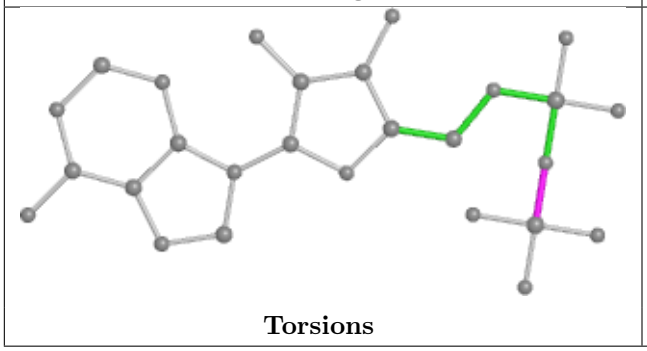

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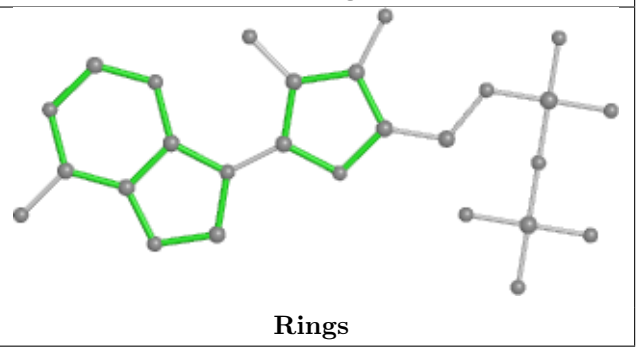
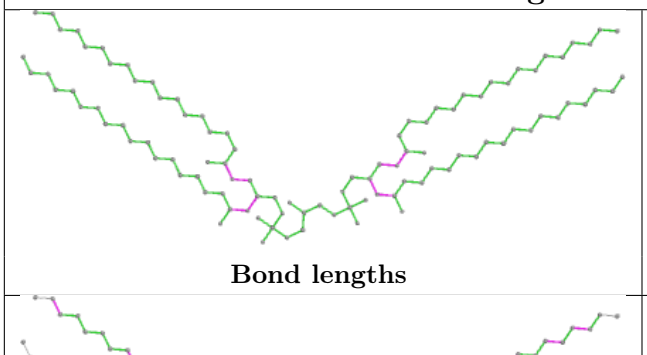


Rings

Ligand CDL L 301



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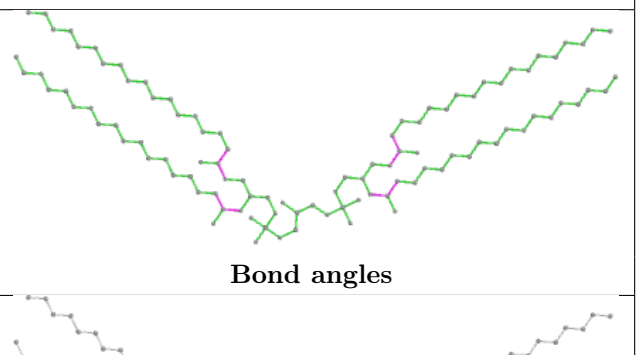
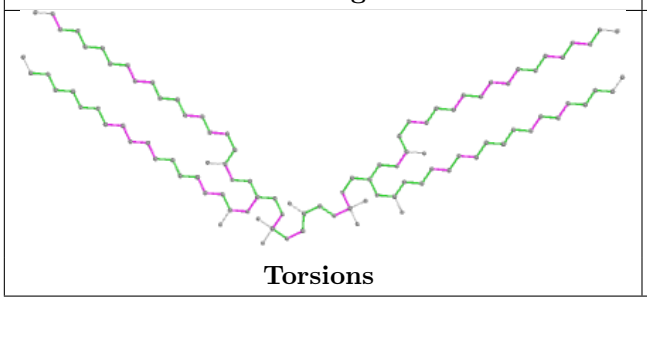


Bond angles



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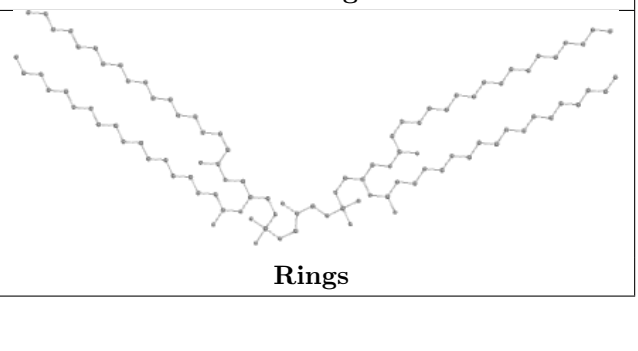
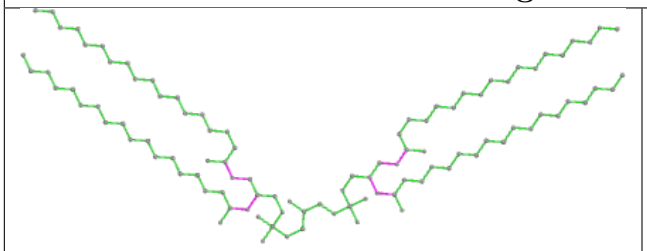
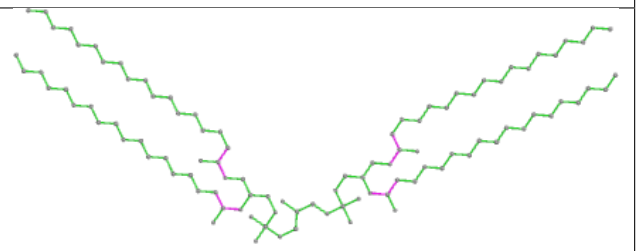


