



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:00 AM UTC

PDB ID : 6YNZ / pdb_00006ynz
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:

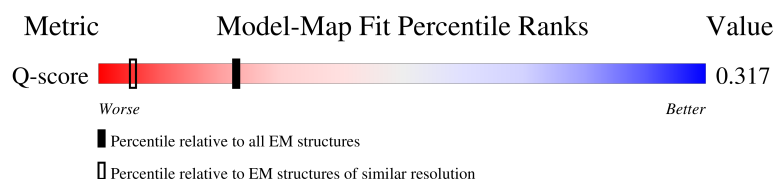
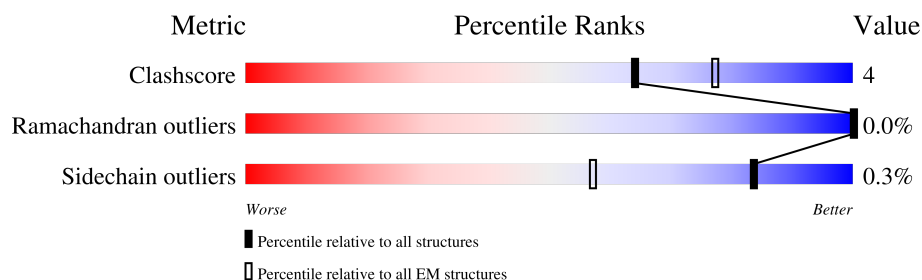
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. 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	92% 5% .
1	A3	446	91% 6% .
1	a	446	90% 7% .
1	a3	446	91% 6% .

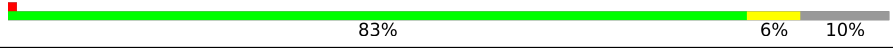
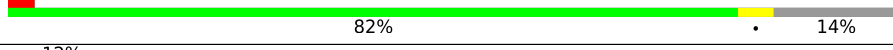
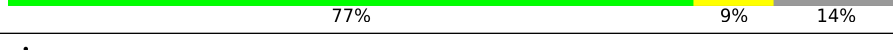
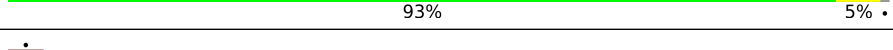
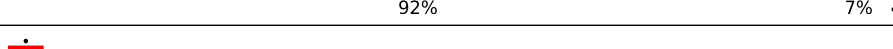
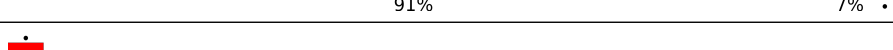
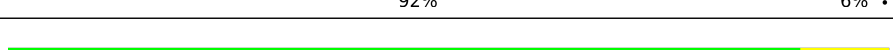
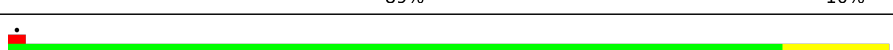
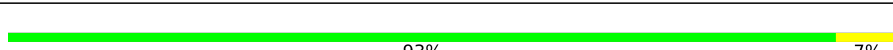
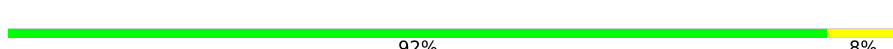
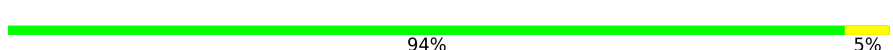
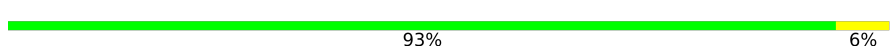
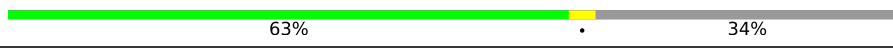
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Mol	Chain	Length	Quality of chain
2	B	381	
2	B3	381	
2	b	381	
2	b3	381	
3	D	234	
3	D3	234	
3	d	234	
3	d3	234	
4	F	204	
4	F3	204	
4	f	204	
4	f3	204	
5	I	209	
5	I3	209	
5	i	209	
5	i3	209	
6	K	179	
6	K3	179	
6	k	179	
6	k3	179	
7	C	100	
7	C3	100	
7	c	100	
7	c3	100	
8	G	286	

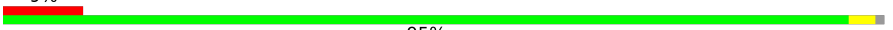
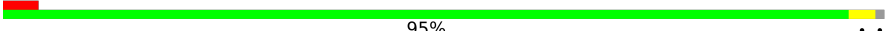
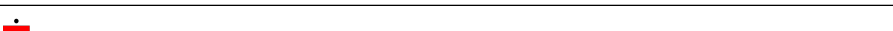
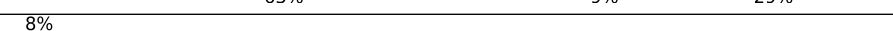
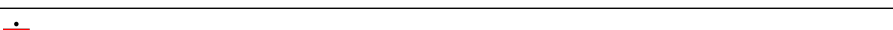
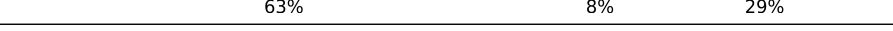
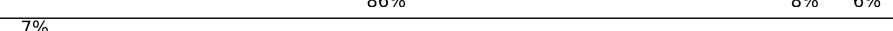
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Mol	Chain	Length	Quality of chain
8	G3	286	
8	g	286	
8	g3	286	
9	H	268	
9	H3	268	
9	h	268	
9	h3	268	
10	J	273	
10	J3	273	
10	j	273	
10	j3	273	
11	L	247	
11	L3	247	
11	l	247	
11	l3	247	
12	M	221	
12	M3	221	
12	m	221	
12	m3	221	
13	N	179	
13	N3	179	
13	n	179	
13	n3	179	
14	O	154	
14	O3	154	

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Mol	Chain	Length	Quality of chain
14	o	154	
14	o3	154	
15	P	152	
15	P3	152	
15	p	152	
15	p3	152	
16	Q	152	
16	Q3	152	
16	q	152	
16	q3	152	
17	R	149	
17	R3	149	
17	r	149	
17	r3	149	
18	S	145	
18	S3	145	
18	s	145	
18	s3	145	
19	E	480	
19	E3	480	
19	e	480	
19	e3	480	
20	i1	108	
20	i2	108	
20	i4	108	

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Mol	Chain	Length	Quality of chain
20	i5	108	
21	t	460	
21	t3	460	
22	G1	219	
22	G2	219	
22	G4	219	
22	G5	219	
23	g1	299	
23	g2	299	
23	g4	299	
23	g5	299	
24	A1	546	
24	A2	546	
24	A4	546	
24	A5	546	
24	B1	546	
24	B2	546	
24	B4	546	
24	B5	546	
24	C1	546	
24	C2	546	
24	C4	546	
24	C5	546	
25	D1	497	
25	D2	497	

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Mol	Chain	Length	Quality of chain
25	D4	497	93% 85%10%5%
25	D5	497	94% 84%11%5%
25	E1	497	85% 83%12%5%
25	E2	497	94% 83%11%5%
25	E4	497	94% 84%11%5%
25	E5	497	86% 81%13%5%
25	F1	497	91% 81%13%6%
25	F2	497	91% 82%12%6%
25	F4	497	92% 81%13%6%
25	F5	497	91% 83%11%6%
26	H1	76	9% 83%16%.
26	H2	76	5% 84%14%.
26	H4	76	7% 87%12%.
26	H5	76	9% 80%18%.
26	I1	76	14% 82%17%.
26	I2	76	. 76%22%.
26	I4	76	5% 80%18%.
26	I5	76	14% 82%17%.
26	J1	76	24% 89%9%.
26	J2	76	8% 83%16%.
26	J4	76	8% 84%14%.
26	J5	76	26% 84%14%.
26	K1	76	32% 87%12%.
26	K2	76	13% 86%13%.
26	K4	76	14% 83%16%.

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Mol	Chain	Length	Quality of chain
26	K5	76	
26	L1	76	
26	L2	76	
26	L4	76	
26	L5	76	
26	M1	76	
26	M2	76	
26	M4	76	
26	M5	76	
26	N1	76	
26	N2	76	
26	N4	76	
26	N5	76	
26	O1	76	
26	O2	76	
26	O4	76	
26	O5	76	
26	P1	76	
26	P2	76	
26	P4	76	
26	P5	76	
26	Q1	76	
26	Q2	76	
26	Q4	76	
26	Q5	76	

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Mol	Chain	Length	Quality of chain
27	d1	158	
27	d2	158	
27	d4	158	
27	d5	158	
28	e1	71	
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 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0

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

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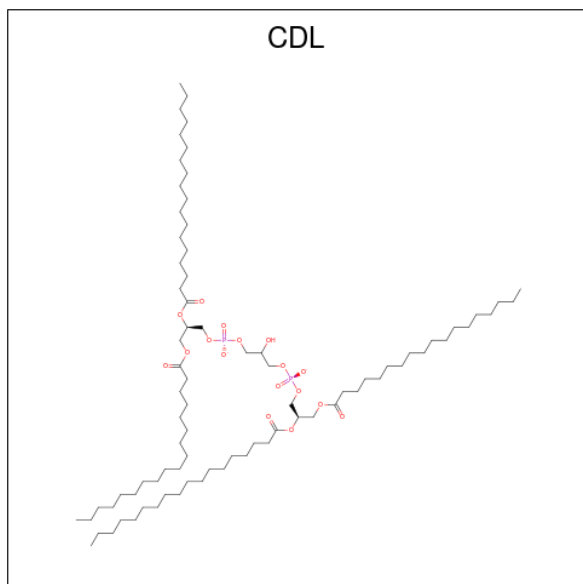
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Mol	Chain	Residues	Atoms						AltConf	Trace
27	d5	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

- 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 (CCD ID: 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
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
29	f	1	Total 256	C 81	H 156	O 17	P 2	0
29	i	1	Total 256	C 81	H 156	O 17	P 2	0
29	k	1	Total 256	C 81	H 156	O 17	P 2	0
29	g	1	Total 256	C 81	H 156	O 17	P 2	0
29	j	1	Total 256	C 81	H 156	O 17	P 2	0
29	j	1	Total 256	C 81	H 156	O 17	P 2	0
29	l	1	Total 256	C 81	H 156	O 17	P 2	0
29	l	1	Total 256	C 81	H 156	O 17	P 2	0
29	p	1	Total 256	C 81	H 156	O 17	P 2	0
29	r	1	Total 256	C 81	H 156	O 17	P 2	0
29	A	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0

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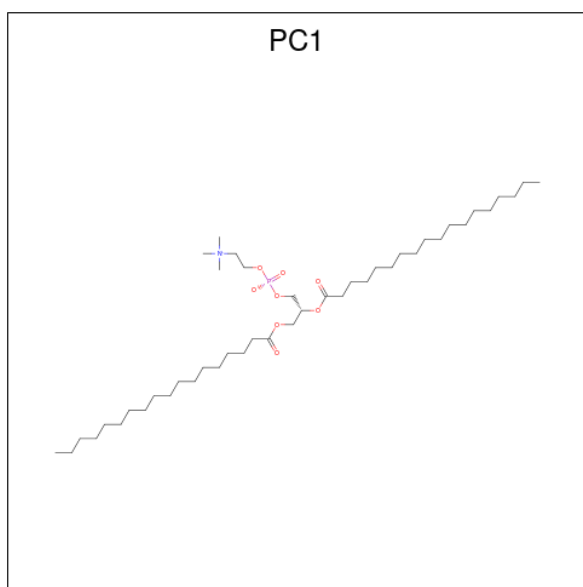
Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	P	1	Total 256	C 81	H 156	O 17	P 2	0
29	a3	1	Total 256	C 81	H 156	O 17	P 2	0
29	a3	1	Total 256	C 81	H 156	O 17	P 2	0
29	b3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	i3	1	Total 256	C 81	H 156	O 17	P 2	0
29	i3	1	Total 256	C 81	H 156	O 17	P 2	0
29	k3	1	Total 256	C 81	H 156	O 17	P 2	0
29	g3	1	Total 256	C 81	H 156	O 17	P 2	0
29	j3	1	Total 256	C 81	H 156	O 17	P 2	0
29	j3	1	Total 256	C 81	H 156	O 17	P 2	0
29	l3	1	Total 256	C 81	H 156	O 17	P 2	0
29	l3	1	Total 256	C 81	H 156	O 17	P 2	0
29	p3	1	Total 256	C 81	H 156	O 17	P 2	0
29	A3	1	Total 256	C 81	H 156	O 17	P 2	0

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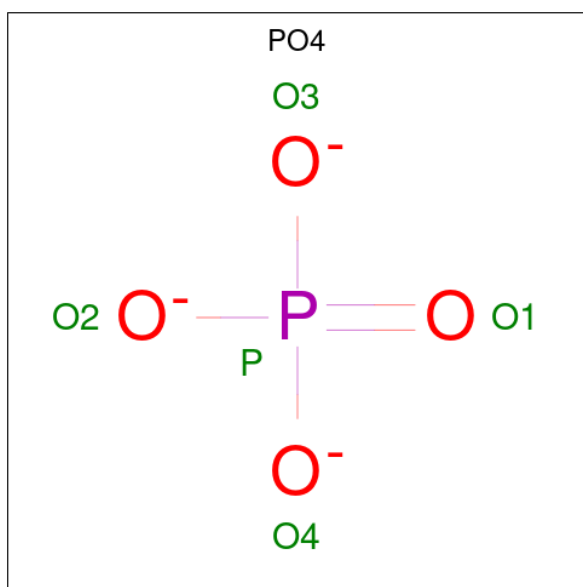
Mol	Chain	Residues	Atoms					AltConf
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	F3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	K3	1	Total 256	C 81	H 156	O 17	P 2	0
29	K3	1	Total 256	C 81	H 156	O 17	P 2	0
29	J3	1	Total 256	C 81	H 156	O 17	P 2	0
29	J3	1	Total 256	C 81	H 156	O 17	P 2	0
29	L3	1	Total 256	C 81	H 156	O 17	P 2	0
29	P3	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



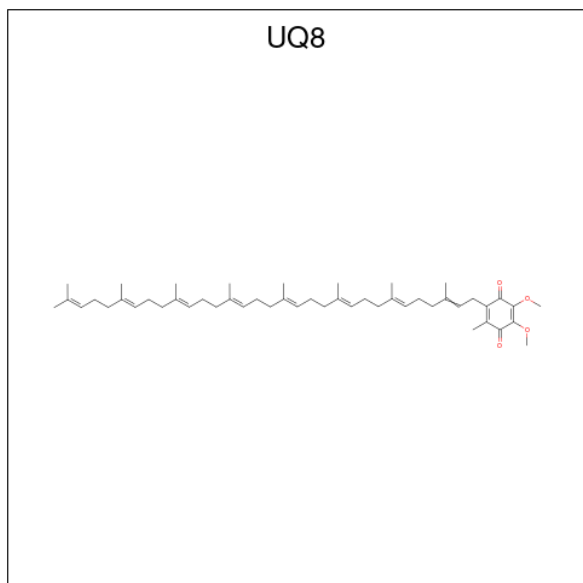
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88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

- Molecule 31 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



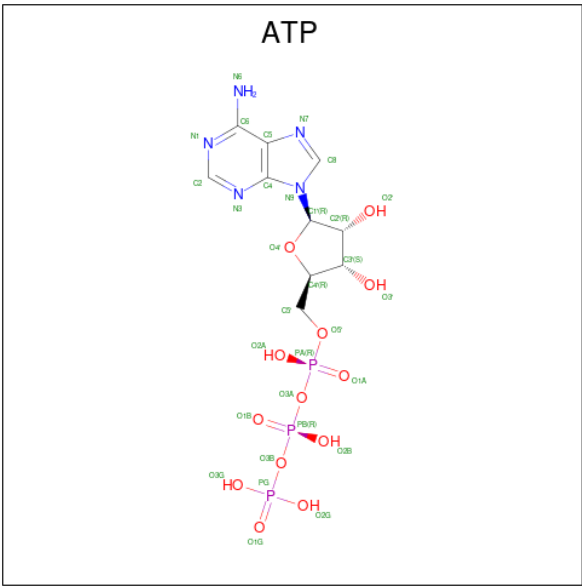
Mol	Chain	Residues	Atoms			AltConf
31	f	1	Total	O	P	0
			5	4	1	
31	F	1	Total	O	P	0
			5	4	1	
31	f3	1	Total	O	P	0
			5	4	1	
31	F3	1	Total	O	P	0
			5	4	1	

- Molecule 32 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

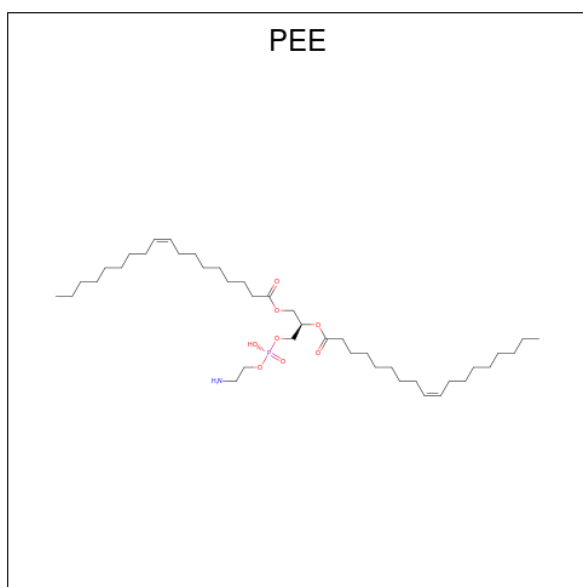
Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total 1	Mg 1	0
34	G	1	Total 1	Mg 1	0
34	C1	1	Total 1	Mg 1	0
34	D1	1	Total 1	Mg 1	0
34	B1	1	Total 1	Mg 1	0
34	A1	1	Total 1	Mg 1	0
34	E1	1	Total 1	Mg 1	0
34	C2	1	Total 1	Mg 1	0
34	D2	1	Total 1	Mg 1	0
34	B2	1	Total 1	Mg 1	0
34	A2	1	Total 1	Mg 1	0

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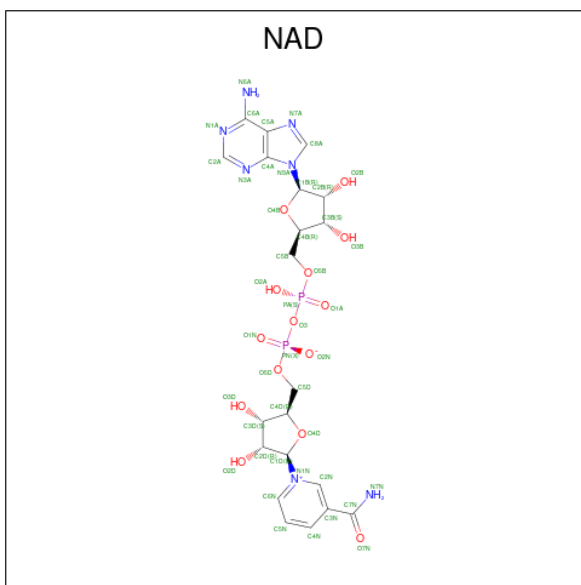
Mol	Chain	Residues	Atoms		AltConf
34	E2	1	Total 1	Mg 1	0
34	g3	1	Total 1	Mg 1	0
34	G3	1	Total 1	Mg 1	0
34	C4	1	Total 1	Mg 1	0
34	D4	1	Total 1	Mg 1	0
34	B4	1	Total 1	Mg 1	0
34	A4	1	Total 1	Mg 1	0
34	E4	1	Total 1	Mg 1	0
34	C5	1	Total 1	Mg 1	0
34	D5	1	Total 1	Mg 1	0
34	B5	1	Total 1	Mg 1	0
34	A5	1	Total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

- Molecule 35 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



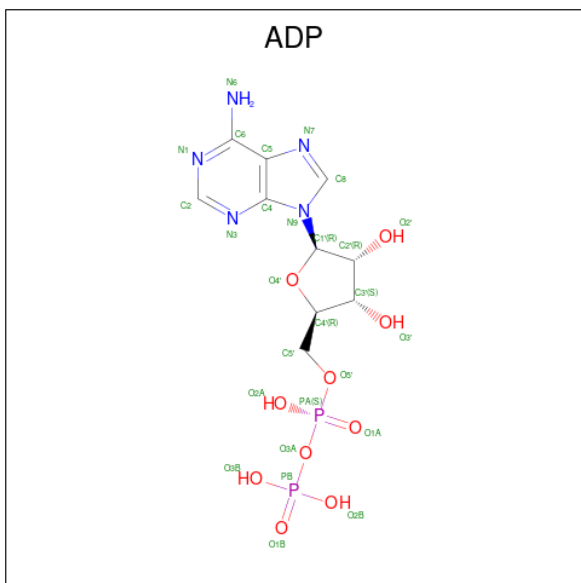
Mol	Chain	Residues	Atoms						AltConf
35	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	a3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	j3	1	Total	C	H	N	O	P	0
			133	41	82	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 (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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

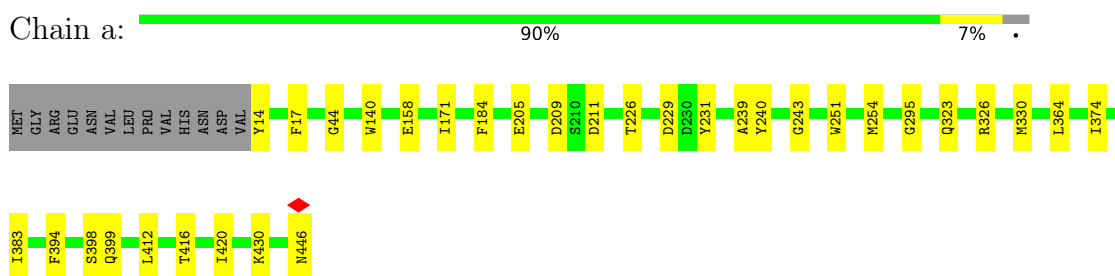


Mol	Chain	Residues	Atoms						AltConf
37	D1	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B1	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D2	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B2	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D5	1	Total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

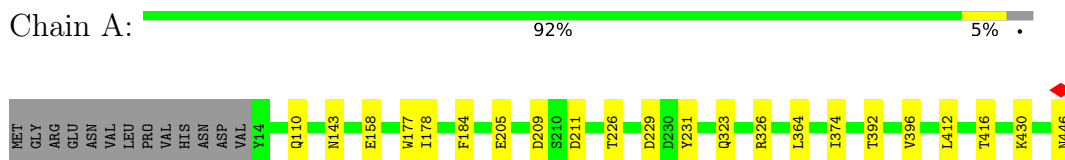
3 Residue-property plots [i](#)

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

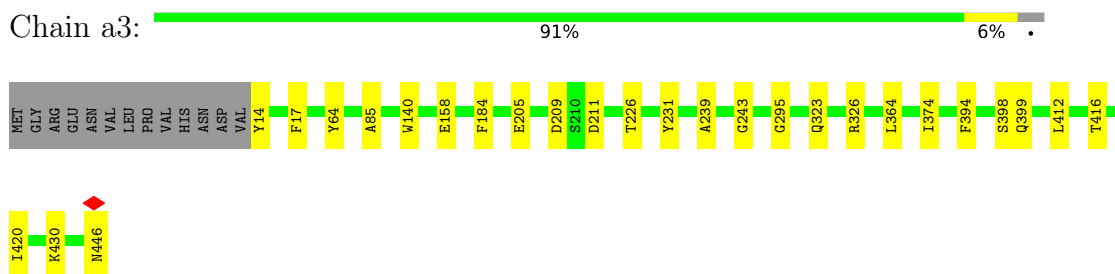
- Molecule 1: Ymf66



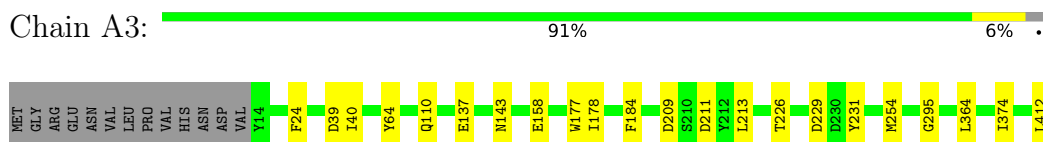
- Molecule 1: Ymf66

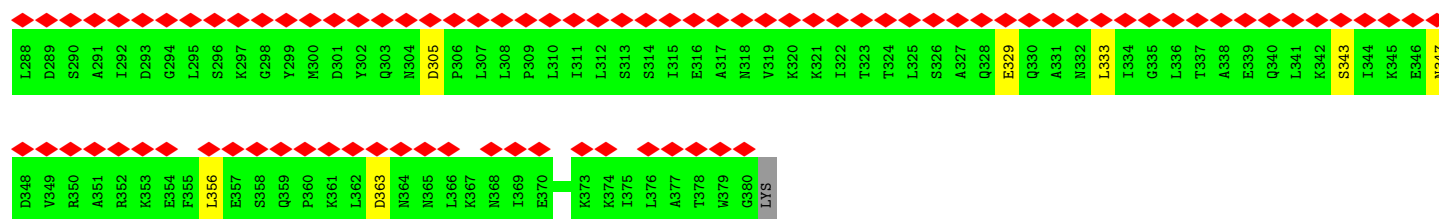


- Molecule 1: Ymf66

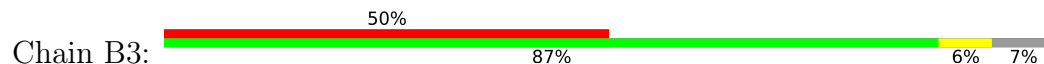


- Molecule 1: Ymf66

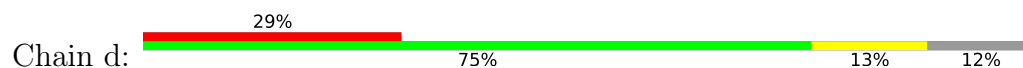




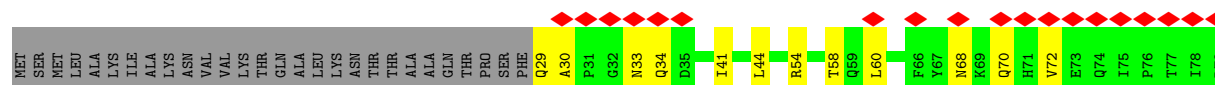
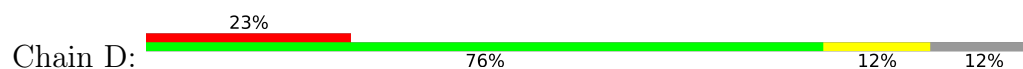
- Molecule 2: subunit b

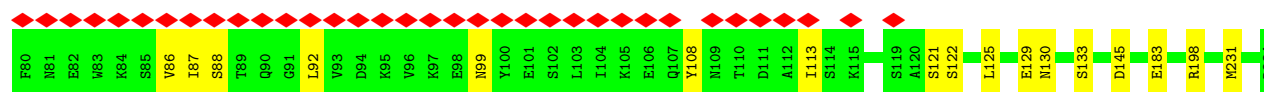


- Molecule 3: subunit d

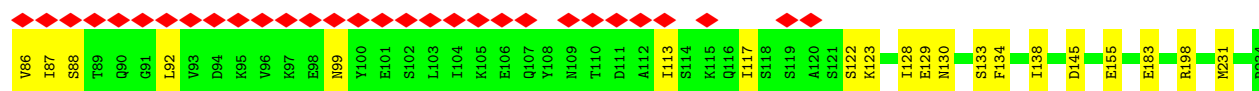
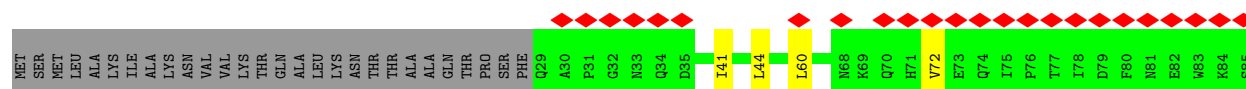
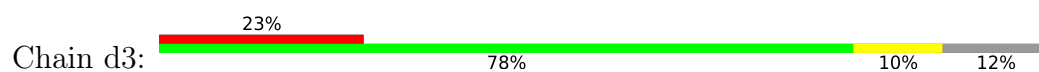


- Molecule 3: subunit d

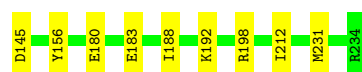
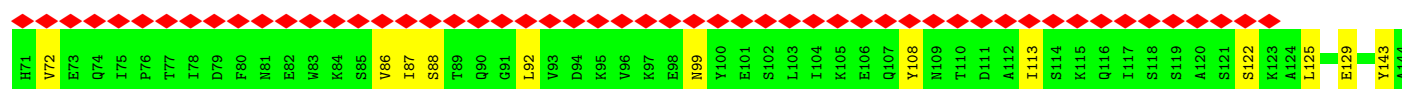
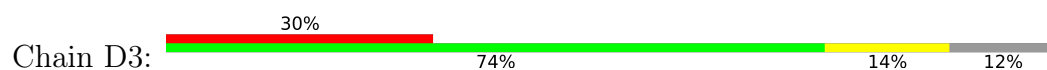




- Molecule 3: subunit d



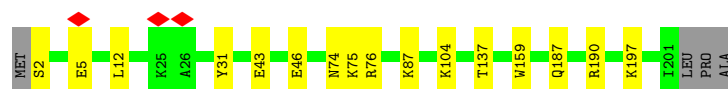
- Molecule 3: subunit d



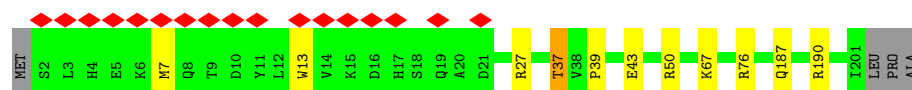
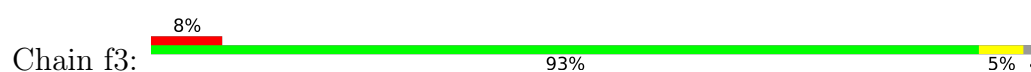
- Molecule 4: subunit f



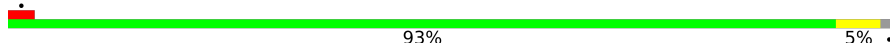
- Molecule 4: subunit f

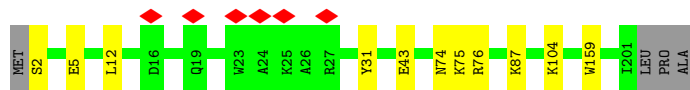


- Molecule 4: subunit f



- Molecule 4: subunit f

Chain F3:  93% 5%



- Molecule 5: subunit i/j

Chain i:  91% 9%

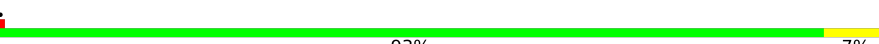


- Molecule 5: subunit i/j

Chain I:  90% 10%



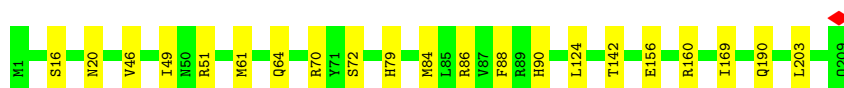
- Molecule 5: subunit i/j

Chain i3:  93% 7%

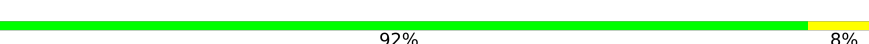


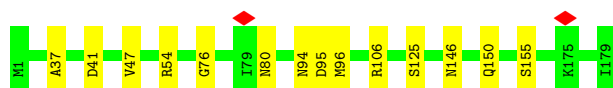
- Molecule 5: subunit i/j

Chain I3:  90% 10%



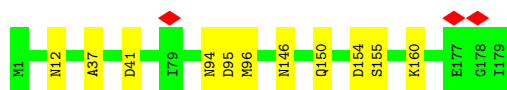
- Molecule 6: subunit k

Chain k:  92% 8%



- Molecule 6: subunit k

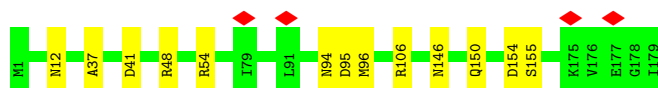
Chain K:  94% 6%



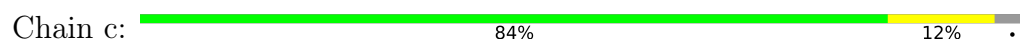
- Molecule 6: subunit k



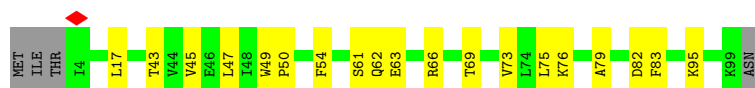
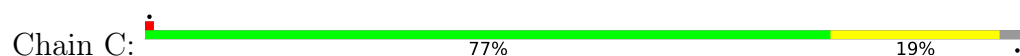
- Molecule 6: subunit k



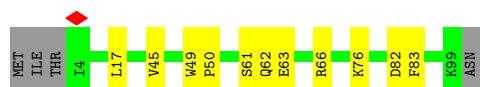
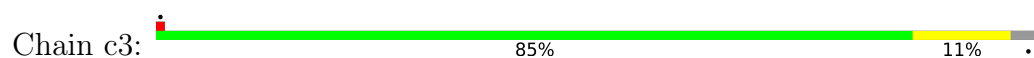
- Molecule 7: Ymf56



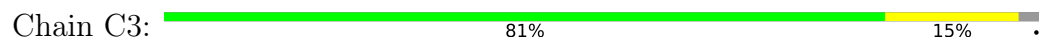
- Molecule 7: Ymf56



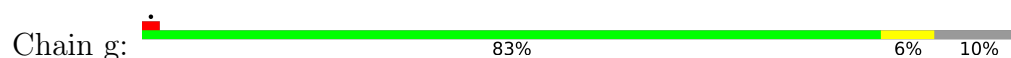
- Molecule 7: Ymf56

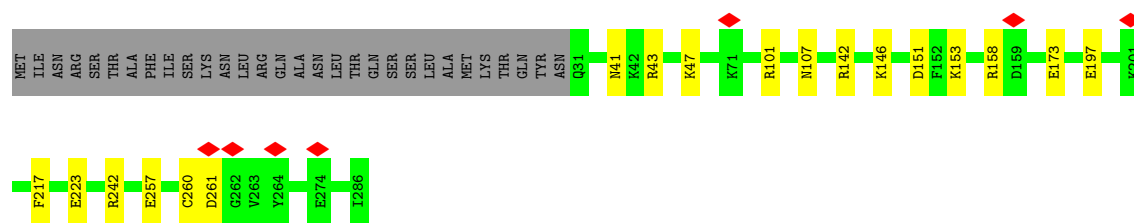


- Molecule 7: Ymf56

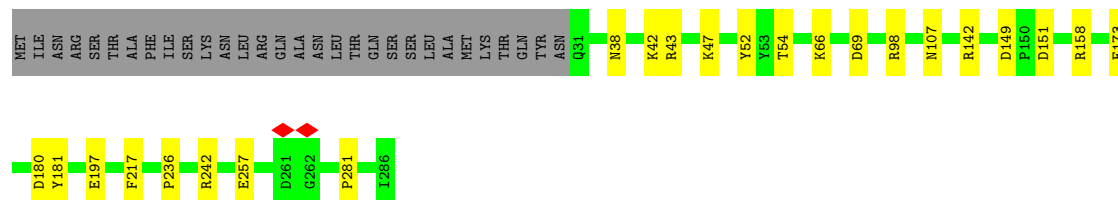
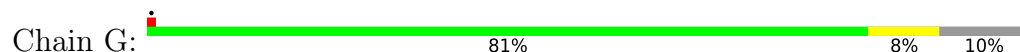


- Molecule 8: ATPPT3

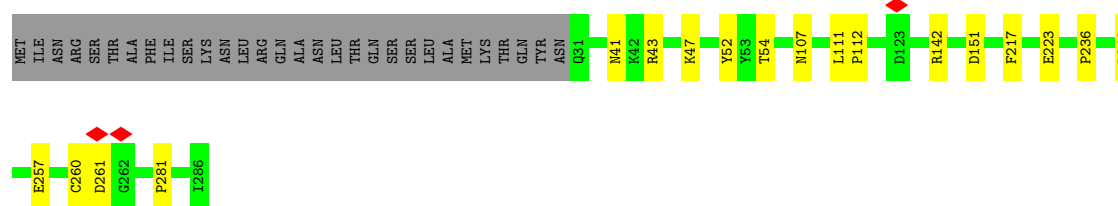
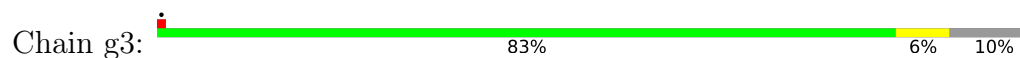




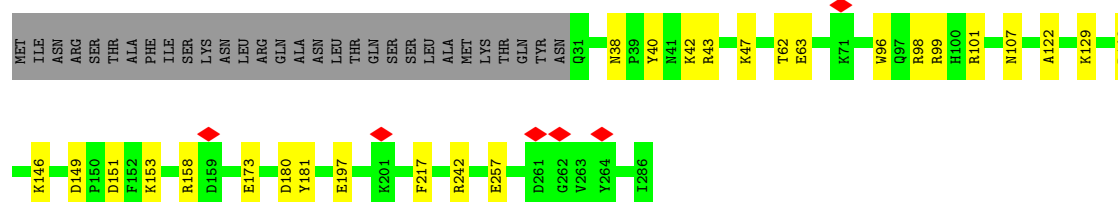
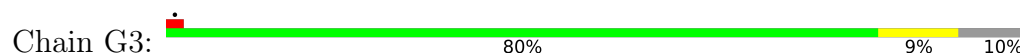
• Molecule 8: ATPTT3



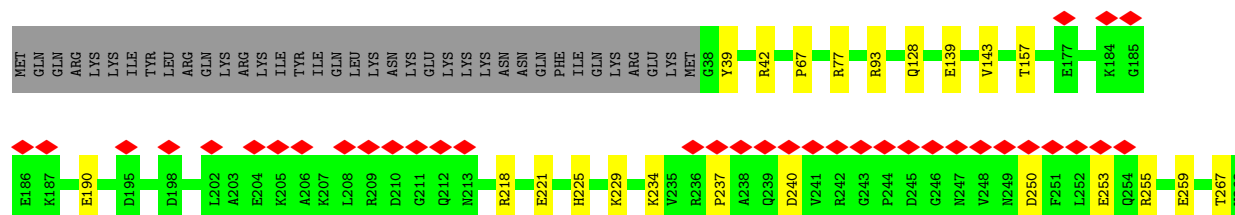
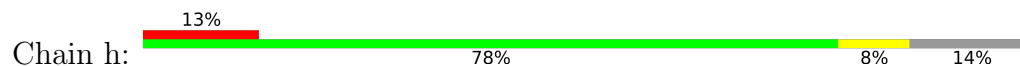
• Molecule 8: ATPTT3



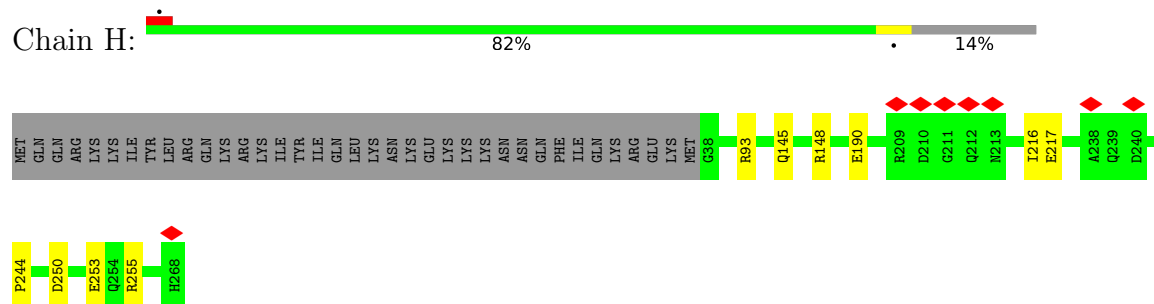
• Molecule 8: ATPTT3



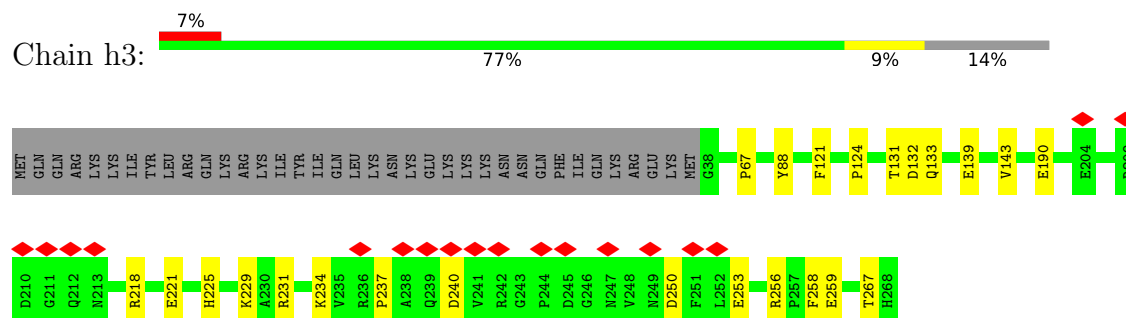
• Molecule 9: ATPTT4



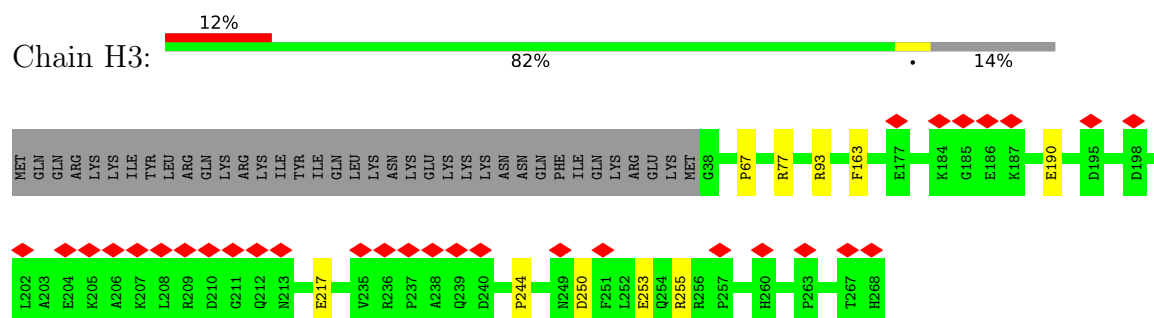
- Molecule 9: ATPTT4



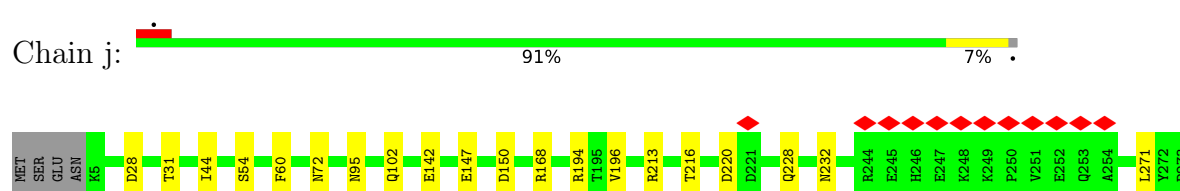
- Molecule 9: ATPTT4



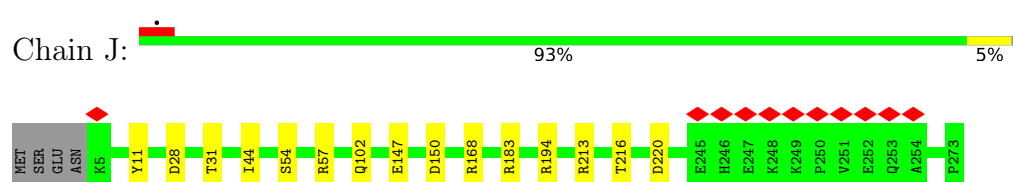
- Molecule 9: ATPTT4



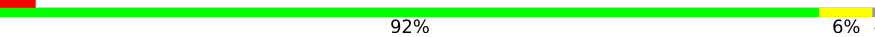
- Molecule 10: ATPTT5

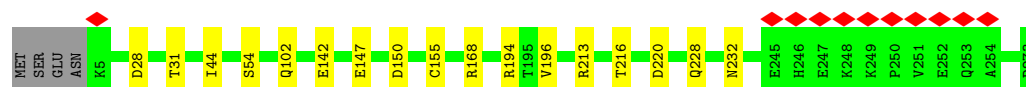


- Molecule 10: ATPTT5

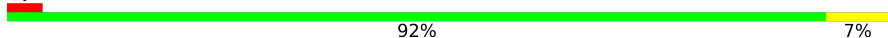


- Molecule 10: ATPTT5

Chain j3:  92% 6%



• Molecule 10: ATPPT5

Chain J3:  92% 7%



• Molecule 11: ATPPT6

Chain l:  89% 11%



• Molecule 11: ATPPT6

Chain L:  89% 10%



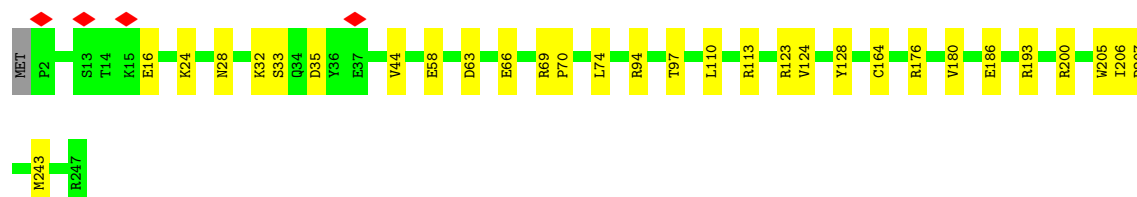
• Molecule 11: ATPPT6

Chain l3:  89% 10%

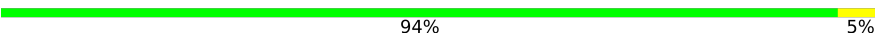


• Molecule 11: ATPPT6

Chain L3:  87% 12%



• Molecule 12: ATPPT7

Chain m:  94% 5%



• Molecule 12: ATPTT7



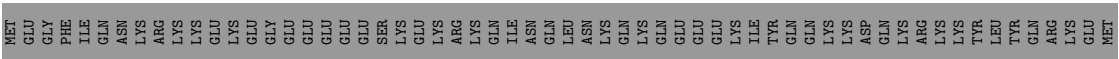
• Molecule 12: ATPTT7



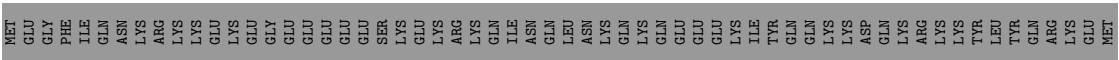
• Molecule 12: ATPTT7



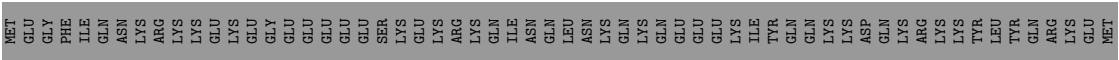
• Molecule 13: ATPTT8

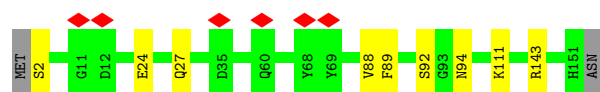


• Molecule 13: ATPTT8

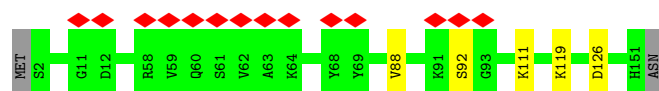


• Molecule 13: ATPTT8

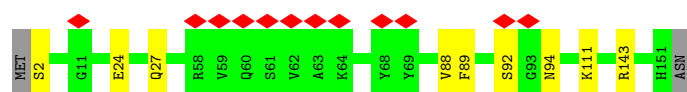




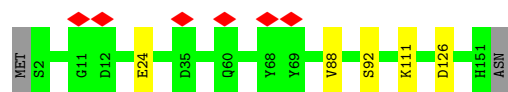
• Molecule 15: ATPTT10



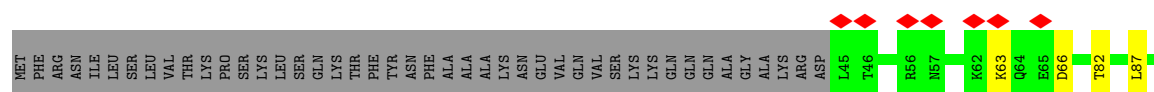
• Molecule 15: ATPTT10



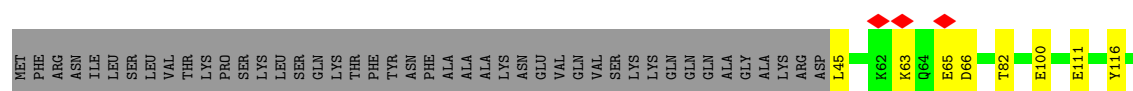
• Molecule 15: ATPTT10



• Molecule 16: ATPTT11

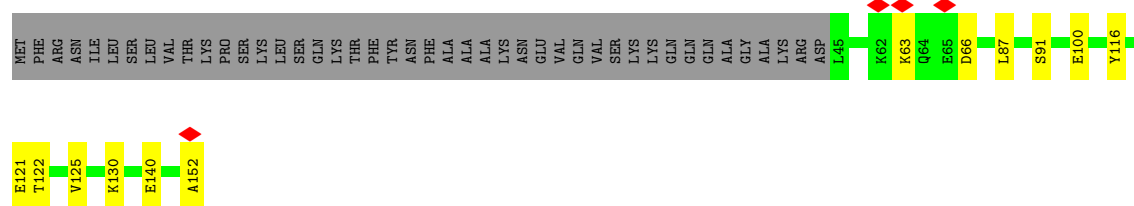


• Molecule 16: ATPTT11



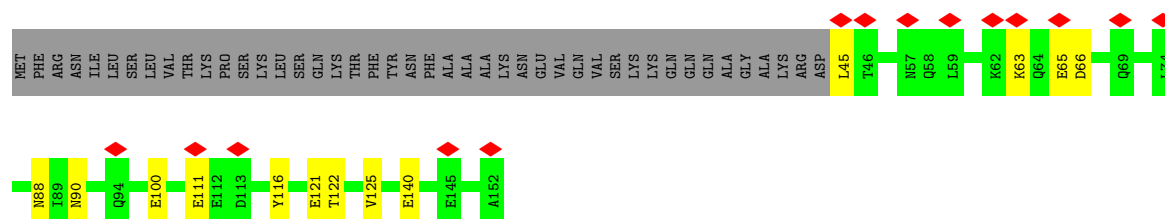
• Molecule 16: ATPTT11

Chain q3: 



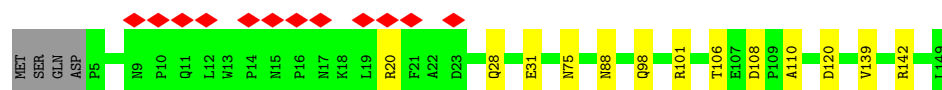
• Molecule 16: ATPPTT11

Chain Q3: 



• Molecule 17: ATPPTT12

Chain r: 



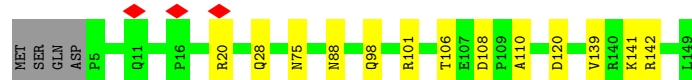
• Molecule 17: ATPPTT12

Chain R: 



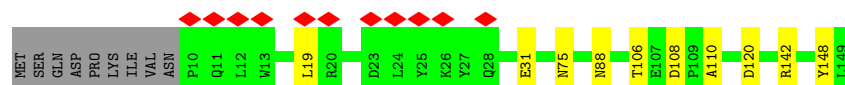
• Molecule 17: ATPPTT12

Chain r3: 

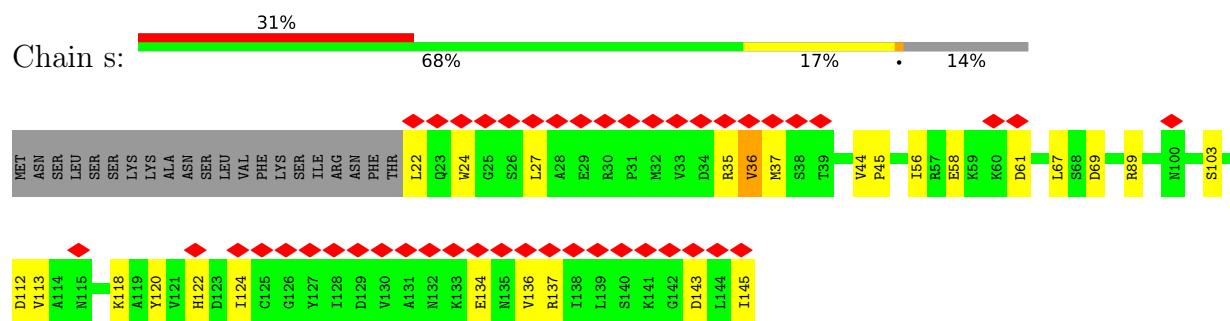


• Molecule 17: ATPPTT12

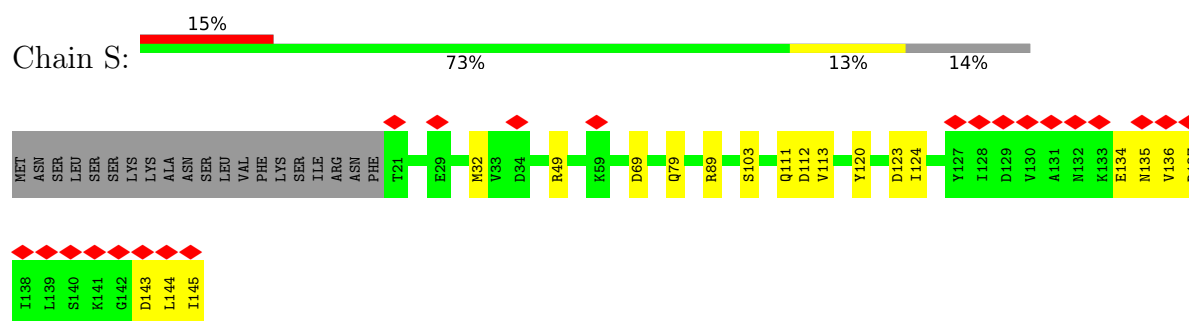
Chain R3: 



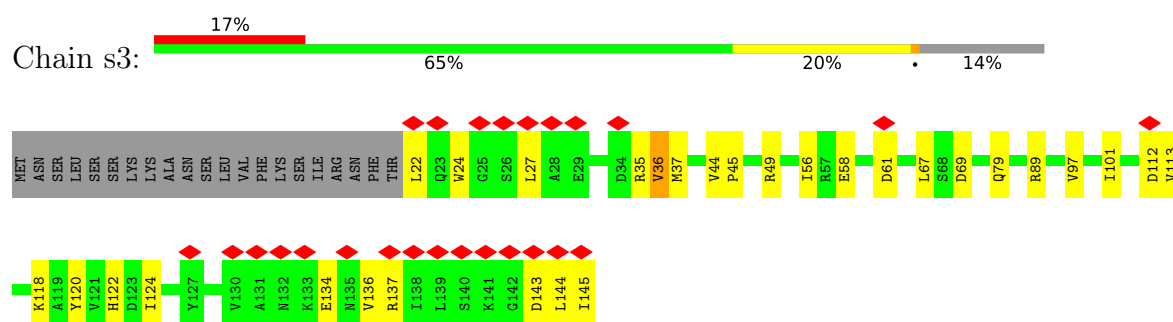
● Molecule 18: ATPTT13



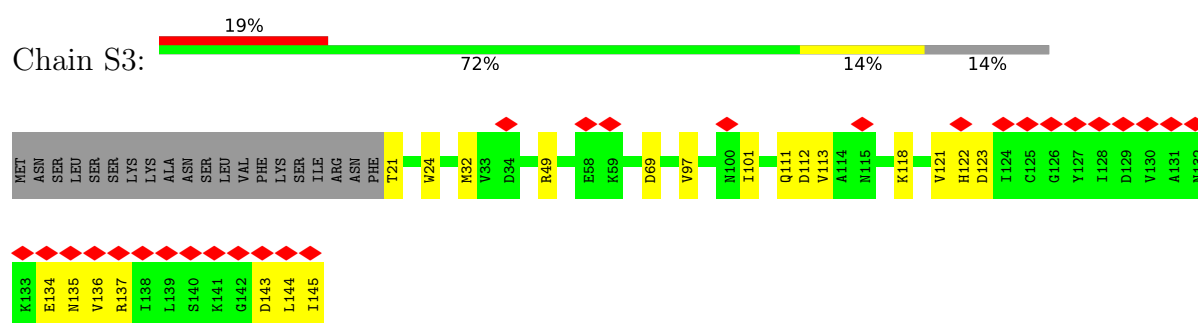
● Molecule 18: ATPTT13



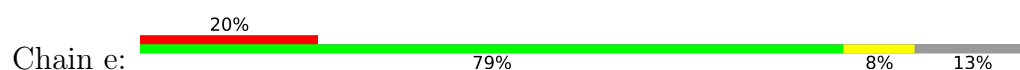
● Molecule 18: ATPTT13

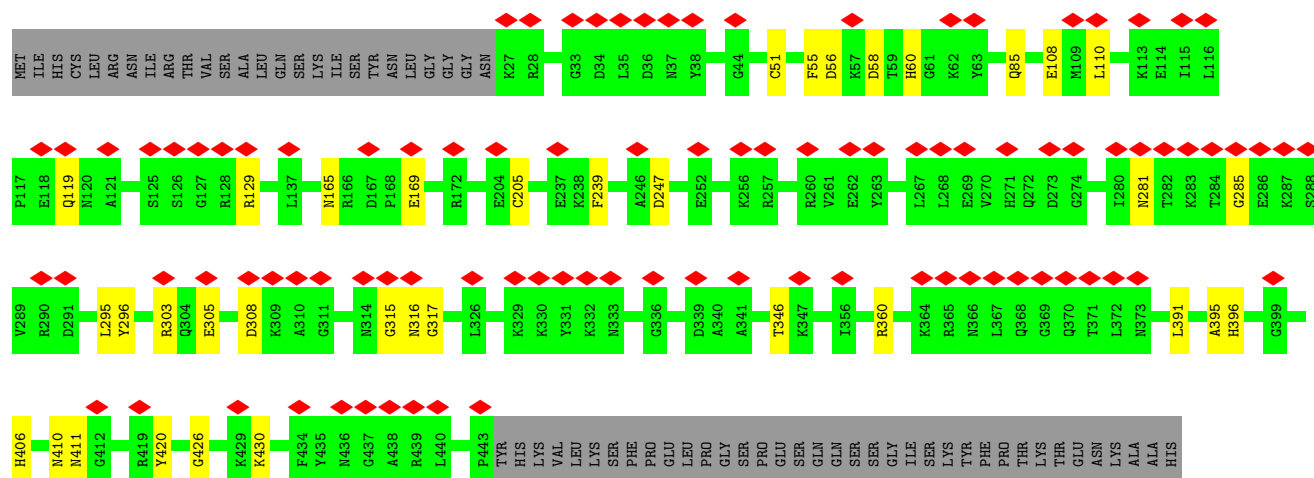


● Molecule 18: ATPTT13

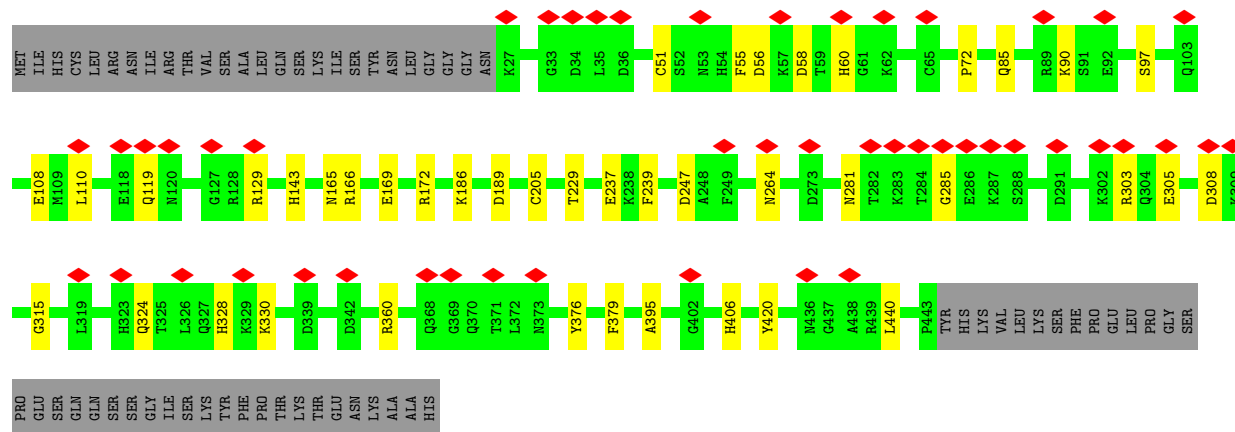
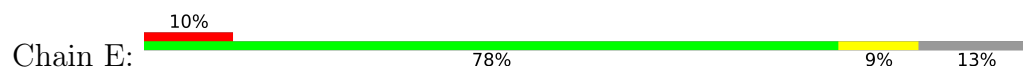


● Molecule 19: ATPTT1

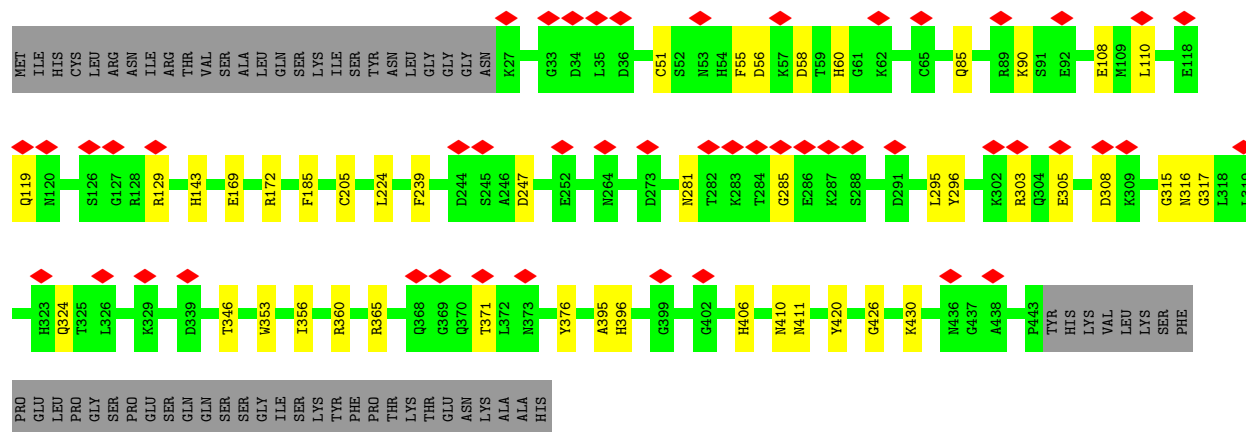
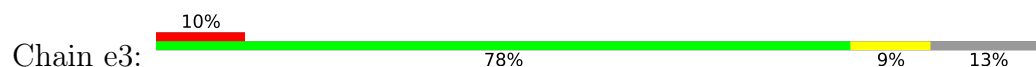




• Molecule 19: ATPPTT1

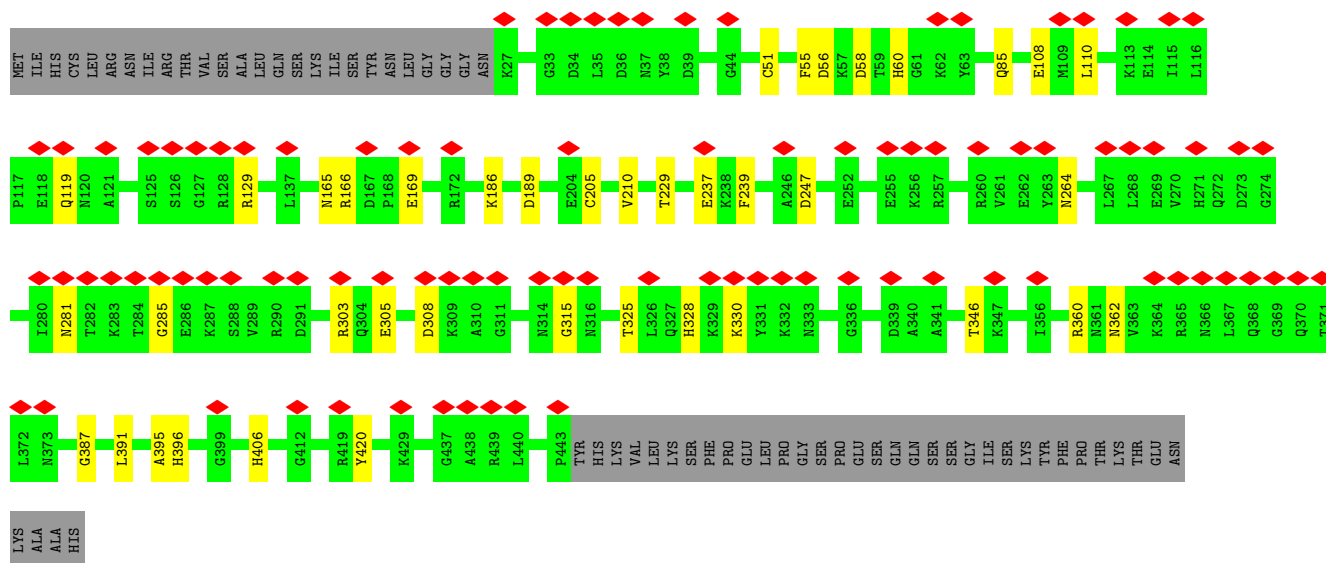


• Molecule 19: ATPPTT1



• Molecule 19: ATPPTT1

Chain E3: 

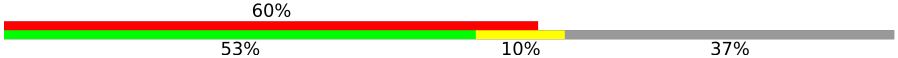


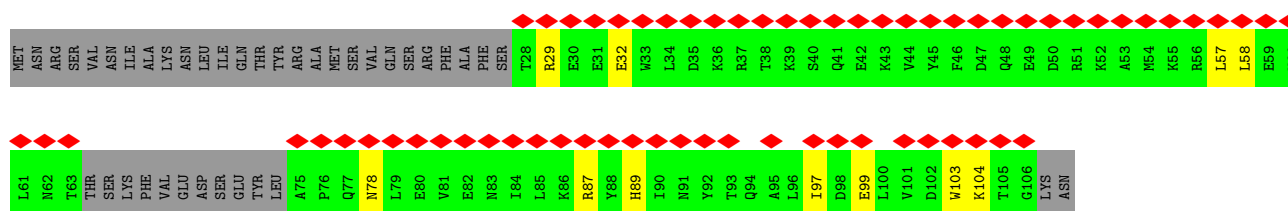
- Molecule 20: Inhibitor of F1 (IF1)

Chain i2: 



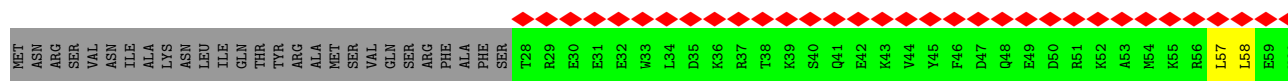
- Molecule 20: Inhibitor of F1 (IF1)

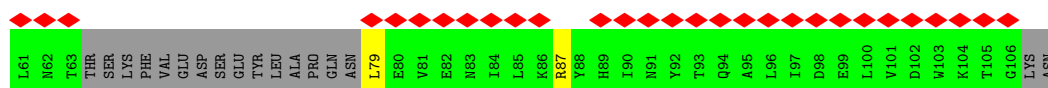
Chain i1: 



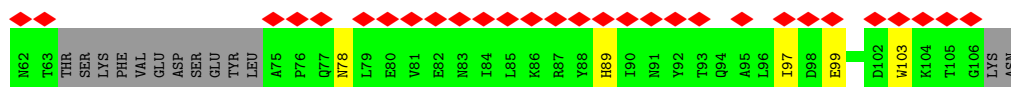
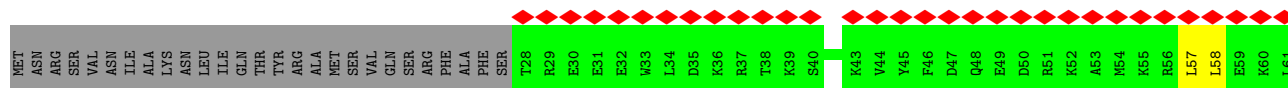
- Molecule 20: Inhibitor of F1 (IF1)

Chain i5: 

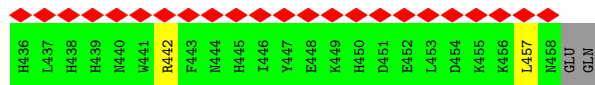
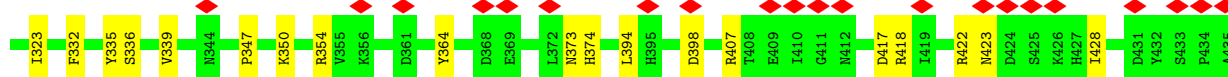
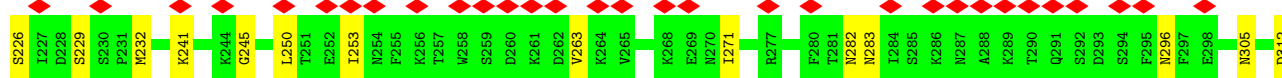
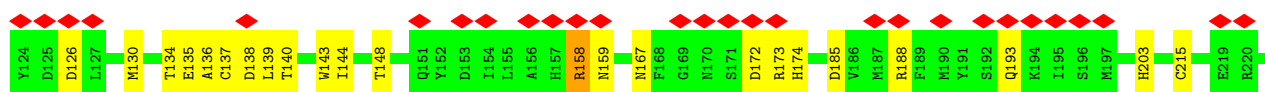
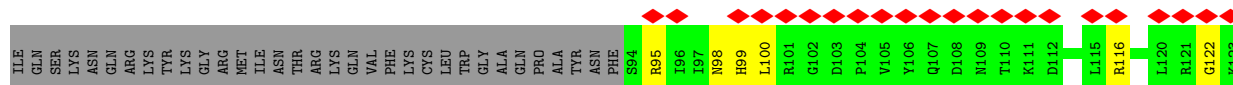
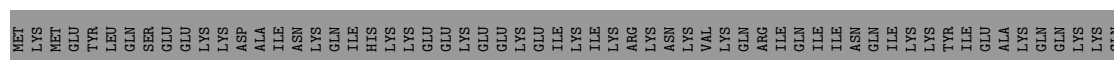




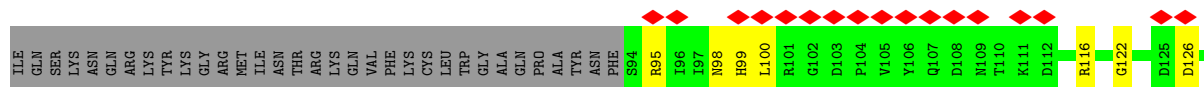
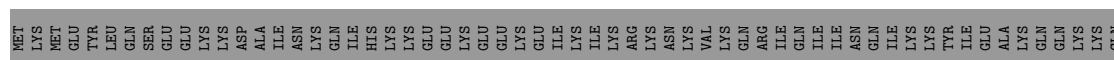
• Molecule 20: Inhibitor of F1 (IF1)