Rings

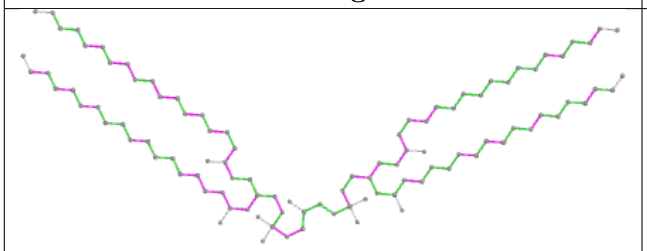
Ligand CDL B3 401



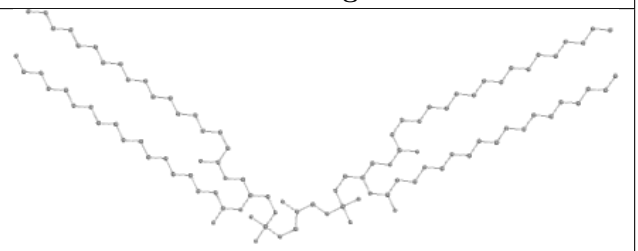
Bond lengths



Bond angles

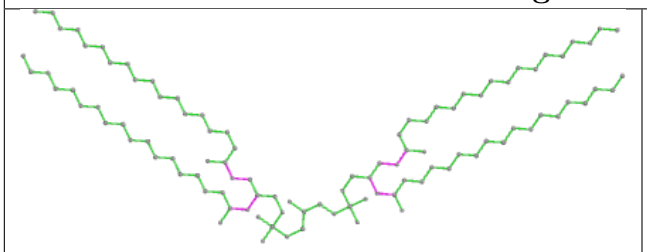


Torsions

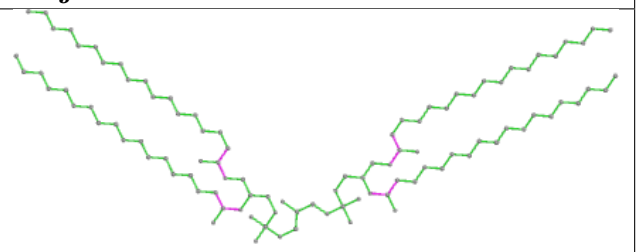


Rings

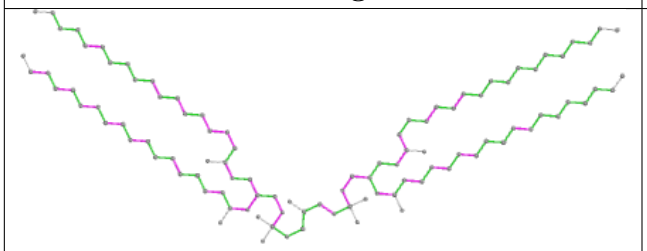
Ligand CDL j 302



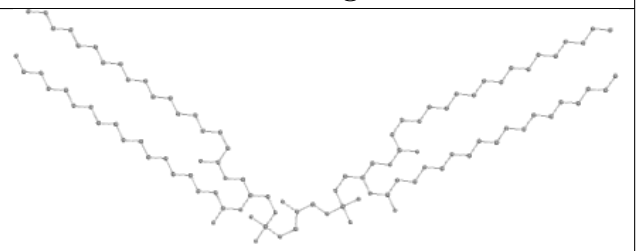
Bond lengths



Bond angles

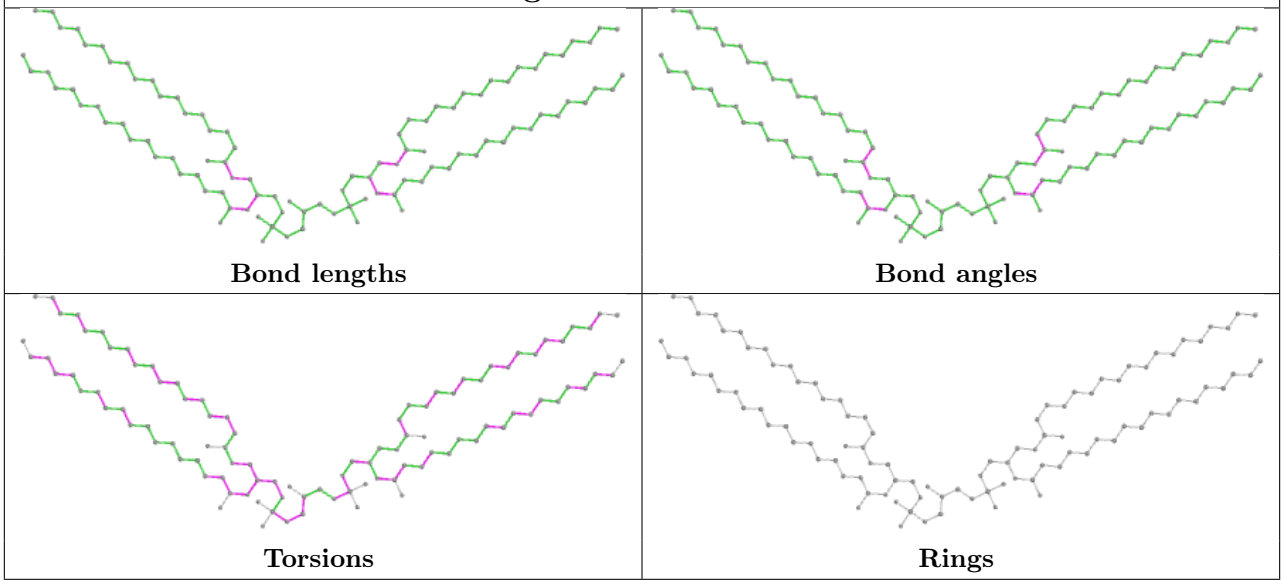


Torsions

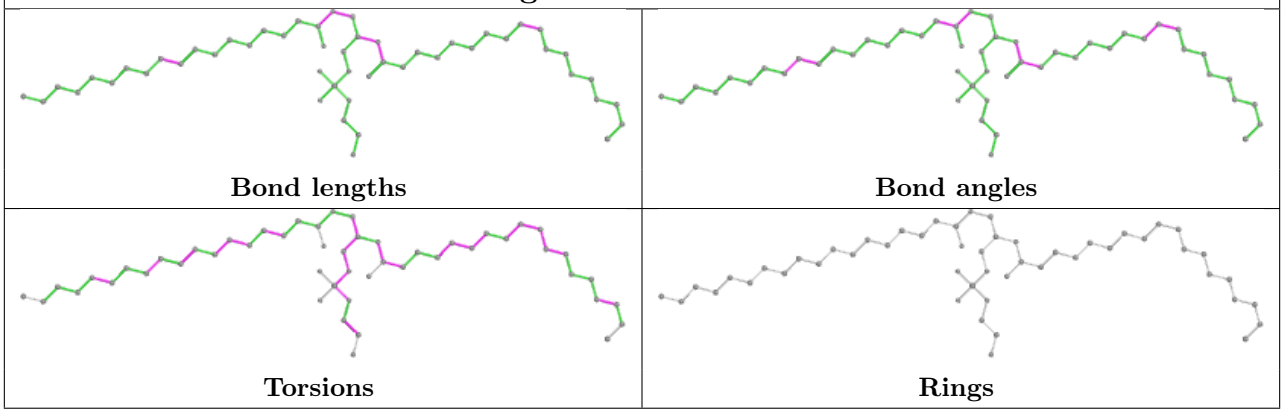


Rings

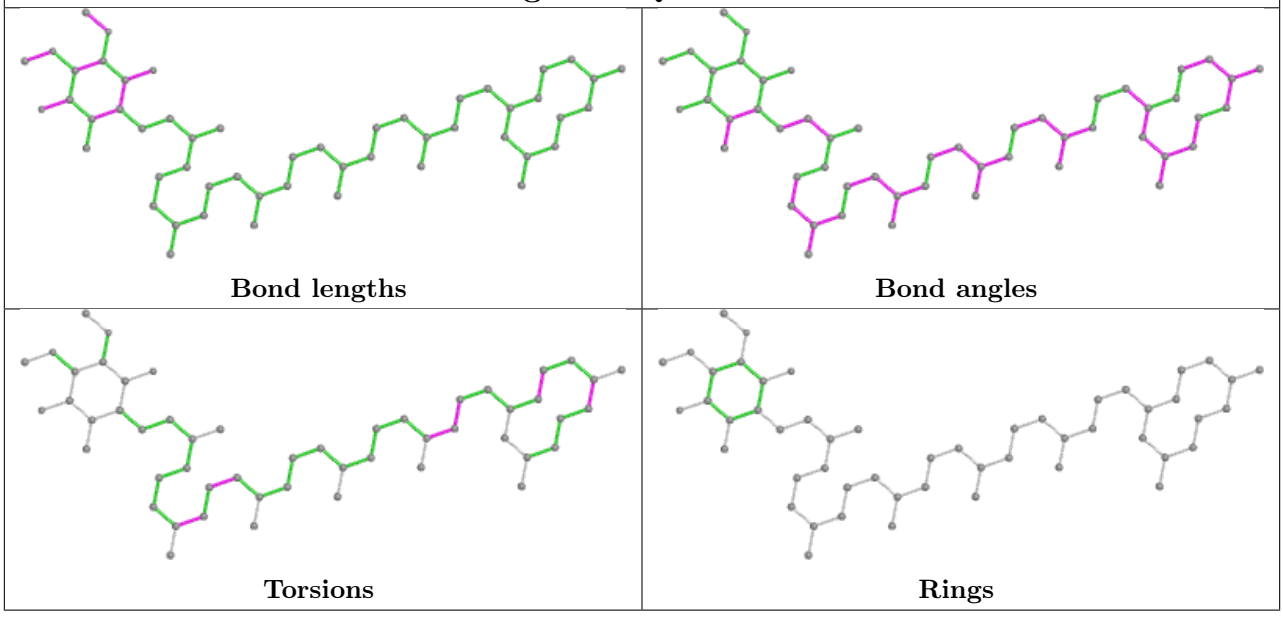
Ligand CDL f3 302



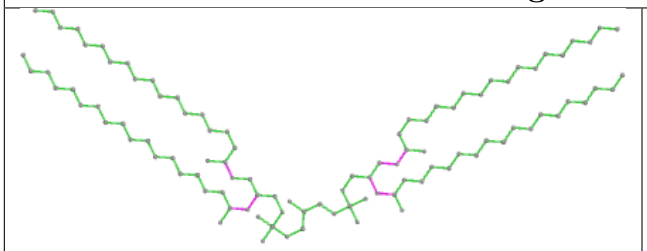
Ligand PEE L3 302



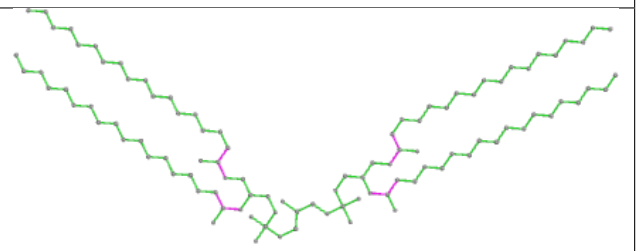
Ligand UQ8 I3 304



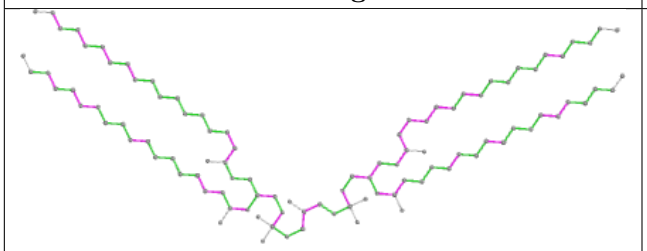
Ligand CDL b 401



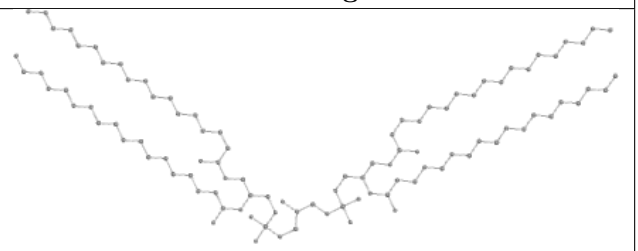
Bond lengths



Bond angles

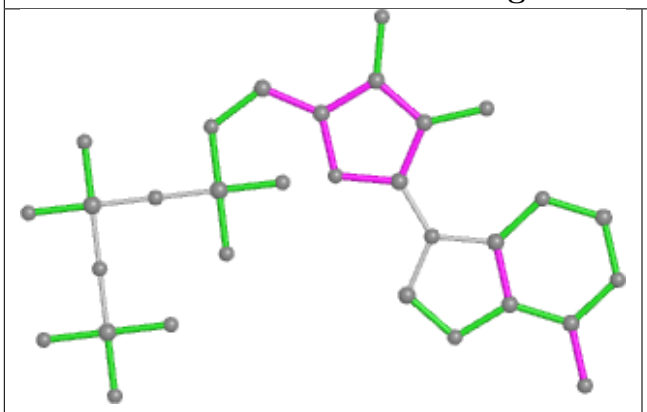


Torsions

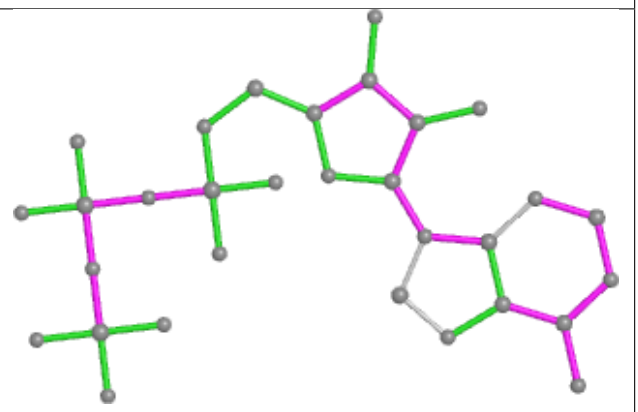


Rings

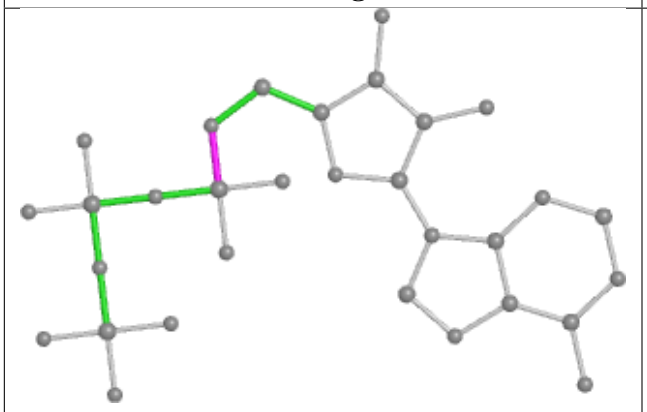
Ligand ATP B2 1003



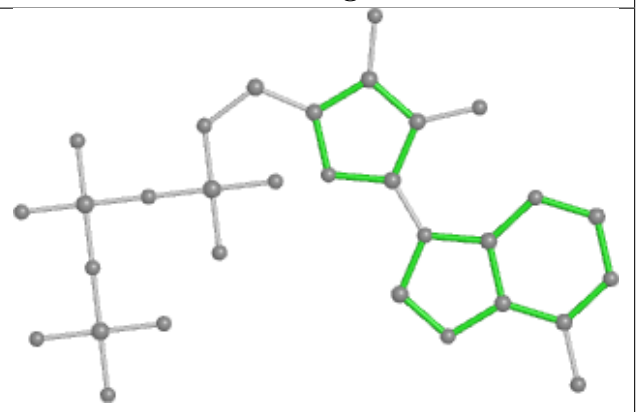
Bond lengths



Bond angles

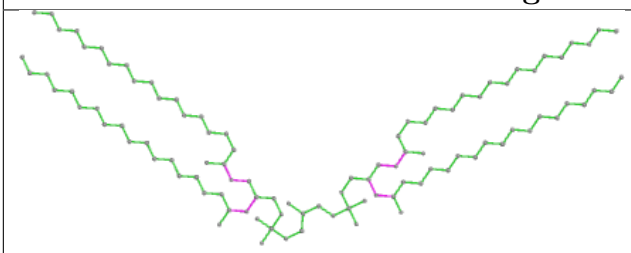


Torsions

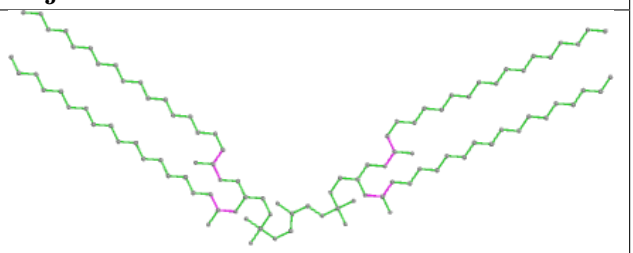


Rings

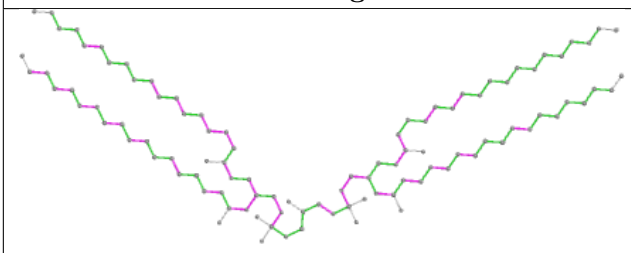
Ligand CDL j3 302



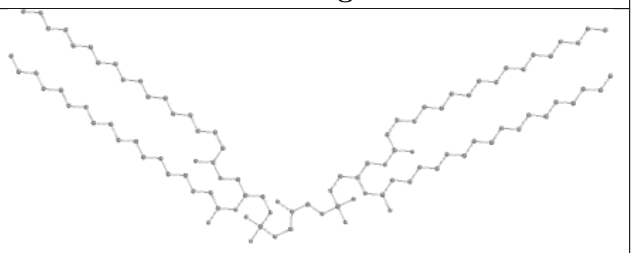
Bond lengths



Bond angles

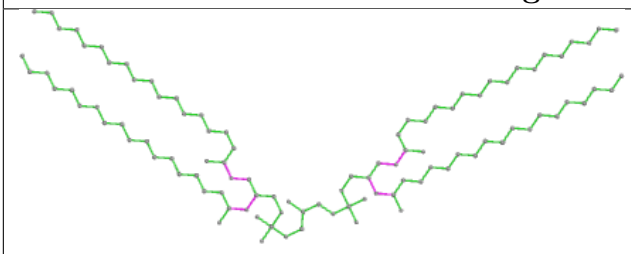


Torsions

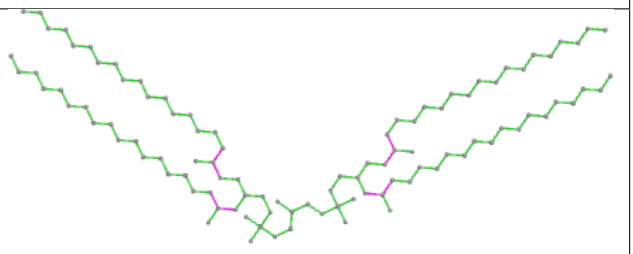


Rings

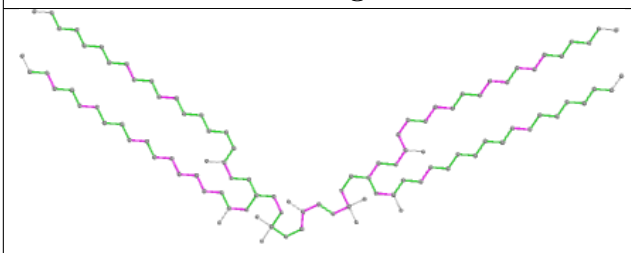
Ligand CDL f3 303



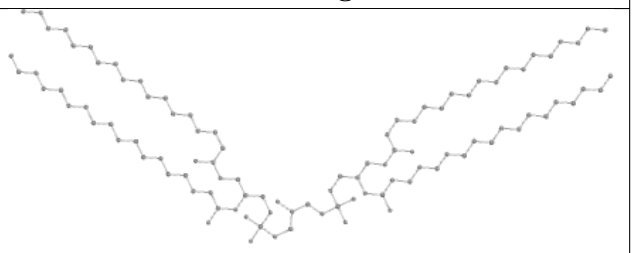
Bond lengths



Bond angles

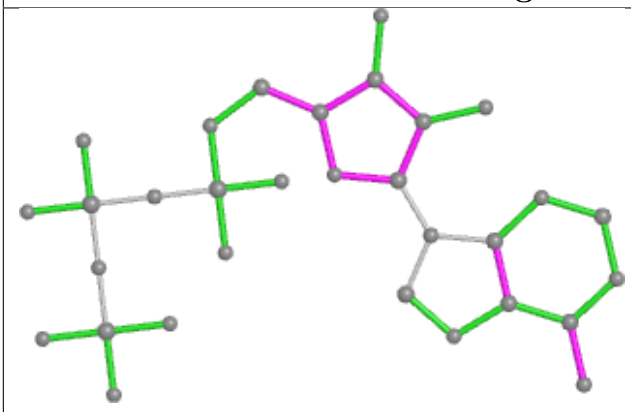


Torsions

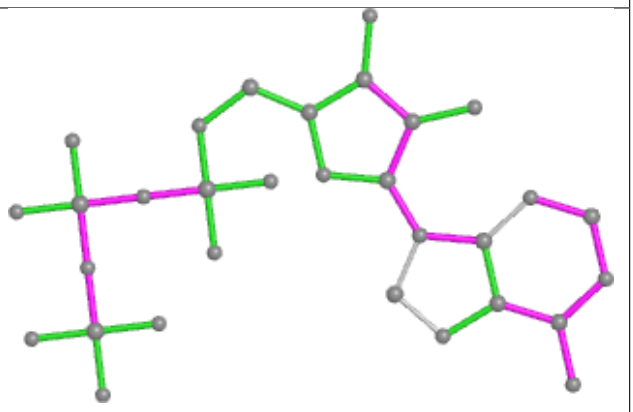


Rings

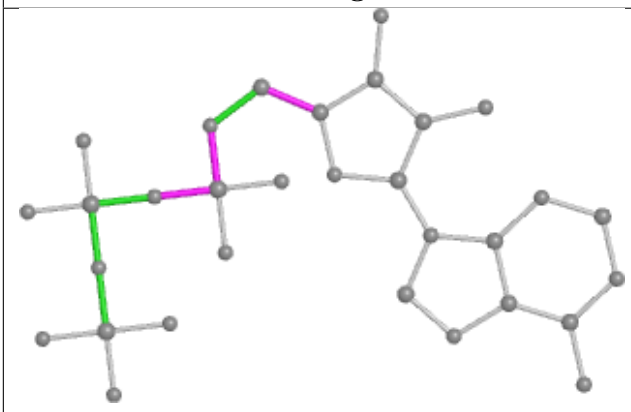
Ligand ATP A1 601



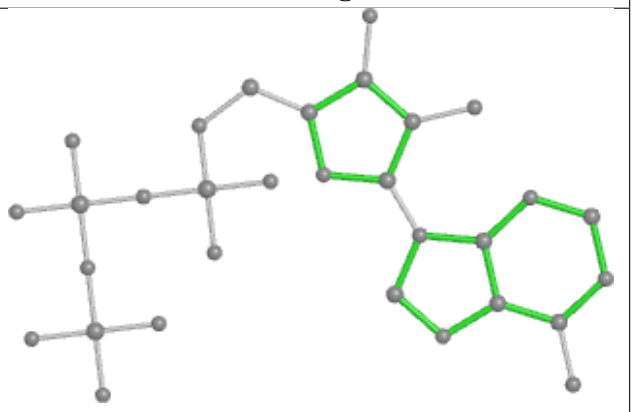
Bond lengths



Bond angles

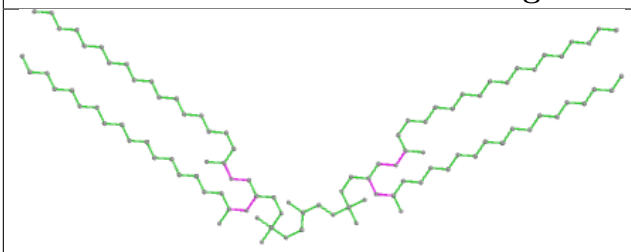


Torsions



Rings

Ligand CDL l3 301



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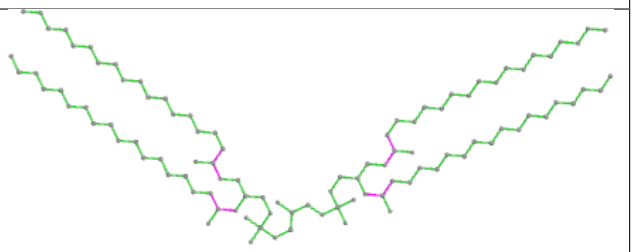
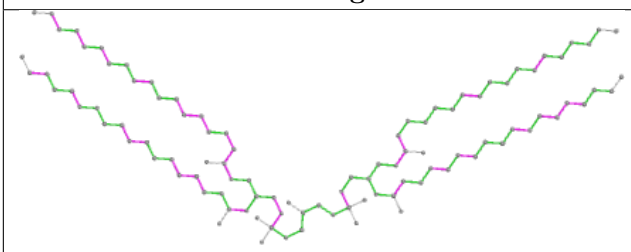
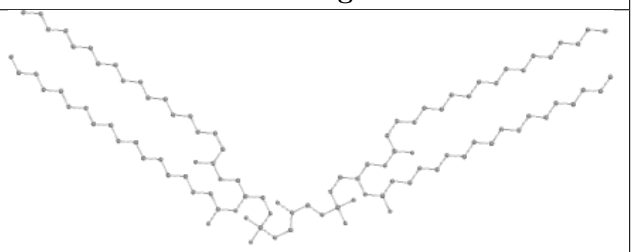


Bond angles

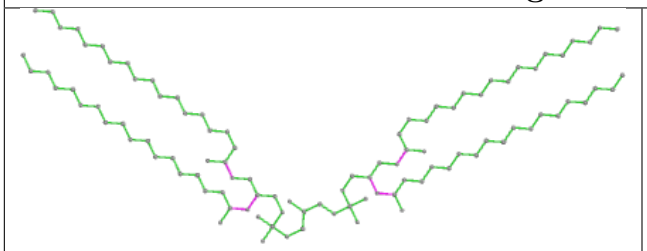


Torsions



Rings

Ligand CDL F 303



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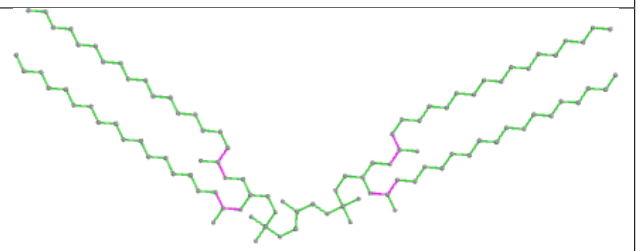
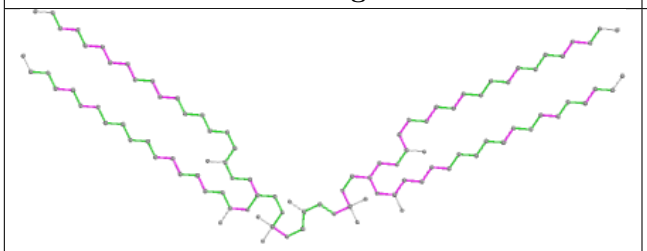
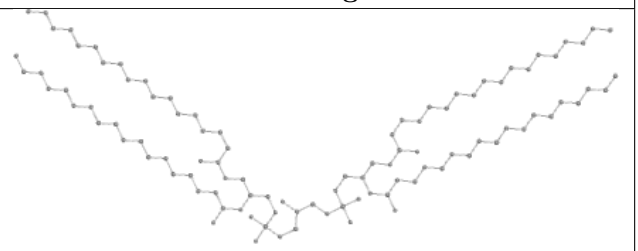