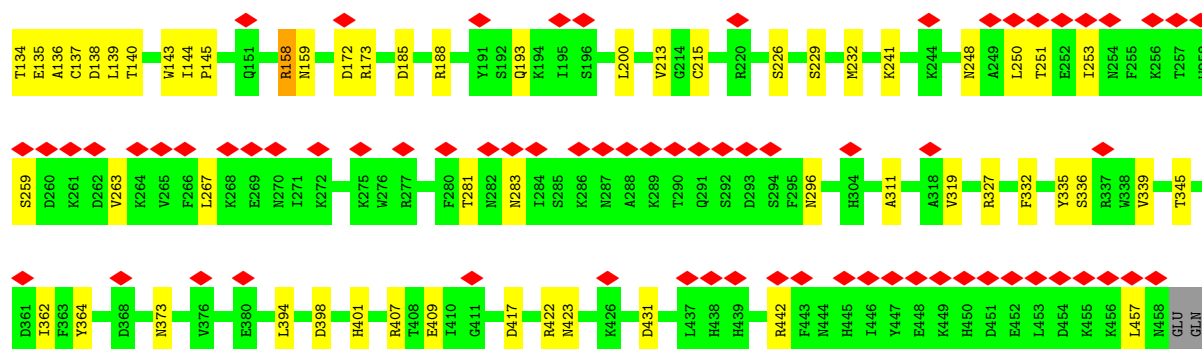


• Molecule 21: ATPPTT2

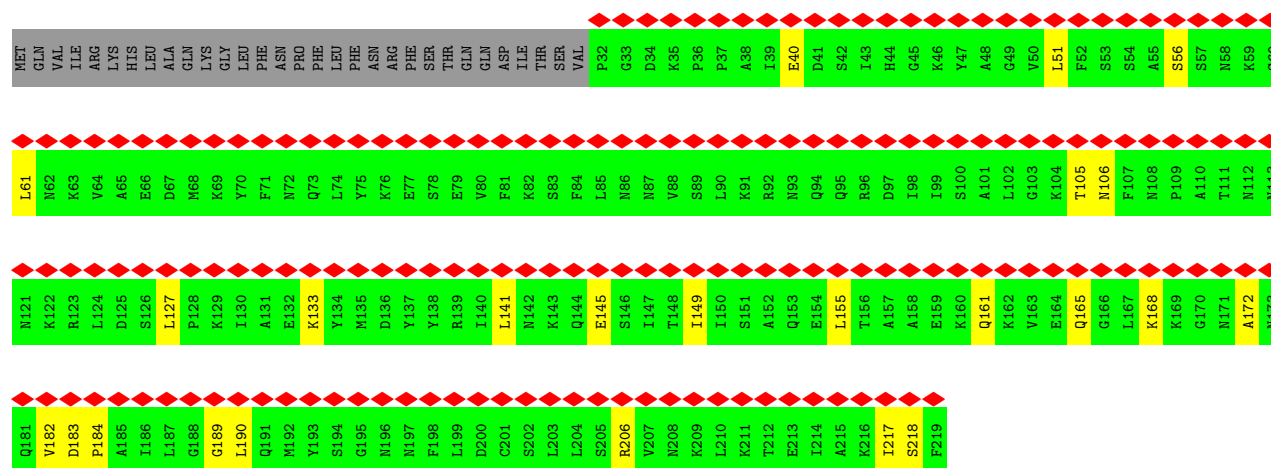
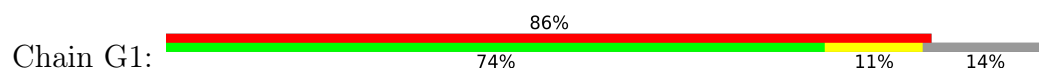


• Molecule 21: ATPPTT2

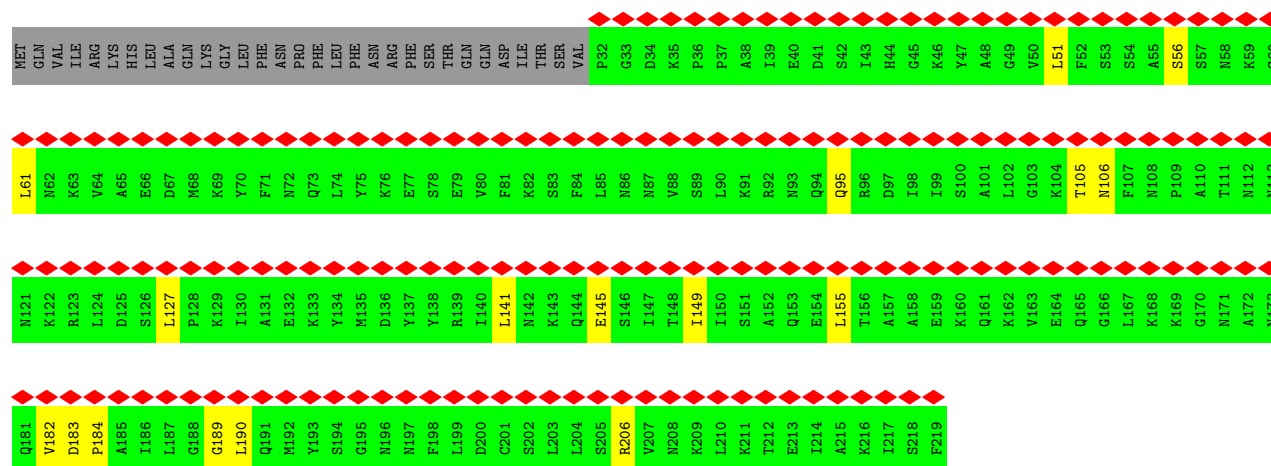
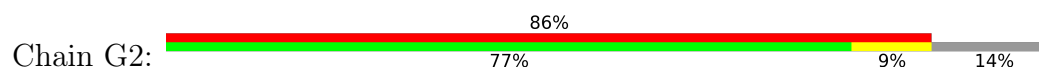




• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

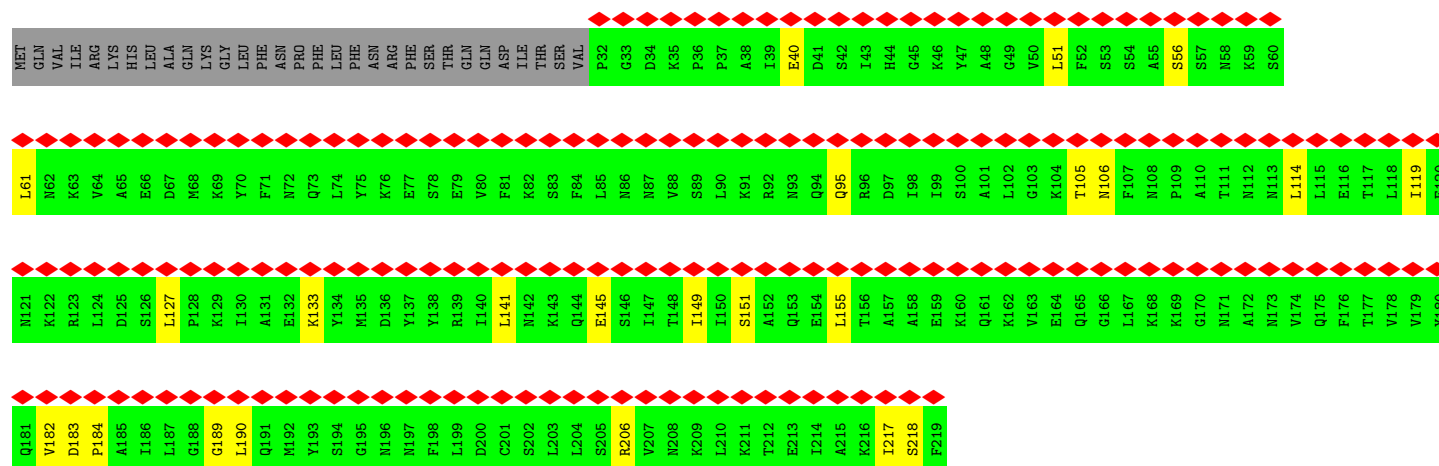


• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)



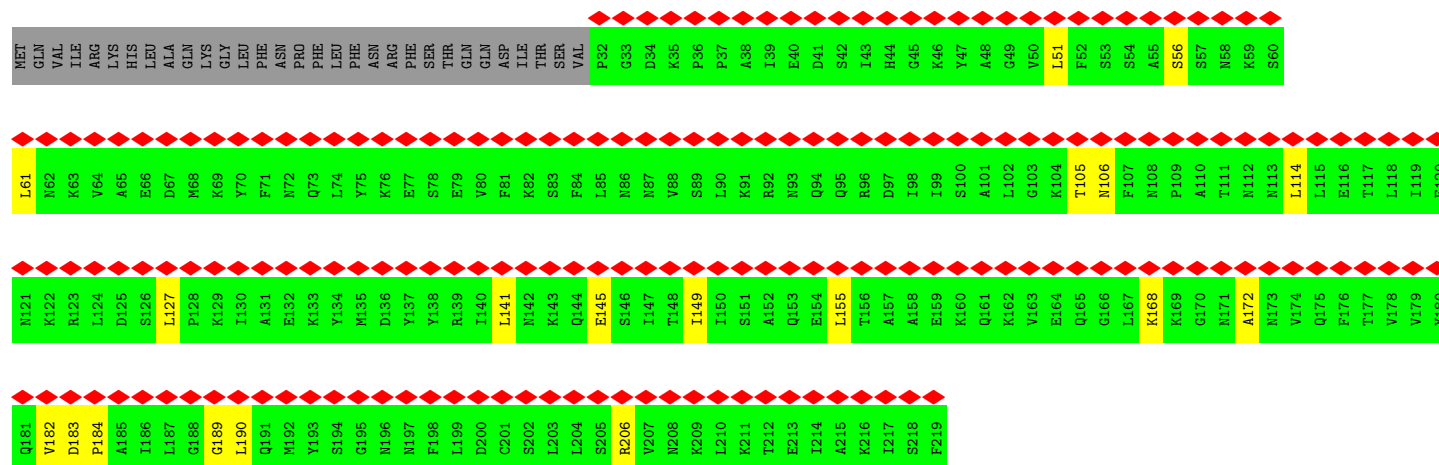
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

Chain G4: 



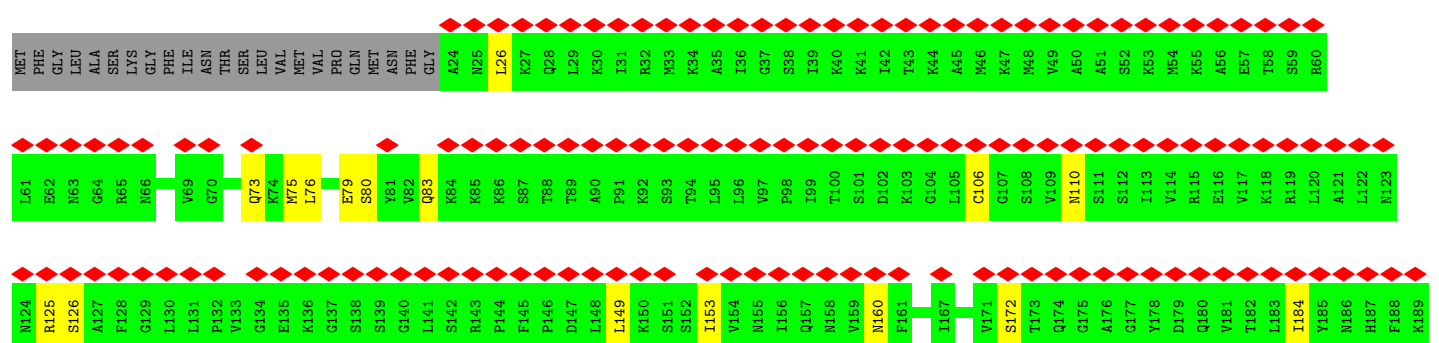
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

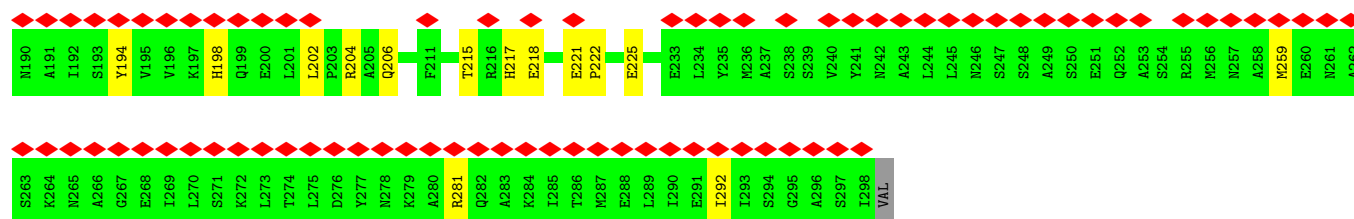
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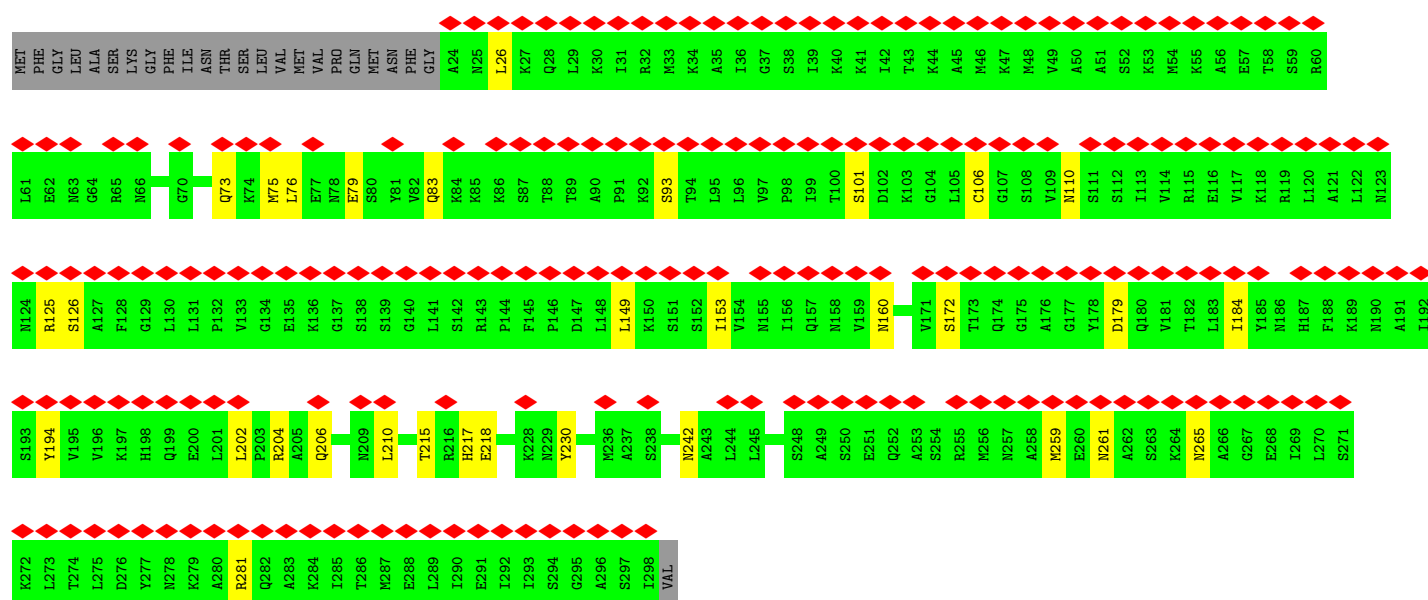
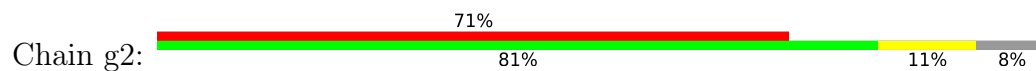
• Molecule 23: ATP synthase subunit gamma

Chain g1: 

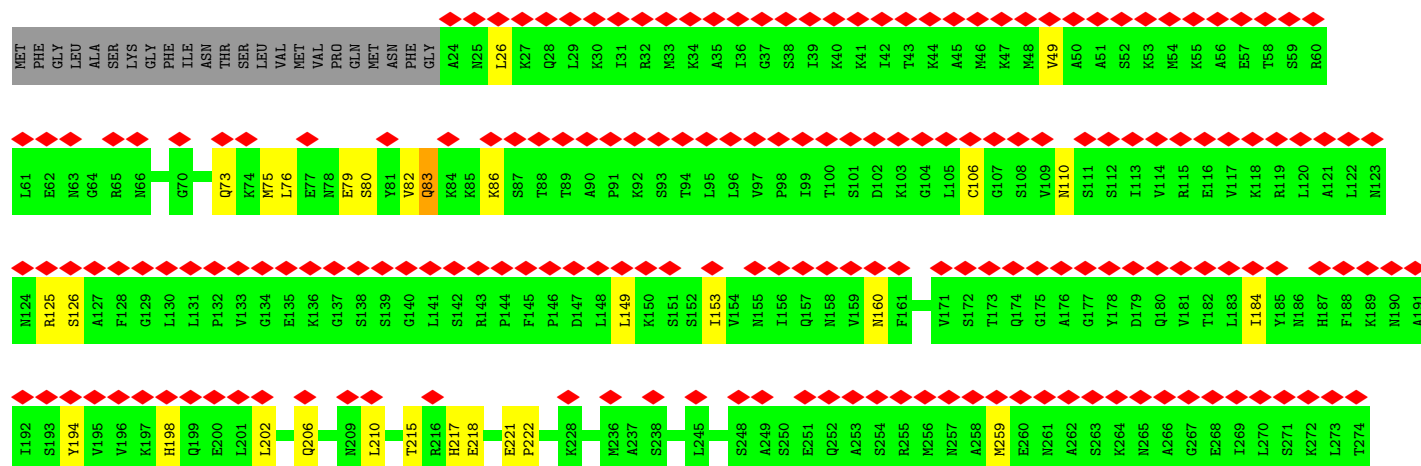
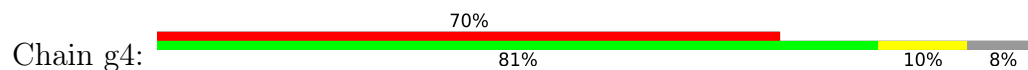


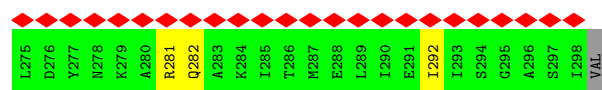


• Molecule 23: ATP synthase subunit gamma

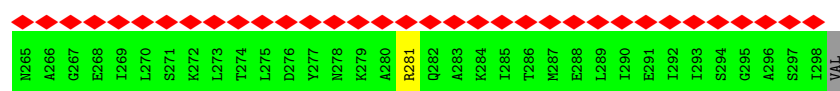
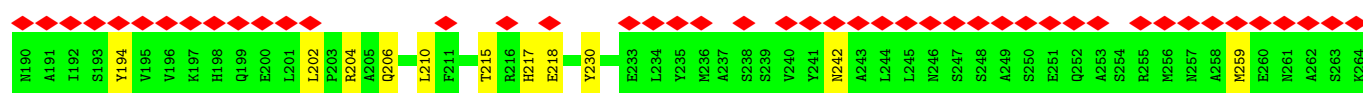
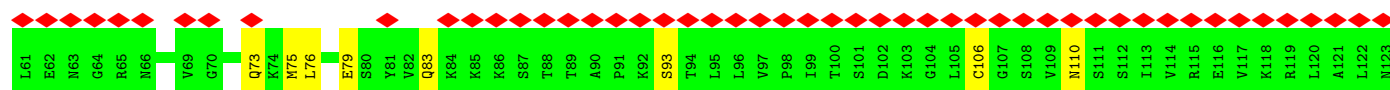
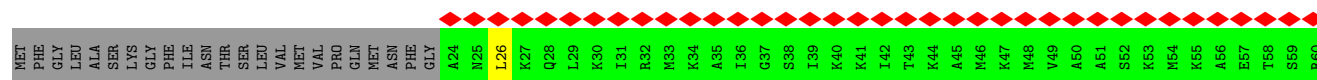
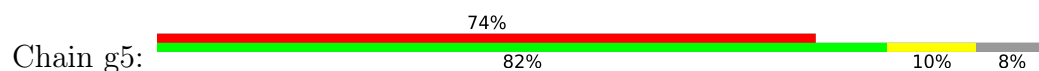


• Molecule 23: ATP synthase subunit gamma

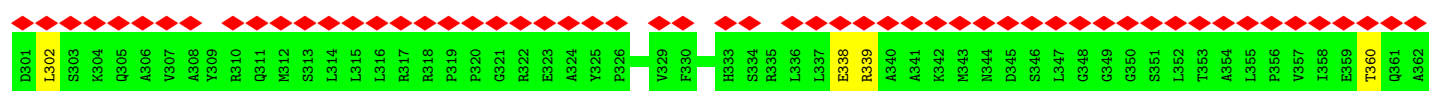
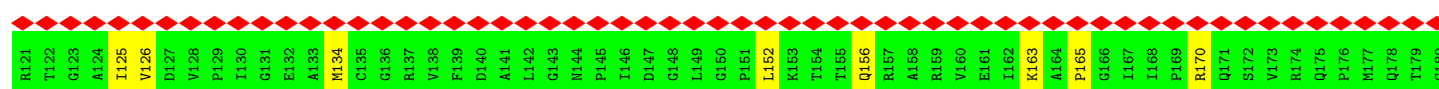
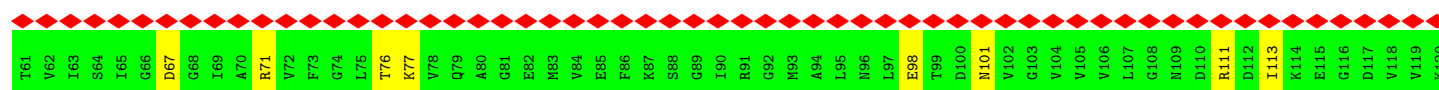
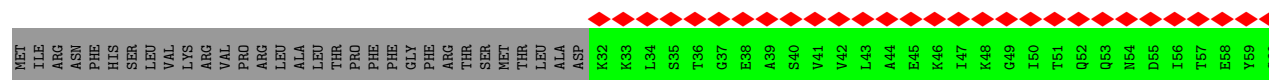
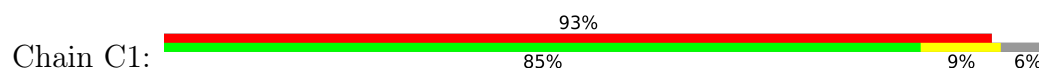


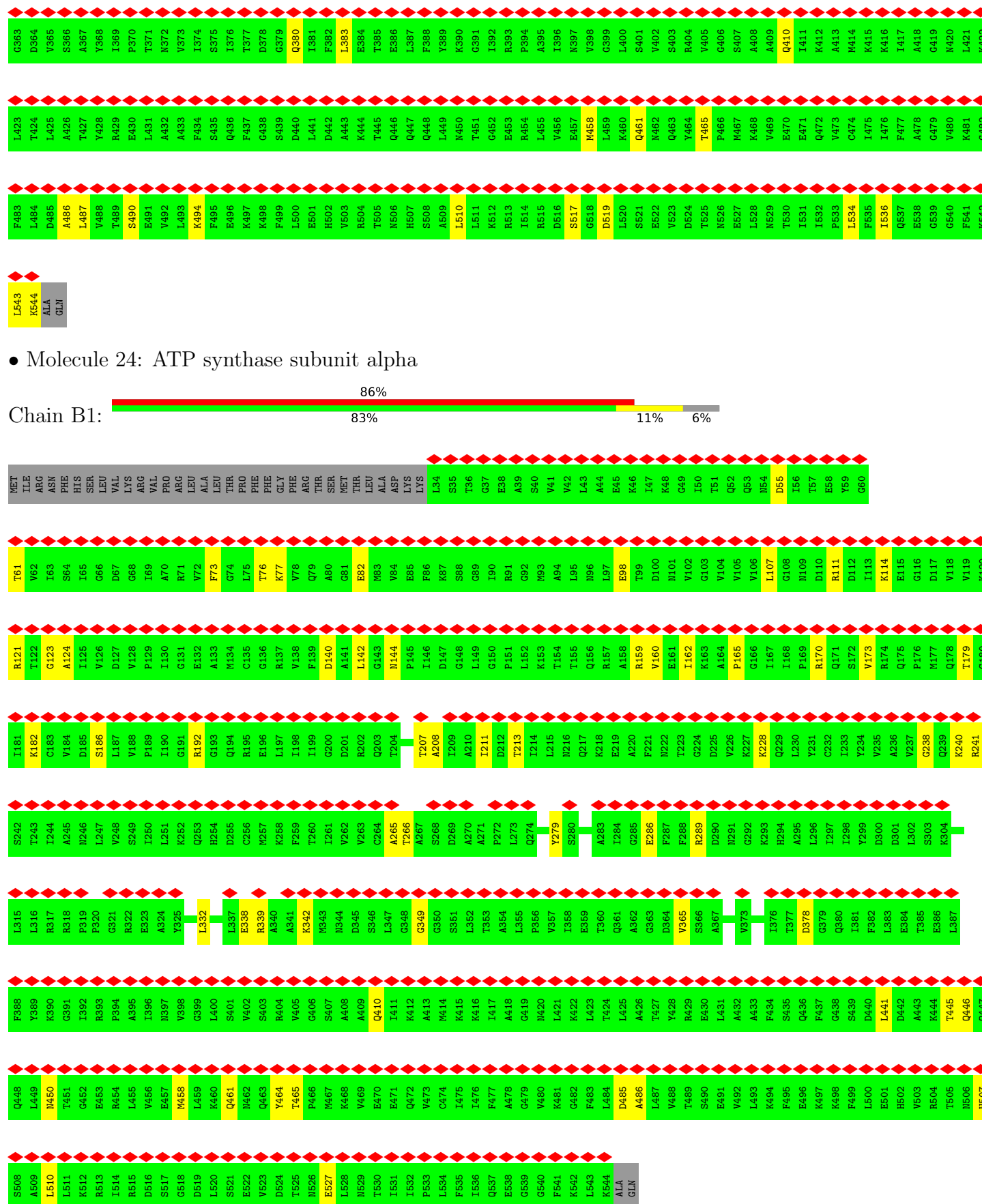


• Molecule 23: ATP synthase subunit gamma



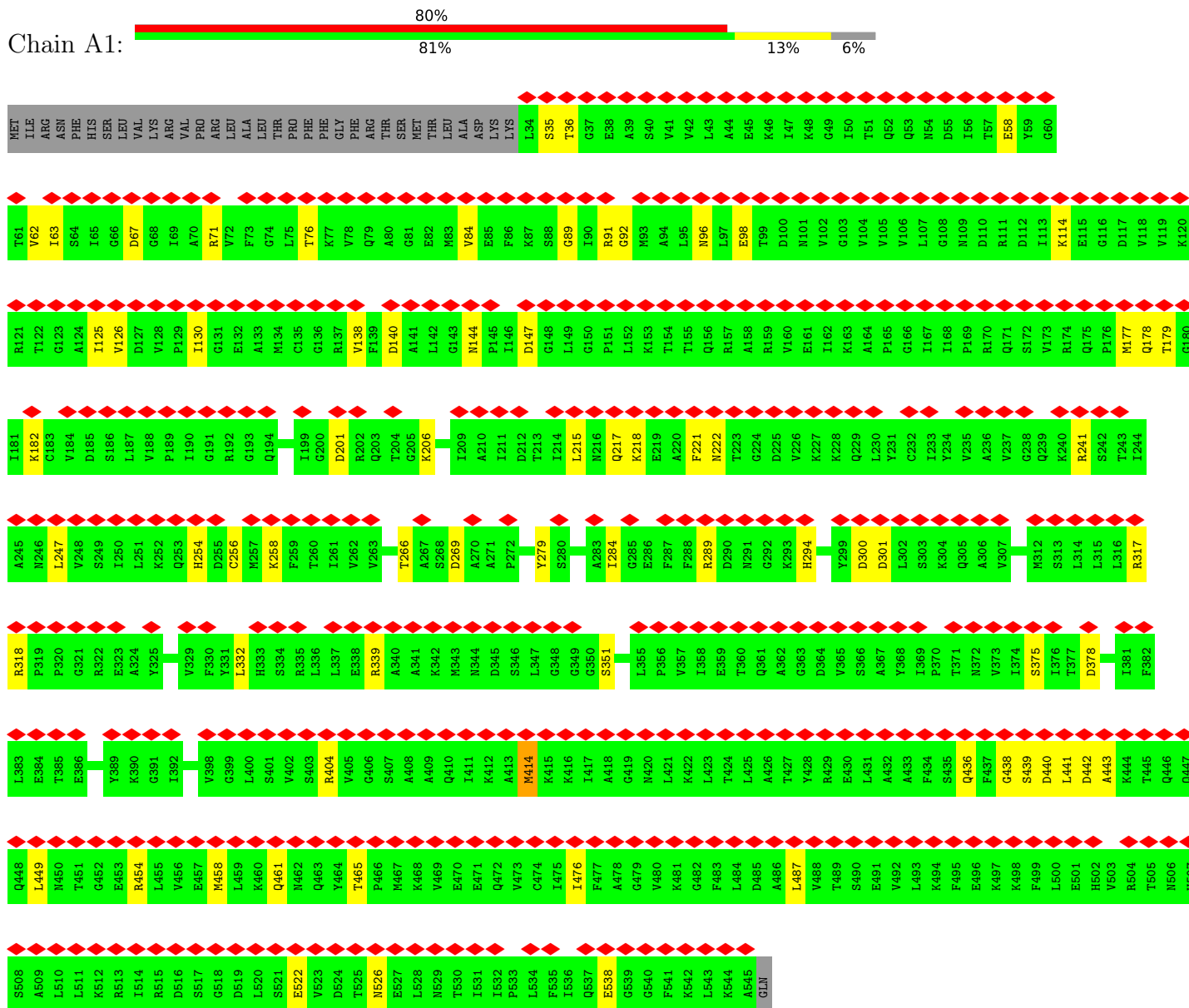
• Molecule 24: ATP synthase subunit alpha





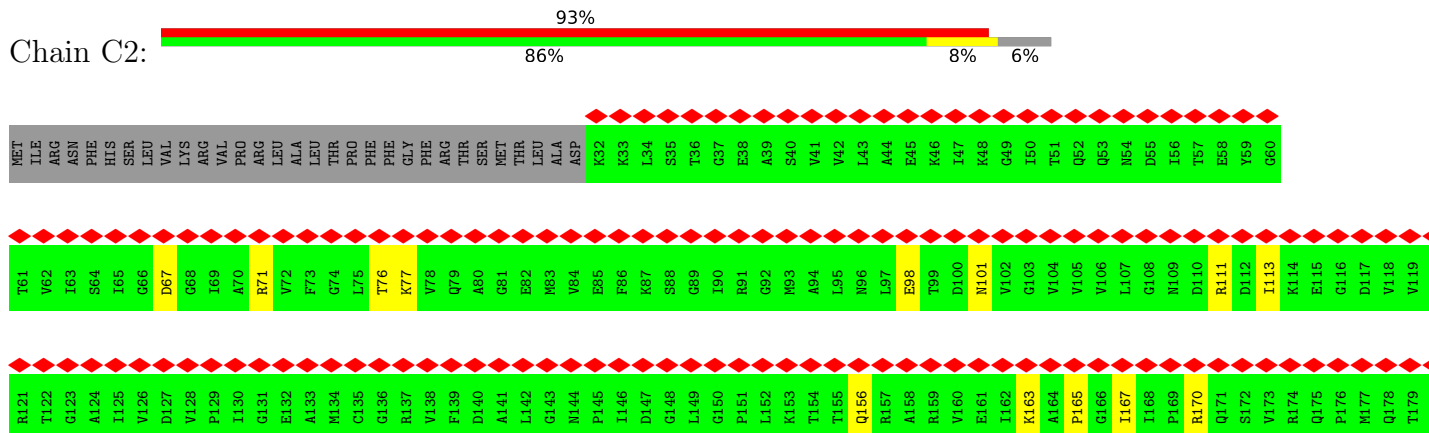
• Molecule 24: ATP synthase subunit alpha

Chain A1:

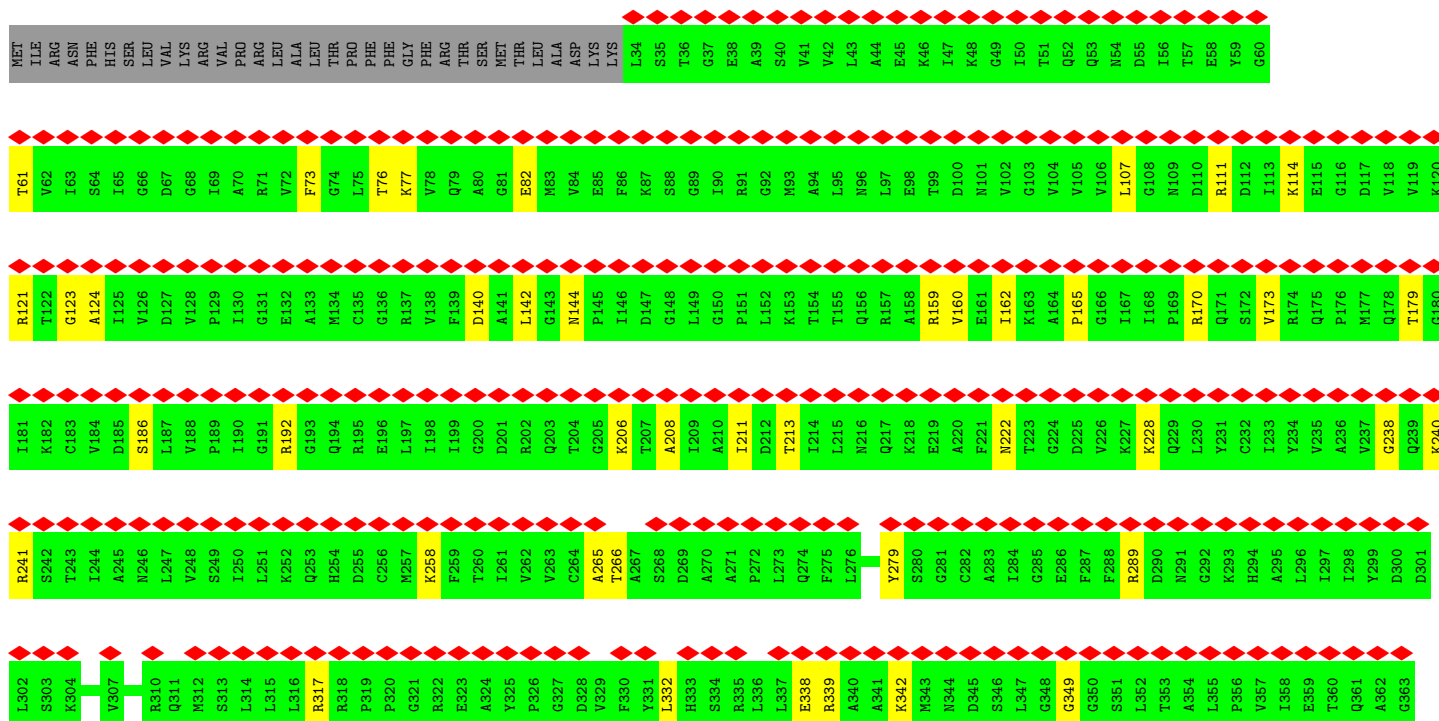
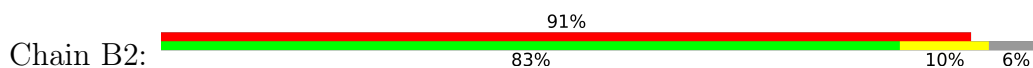


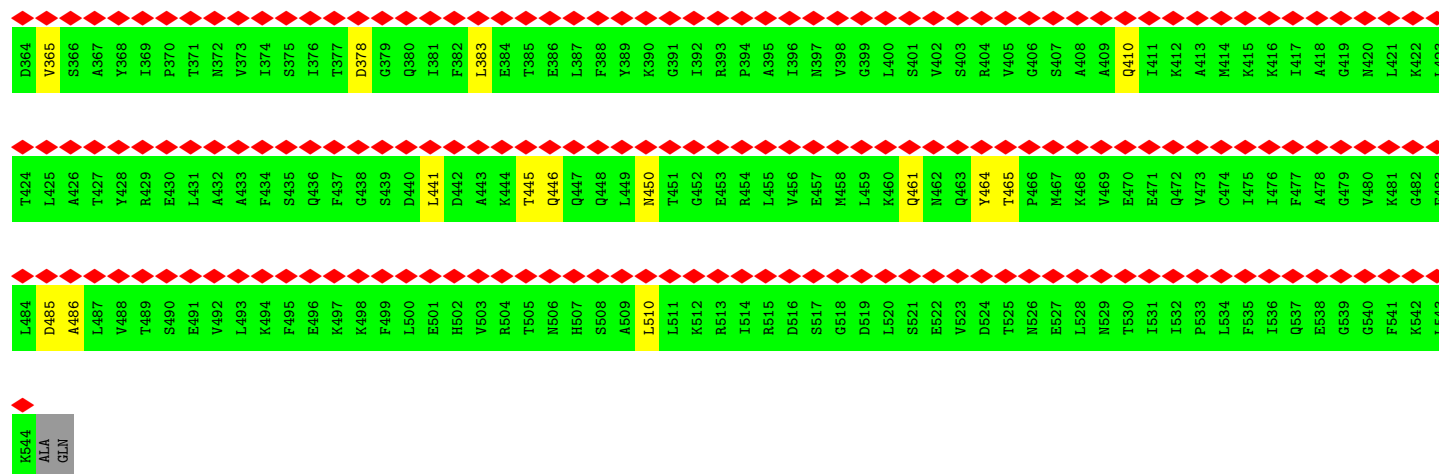
• Molecule 24: ATP synthase subunit alpha

Chain C2:

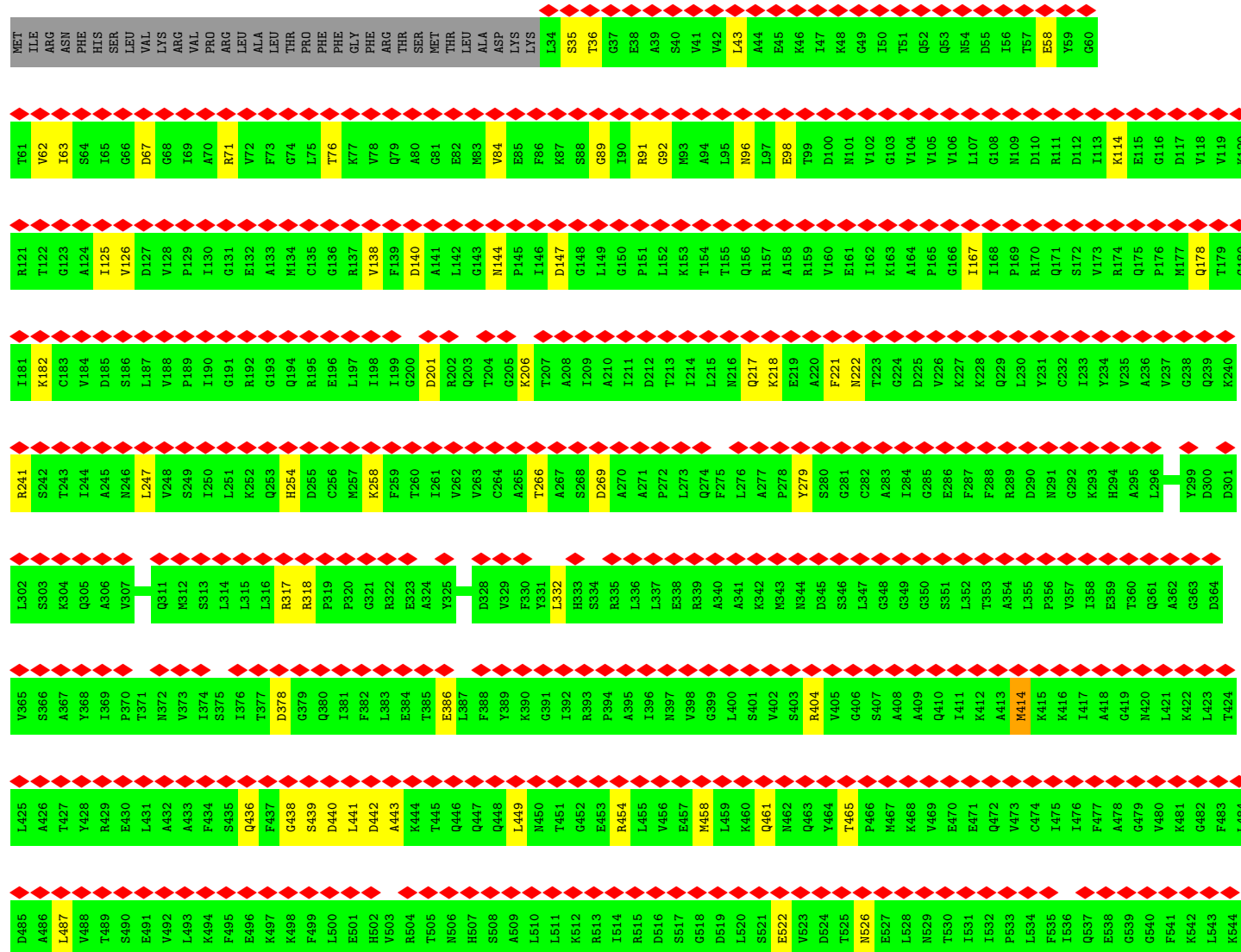
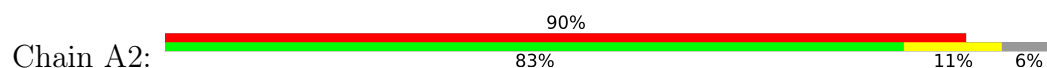


- Molecule 24: ATP synthase subunit alpha



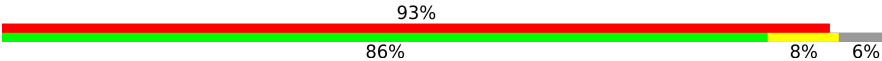


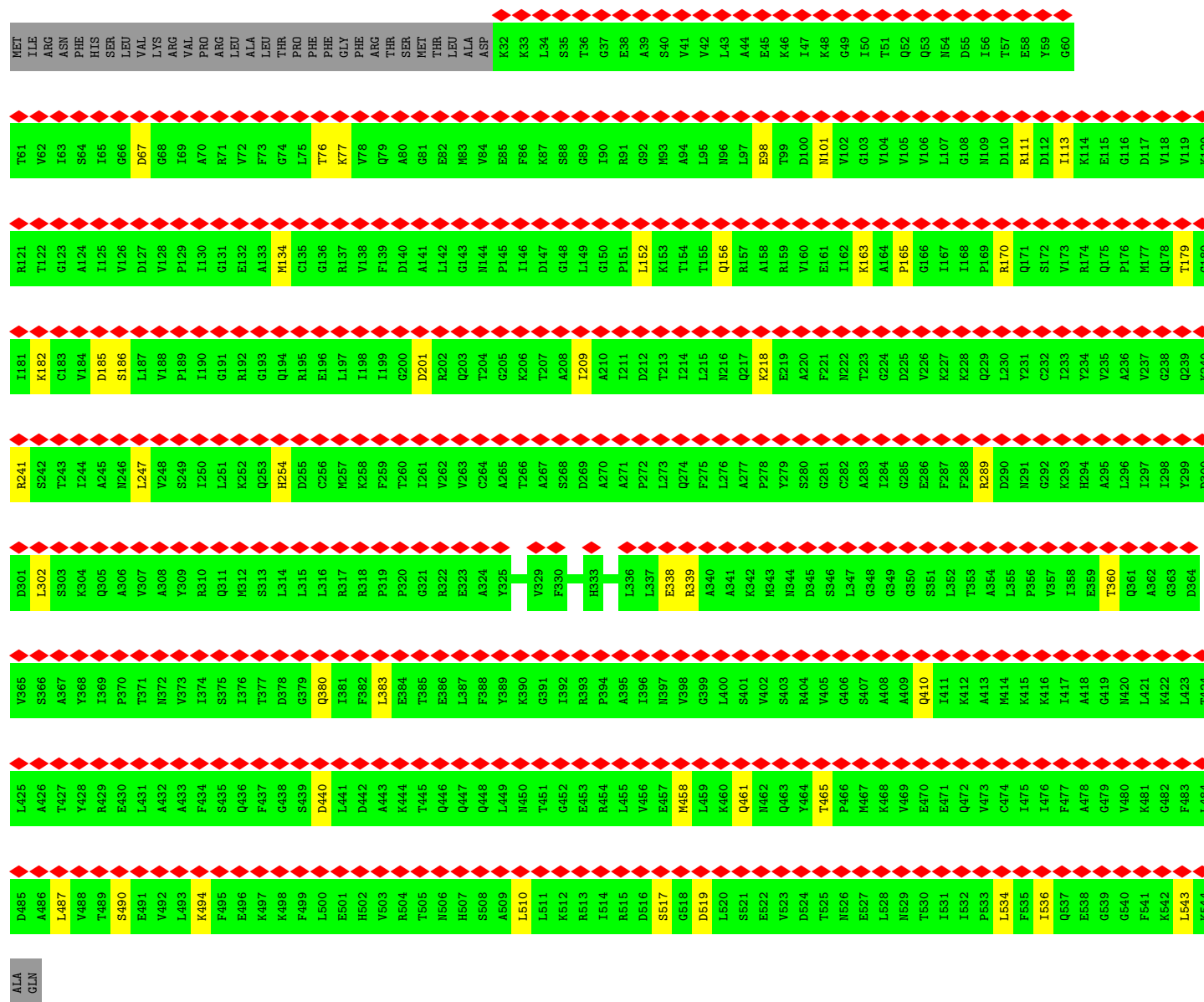
• Molecule 24: ATP synthase subunit alpha



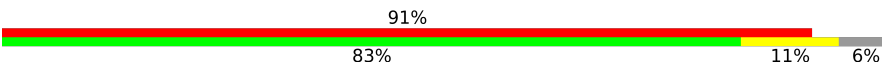


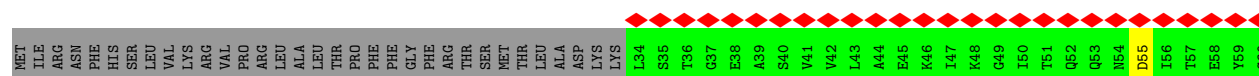
• Molecule 24: ATP synthase subunit alpha

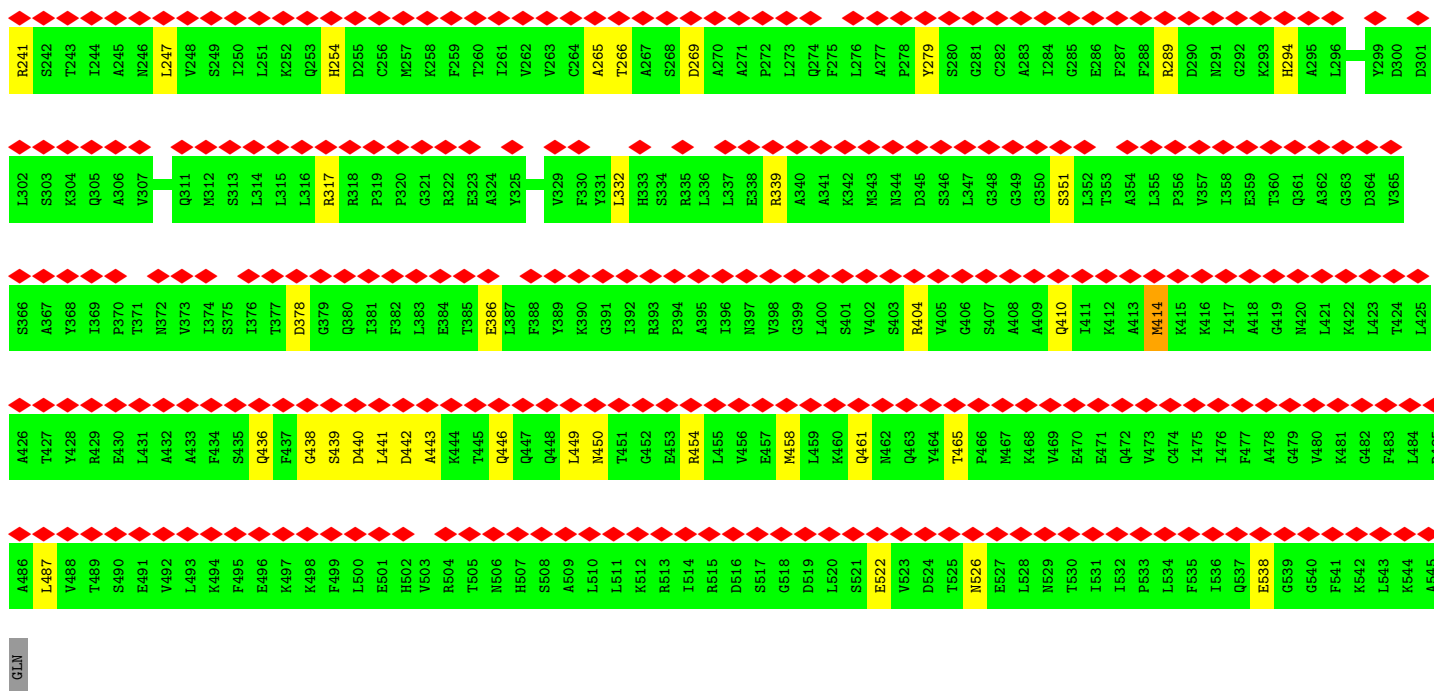
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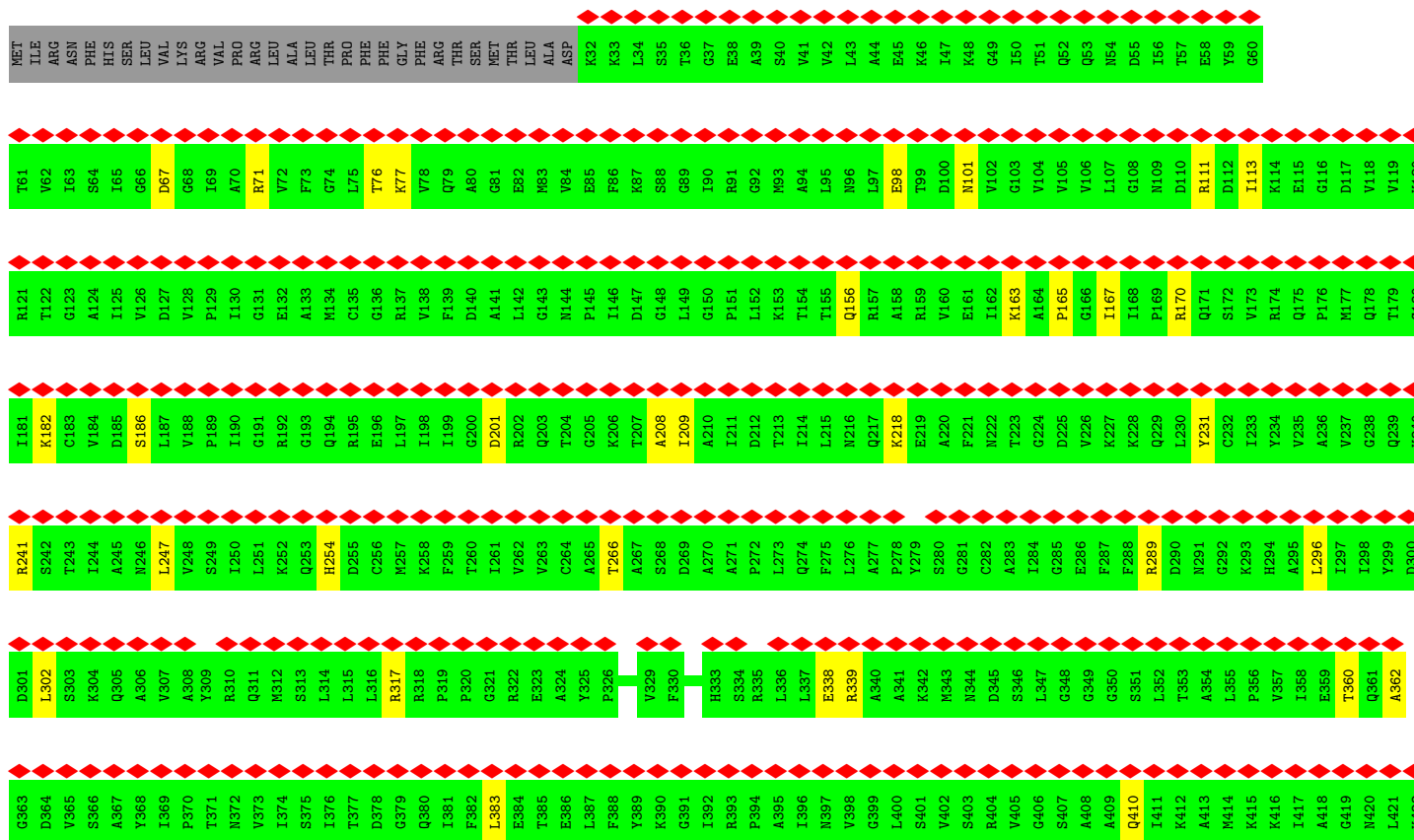
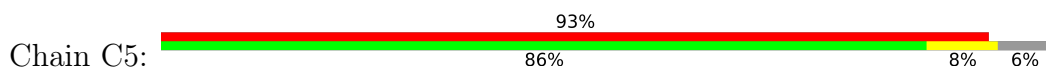
• Molecule 24: ATP synthase subunit alpha

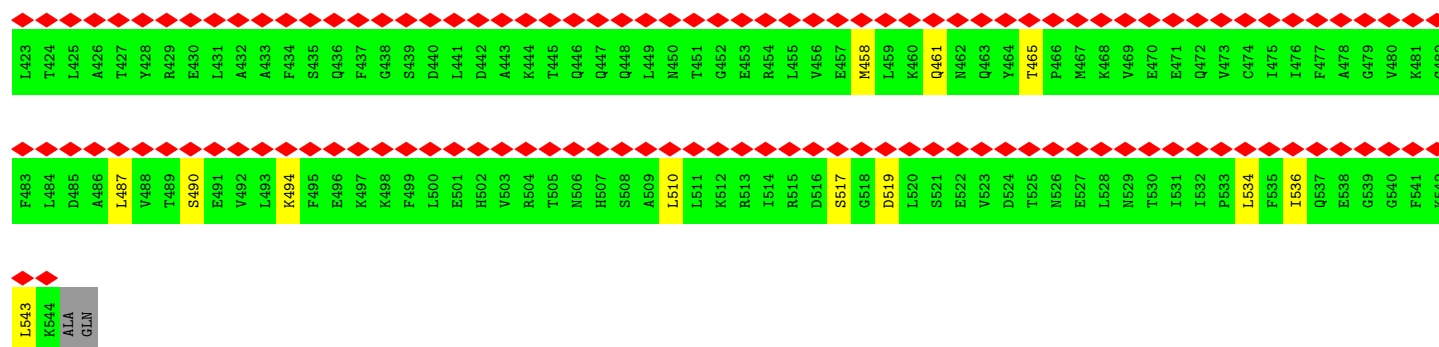
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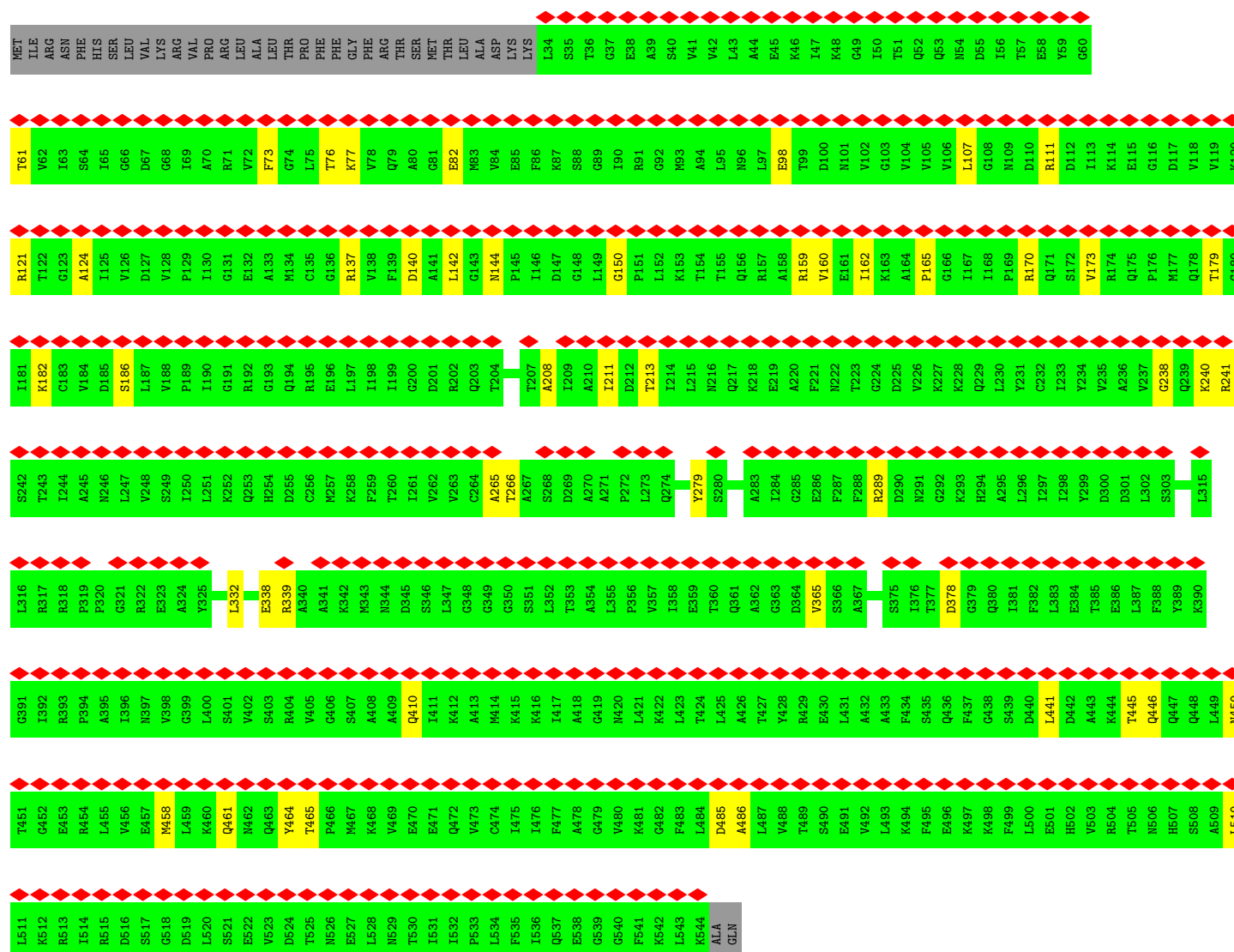
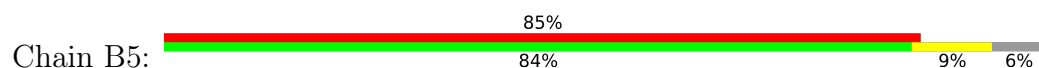


• Molecule 24: ATP synthase subunit alpha

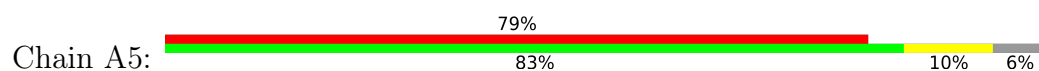


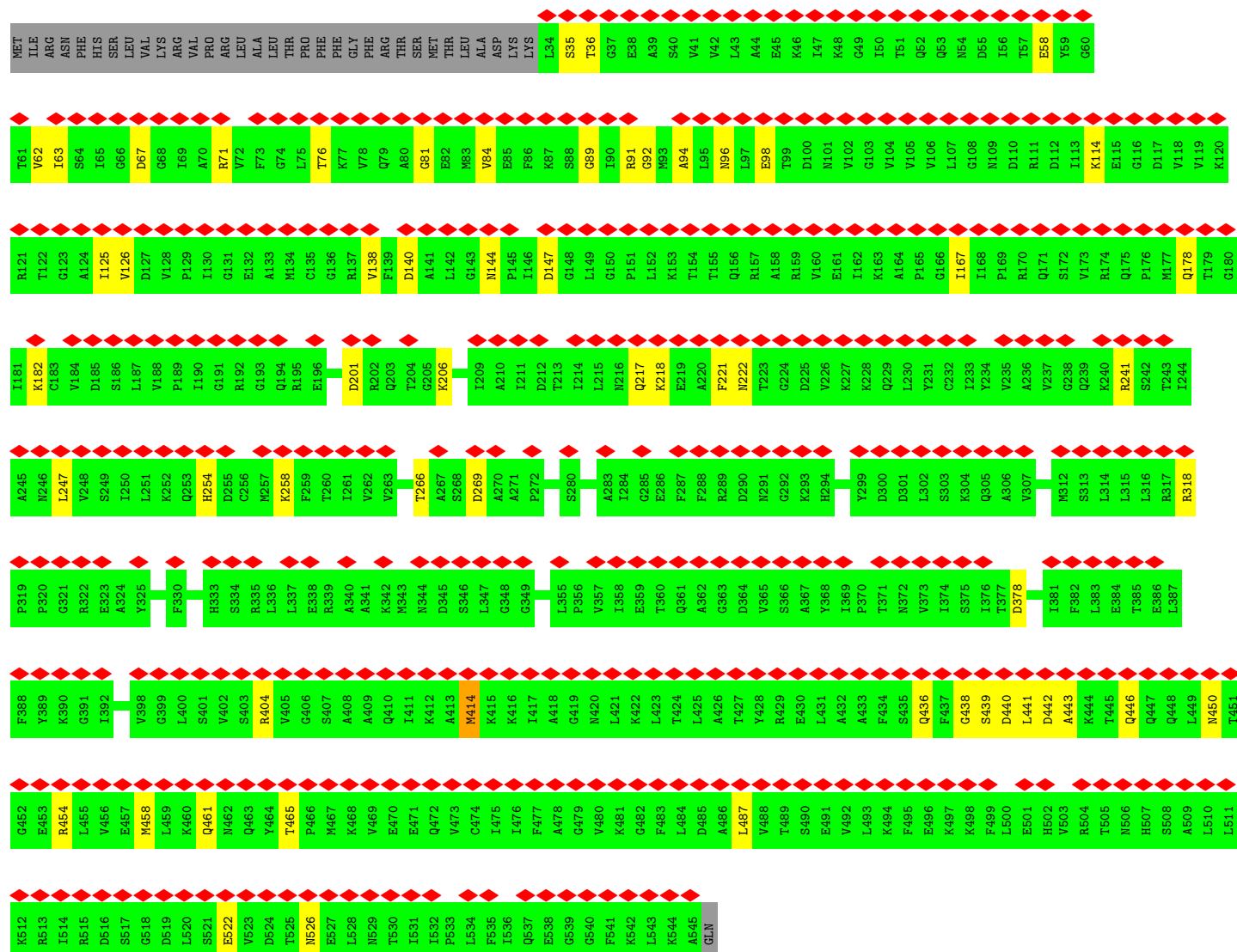


• Molecule 24: ATP synthase subunit alpha

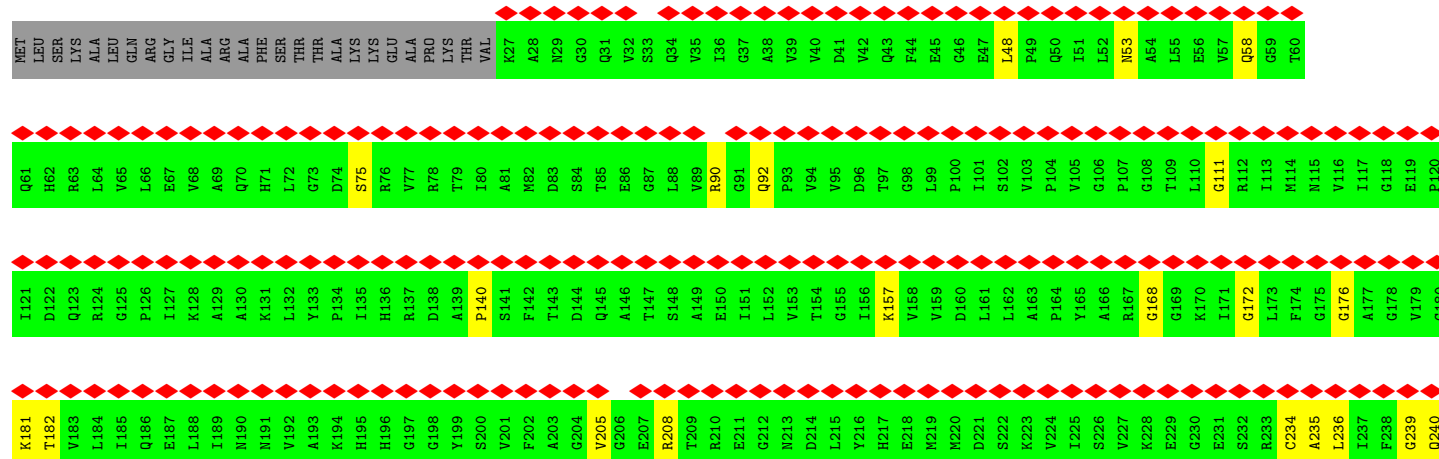
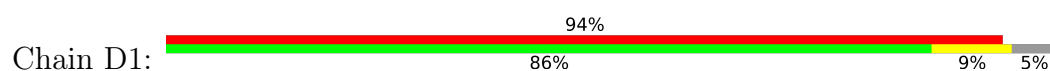


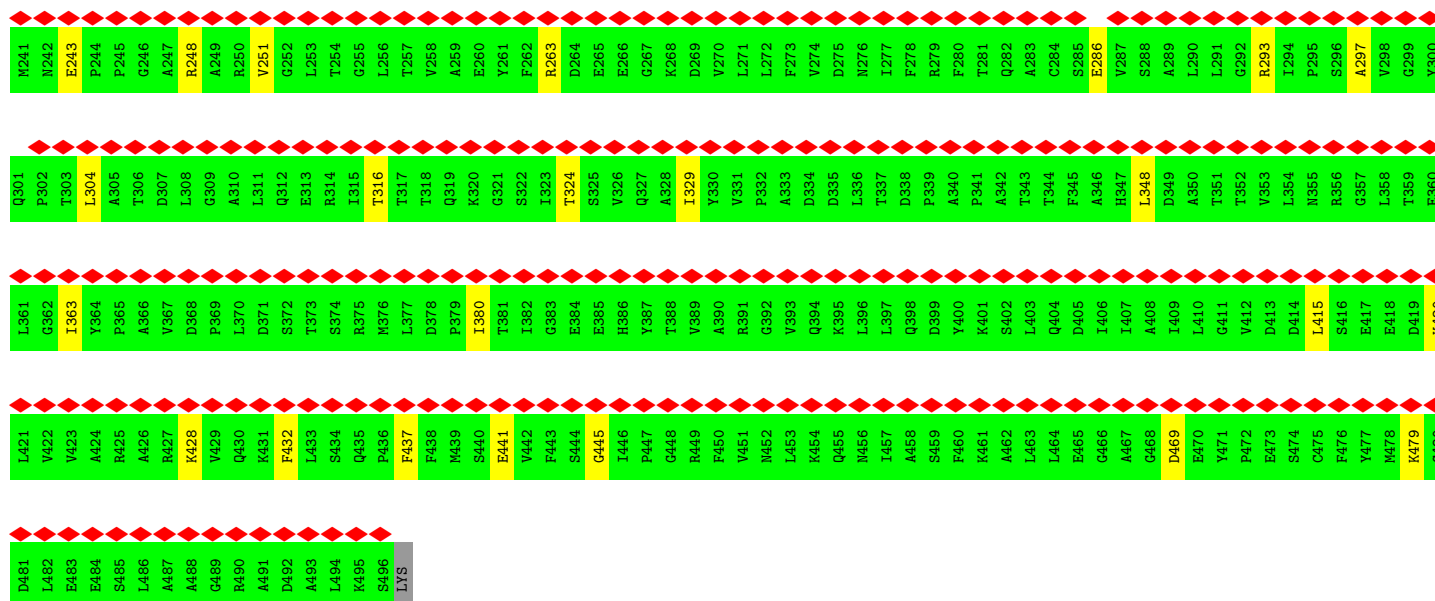
• Molecule 24: ATP synthase subunit alpha



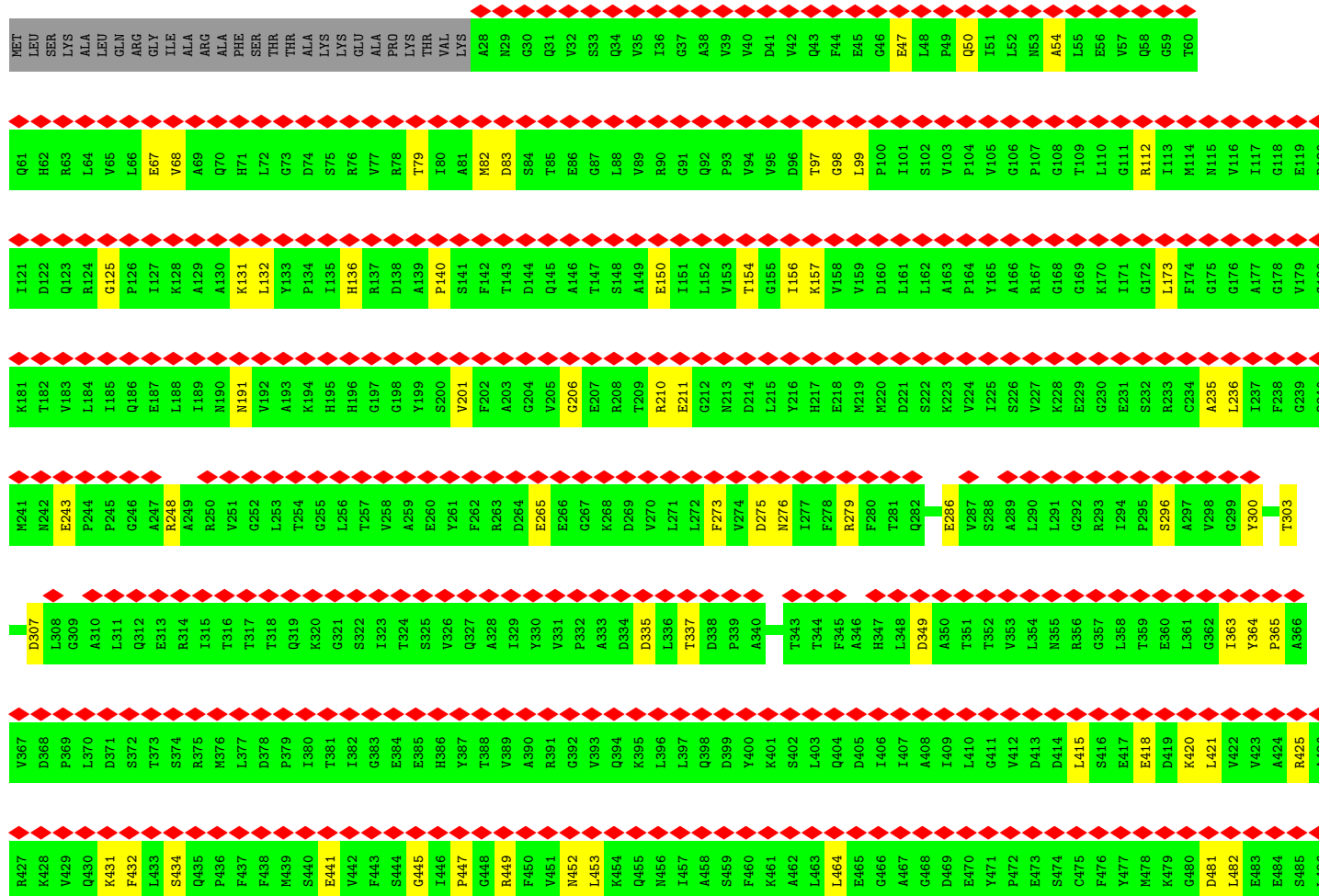
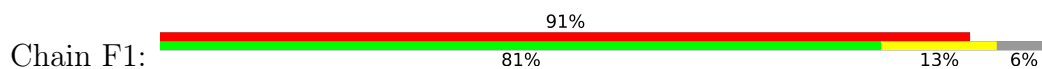


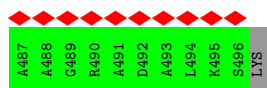
• Molecule 25: ATP synthase subunit beta





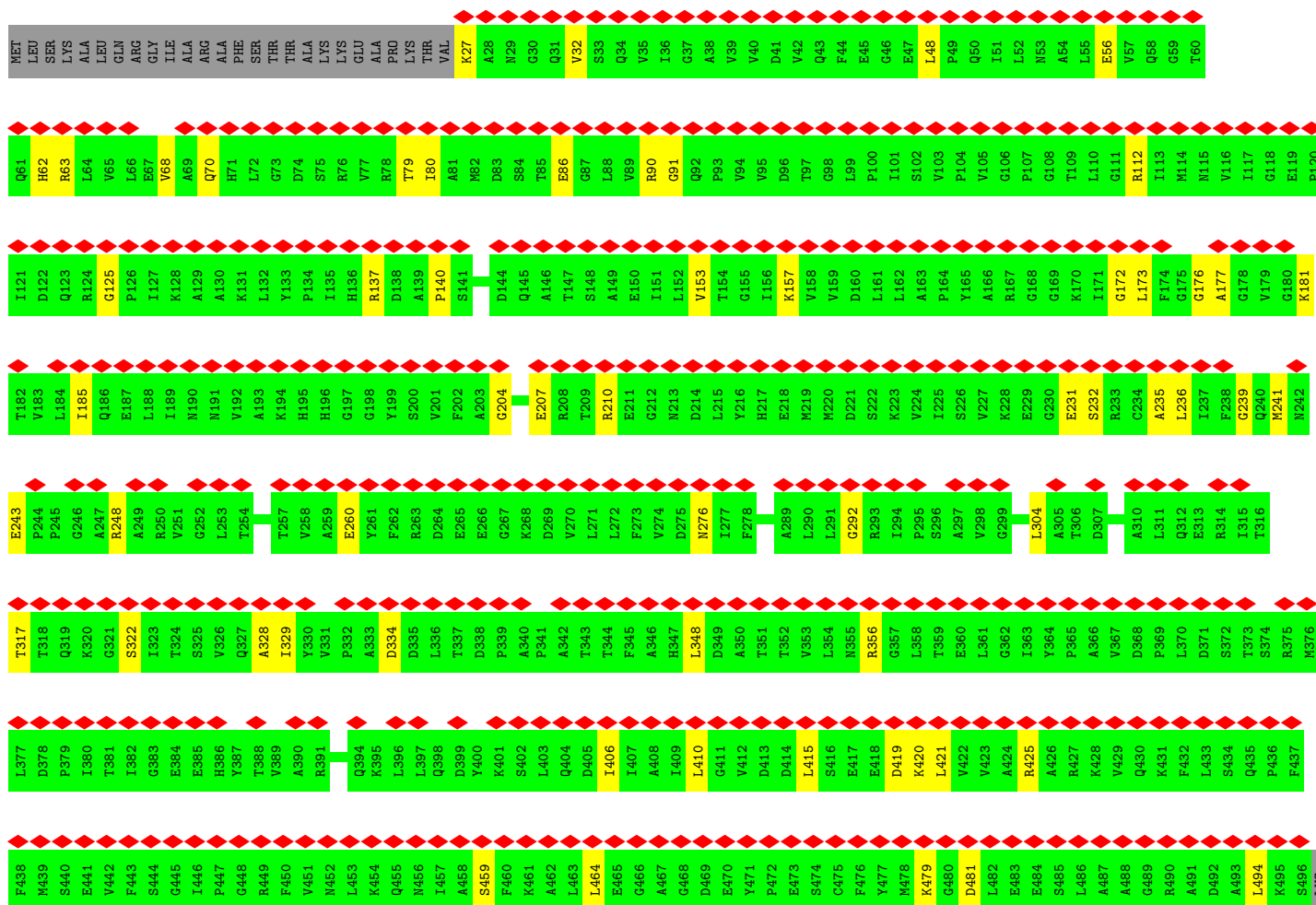
• Molecule 25: ATP synthase subunit beta



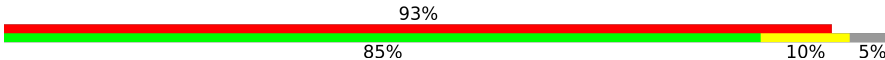


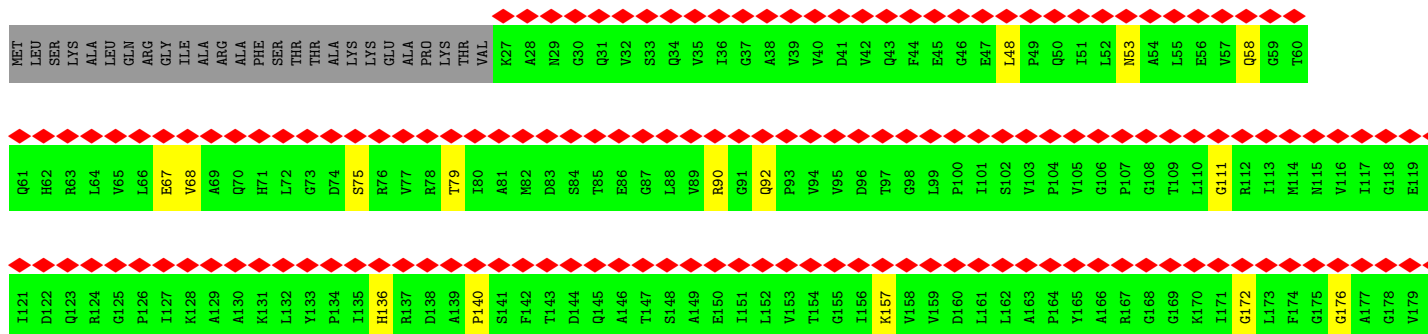
● Molecule 25: ATP synthase subunit beta

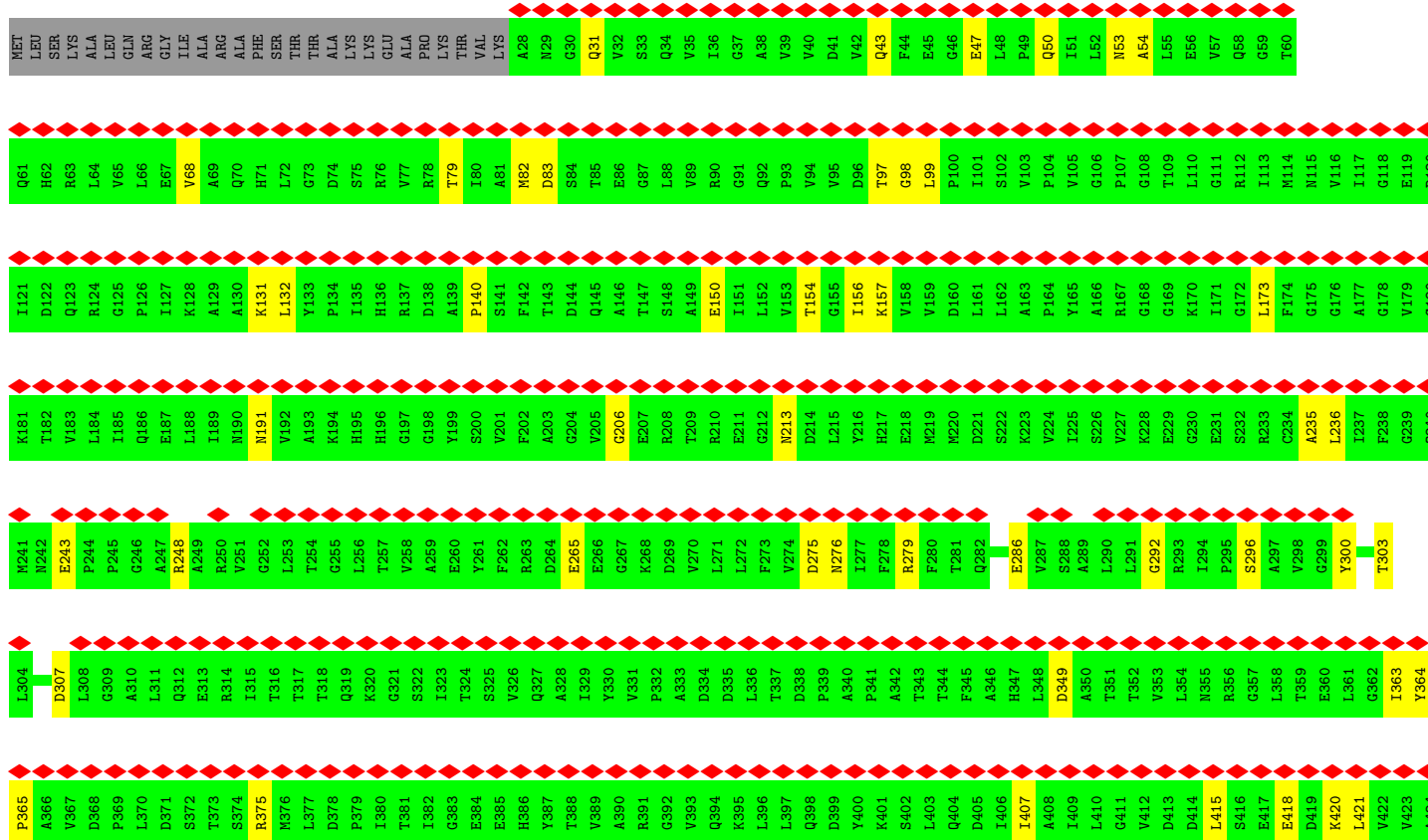
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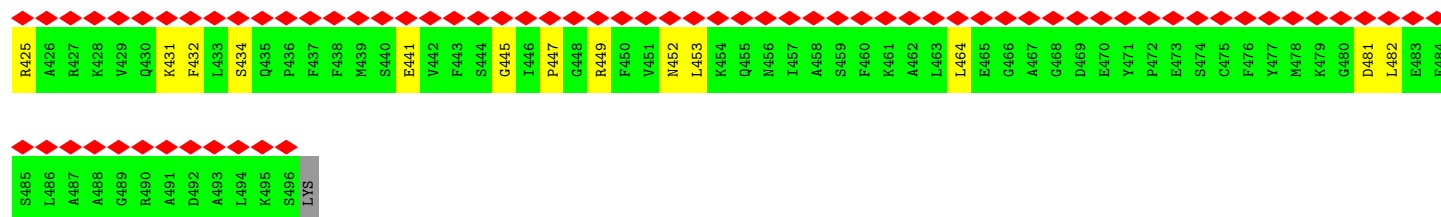


● Molecule 25: ATP synthase subunit beta

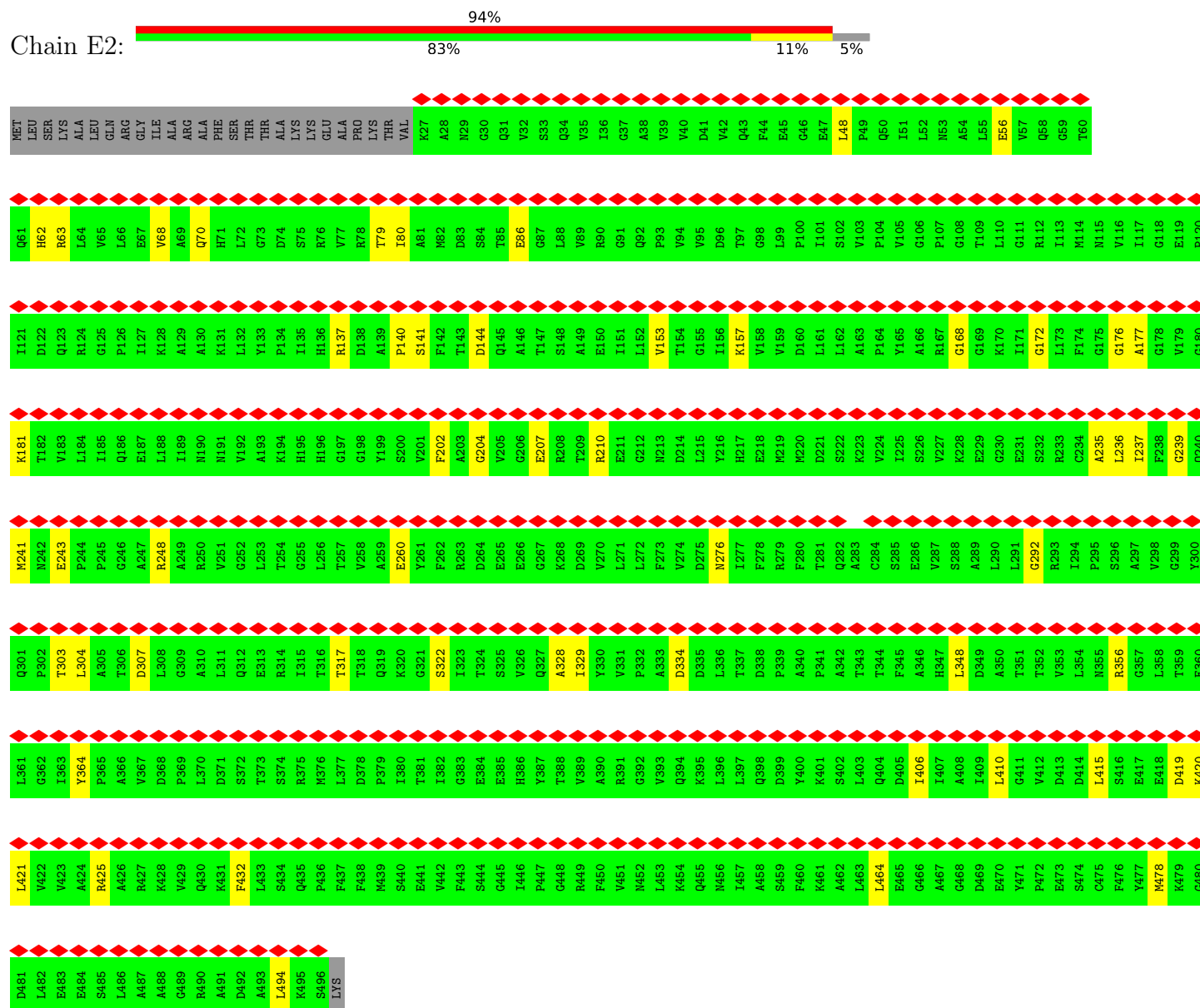
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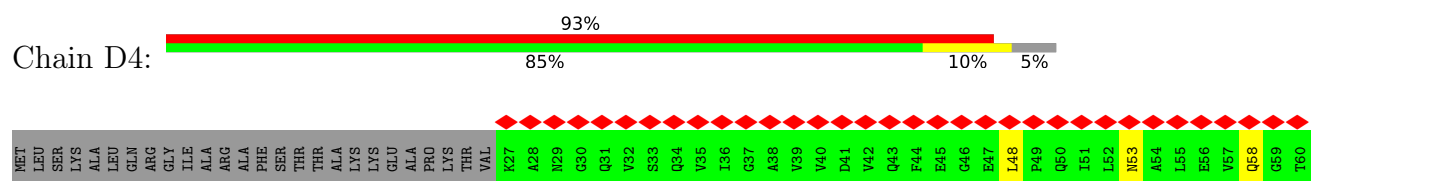


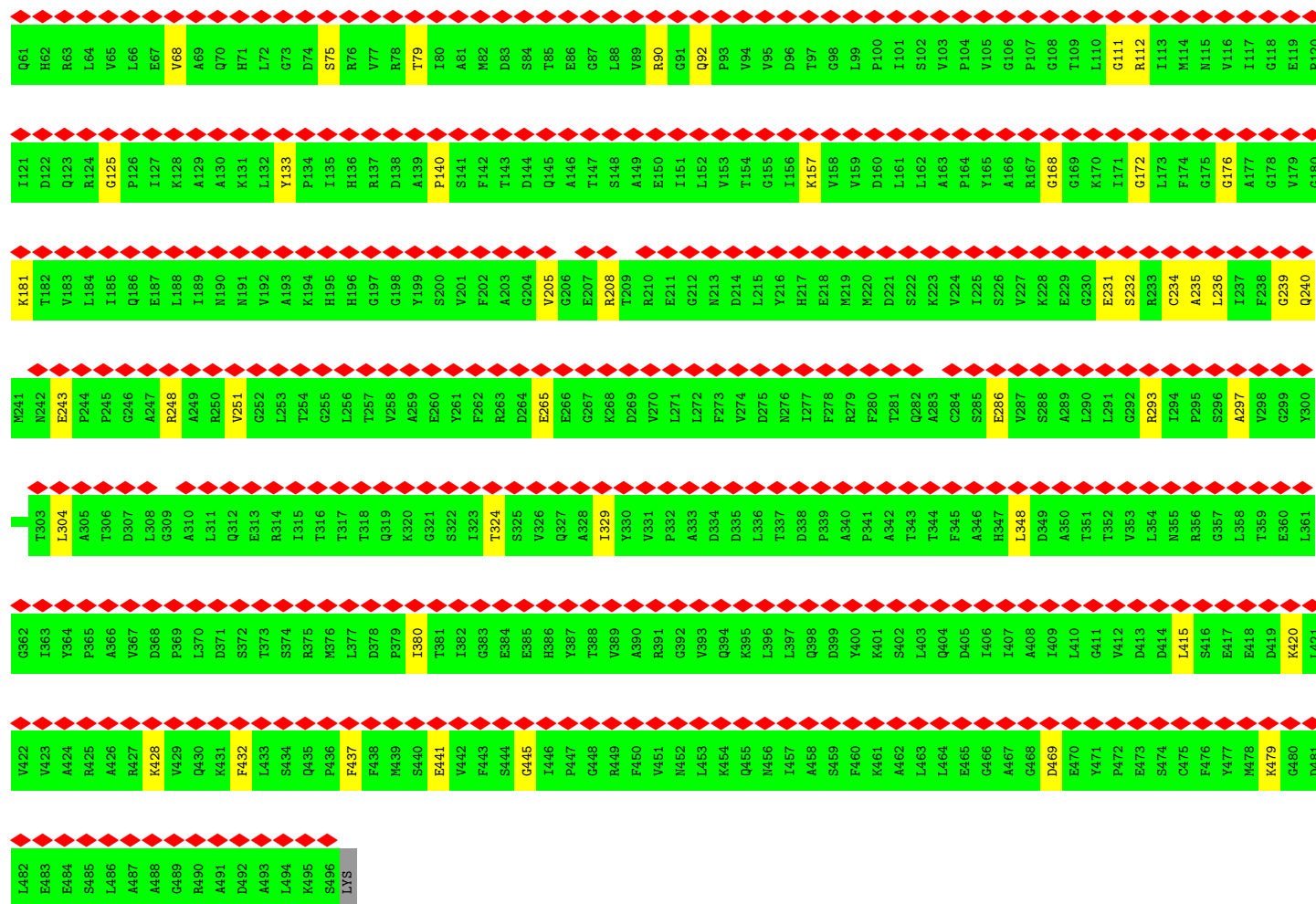


• Molecule 25: ATP synthase subunit beta

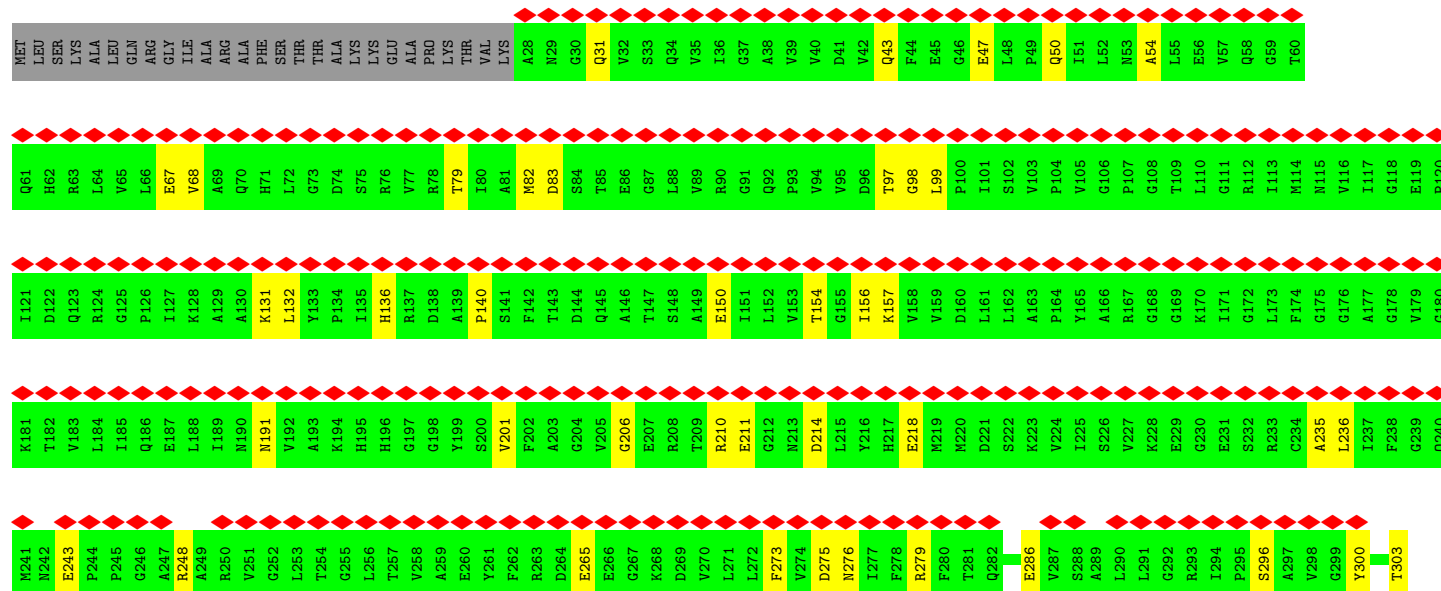
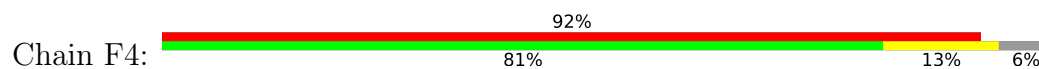


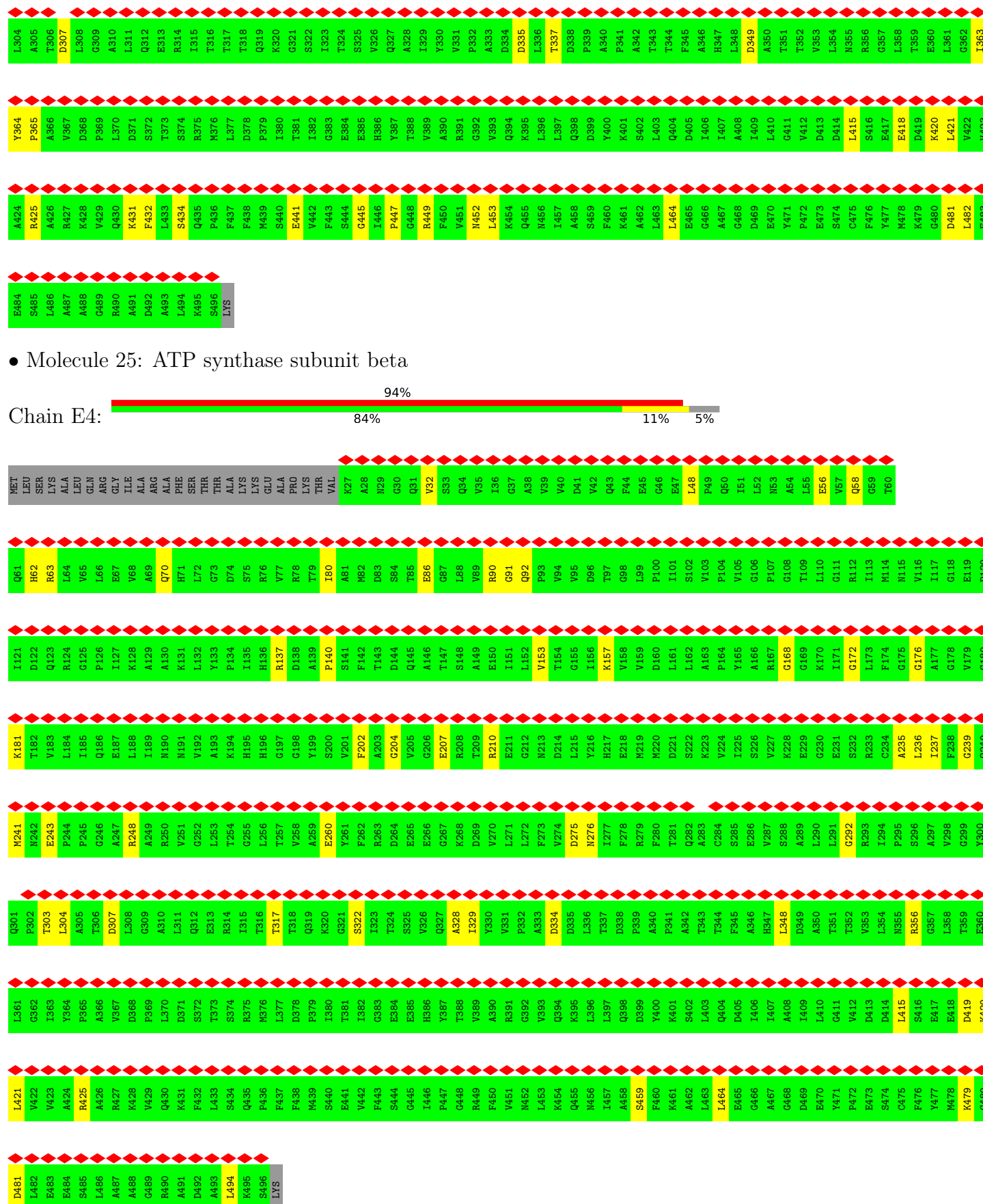
• Molecule 25: ATP synthase subunit beta





● Molecule 25: ATP synthase subunit beta





• Molecule 25: ATP synthase subunit beta

94%

Chain E4:

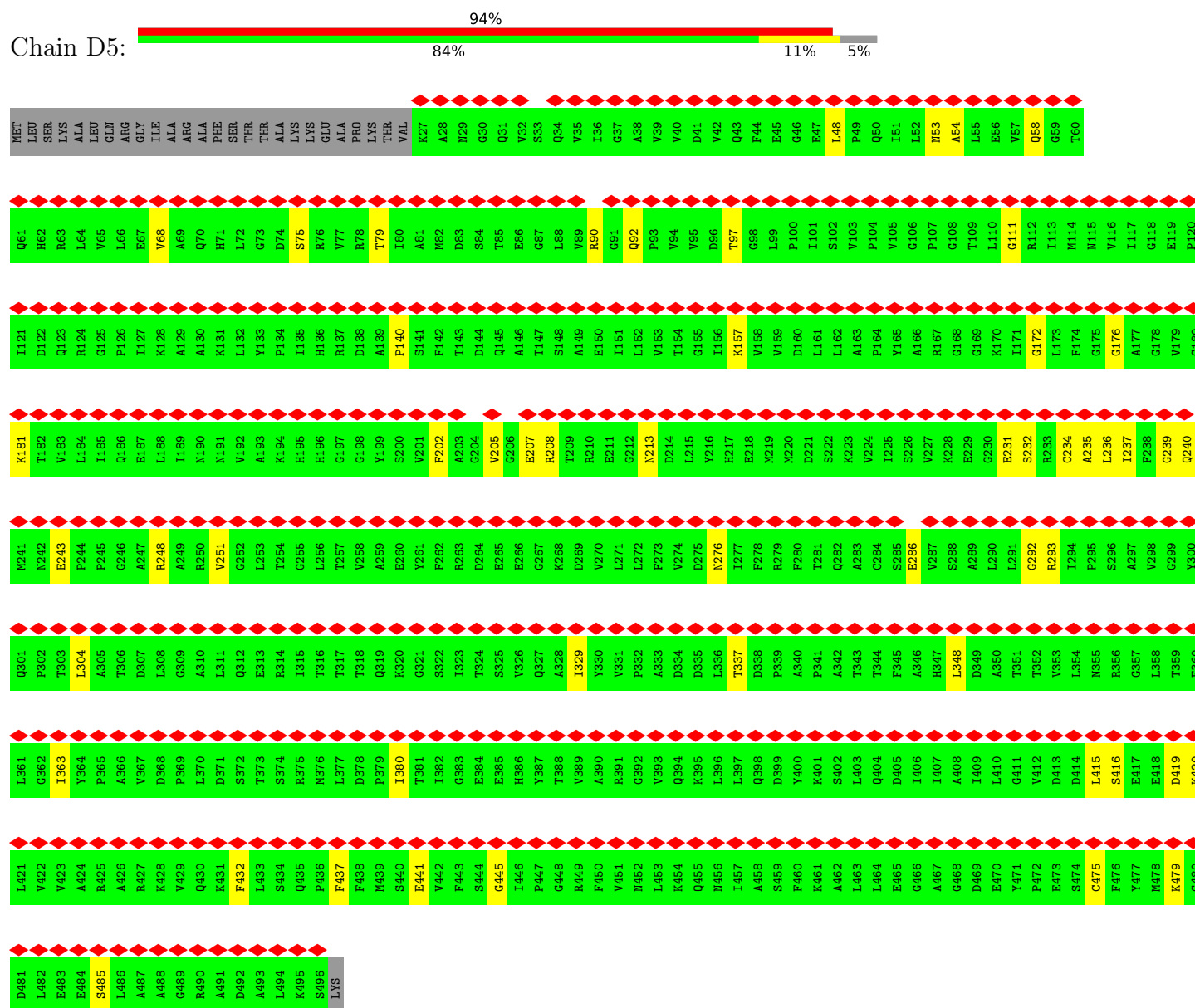
84%

11%

5%

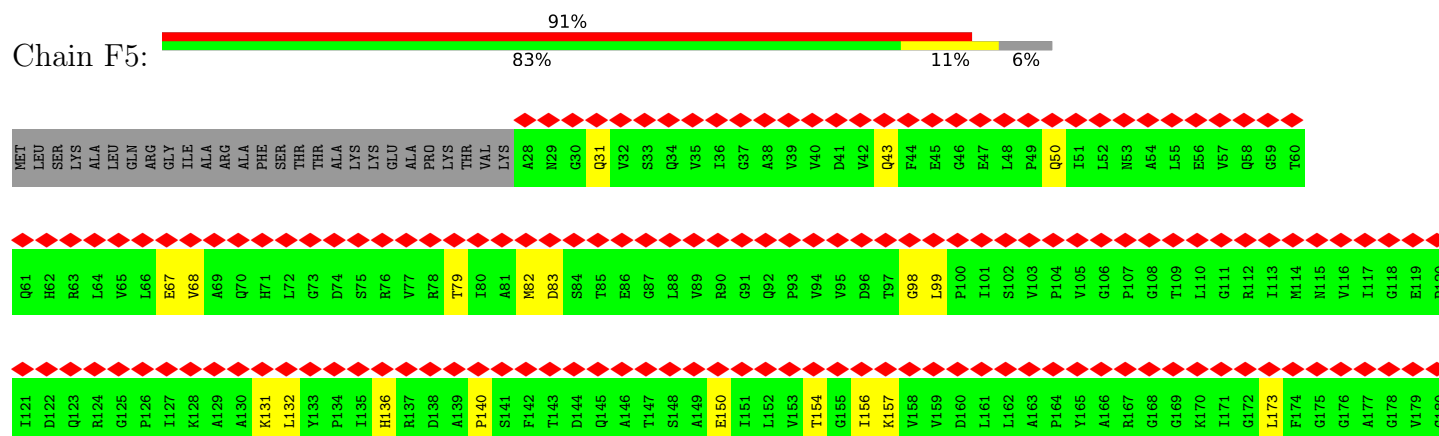
• Molecule 25: ATP synthase subunit beta

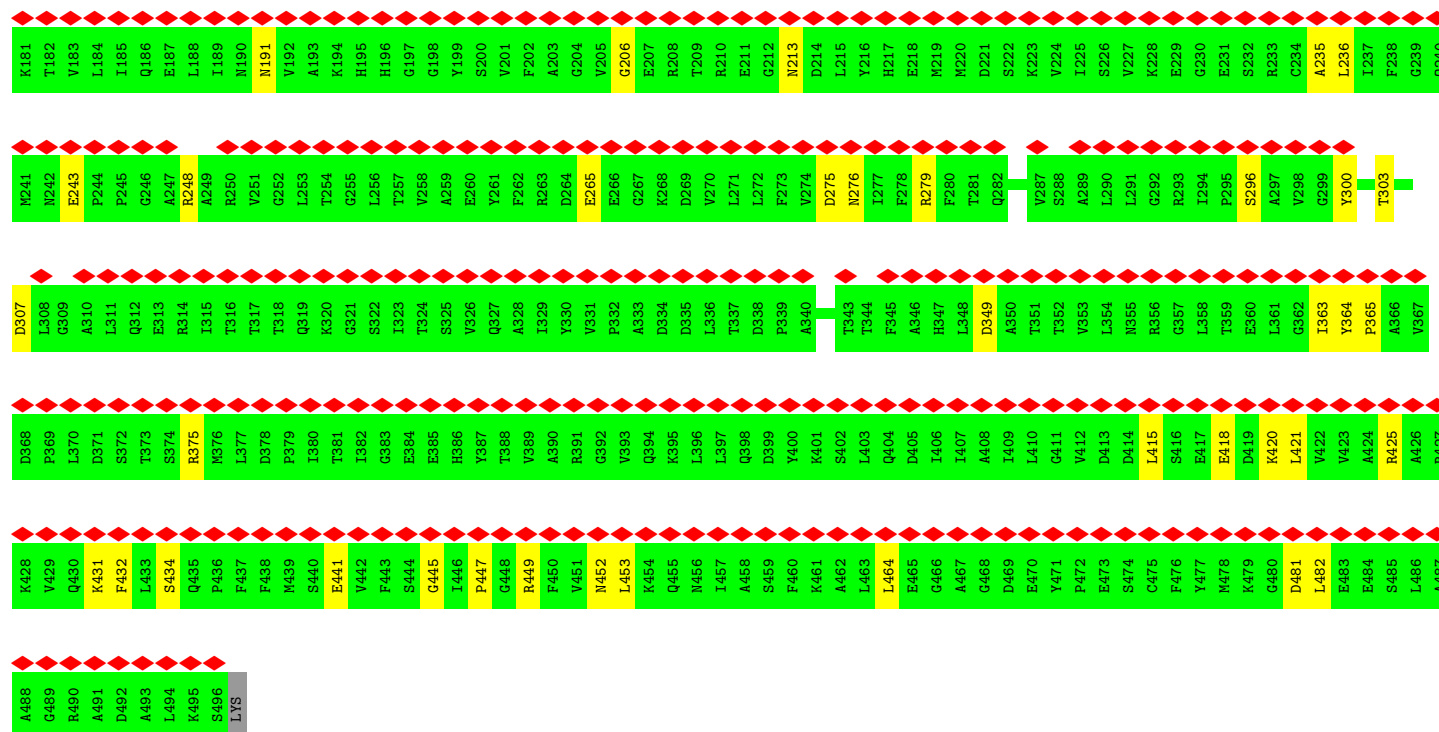
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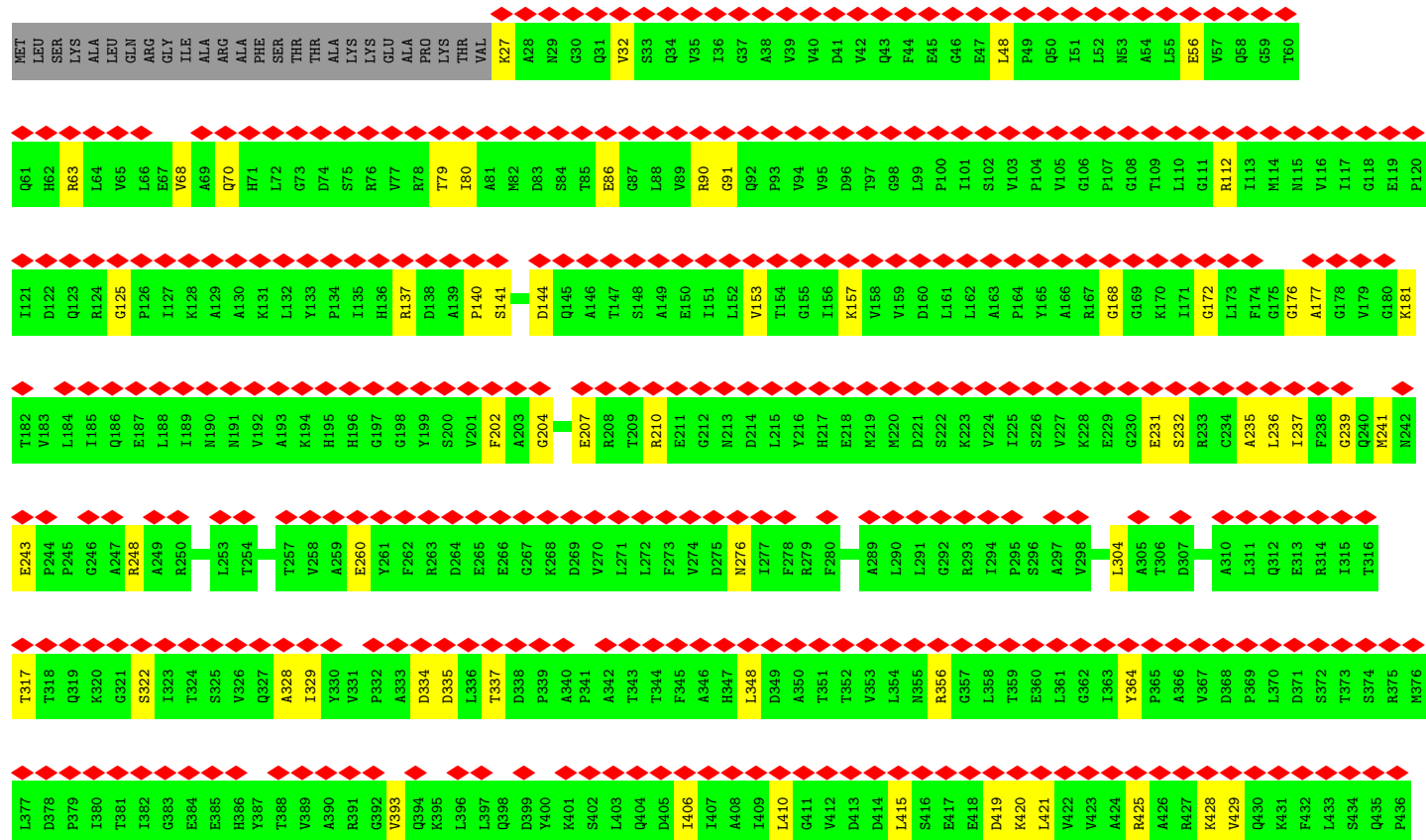
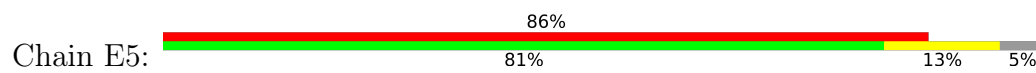
• Molecule 25: ATP synthase subunit beta

Chain F5:





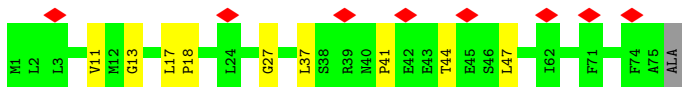
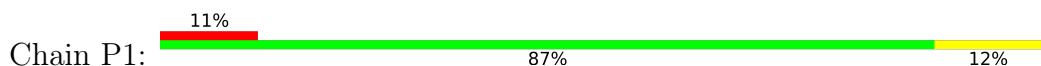
● Molecule 25: ATP synthase subunit beta



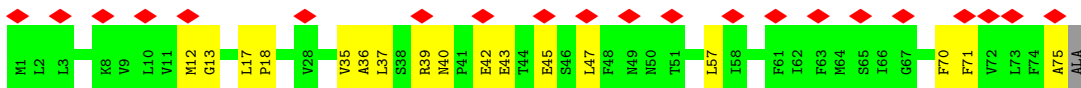
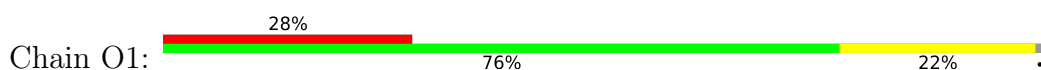


LYS

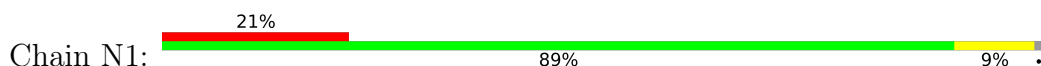
- Molecule 26: ATP synthase F0 subunit 9



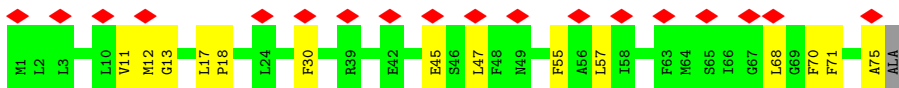
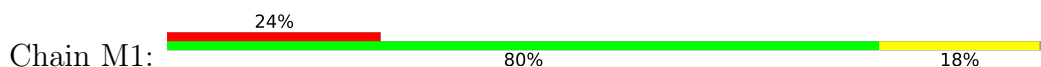
- Molecule 26: ATP synthase F0 subunit 9



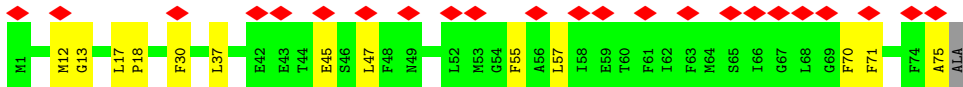
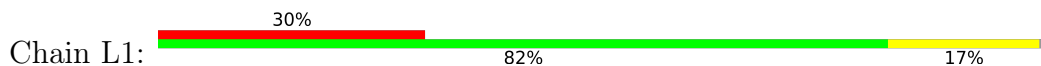
- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9

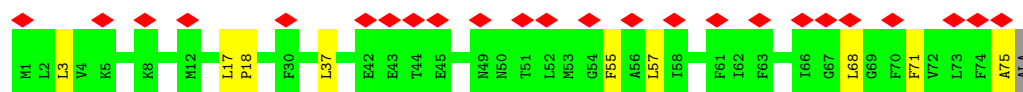


- Molecule 26: ATP synthase F0 subunit 9

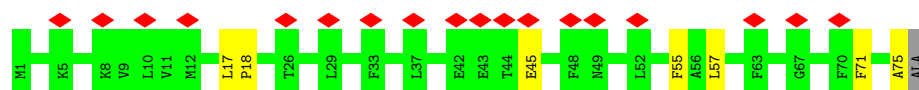
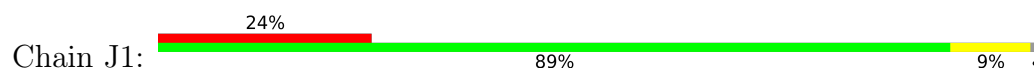


- Molecule 26: ATP synthase F0 subunit 9

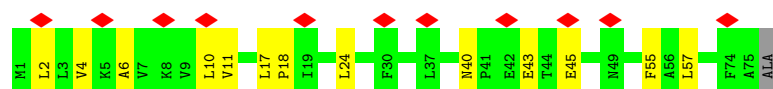
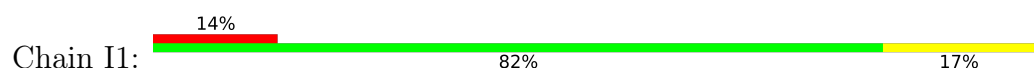




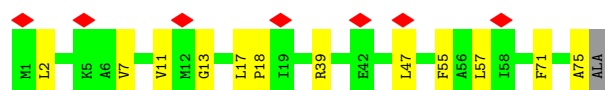
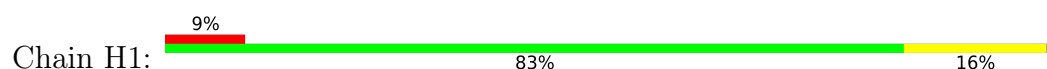
- Molecule 26: ATP synthase F0 subunit 9



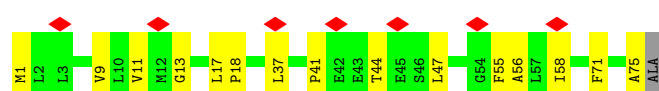
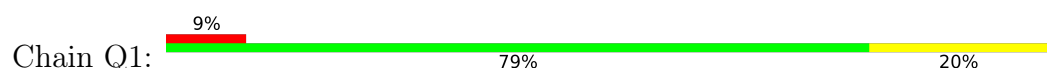
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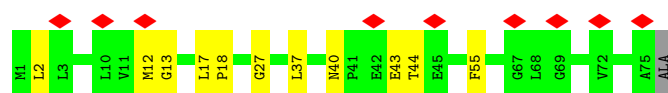
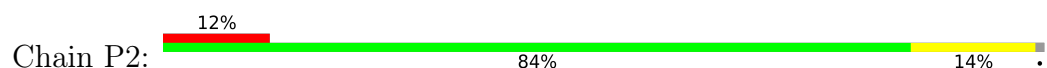
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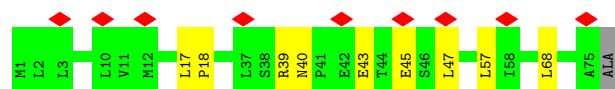
- Molecule 26: ATP synthase F0 subunit 9



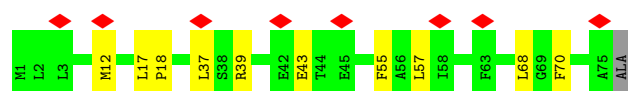
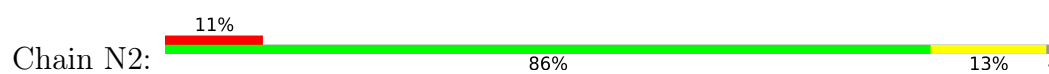
- Molecule 26: ATP synthase F0 subunit 9



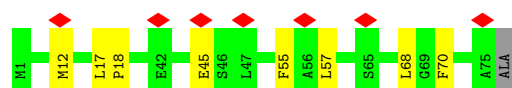
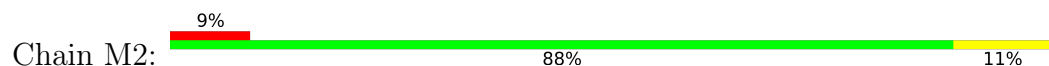
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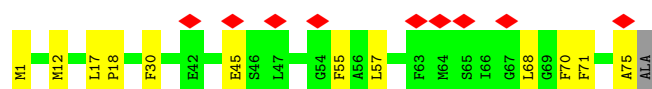
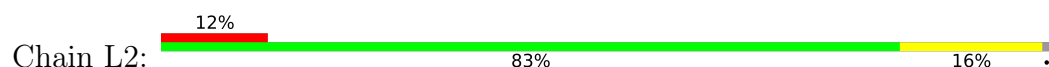
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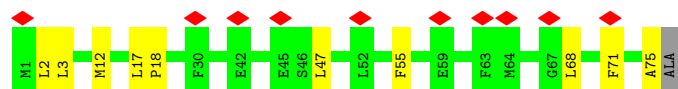
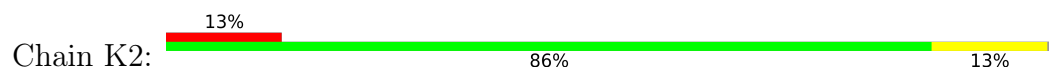
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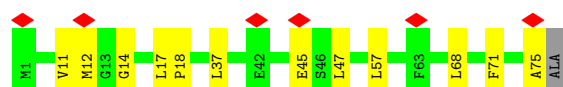
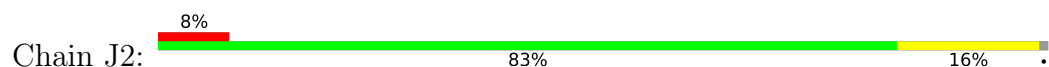
- Molecule 26: ATP synthase F0 subunit 9



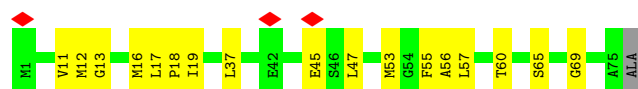
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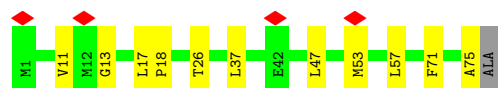
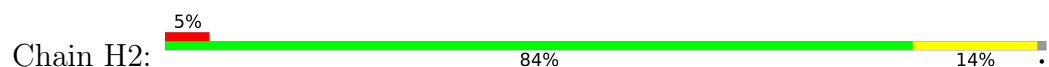
- Molecule 26: ATP synthase F0 subunit 9



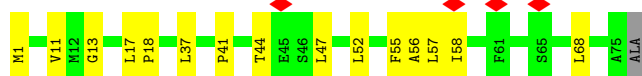
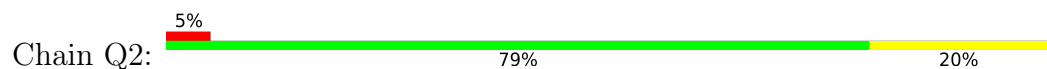
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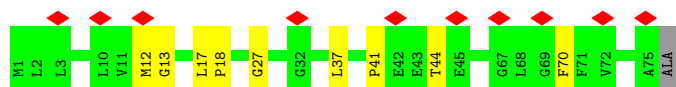
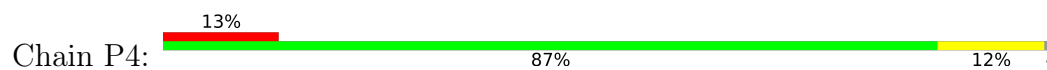
- Molecule 26: ATP synthase F0 subunit 9



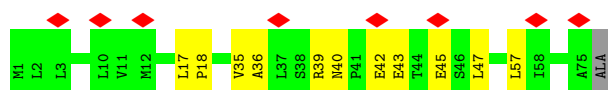
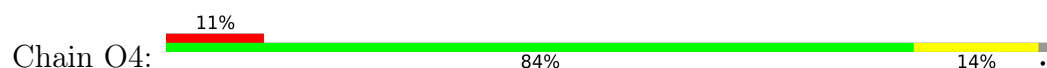
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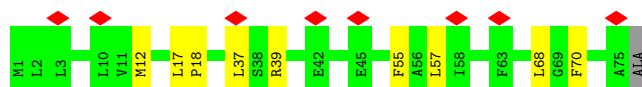
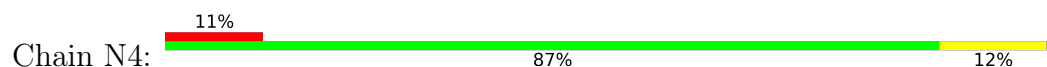
- Molecule 26: ATP synthase F0 subunit 9



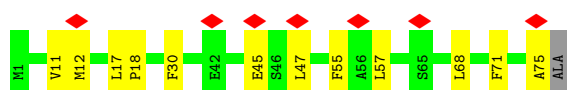
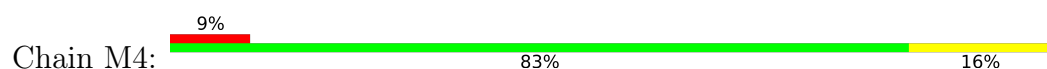
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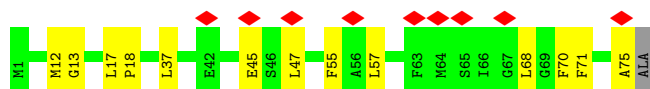
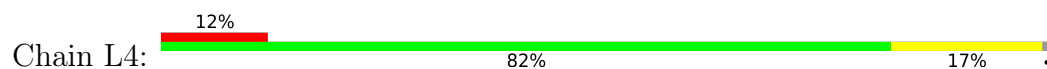
- Molecule 26: ATP synthase F0 subunit 9



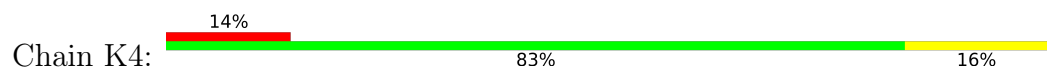
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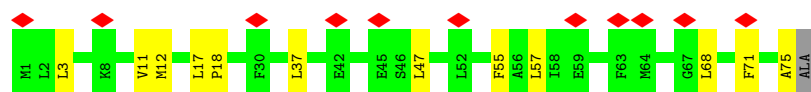


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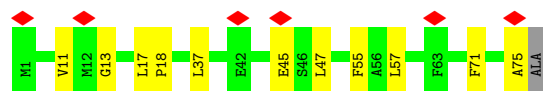
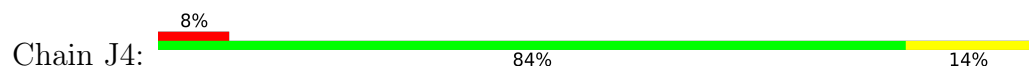


- Molecule 26: ATP synthase F0 subunit 9

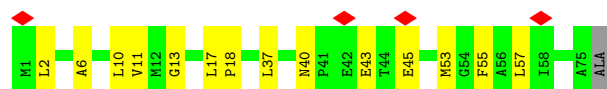
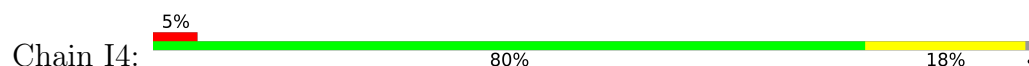




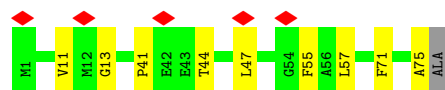
- Molecule 26: ATP synthase F0 subunit 9



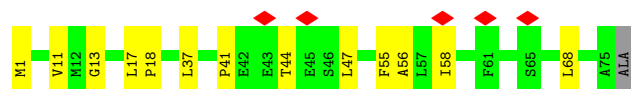
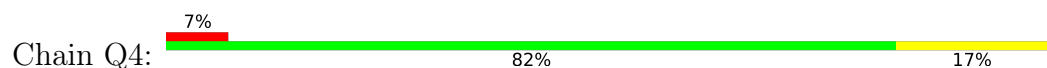
- Molecule 26: ATP synthase F0 subunit 9



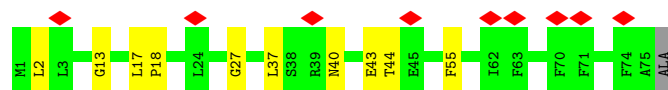
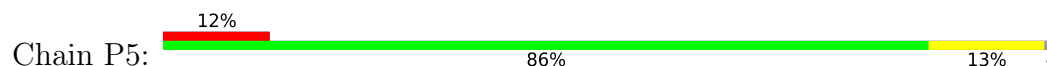
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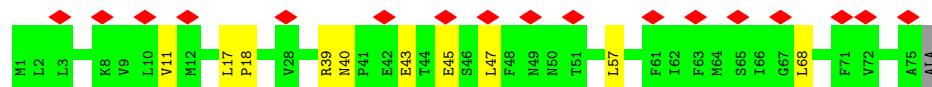
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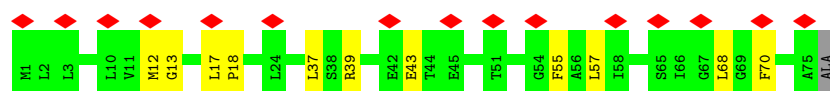
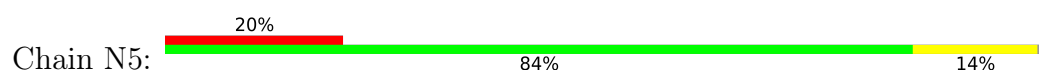
- Molecule 26: ATP synthase F0 subunit 9



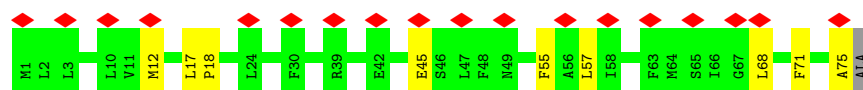
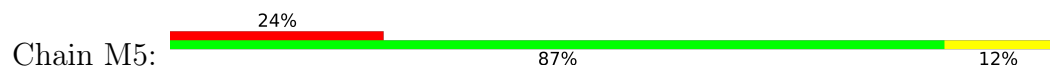
- Molecule 26: ATP synthase F0 subunit 9



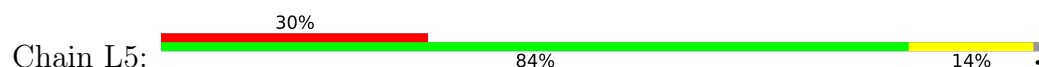
- Molecule 26: ATP synthase F0 subunit 9



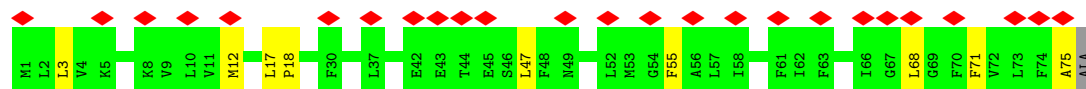
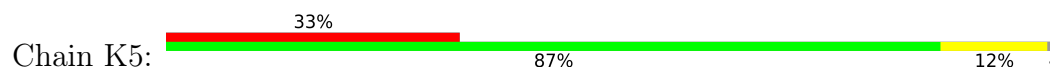
- Molecule 26: ATP synthase F0 subunit 9



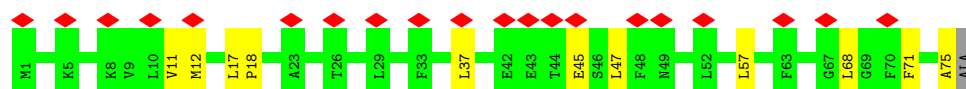
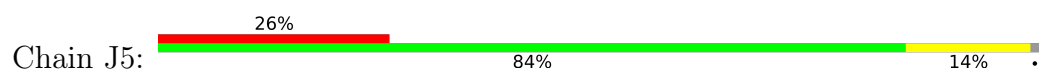
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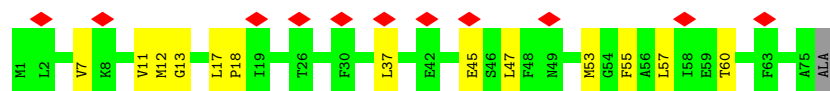
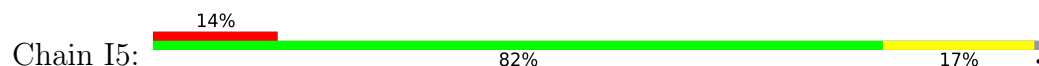
- Molecule 26: ATP synthase F0 subunit 9



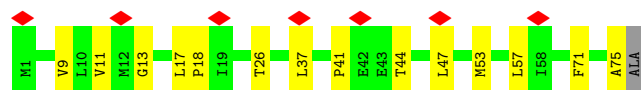
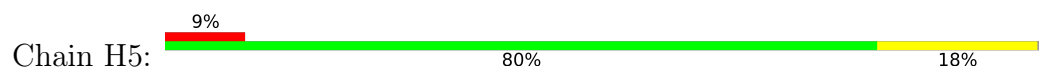
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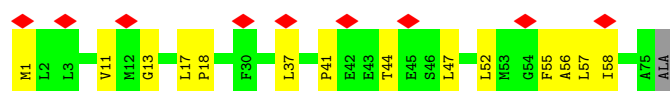
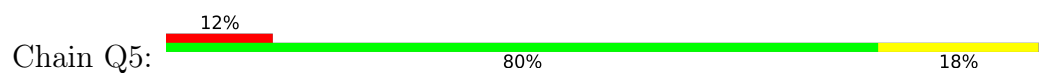
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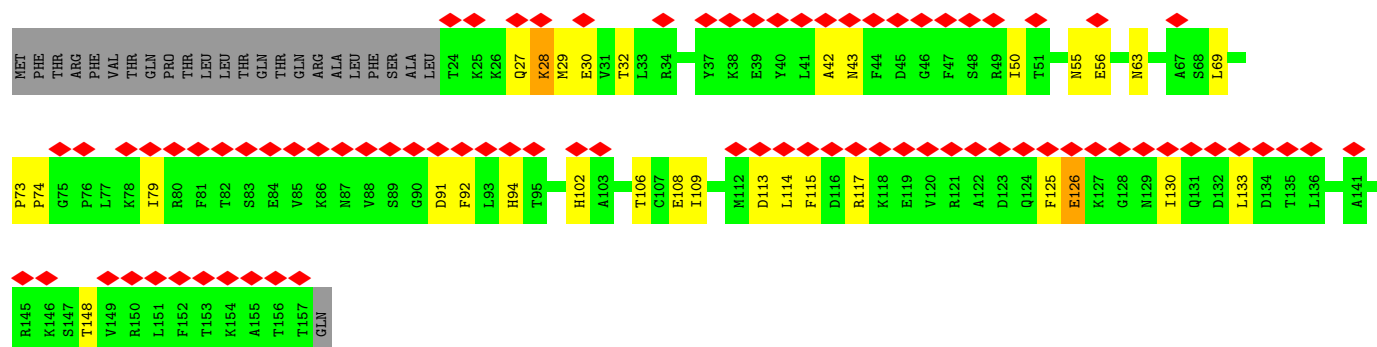
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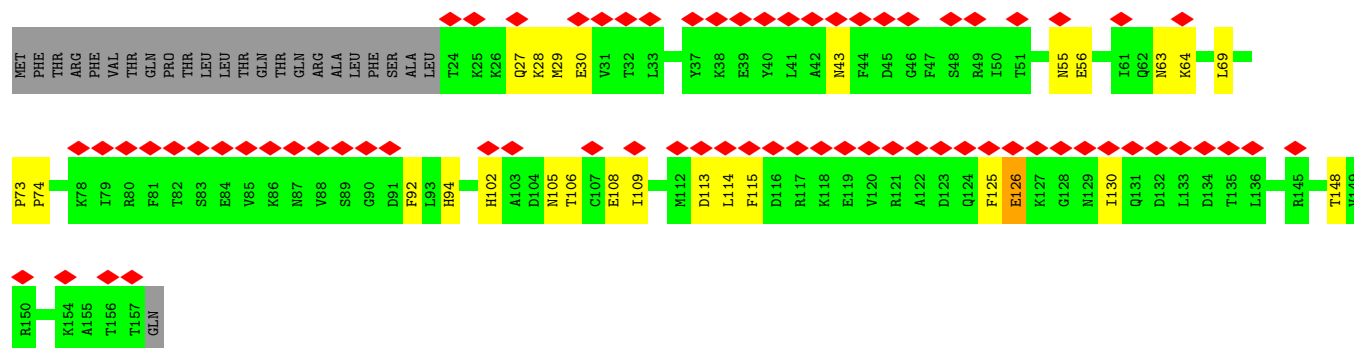
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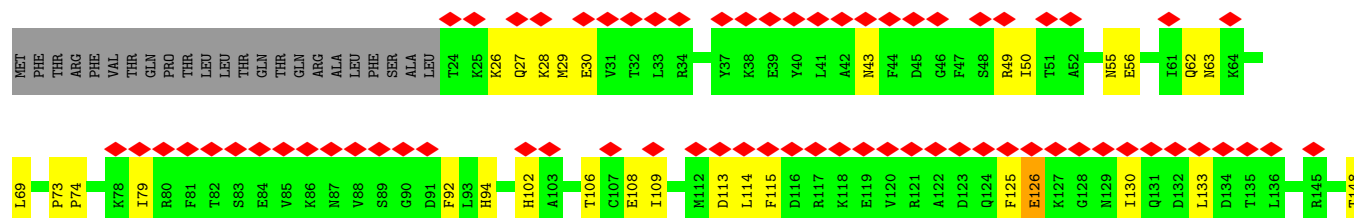
- Molecule 27: subunit delta

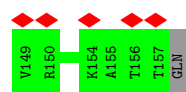


- Molecule 27: subunit delta

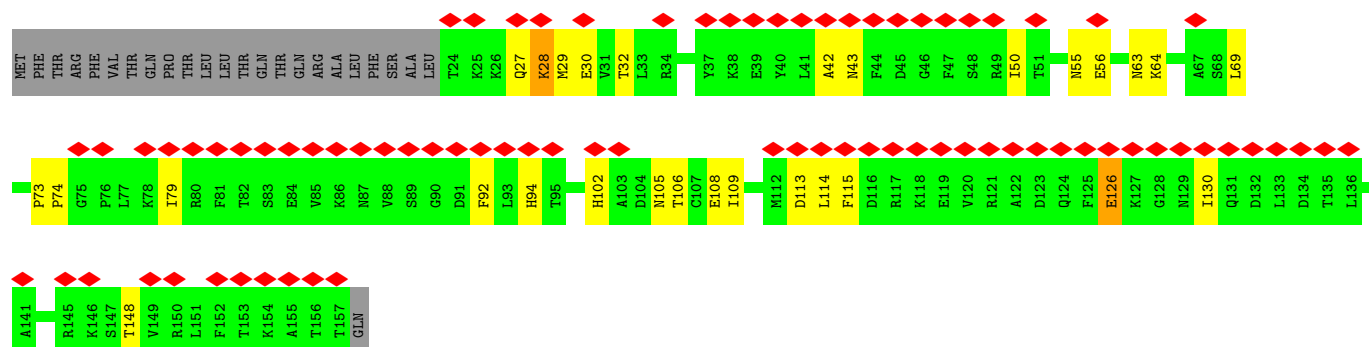


- Molecule 27: subunit delta





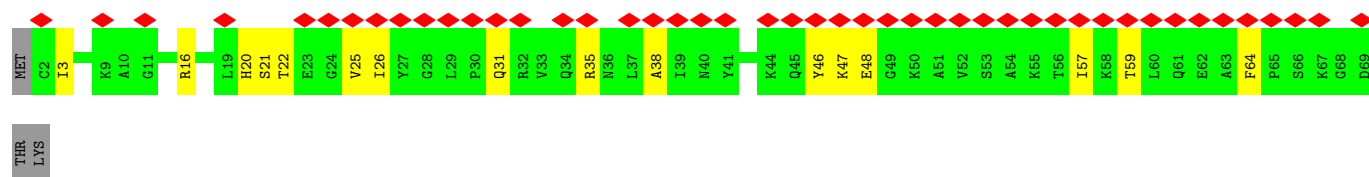
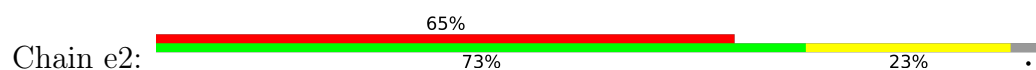
- Molecule 27: subunit delta



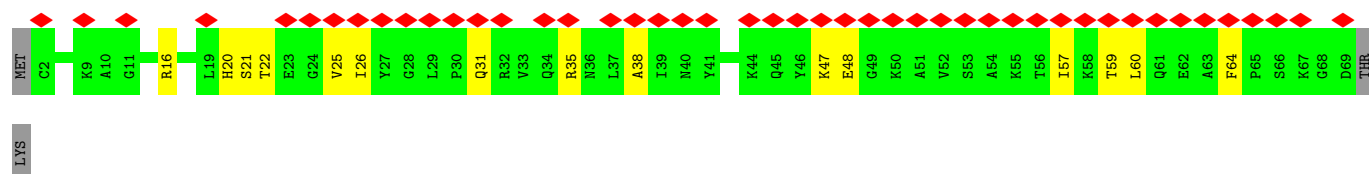
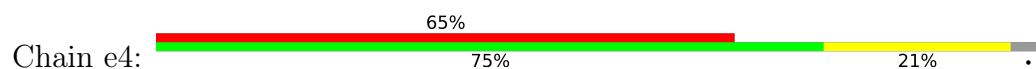
- Molecule 28: subunit epsilon



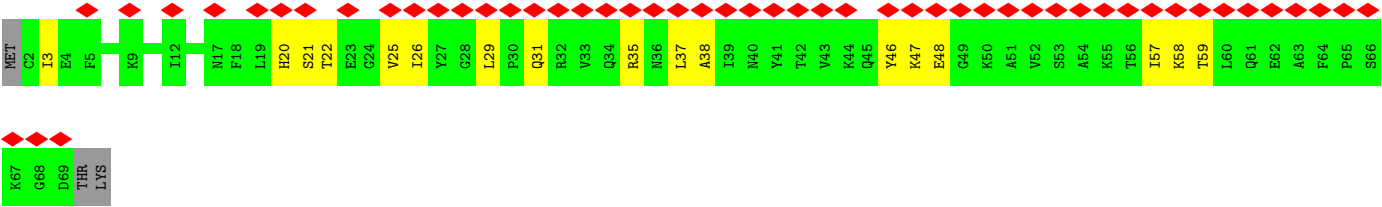
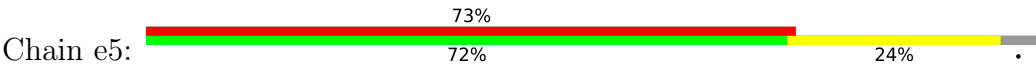
- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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: UQ8, CDL, PO4, MG, ADP, NAD, PC1, PEE, ATP

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	0.16	0/3752	0.23	0/5109
1	A3	0.15	0/3752	0.23	0/5109
1	a	0.15	0/3752	0.23	0/5109
1	a3	0.16	0/3752	0.24	0/5109
2	B	0.13	0/2940	0.23	0/3969
2	B3	0.12	0/2940	0.22	0/3969
2	b	0.12	0/2940	0.23	0/3969
2	b3	0.13	0/2940	0.23	0/3969
3	D	0.12	0/1715	0.21	0/2321
3	D3	0.11	0/1715	0.21	0/2321
3	d	0.11	0/1715	0.21	0/2321
3	d3	0.12	0/1715	0.21	0/2321
4	F	0.18	0/1733	0.26	0/2327
4	F3	0.17	0/1733	0.27	0/2327
4	f	0.17	0/1733	0.26	0/2327
4	f3	0.18	0/1733	0.25	0/2327
5	I	0.16	0/1771	0.27	0/2394
5	I3	0.15	0/1771	0.27	0/2394
5	i	0.16	0/1771	0.28	0/2394
5	i3	0.16	0/1771	0.26	0/2394
6	K	0.11	0/1508	0.24	0/2024
6	K3	0.11	0/1508	0.24	0/2024
6	k	0.11	0/1508	0.23	0/2024
6	k3	0.11	0/1508	0.23	0/2024
7	C	0.15	0/866	0.26	0/1176
7	C3	0.14	0/866	0.25	0/1176
7	c	0.14	0/866	0.25	0/1176
7	c3	0.15	0/866	0.26	0/1176
8	G	0.12	0/2302	0.25	0/3115
8	G3	0.11	0/2302	0.25	0/3115
8	g	0.11	0/2302	0.25	0/3115
8	g3	0.12	0/2302	0.25	0/3115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	H	0.14	0/2006	0.26	0/2704
9	H3	0.13	0/2006	0.26	0/2704
9	h	0.13	0/2006	0.25	0/2704
9	h3	0.13	0/2006	0.25	0/2704
10	J	0.16	0/2256	0.26	0/3069
10	J3	0.15	0/2256	0.25	0/3069
10	j	0.15	0/2256	0.25	0/3069
10	j3	0.16	0/2256	0.25	0/3069
11	L	0.17	0/2140	0.26	0/2903
11	L3	0.16	0/2140	0.27	0/2903
11	l	0.16	0/2140	0.27	0/2903
11	l3	0.17	0/2140	0.26	0/2903
12	M	0.16	0/1912	0.24	0/2598
12	M3	0.14	0/1912	0.24	0/2598
12	m	0.14	0/1912	0.24	0/2598
12	m3	0.15	0/1912	0.23	0/2598
13	N	0.16	0/1030	0.22	0/1393
13	N3	0.15	0/1030	0.23	0/1393
13	n	0.15	0/1030	0.23	0/1393
13	n3	0.16	0/1030	0.23	0/1393
14	O	0.13	0/821	0.22	0/1104
14	O3	0.13	0/821	0.22	0/1104
14	o	0.13	0/821	0.22	0/1104
14	o3	0.13	0/821	0.22	0/1104
15	P	0.10	0/1249	0.21	0/1695
15	P3	0.09	0/1249	0.21	0/1695
15	p	0.09	0/1249	0.21	0/1695
15	p3	0.10	0/1249	0.20	0/1695
16	Q	0.11	0/888	0.21	0/1200
16	Q3	0.09	0/888	0.21	0/1200
16	q	0.10	0/888	0.21	0/1200
16	q3	0.11	0/888	0.21	0/1200
17	R	0.15	0/1185	0.23	0/1594
17	R3	0.13	0/1185	0.23	0/1594
17	r	0.13	0/1225	0.24	0/1649
17	r3	0.15	0/1225	0.24	0/1649
18	S	0.14	0/1044	0.26	0/1414
18	S3	0.13	0/1044	0.25	0/1414
18	s	0.12	0/1037	0.25	0/1404
18	s3	0.13	0/1037	0.26	0/1404
19	E	0.09	0/3492	0.22	0/4720
19	E3	0.08	0/3492	0.21	0/4720
19	e	0.08	0/3492	0.21	0/4720