Bond angles

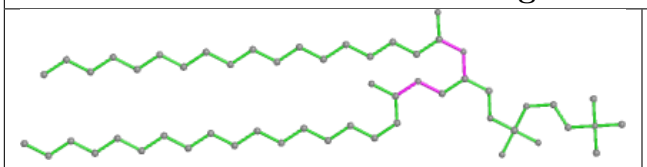


Torsions

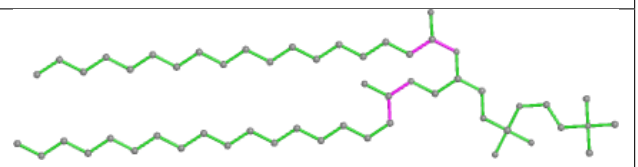


Rings

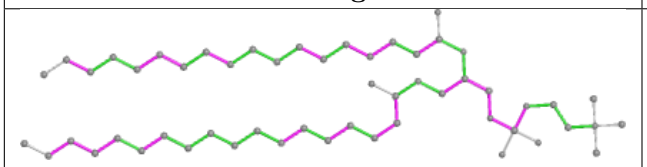
Ligand PC1 G3 303



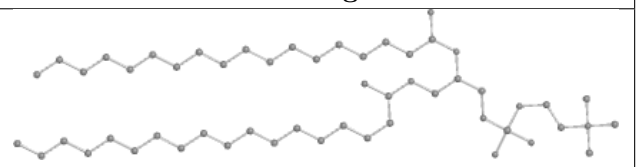
Bond lengths



Bond angles

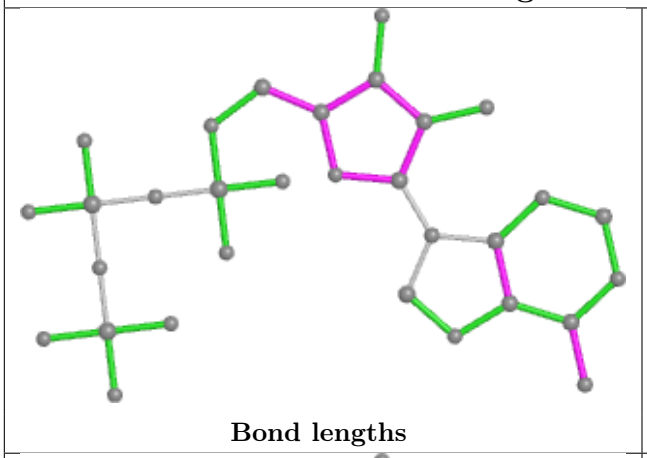


Torsions

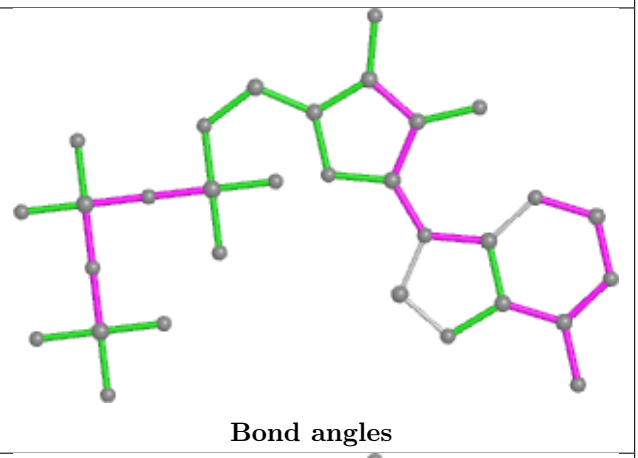


Rings

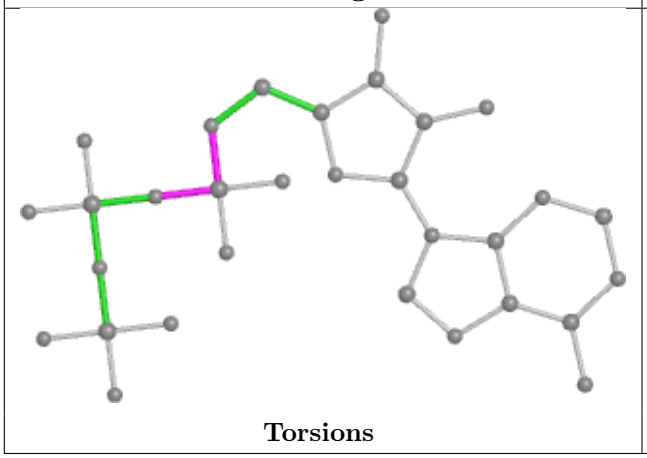
Ligand ATP C2 601



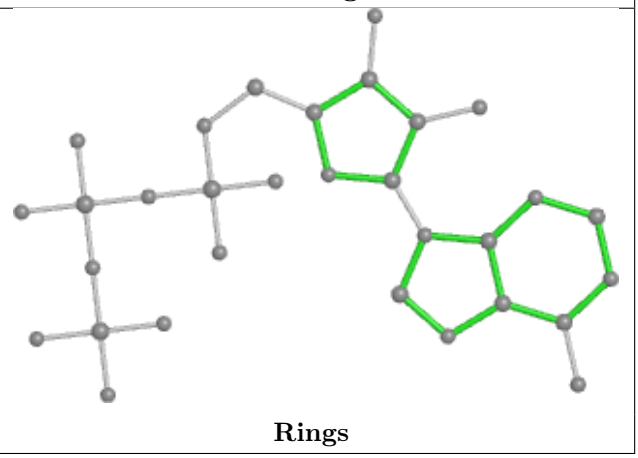
Bond lengths



Bond angles

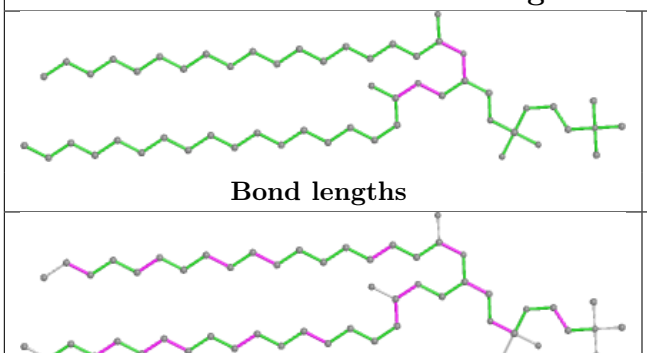


Torsions

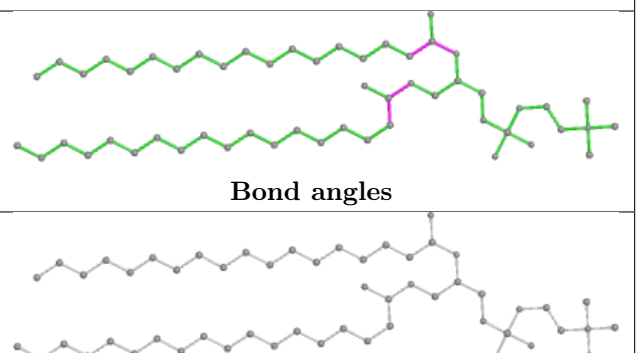


Rings

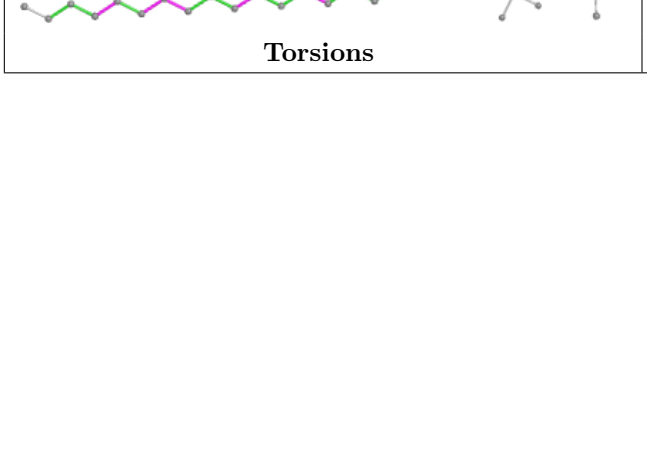
Ligand PC1 G 304



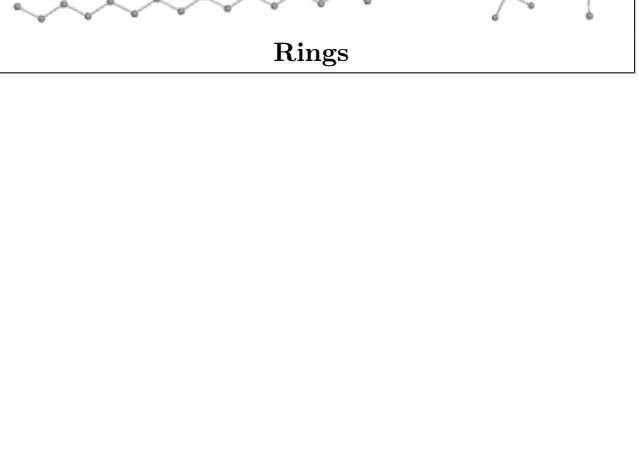
Bond lengths



Bond angles

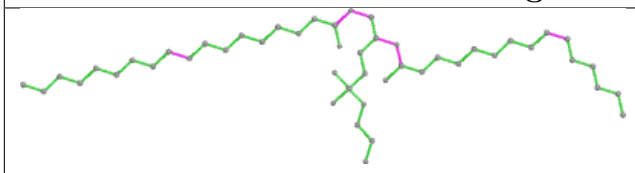


Torsions

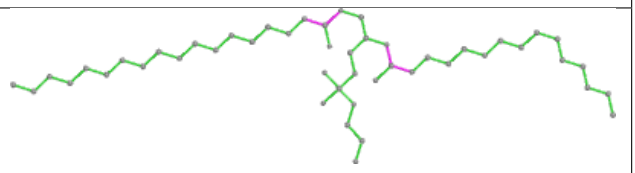


Rings

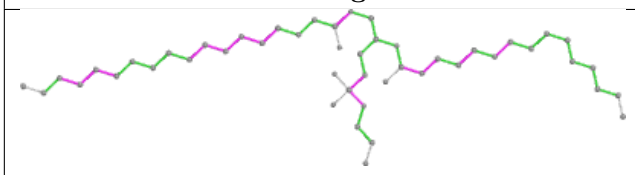
Ligand PEE l3 302



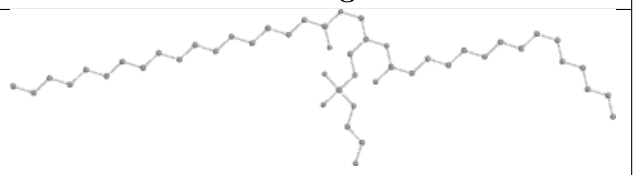
Bond lengths



Bond angles

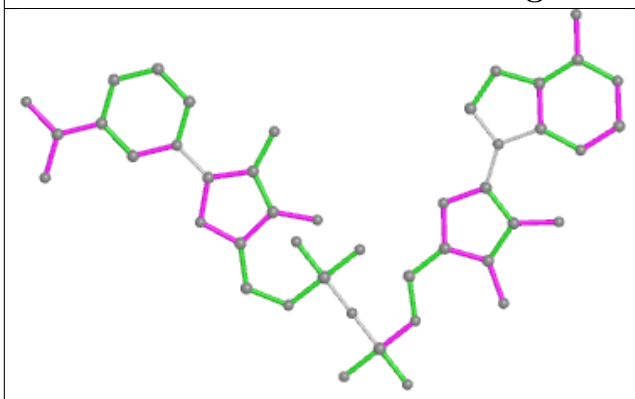


Torsions

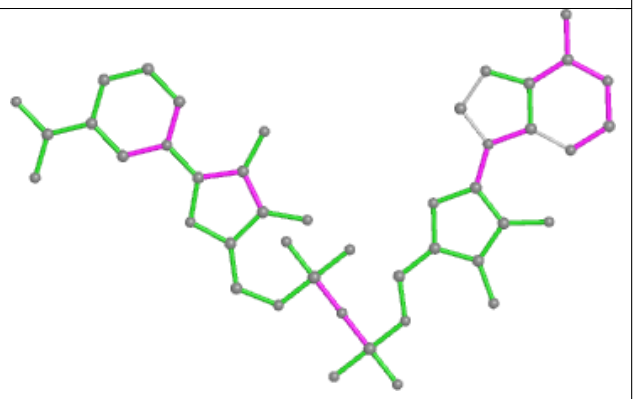


Rings

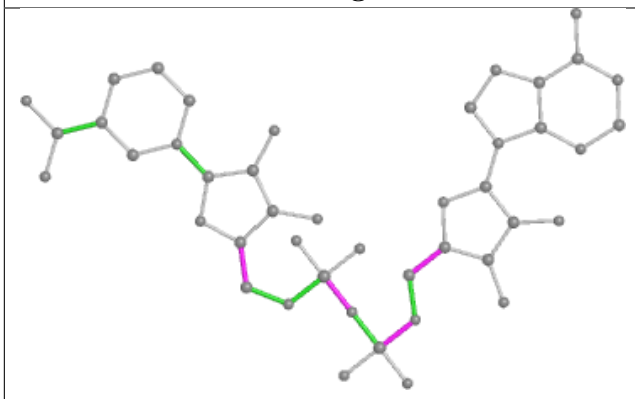
Ligand NAD e 900



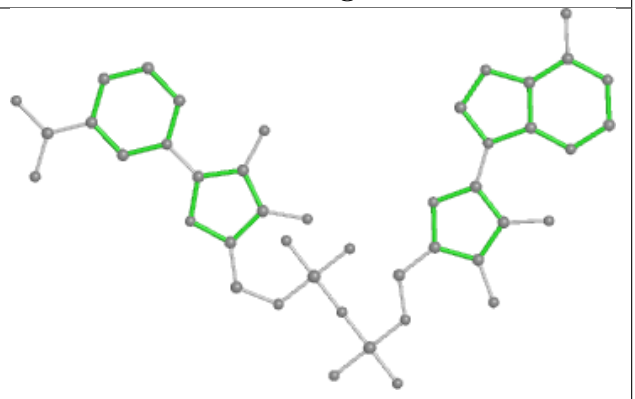
Bond lengths



Bond angles

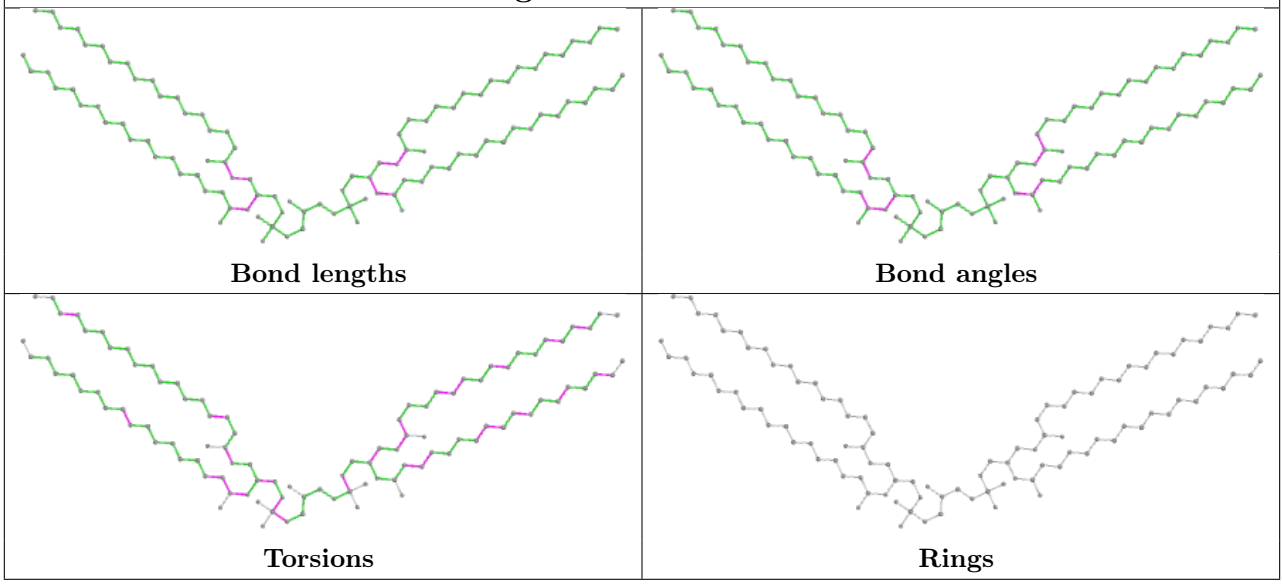


Torsions

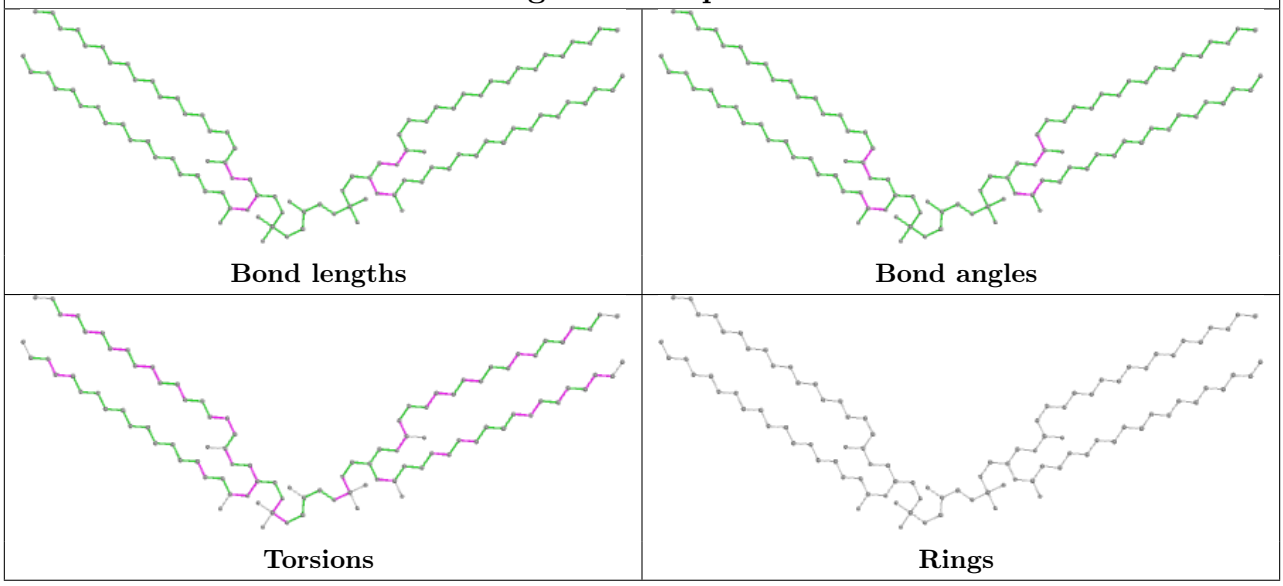


Rings

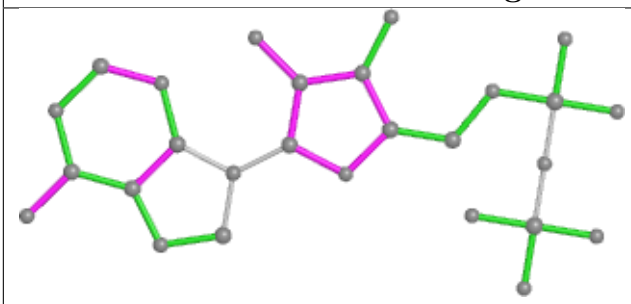
Ligand CDL K3 202



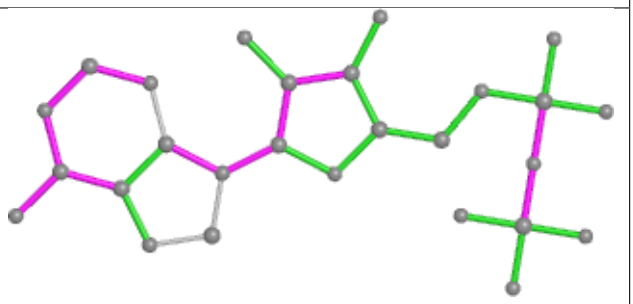
Ligand CDL p 201



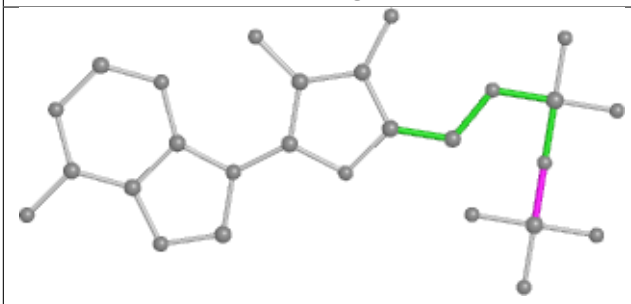
Ligand ADP B5 1002



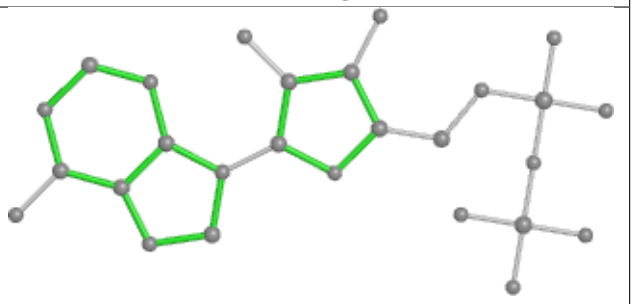
Bond lengths



Bond angles

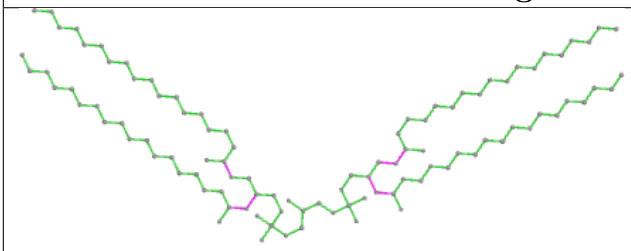


Torsions

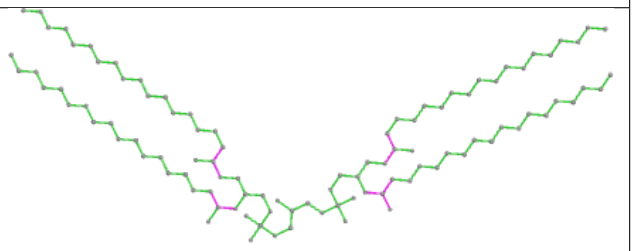


Rings

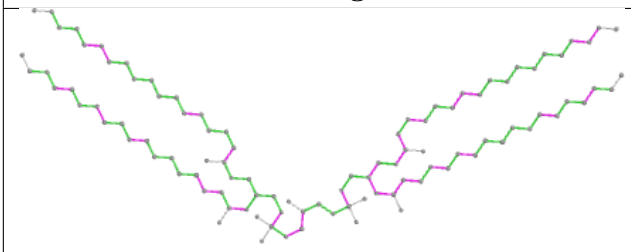
Ligand CDL B3 402



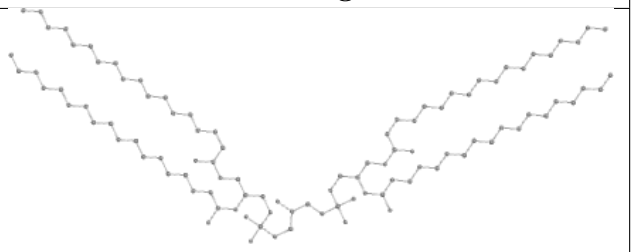
Bond lengths



Bond angles

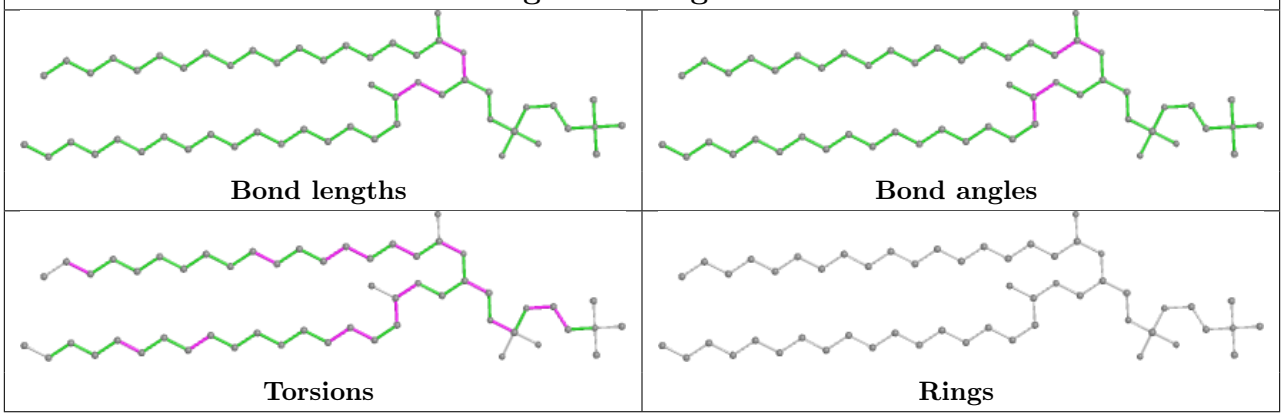


Torsions

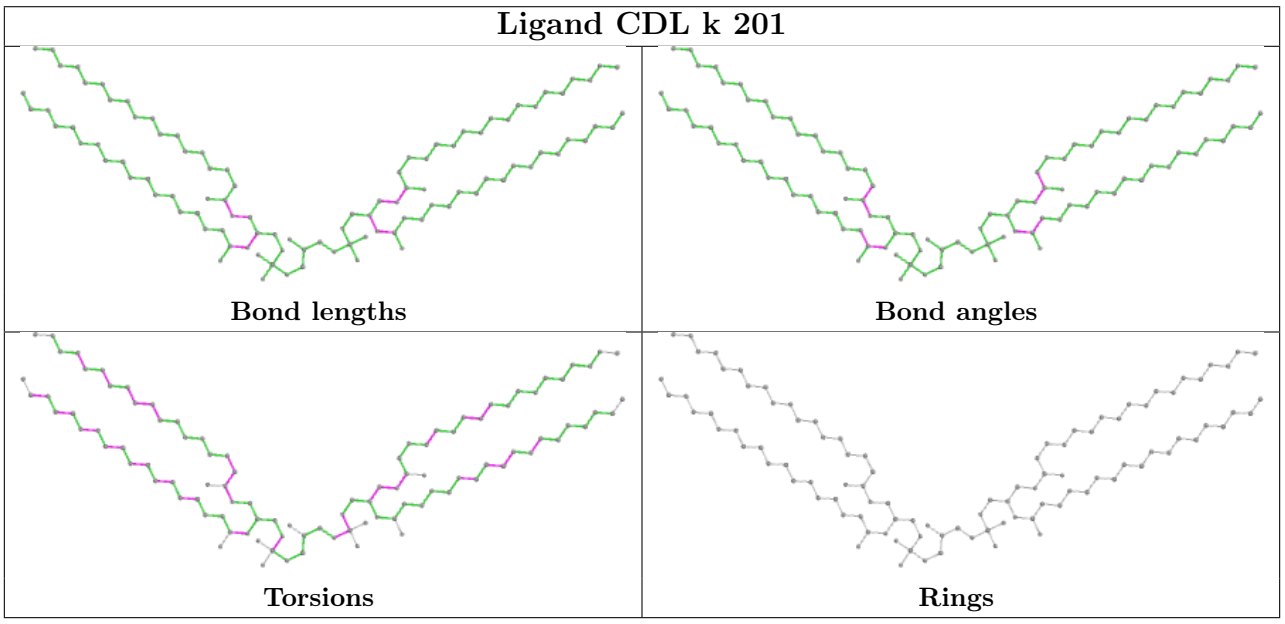


Rings

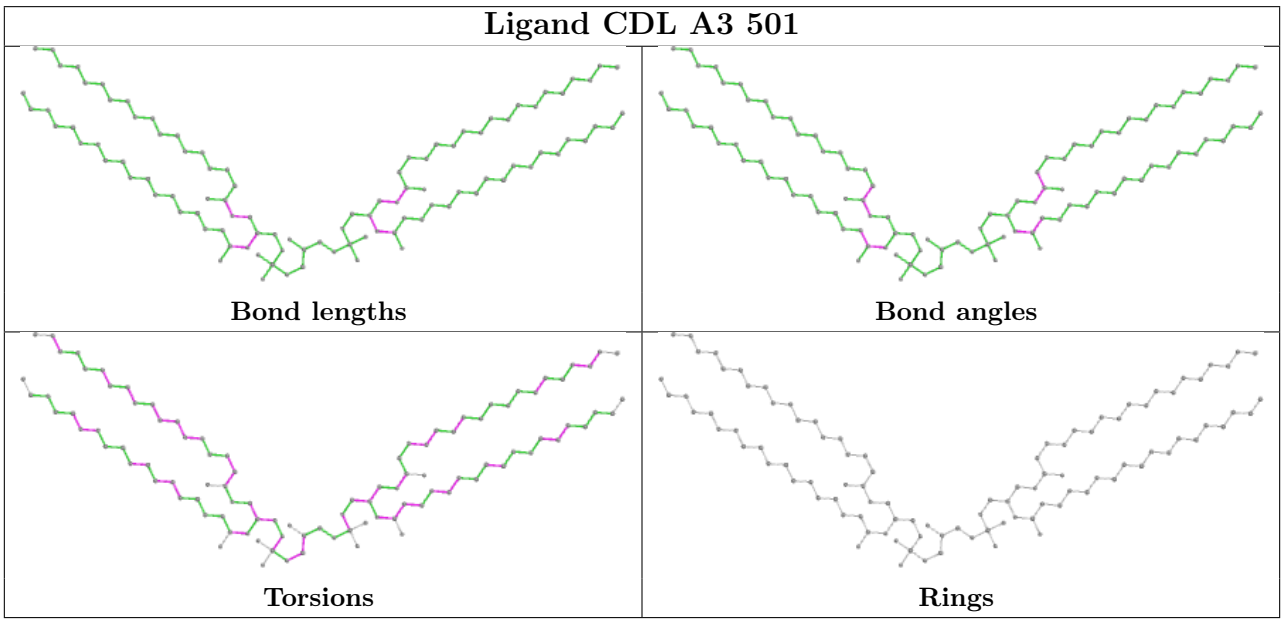
Ligand PC1 g3 304



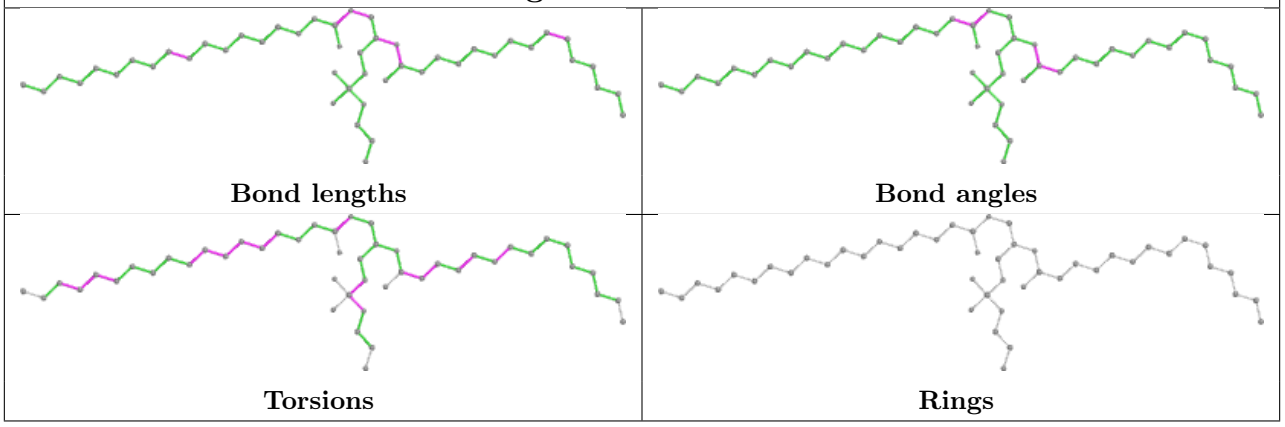
Ligand CDL k 201



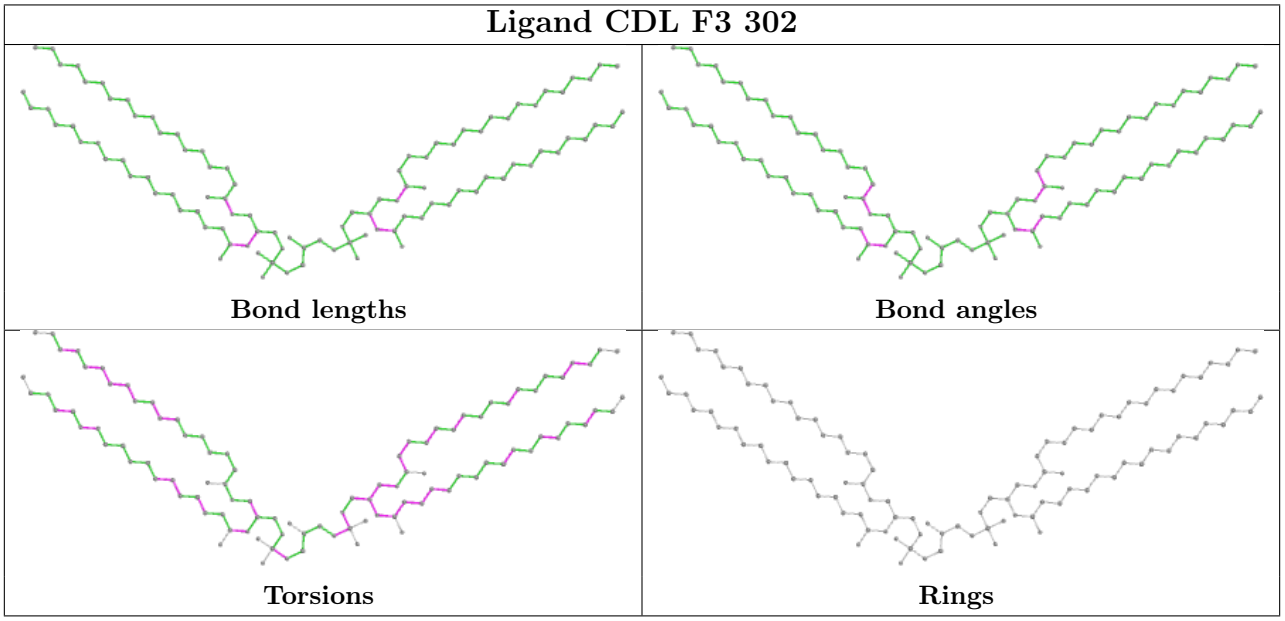
Ligand CDL A3 501



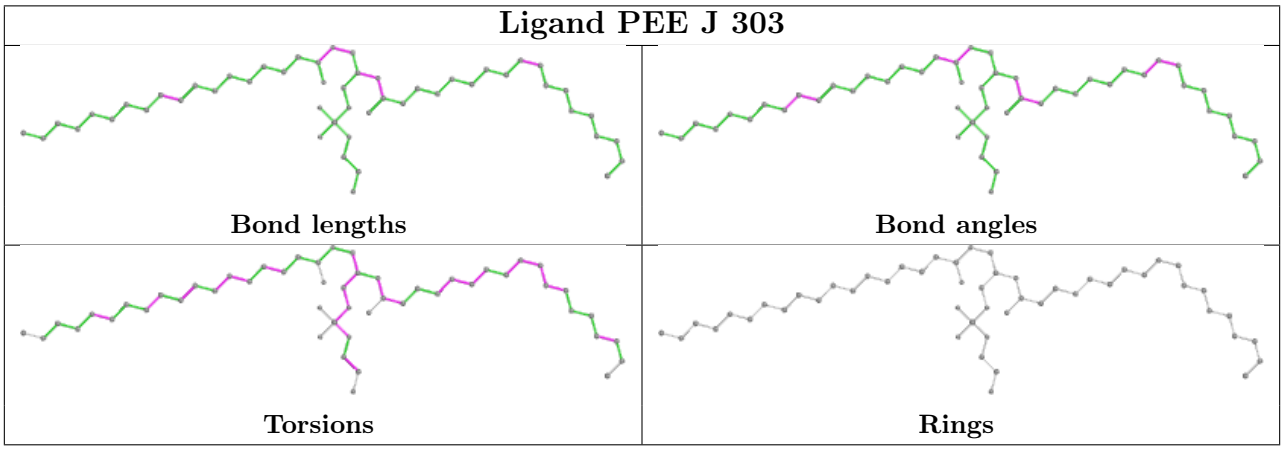
Ligand PEE A 501



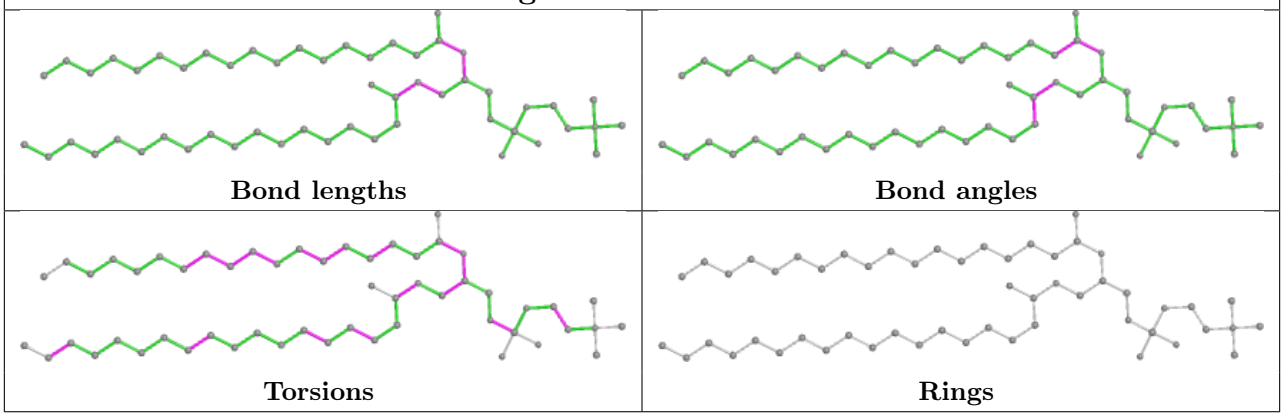
Ligand CDL F3 302



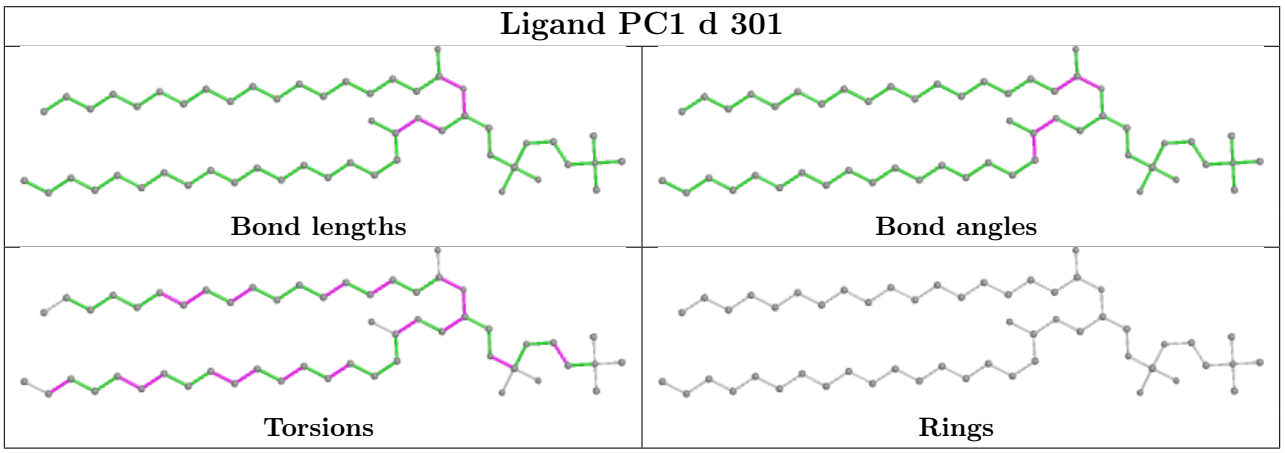
Ligand PEE J 303



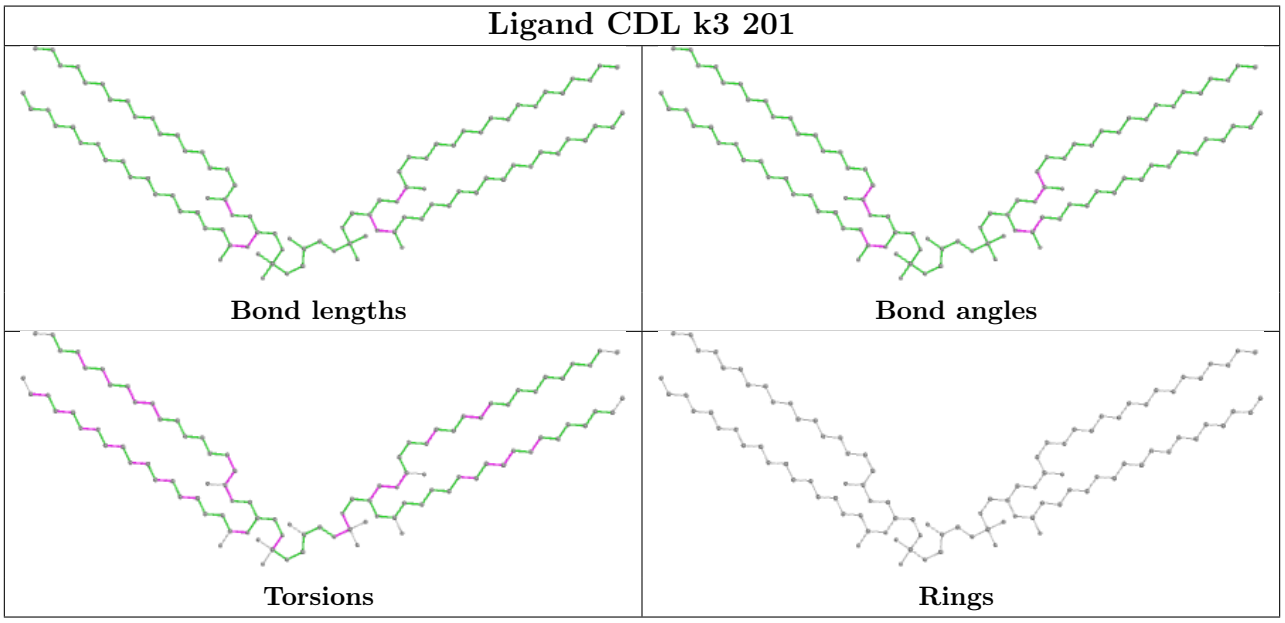
Ligand PC1 D3 301



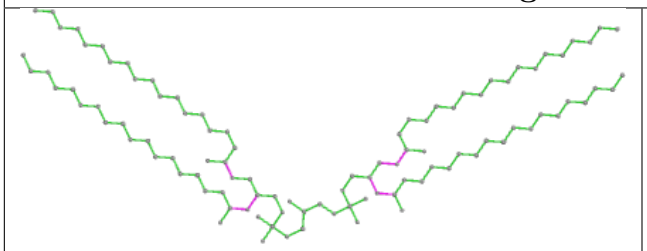
Ligand PC1 d 301



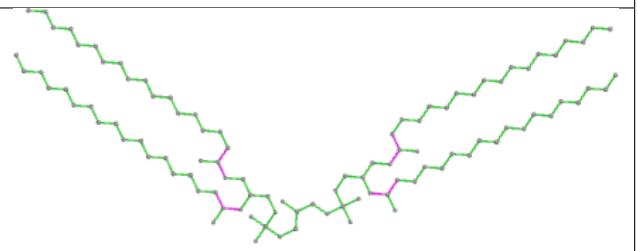
Ligand CDL k3 201



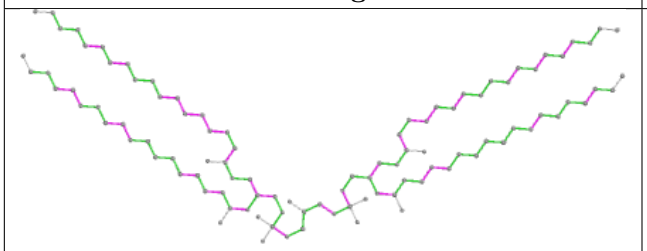
Ligand CDL J3 301



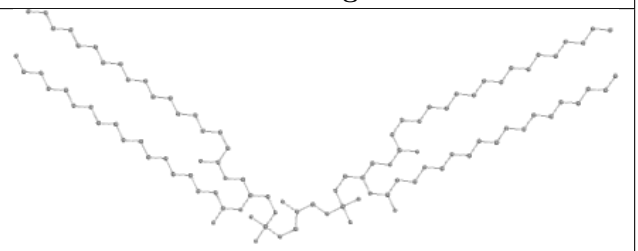
Bond lengths



Bond angles

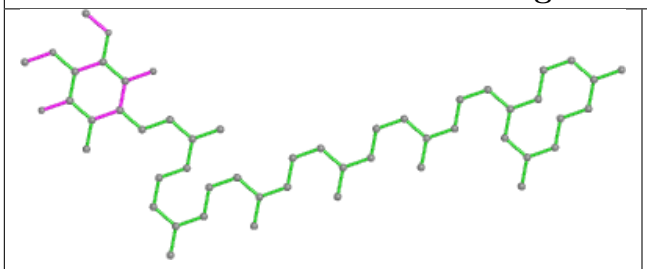


Torsions

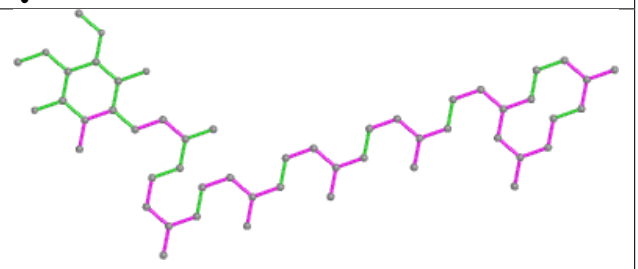


Rings

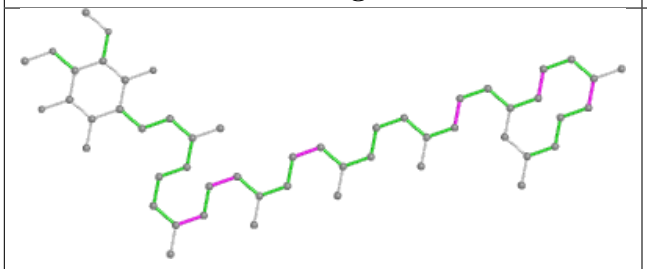
Ligand UQ8 i 302



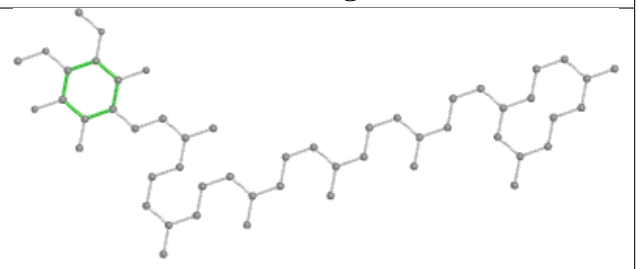
Bond lengths



Bond angles

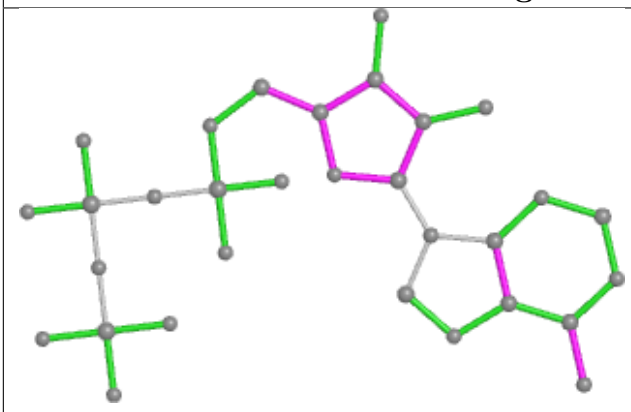


Torsions



Rings

Ligand ATP A2 601



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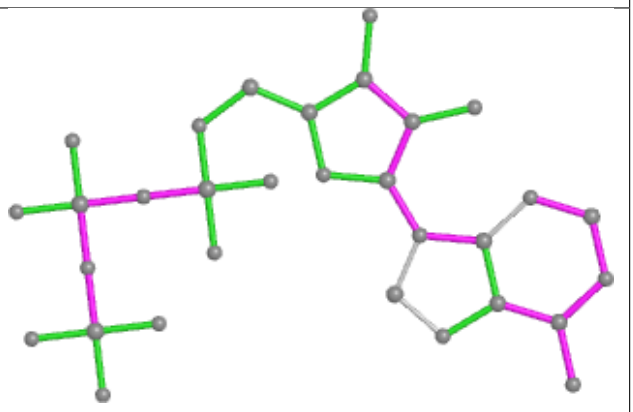
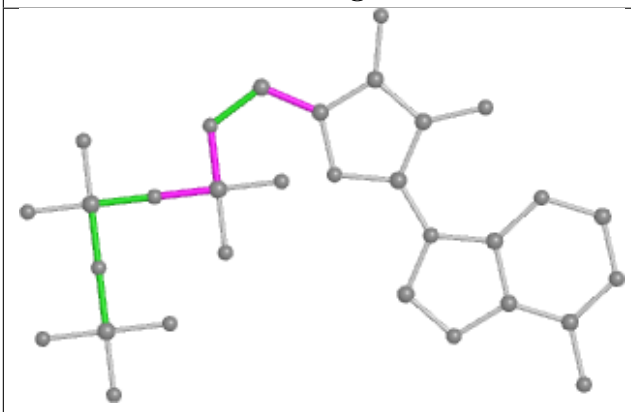
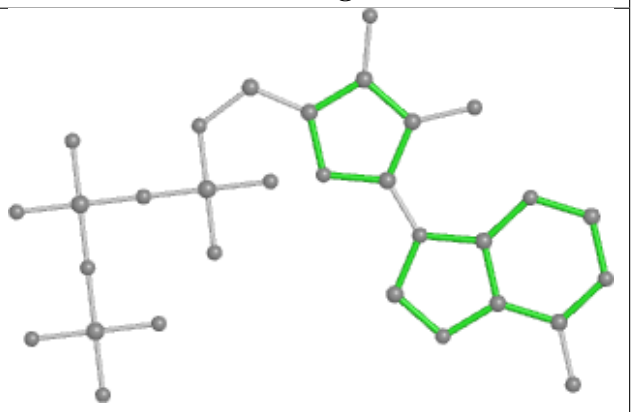