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	e3	0.09	0/3492	0.21	0/4720
20	i1	0.08	0/593	0.20	0/795
20	i2	0.07	0/563	0.19	0/753
20	i4	0.08	0/593	0.20	0/795
20	i5	0.08	0/563	0.20	0/753
21	t	0.10	0/3103	0.26	0/4200
21	t3	0.11	0/3103	0.25	0/4200
22	G1	0.07	0/1507	0.22	0/2027
22	G2	0.07	0/1507	0.21	0/2027
22	G4	0.07	0/1507	0.22	0/2027
22	G5	0.07	0/1507	0.21	0/2027
23	g1	0.07	0/2156	0.22	0/2900
23	g2	0.07	0/2156	0.21	0/2900
23	g4	0.07	0/2156	0.22	0/2900
23	g5	0.07	0/2156	0.22	0/2900
24	A1	0.07	0/3961	0.21	0/5346
24	A2	0.07	0/3961	0.21	0/5346
24	A4	0.07	0/3961	0.21	0/5346
24	A5	0.07	0/3961	0.21	0/5346
24	B1	0.07	0/3956	0.21	0/5339
24	B2	0.07	0/3956	0.21	0/5339
24	B4	0.07	0/3956	0.21	0/5339
24	B5	0.07	0/3956	0.21	0/5339
24	C1	0.07	0/3974	0.21	0/5361
24	C2	0.07	0/3974	0.21	0/5361
24	C4	0.07	0/3974	0.21	0/5361
24	C5	0.07	0/3974	0.21	0/5361
25	D1	0.07	0/3613	0.21	0/4900
25	D2	0.07	0/3613	0.21	0/4900
25	D4	0.07	0/3613	0.21	0/4900
25	D5	0.07	0/3613	0.21	0/4900
25	E1	0.07	0/3613	0.21	0/4900
25	E2	0.07	0/3613	0.21	0/4900
25	E4	0.07	0/3613	0.21	0/4900
25	E5	0.07	0/3613	0.21	0/4900
25	F1	0.07	0/3604	0.22	0/4889
25	F2	0.07	0/3604	0.21	0/4889
25	F4	0.07	0/3604	0.21	0/4889
25	F5	0.07	0/3604	0.21	0/4889
26	H1	0.09	0/572	0.20	0/771
26	H2	0.09	0/572	0.21	0/771
26	H4	0.09	0/572	0.20	0/771
26	H5	0.09	0/572	0.21	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	I1	0.09	0/572	0.21	0/771
26	I2	0.11	0/572	0.25	0/771
26	I4	0.09	0/572	0.21	0/771
26	I5	0.11	0/572	0.25	0/771
26	J1	0.08	0/572	0.19	0/771
26	J2	0.09	0/572	0.20	0/771
26	J4	0.08	0/572	0.20	0/771
26	J5	0.08	0/572	0.19	0/771
26	K1	0.07	0/572	0.19	0/771
26	K2	0.08	0/572	0.18	0/771
26	K4	0.08	0/572	0.19	0/771
26	K5	0.07	0/572	0.18	0/771
26	L1	0.07	0/572	0.18	0/771
26	L2	0.07	0/572	0.19	0/771
26	L4	0.07	0/572	0.18	0/771
26	L5	0.07	0/572	0.18	0/771
26	M1	0.07	0/572	0.18	0/771
26	M2	0.07	0/572	0.18	0/771
26	M4	0.07	0/572	0.18	0/771
26	M5	0.07	0/572	0.18	0/771
26	N1	0.07	0/572	0.18	0/771
26	N2	0.07	0/572	0.18	0/771
26	N4	0.07	0/572	0.18	0/771
26	N5	0.07	0/572	0.18	0/771
26	O1	0.07	0/572	0.19	0/771
26	O2	0.07	0/572	0.19	0/771
26	O4	0.07	0/572	0.19	0/771
26	O5	0.07	0/572	0.19	0/771
26	P1	0.08	0/572	0.19	0/771
26	P2	0.08	0/572	0.20	0/771
26	P4	0.07	0/572	0.20	0/771
26	P5	0.08	0/572	0.19	0/771
26	Q1	0.08	0/572	0.19	0/771
26	Q2	0.08	0/572	0.19	0/771
26	Q4	0.08	0/572	0.19	0/771
26	Q5	0.08	0/572	0.19	0/771
27	d1	0.09	0/1081	0.26	0/1459
27	d2	0.09	0/1081	0.26	0/1459
27	d4	0.09	0/1081	0.26	0/1459
27	d5	0.09	0/1081	0.27	0/1459
28	e1	0.08	0/547	0.24	0/735
28	e2	0.08	0/547	0.26	0/735
28	e4	0.09	0/547	0.25	0/735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	e5	0.08	0/547	0.25	0/735
All	All	0.11	0/281952	0.23	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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	3529	3529	18	0
1	A3	3628	3529	3529	22	0
1	a	3628	3527	3529	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a3	3628	3527	3529	26	0
2	B	2875	2849	2850	22	0
2	B3	2875	2849	2850	22	0
2	b	2875	2851	2851	20	0
2	b3	2875	2851	2851	17	0
3	D	1676	1598	1598	27	0
3	D3	1676	1598	1598	28	0
3	d	1676	1598	1598	25	0
3	d3	1676	1598	1598	22	0
4	F	1682	1692	1692	12	0
4	F3	1682	1692	1692	9	0
4	f	1682	1691	1691	13	0
4	f3	1682	1691	1690	10	0
5	I	1720	1740	1740	15	0
5	I3	1720	1740	1740	14	0
5	i	1720	1742	1741	16	0
5	i3	1720	1742	1741	13	0
6	K	1473	1430	1430	8	0
6	K3	1473	1430	1430	10	0
6	k	1473	1429	1429	10	0
6	k3	1473	1429	1429	11	0
7	C	841	830	830	15	0
7	C3	841	830	830	11	0
7	c	841	830	830	8	0
7	c3	841	830	830	9	0
8	G	2220	2118	2118	14	0
8	G3	2220	2118	2118	17	0
8	g	2220	2118	2119	12	0
8	g3	2220	2118	2118	11	0
9	H	1953	1883	1882	8	0
9	H3	1953	1883	1882	9	0
9	h	1953	1883	1882	20	0
9	h3	1953	1883	1882	20	0
10	J	2199	2147	2147	14	0
10	J3	2199	2147	2147	15	0
10	j	2199	2147	2147	16	0
10	j3	2199	2147	2147	15	0
11	L	2071	1999	2000	23	0
11	L3	2071	1999	2000	28	0
11	l	2071	1999	2000	25	0
11	l3	2071	1999	2000	23	0
12	M	1861	1835	1835	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M3	1861	1835	1835	13	0
12	m	1861	1835	1835	10	0
12	m3	1861	1835	1835	11	0
13	N	998	962	962	5	0
13	N3	998	962	962	10	0
13	n	998	962	962	7	0
13	n3	998	962	962	4	0
14	O	805	794	794	0	0
14	O3	805	794	794	0	0
14	o	805	794	794	3	0
14	o3	805	794	794	2	0
15	P	1217	1196	1196	4	0
15	P3	1217	1196	1196	4	0
15	p	1217	1196	1196	6	0
15	p3	1217	1196	1196	6	0
16	Q	875	874	874	9	0
16	Q3	875	874	874	10	0
16	q	875	874	874	10	0
16	q3	875	874	874	8	0
17	R	1154	1134	1134	11	0
17	R3	1154	1134	1134	9	0
17	r	1193	1180	1180	12	0
17	r3	1193	1180	1180	13	0
18	S	1023	1016	1016	17	0
18	S3	1023	1016	1016	17	0
18	s	1016	1009	1009	21	0
18	s3	1016	1009	1009	23	0
19	E	3395	3286	3285	25	0
19	E3	3395	3286	3285	23	0
19	e	3395	3286	3285	20	0
19	e3	3395	3286	3285	25	0
20	i1	585	582	582	9	0
20	i2	556	556	556	4	0
20	i4	585	582	582	6	0
20	i5	556	556	556	3	0
21	t	3013	2876	2876	46	0
21	t3	3013	2876	2876	46	0
22	G1	1485	1515	1515	18	0
22	G2	1485	1515	1515	15	0
22	G4	1485	1515	1515	18	0
22	G5	1485	1515	1515	15	0
23	g1	2126	2206	2206	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	g2	2126	2206	2206	26	0
23	g4	2126	2206	2206	27	0
23	g5	2126	2206	2206	22	0
24	A1	3909	4037	4037	45	0
24	A2	3909	4037	4037	39	0
24	A4	3909	4037	4037	39	0
24	A5	3909	4037	4037	37	0
24	B1	3904	4030	4030	39	0
24	B2	3904	4030	4030	38	0
24	B4	3904	4030	4030	38	0
24	B5	3904	4030	4030	33	0
24	C1	3922	4058	4058	31	0
24	C2	3922	4058	4058	30	0
24	C4	3922	4058	4058	29	0
24	C5	3922	4058	4058	33	0
25	D1	3554	3581	3581	30	0
25	D2	3554	3581	3581	31	0
25	D4	3554	3581	3581	29	0
25	D5	3554	3581	3581	33	0
25	E1	3554	3581	3581	38	0
25	E2	3554	3581	3581	37	0
25	E4	3554	3581	3581	37	0
25	E5	3554	3581	3581	42	0
25	F1	3545	3568	3568	41	0
25	F2	3545	3568	3568	43	0
25	F4	3545	3568	3568	42	0
25	F5	3545	3568	3568	38	0
26	H1	561	587	587	16	0
26	H2	561	587	587	13	0
26	H4	561	587	587	11	0
26	H5	561	587	587	13	0
26	I1	561	587	587	14	0
26	I2	561	587	587	24	0
26	I4	561	587	587	14	0
26	I5	561	587	587	19	0
26	J1	561	587	587	6	0
26	J2	561	587	587	13	0
26	J4	561	587	587	10	0
26	J5	561	587	587	10	0
26	K1	561	587	587	8	0
26	K2	561	587	587	10	0
26	K4	561	587	587	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	K5	561	587	587	9	0
26	L1	561	587	587	14	0
26	L2	561	587	587	13	0
26	L4	561	587	587	14	0
26	L5	561	587	587	11	0
26	M1	561	587	587	14	0
26	M2	561	587	587	10	0
26	M4	561	587	587	13	0
26	M5	561	587	587	9	0
26	N1	561	587	587	9	0
26	N2	561	587	587	11	0
26	N4	561	587	587	10	0
26	N5	561	587	587	12	0
26	O1	561	587	587	13	0
26	O2	561	587	587	8	0
26	O4	561	587	587	9	0
26	O5	561	587	587	9	0
26	P1	561	587	587	8	0
26	P2	561	587	587	11	0
26	P4	561	587	587	8	0
26	P5	561	587	587	11	0
26	Q1	561	587	587	17	0
26	Q2	561	587	587	17	0
26	Q4	561	587	587	15	0
26	Q5	561	587	587	15	0
27	d1	1062	1082	1082	27	0
27	d2	1062	1082	1082	23	0
27	d4	1062	1082	1082	25	0
27	d5	1062	1082	1082	25	0
28	e1	537	559	559	13	0
28	e2	537	559	559	11	0
28	e4	537	559	559	12	0
28	e5	537	559	559	11	0
29	A	100	156	156	0	0
29	A3	100	156	156	1	0
29	B	400	624	624	8	0
29	B3	400	624	624	8	0
29	F	200	312	312	14	0
29	F3	100	156	156	2	0
29	I	200	312	312	3	0
29	I3	300	468	468	13	0
29	J	200	312	312	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	J3	200	312	312	0	0
29	K	200	312	312	1	0
29	K3	200	312	312	2	0
29	L	200	312	312	8	0
29	L3	100	156	156	1	0
29	P	100	156	156	0	0
29	P3	100	156	156	0	0
29	a	100	156	156	2	0
29	a3	200	312	312	14	0
29	b	100	156	156	1	0
29	b3	100	156	156	1	0
29	f	300	468	468	4	0
29	f3	300	468	468	2	0
29	g	100	156	156	1	0
29	g3	100	156	156	1	0
29	i	100	156	156	0	0
29	i3	200	312	312	2	0
29	j	200	312	312	0	0
29	j3	200	312	312	0	0
29	k	100	156	156	1	0
29	k3	100	156	156	1	0
29	l	200	312	312	7	0
29	l3	200	312	312	7	0
29	p	100	156	156	0	0
29	p3	100	156	156	0	0
29	r	100	156	156	1	0
30	D	54	88	88	0	0
30	D3	54	88	88	1	0
30	G	108	176	176	1	0
30	G3	108	176	176	1	0
30	d	54	88	88	0	0
30	d3	54	88	88	0	0
30	g	108	176	176	0	0
30	g3	108	176	176	0	0
31	F	5	0	0	0	0
31	F3	5	0	0	0	0
31	f	5	0	0	1	0
31	f3	5	0	0	0	0
32	I	53	74	74	8	0
32	I3	53	74	74	7	0
32	i	53	74	74	5	0
32	i3	53	74	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A1	31	11	12	1	0
33	A2	31	11	12	0	0
33	A4	31	11	12	0	0
33	A5	31	11	12	0	0
33	B1	31	11	12	2	0
33	B2	31	11	12	2	0
33	B4	31	11	12	2	0
33	B5	31	11	12	2	0
33	C1	31	11	12	0	0
33	C2	31	11	12	1	0
33	C4	31	11	12	0	0
33	C5	31	11	12	1	0
33	G	31	11	12	1	0
33	G3	31	11	12	2	0
33	g	31	11	12	1	0
33	g3	31	11	12	1	0
34	A1	1	0	0	0	0
34	A2	1	0	0	0	0
34	A4	1	0	0	0	0
34	A5	1	0	0	0	0
34	B1	1	0	0	0	0
34	B2	1	0	0	0	0
34	B4	1	0	0	0	0
34	B5	1	0	0	0	0
34	C1	1	0	0	0	0
34	C2	1	0	0	0	0
34	C4	1	0	0	0	0
34	C5	1	0	0	0	0
34	D1	1	0	0	0	0
34	D2	1	0	0	0	0
34	D4	1	0	0	0	0
34	D5	1	0	0	0	0
34	E1	1	0	0	0	0
34	E2	1	0	0	0	0
34	E4	1	0	0	0	0
34	E5	1	0	0	0	0
34	G	1	0	0	0	0
34	G3	1	0	0	0	0
34	g	1	0	0	0	0
34	g3	1	0	0	0	0
35	A	48	75	73	0	0
35	J	51	82	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	48	75	73	1	0
35	L3	51	82	82	0	0
35	a3	48	75	73	1	0
35	j3	51	82	82	0	0
35	l3	48	75	73	0	0
35	m	51	82	82	0	0
36	E	44	26	25	1	0
36	E3	44	26	25	0	0
36	e	44	26	25	0	0
36	e3	44	26	25	2	0
37	B1	27	11	12	0	0
37	B2	27	11	12	0	0
37	B4	27	11	12	0	0
37	B5	27	11	12	0	0
37	D1	27	11	11	2	0
37	D2	27	11	11	0	0
37	D4	27	11	11	0	0
37	D5	27	11	11	0	0
All	All	284056	287810	287818	2332	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 2332 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s3:36:VAL:O	21:t3:407:ARG:NH2	2.00	0.94
26:H2:47:LEU:HD23	26:Q2:37:LEU:HD23	1.52	0.91
18:s3:36:VAL:O	21:t3:407:ARG:NH2	2.08	0.87
1:a3:374:ILE:O	11:L3:128:TYR:OH	1.94	0.86
24:B2:289:ARG:NH1	24:B2:339:ARG:O	2.09	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	43	73
24	B2	509/546 (93%)	500 (98%)	9 (2%)	0	100	100
24	B4	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	43	73
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%)	396 (100%)	1 (0%)	86	87
1	A3	397/409 (97%)	395 (100%)	2 (0%)	81	85
1	a	397/409 (97%)	396 (100%)	1 (0%)	86	87
1	a3	397/409 (97%)	395 (100%)	2 (0%)	81	85
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%)	182 (100%)	1 (0%)	81	85
3	d3	183/206 (89%)	182 (100%)	1 (0%)	81	85
4	F	175/178 (98%)	173 (99%)	2 (1%)	65	78
4	F3	175/178 (98%)	173 (99%)	2 (1%)	65	78
4	f	175/178 (98%)	174 (99%)	1 (1%)	78	83
4	f3	175/178 (98%)	173 (99%)	2 (1%)	65	78
5	I	182/182 (100%)	180 (99%)	2 (1%)	65	78
5	I3	182/182 (100%)	180 (99%)	2 (1%)	65	78
5	i	182/182 (100%)	181 (100%)	1 (0%)	81	85
5	i3	182/182 (100%)	182 (100%)	0	100	100
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%)	152 (100%)	0	100	100
6	k3	152/152 (100%)	152 (100%)	0	100	100
7	C	93/97 (96%)	93 (100%)	0	100	100
7	C3	93/97 (96%)	93 (100%)	0	100	100
7	c	93/97 (96%)	93 (100%)	0	100	100
7	c3	93/97 (96%)	93 (100%)	0	100	100
8	G	235/262 (90%)	234 (100%)	1 (0%)	84	86
8	G3	235/262 (90%)	234 (100%)	1 (0%)	84	86
8	g	235/262 (90%)	234 (100%)	1 (0%)	84	86
8	g3	235/262 (90%)	234 (100%)	1 (0%)	84	86
9	H	208/245 (85%)	208 (100%)	0	100	100
9	H3	208/245 (85%)	208 (100%)	0	100	100
9	h	208/245 (85%)	208 (100%)	0	100	100
9	h3	208/245 (85%)	208 (100%)	0	100	100
10	J	235/239 (98%)	235 (100%)	0	100	100
10	J3	235/239 (98%)	235 (100%)	0	100	100
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%)	218 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L3	219/220 (100%)	218 (100%)	1 (0%)	81	85
11	l	219/220 (100%)	218 (100%)	1 (0%)	81	85
11	l3	219/220 (100%)	218 (100%)	1 (0%)	81	85
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%)	81	85
12	m3	202/202 (100%)	201 (100%)	1 (0%)	81	85
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%)	104 (100%)	0	100	100
13	n3	104/162 (64%)	104 (100%)	0	100	100
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%)	73	81
17	R3	120/129 (93%)	119 (99%)	1 (1%)	73	81
17	r	125/129 (97%)	124 (99%)	1 (1%)	73	81
17	r3	125/129 (97%)	124 (99%)	1 (1%)	73	81
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%)	108 (97%)	3 (3%)	39	67
18	s3	111/131 (85%)	108 (97%)	3 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	E	359/414 (87%)	359 (100%)	0	100	100
19	E3	359/414 (87%)	359 (100%)	0	100	100
19	e	359/414 (87%)	359 (100%)	0	100	100
19	e3	359/414 (87%)	359 (100%)	0	100	100
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%)	321 (99%)	4 (1%)	63	78
21	t3	325/414 (78%)	321 (99%)	4 (1%)	63	78
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%)	233 (100%)	1 (0%)	84	86
23	g2	234/254 (92%)	232 (99%)	2 (1%)	70	80
23	g4	234/254 (92%)	232 (99%)	2 (1%)	70	80
23	g5	234/254 (92%)	232 (99%)	2 (1%)	70	80
24	A1	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	A2	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	A4	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	A5	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	B1	422/453 (93%)	422 (100%)	0	100	100
24	B2	422/453 (93%)	422 (100%)	0	100	100
24	B4	422/453 (93%)	422 (100%)	0	100	100
24	B5	422/453 (93%)	422 (100%)	0	100	100
24	C1	424/453 (94%)	423 (100%)	1 (0%)	87	89
24	C2	424/453 (94%)	423 (100%)	1 (0%)	87	89
24	C4	424/453 (94%)	423 (100%)	1 (0%)	87	89
24	C5	424/453 (94%)	423 (100%)	1 (0%)	87	89
25	D1	381/402 (95%)	380 (100%)	1 (0%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D2	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	D4	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	D5	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	E1	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	E2	381/402 (95%)	381 (100%)	0	100	100
25	E4	381/402 (95%)	381 (100%)	0	100	100
25	E5	381/402 (95%)	380 (100%)	1 (0%)	86	87
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%)	58 (98%)	1 (2%)	53	74
26	I2	59/59 (100%)	59 (100%)	0	100	100
26	I4	59/59 (100%)	58 (98%)	1 (2%)	53	74
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%)	59 (100%)	0	100	100
26	K4	59/59 (100%)	59 (100%)	0	100	100
26	K5	59/59 (100%)	59 (100%)	0	100	100
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%)	115 (98%)	2 (2%)	53	74
27	d2	117/139 (84%)	116 (99%)	1 (1%)	70	80
27	d4	117/139 (84%)	116 (99%)	1 (1%)	70	80
27	d5	117/139 (84%)	115 (98%)	2 (2%)	53	74
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%)	29519 (100%)	81 (0%)	84	87

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G3	217	PHE
27	d4	126	GLU
17	R3	19	LEU
23	g4	194	TYR
25	D5	437	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
10	j3	130	GLN
5	I3	20	ASN
24	A5	506	ASN
11	l3	183	ASN
15	p3	150	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 oligosaccharides 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
32	UQ8	I	303	-	53,53,53	1.85	7 (13%)	66,67,67	1.66	16 (24%)
35	PEE	L	303	-	47,47,50	1.19	6 (12%)	50,52,55	1.19	5 (10%)
29	CDL	B3	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
33	ATP	G	301	34	32,33,33	3.54	13 (40%)	48,52,52	2.22	14 (29%)
29	CDL	f	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	5 (4%)
30	PC1	G3	304	-	53,53,53	0.96	4 (7%)	59,61,61	1.01	2 (3%)
36	NAD	e3	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.10	13 (20%)
33	ATP	C5	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
29	CDL	b3	401	-	99,99,99	0.89	8 (8%)	105,111,111	1.13	4 (3%)
29	CDL	K3	202	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	5 (4%)
29	CDL	A	502	-	99,99,99	0.90	8 (8%)	105,111,111	1.11	4 (3%)
35	PEE	m	301	-	50,50,50	1.16	6 (12%)	53,55,55	1.12	5 (9%)
32	UQ8	i3	303	-	53,53,53	1.85	7 (13%)	66,67,67	1.60	16 (24%)
30	PC1	g	304	-	53,53,53	0.97	4 (7%)	59,61,61	0.96	3 (5%)
33	ATP	A4	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	13 (27%)
29	CDL	I3	303	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	B1	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.27	17 (39%)
29	CDL	j3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	A3	501	-	99,99,99	0.90	8 (8%)	105,111,111	1.09	4 (3%)
29	CDL	J	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	F	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	5 (4%)
29	CDL	L	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	i	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.08	4 (3%)
29	CDL	l3	303	-	99,99,99	0.90	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	a	501	-	99,99,99	0.90	8 (8%)	105,111,111	1.07	5 (4%)
29	CDL	B	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.98	4 (3%)
33	ATP	g3	301	34	32,33,33	3.54	13 (40%)	48,52,52	2.22	14 (29%)
33	ATP	g	301	34	32,33,33	3.55	13 (40%)	48,52,52	2.21	13 (27%)
37	ADP	D5	501	34	28,29,29	3.42	10 (35%)	43,45,45	3.26	15 (34%)
29	CDL	I	301	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
33	ATP	G3	301	34	32,33,33	3.54	13 (40%)	48,52,52	2.22	13 (27%)
29	CDL	r	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	J3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	i3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
29	CDL	k3	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PC1	D3	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.10	2 (3%)
29	CDL	f3	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
29	CDL	f	304	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
30	PC1	g3	303	-	53,53,53	0.97	4 (7%)	59,61,61	1.01	2 (3%)
35	PEE	A	501	-	47,47,50	1.20	6 (12%)	50,52,55	1.23	4 (8%)
29	CDL	p	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	j	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	I3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
30	PC1	g	303	-	53,53,53	0.97	4 (7%)	59,61,61	0.99	2 (3%)
33	ATP	C4	601	34	32,33,33	3.58	13 (40%)	48,52,52	2.19	13 (27%)
29	CDL	i3	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	B5	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.28	16 (37%)
29	CDL	a3	502	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	5 (4%)
35	PEE	l3	302	-	47,47,50	1.19	6 (12%)	50,52,55	1.23	4 (8%)
29	CDL	K	202	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	4 (3%)
31	PO4	f	301	-	4,4,4	1.01	0	6,6,6	0.44	0
29	CDL	B	403	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	f3	304	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
30	PC1	g3	304	-	53,53,53	0.97	4 (7%)	59,61,61	0.93	2 (3%)
31	PO4	F	301	-	4,4,4	1.03	0	6,6,6	0.48	0
29	CDL	B3	404	-	99,99,99	0.90	8 (8%)	105,111,111	1.12	5 (4%)
33	ATP	B5	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.21	14 (29%)
33	ATP	B4	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	14 (29%)
29	CDL	B3	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.13	5 (4%)
36	NAD	E3	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.11	13 (20%)
29	CDL	g	305	-	99,99,99	0.90	8 (8%)	105,111,111	1.09	4 (3%)
29	CDL	I3	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.03	4 (3%)
30	PC1	G	304	-	53,53,53	0.96	4 (7%)	59,61,61	0.99	2 (3%)
29	CDL	b	401	-	99,99,99	0.88	7 (7%)	105,111,111	1.11	5 (4%)
37	ADP	D2	501	34	28,29,29	3.43	10 (35%)	43,45,45	3.25	15 (34%)
29	CDL	j	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	I	302	-	99,99,99	0.89	7 (7%)	105,111,111	1.06	4 (3%)
33	ATP	B1	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.19	14 (29%)
36	NAD	e	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.12	13 (20%)
29	CDL	f	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	l	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	4 (3%)
30	PC1	d3	301	-	53,53,53	0.96	4 (7%)	59,61,61	1.08	2 (3%)
33	ATP	A5	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
29	CDL	l	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	J	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.06	4 (3%)
29	CDL	L	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
33	ATP	B2	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.21	14 (29%)
29	CDL	B	404	-	99,99,99	0.90	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	P	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.03	5 (4%)
29	CDL	P3	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	5 (4%)
35	PEE	L3	302	-	50,50,50	1.17	6 (12%)	53,55,55	1.17	4 (7%)
30	PC1	G	303	-	53,53,53	0.97	4 (7%)	59,61,61	1.01	2 (3%)
33	ATP	A1	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
30	PC1	d	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.08	2 (3%)
29	CDL	l3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	5 (4%)
29	CDL	J3	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	B	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.13	6 (5%)
29	CDL	g3	305	-	99,99,99	0.89	8 (8%)	105,111,111	1.11	4 (3%)
29	CDL	K	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	B3	403	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	F	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)
33	ATP	C2	601	34	32,33,33	3.58	13 (40%)	48,52,52	2.20	13 (27%)
29	CDL	f3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
37	ADP	B2	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.28	17 (39%)
29	CDL	p3	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	D1	501	34	28,29,29	3.42	11 (39%)	43,45,45	3.46	16 (37%)
31	PO4	F3	301	-	4,4,4	1.01	0	6,6,6	0.46	0
29	CDL	K3	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
29	CDL	F3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
35	PEE	a3	503	-	47,47,50	1.20	6 (12%)	50,52,55	1.19	5 (10%)
32	UQ8	I3	304	-	53,53,53	1.87	7 (13%)	66,67,67	1.63	16 (24%)
33	ATP	C1	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.18	12 (25%)
35	PEE	j3	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.11	5 (9%)
36	NAD	E	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.09	13 (20%)
29	CDL	L3	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.00	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	j3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
32	UQ8	i	302	-	53,53,53	1.86	7 (13%)	66,67,67	1.59	17 (25%)
37	ADP	D4	501	34	28,29,29	3.43	11 (39%)	43,45,45	3.46	15 (34%)
29	CDL	k	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
37	ADP	B4	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.28	17 (39%)
29	CDL	a3	501	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	5 (4%)
35	PEE	J	303	-	50,50,50	1.17	6 (12%)	53,55,55	1.17	5 (9%)
30	PC1	G3	303	-	53,53,53	0.97	4 (7%)	59,61,61	1.00	2 (3%)
33	ATP	A2	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	13 (27%)
31	PO4	f3	301	-	4,4,4	1.03	0	6,6,6	0.48	0
30	PC1	D	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.09	2 (3%)

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
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
35	PEE	L	303	-	-	21/51/51/54	-
29	CDL	B3	401	-	-	44/110/110/110	-
33	ATP	G	301	34	-	0/22/38/38	0/3/3/3
29	CDL	f	303	-	-	42/110/110/110	-
30	PC1	G3	304	-	-	19/57/57/57	-
36	NAD	e3	900	-	-	9/30/62/62	0/5/5/5
33	ATP	C5	601	34	-	4/22/38/38	0/3/3/3
29	CDL	b3	401	-	-	43/110/110/110	-
29	CDL	K3	202	-	-	35/110/110/110	-
29	CDL	A	502	-	-	46/110/110/110	-
35	PEE	m	301	-	-	24/54/54/54	-
32	UQ8	i3	303	-	-	8/51/75/75	0/1/1/1
30	PC1	g	304	-	-	19/57/57/57	-
33	ATP	A4	601	34	-	5/22/38/38	0/3/3/3
29	CDL	I3	303	-	-	38/110/110/110	-
37	ADP	B1	1002	34	-	1/16/32/32	0/3/3/3
29	CDL	j3	302	-	-	41/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	A3	501	-	-	45/110/110/110	-
29	CDL	J	302	-	-	37/110/110/110	-
29	CDL	F	302	-	-	38/110/110/110	-
29	CDL	L	302	-	-	44/110/110/110	-
29	CDL	i	301	-	-	38/110/110/110	-
29	CDL	l3	303	-	-	40/110/110/110	-
29	CDL	a	501	-	-	34/110/110/110	-
29	CDL	B	401	-	-	44/110/110/110	-
33	ATP	g3	301	34	-	0/22/38/38	0/3/3/3
33	ATP	g	301	34	-	0/22/38/38	0/3/3/3
37	ADP	D5	501	34	-	1/16/32/32	0/3/3/3
29	CDL	I	301	-	-	45/110/110/110	-
33	ATP	G3	301	34	-	0/22/38/38	0/3/3/3
29	CDL	r	201	-	-	36/110/110/110	-
29	CDL	J3	302	-	-	40/110/110/110	-
29	CDL	i3	302	-	-	37/110/110/110	-
29	CDL	k3	201	-	-	36/110/110/110	-
30	PC1	D3	301	-	-	22/57/57/57	-
29	CDL	f3	303	-	-	42/110/110/110	-
29	CDL	f	304	-	-	47/110/110/110	-
30	PC1	g3	303	-	-	20/57/57/57	-
35	PEE	A	501	-	-	20/51/51/54	-
29	CDL	p	201	-	-	44/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
29	CDL	I3	301	-	-	43/110/110/110	-
30	PC1	g	303	-	-	20/57/57/57	-
33	ATP	C4	601	34	-	5/22/38/38	0/3/3/3
29	CDL	i3	301	-	-	36/110/110/110	-
37	ADP	B5	1002	34	-	2/16/32/32	0/3/3/3
29	CDL	a3	502	-	-	38/110/110/110	-
35	PEE	l3	302	-	-	20/51/51/54	-
29	CDL	K	202	-	-	34/110/110/110	-
29	CDL	B	403	-	-	33/110/110/110	-
29	CDL	f3	304	-	-	47/110/110/110	-
30	PC1	g3	304	-	-	17/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	B3	404	-	-	44/110/110/110	-
33	ATP	B5	1003	34	-	1/22/38/38	0/3/3/3
33	ATP	B4	1003	34	-	1/22/38/38	0/3/3/3
29	CDL	B3	402	-	-	39/110/110/110	-
36	NAD	E3	900	-	-	7/30/62/62	0/5/5/5
29	CDL	g	305	-	-	34/110/110/110	-
29	CDL	I3	302	-	-	44/110/110/110	-
30	PC1	G	304	-	-	19/57/57/57	-
29	CDL	b	401	-	-	44/110/110/110	-
37	ADP	D2	501	34	-	1/16/32/32	0/3/3/3
29	CDL	j	301	-	-	38/110/110/110	-
29	CDL	I	302	-	-	38/110/110/110	-
33	ATP	B1	1003	34	-	1/22/38/38	0/3/3/3
36	NAD	e	900	-	-	8/30/62/62	0/5/5/5
29	CDL	f	302	-	-	53/110/110/110	-
29	CDL	l	302	-	-	40/110/110/110	-
30	PC1	d3	301	-	-	23/57/57/57	-
33	ATP	A5	601	34	-	6/22/38/38	0/3/3/3
29	CDL	l	301	-	-	38/110/110/110	-
29	CDL	J	301	-	-	40/110/110/110	-
29	CDL	L	301	-	-	37/110/110/110	-
33	ATP	B2	1003	34	-	1/22/38/38	0/3/3/3
29	CDL	B	404	-	-	45/110/110/110	-
29	CDL	P	201	-	-	36/110/110/110	-
29	CDL	P3	201	-	-	36/110/110/110	-
35	PEE	L3	302	-	-	28/54/54/54	-
30	PC1	G	303	-	-	28/57/57/57	-
33	ATP	A1	601	34	-	5/22/38/38	0/3/3/3
30	PC1	d	301	-	-	23/57/57/57	-
29	CDL	l3	301	-	-	38/110/110/110	-
29	CDL	J3	301	-	-	41/110/110/110	-
29	CDL	B	402	-	-	38/110/110/110	-
29	CDL	g3	305	-	-	34/110/110/110	-
29	CDL	K	201	-	-	28/110/110/110	-
29	CDL	B3	403	-	-	32/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	F	303	-	-	46/110/110/110	-
33	ATP	C2	601	34	-	4/22/38/38	0/3/3/3
29	CDL	f3	302	-	-	53/110/110/110	-
37	ADP	B2	1002	34	-	2/16/32/32	0/3/3/3
29	CDL	p3	201	-	-	43/110/110/110	-
37	ADP	D1	501	34	-	3/16/32/32	0/3/3/3
29	CDL	K3	201	-	-	28/110/110/110	-
29	CDL	F3	302	-	-	45/110/110/110	-
35	PEE	a3	503	-	-	21/51/51/54	-
32	UQ8	I3	304	-	-	9/51/75/75	0/1/1/1
33	ATP	C1	601	34	-	5/22/38/38	0/3/3/3
35	PEE	j3	303	-	-	24/54/54/54	-
36	NAD	E	900	-	-	8/30/62/62	0/5/5/5
29	CDL	L3	301	-	-	37/110/110/110	-
29	CDL	j3	301	-	-	39/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
37	ADP	D4	501	34	-	3/16/32/32	0/3/3/3
29	CDL	k	201	-	-	36/110/110/110	-
37	ADP	B4	1002	34	-	1/16/32/32	0/3/3/3
29	CDL	a3	501	-	-	34/110/110/110	-
35	PEE	J	303	-	-	28/54/54/54	-
30	PC1	G3	303	-	-	28/57/57/57	-
33	ATP	A2	601	34	-	6/22/38/38	0/3/3/3
30	PC1	D	301	-	-	22/57/57/57	-

The worst 5 of 972 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D2	501	ADP	C2'-C3'	-10.64	1.24	1.53
37	D5	501	ADP	C2'-C3'	-10.59	1.24	1.53
37	B2	1002	ADP	C2'-C3'	-10.58	1.24	1.53
37	D1	501	ADP	C2'-C3'	-10.58	1.24	1.53
37	B4	1002	ADP	C2'-C3'	-10.56	1.24	1.53

The worst 5 of 772 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D4	501	ADP	C1'-N9-C8	-13.42	97.31	127.09
37	D1	501	ADP	C1'-N9-C8	-13.38	97.40	127.09
37	B5	1002	ADP	C1'-N9-C8	-12.29	99.81	127.09
37	B1	1002	ADP	C1'-N9-C8	-12.27	99.87	127.09
37	B4	1002	ADP	C1'-N9-C8	-12.25	99.91	127.09

There are no chirality outliers.

5 of 2956 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-OB2
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4

There are no ring outliers.

61 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	I	303	UQ8	8	0
35	L	303	PEE	1	0
33	G	301	ATP	1	0
29	f	303	CDL	3	0
36	e3	900	NAD	2	0
33	C5	601	ATP	1	0
29	b3	401	CDL	1	0
29	K3	202	CDL	1	0
32	i3	303	UQ8	5	0
29	A3	501	CDL	1	0
29	F	302	CDL	12	0
29	L	302	CDL	7	0
29	l3	303	CDL	3	0
29	a	501	CDL	2	0
33	g3	301	ATP	1	0
33	g	301	ATP	1	0
29	I	301	CDL	3	0
33	G3	301	ATP	2	0
29	r	201	CDL	1	0
29	k3	201	CDL	1	0
30	D3	301	PC1	1	0
29	f3	303	CDL	2	0

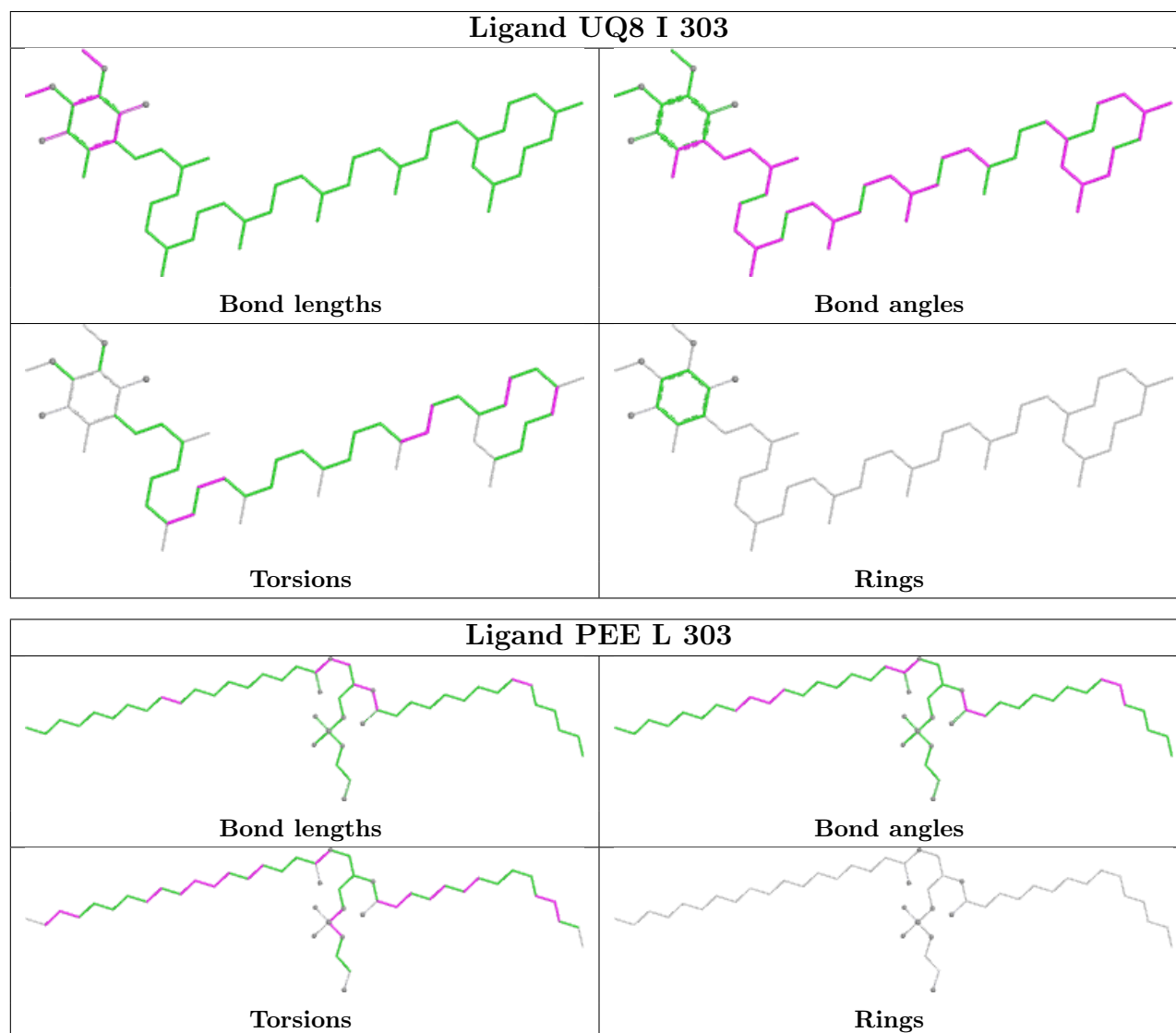
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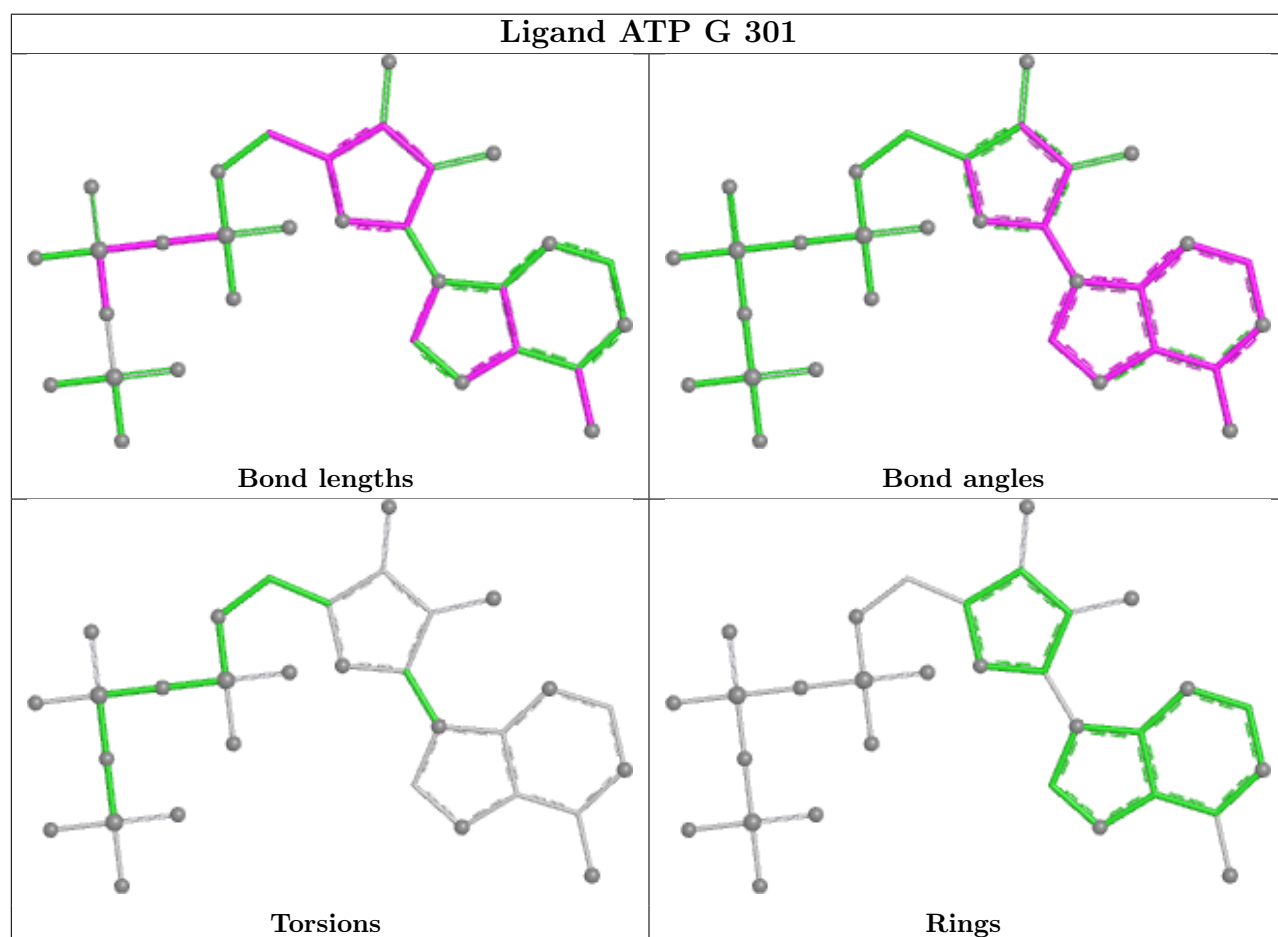
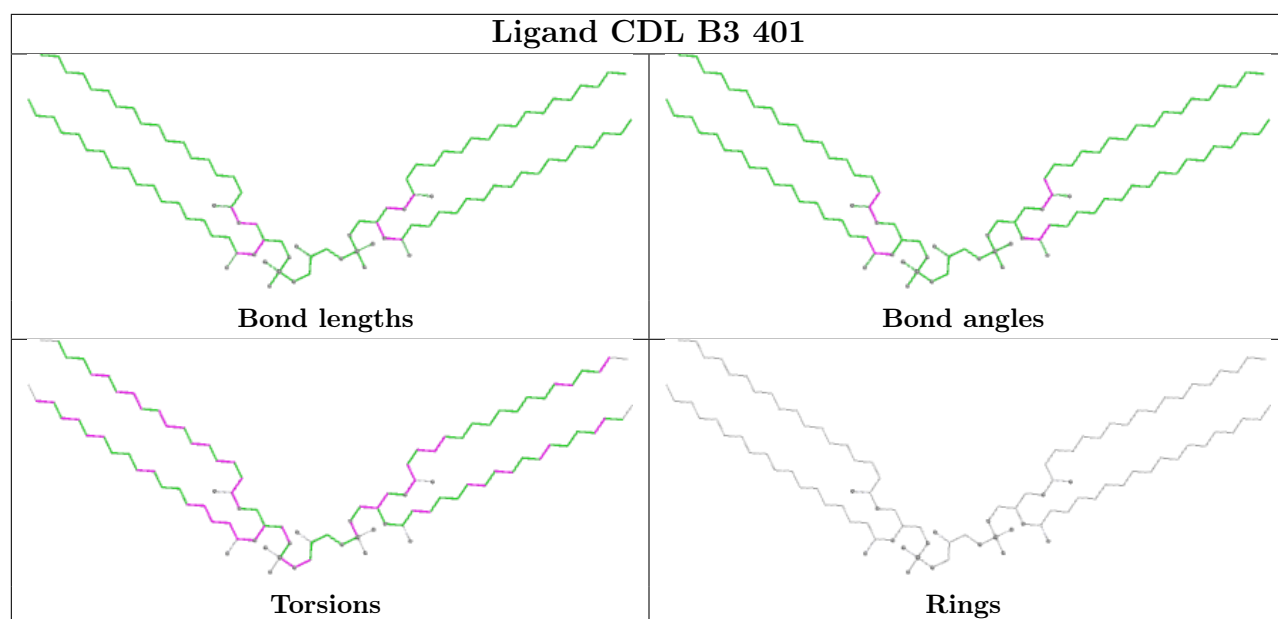
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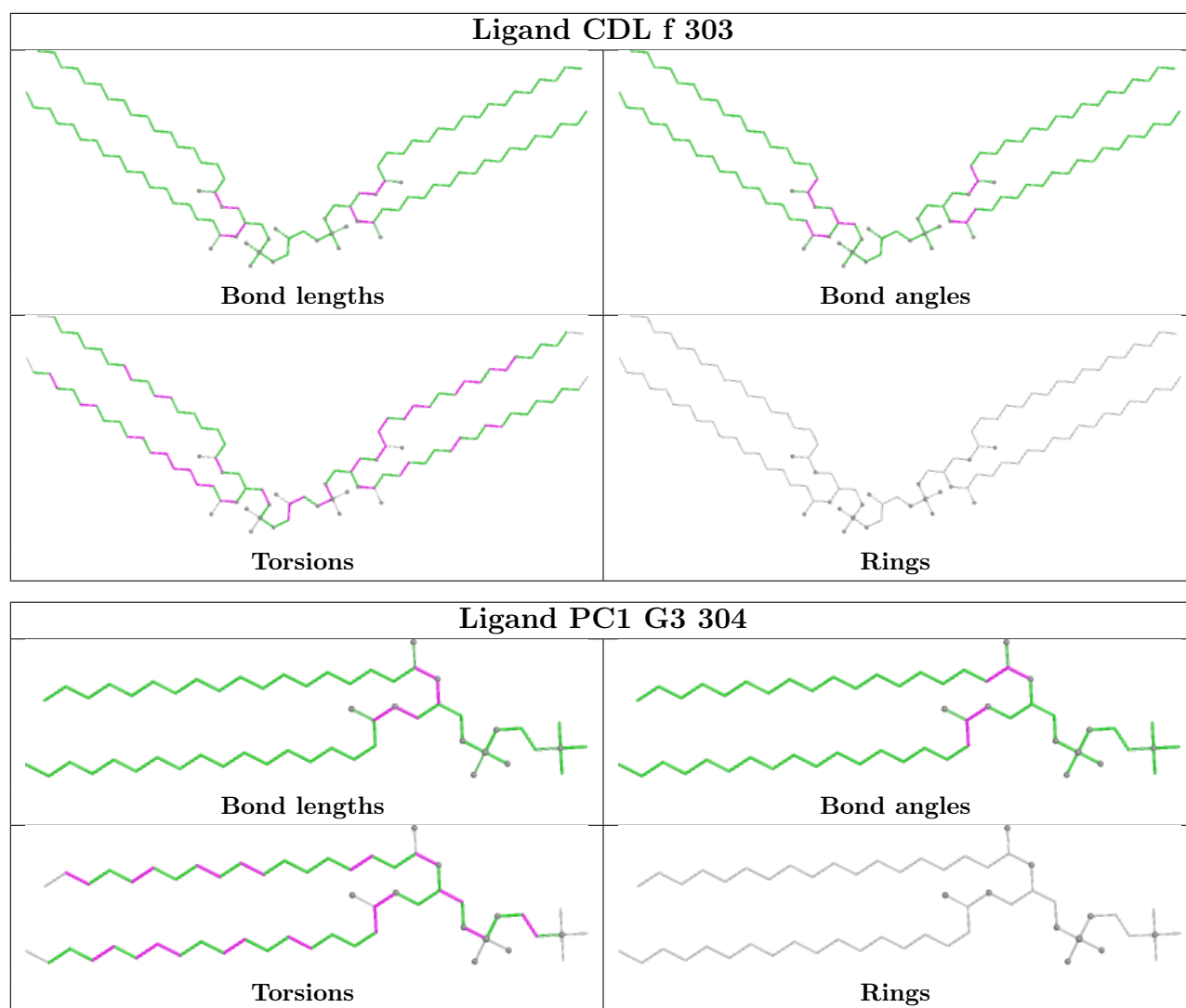
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	f	304	CDL	1	0
29	I3	301	CDL	5	0
29	i3	301	CDL	2	0
29	a3	502	CDL	14	0
31	f	301	PO4	1	0
29	B	403	CDL	1	0
29	B3	404	CDL	3	0
33	B5	1003	ATP	2	0
33	B4	1003	ATP	2	0
29	B3	402	CDL	3	0
29	g	305	CDL	1	0
29	I3	302	CDL	9	0
29	b	401	CDL	1	0
33	B1	1003	ATP	2	0
29	l	302	CDL	3	0
29	l	301	CDL	4	0
29	L	301	CDL	1	0
33	B2	1003	ATP	2	0
29	B	404	CDL	4	0
30	G	303	PC1	1	0
33	A1	601	ATP	1	0
29	l3	301	CDL	4	0
29	B	402	CDL	3	0
29	g3	305	CDL	1	0
29	K	201	CDL	1	0
29	B3	403	CDL	2	0
29	F	303	CDL	2	0
33	C2	601	ATP	1	0
37	D1	501	ADP	2	0
29	K3	201	CDL	1	0
29	F3	302	CDL	2	0
35	a3	503	PEE	1	0
32	I3	304	UQ8	7	0
36	E	900	NAD	1	0
29	L3	301	CDL	1	0
32	i	302	UQ8	5	0
29	k	201	CDL	1	0
35	J	303	PEE	1	0
30	G3	303	PC1	1	0

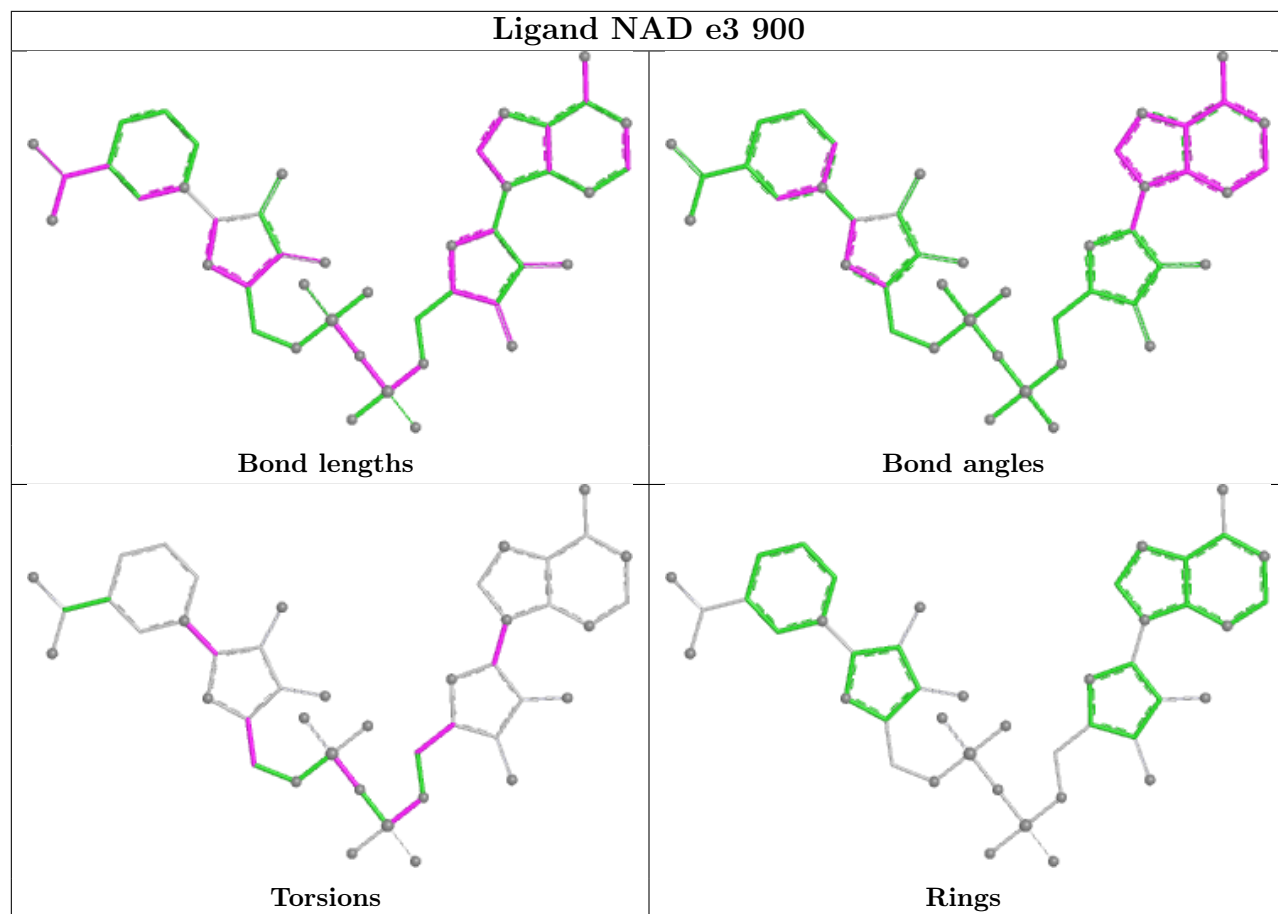
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

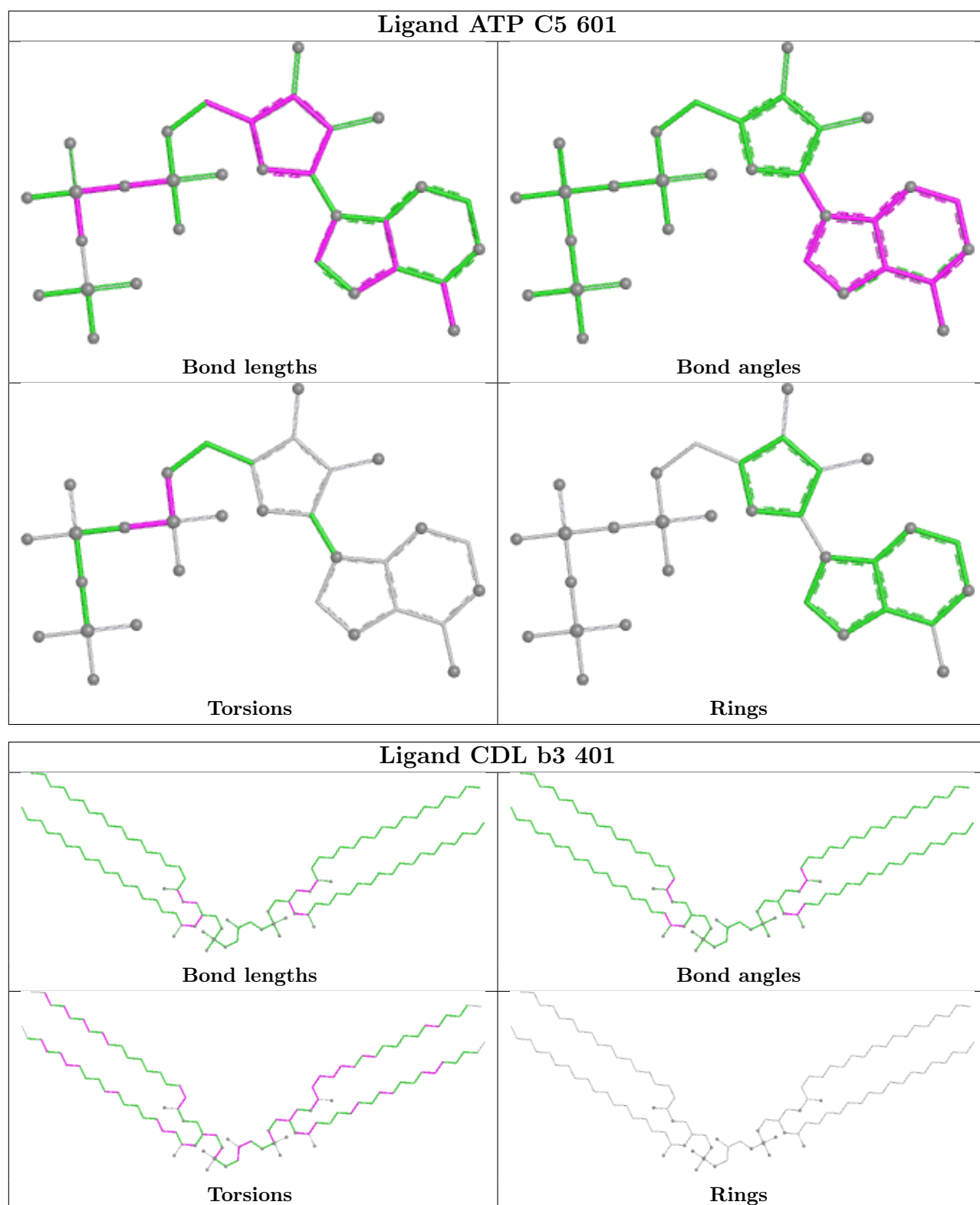
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

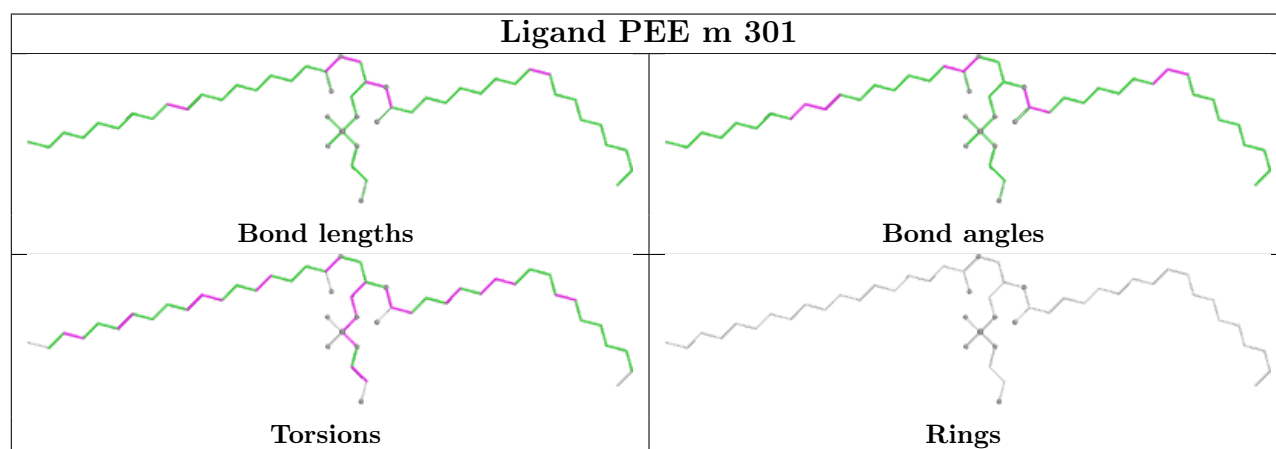
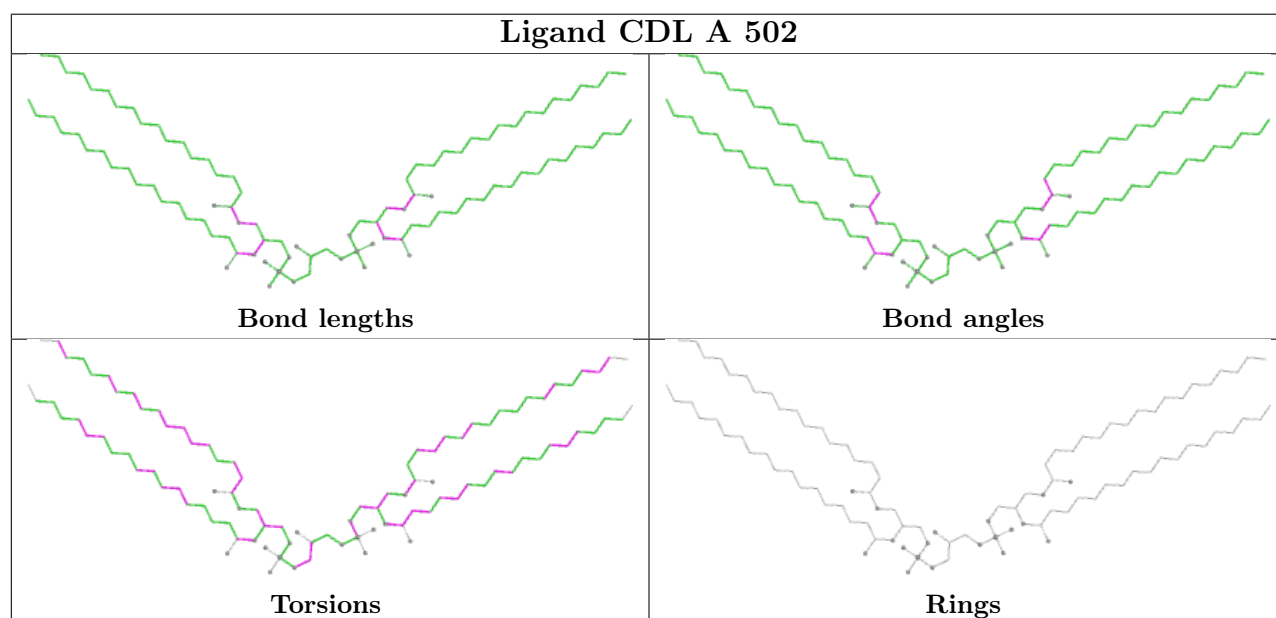
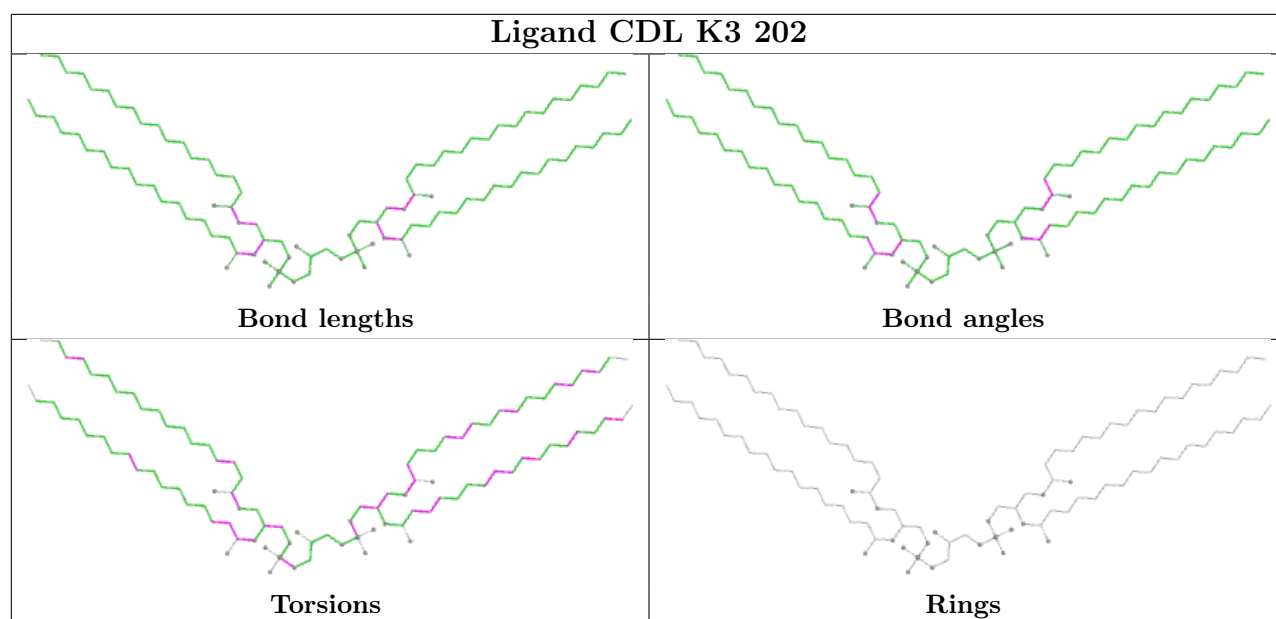


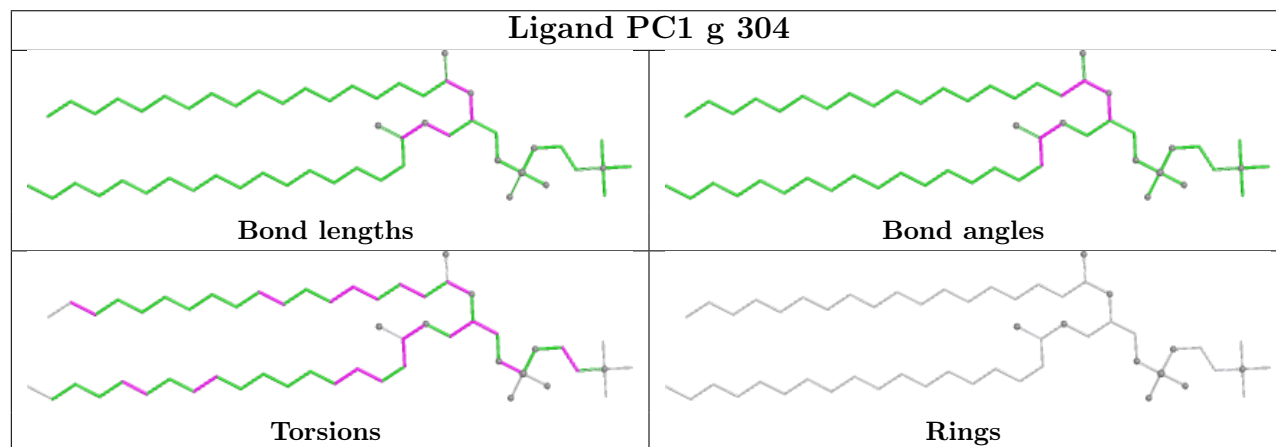
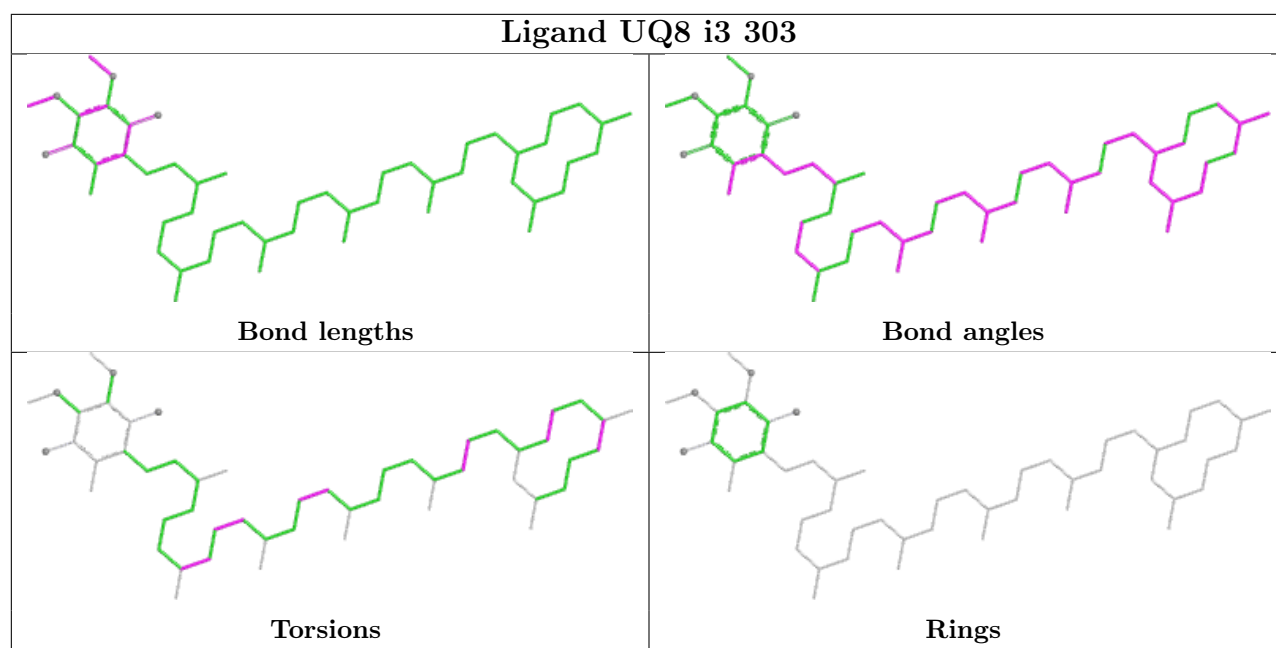