Bond angles

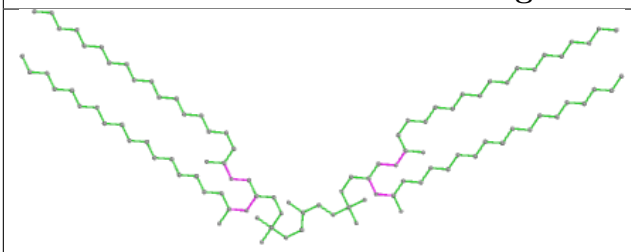


Torsions

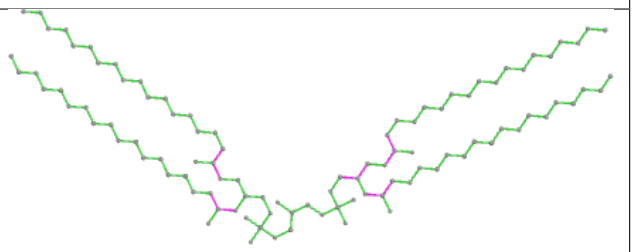


Rings

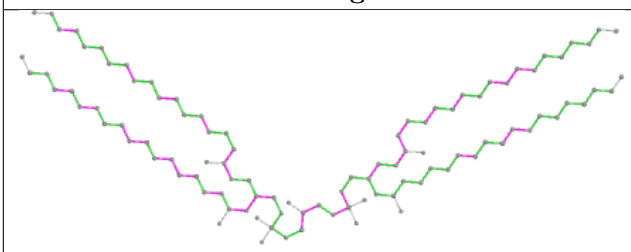
Ligand CDL B3 404



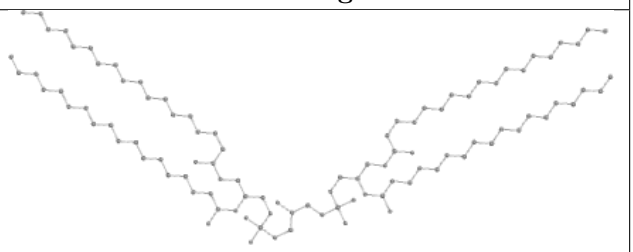
Bond lengths



Bond angles

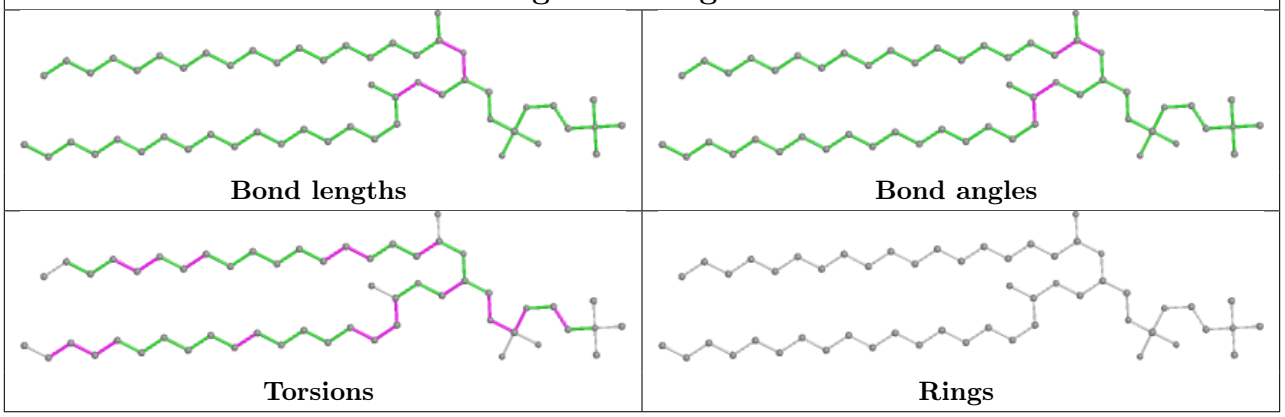


Torsions

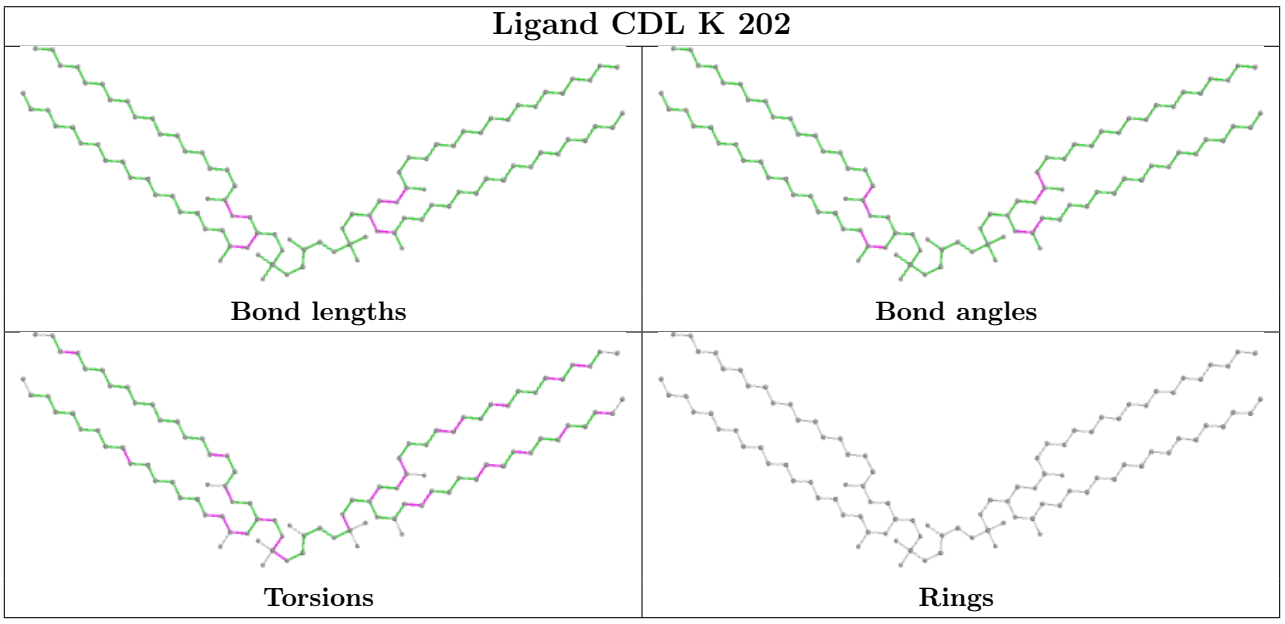


Rings

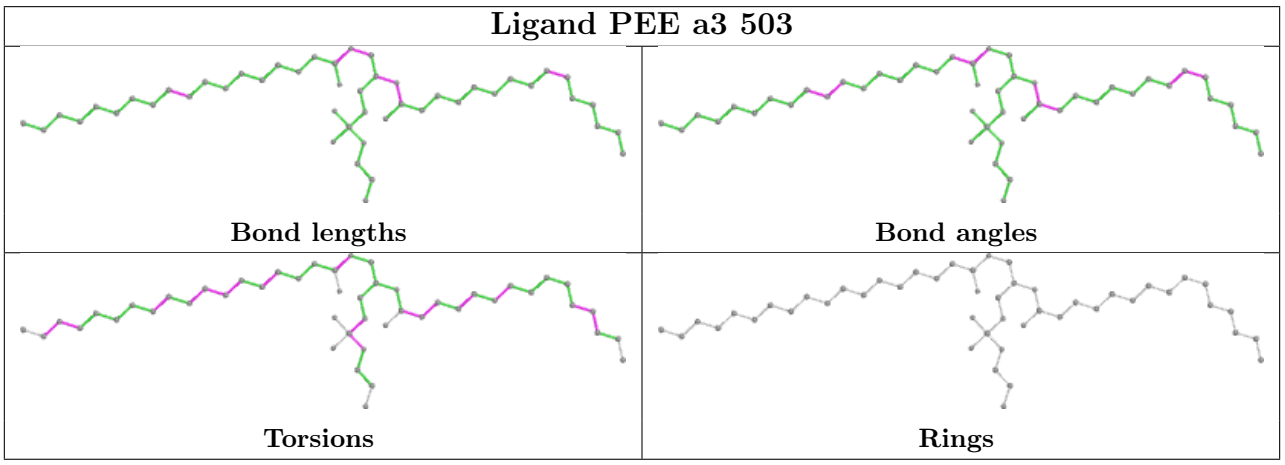
Ligand PC1 g 303



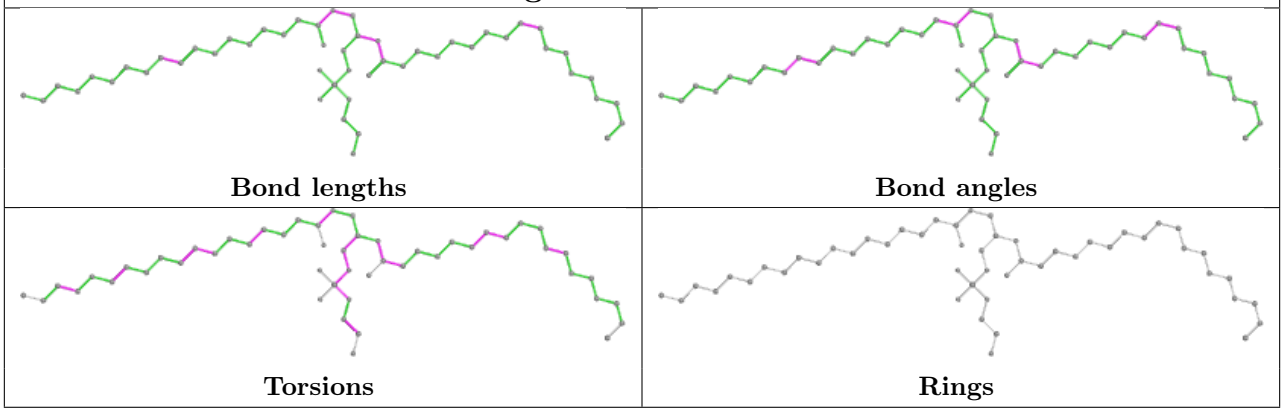
Ligand CDL K 202



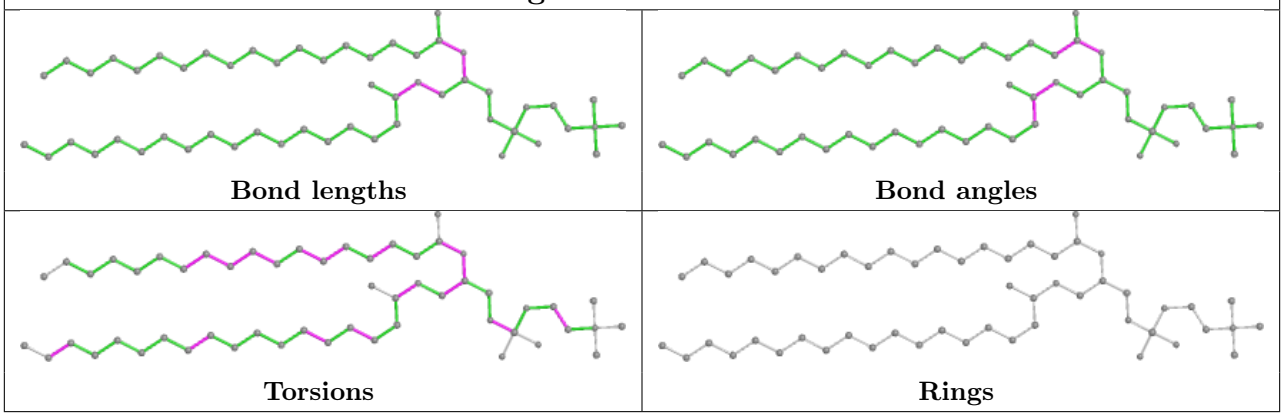
Ligand PEE a3 503



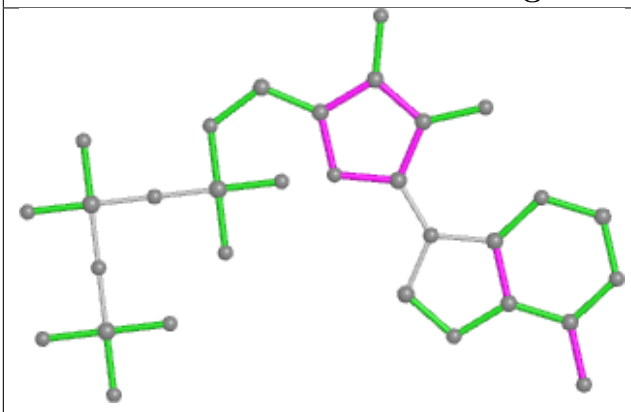
Ligand PEE m 301



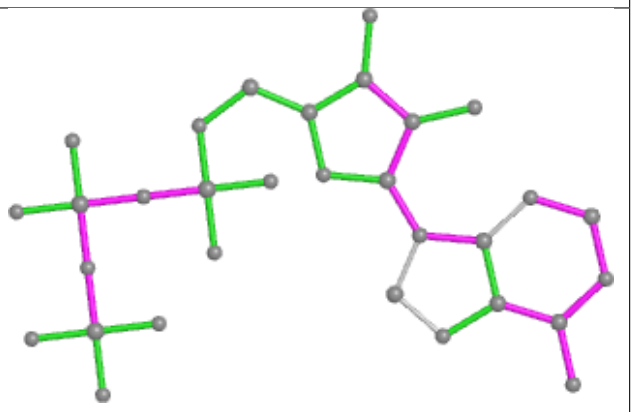
Ligand PC1 D 301



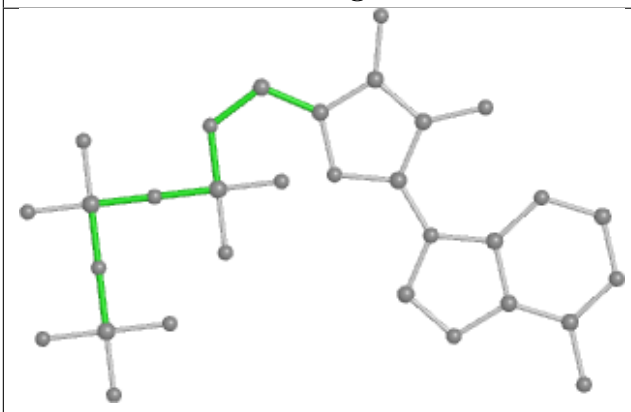
Ligand ATP G 301



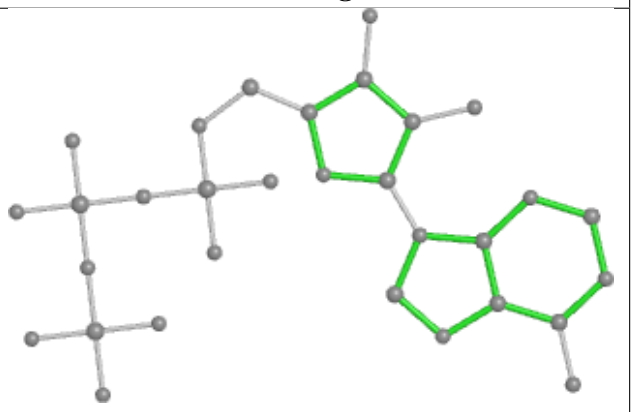
Bond lengths



Bond angles

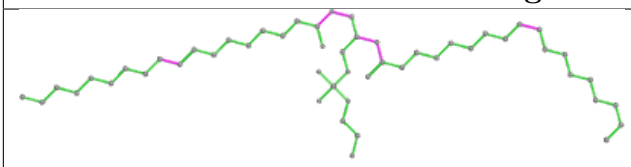


Torsions



Rings

Ligand PEE j3 303



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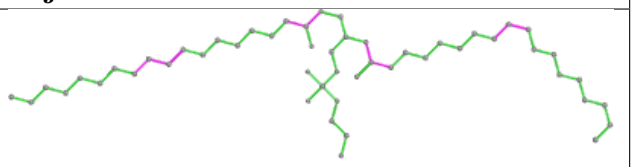
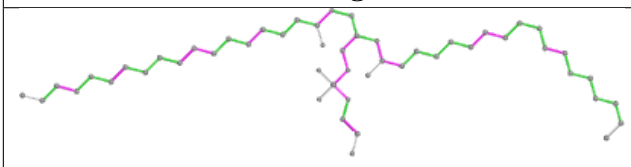
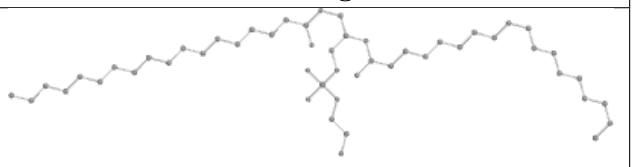


Bond angles

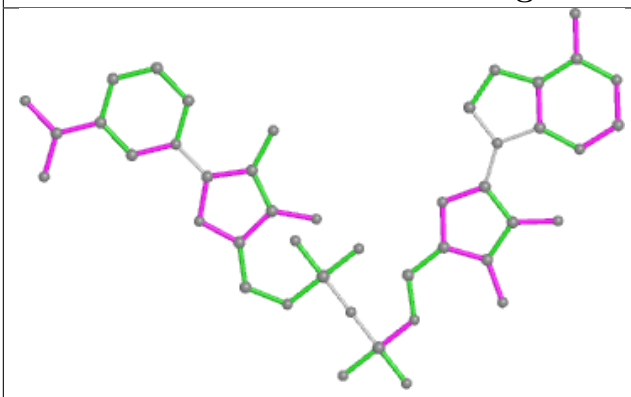


Torsions

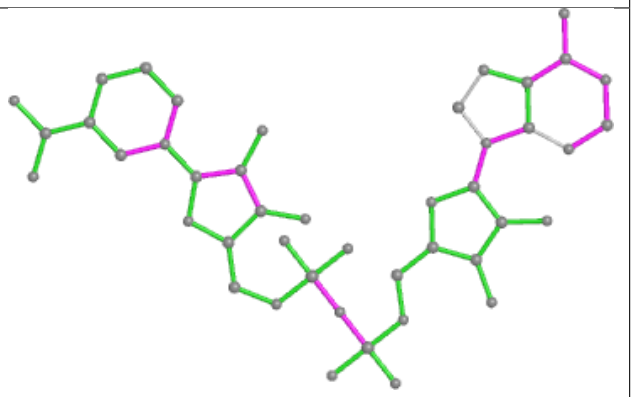


Rings

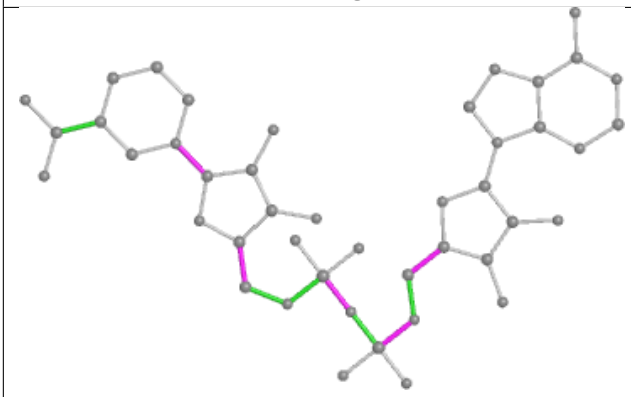
Ligand NAD e3 900



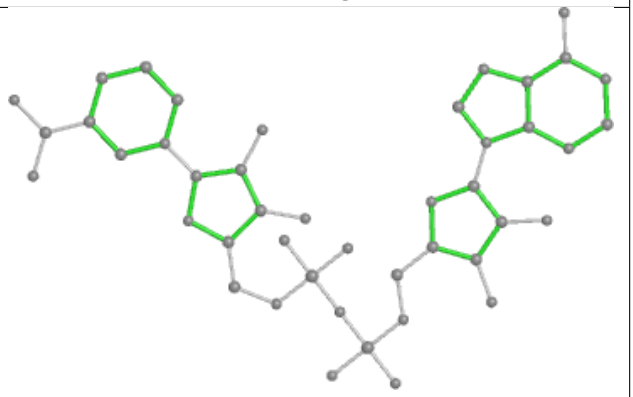
Bond lengths



Bond angles

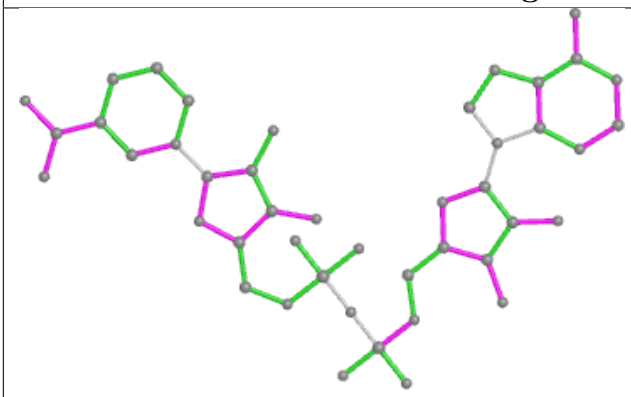


Torsions



Rings

Ligand NAD E 900



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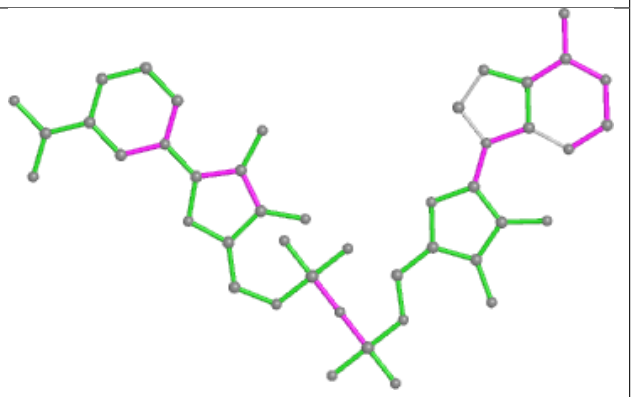
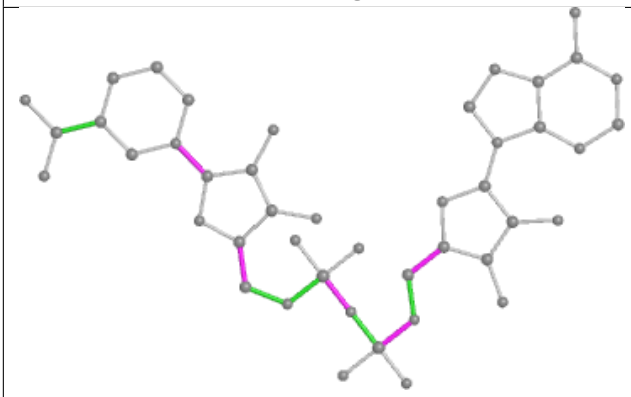
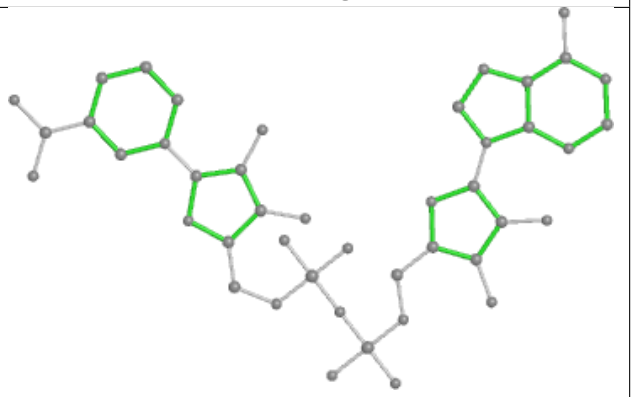


Bond angles

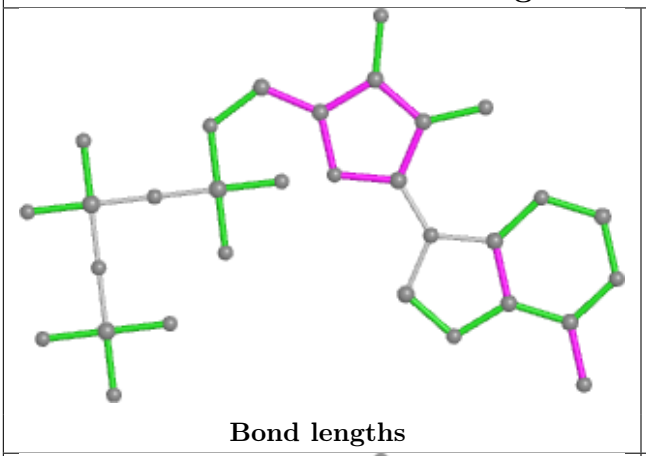


Torsions

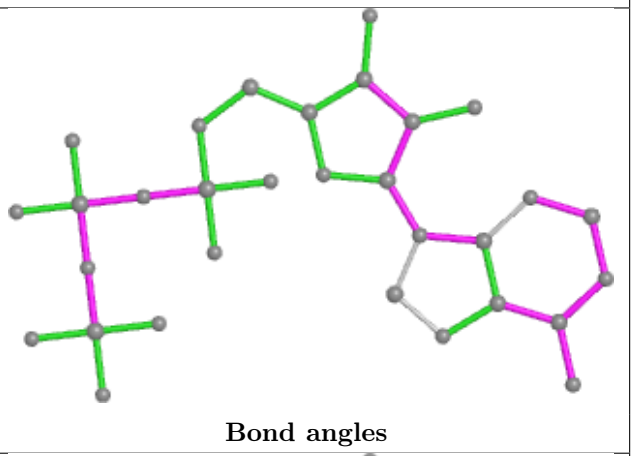


Rings

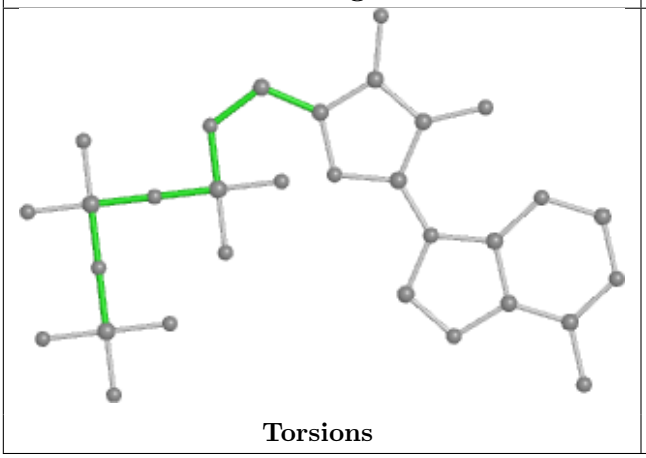
Ligand ATP G3 301



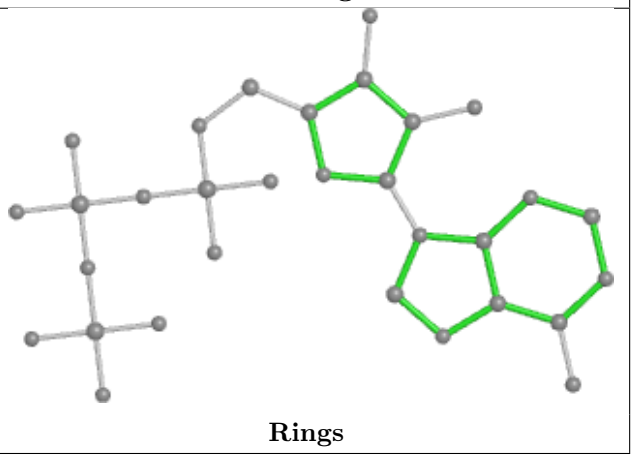
Bond lengths



Bond angles

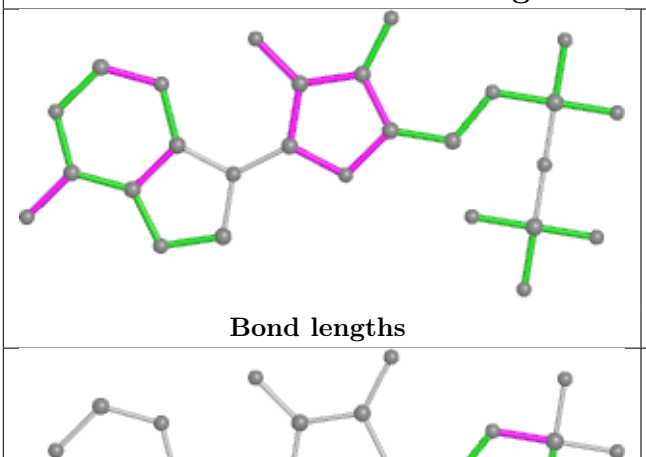


Torsions

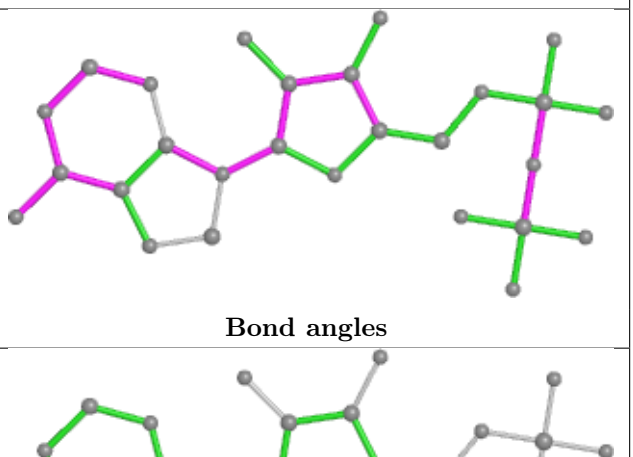


Rings

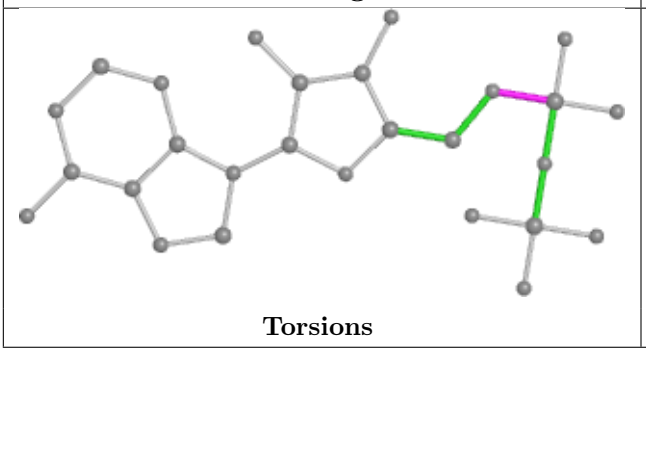
Ligand ADP D2 501



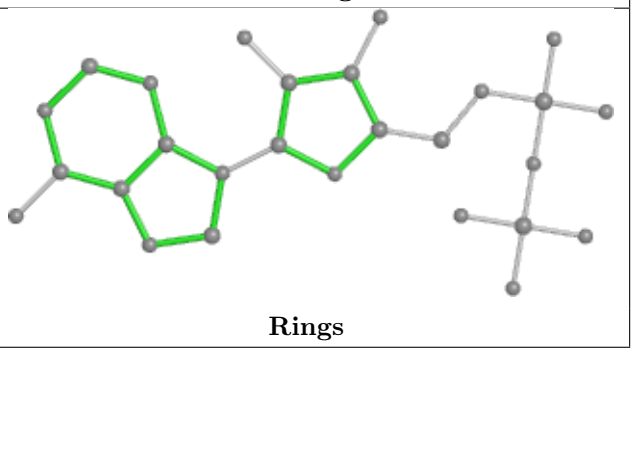
Bond lengths



Bond angles

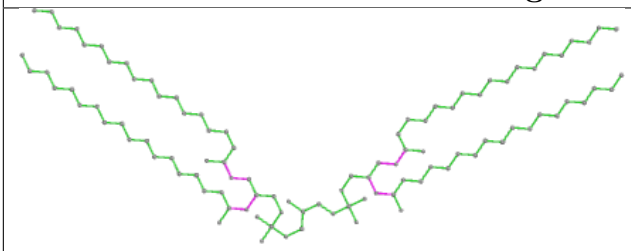


Torsions



Rings

Ligand CDL F 302



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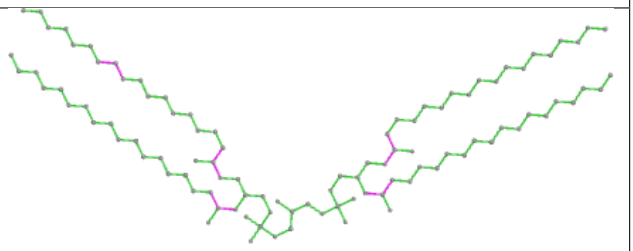
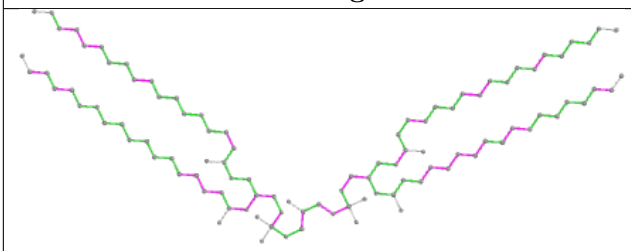


Bond angles



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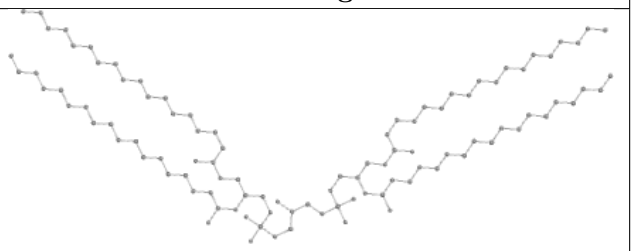
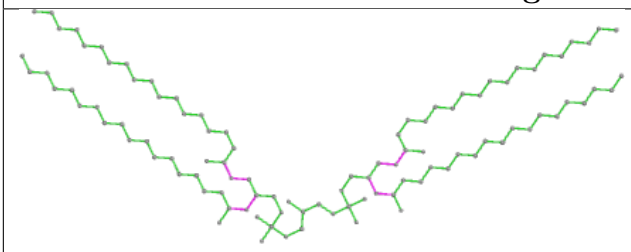
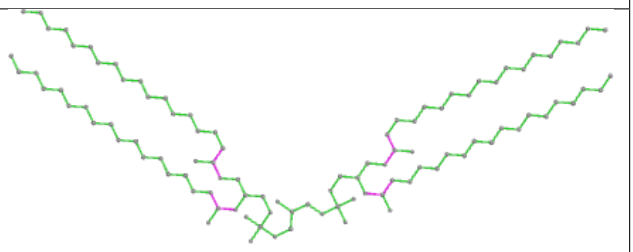


Rings

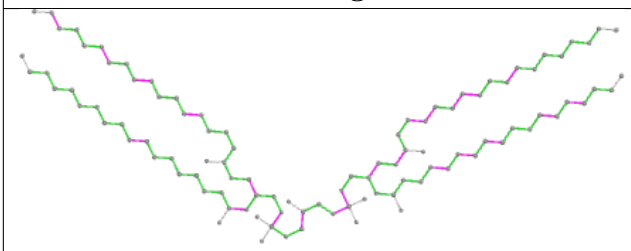
Ligand CDL K 201



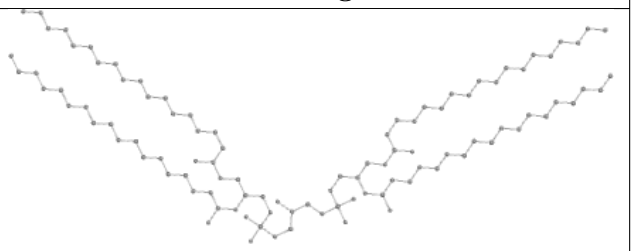
Bond lengths



Bond angles

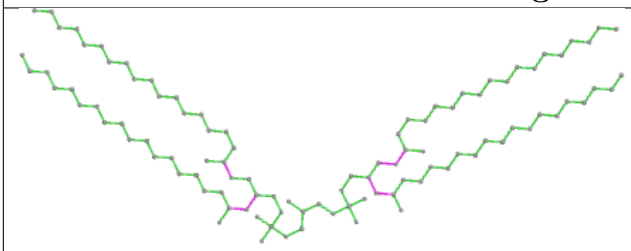


Torsions

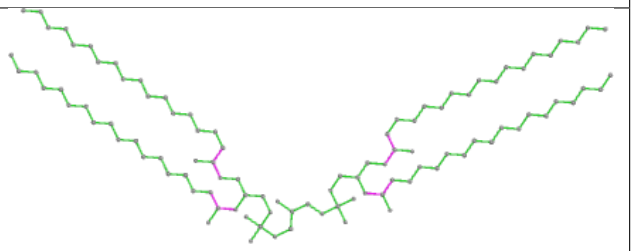


Rings

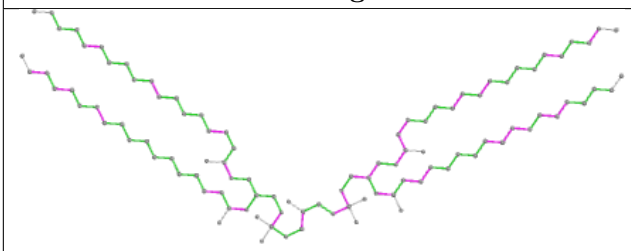
Ligand CDL i 301



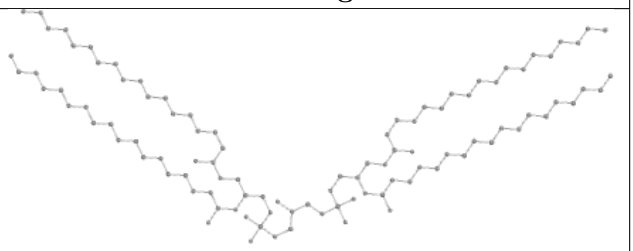
Bond lengths



Bond angles

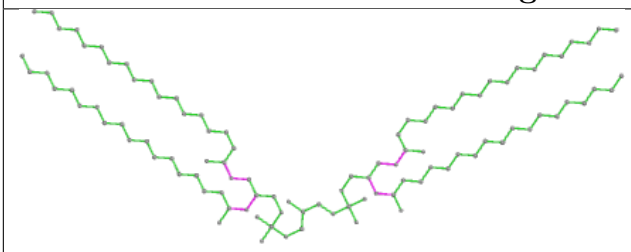


Torsions



Rings

Ligand CDL a3 502



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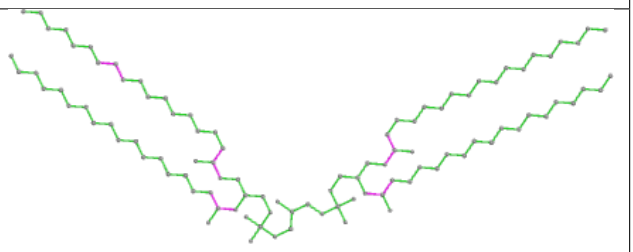
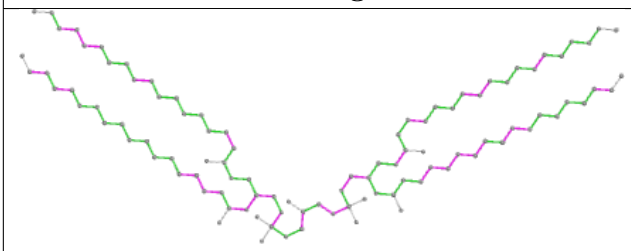
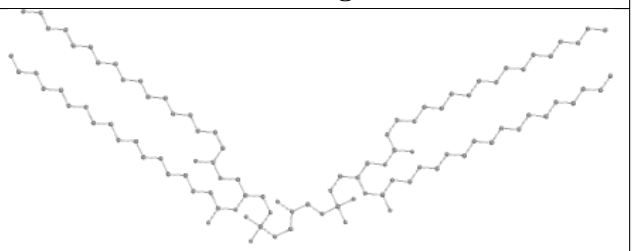