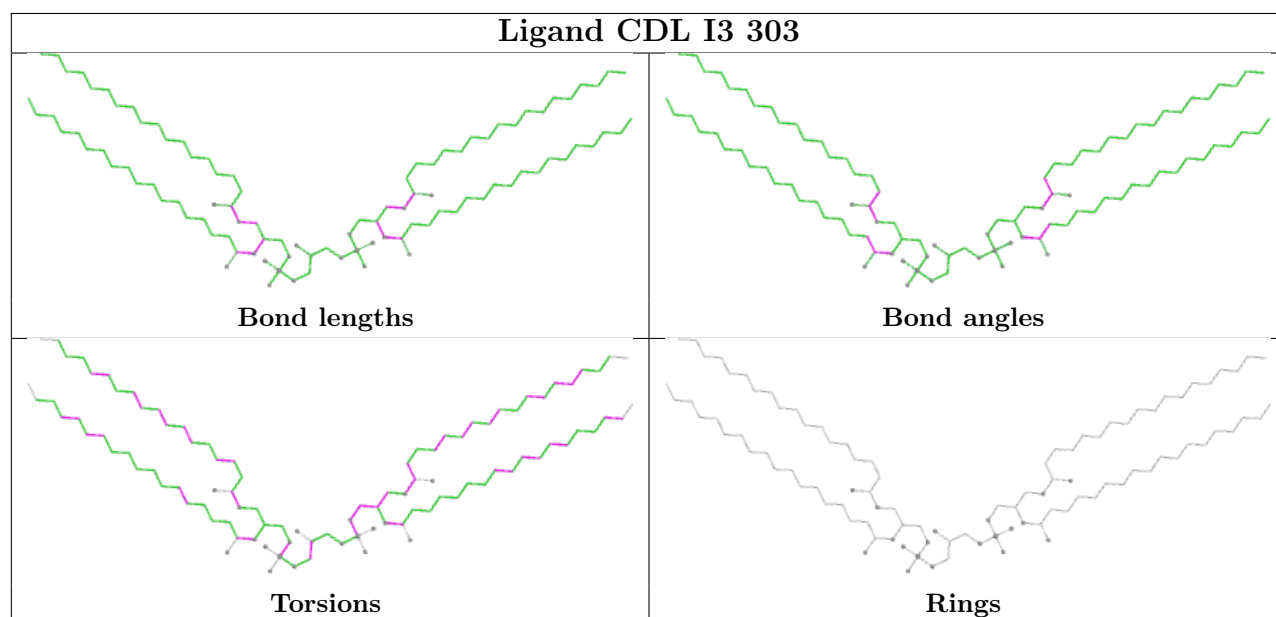
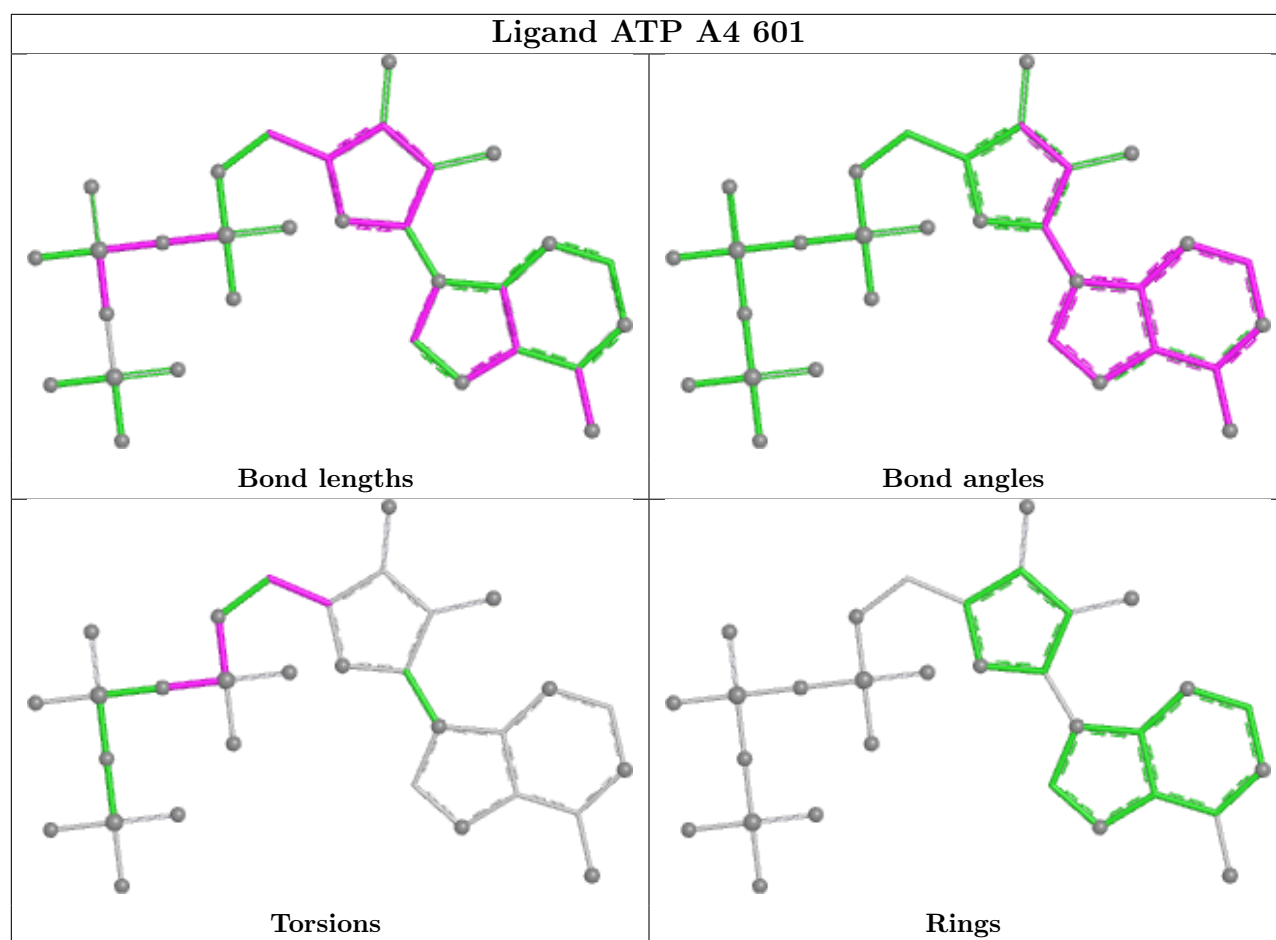


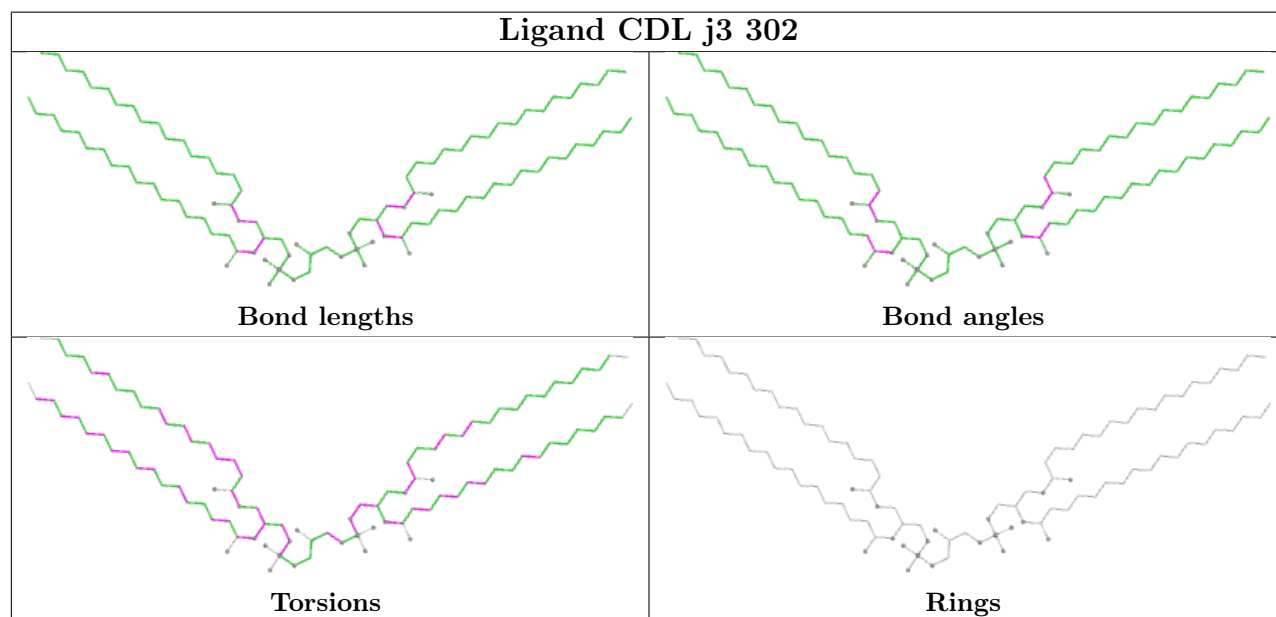
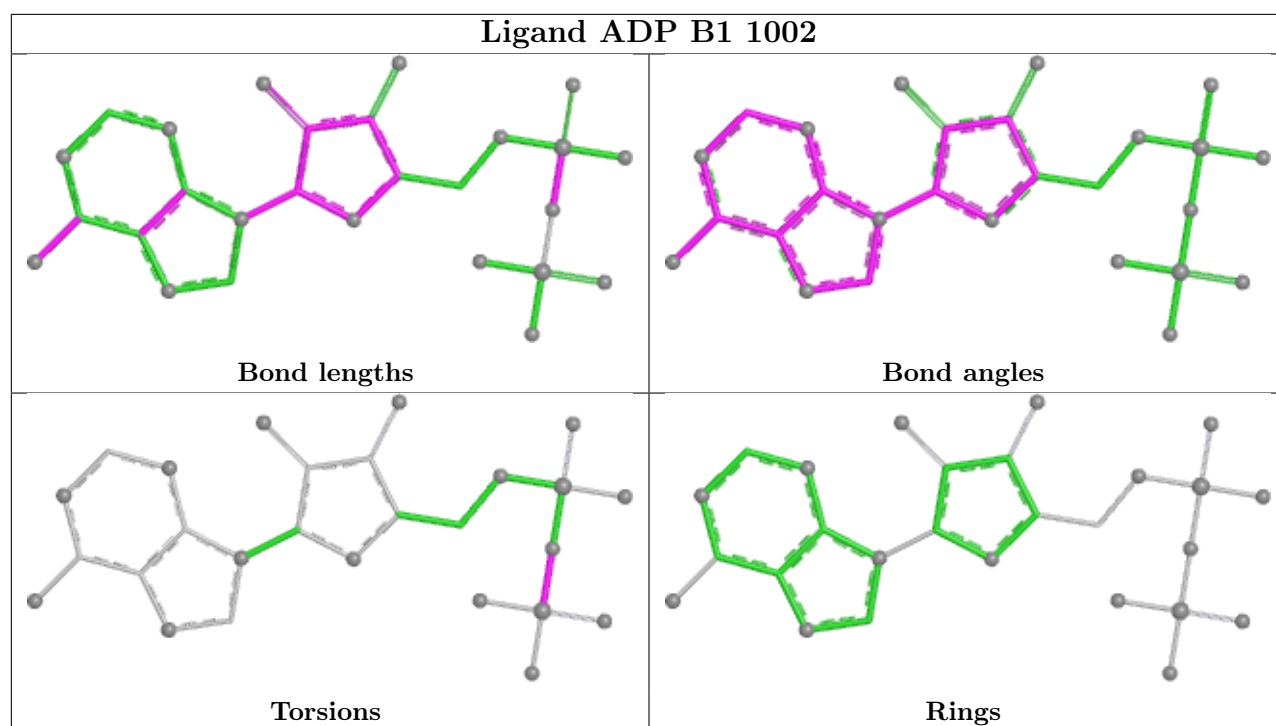


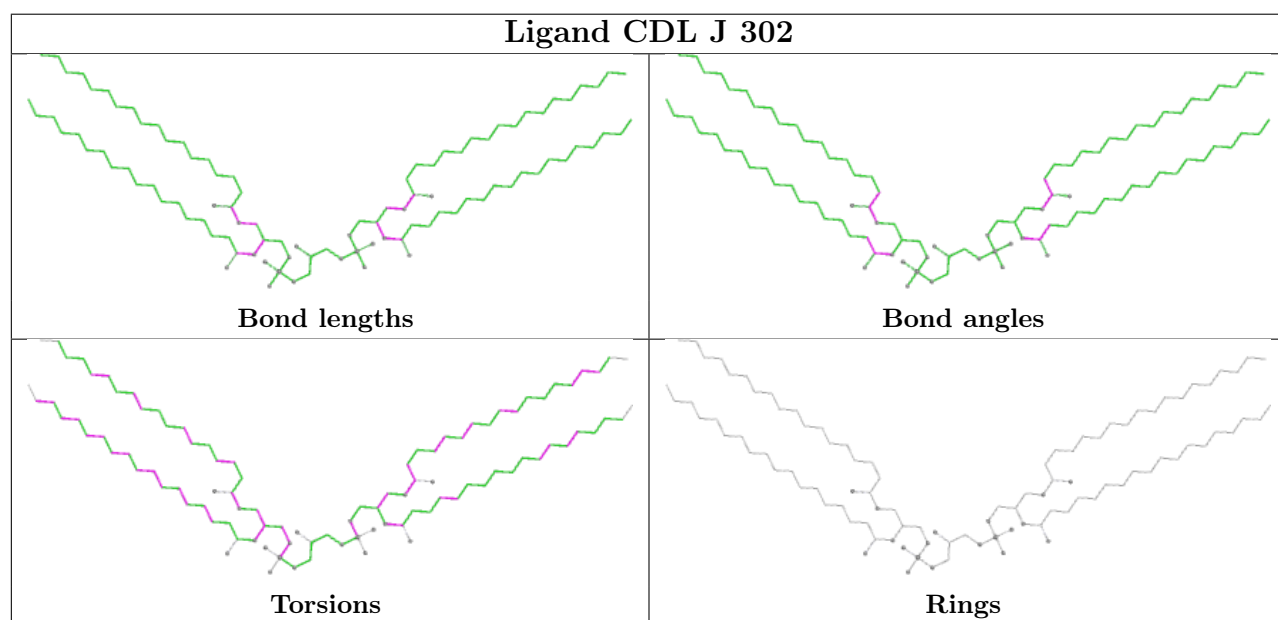
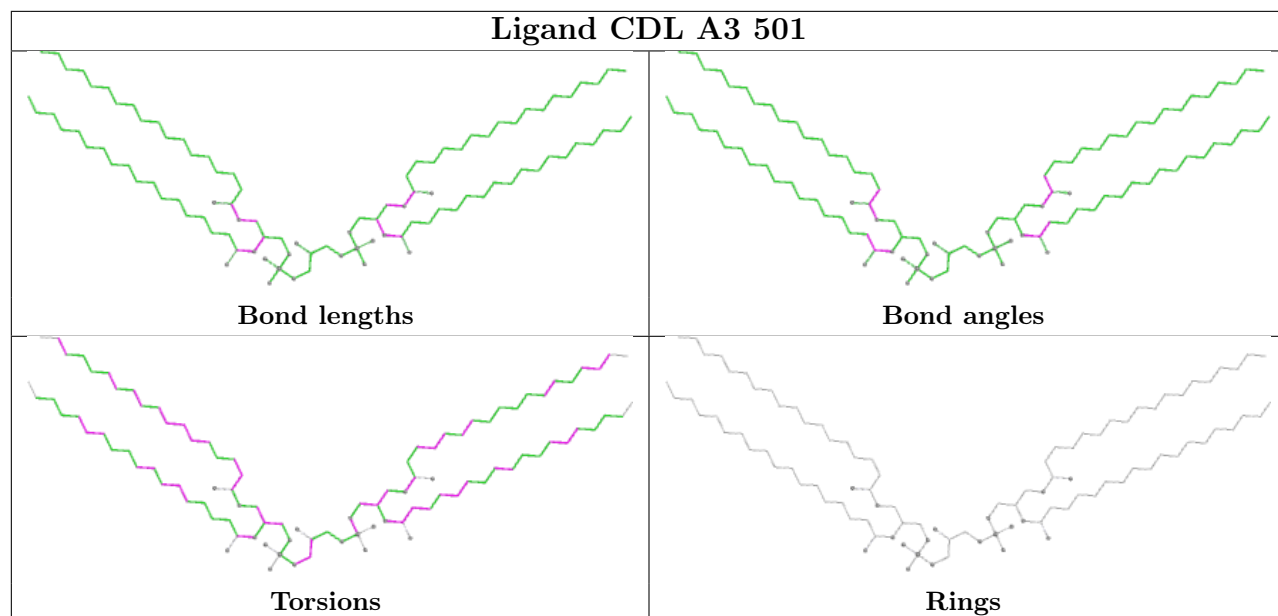


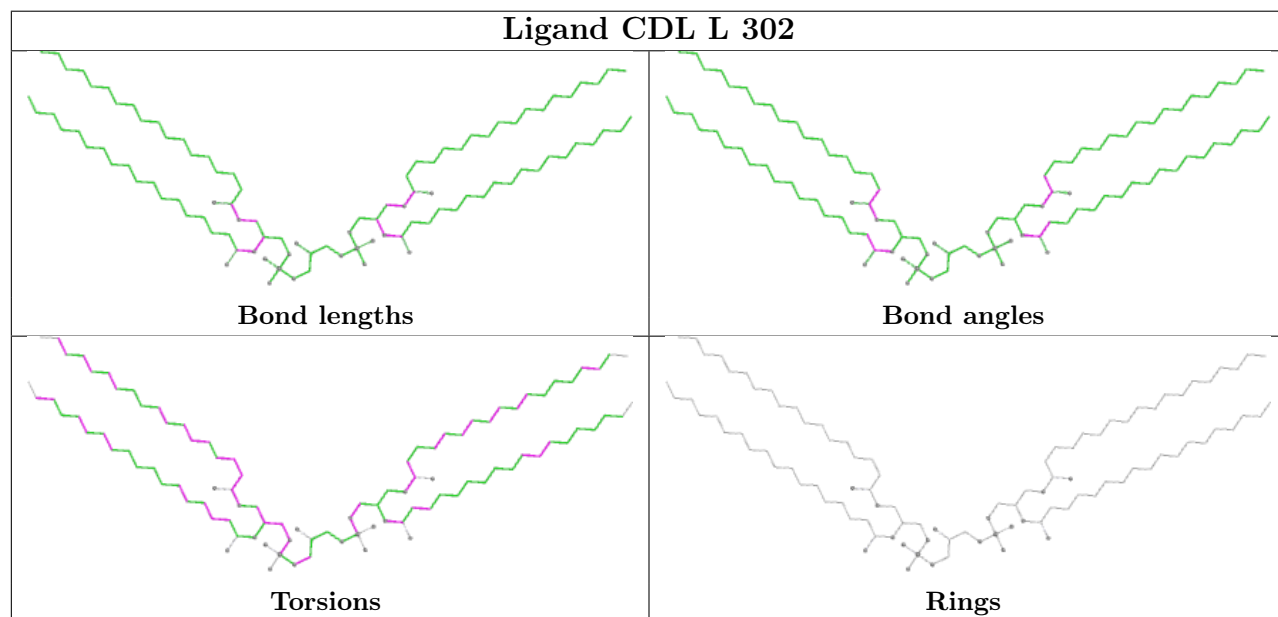
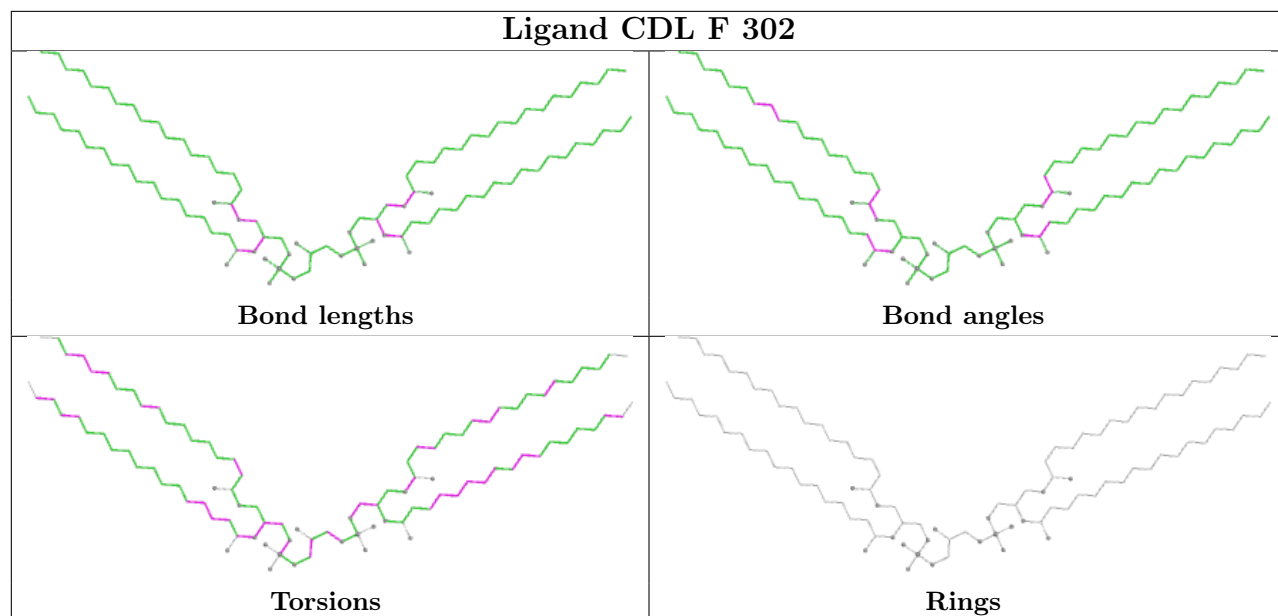


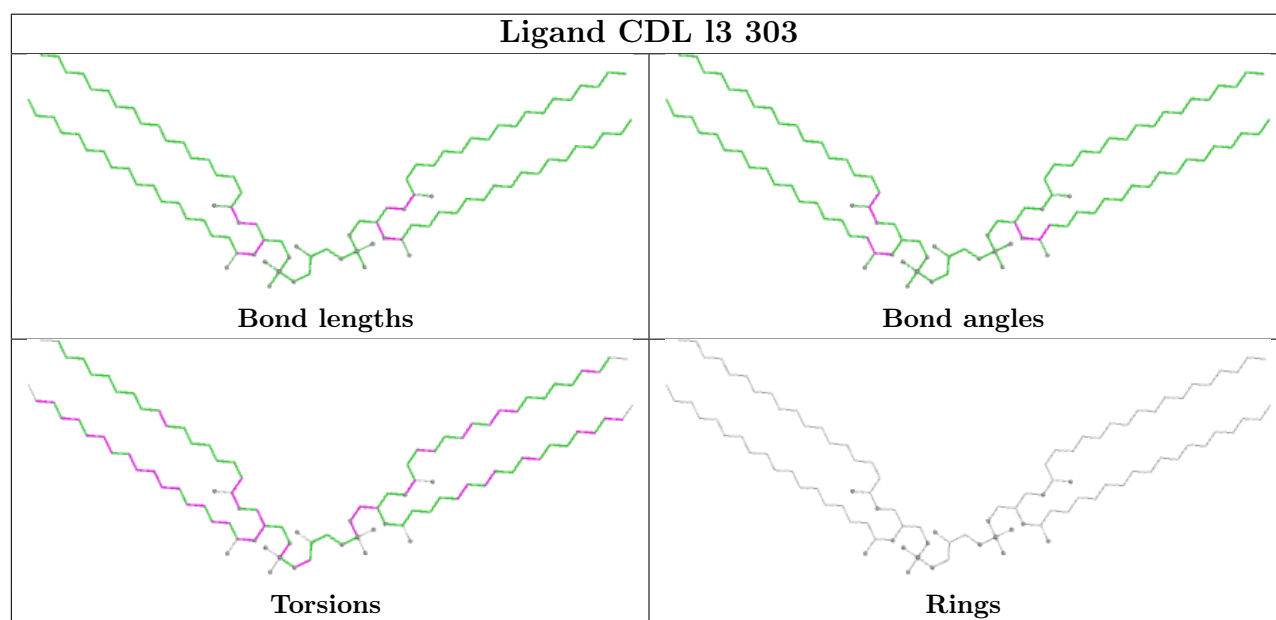
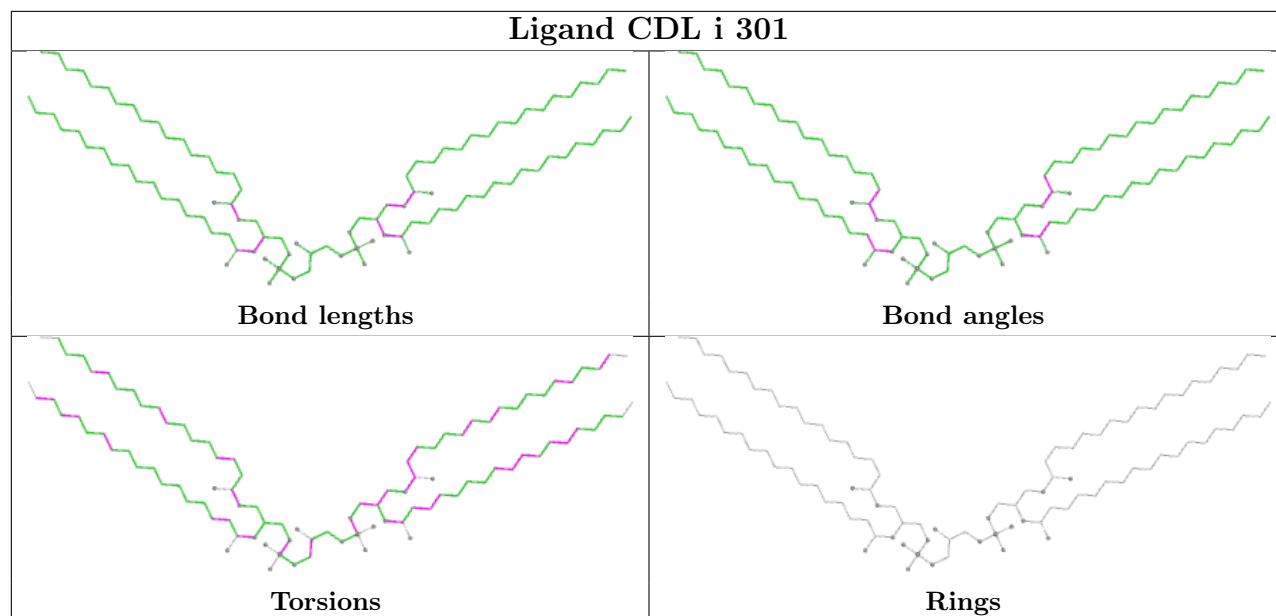


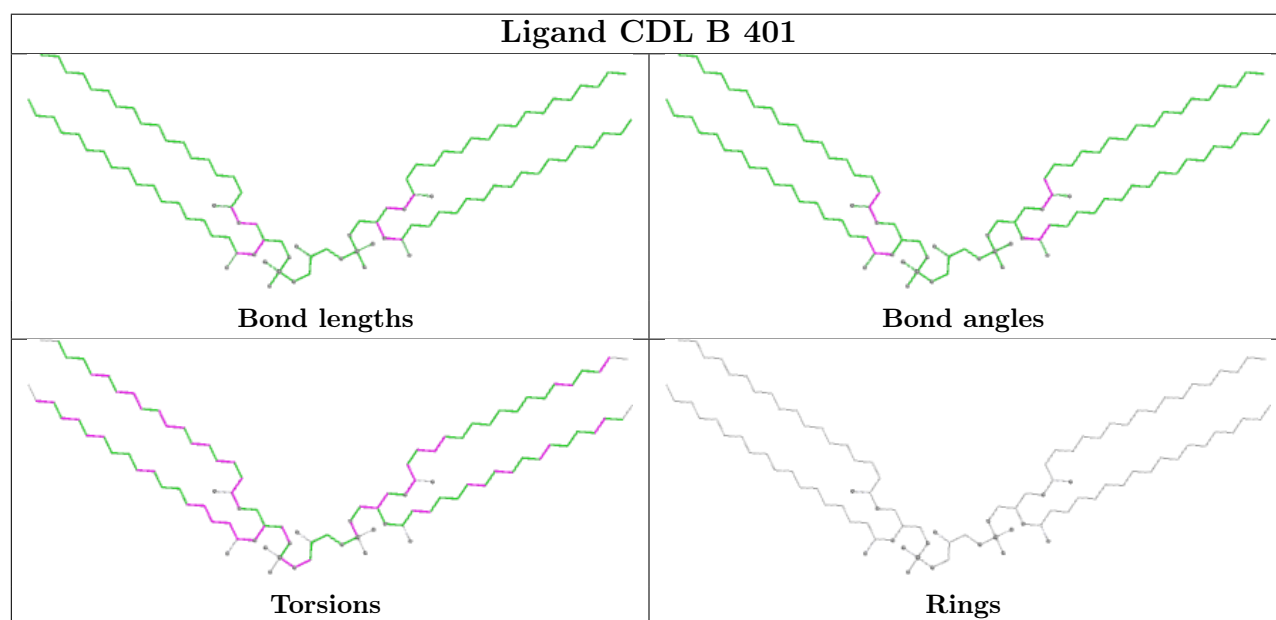
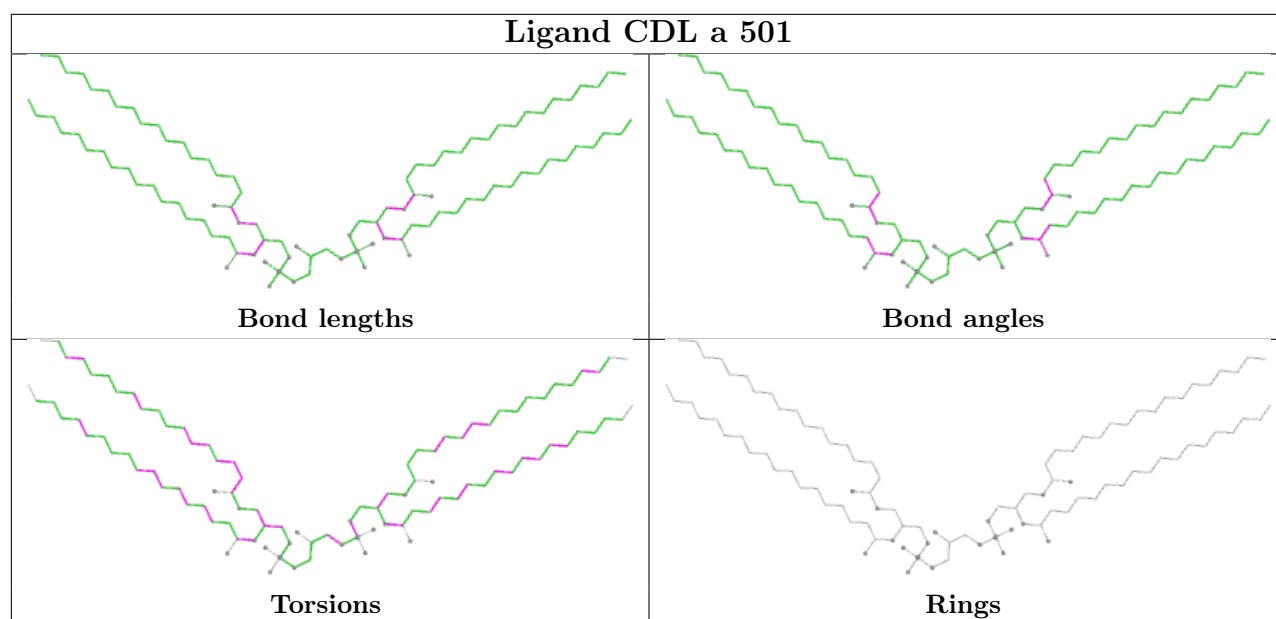


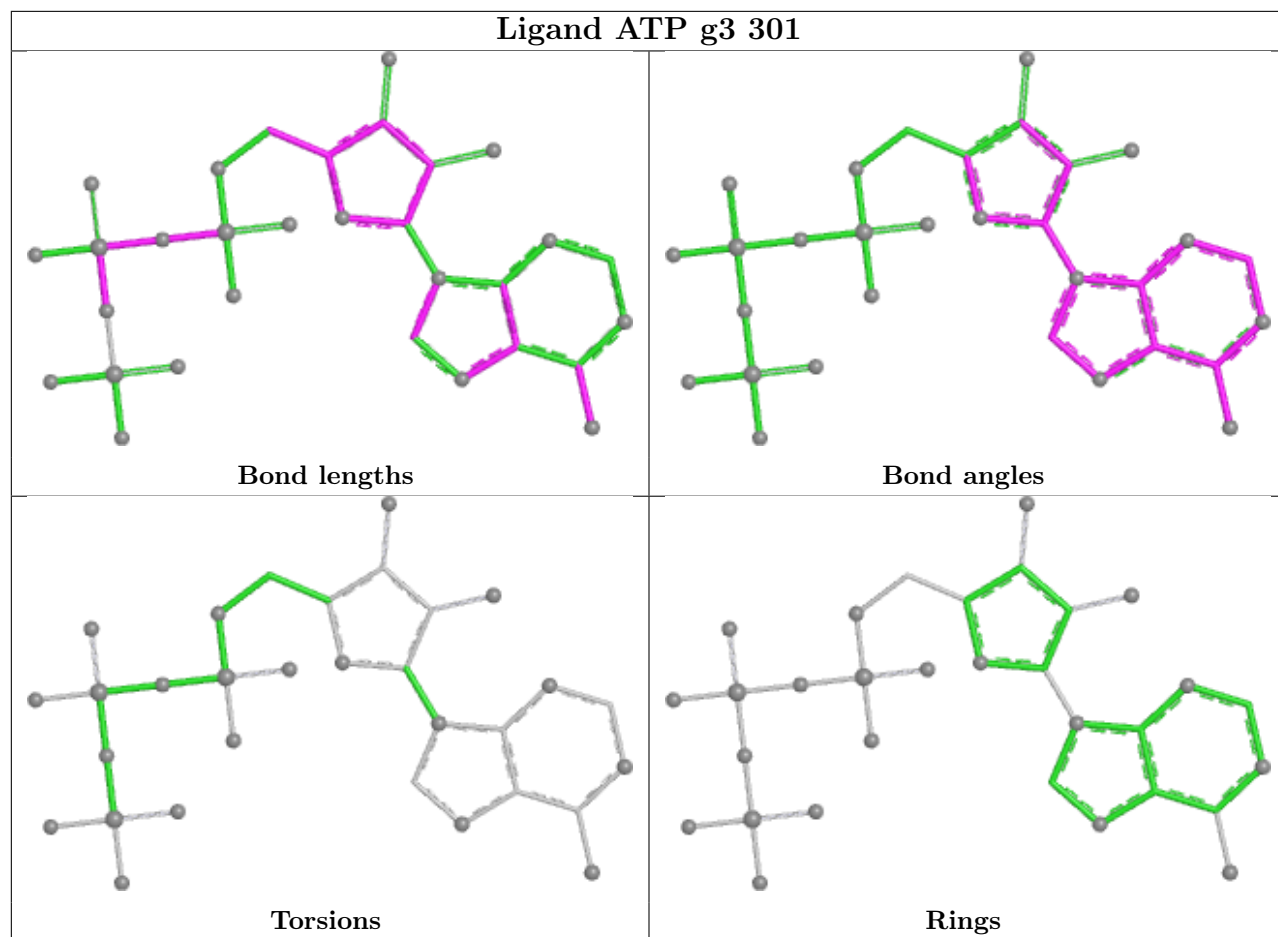


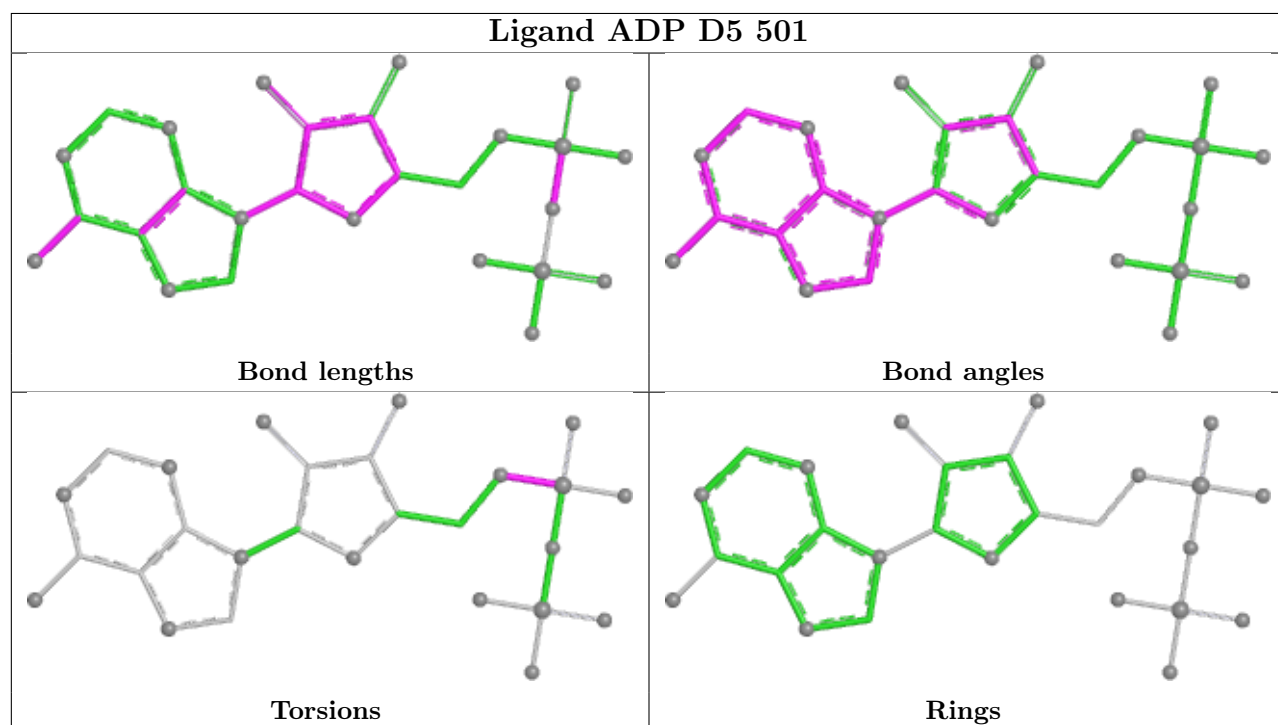
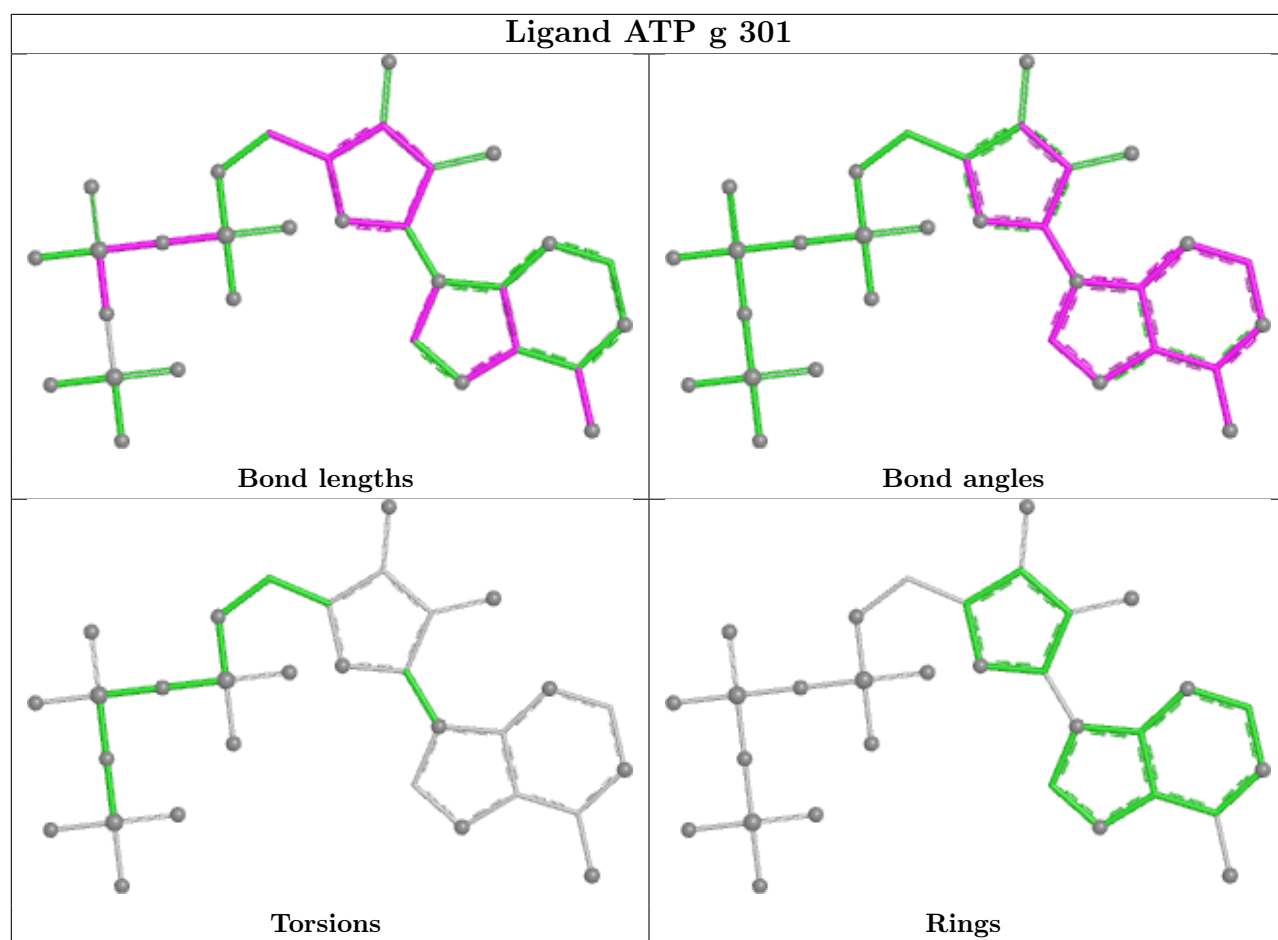


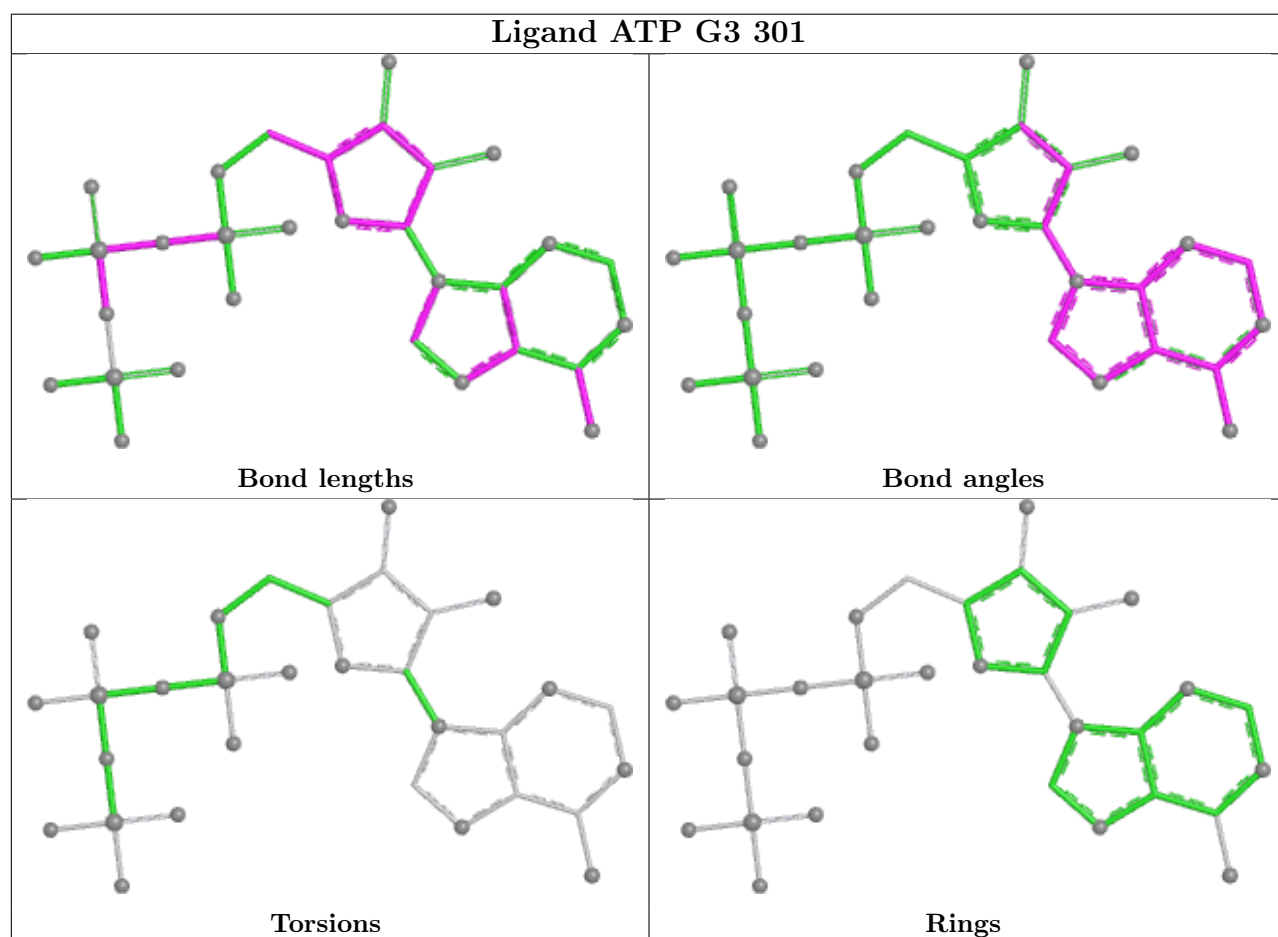
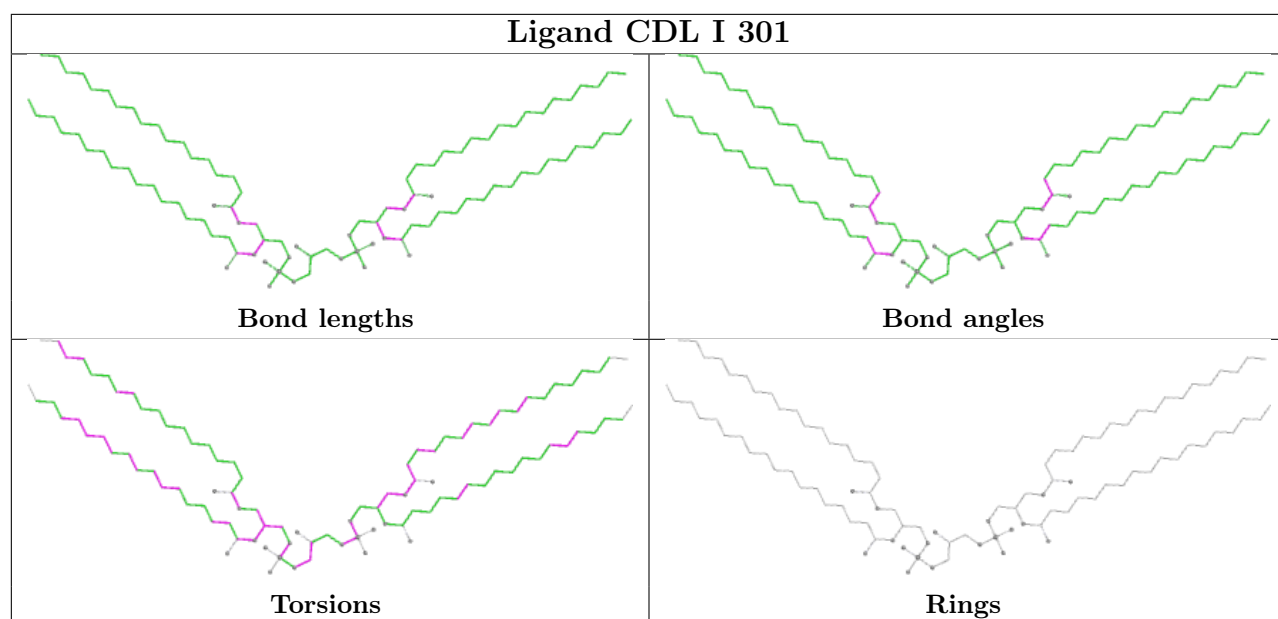


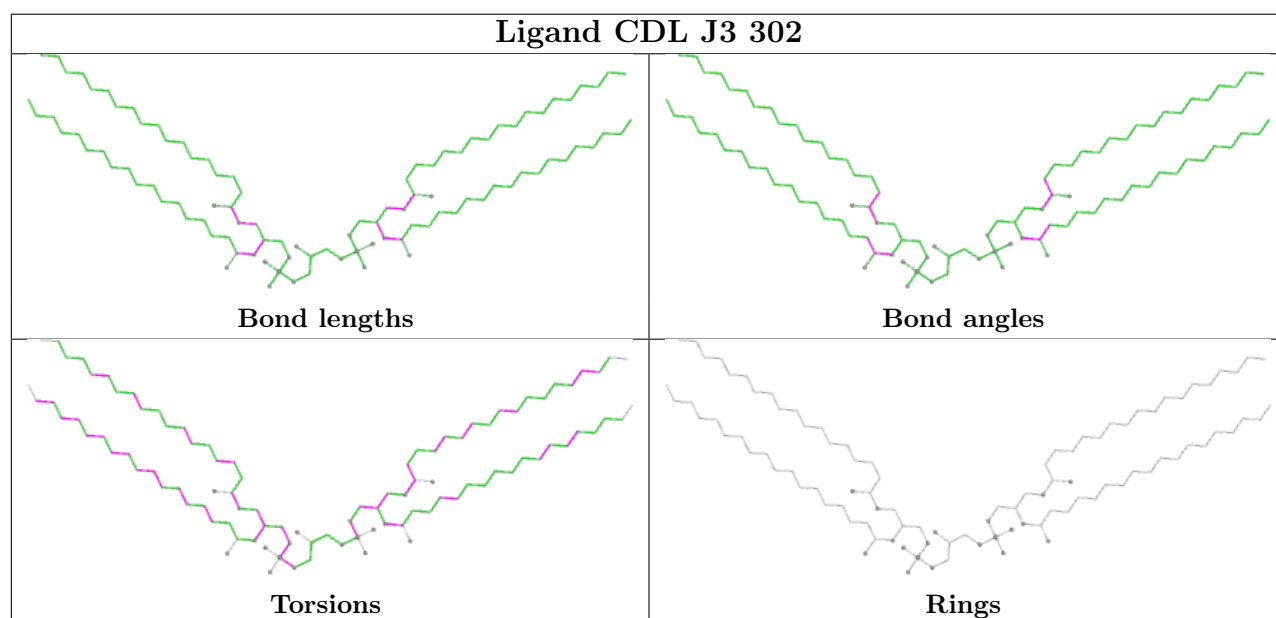
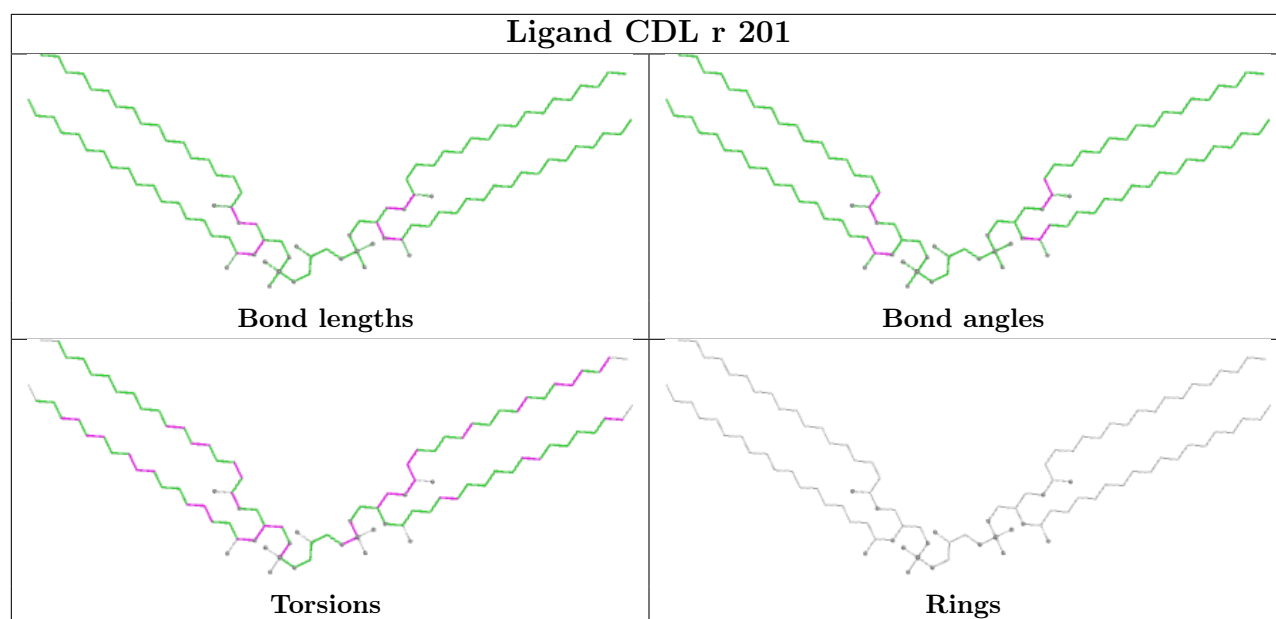


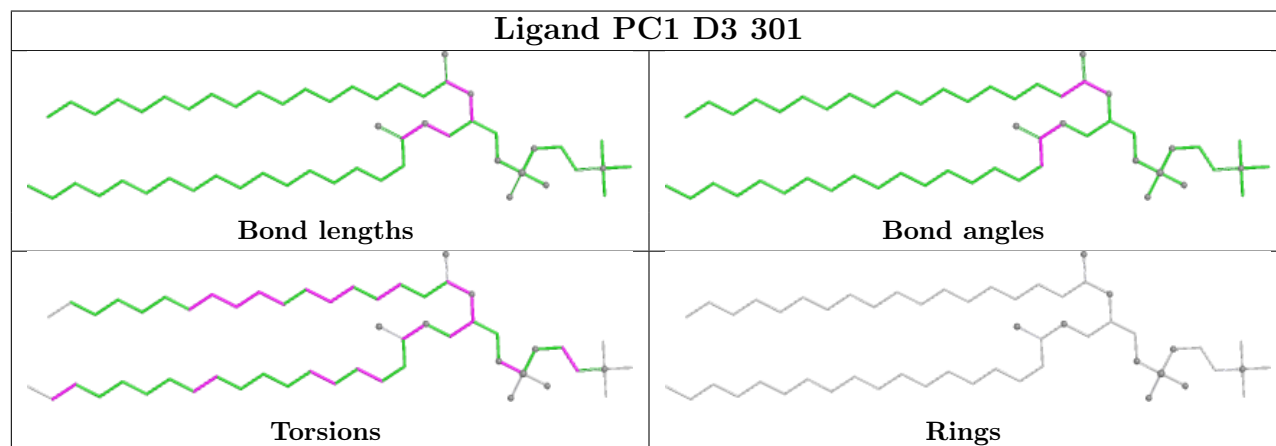
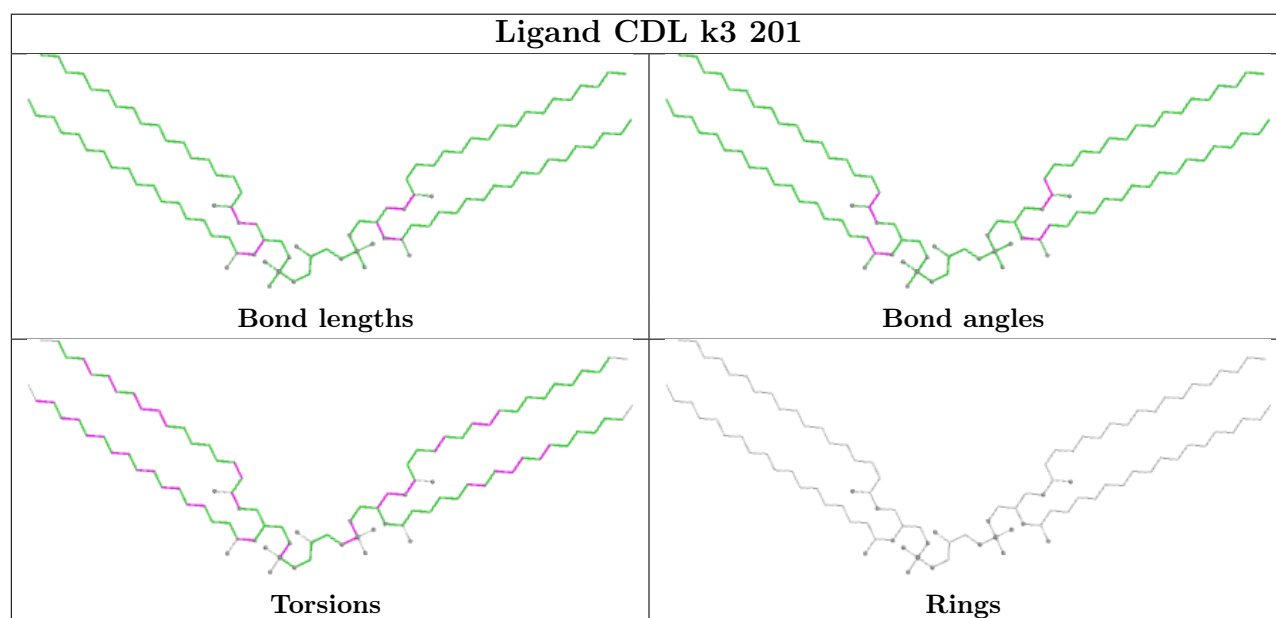
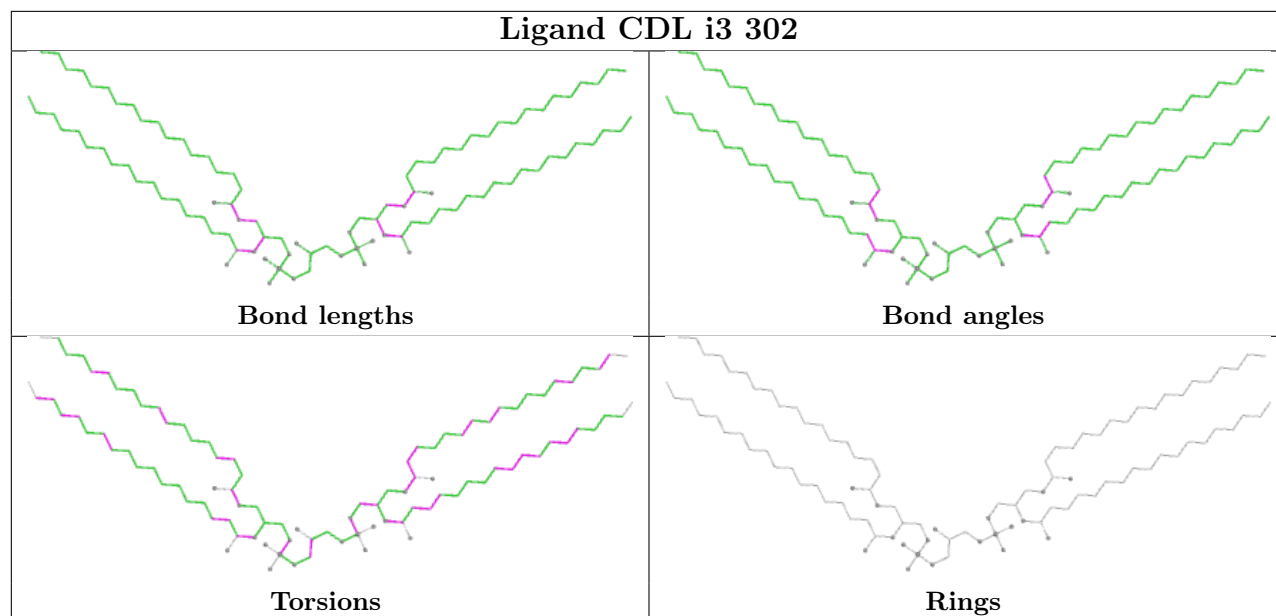


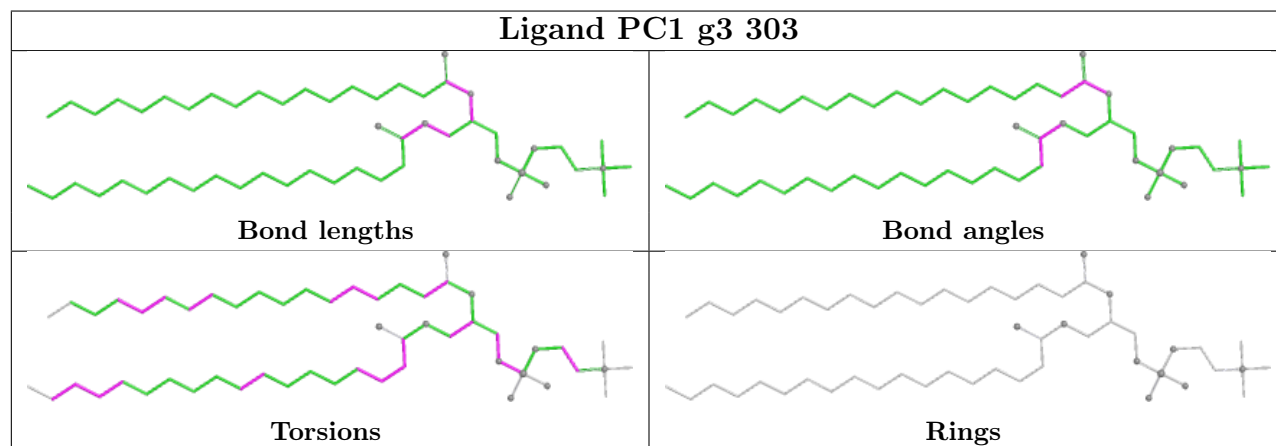
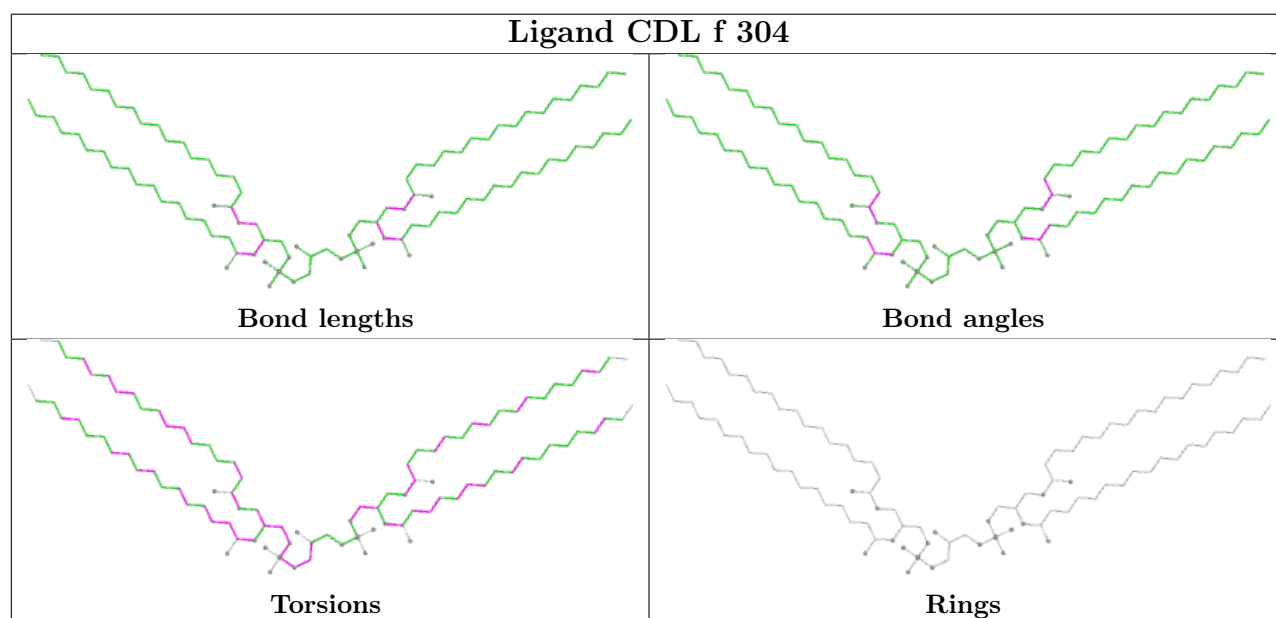
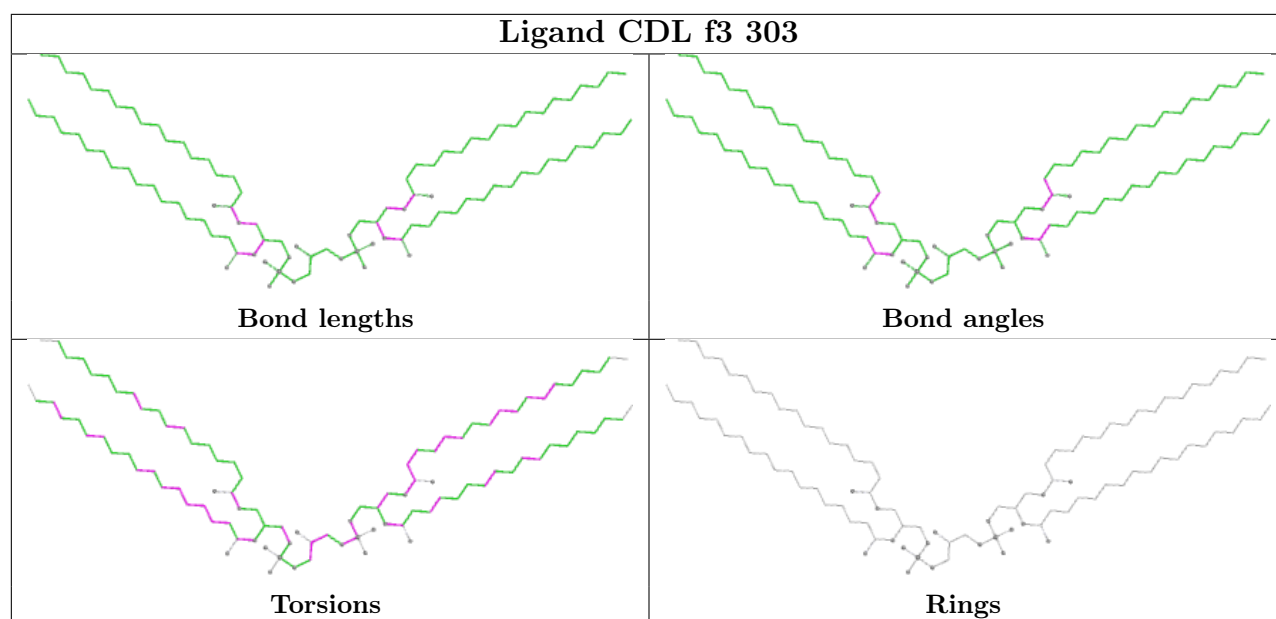


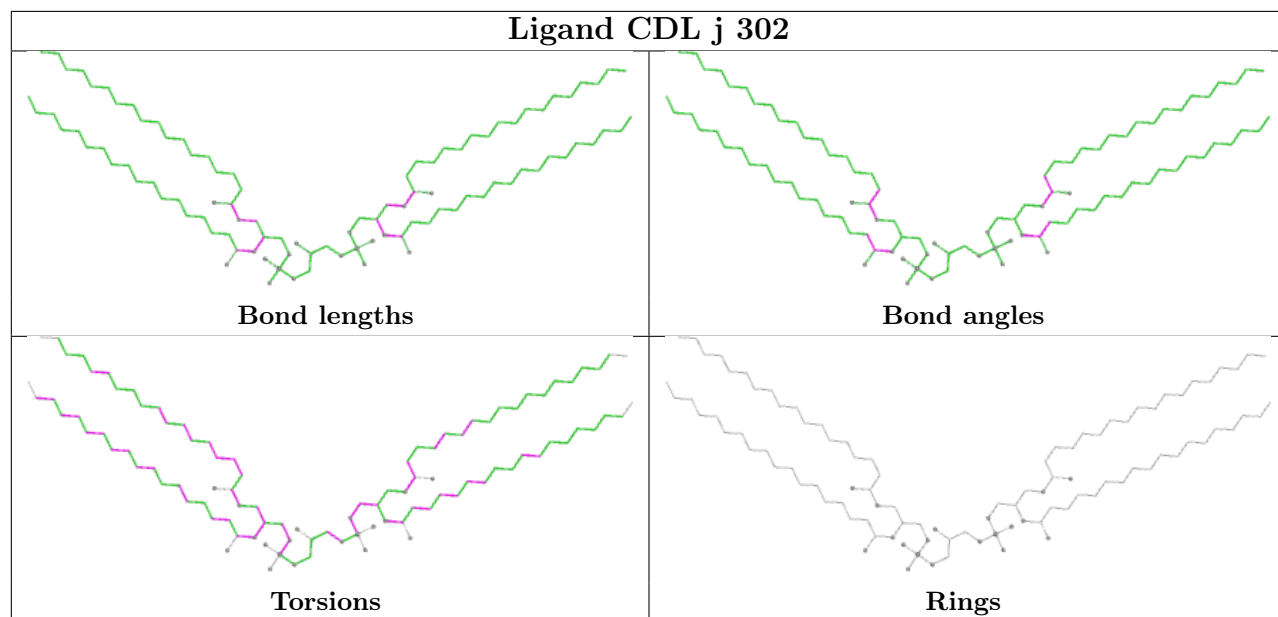
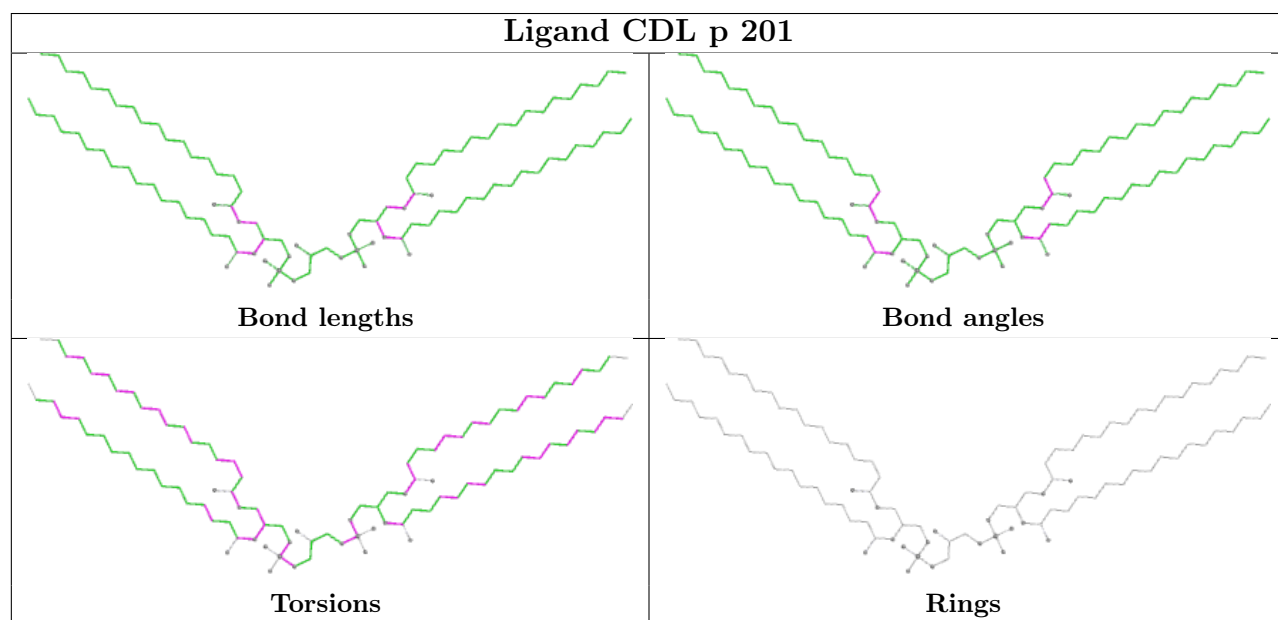
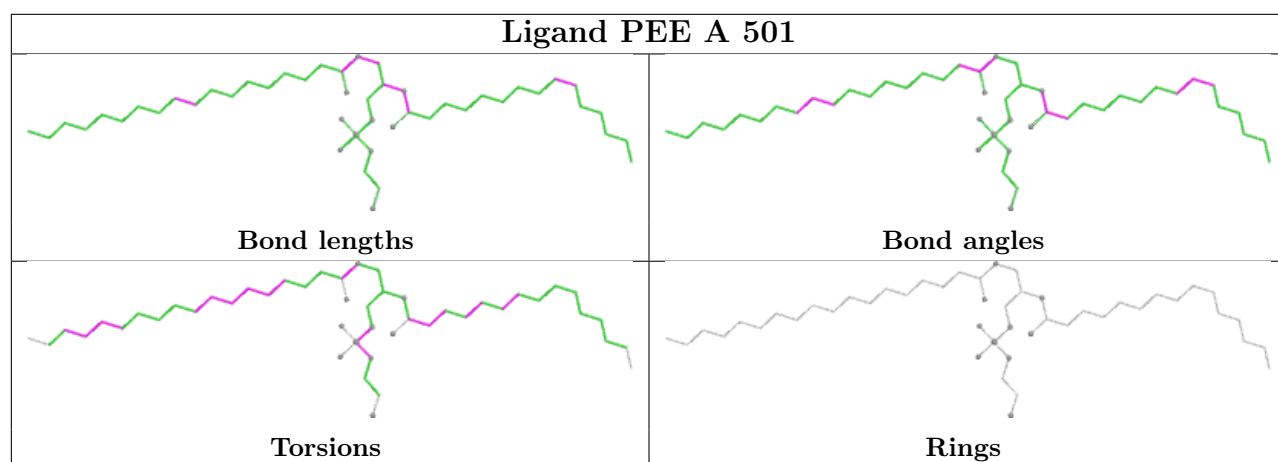