Bond angles

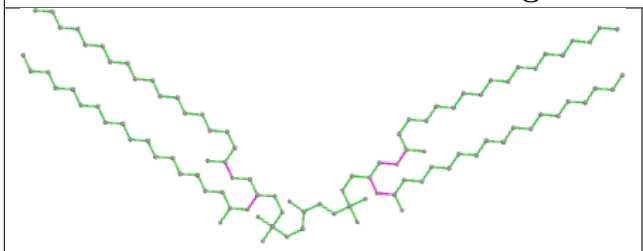


Torsions

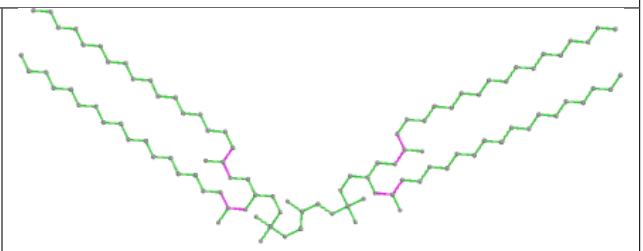


Rings

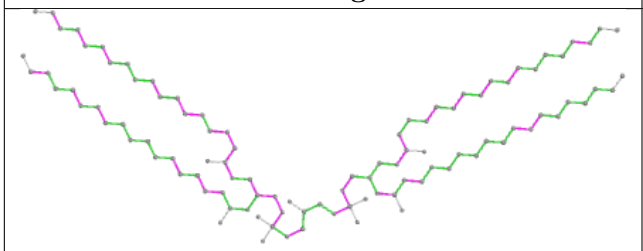
Ligand CDL I3 302



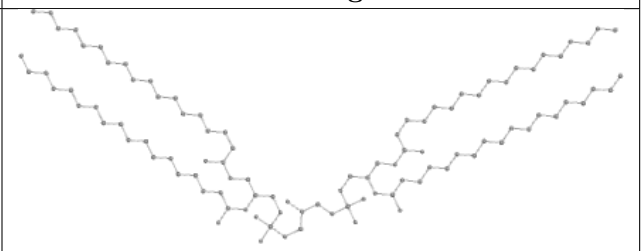
Bond lengths



Bond angles

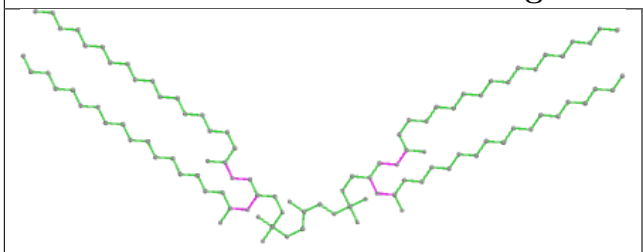


Torsions

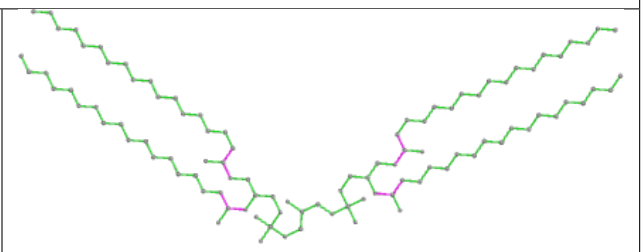


Rings

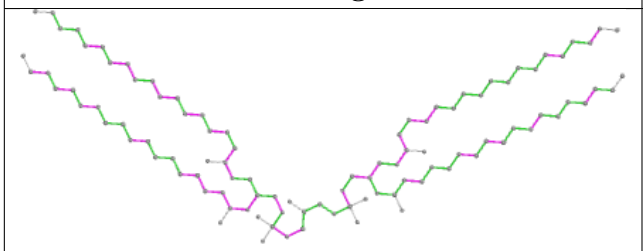
Ligand CDL B 401



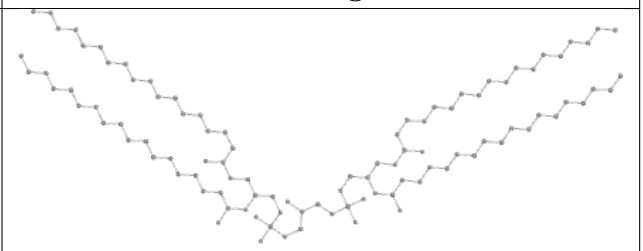
Bond lengths



Bond angles

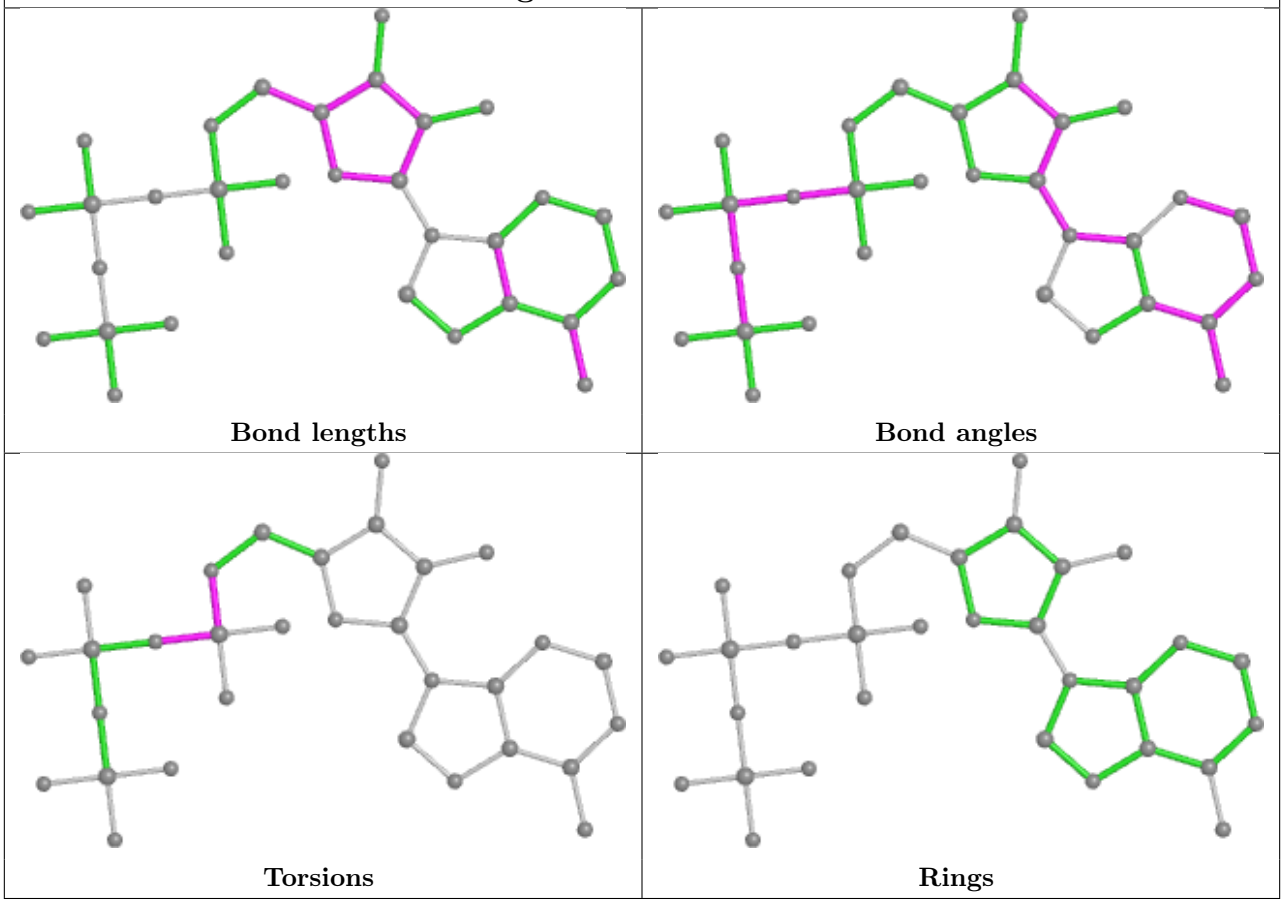


Torsions

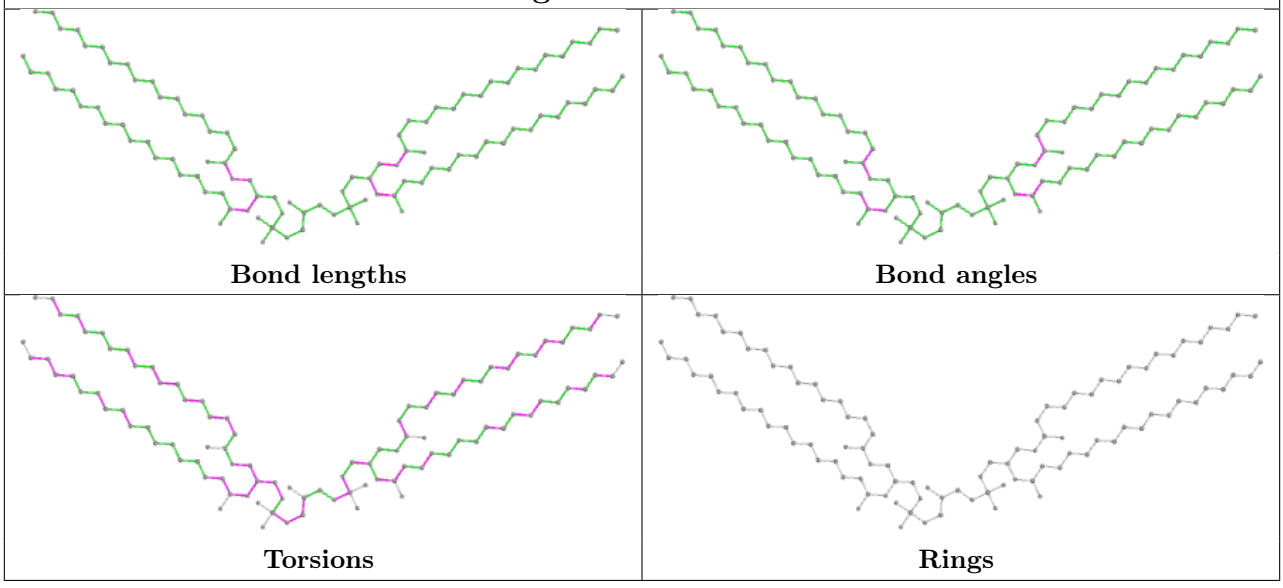


Rings

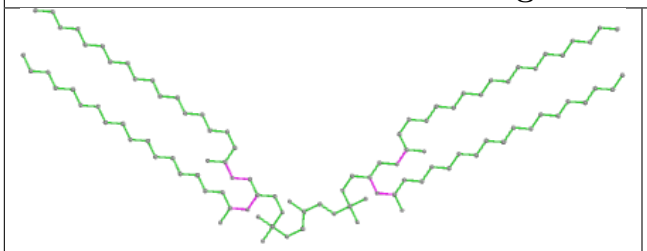
Ligand ATP C5 601



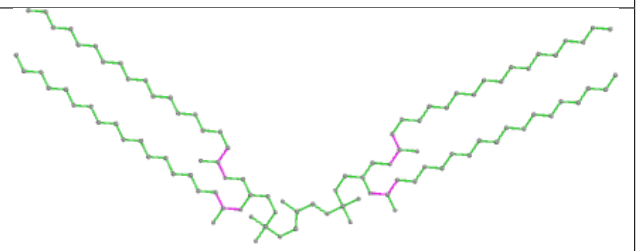
Ligand CDL f 302



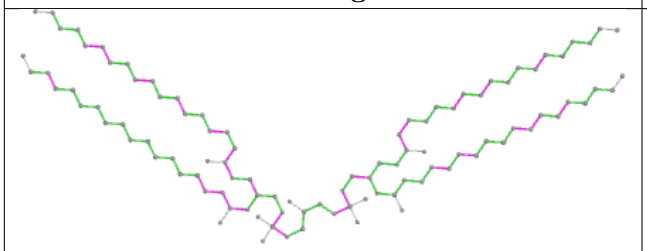
Ligand CDL P3 201



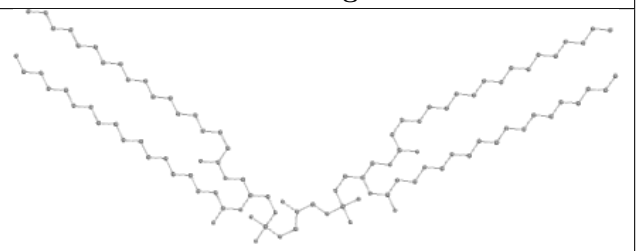
Bond lengths



Bond angles

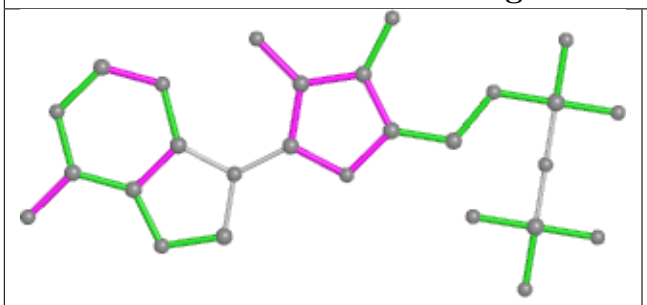


Torsions

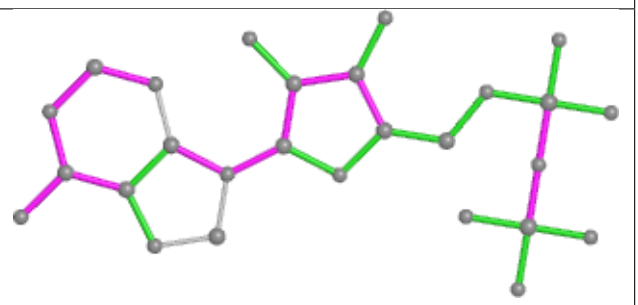


Rings

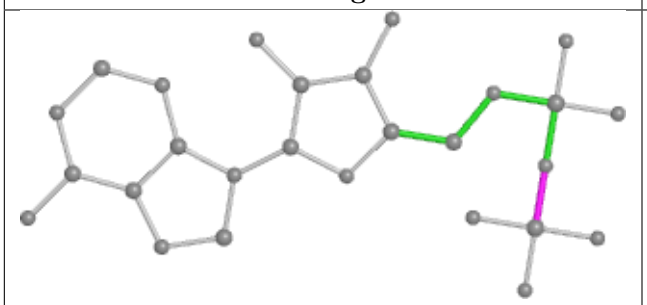
Ligand ADP B1 1002



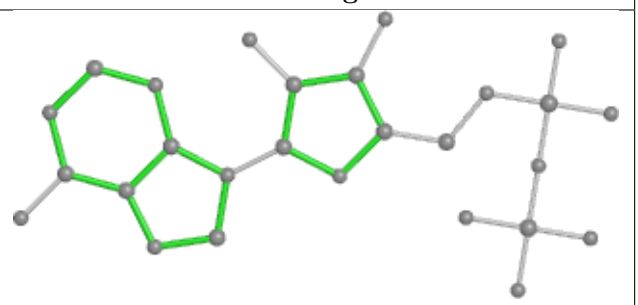
Bond lengths



Bond angles

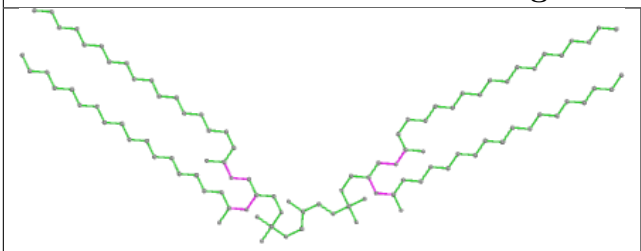


Torsions

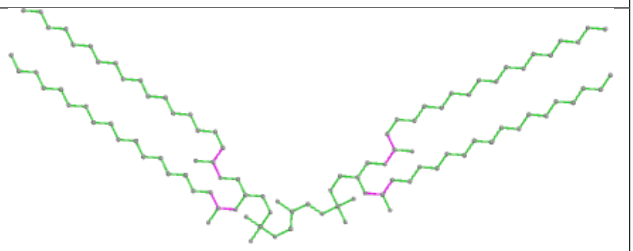


Rings

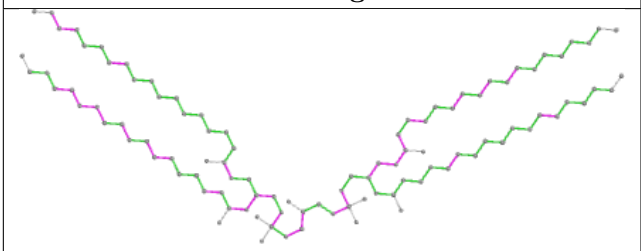
Ligand CDL I 301



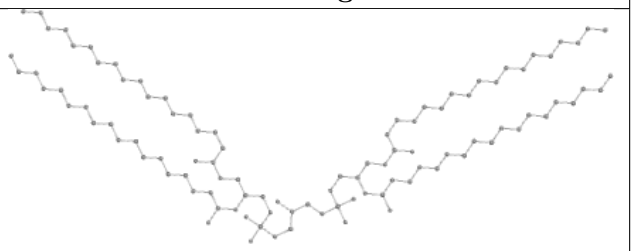
Bond lengths



Bond angles

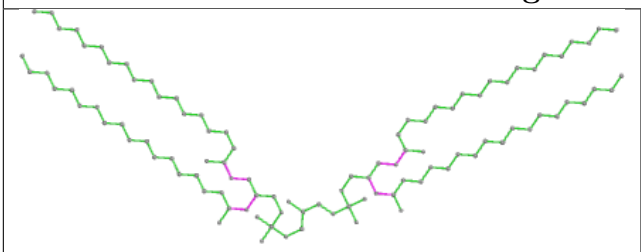


Torsions

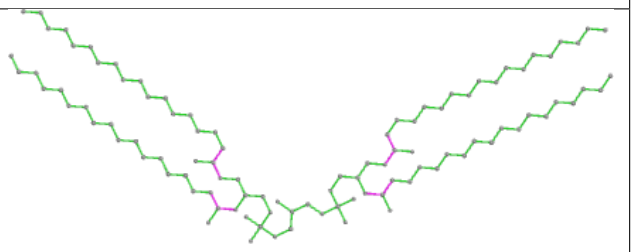


Rings

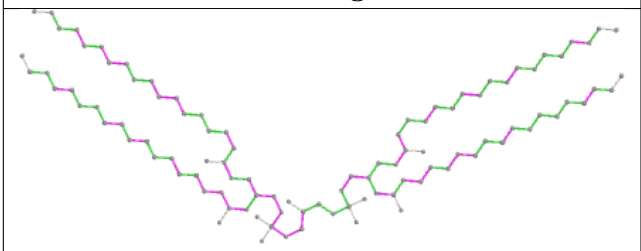
Ligand CDL f3 304



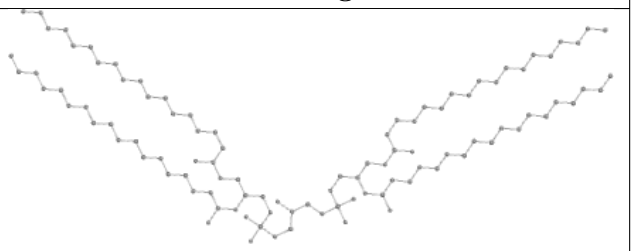
Bond lengths



Bond angles

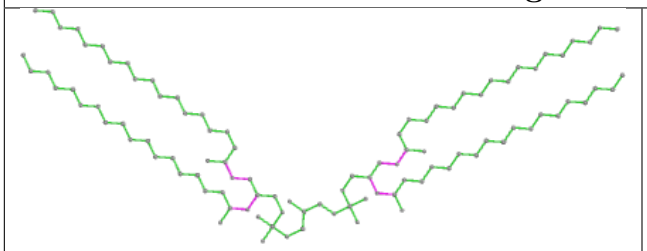


Torsions

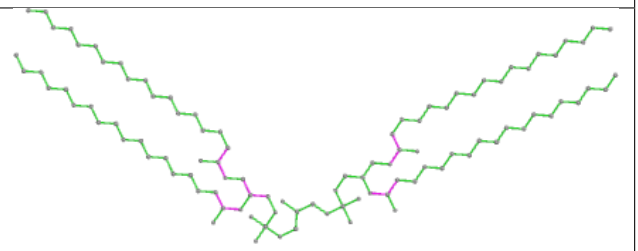


Rings

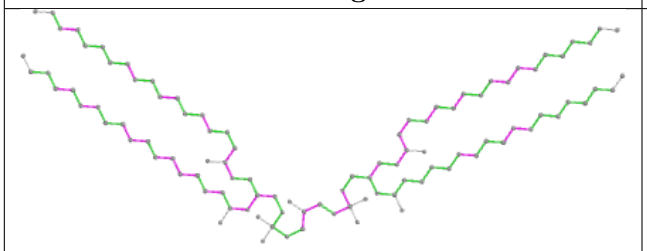
Ligand CDL B 404



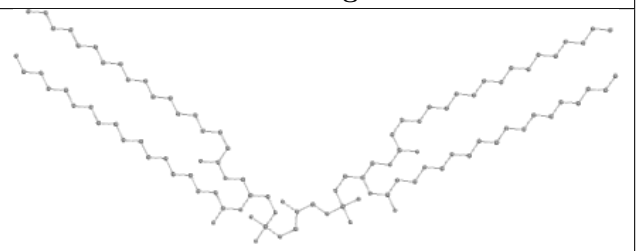
Bond lengths



Bond angles

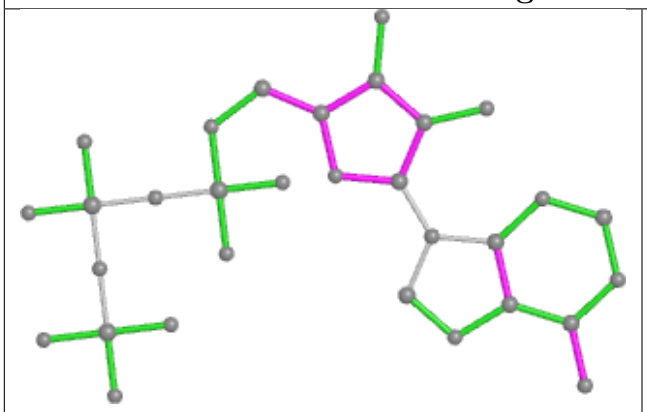


Torsions

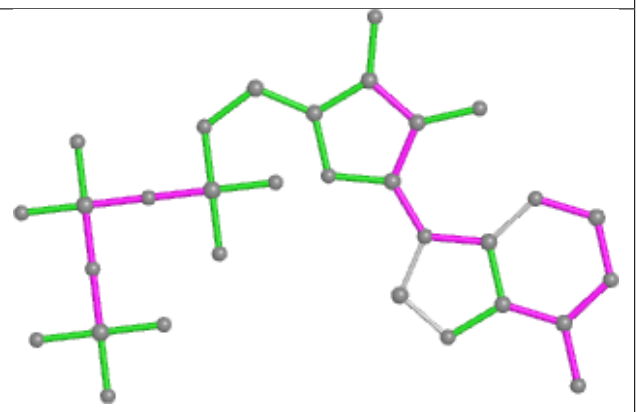


Rings

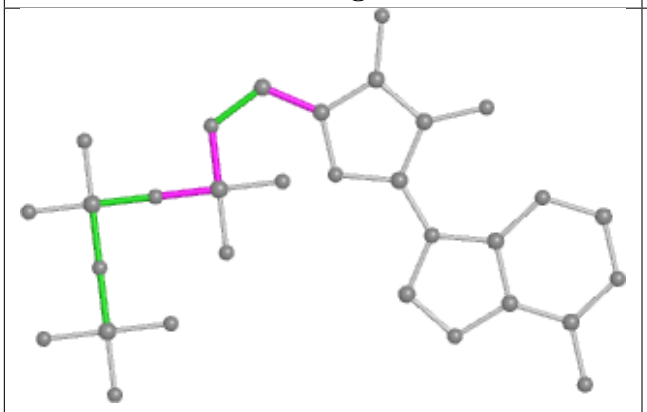
Ligand ATP A5 601



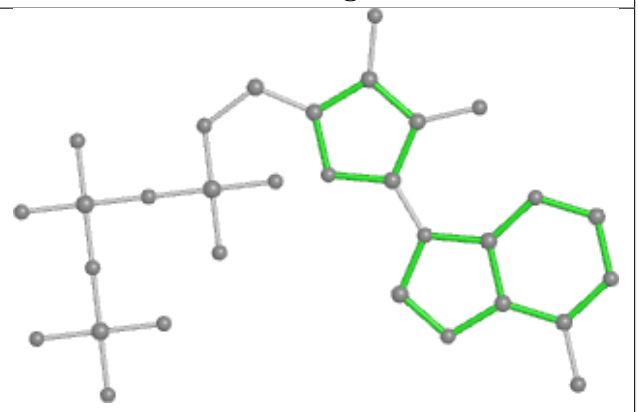
Bond lengths



Bond angles

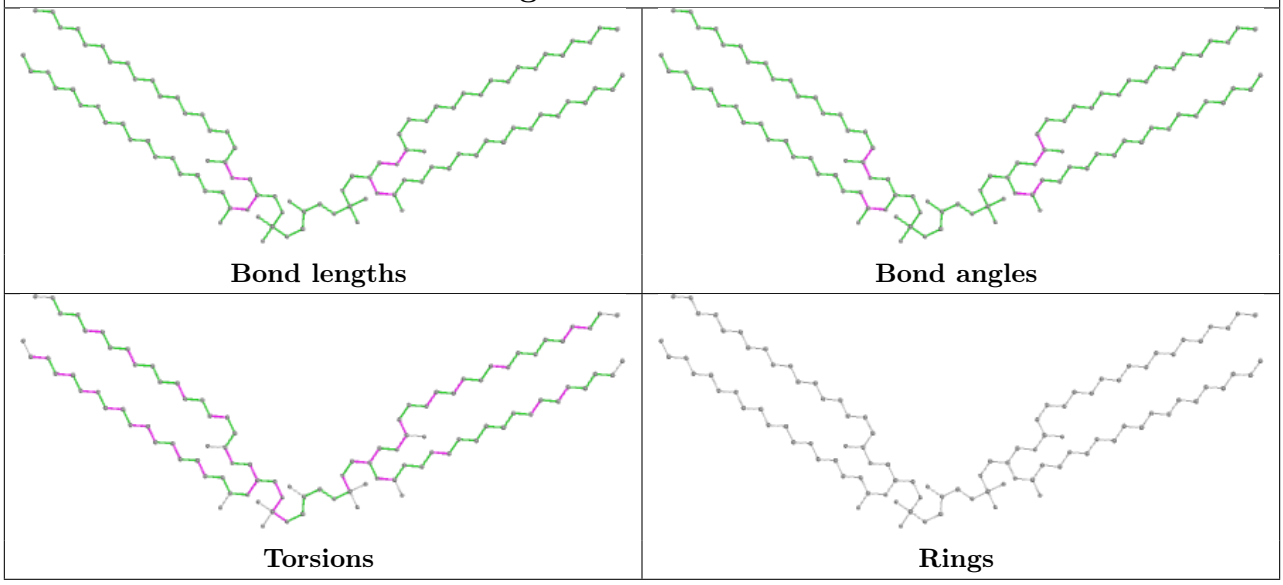


Torsions

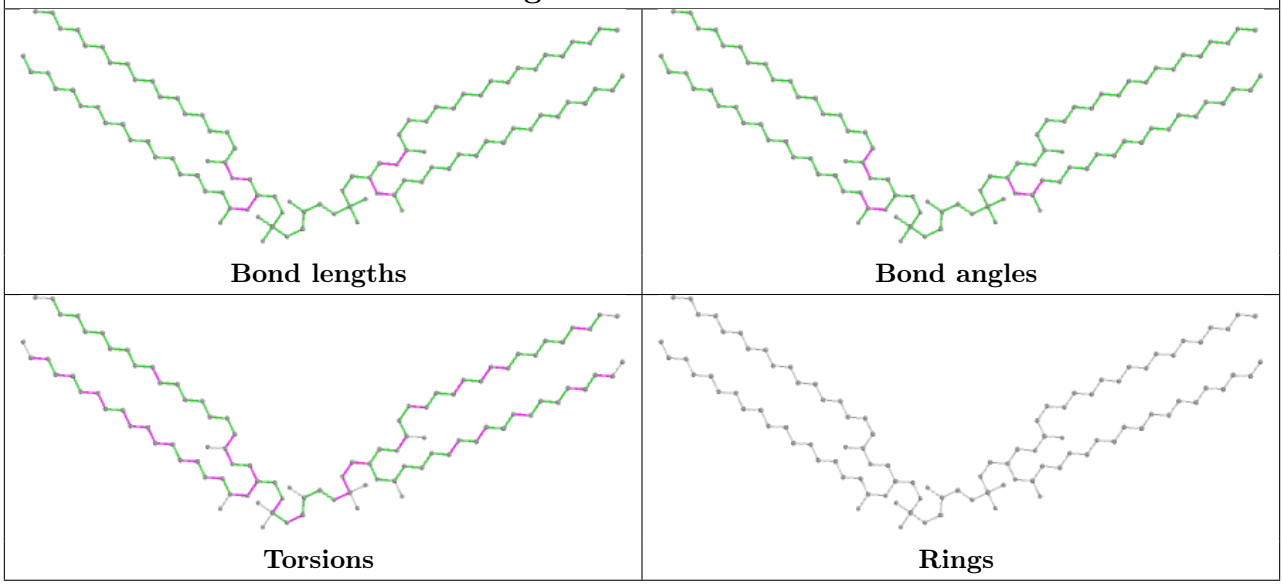


Rings

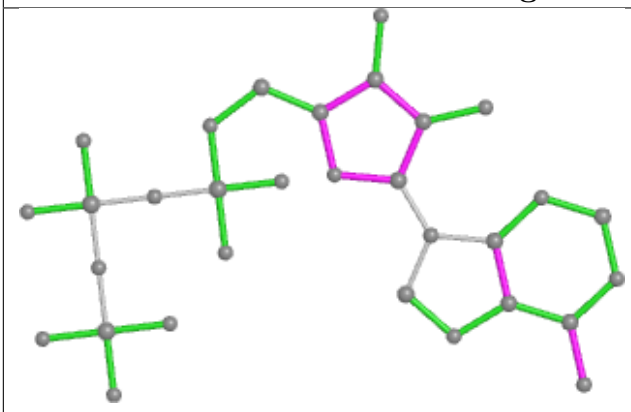
Ligand CDL J3 302



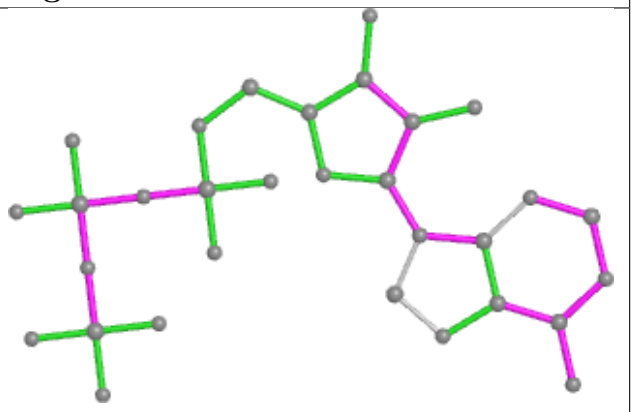
Ligand CDL l3 303



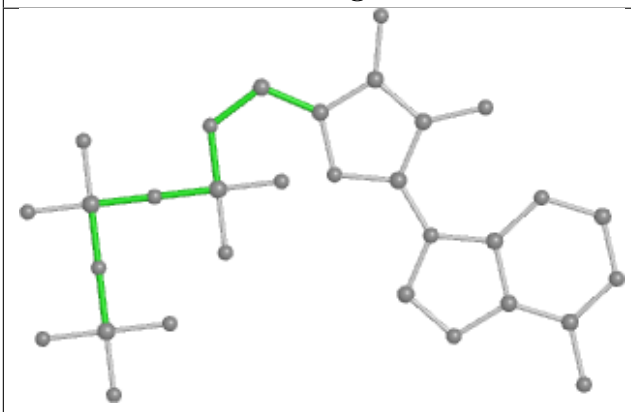
Ligand ATP g3 301



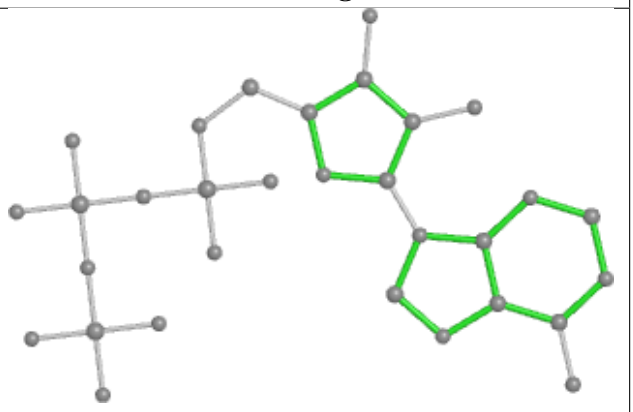
Bond lengths



Bond angles

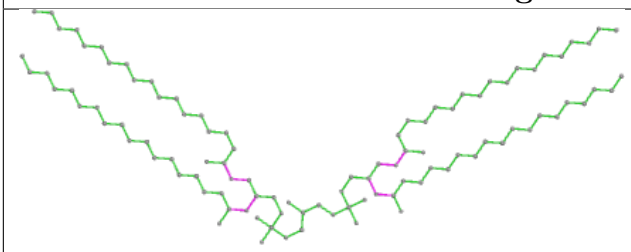


Torsions

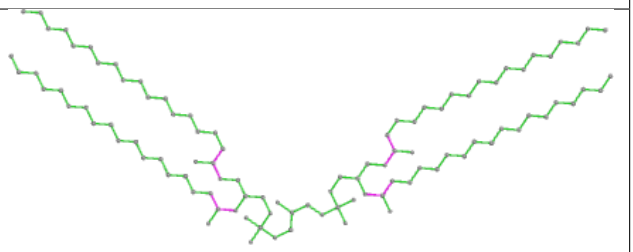


Rings

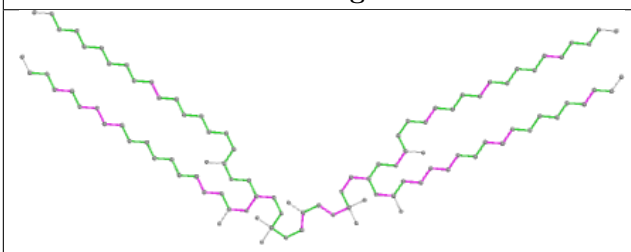
Ligand CDL B3 403



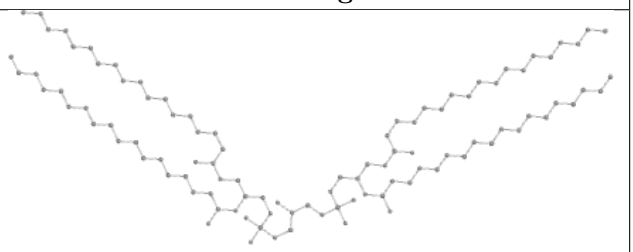
Bond lengths



Bond angles

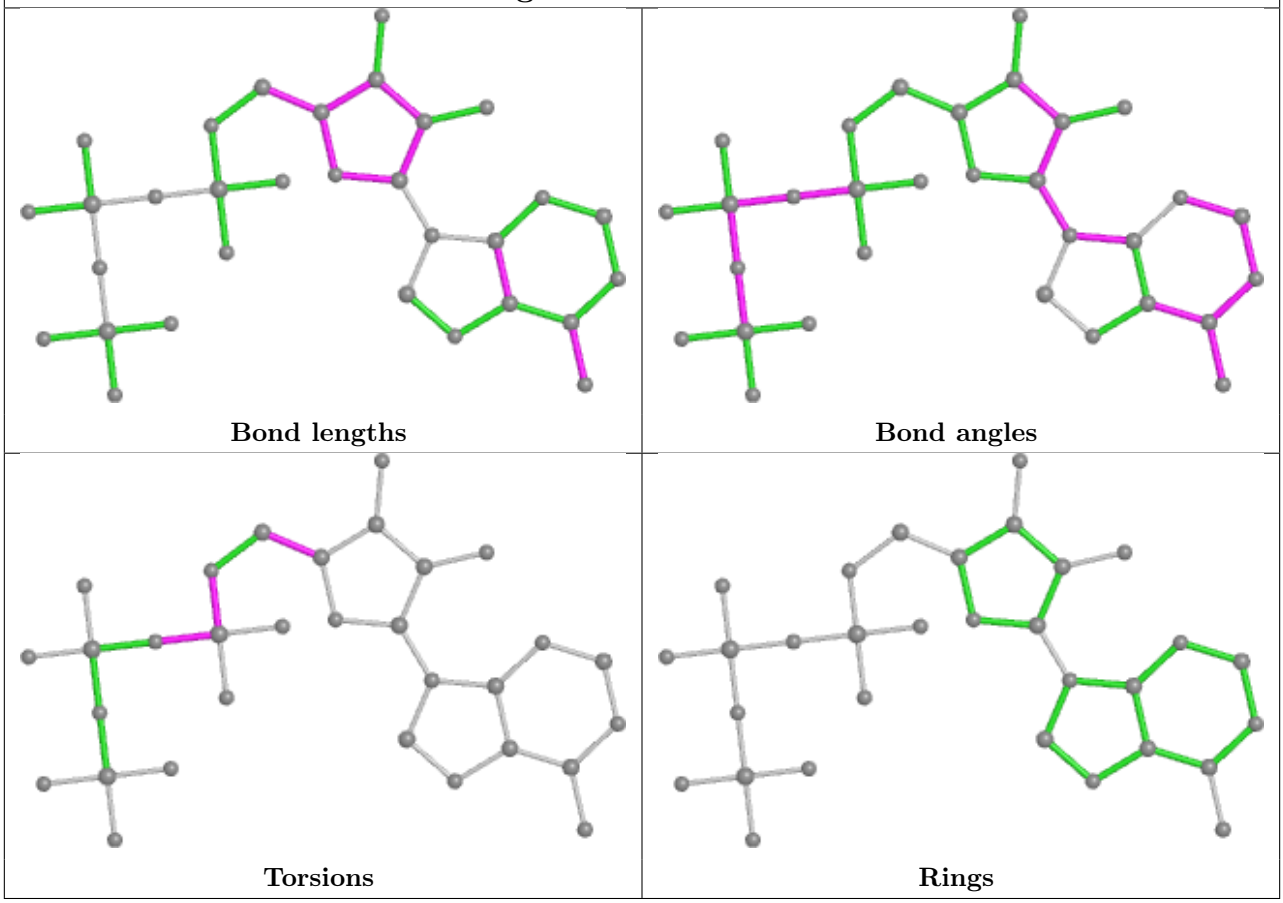


Torsions

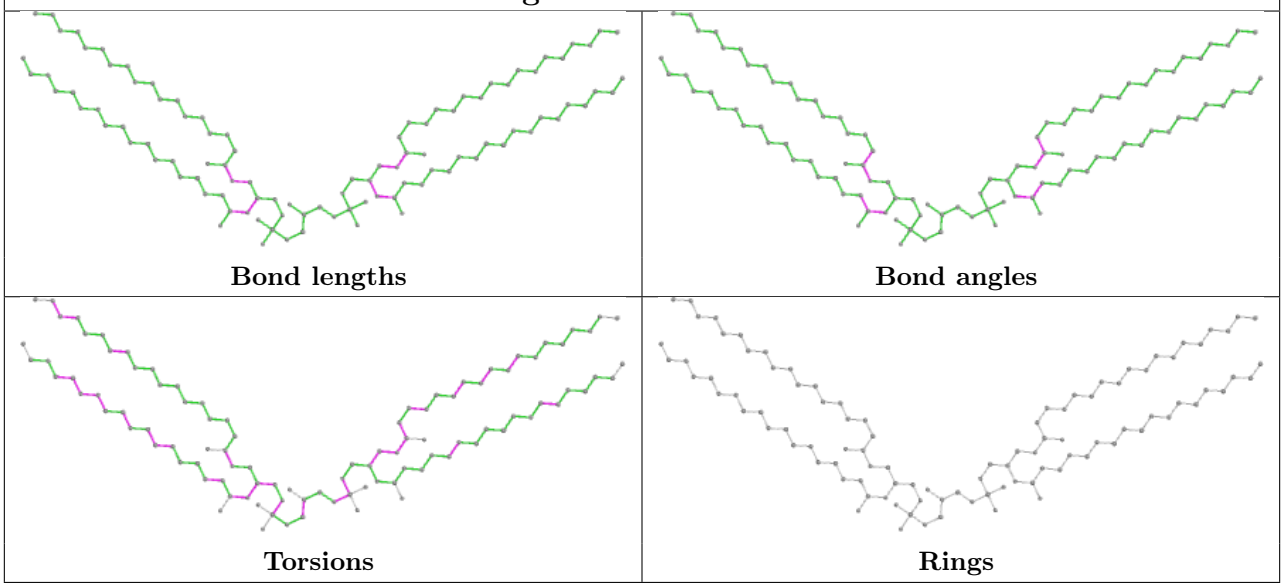


Rings