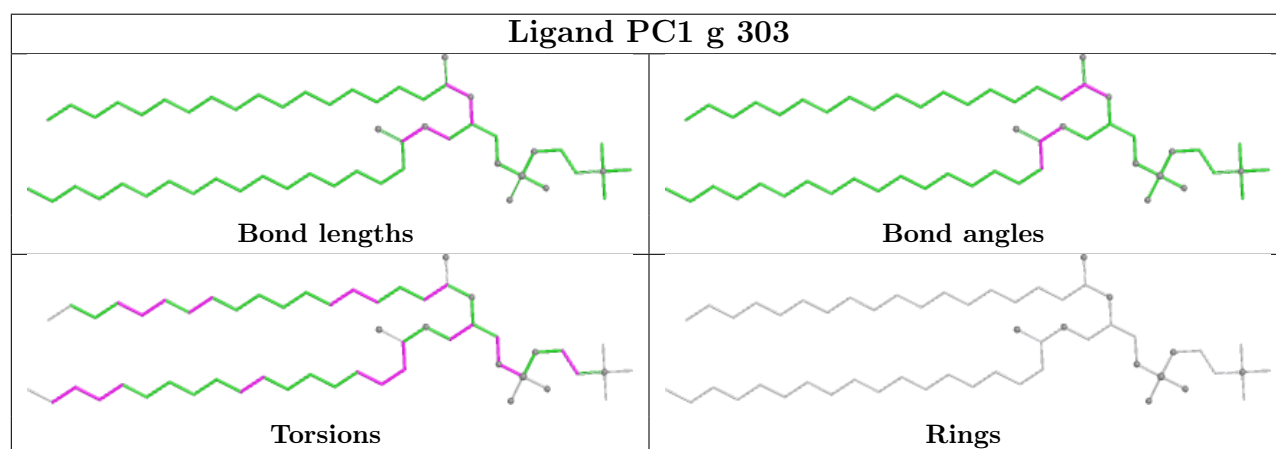
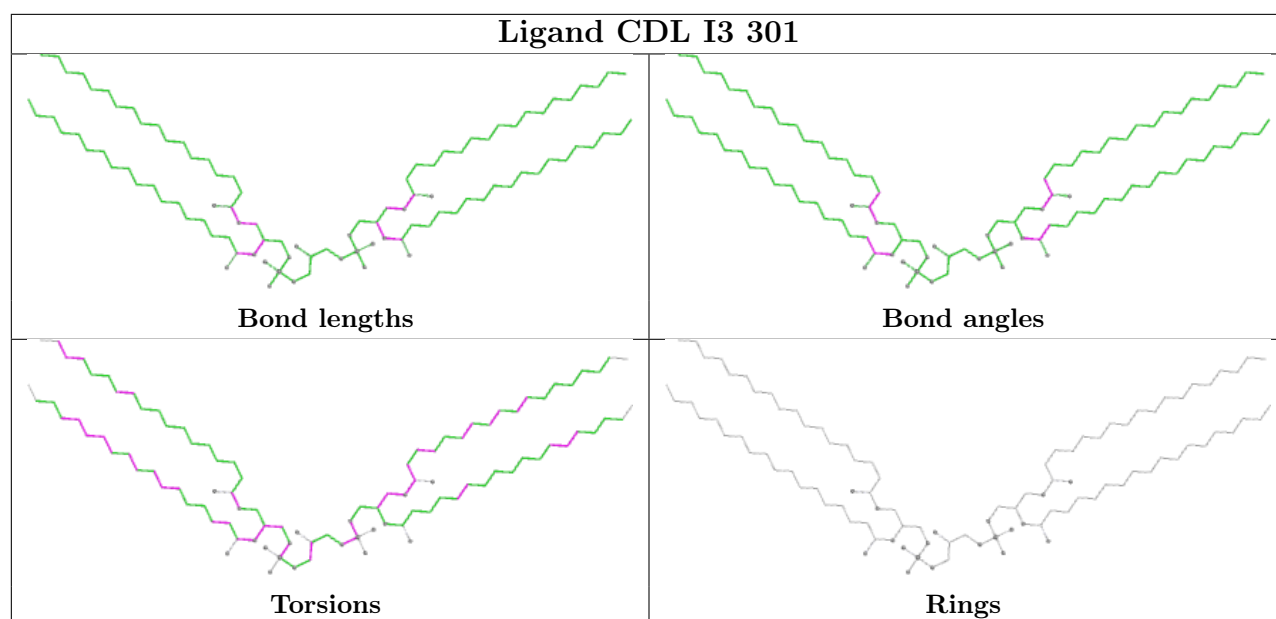


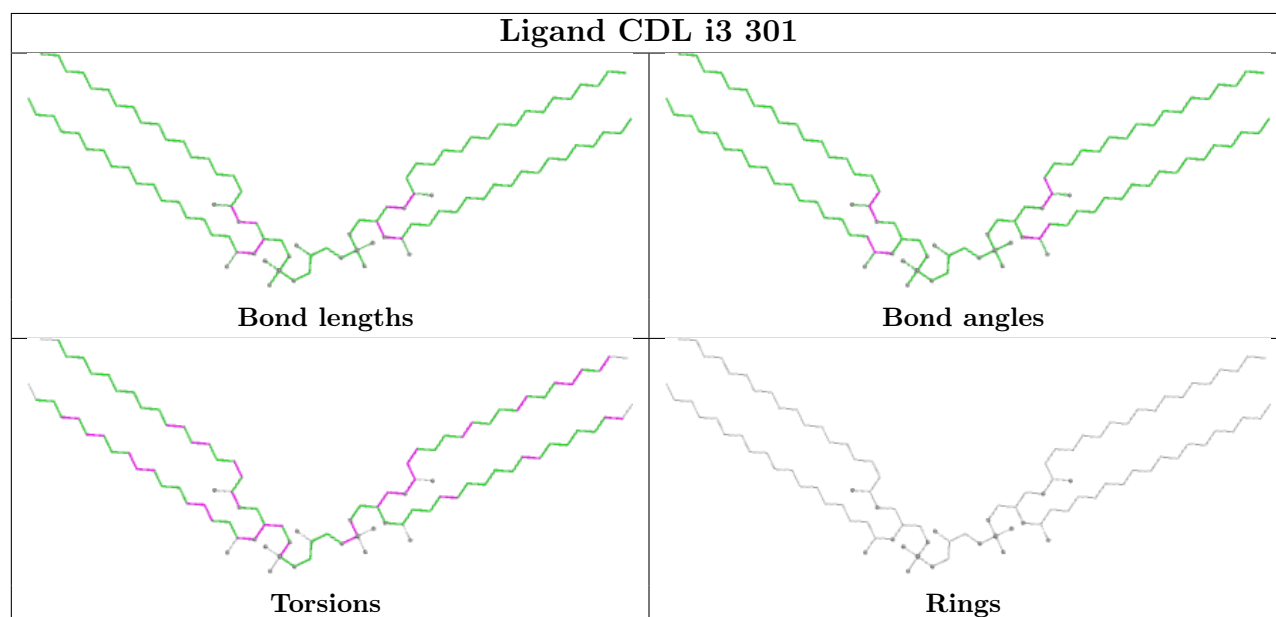
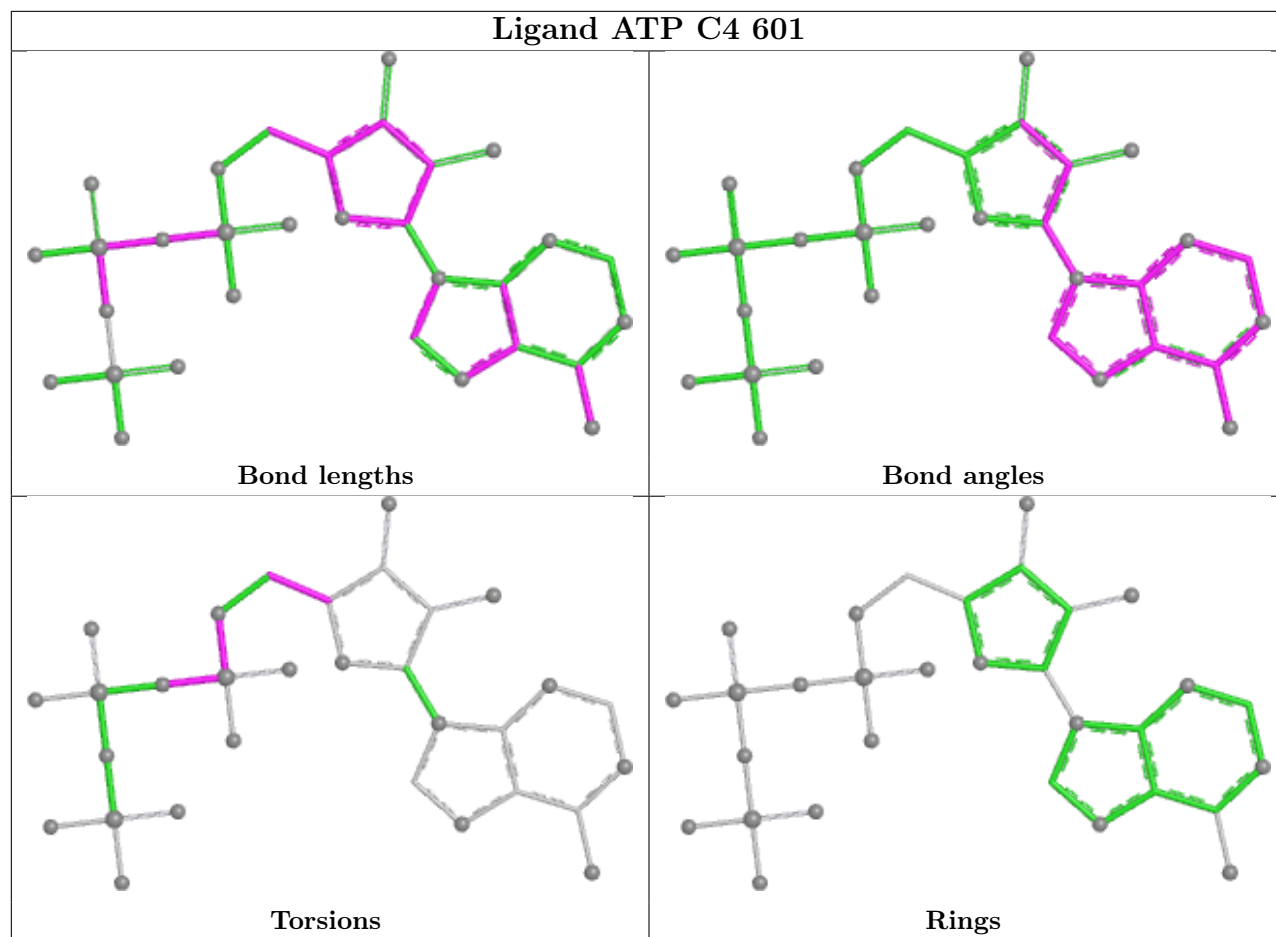


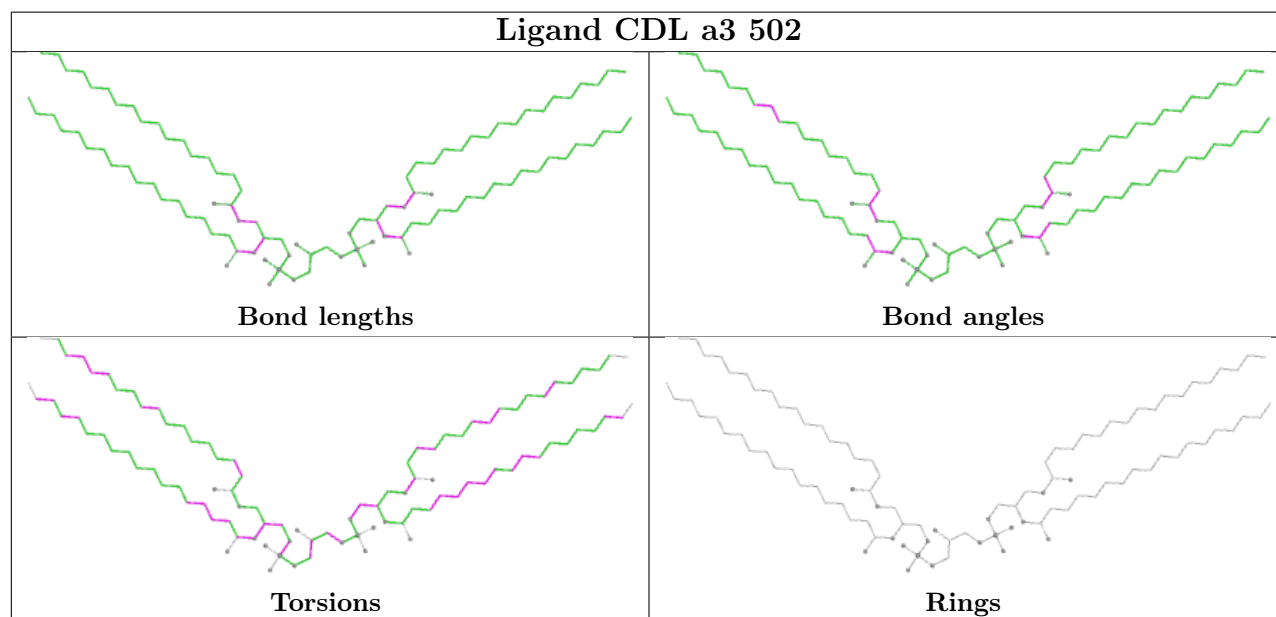
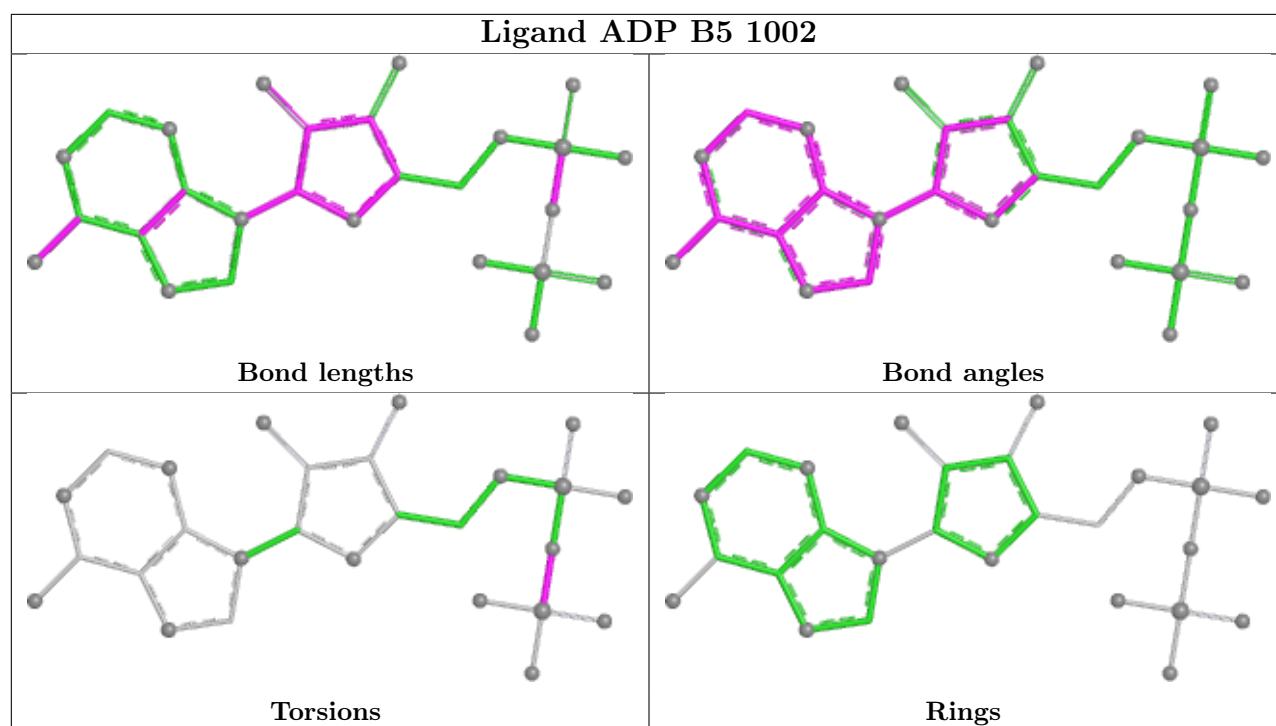


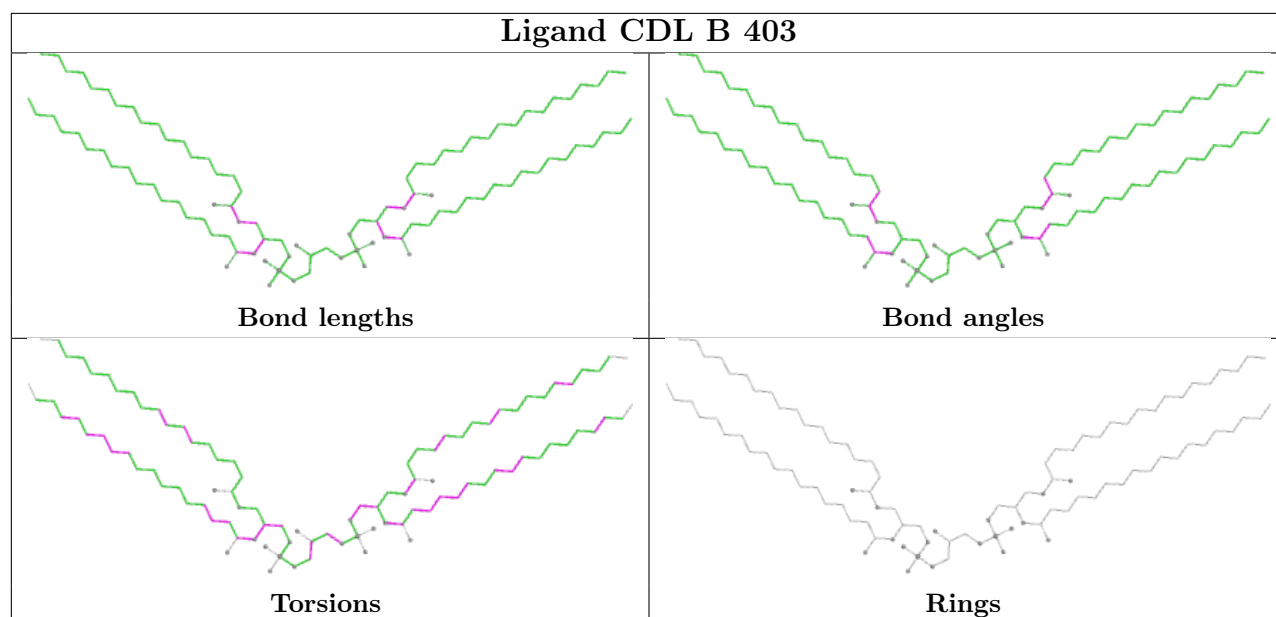
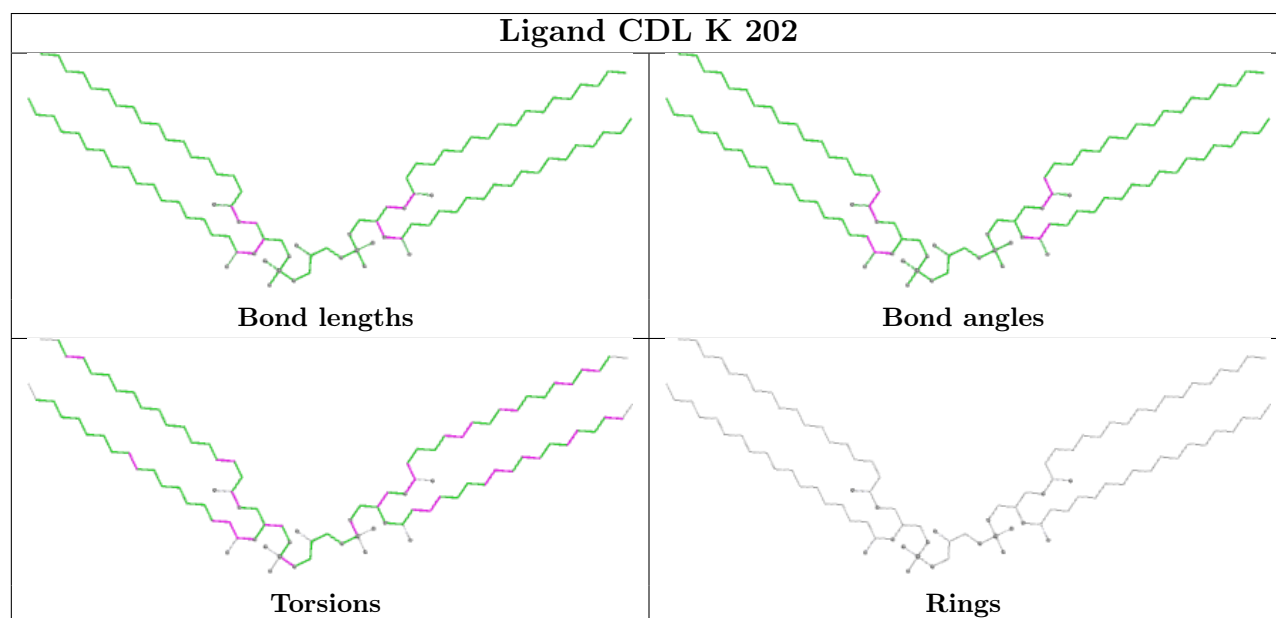
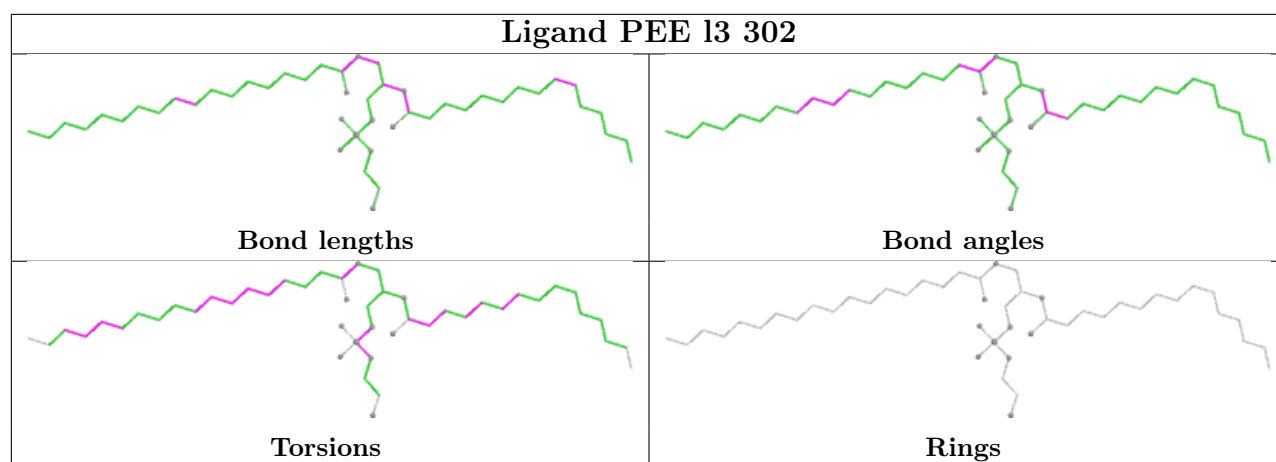


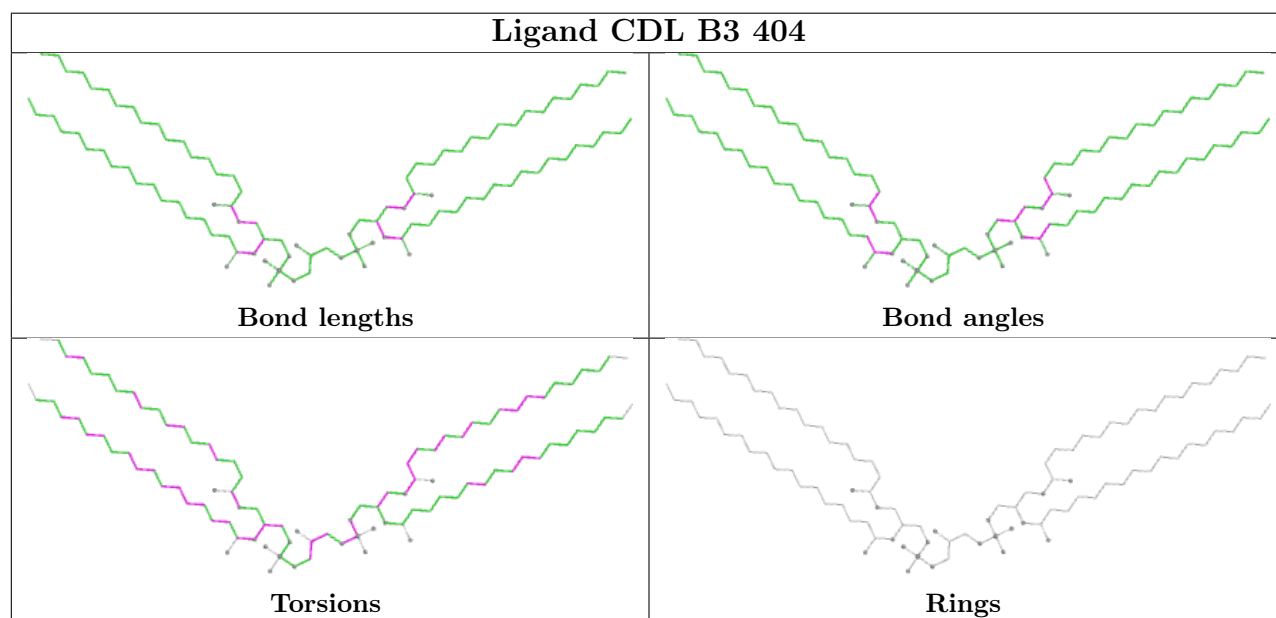
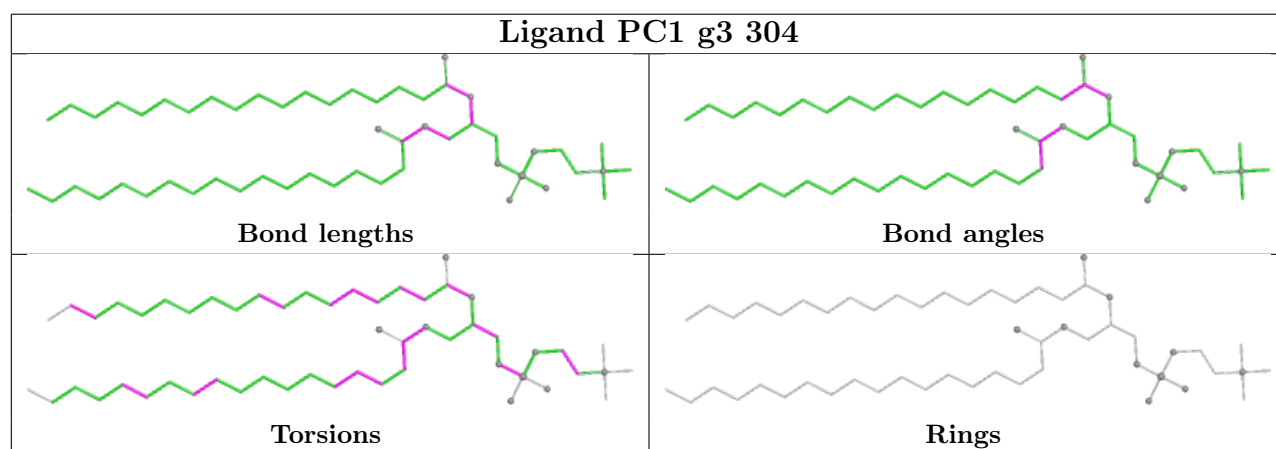
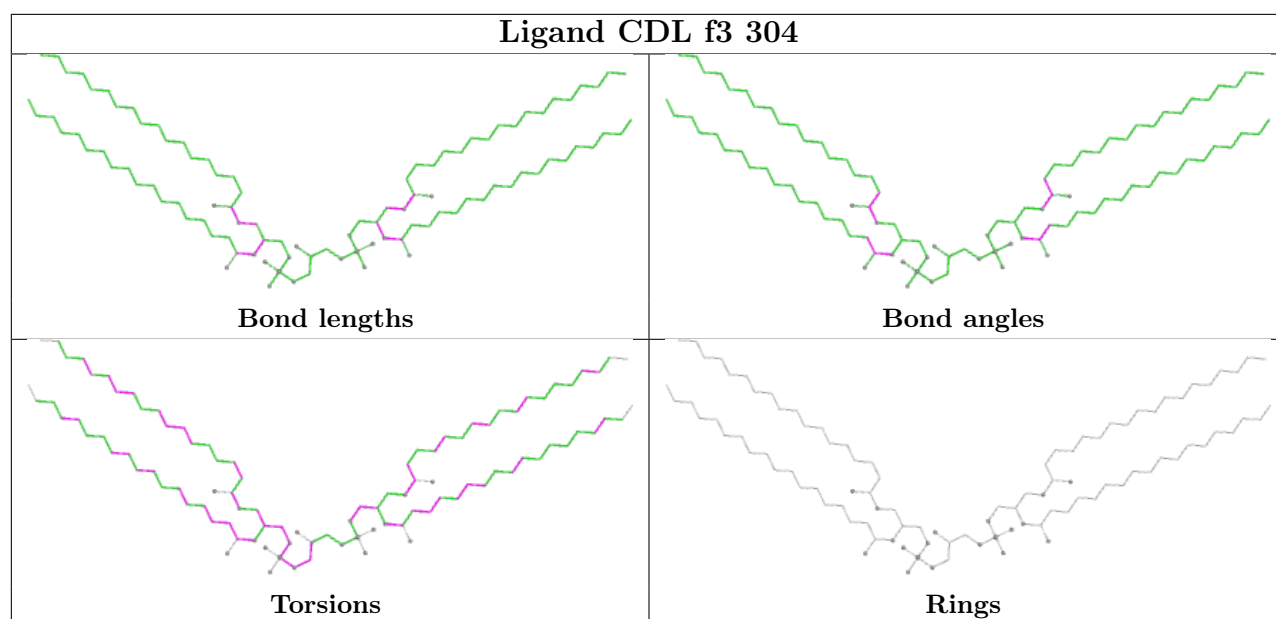




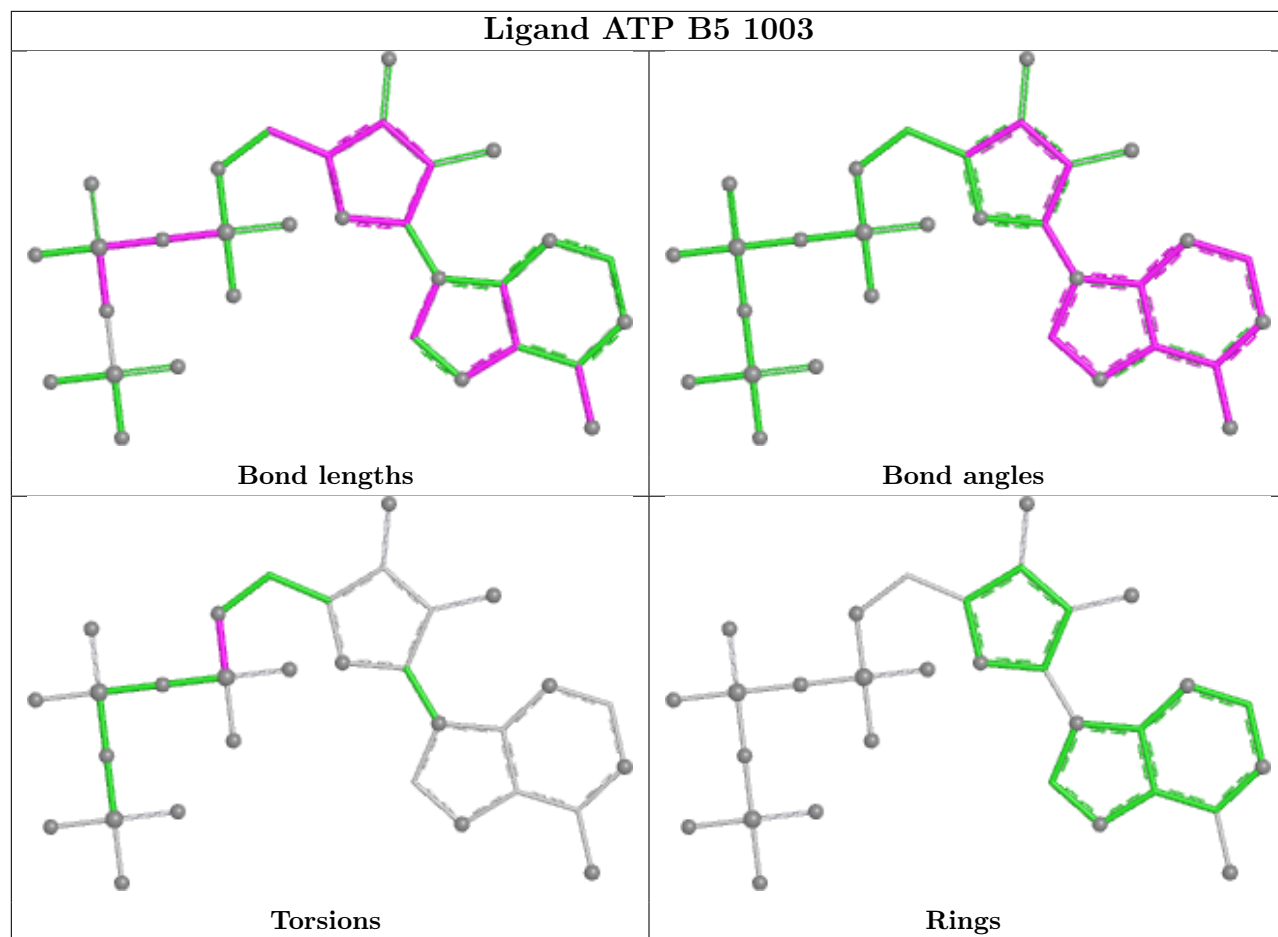


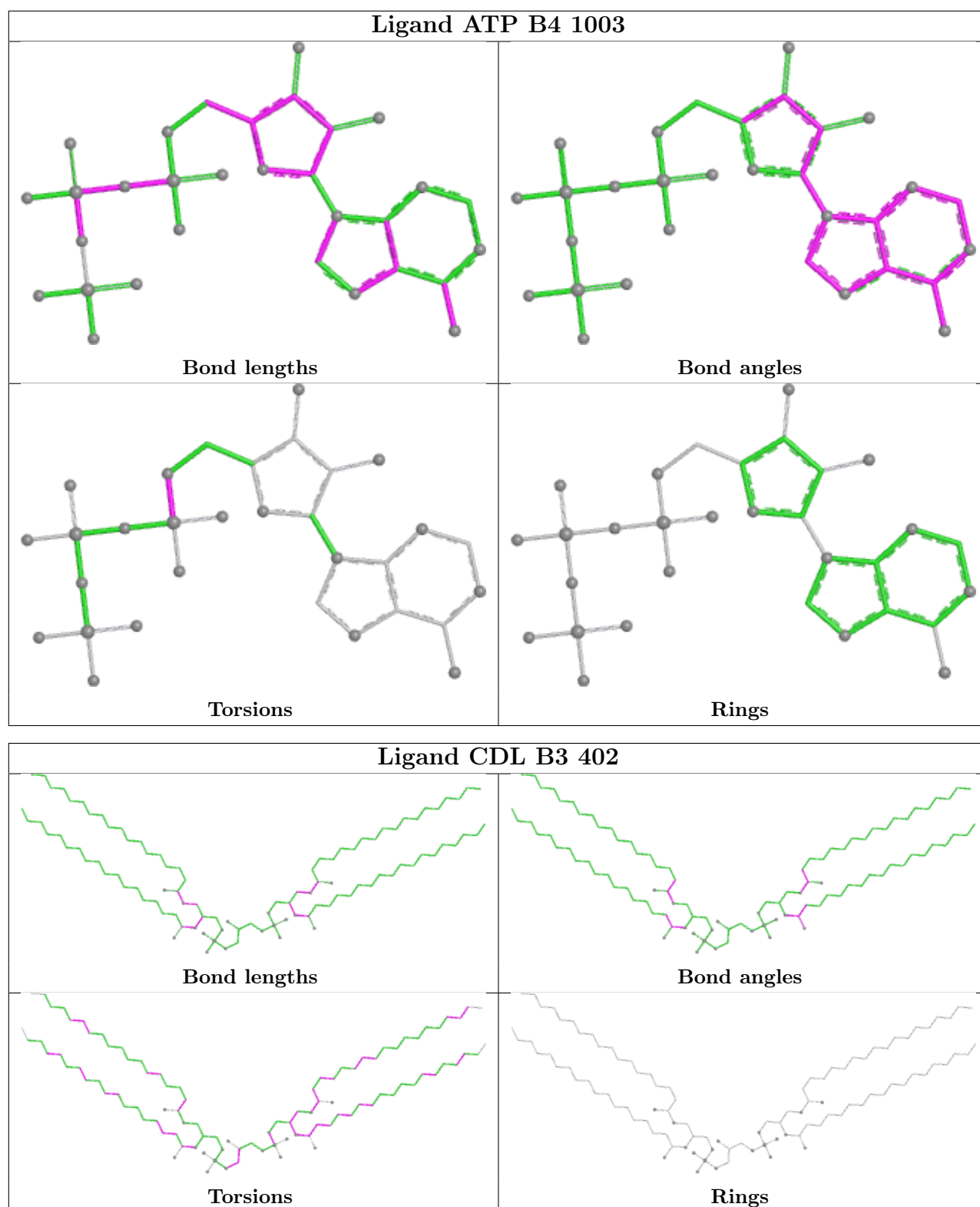


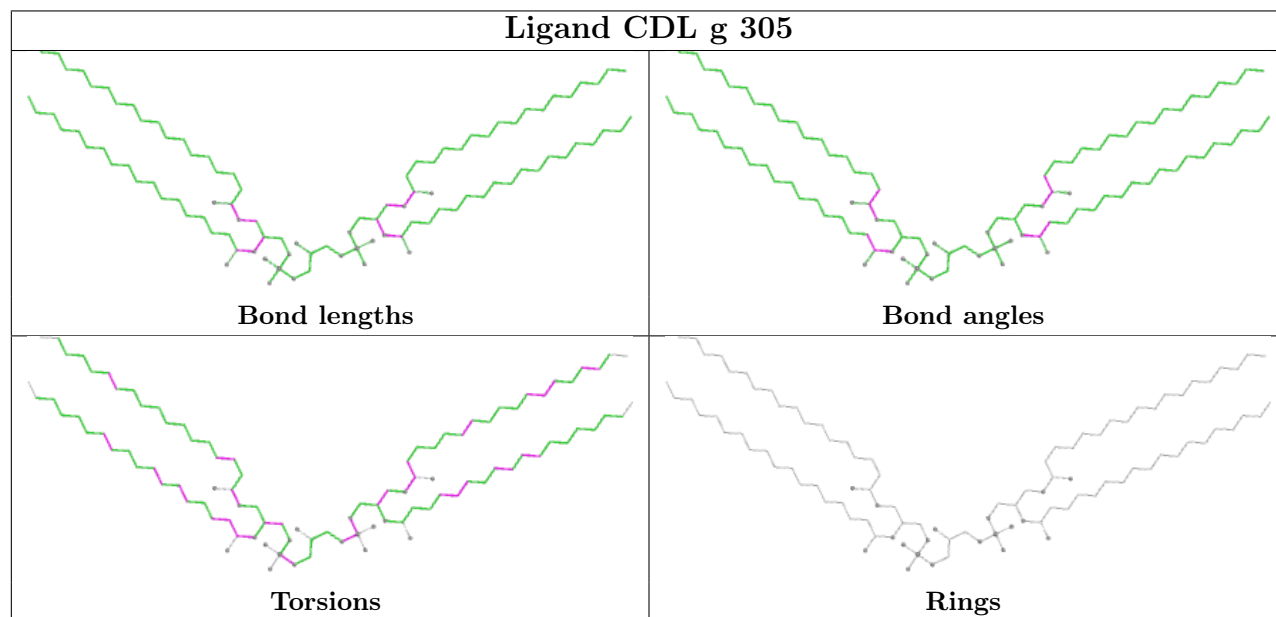
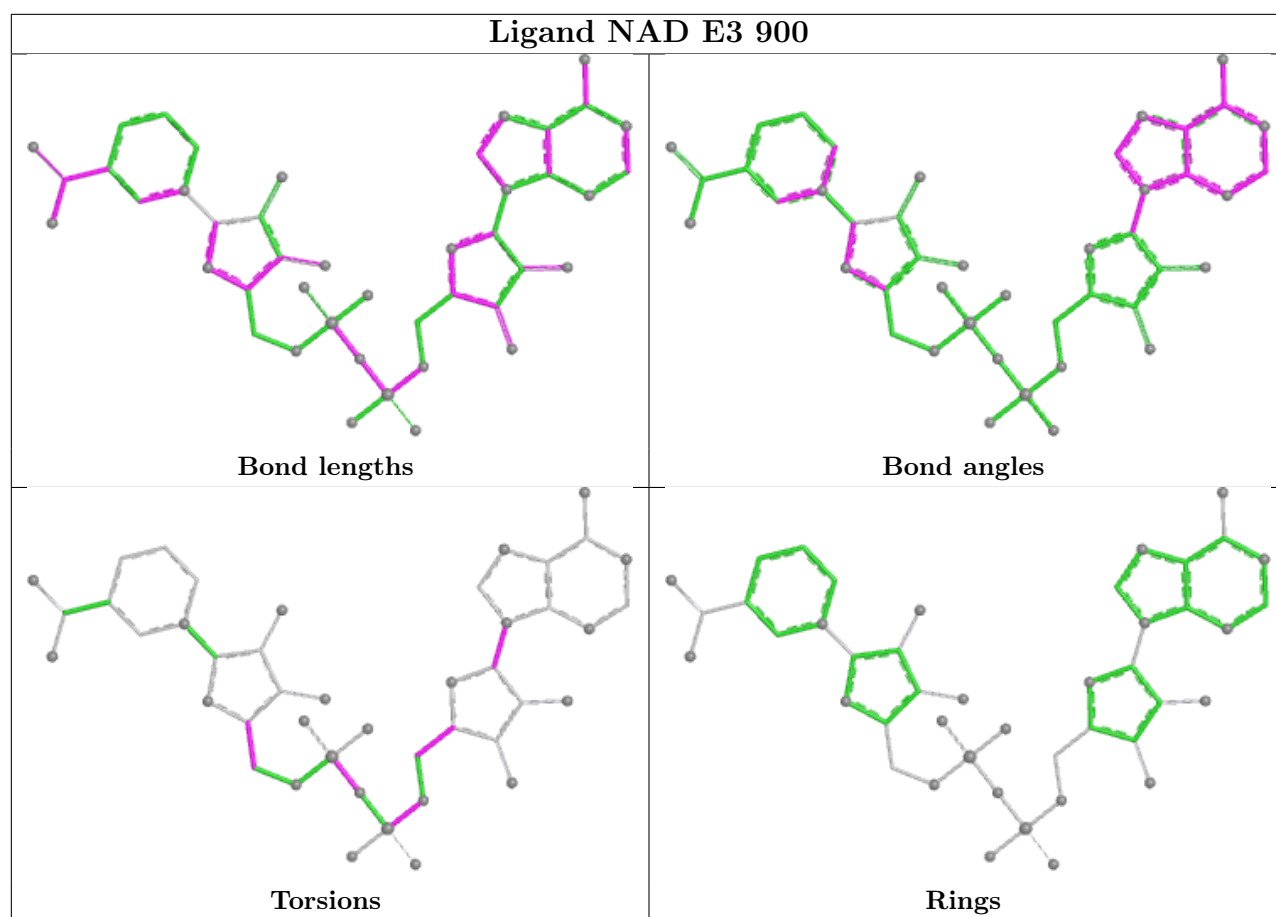


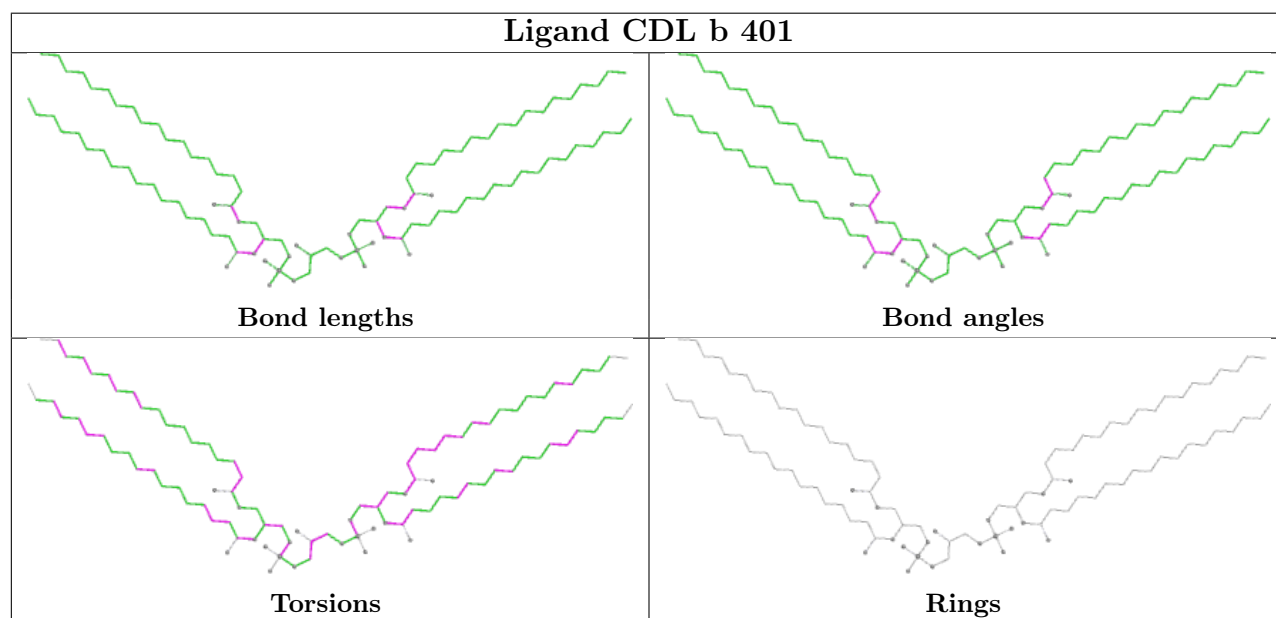
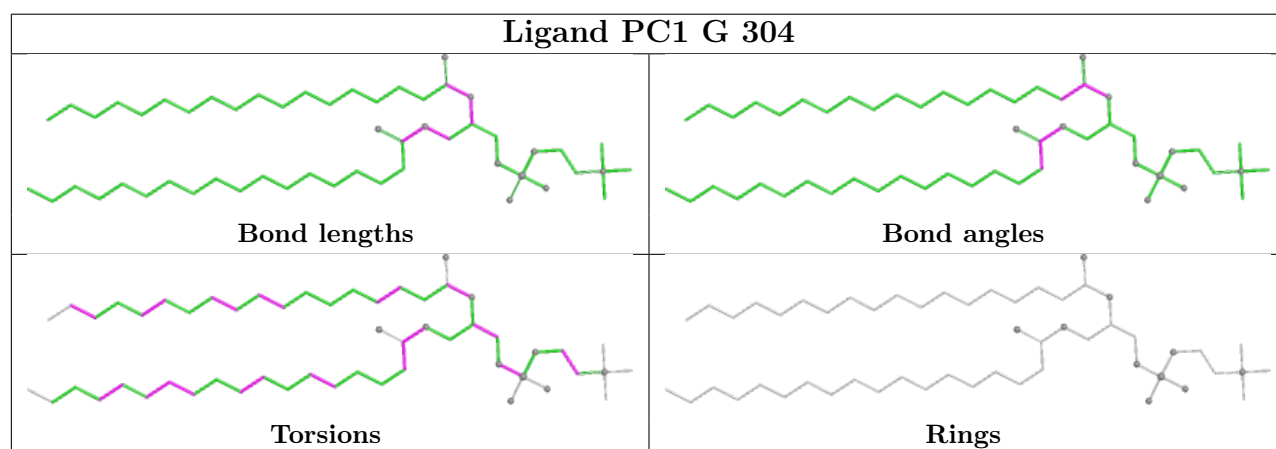
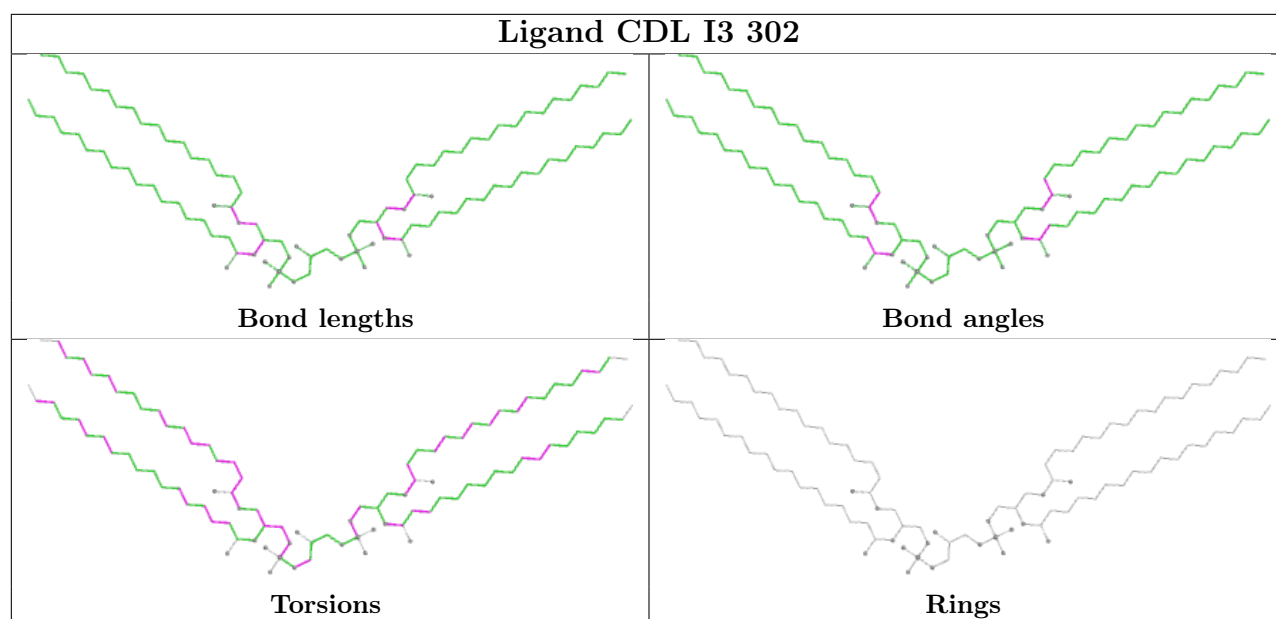


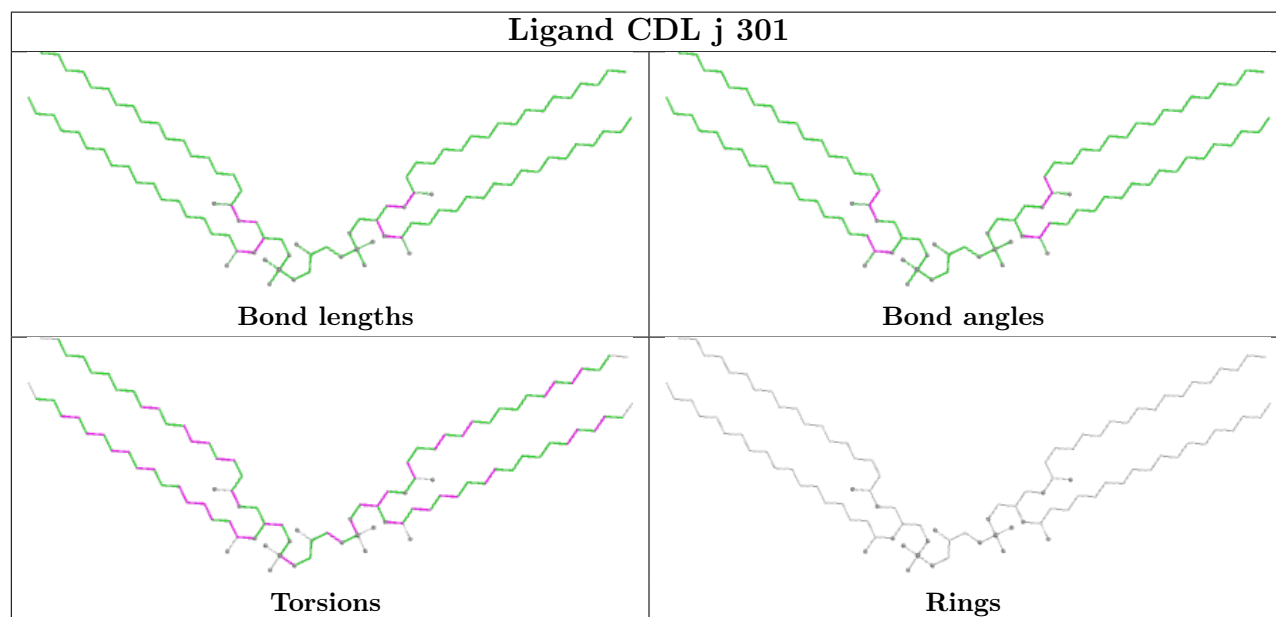
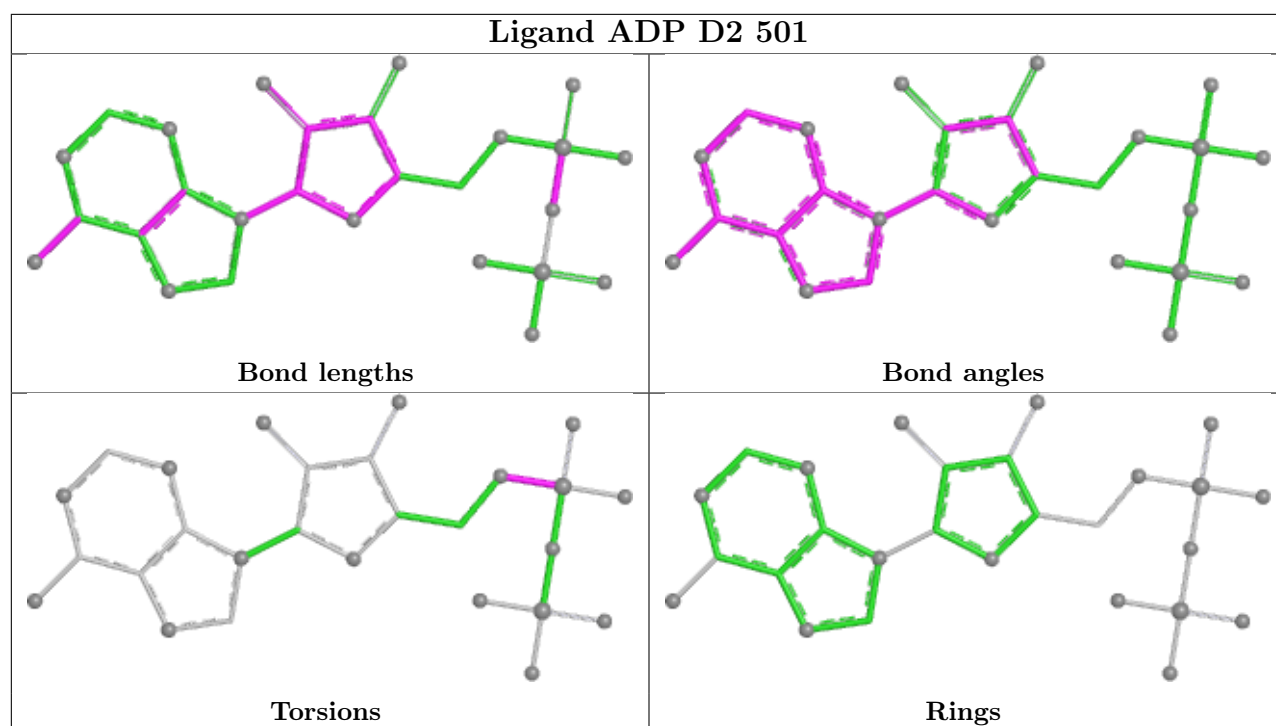
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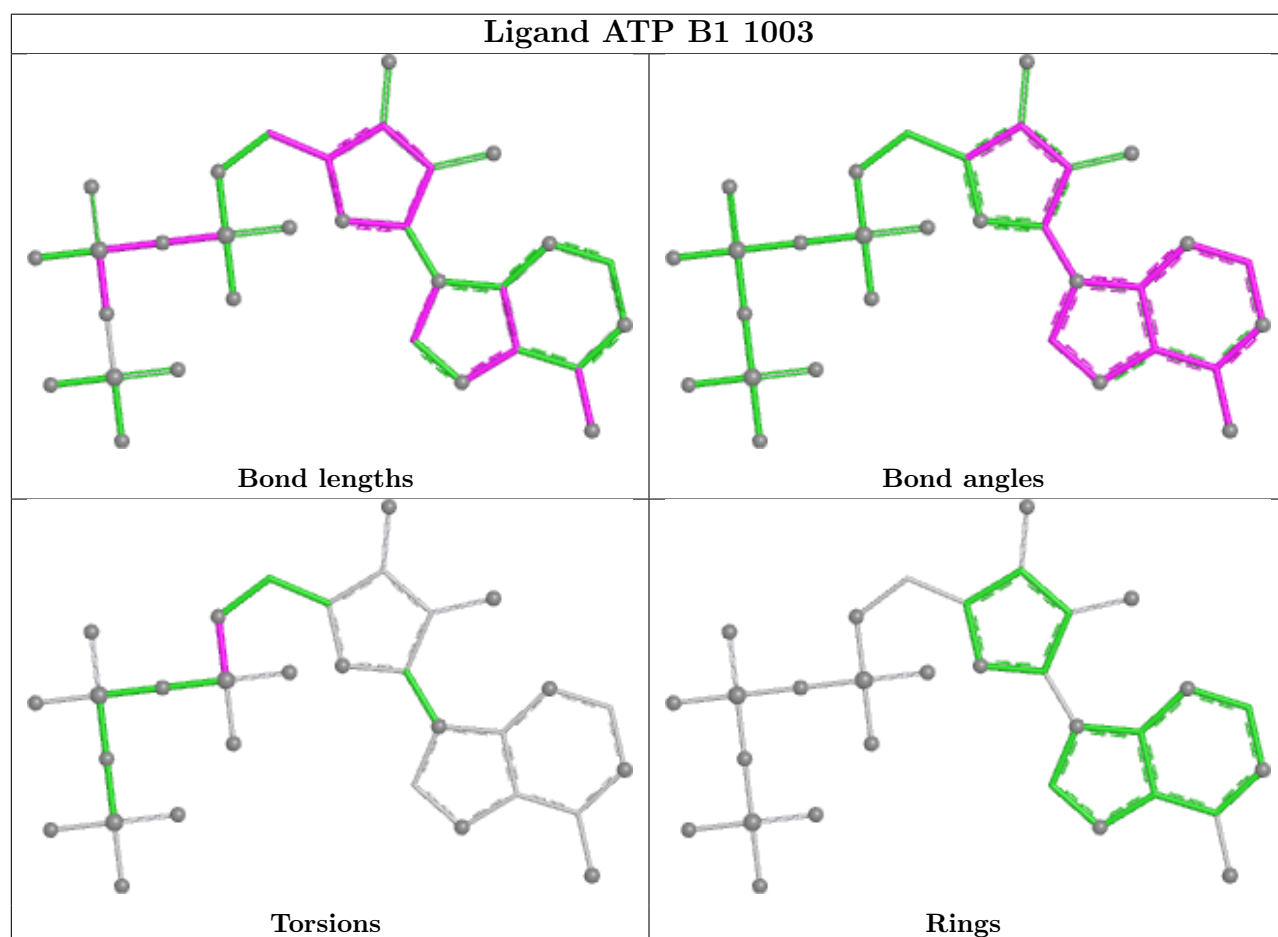
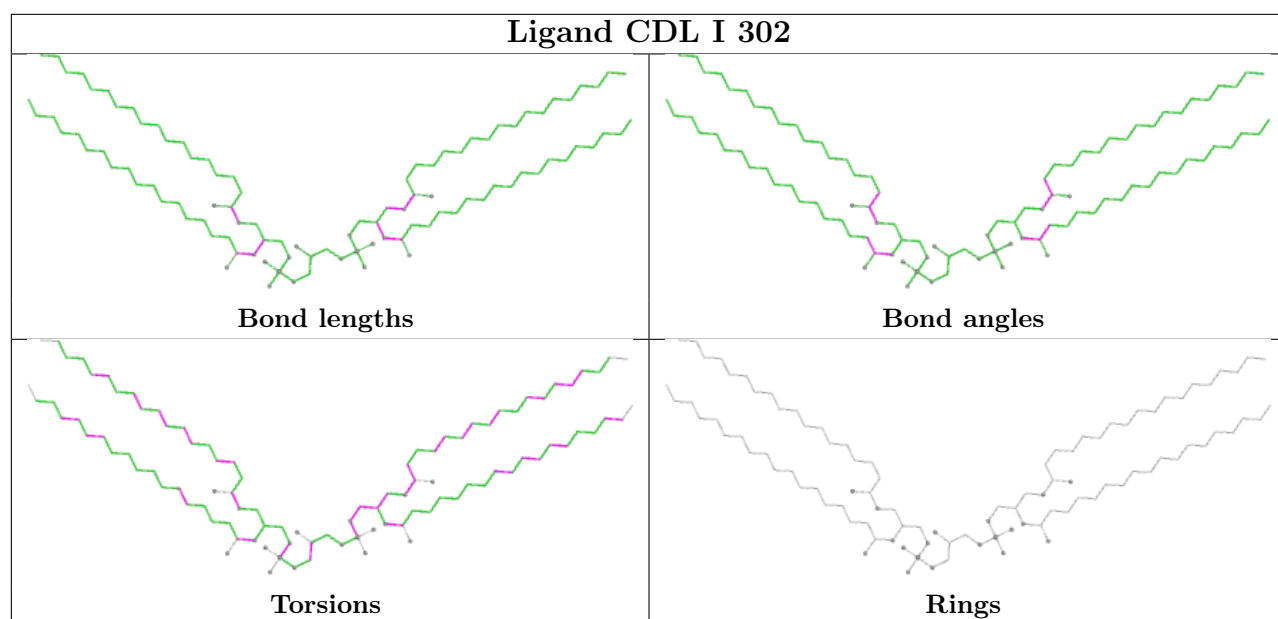


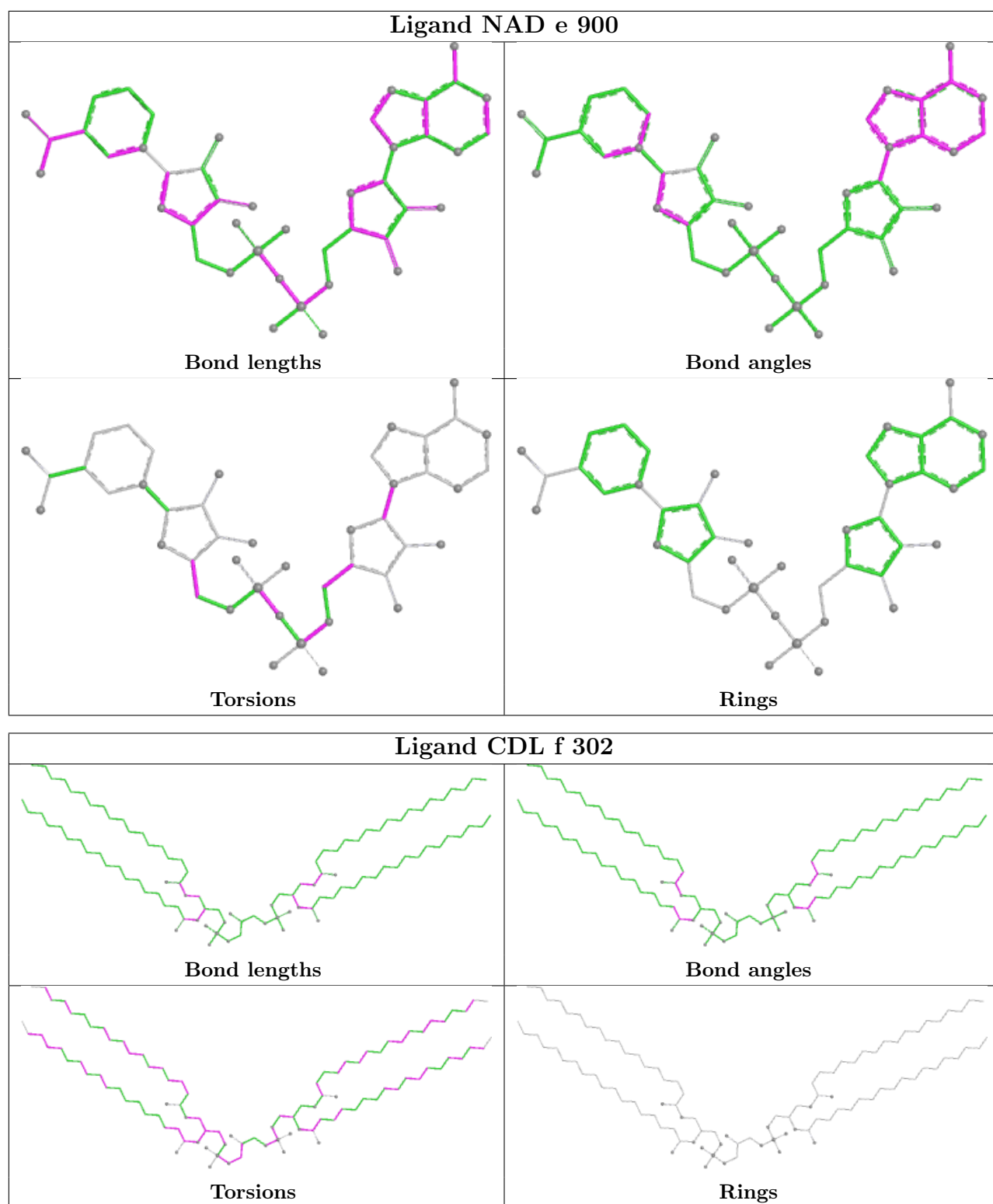


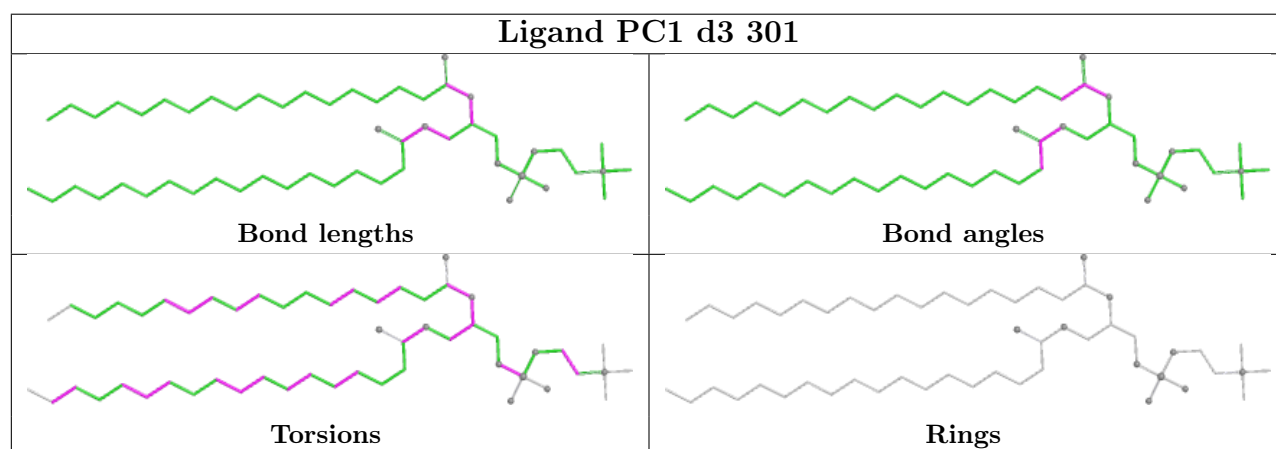
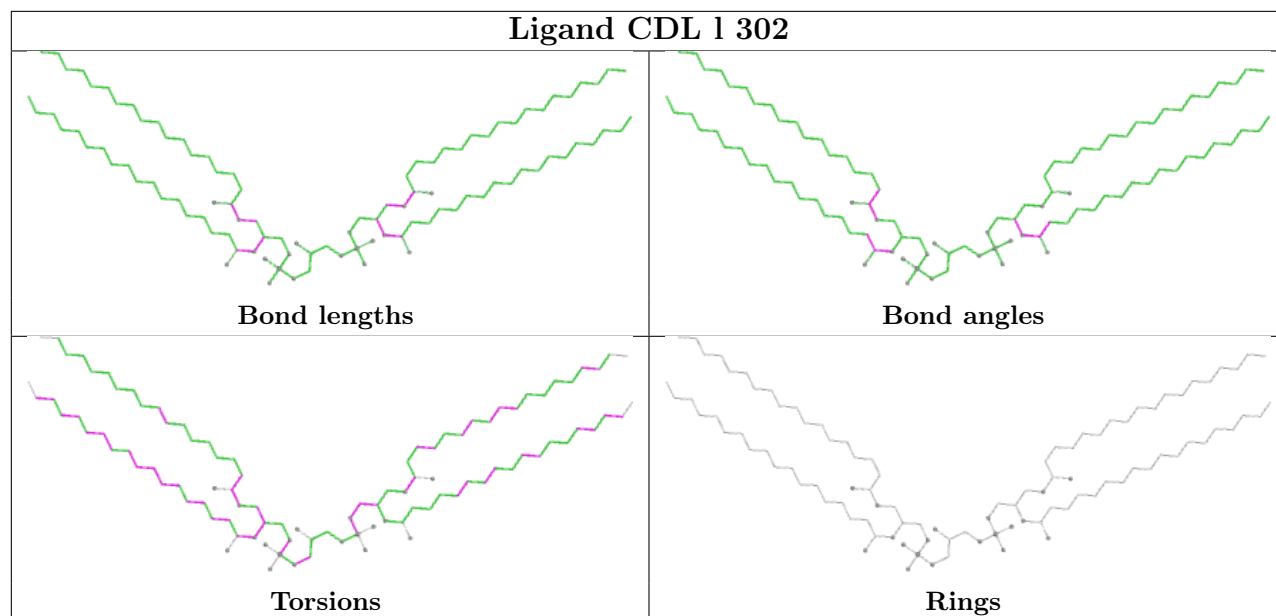


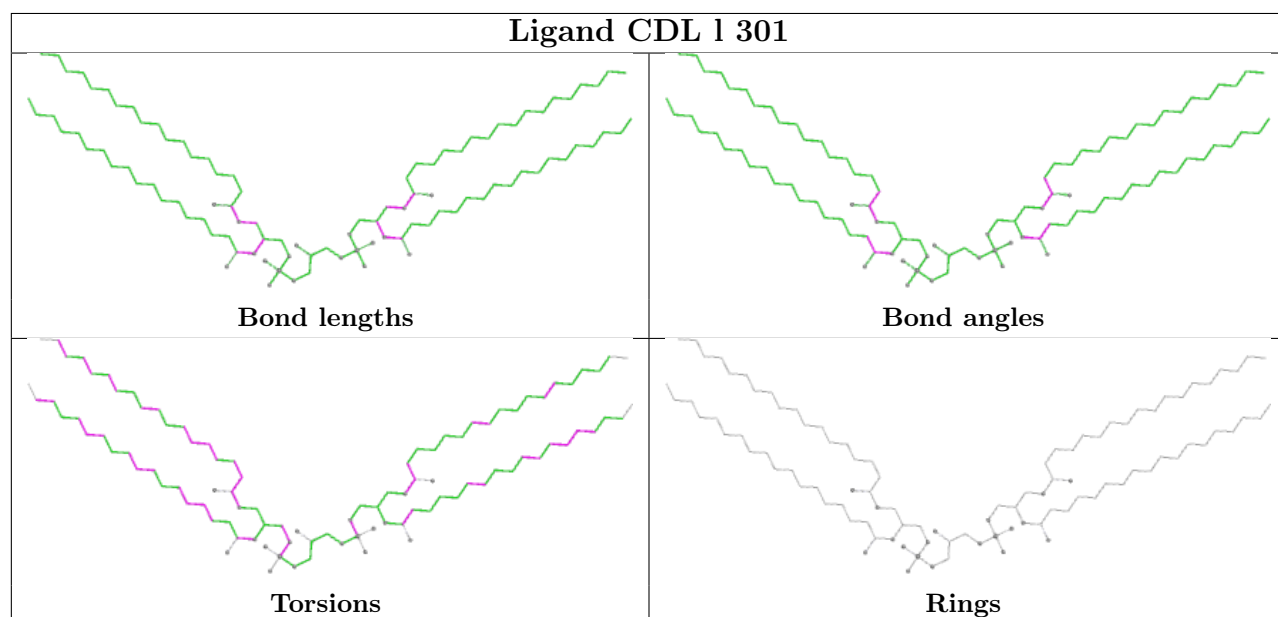
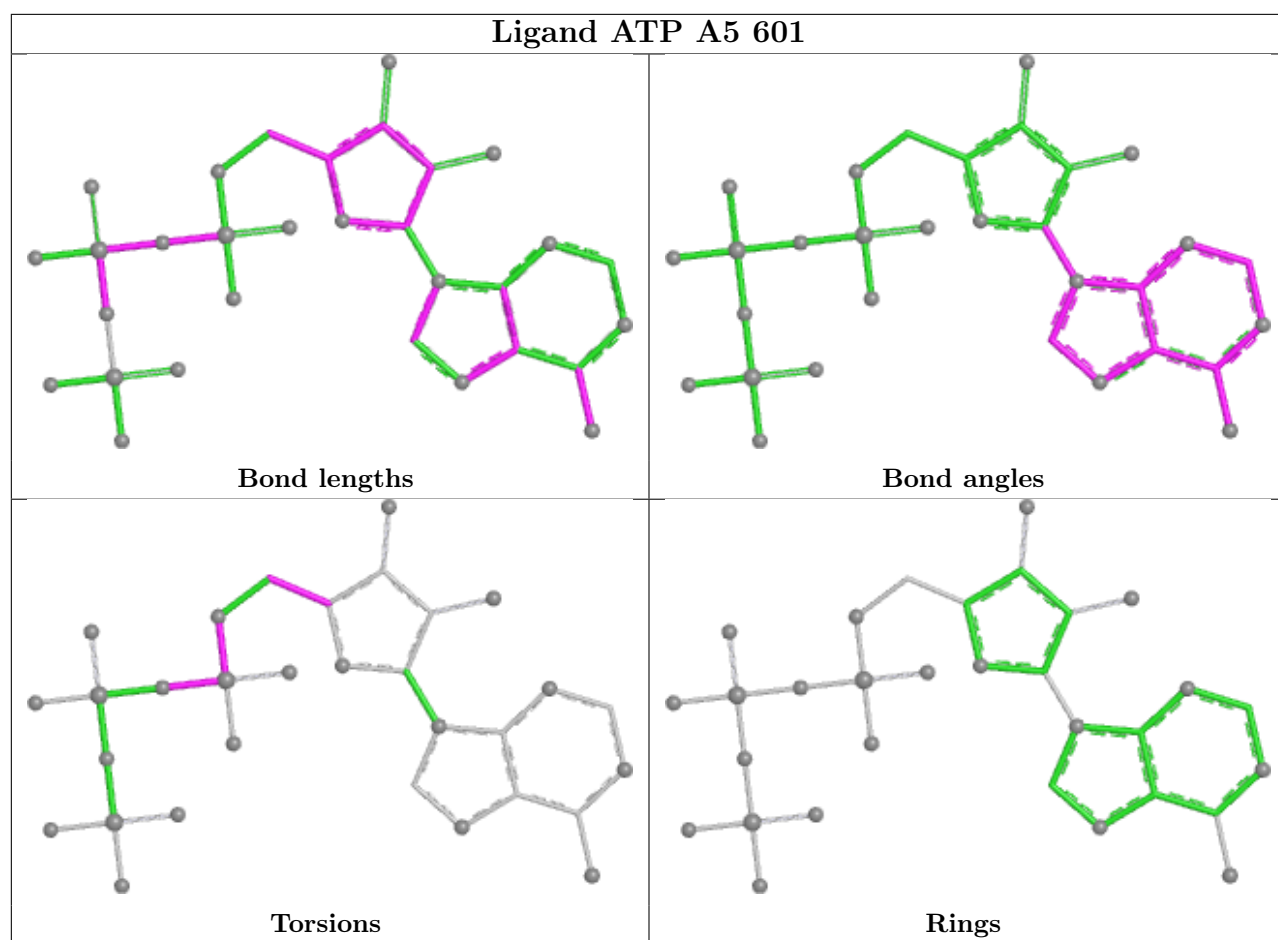


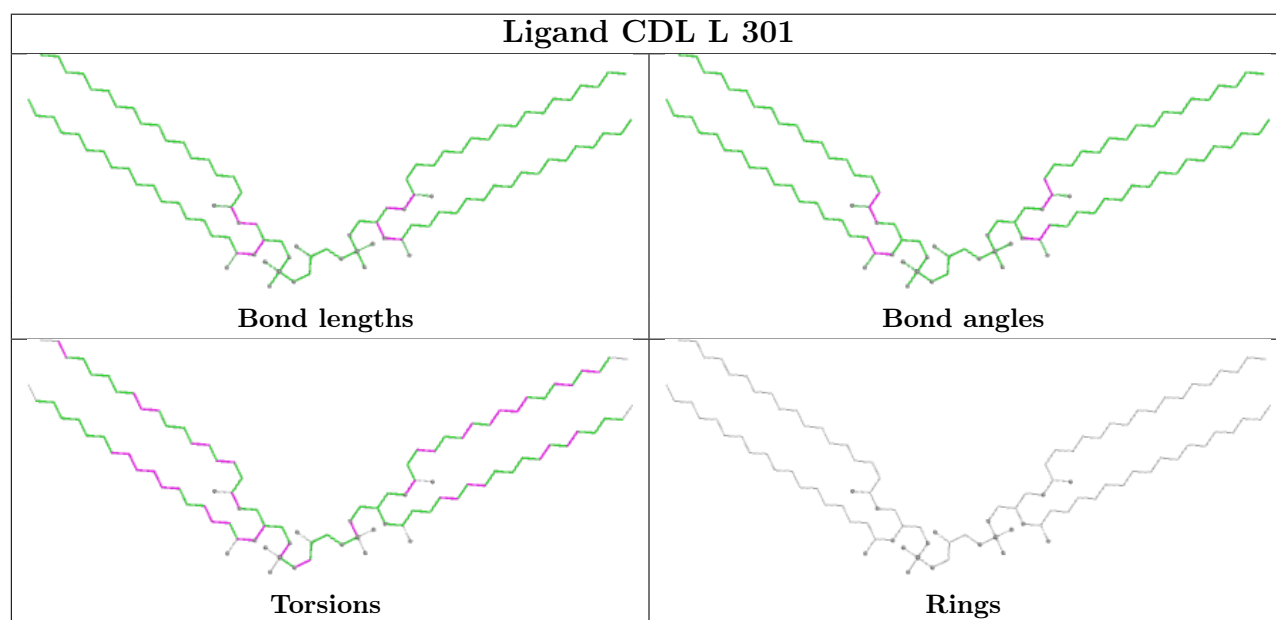
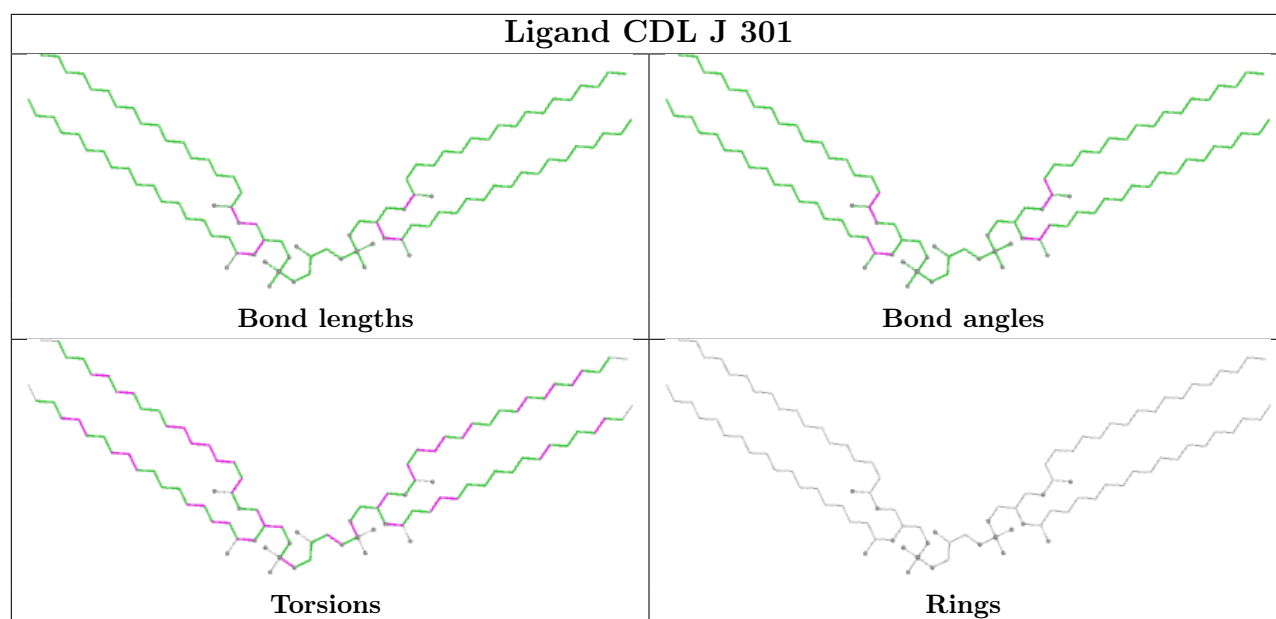


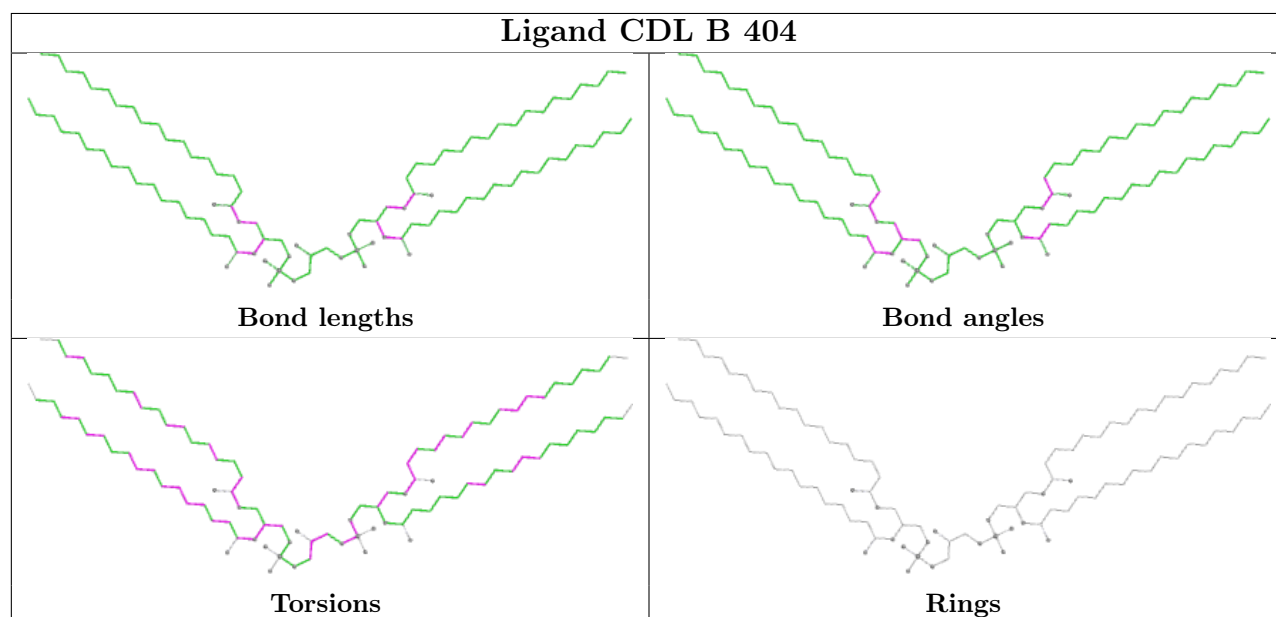
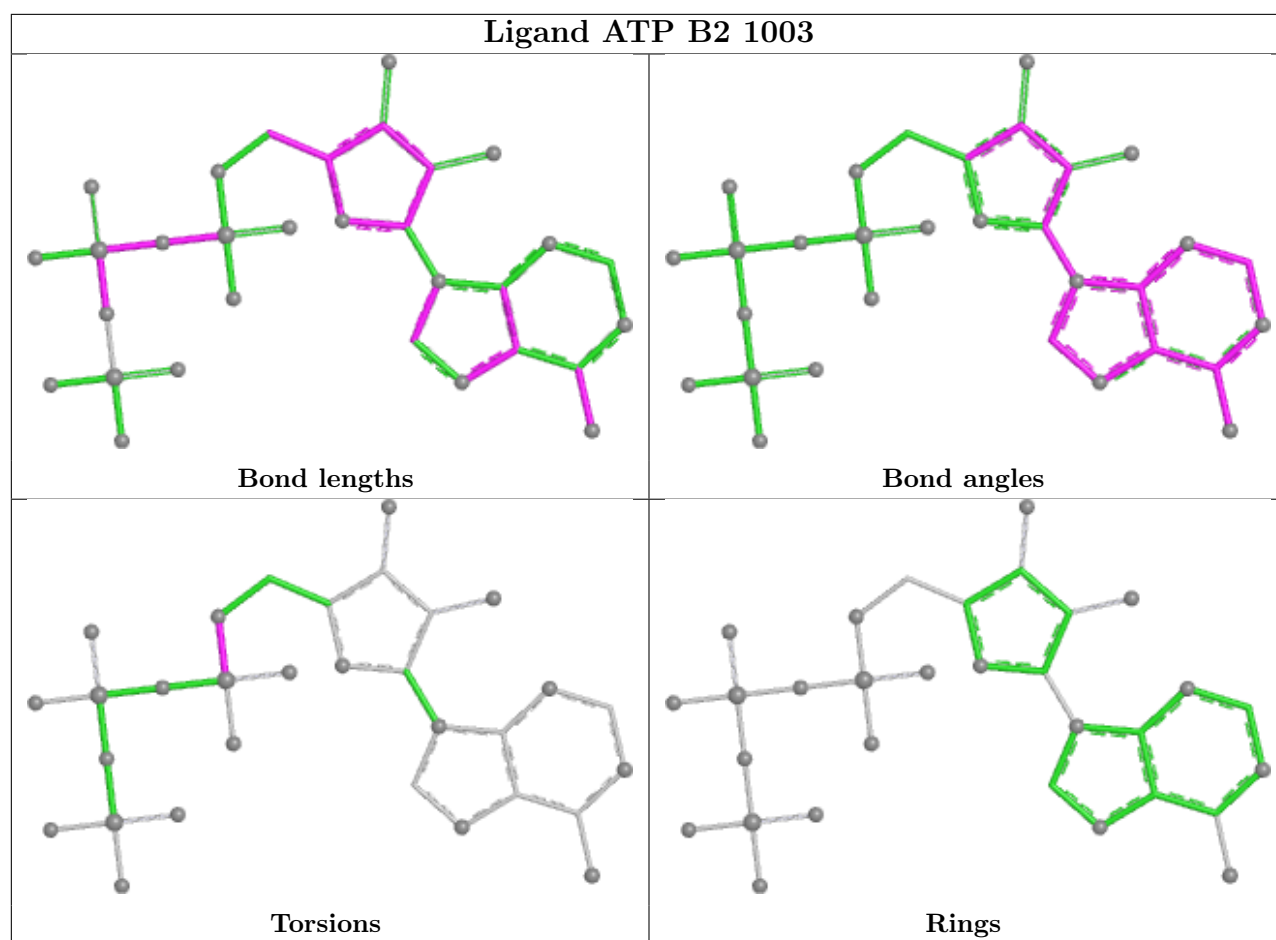


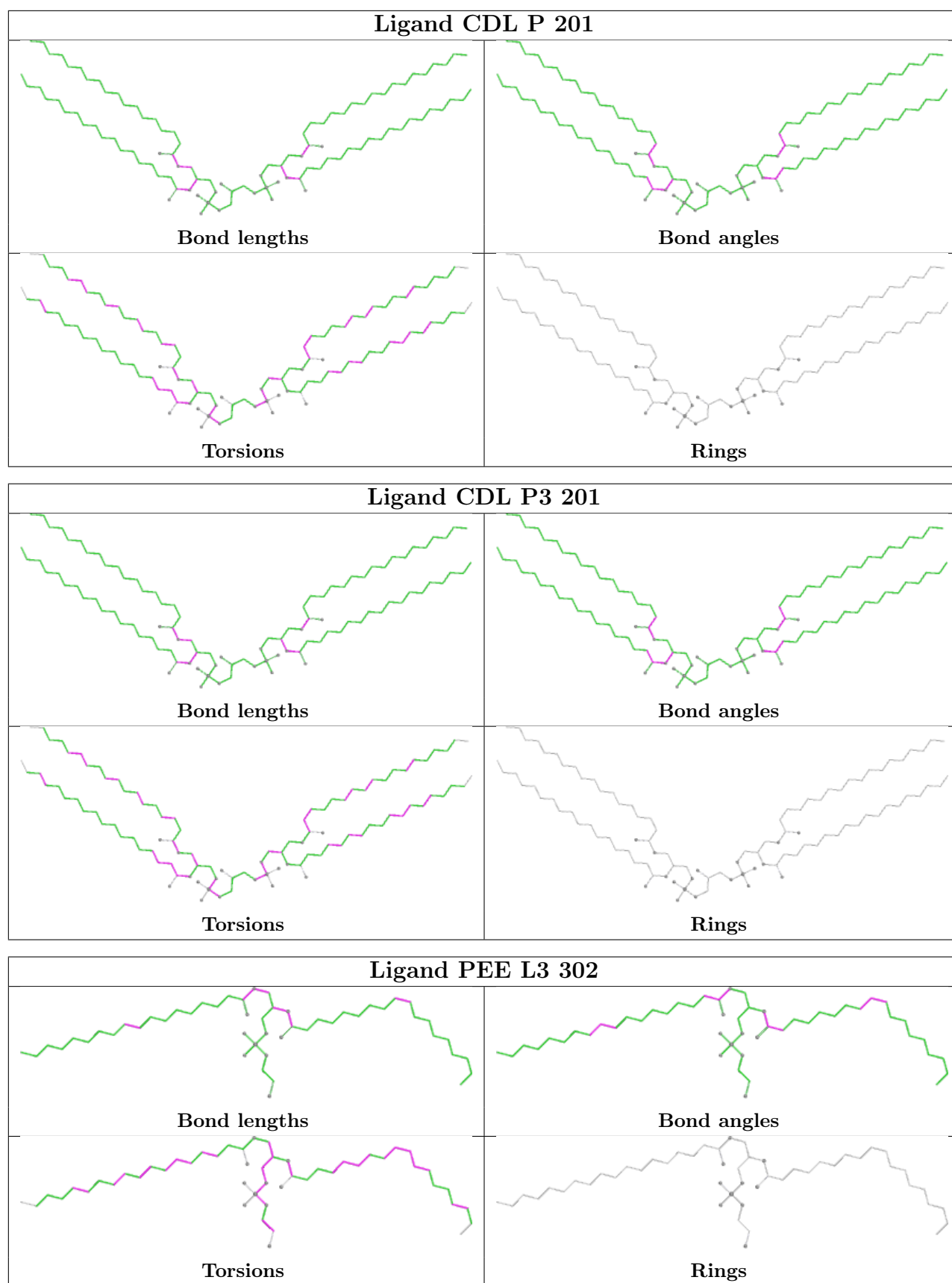


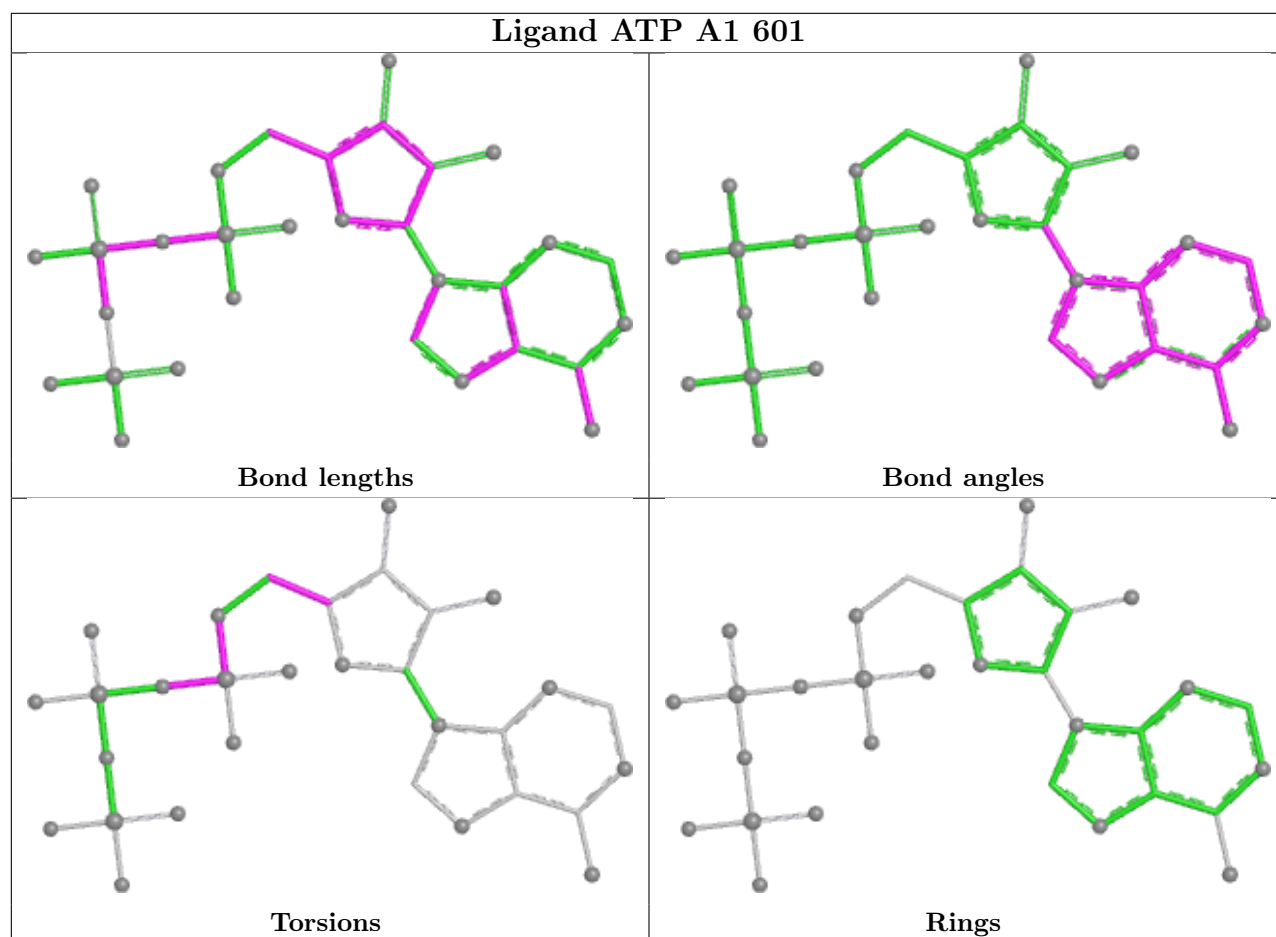
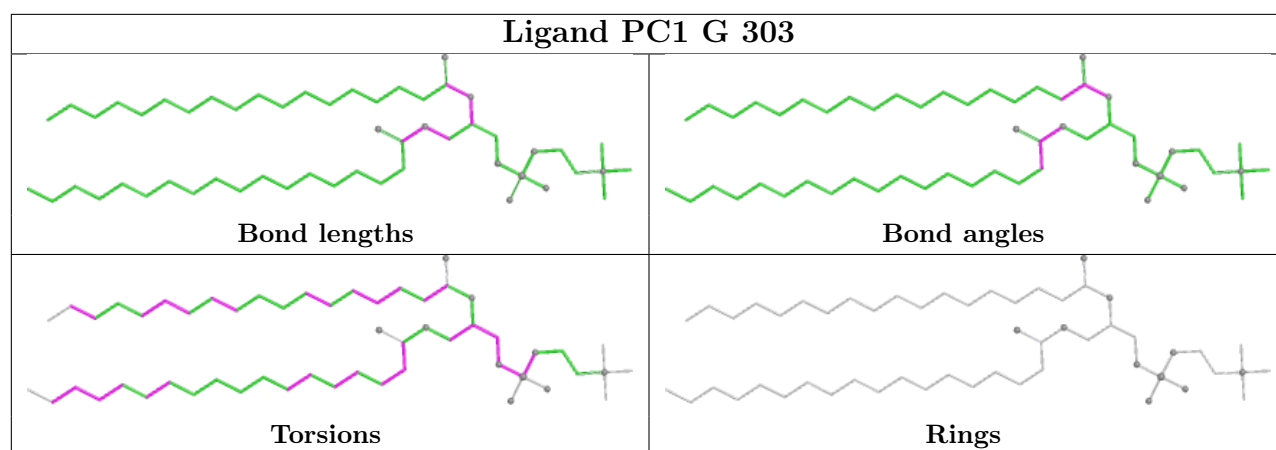


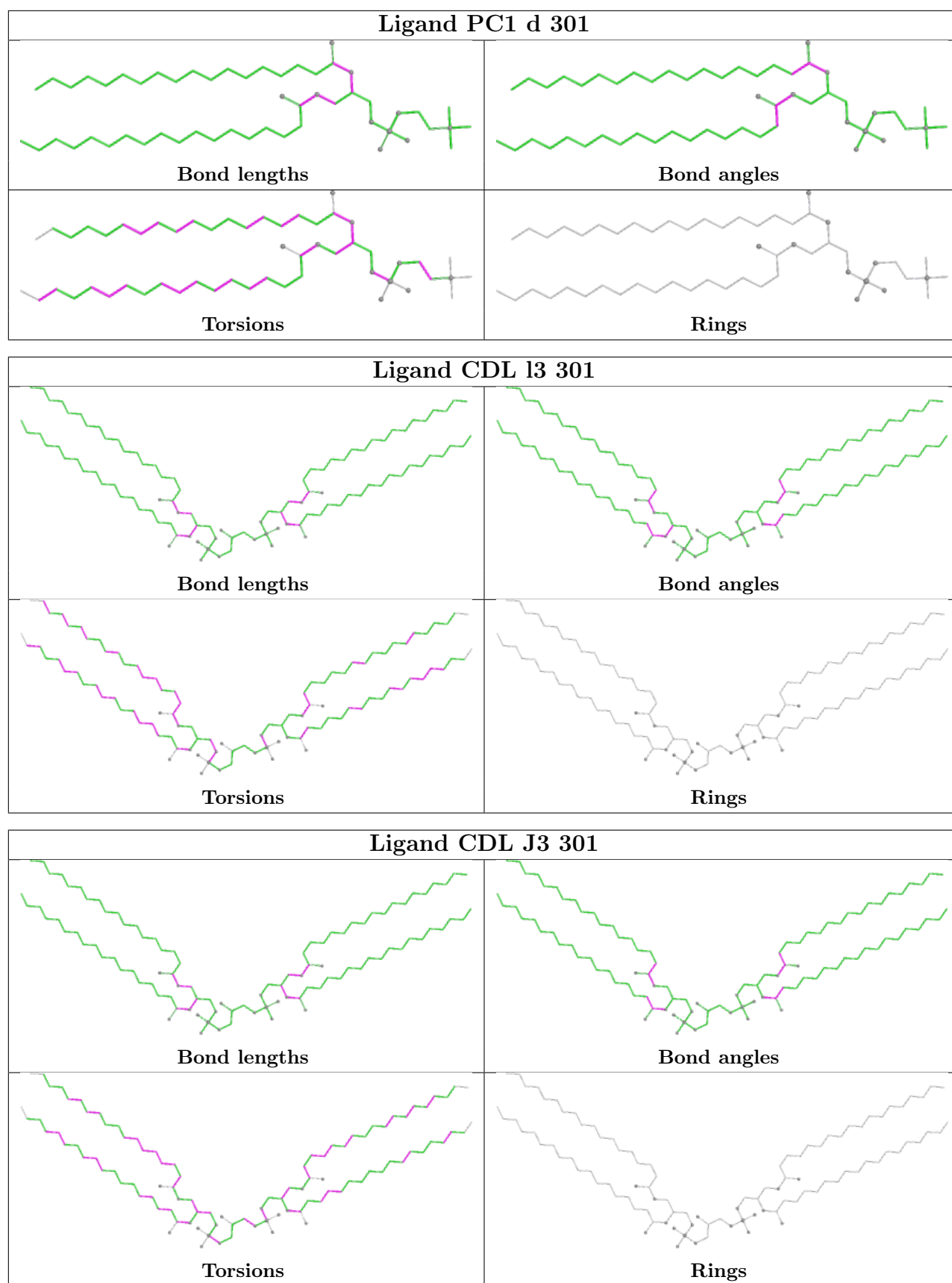


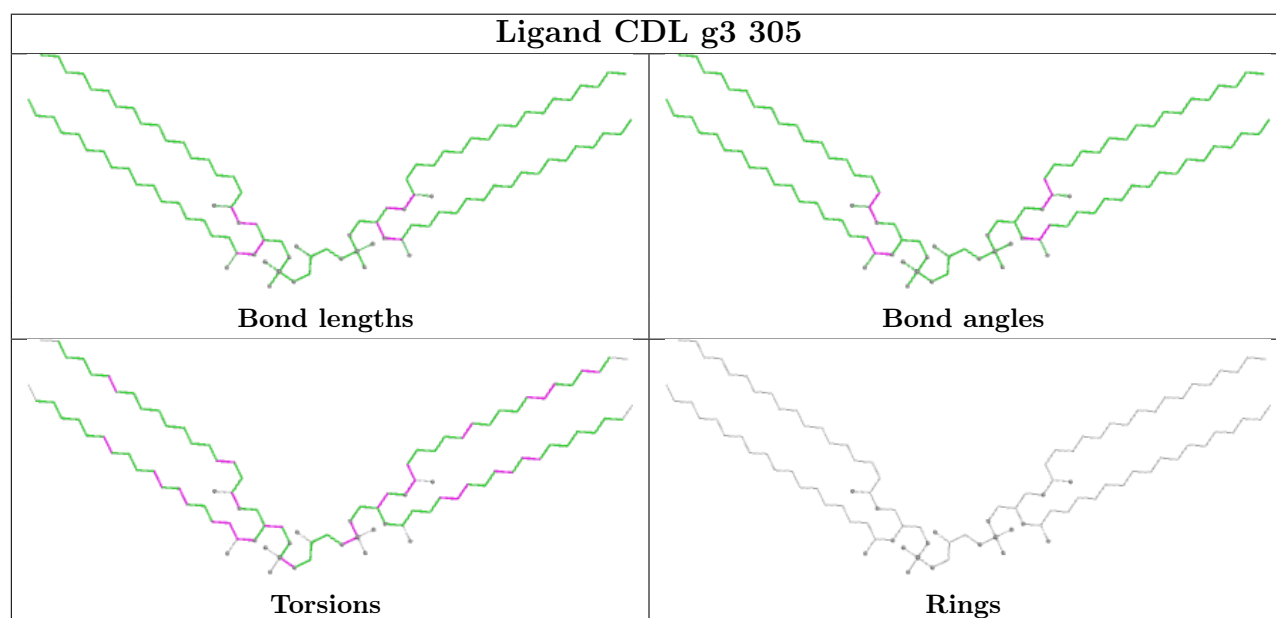
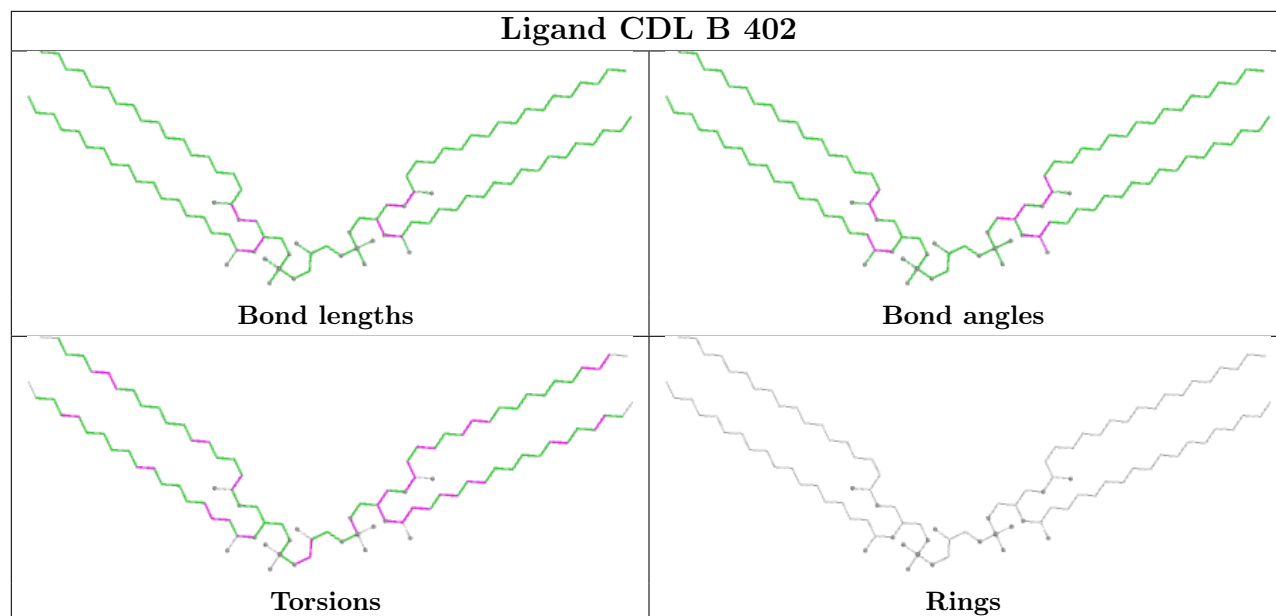


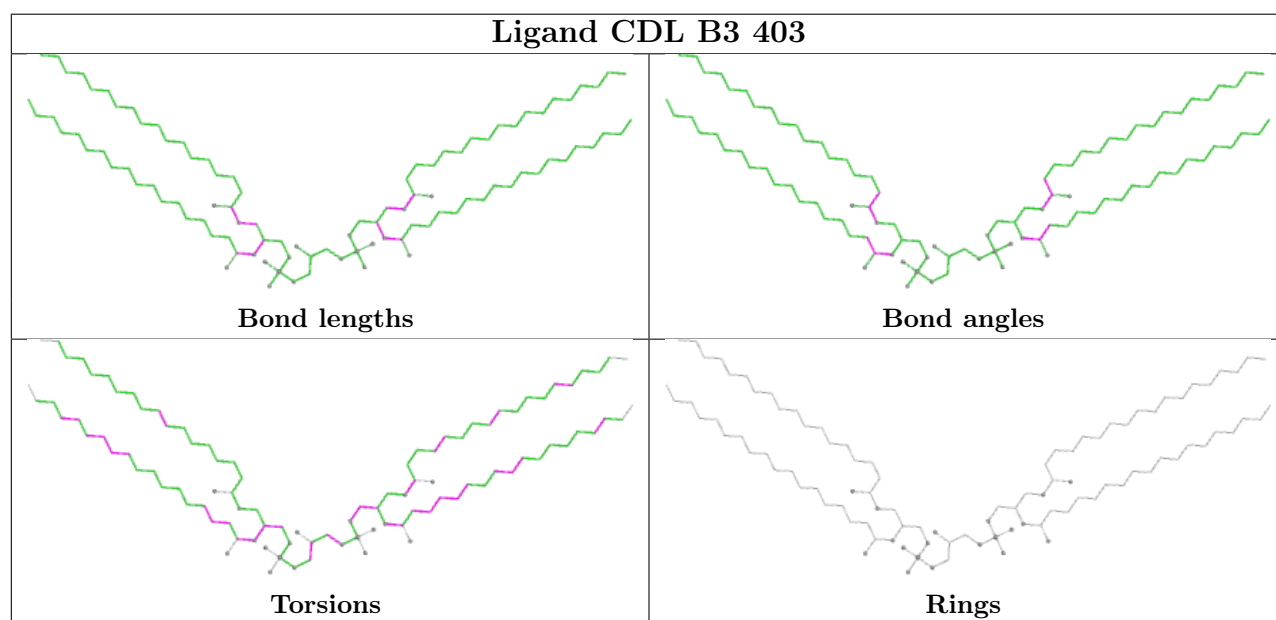
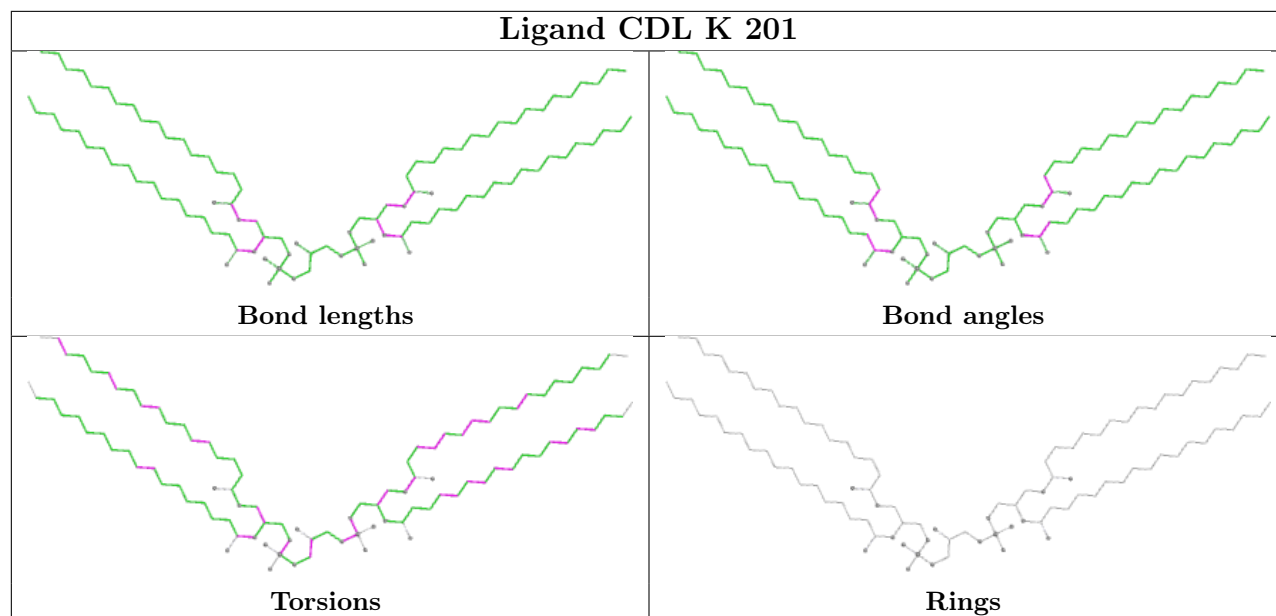


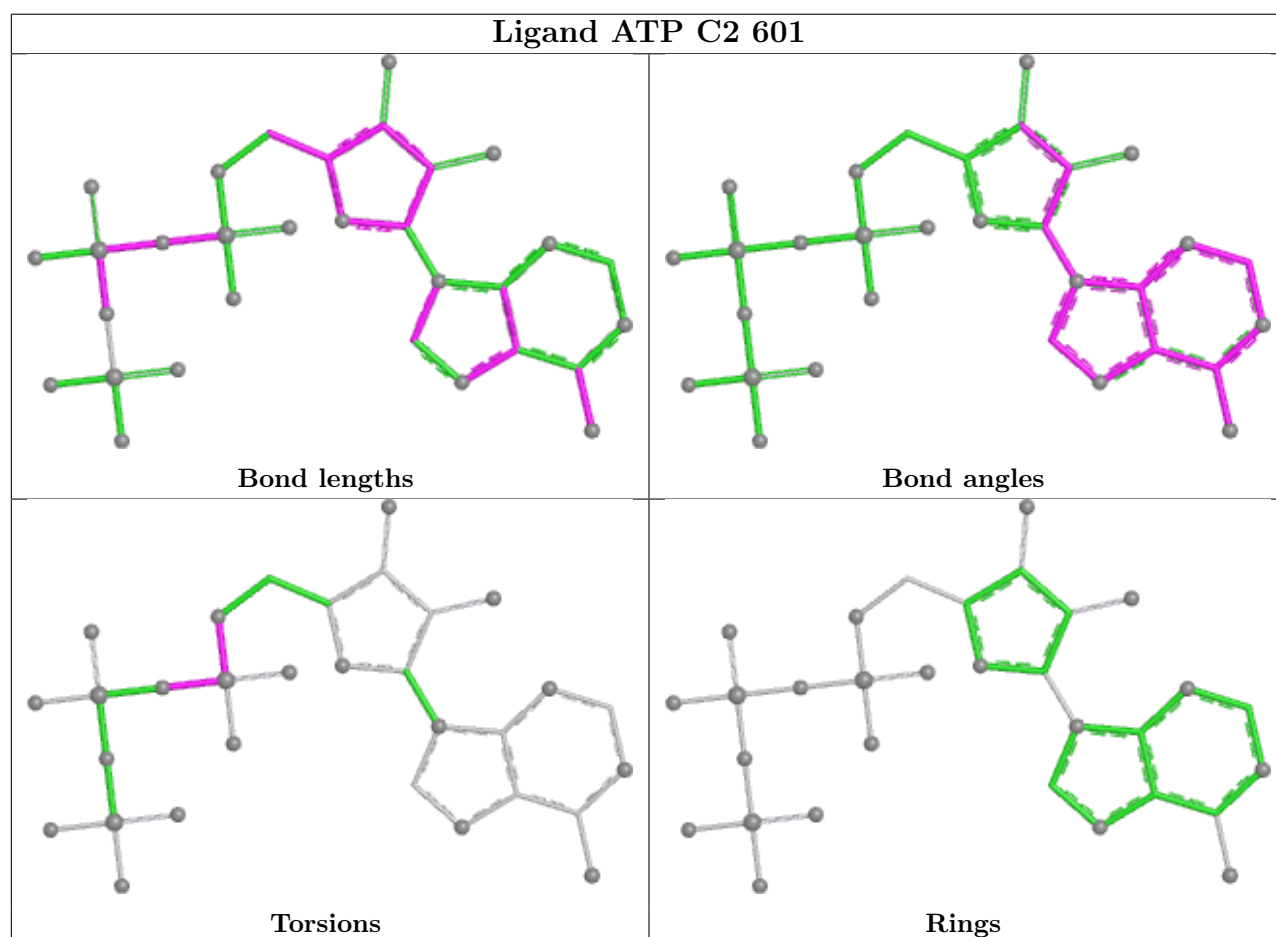
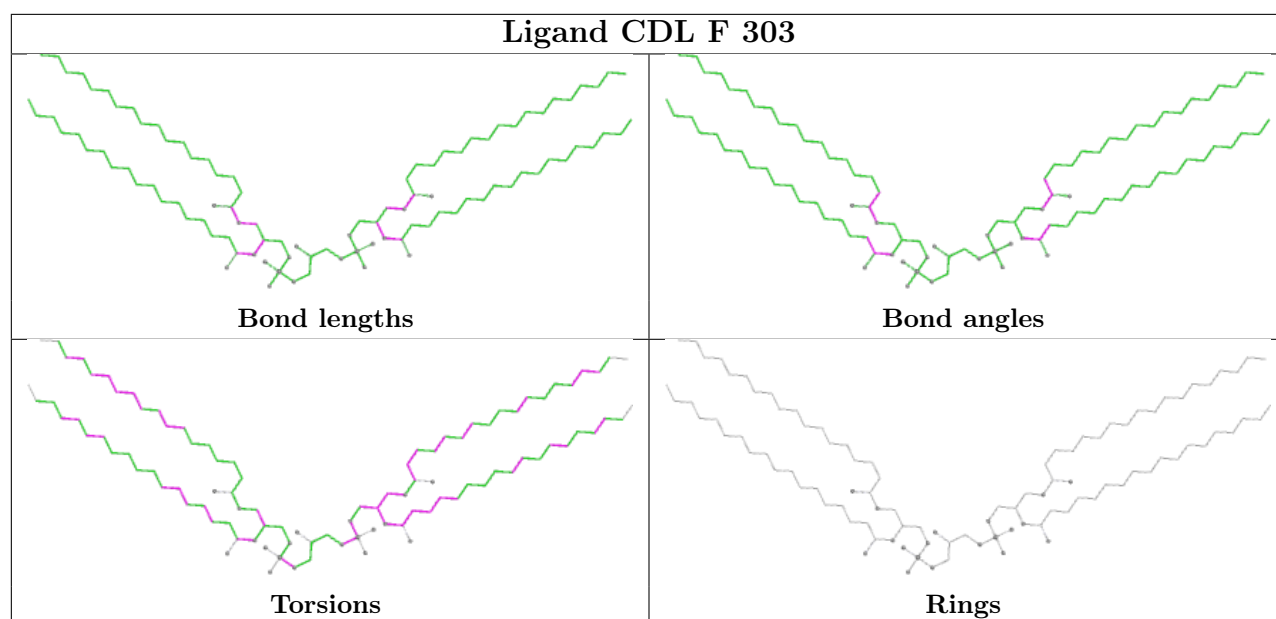


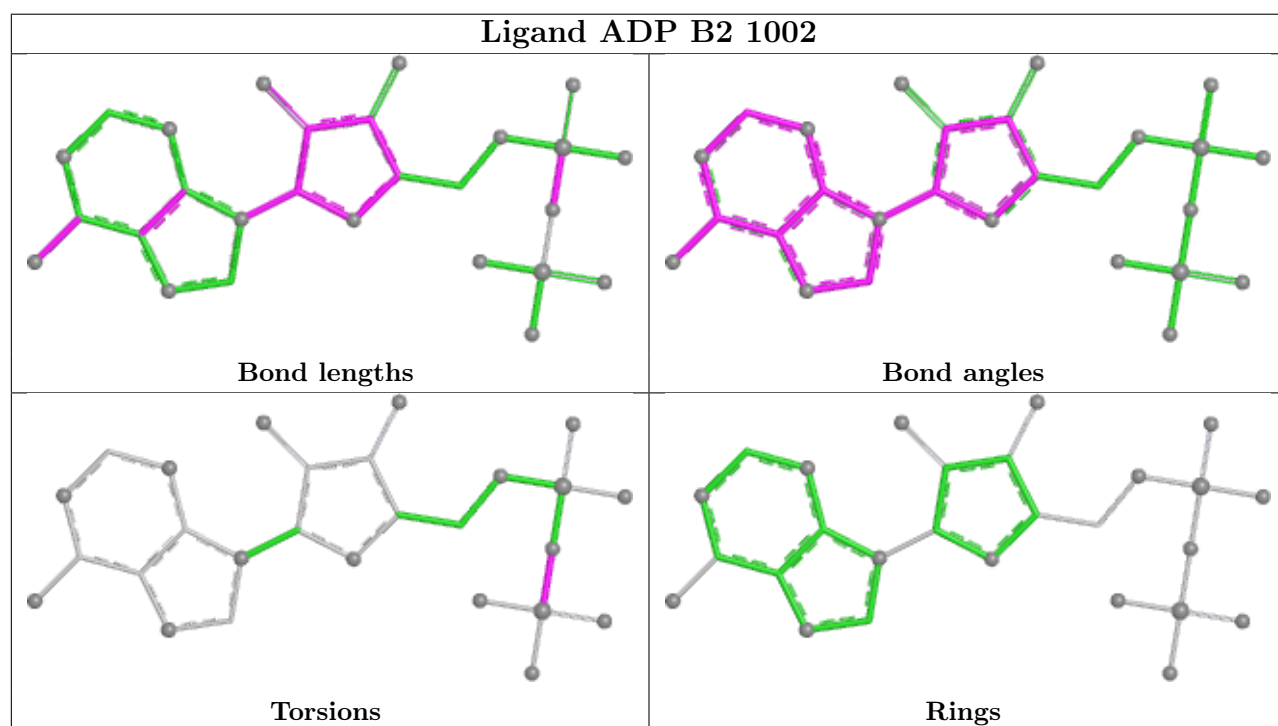
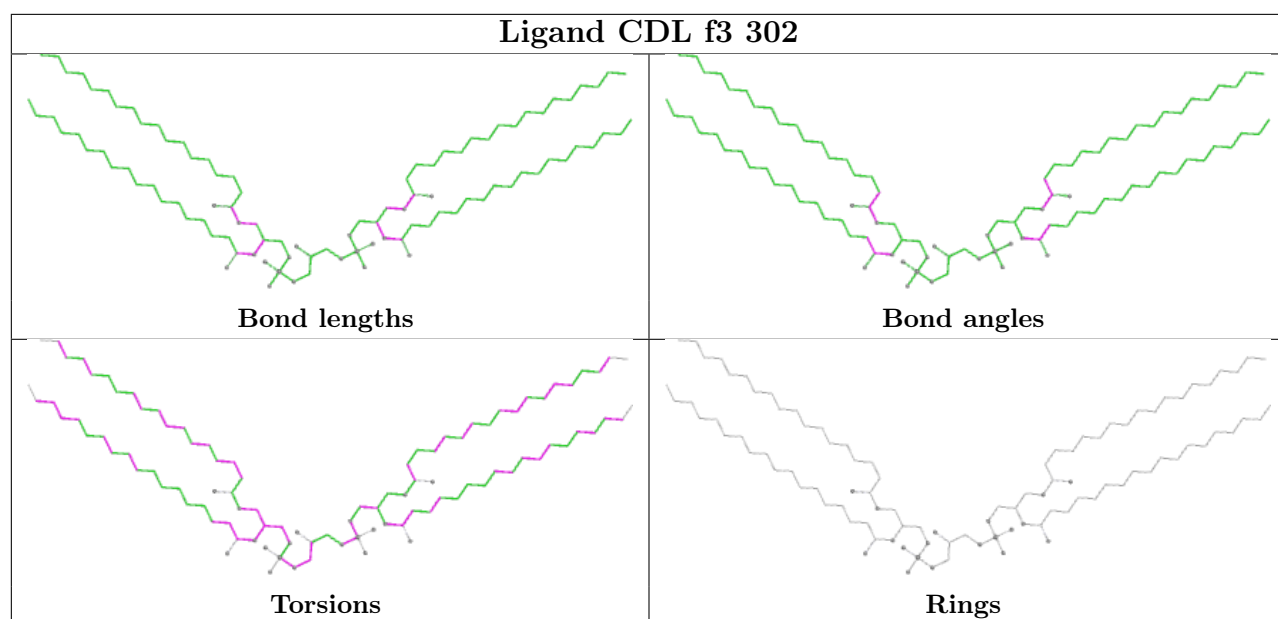


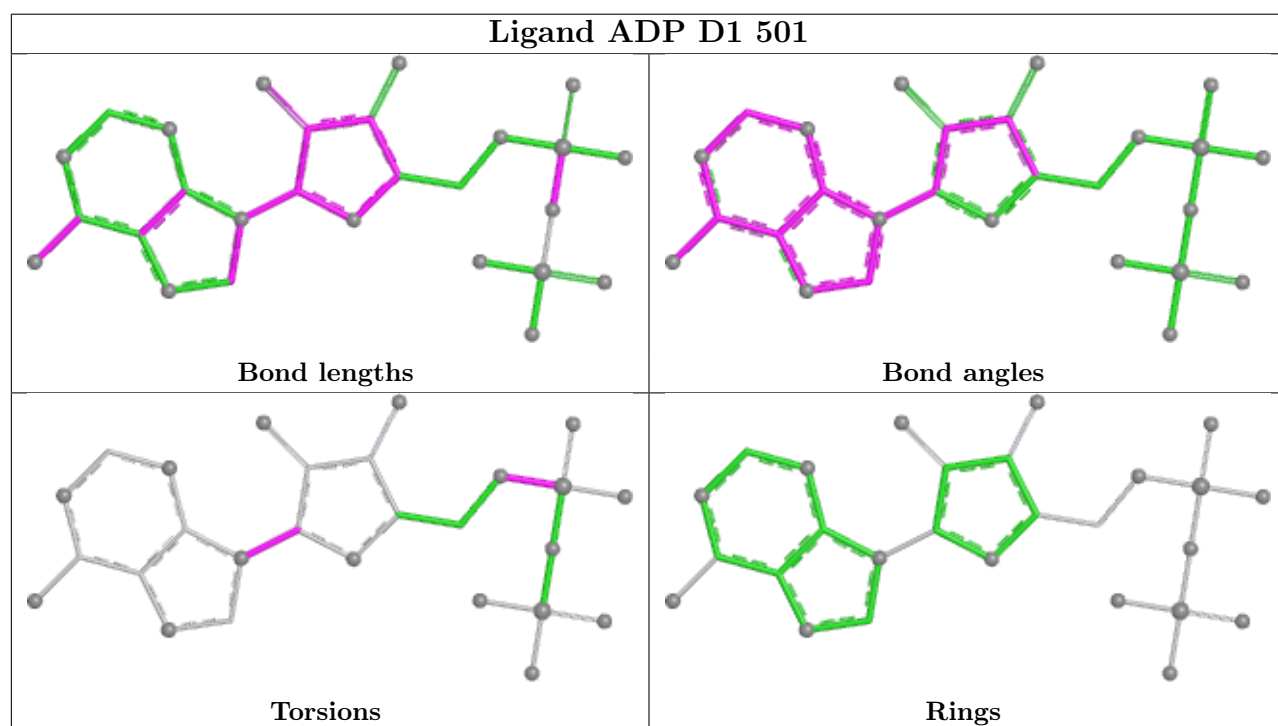
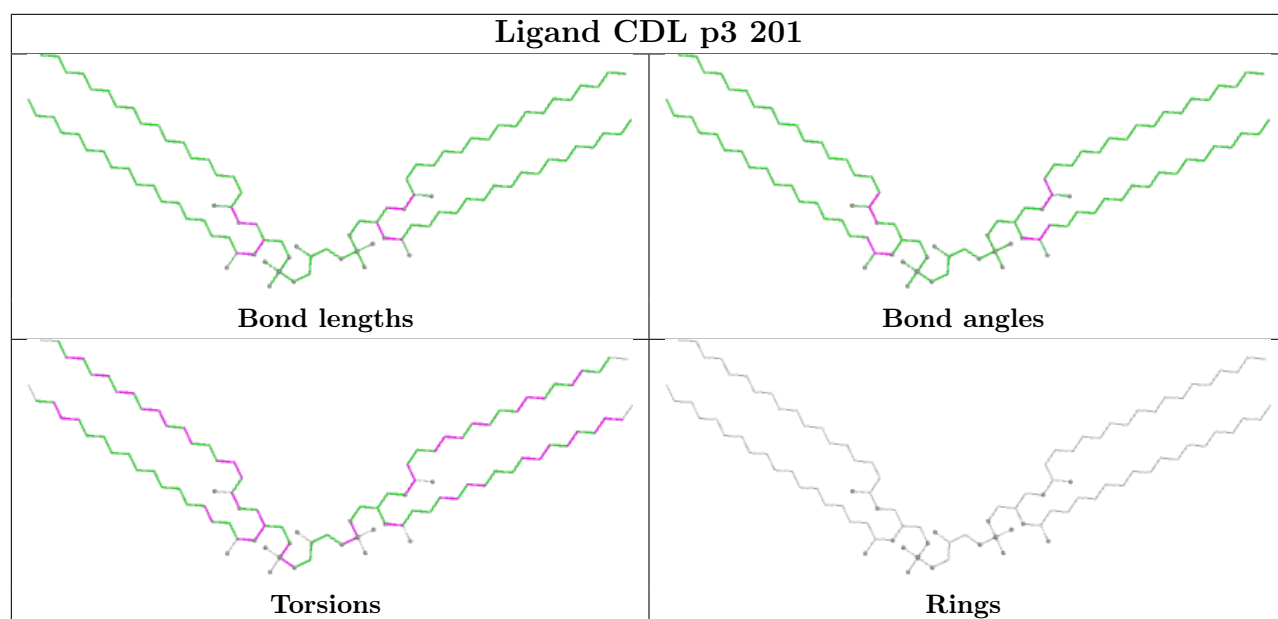


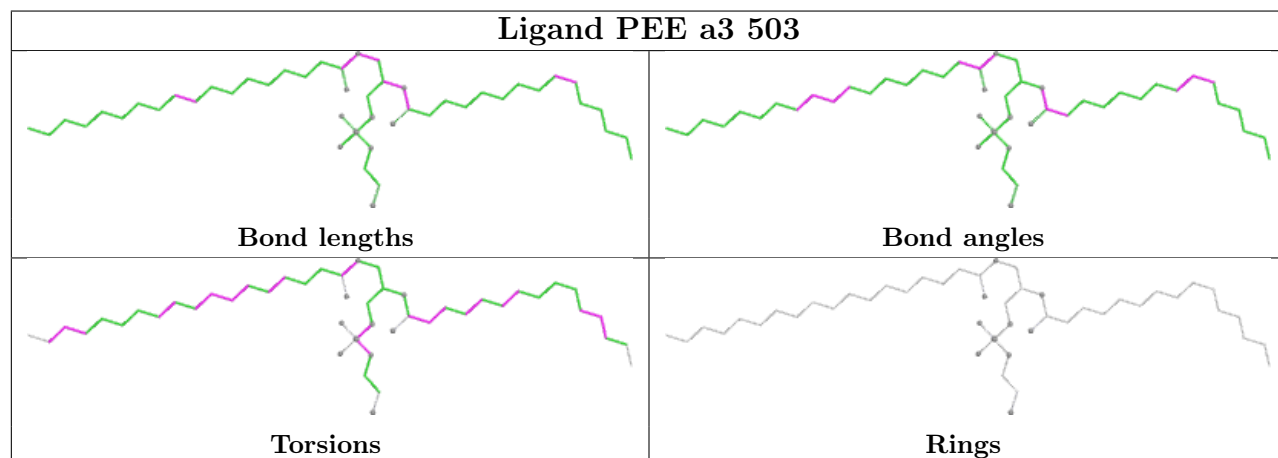
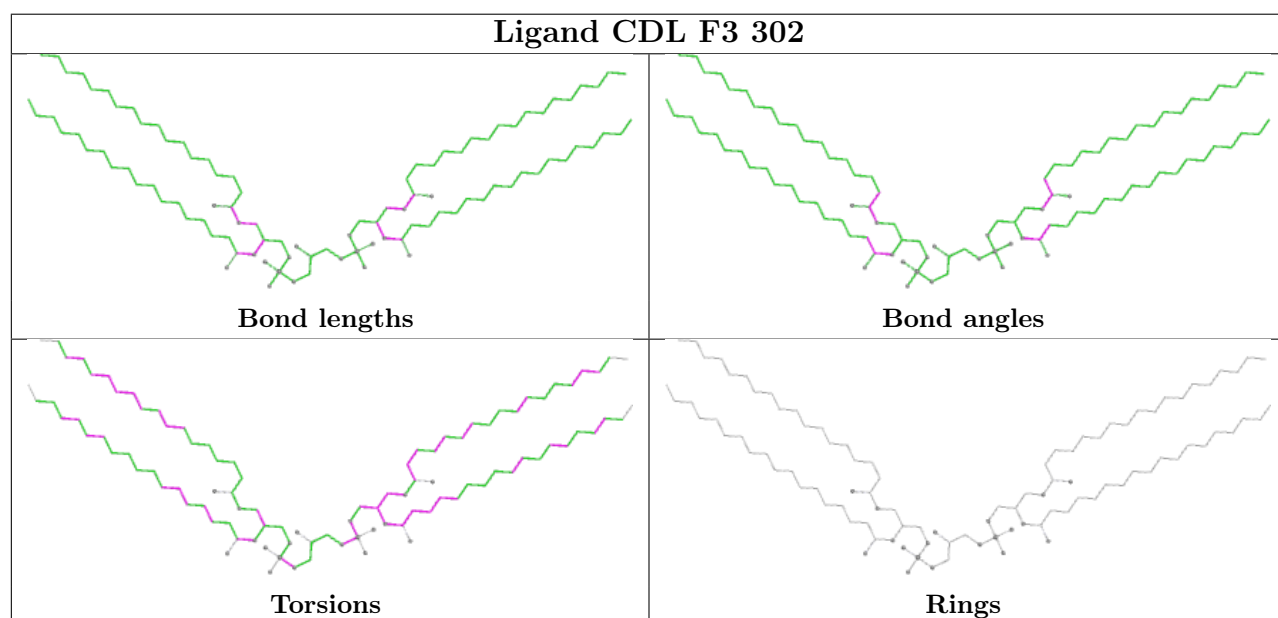
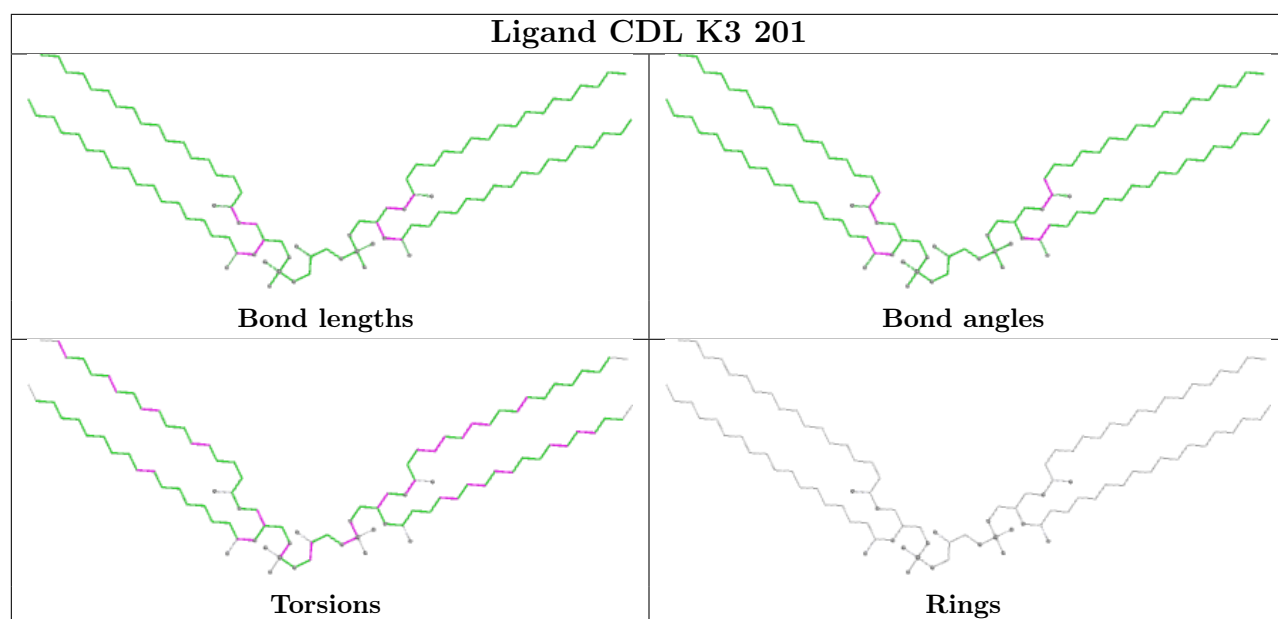


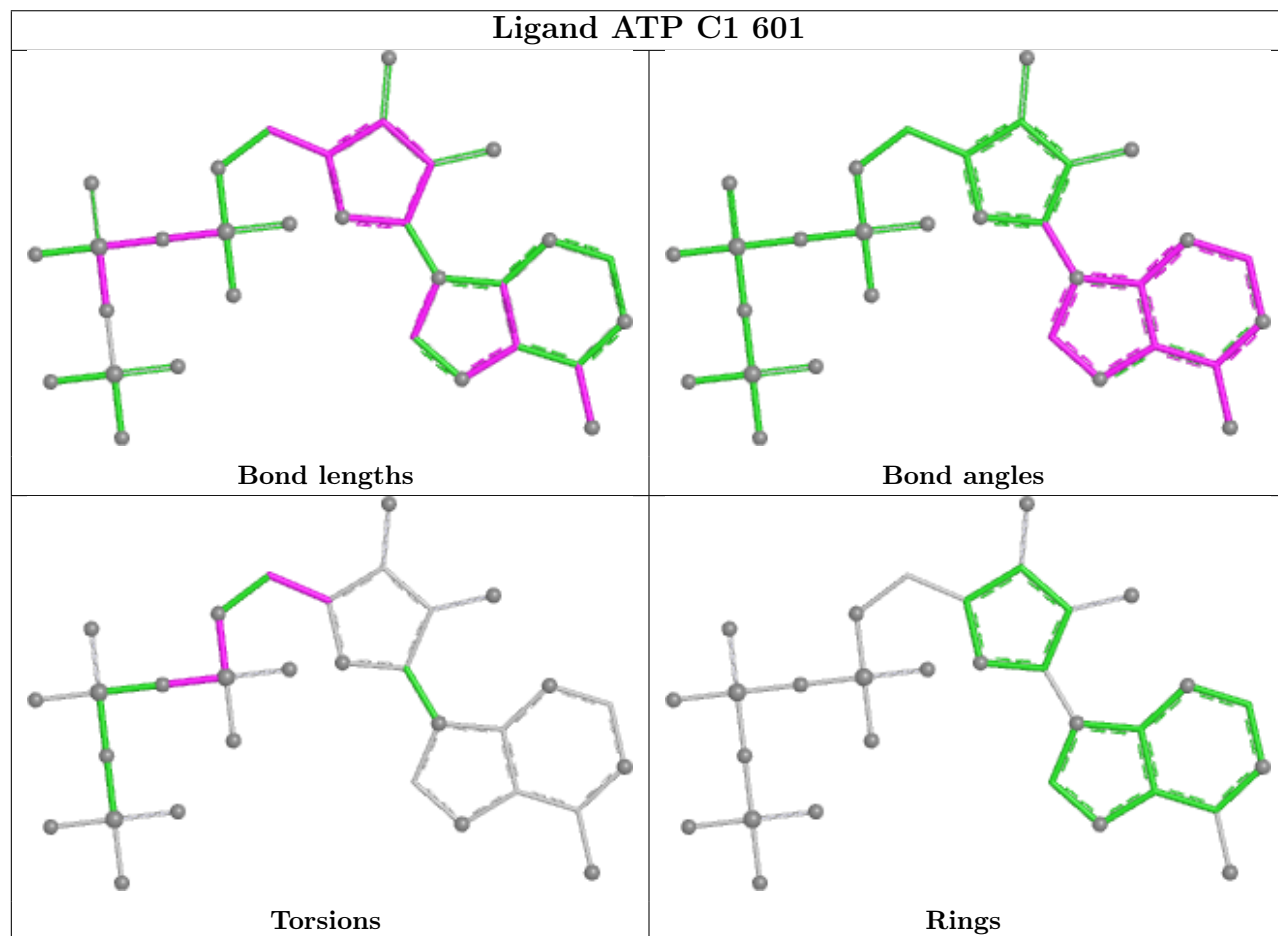
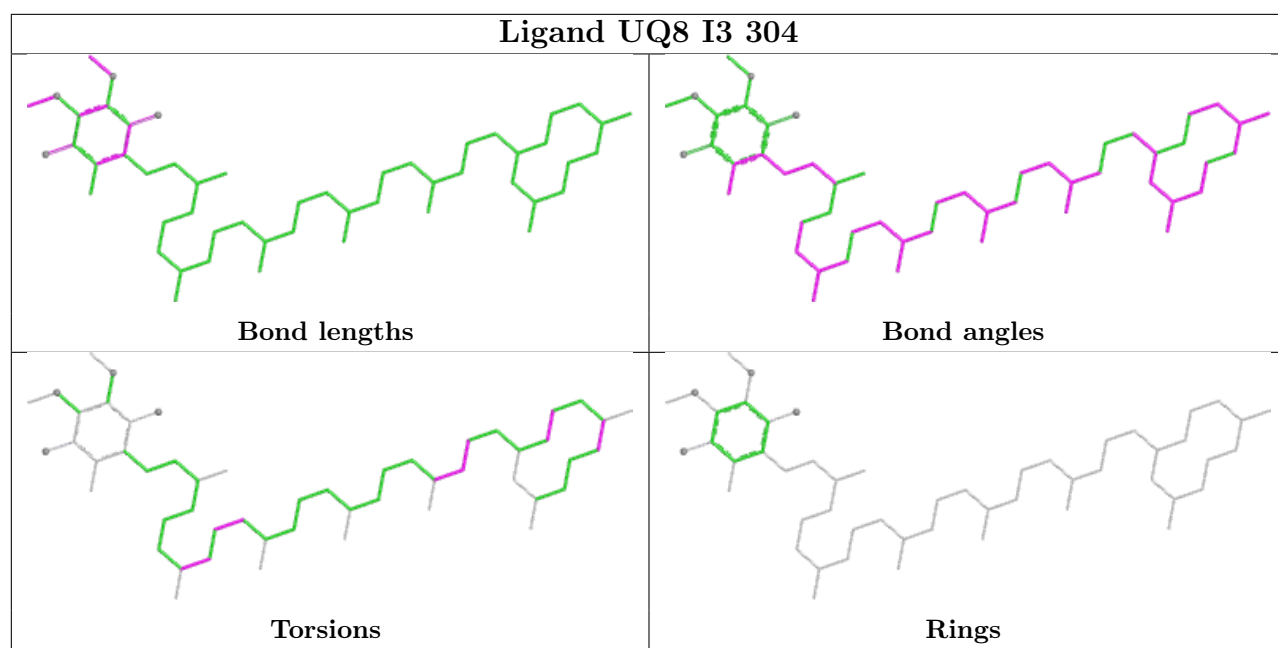


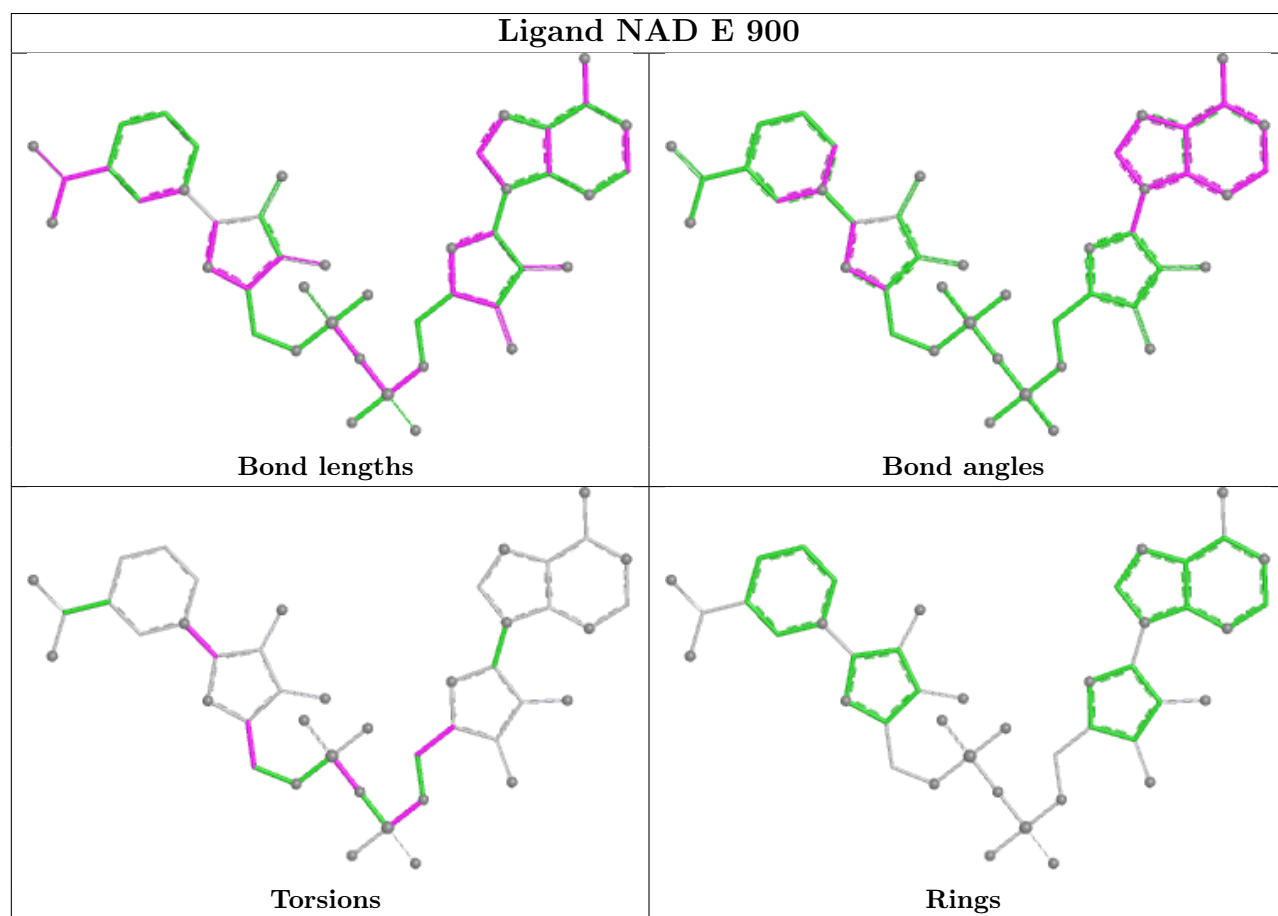
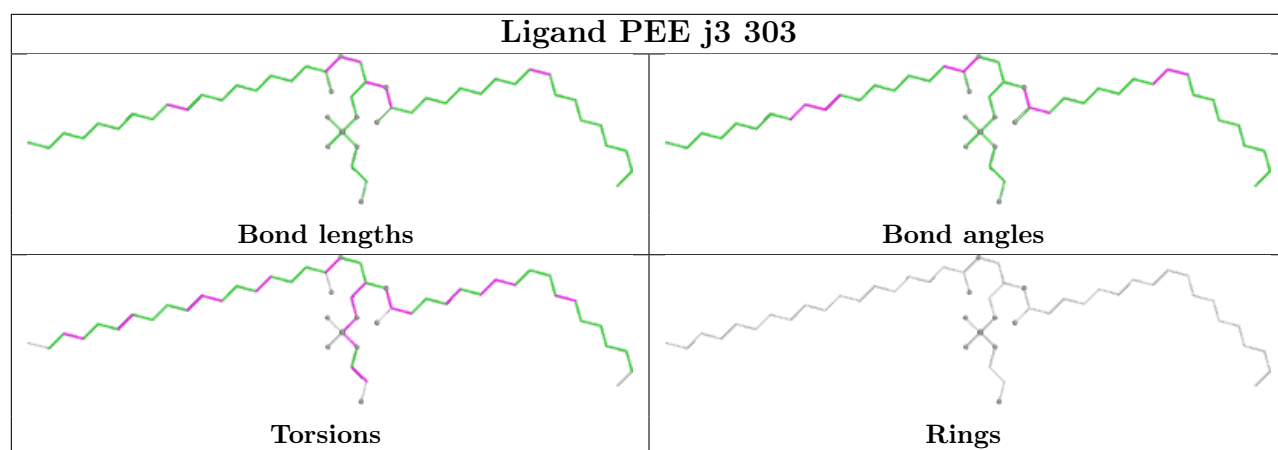