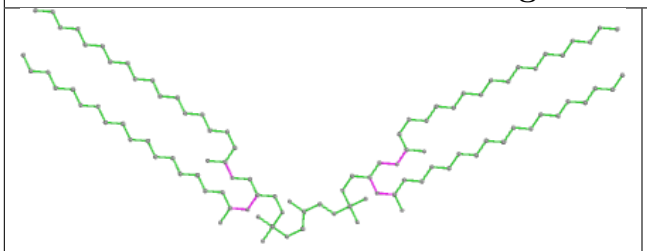
Ligand ATP A4 601



Ligand CDL I3 301



Ligand CDL b3 401



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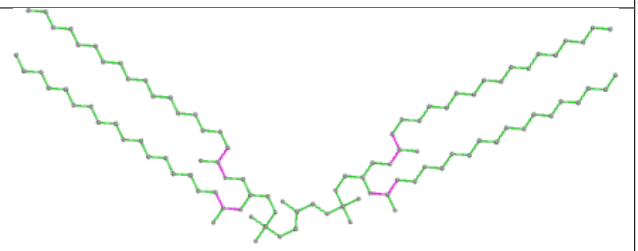
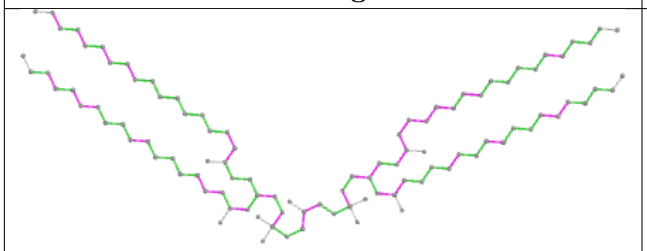
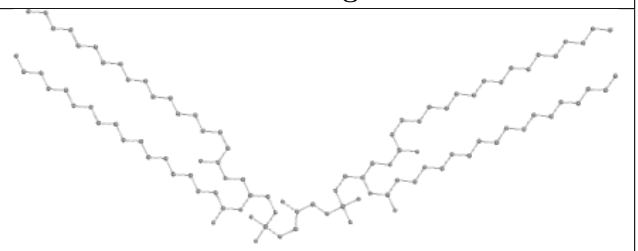


Bond angles

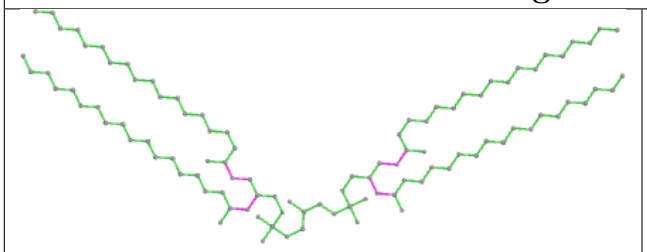


Torsions

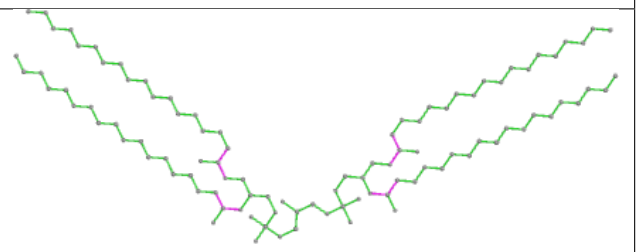


Rings

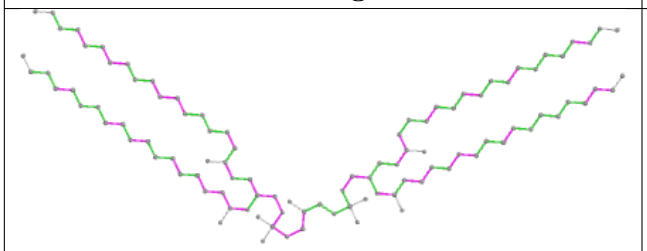
Ligand CDL f 304



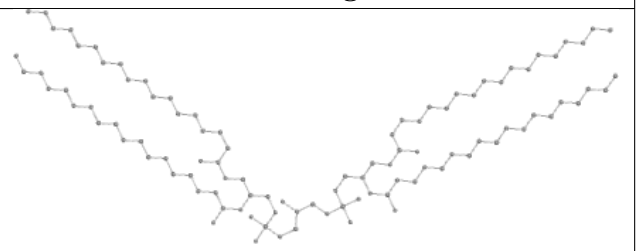
Bond lengths



Bond angles

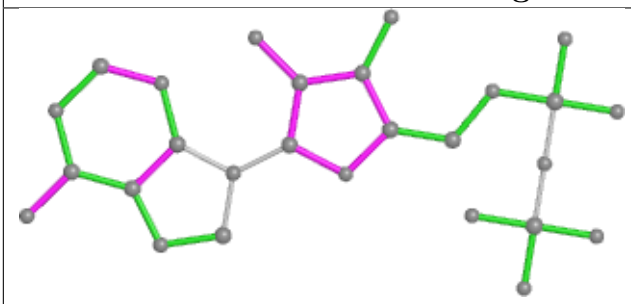


Torsions

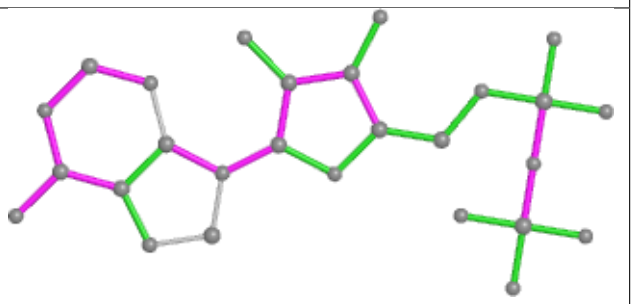


Rings

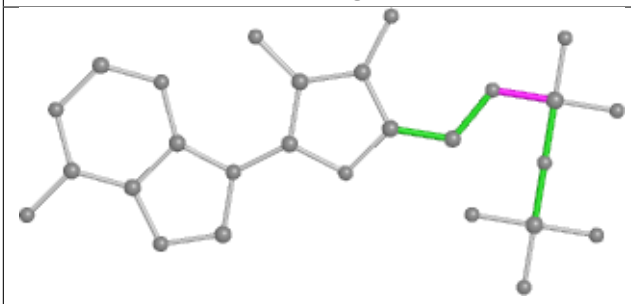
Ligand ADP D4 501



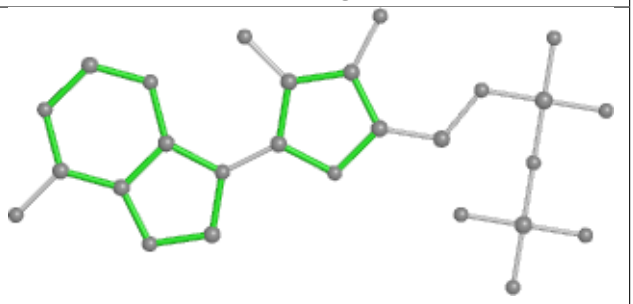
Bond lengths



Bond angles

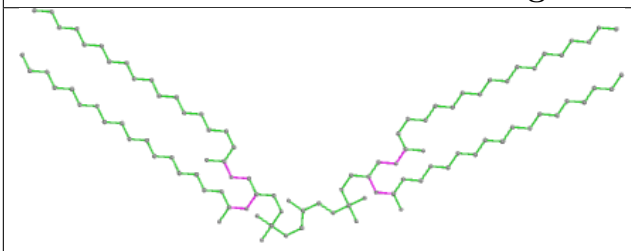


Torsions

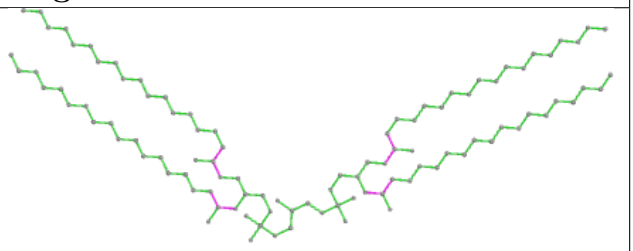


Rings

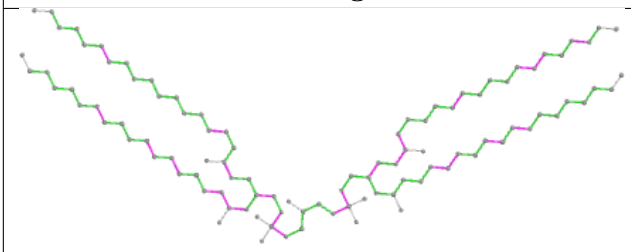
Ligand CDL g 305



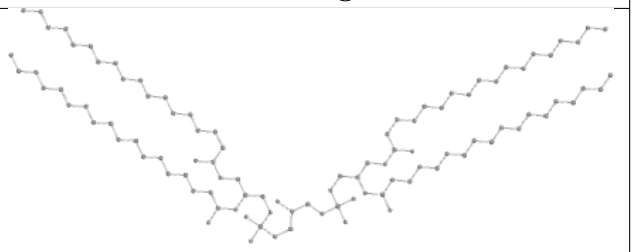
Bond lengths



Bond angles

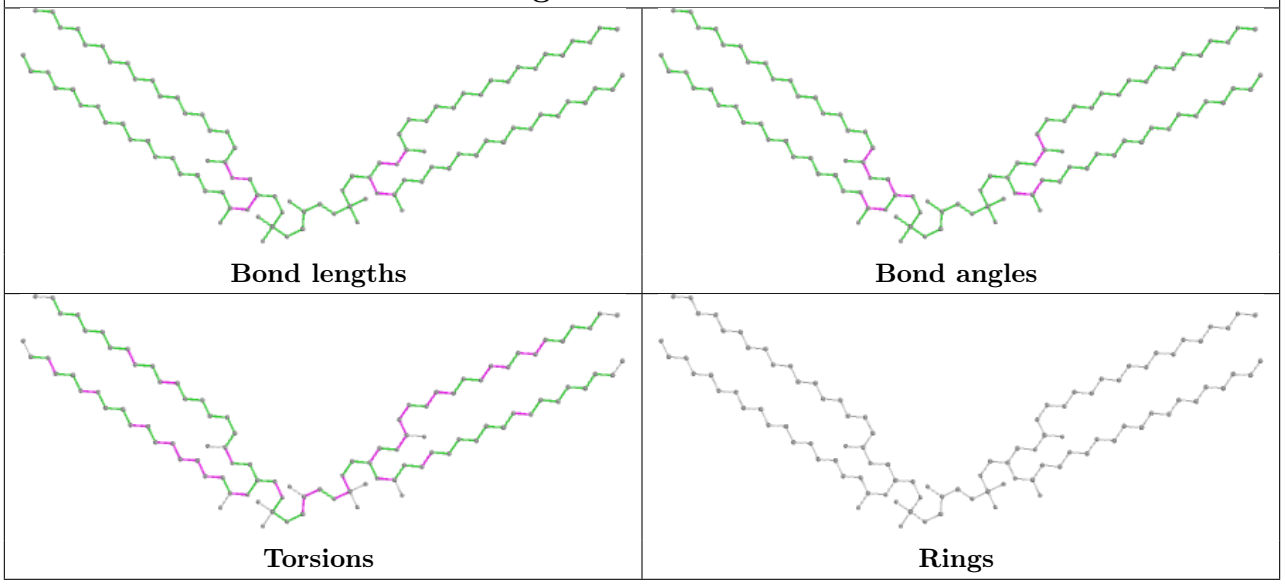


Torsions



Rings

Ligand CDL f 303



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

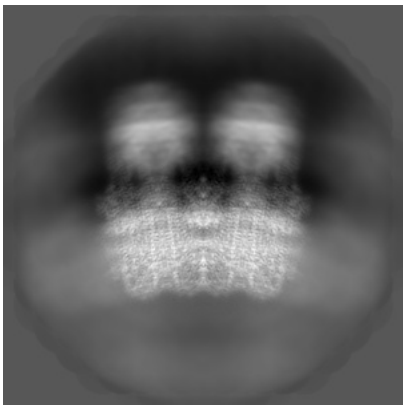
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10861. These allow visual inspection of the internal detail of the map and identification of artifacts.

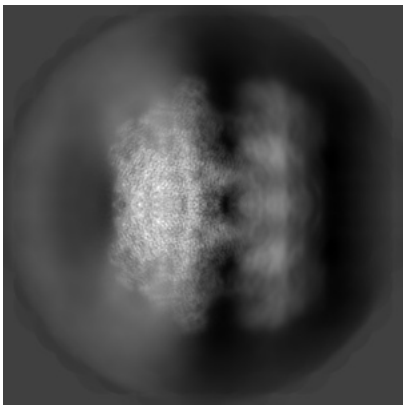
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

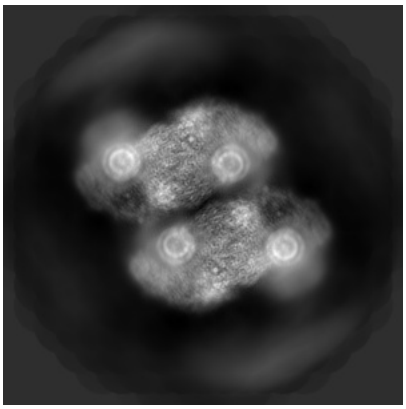
6.1.1 Primary map



X

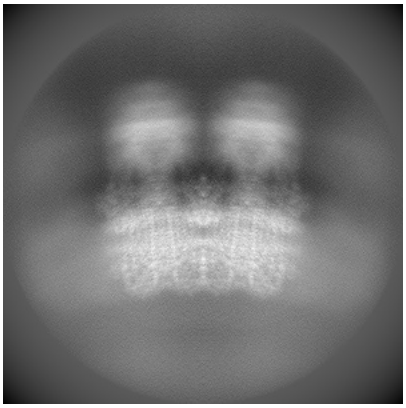


Y

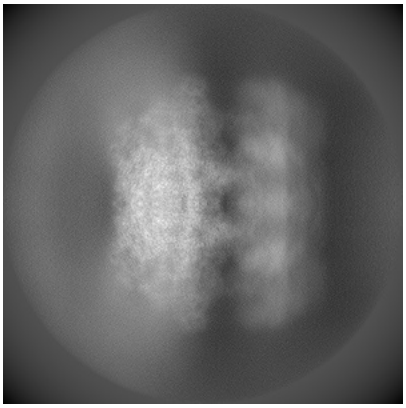


Z

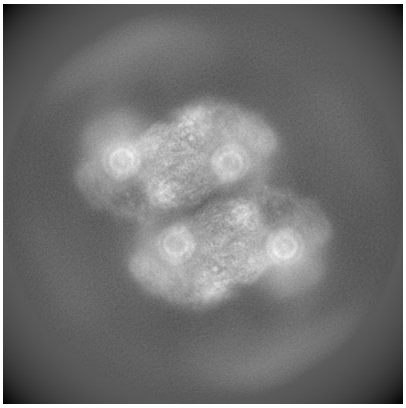
6.1.2 Raw map



X



Y

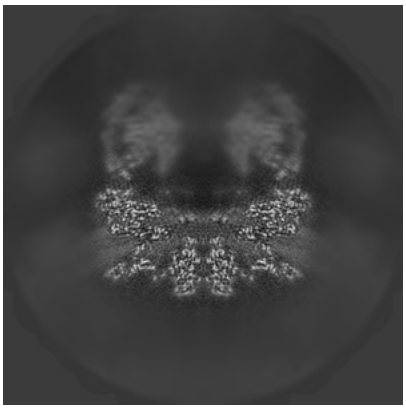


Z

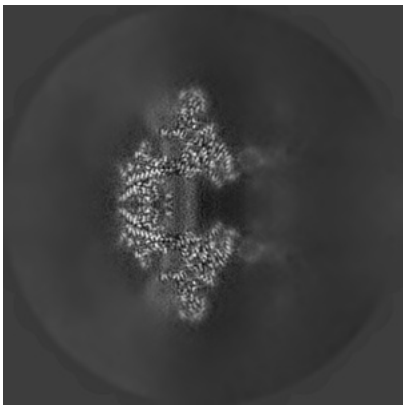
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

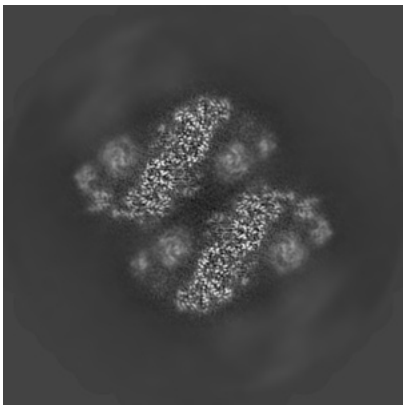
6.2.1 Primary map



X Index: 300

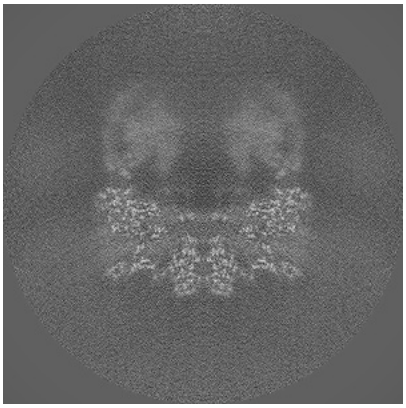


Y Index: 300

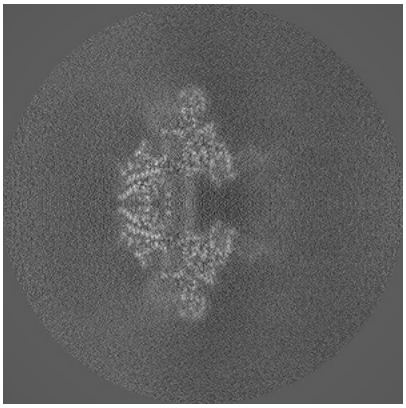


Z Index: 300

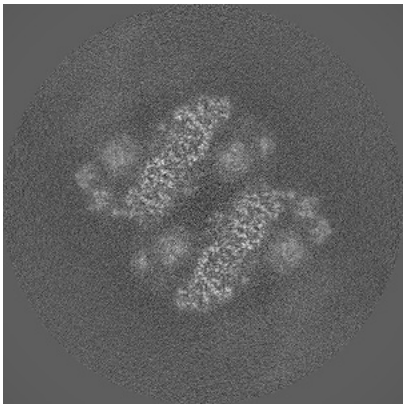
6.2.2 Raw map



X Index: 300



Y Index: 300

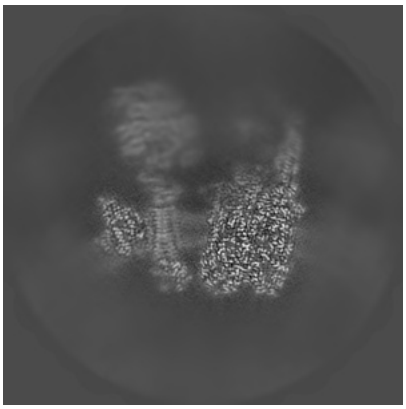


Z Index: 300

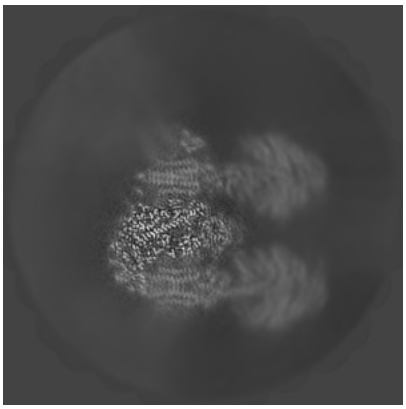
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

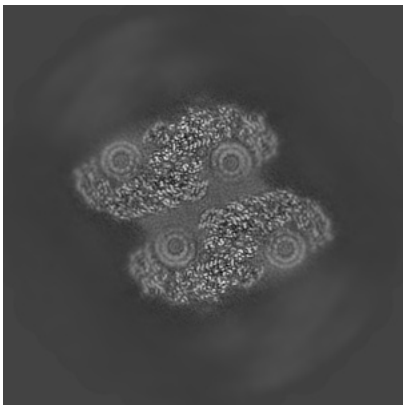
6.3.1 Primary map



X Index: 275

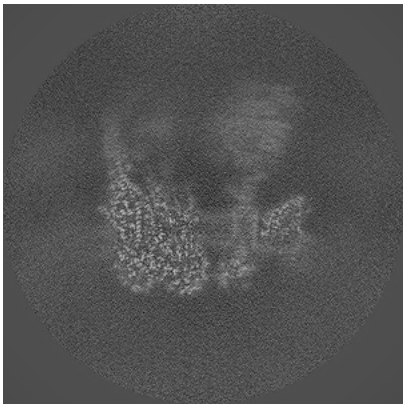


Y Index: 376

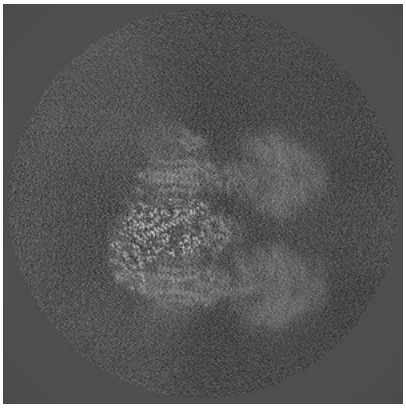


Z Index: 278

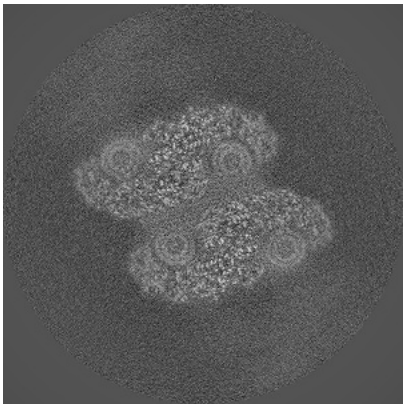
6.3.2 Raw map



X Index: 320



Y Index: 376

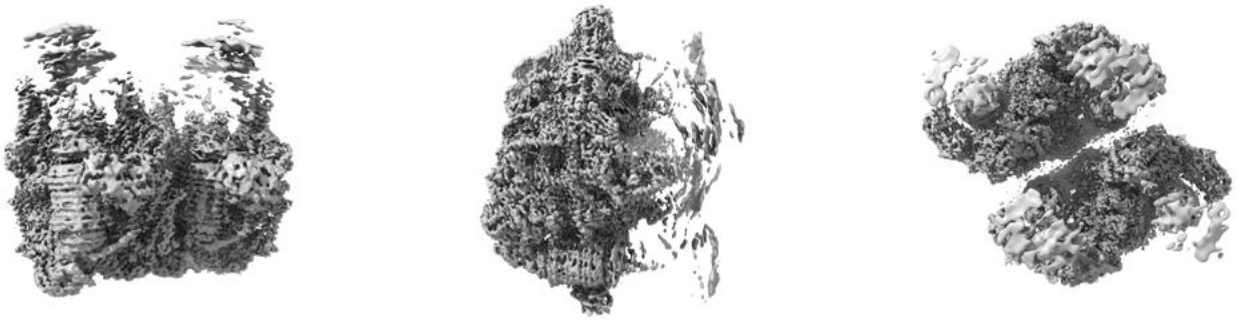


Z Index: 278

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

6.4 Orthogonal surface views (i)

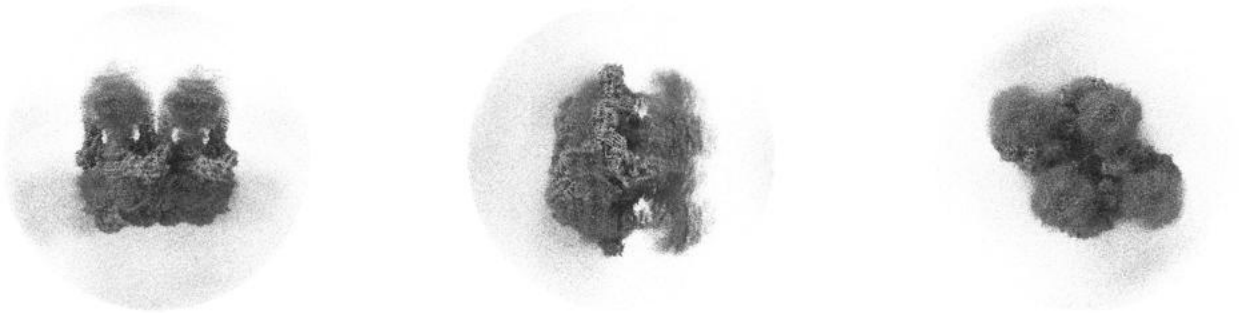
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