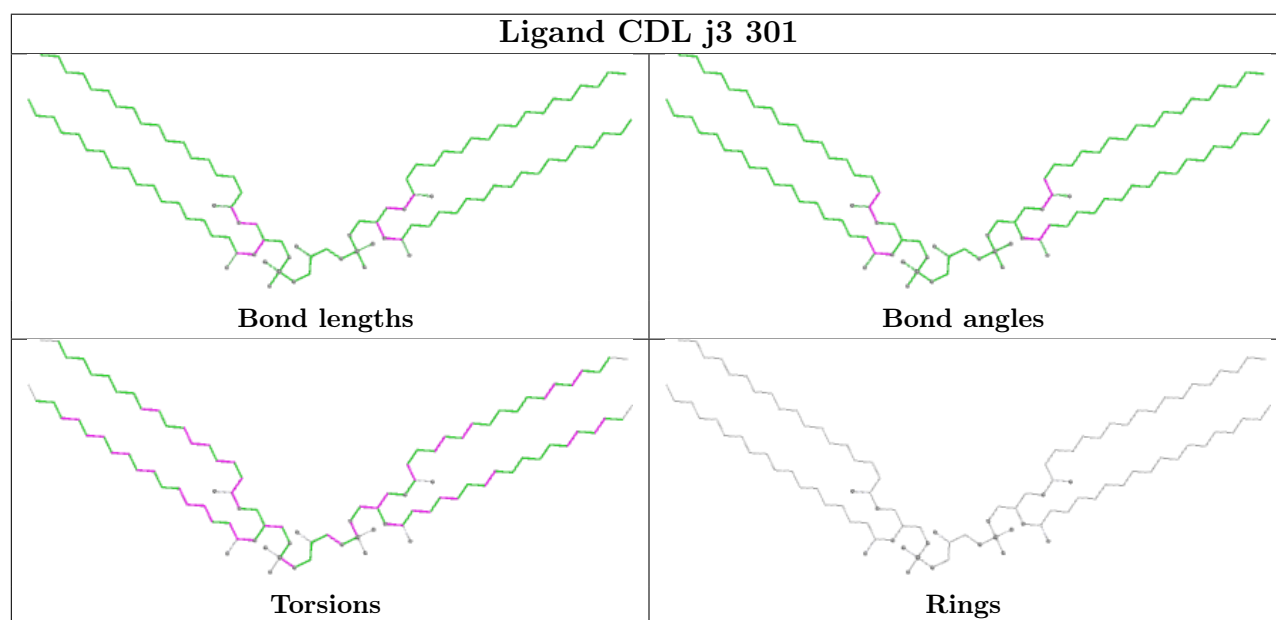
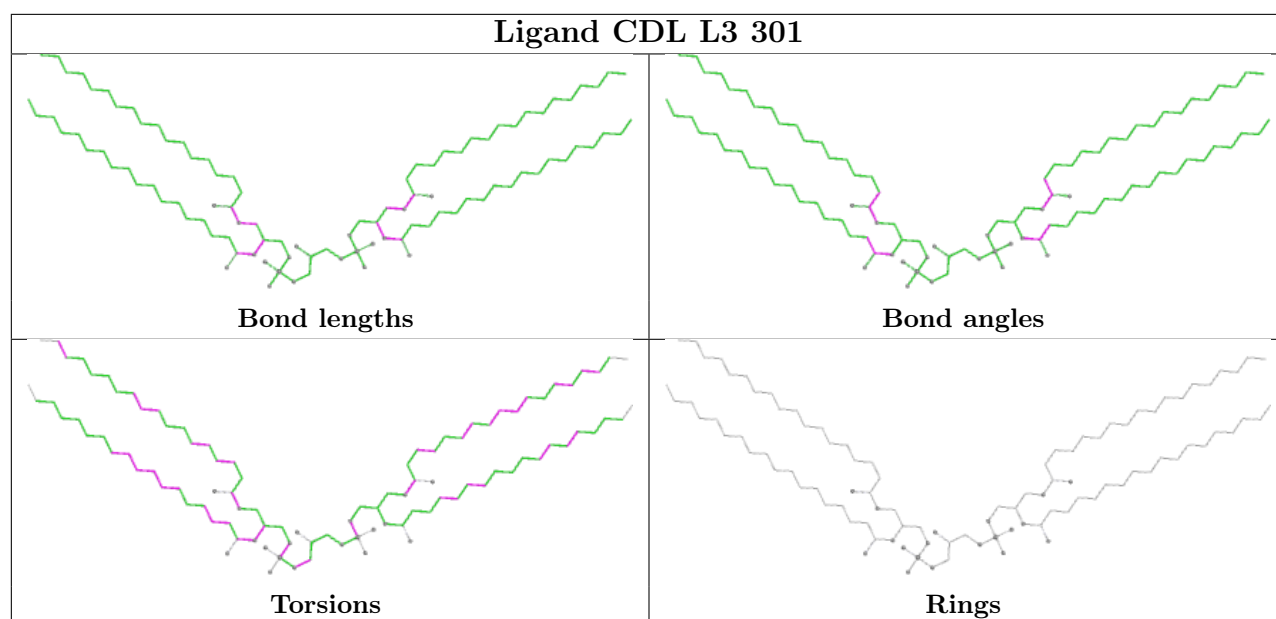


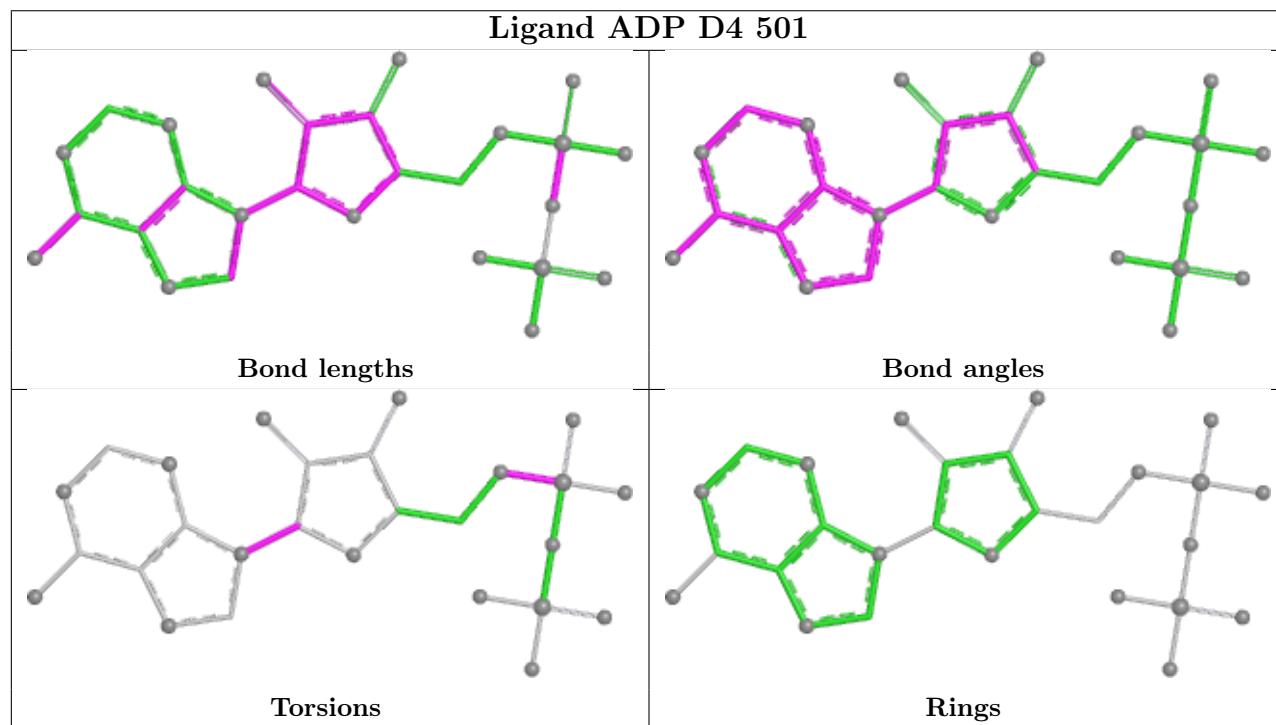
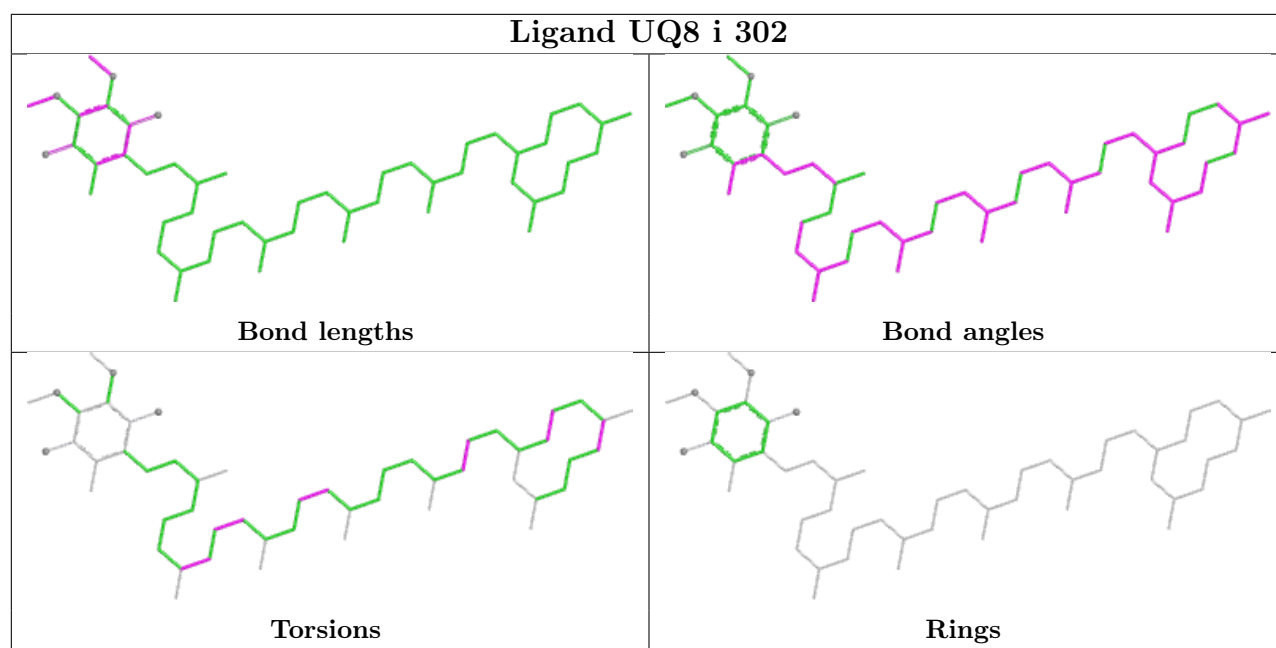


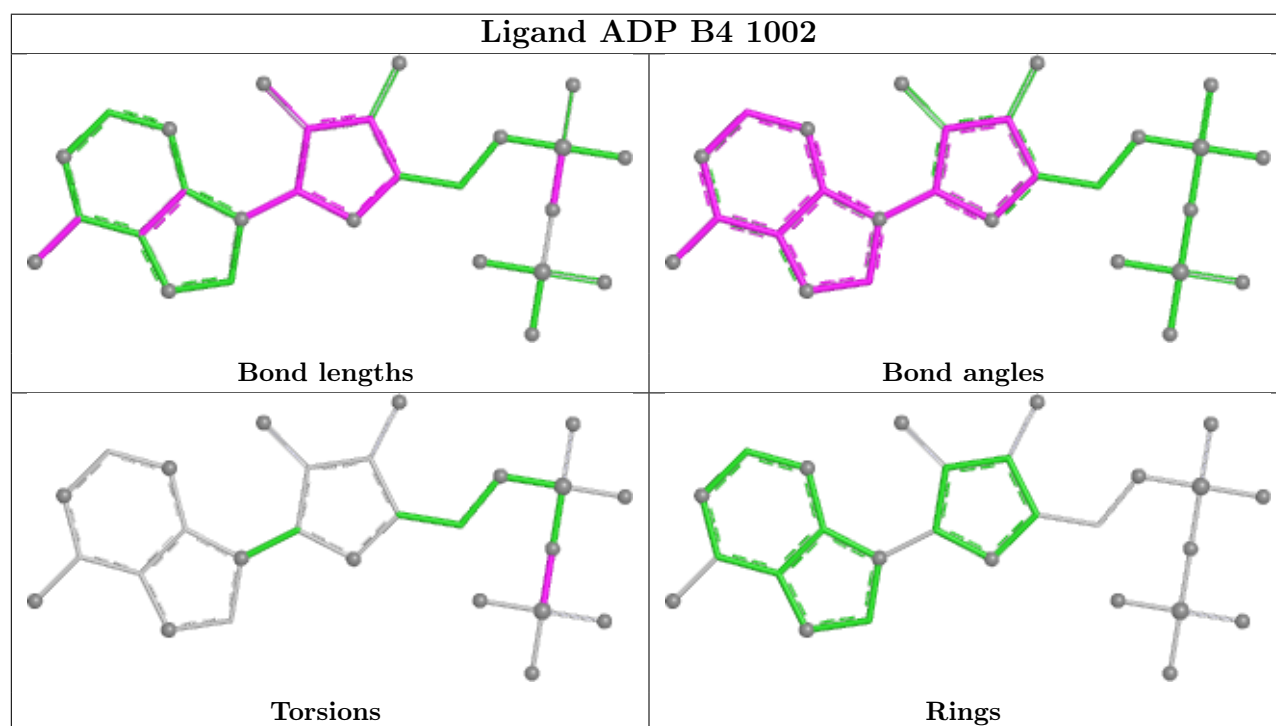
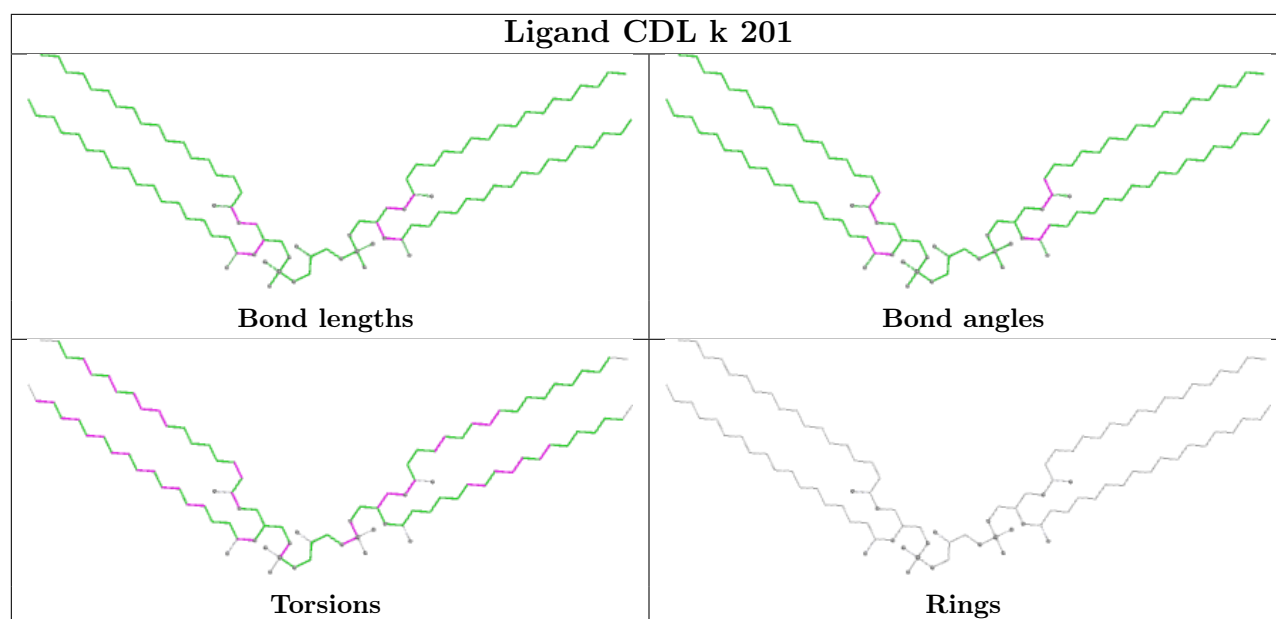


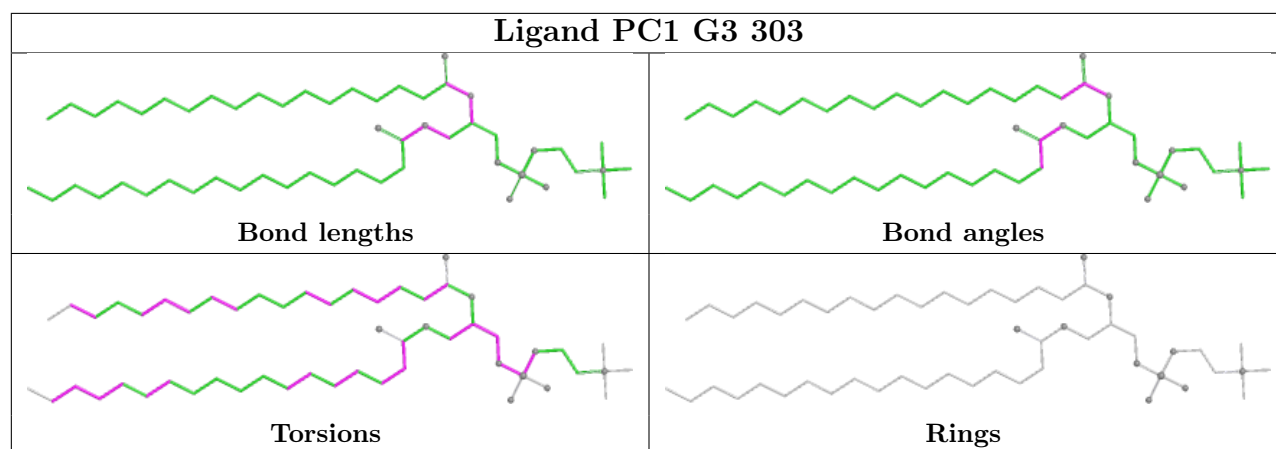
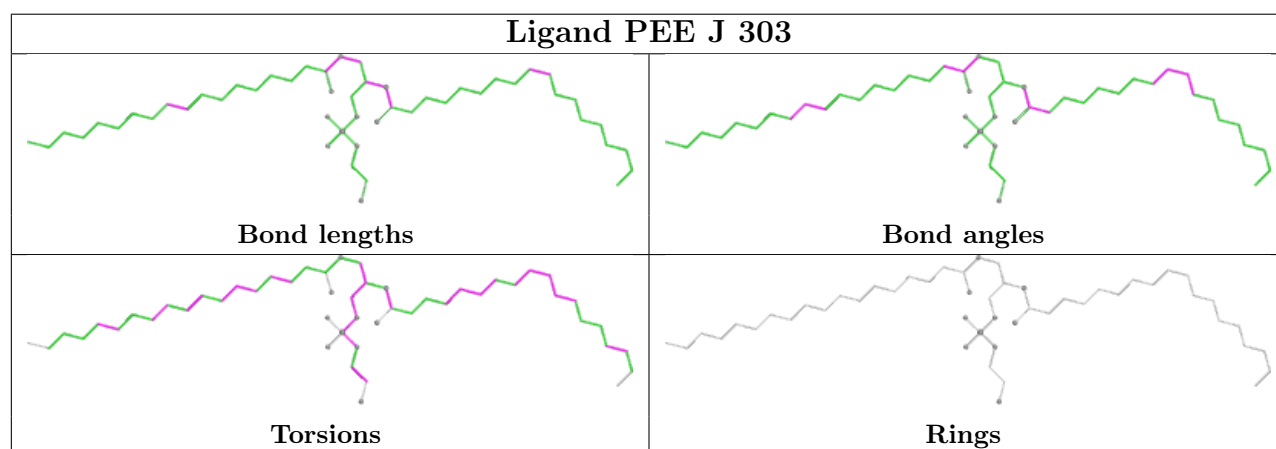
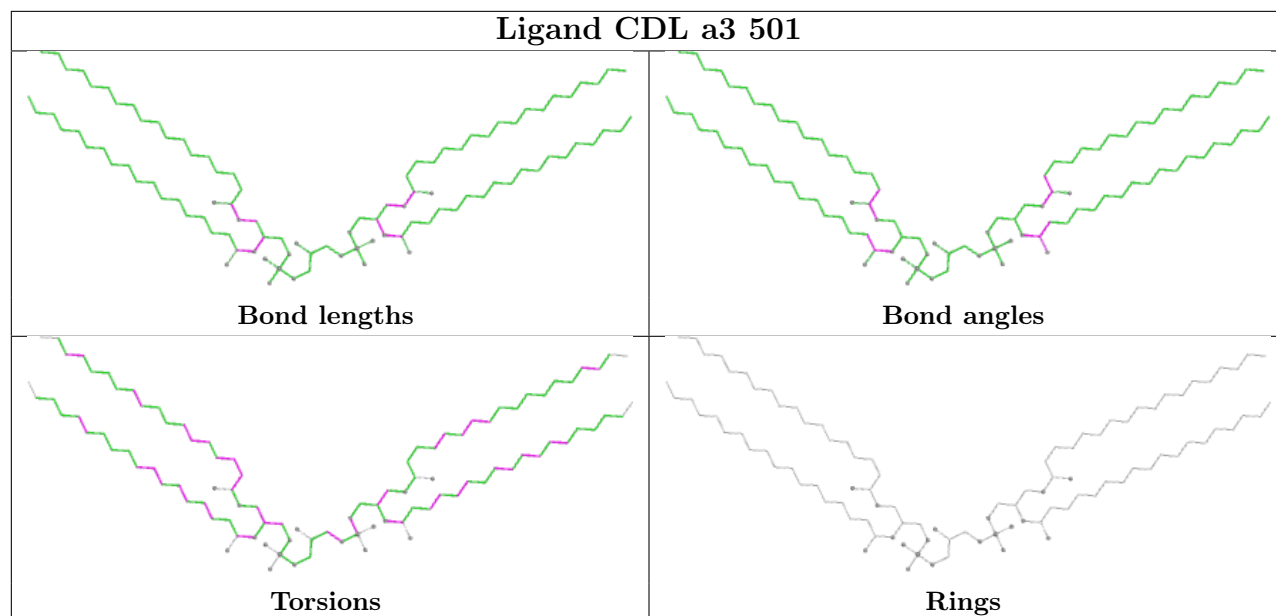


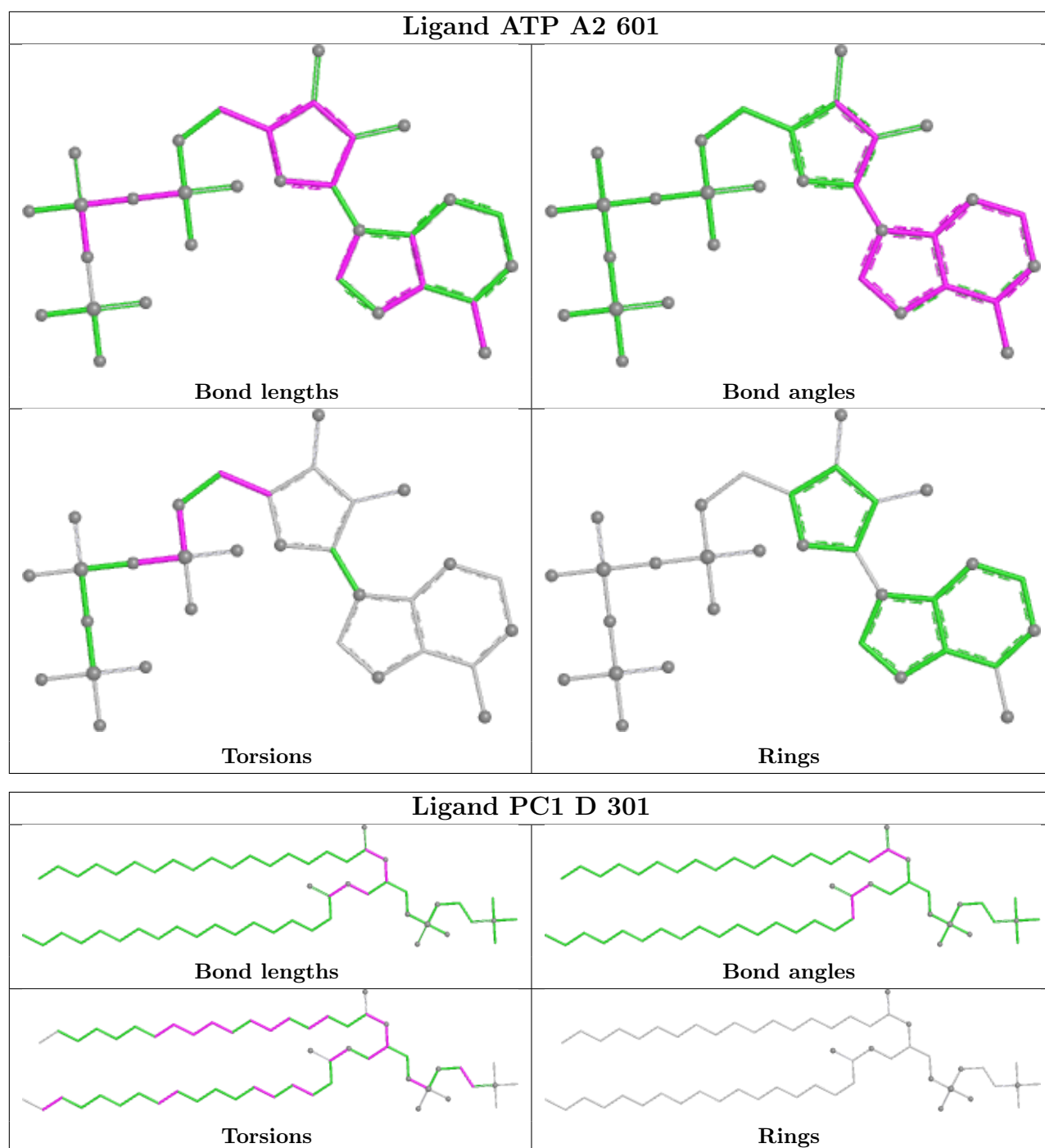












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

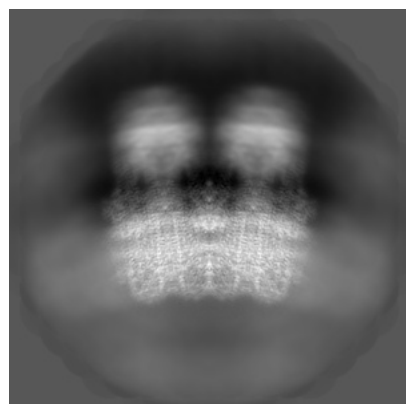
6 Map visualisation [i](#)

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

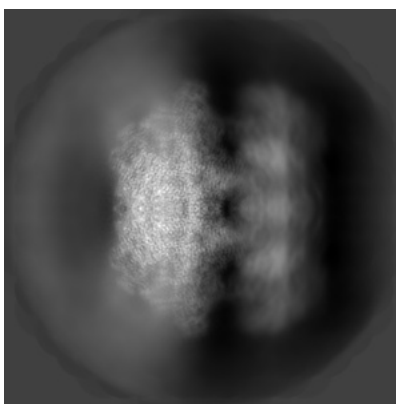
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

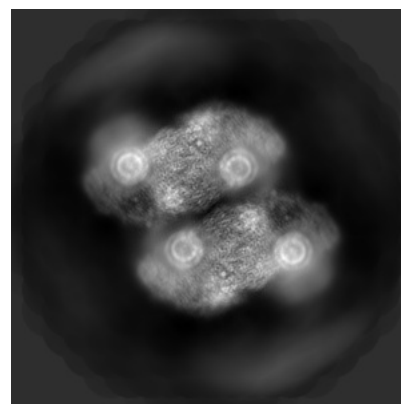
6.1.1 Primary map



X

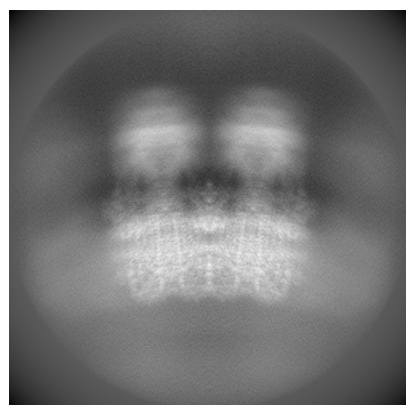


Y

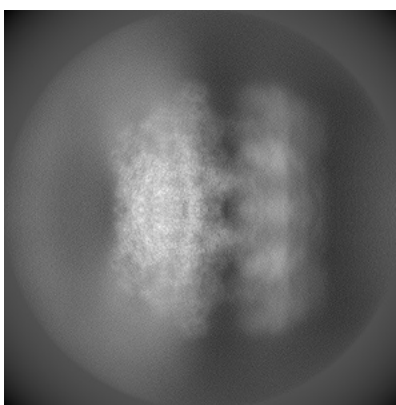


Z

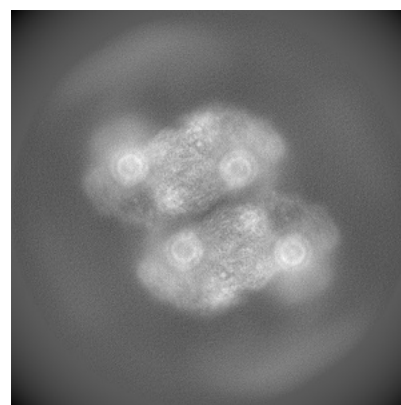
6.1.2 Raw map



X



Y

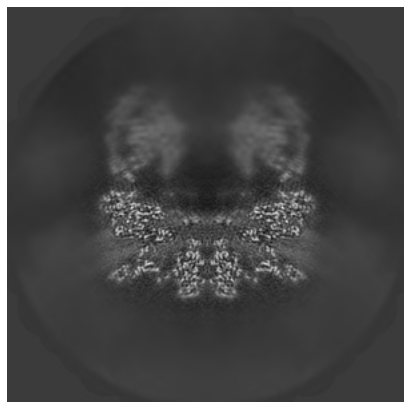


Z

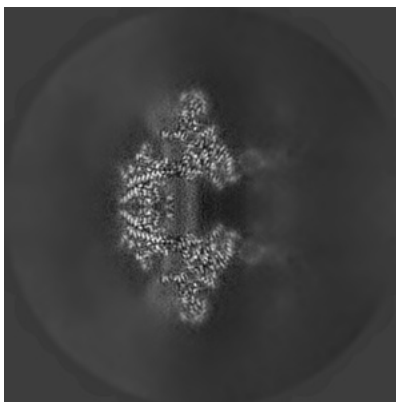
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

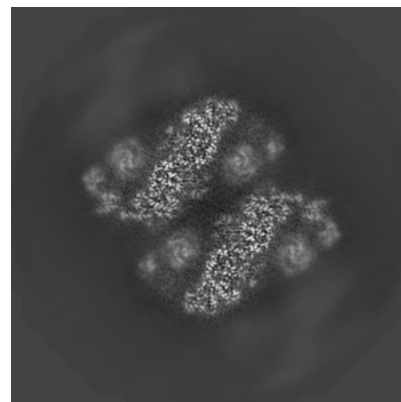
6.2.1 Primary map



X Index: 300

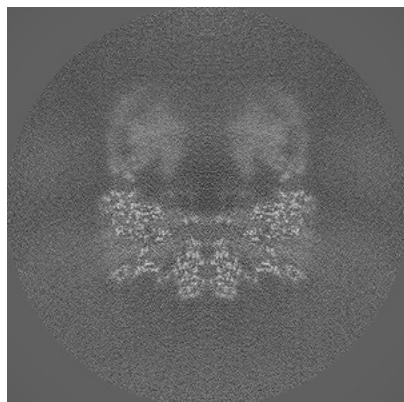


Y Index: 300

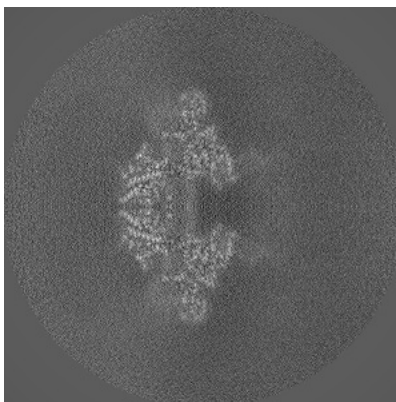


Z Index: 300

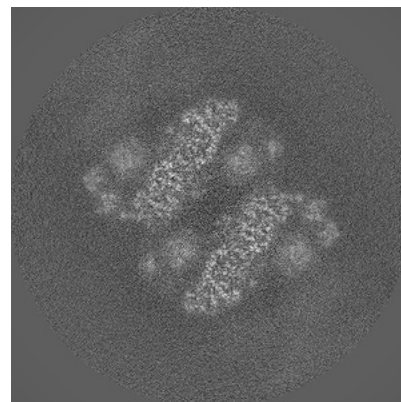
6.2.2 Raw map



X Index: 300



Y Index: 300

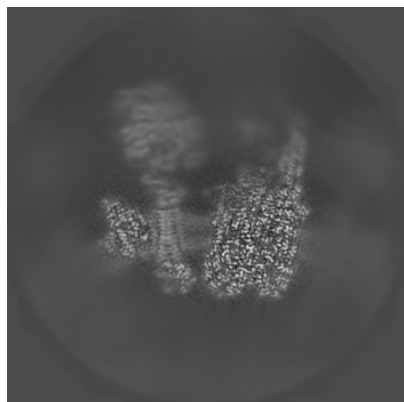


Z Index: 300

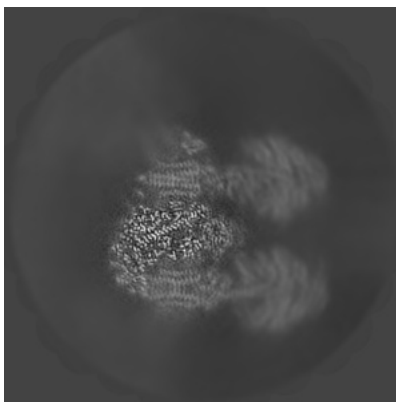
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

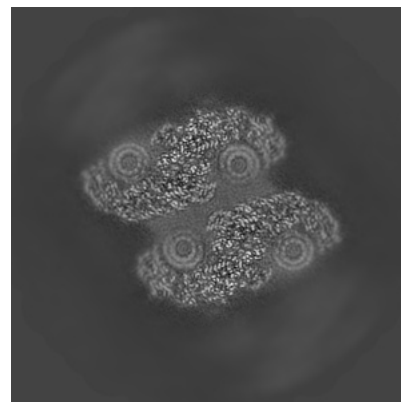
6.3.1 Primary map



X Index: 275

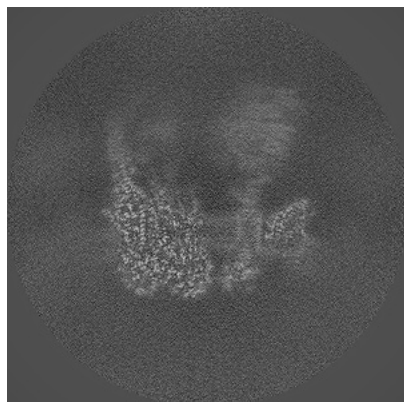


Y Index: 376

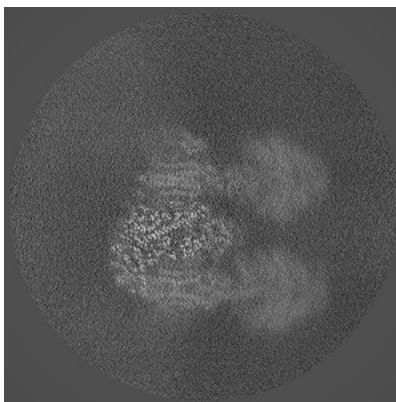


Z Index: 278

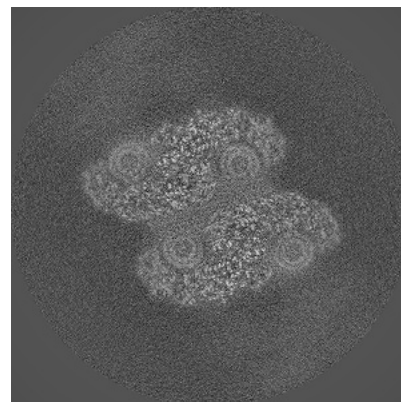
6.3.2 Raw map



X Index: 320



Y Index: 376

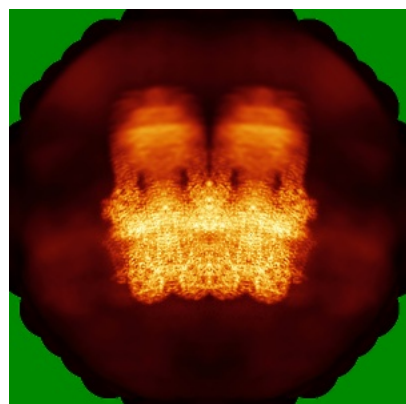


Z Index: 278

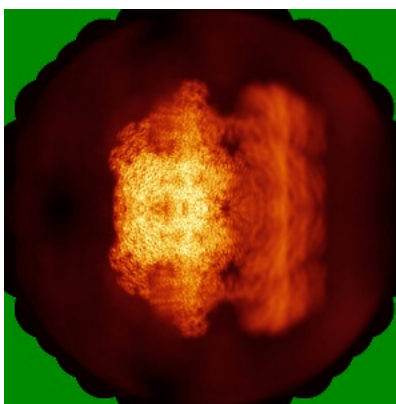
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

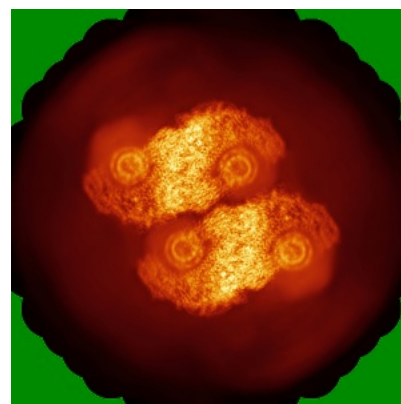
6.4.1 Primary map



X

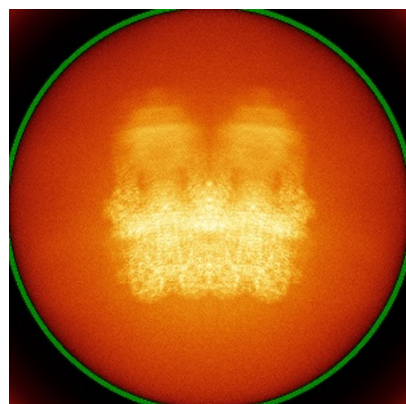


Y

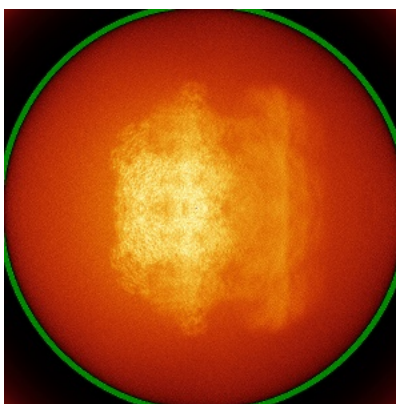


Z

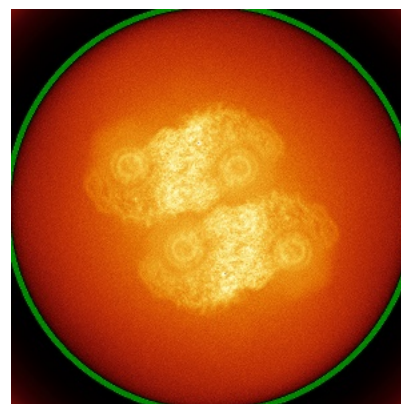
6.4.2 Raw map



X



Y



Z

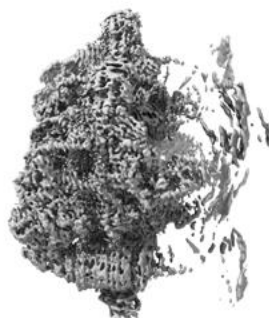
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

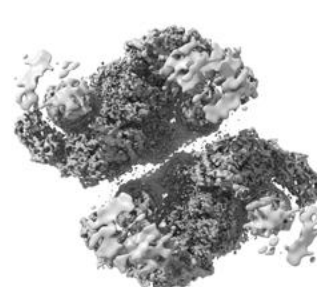
6.5.1 Primary map



X



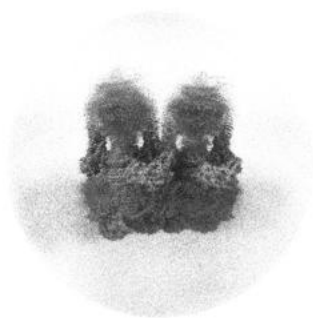
Y



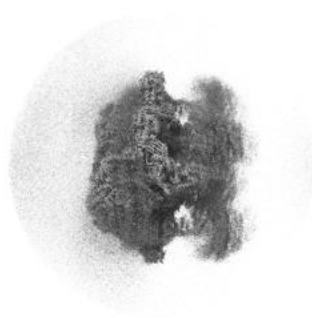
Z

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

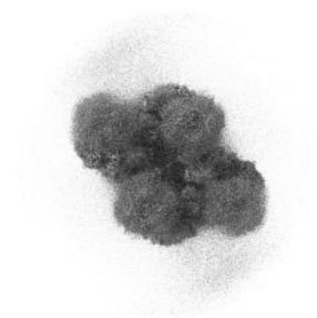
6.5.2 Raw map



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.

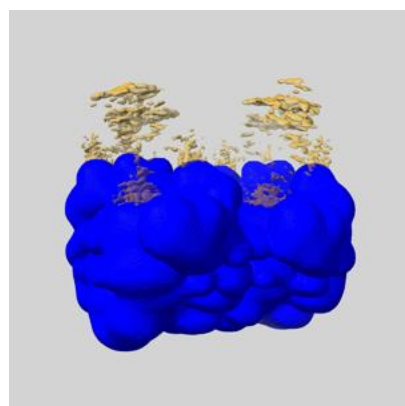
6.6 Mask visualisation [i](#)

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

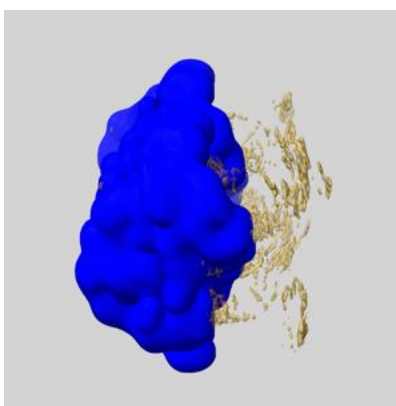
A mask typically either:

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

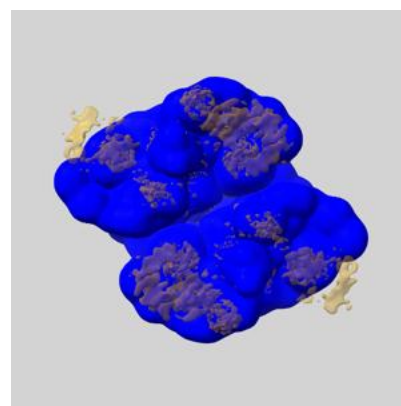
6.6.1 emd_10861_msk_1.map [i](#)



X



Y

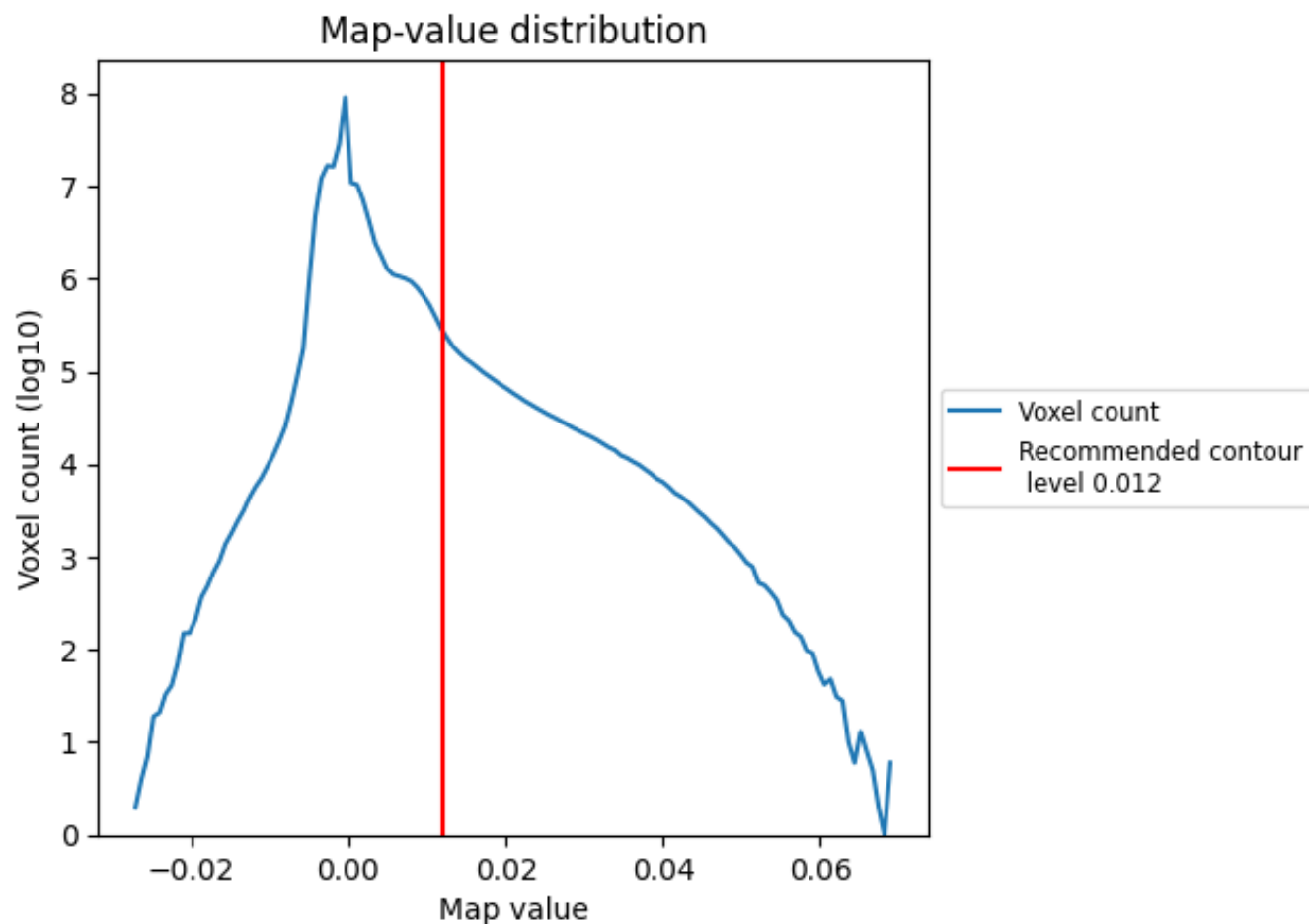


Z

7 Map analysis [i](#)

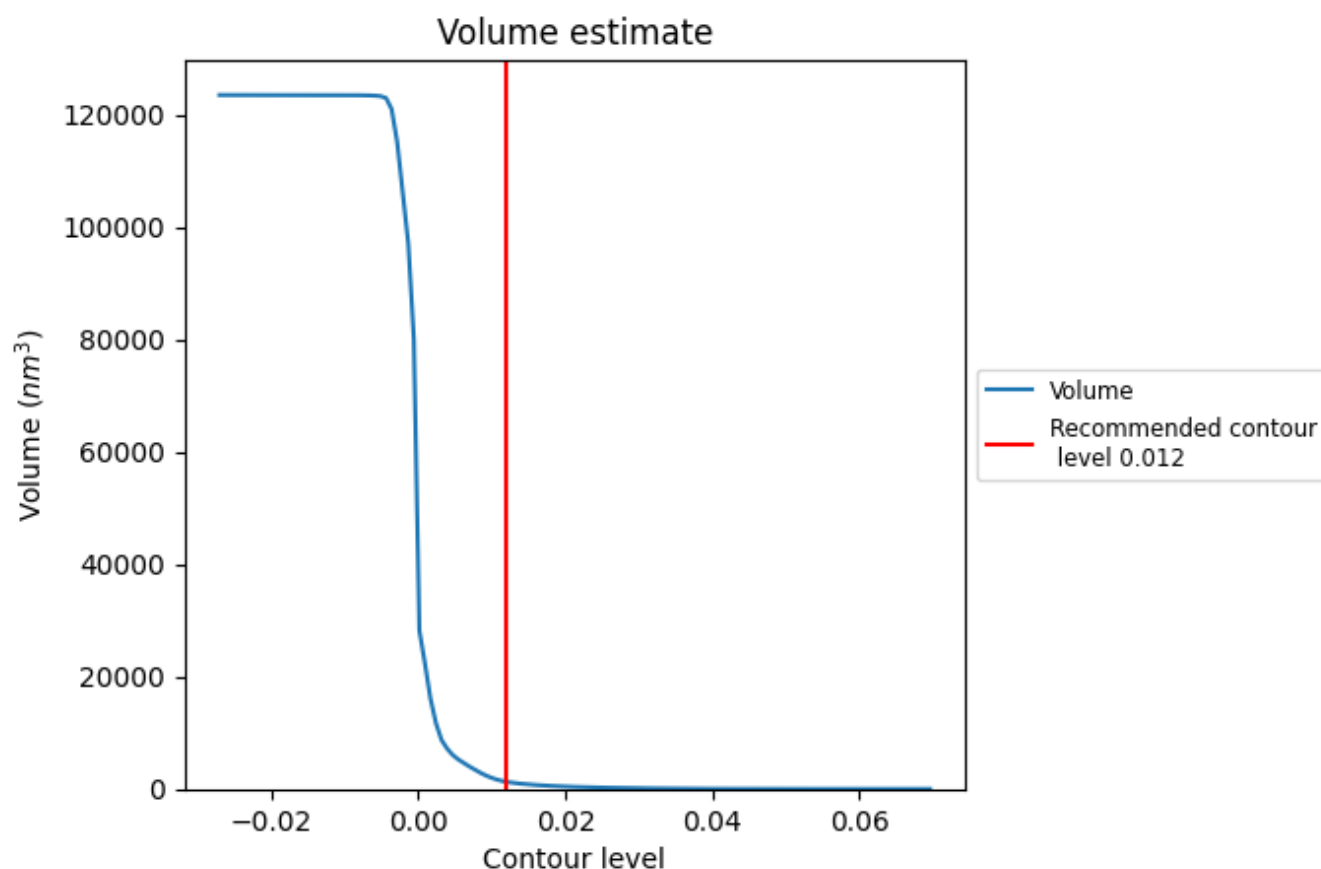
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

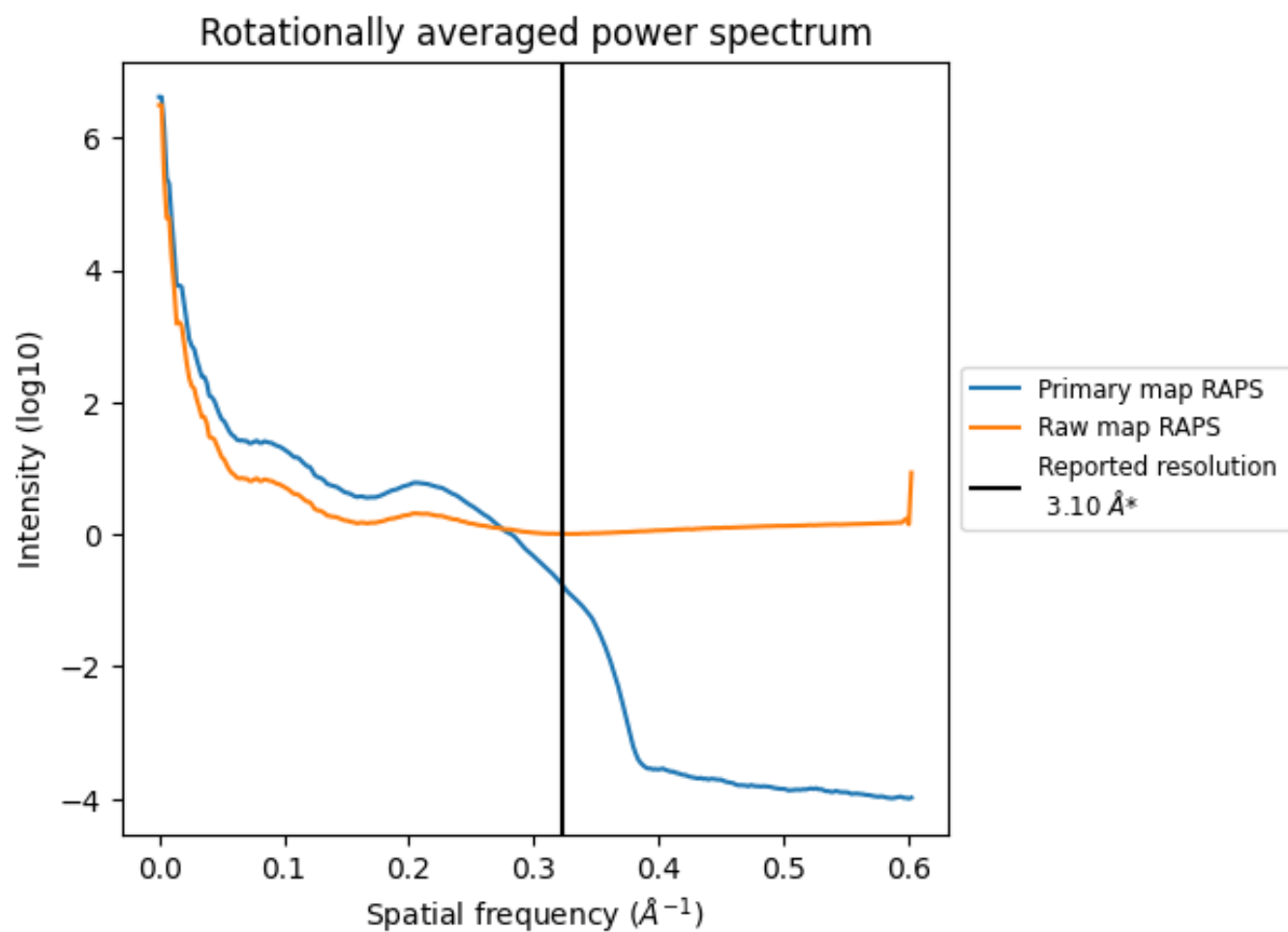
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

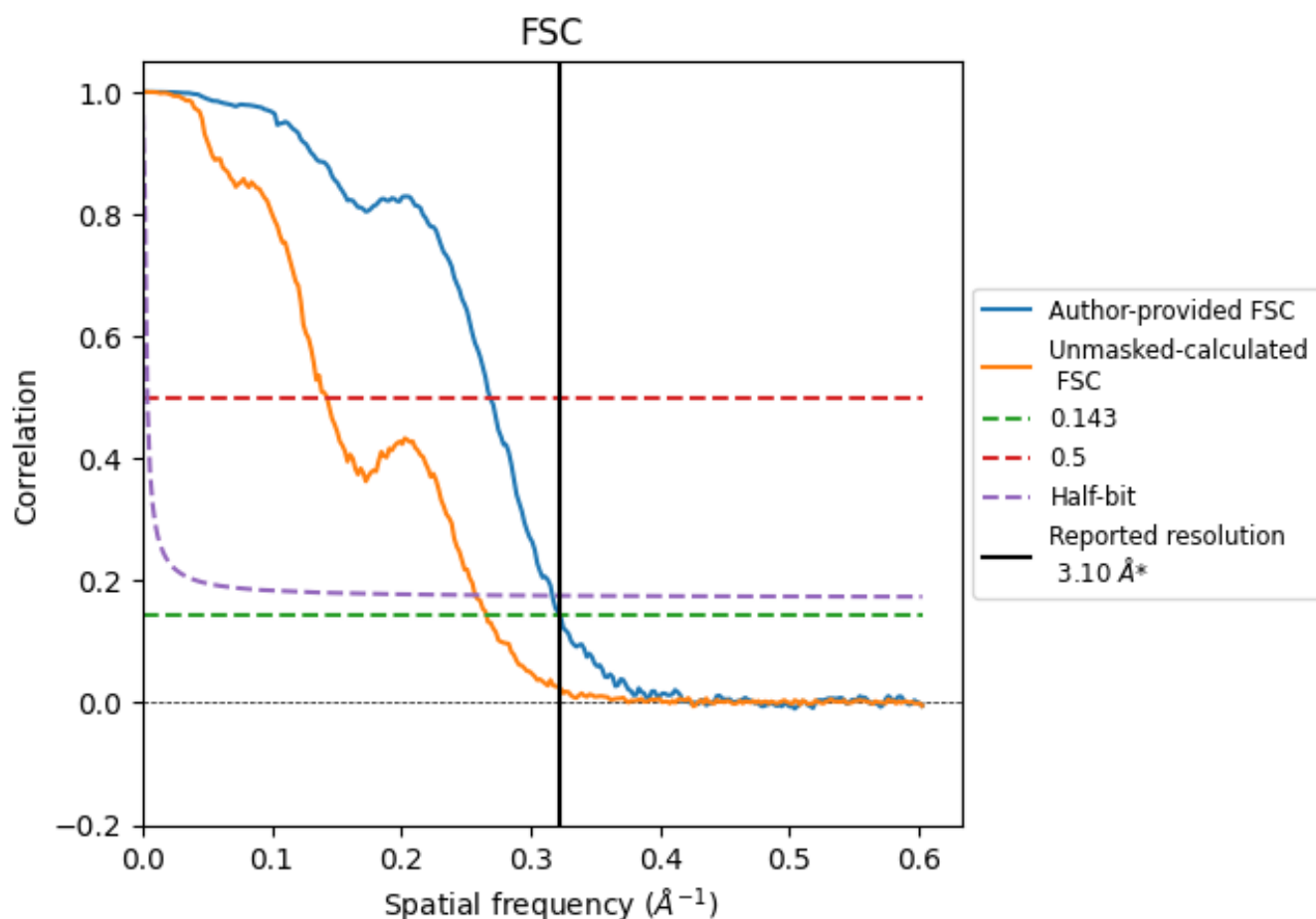


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

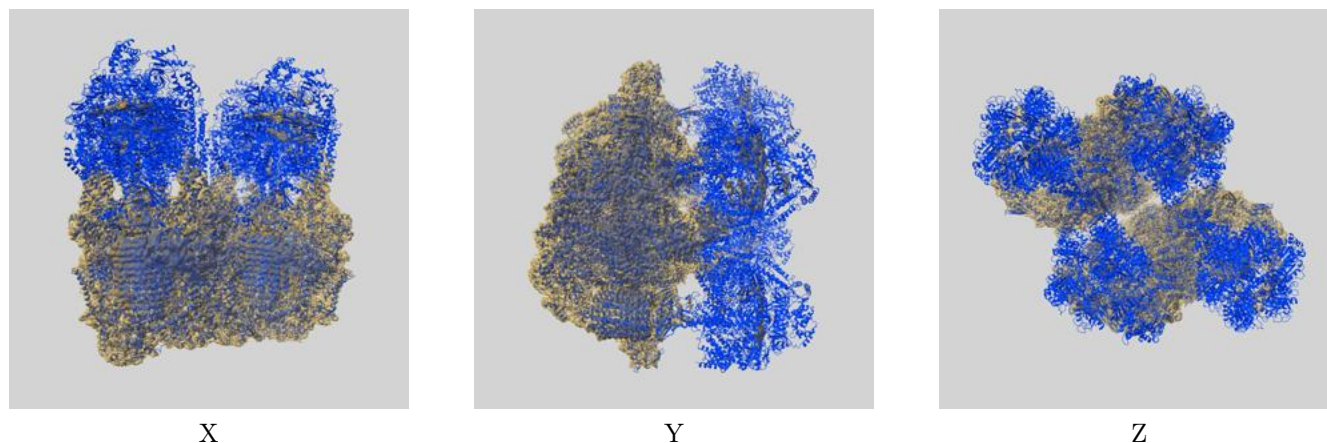
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.72	3.16
Unmasked-calculated*	3.76	7.01	3.89

*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 [i](#)

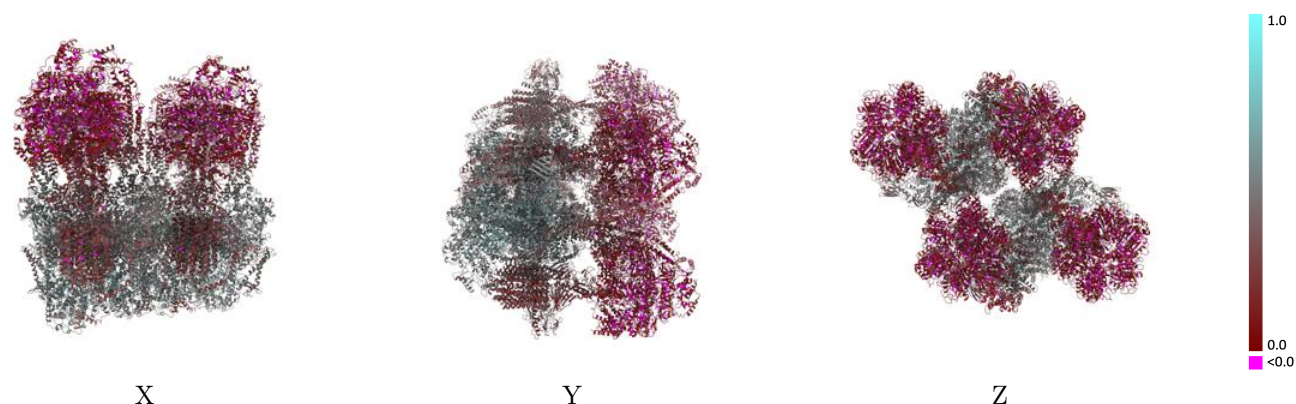
This section contains information regarding the fit between EMDB map EMD-10861 and PDB model 6YNZ. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



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](#)

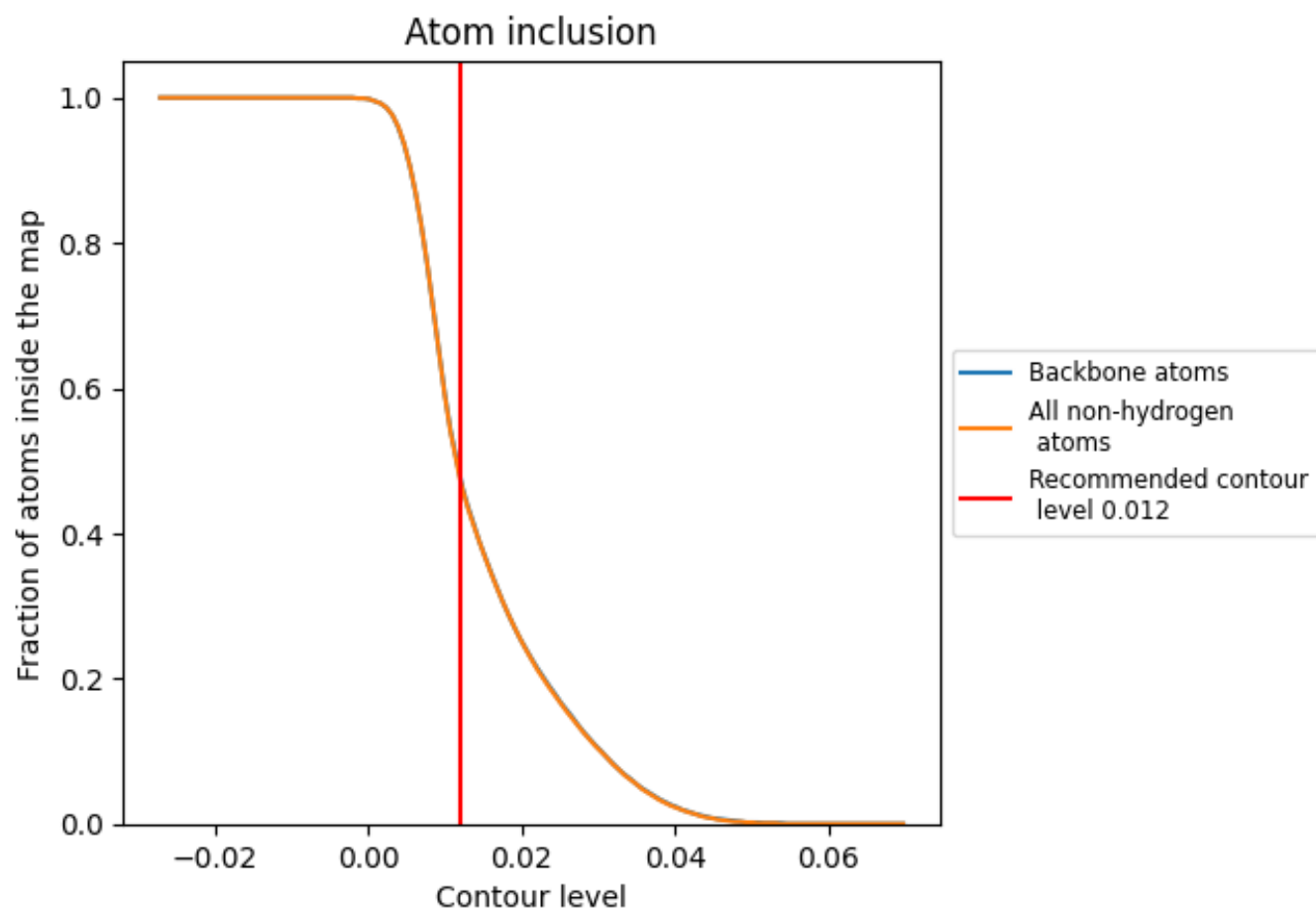


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

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	Q-score
All	0.4740	0.3170
A	0.8900	0.5390
A1	0.1400	0.1480
A2	0.0490	0.1350
A3	0.8860	0.5350
A4	0.0500	0.1360
A5	0.1440	0.1460
B	0.4990	0.3720
B1	0.0720	0.1030
B2	0.0260	0.0960
B3	0.4380	0.3590
B4	0.0260	0.0910
B5	0.0750	0.1090
C	0.9210	0.5390
C1	0.0110	0.1020
C2	0.0100	0.0850
C3	0.9010	0.5170
C4	0.0100	0.0910
C5	0.0110	0.0980
D	0.6370	0.4190
D1	0.0110	0.1130
D2	0.0140	0.1060
D3	0.5740	0.4000
D4	0.0150	0.1120
D5	0.0110	0.1070
E	0.6940	0.3810
E1	0.0850	0.1090
E2	0.0070	0.0990
E3	0.5910	0.3760
E4	0.0060	0.0930
E5	0.0840	0.1120
F	0.8620	0.5330
F1	0.0330	0.1050
F2	0.0300	0.0930
F3	0.8620	0.5410



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Chain	Atom inclusion	Q-score
F4	 0.0270	 0.0900
F5	 0.0340	 0.1070
G	 0.8260	 0.4910
G1	 0.0000	 0.1100
G2	 0.0000	 0.1040
G3	 0.7570	 0.4600
G4	 0.0000	 0.1020
G5	 0.0000	 0.1110
H	 0.8440	 0.4920
H1	 0.7070	 0.3200
H2	 0.7480	 0.3540
H3	 0.7470	 0.4600
H4	 0.7370	 0.3510
H5	 0.7070	 0.3140
I	 0.8520	 0.5090
I1	 0.6670	 0.3080
I2	 0.7480	 0.3210
I3	 0.7920	 0.4940
I4	 0.7480	 0.3170
I5	 0.6640	 0.3040
J	 0.8320	 0.4970
J1	 0.5780	 0.3010
J2	 0.7500	 0.3050
J3	 0.8030	 0.4820
J4	 0.7420	 0.3020
J5	 0.5730	 0.3020
K	 0.7860	 0.4370
K1	 0.5560	 0.2960
K2	 0.6910	 0.2760
K3	 0.7690	 0.4430
K4	 0.6960	 0.2740
K5	 0.5510	 0.2980
L	 0.8910	 0.5260
L1	 0.5580	 0.3000
L2	 0.7080	 0.2540
L3	 0.8580	 0.5160
L4	 0.7000	 0.2520
L5	 0.5730	 0.3000
M	 0.9330	 0.5270
M1	 0.6370	 0.2900
M2	 0.7510	 0.2800
M3	 0.9140	 0.5170

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Chain	Atom inclusion	Q-score
M4	 0.7580	 0.2820
M5	 0.6350	 0.2930
N	 0.9300	 0.5530
N1	 0.6210	 0.2830
N2	 0.7460	 0.2890
N3	 0.9090	 0.5410
N4	 0.7530	 0.2920
N5	 0.6230	 0.2860
O	 0.8700	 0.4970
O1	 0.6400	 0.2950
O2	 0.6960	 0.2760
O3	 0.8960	 0.4930
O4	 0.6920	 0.2730
O5	 0.6420	 0.2900
P	 0.7080	 0.4440
P1	 0.6820	 0.3080
P2	 0.6800	 0.3040
P3	 0.7280	 0.4340
P4	 0.6780	 0.3030
P5	 0.6890	 0.3090
Q	 0.7870	 0.4740
Q1	 0.6800	 0.3010
Q2	 0.7120	 0.3370
Q3	 0.6750	 0.4400
Q4	 0.7190	 0.3330
Q5	 0.6670	 0.3010
R	 0.8680	 0.5130
R3	 0.8260	 0.5040
S	 0.7340	 0.4300
S3	 0.6440	 0.4040
a	 0.8850	 0.5360
a3	 0.8680	 0.5290
b	 0.4400	 0.3580
b3	 0.5050	 0.3720
c	 0.8960	 0.5180
c3	 0.9180	 0.5400
d	 0.5720	 0.3980
d1	 0.2940	 0.2560
d2	 0.3590	 0.2310
d3	 0.6370	 0.4210
d4	 0.3510	 0.2340
d5	 0.2900	 0.2610

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Chain	Atom inclusion	Q-score
e	 0.5840	 0.3730
e1	 0.2350	 0.2080
e2	 0.2600	 0.2250
e3	 0.6960	 0.3810
e4	 0.2630	 0.2310
e5	 0.2270	 0.2020
f	 0.7670	 0.5250
f3	 0.8120	 0.5360
g	 0.7460	 0.4620
g1	 0.1590	 0.2070
g2	 0.1950	 0.2080
g3	 0.8180	 0.4890
g4	 0.1970	 0.2050
g5	 0.1610	 0.2050
h	 0.7220	 0.4690
h3	 0.8190	 0.5010
i	 0.8250	 0.4940
i1	 0.0400	 0.1780
i2	 0.0700	 0.1820
i3	 0.8470	 0.5160
i4	 0.0910	 0.2000
i5	 0.0300	 0.1910
j	 0.8010	 0.4810
j3	 0.8380	 0.4910
k	 0.7840	 0.4400
k3	 0.7920	 0.4370
l	 0.8520	 0.5170
l3	 0.8930	 0.5230
m	 0.9040	 0.5140
m3	 0.9320	 0.5230
n	 0.9070	 0.5410
n3	 0.9280	 0.5530
o	 0.8960	 0.4970
o3	 0.8580	 0.4950
p	 0.7170	 0.4310
p3	 0.7090	 0.4430
q	 0.6780	 0.4440
q3	 0.7860	 0.4720
r	 0.7860	 0.4940
r3	 0.8700	 0.5200
s	 0.5440	 0.3940
s3	 0.7000	 0.4300

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Chain	Atom inclusion	Q-score
t	 0.5330	 0.3790
t3	 0.6050	 0.4000