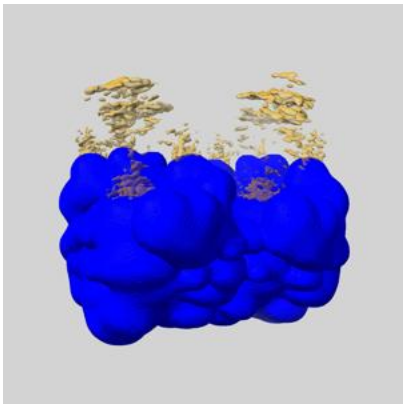
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

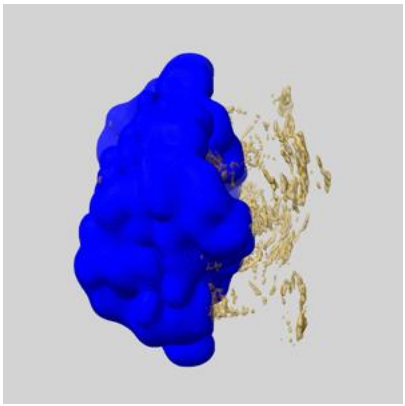
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

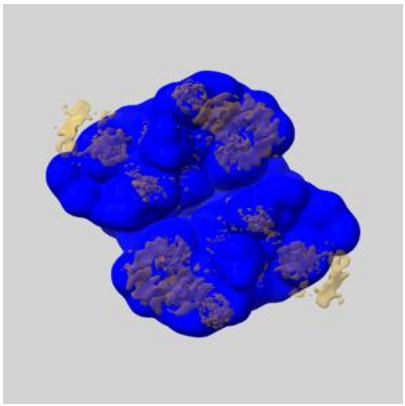
6.5.1 emd_10861_msk_1.map



X



Y

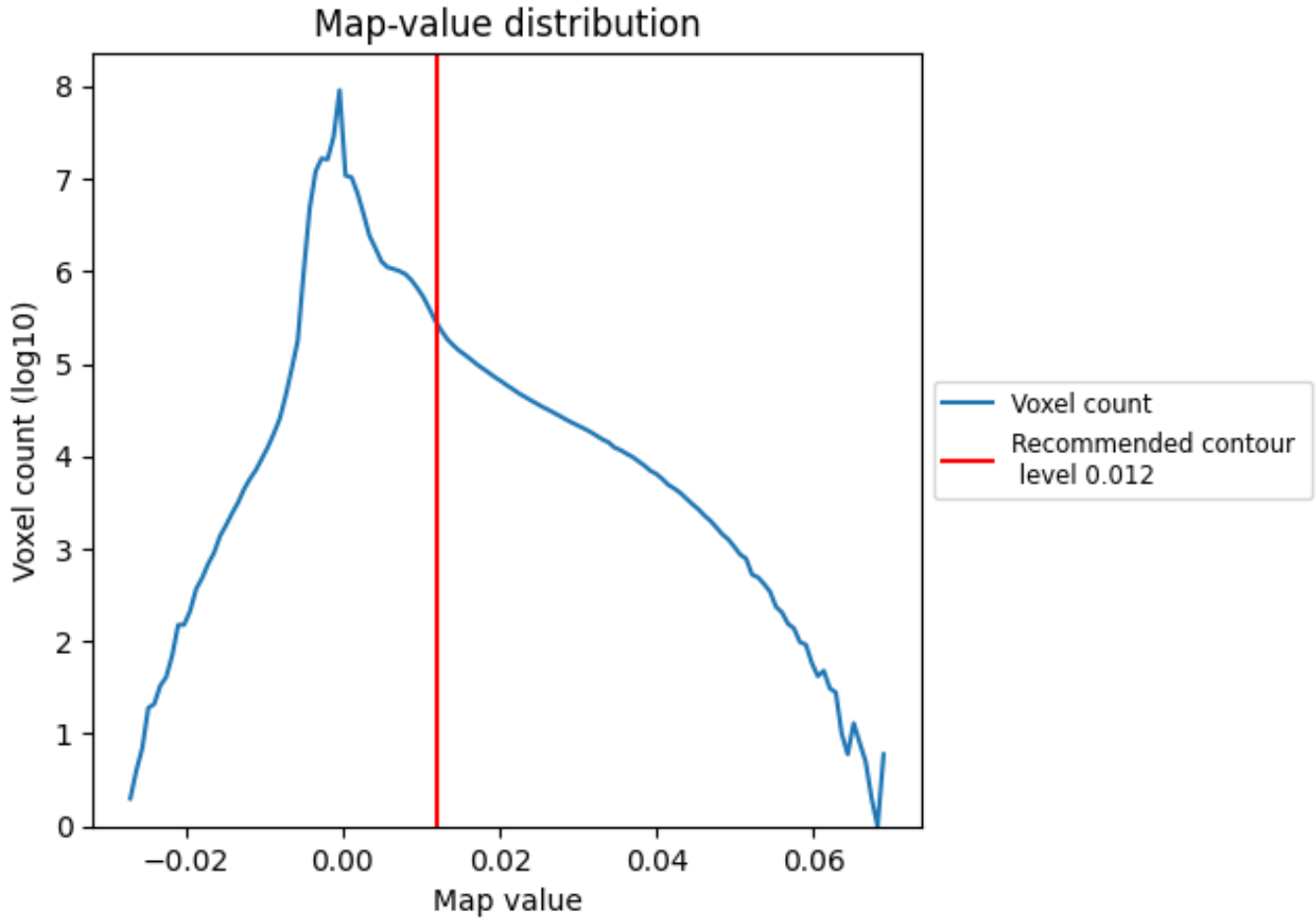


Z

7 Map analysis

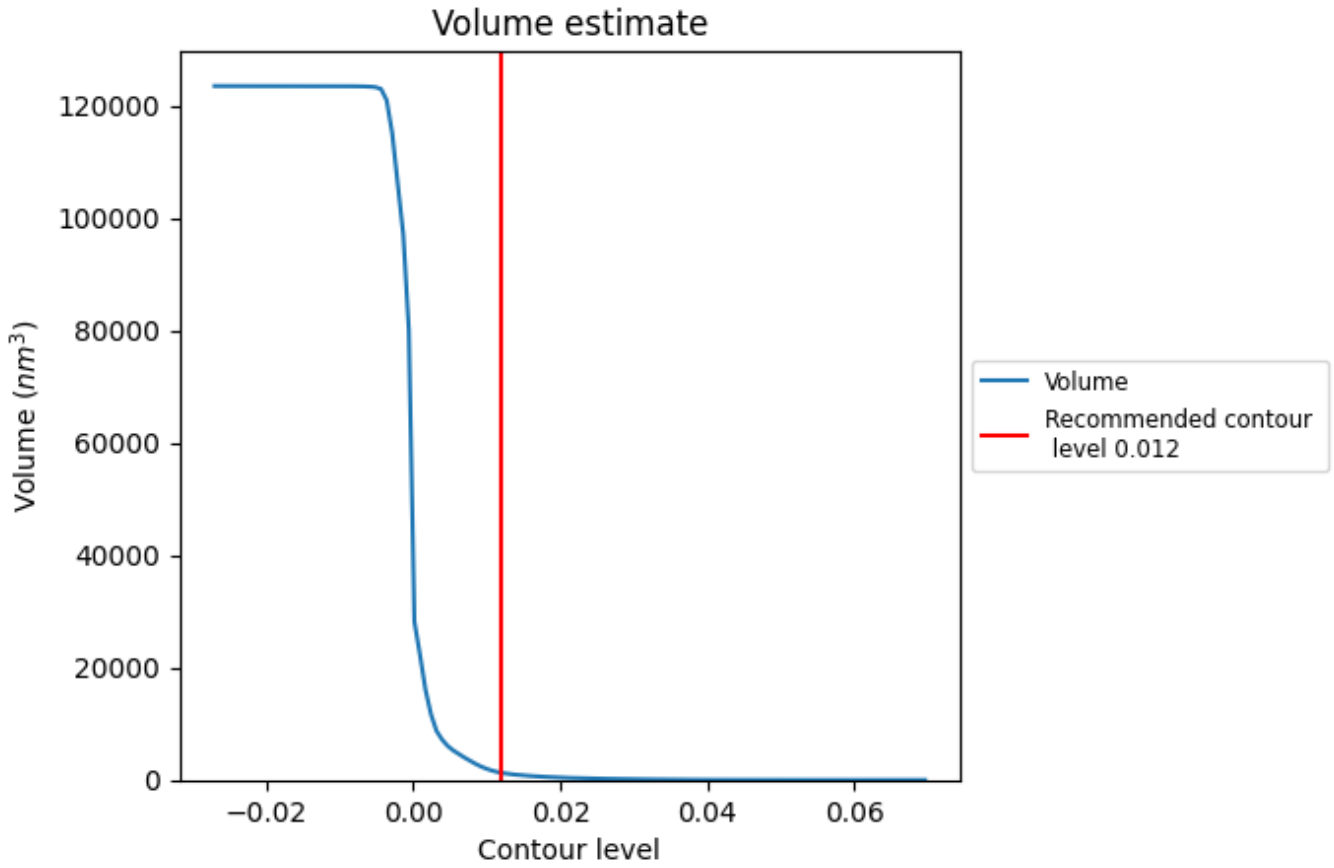
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

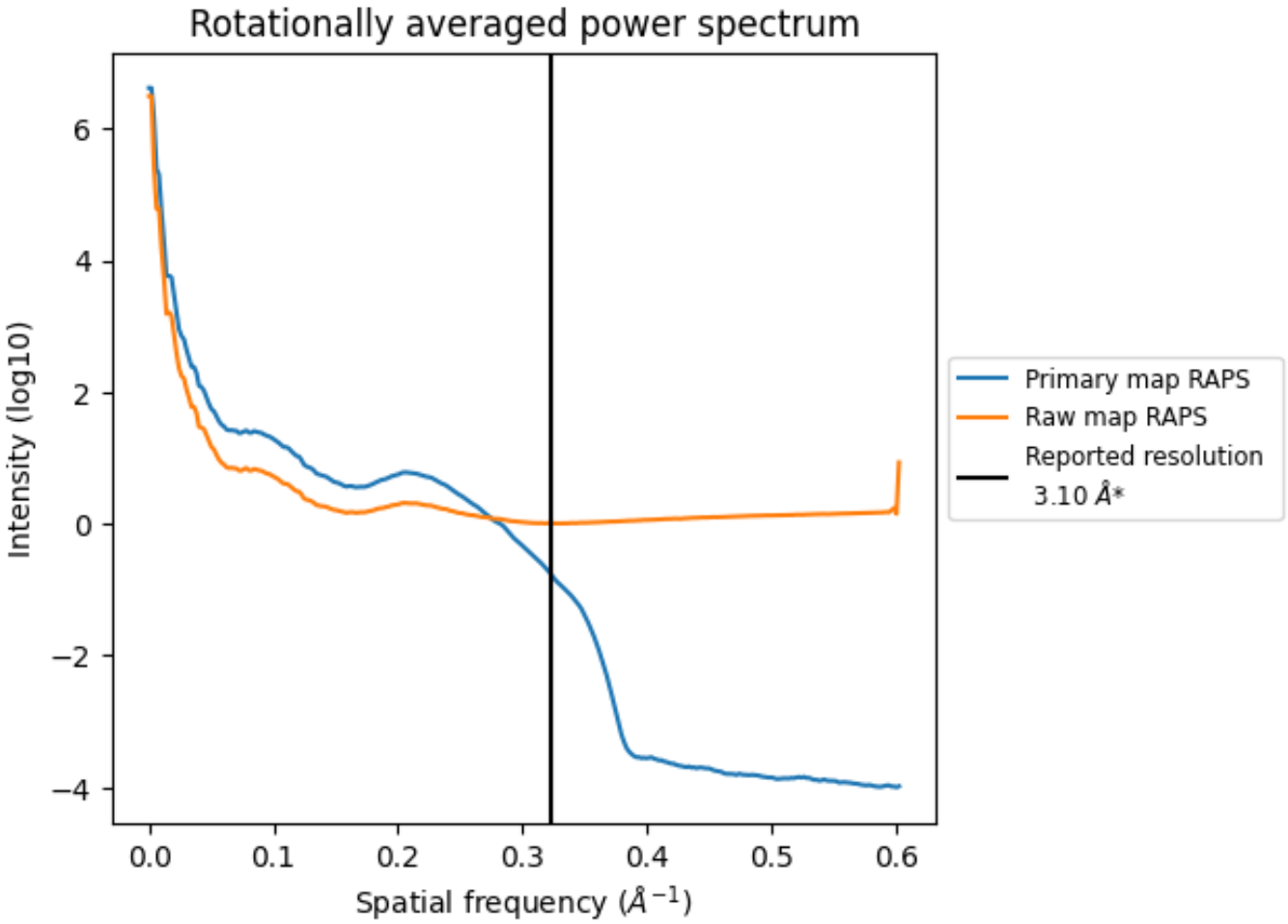
7.2 Volume estimate



The volume at the recommended contour level is 1280 nm^3; this corresponds to an approximate mass of 1157 kDa.

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

7.3 Rotationally averaged power spectrum (i)

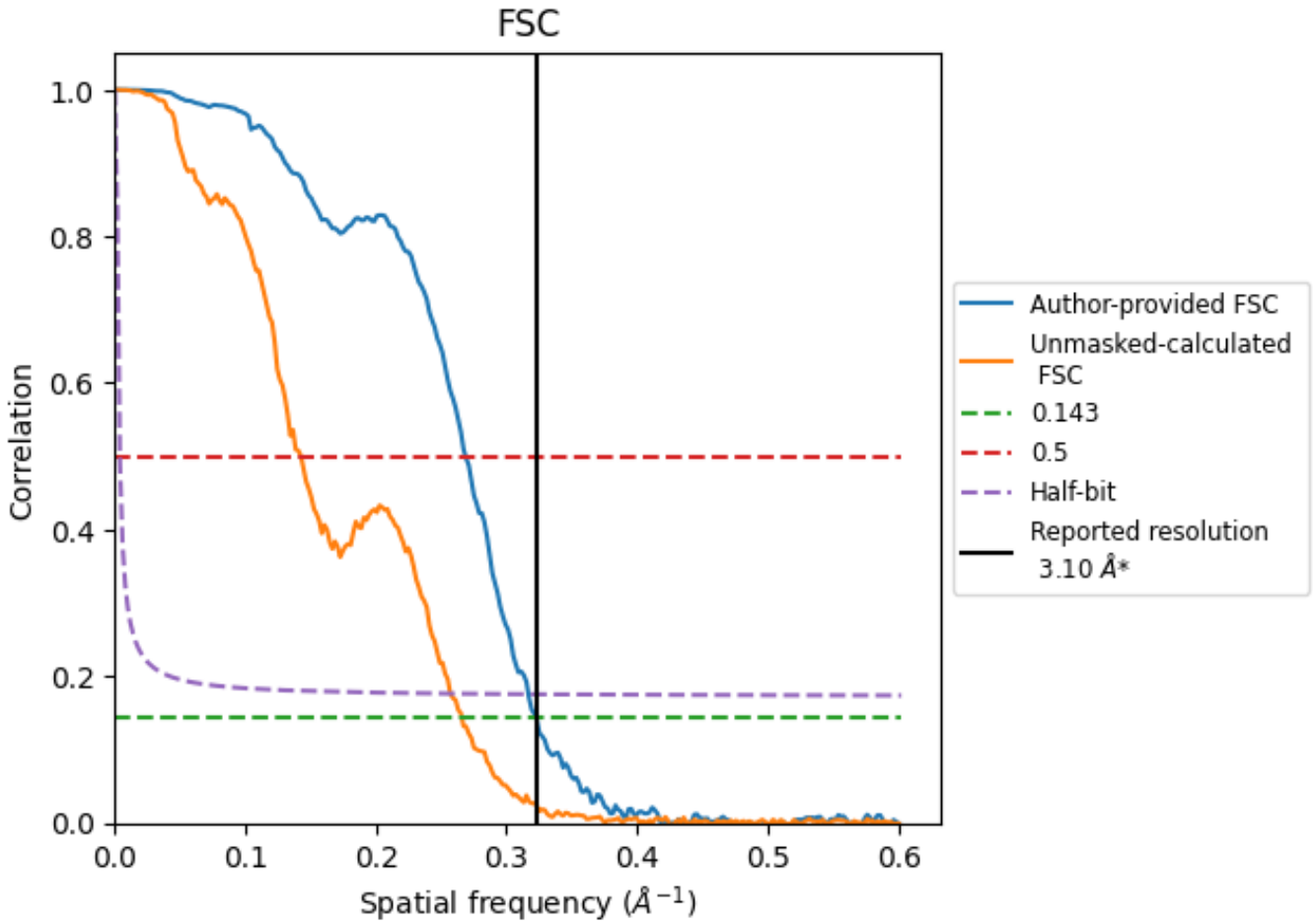


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

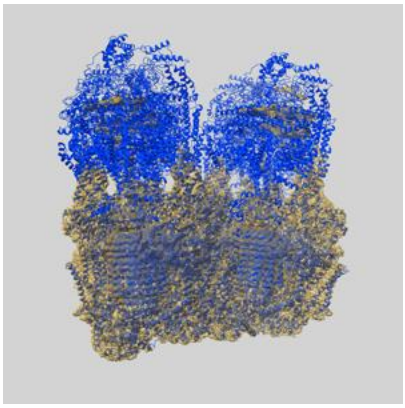
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.72	3.16
Unmasked-calculated*	3.76	7.01	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.1 by more than 10 %

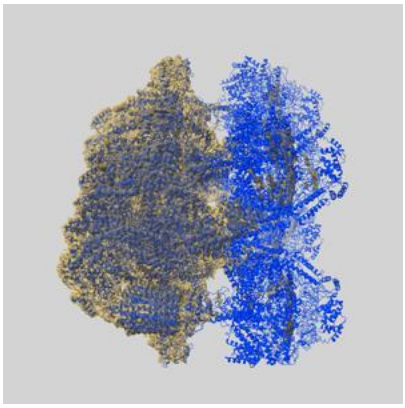
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10861 and PDB model 6YNZ. Per-residue inclusion information can be found in section 3 on page 32.

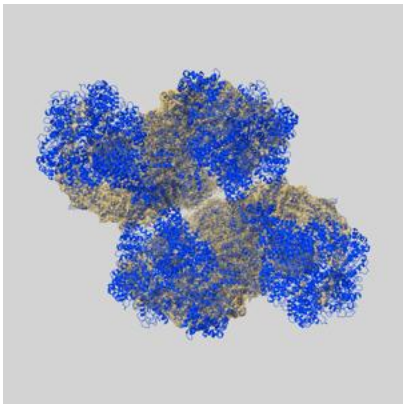
9.1 Map-model overlay



X



Y



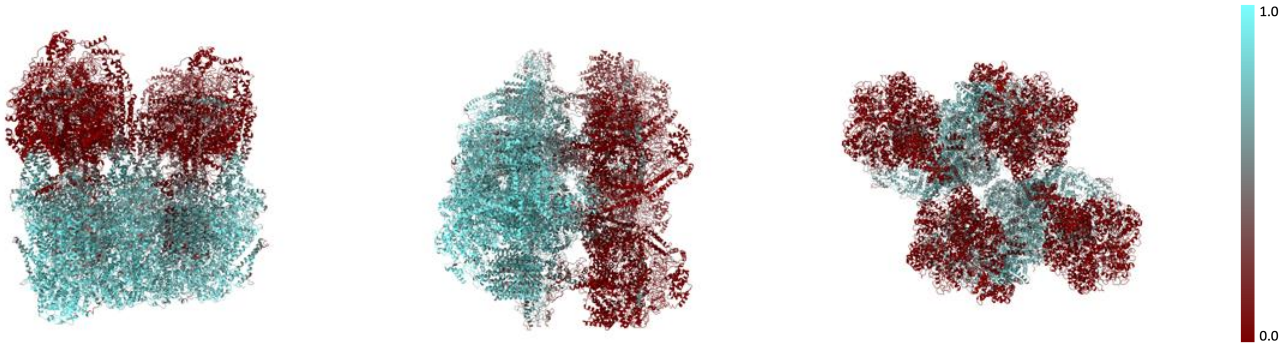
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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)

This section was not generated.

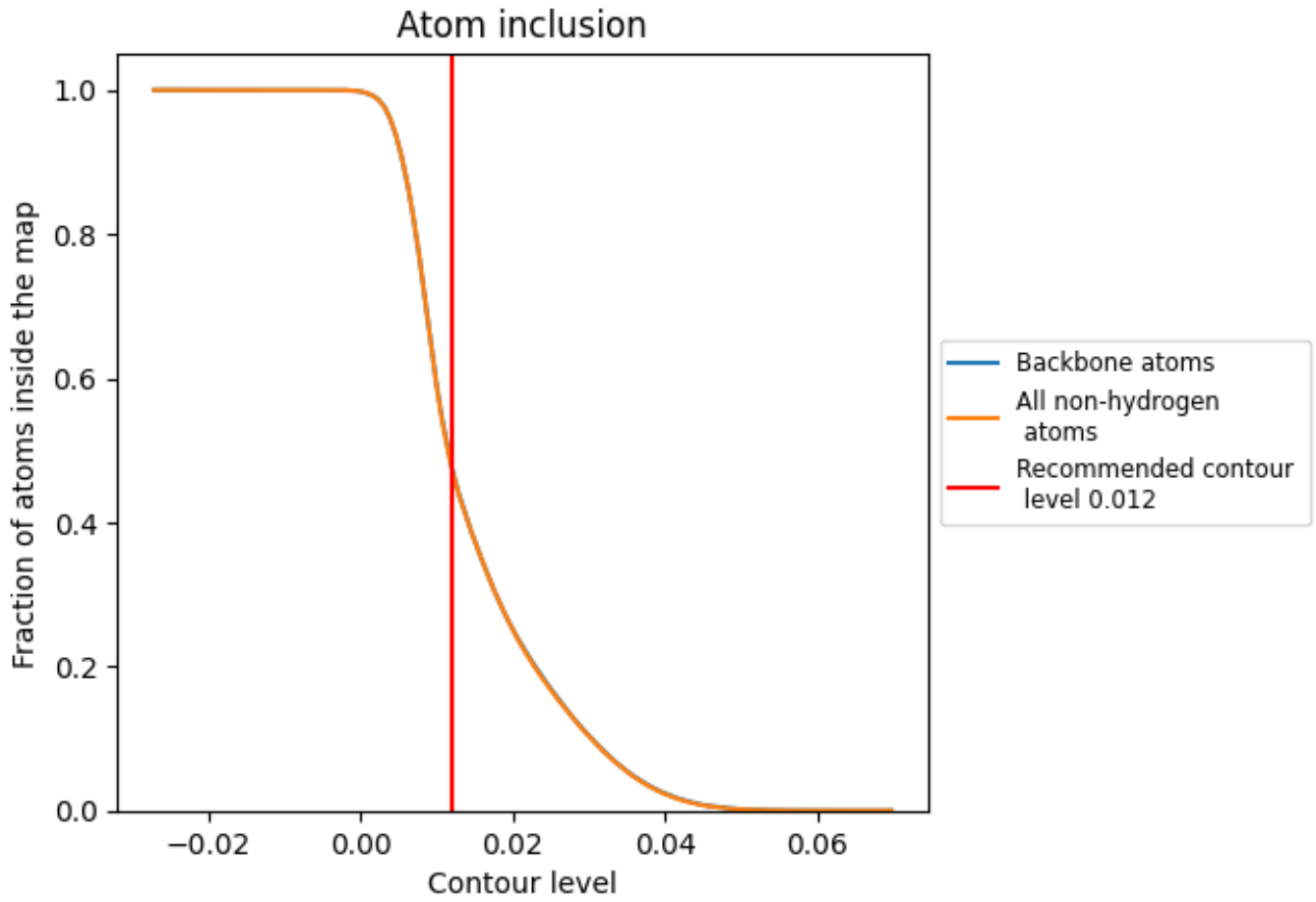
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.4739
A	0.8901
A1	0.1404
A2	0.0485
A3	0.8862
A4	0.0501
A5	0.1437
B	0.4995
B1	0.0719
B2	0.0262
B3	0.4381
B4	0.0262
B5	0.0749
C	0.9208
C1	0.0113
C2	0.0098
C3	0.9013
C4	0.0103
C5	0.0111
D	0.6371
D1	0.0111
D2	0.0136
D3	0.5743
D4	0.0150
D5	0.0108
E	0.6939
E1	0.0853
E2	0.0066
E3	0.5909
E4	0.0063
E5	0.0835
F	0.8620
F1	0.0330
F2	0.0296
F3	0.8621

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Chain	Atom inclusion
F4	0.0270
F5	0.0341
G	0.8262
G1	0.0000
G2	0.0000
G3	0.7566
G4	0.0000
G5	0.0000
H	0.8439
H1	0.7066
H2	0.7478
H3	0.7468
H4	0.7370
H5	0.7066
I	0.8517
I1	0.6673
I2	0.7478
I3	0.7925
I4	0.7478
I5	0.6637
J	0.8316
J1	0.5778
J2	0.7496
J3	0.8035
J4	0.7424
J5	0.5725
K	0.7865
K1	0.5564
K2	0.6905
K3	0.7693
K4	0.6959
K5	0.5510
L	0.8909
L1	0.5581
L2	0.7084
L3	0.8579
L4	0.6995
L5	0.5725
M	0.9334
M1	0.6369
M2	0.7513
M3	0.9141

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Chain	Atom inclusion
M4	0.7585
M5	0.6351
N	0.9305
N1	0.6208
N2	0.7460
N3	0.9091
N4	0.7531
N5	0.6225
O	0.8698
O1	0.6404
O2	0.6959
O3	0.8963
O4	0.6923
O5	0.6422
P	0.7076
P1	0.6816
P2	0.6798
P3	0.7284
P4	0.6780
P5	0.6887
Q	0.7870
Q1	0.6798
Q2	0.7120
Q3	0.6748
Q4	0.7191
Q5	0.6673
R	0.8681
R3	0.8257
S	0.7339
S3	0.6436
a	0.8853
a3	0.8683
b	0.4400
b3	0.5046
c	0.8965
c3	0.9184
d	0.5719
d1	0.2943
d2	0.3586
d3	0.6371
d4	0.3509
d5	0.2905

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Chain	Atom inclusion
e	0.5841
e1	0.2348
e2	0.2595
e3	0.6959
e4	0.2633
e5	0.2273
f	0.7666
f3	0.8120
g	0.7459
g1	0.1585
g2	0.1953
g3	0.8176
g4	0.1972
g5	0.1605
h	0.7220
h3	0.8186
i	0.8245
i1	0.0404
i2	0.0702
i3	0.8471
i4	0.0912
i5	0.0296
j	0.8009
j3	0.8379
k	0.7843
k3	0.7922
l	0.8520
l3	0.8931
m	0.9036
m3	0.9323
n	0.9070
n3	0.9285
o	0.8963
o3	0.8584
p	0.7168
p3	0.7091
q	0.6782
q3	0.7859
r	0.7857
r3	0.8700
s	0.5440
s3	0.6997

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Chain	Atom inclusion
t	0.5329
t3	0.6047