



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:54 AM UTC

PDB ID : 7W5Z / pdb_00007w5z
EMDB ID : EMD-32325
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial complex IV, composite dimer model
Authors : Zhou, L.; Maldonado, M.; Padavannil, A.; Letts, J.
Deposited on : 2021-11-30
Resolution : 3.02 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:

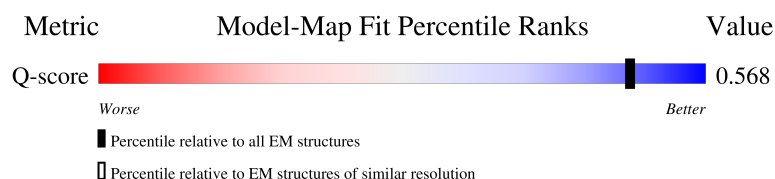
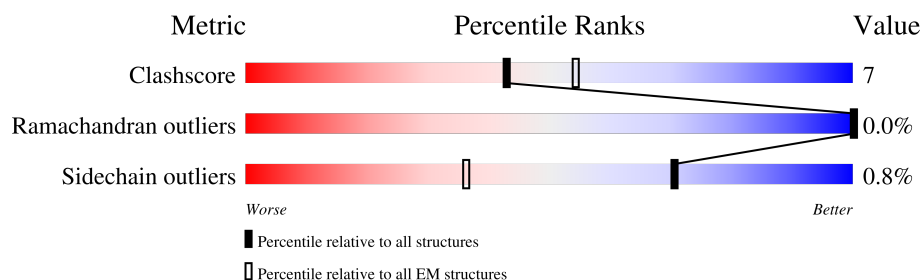
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

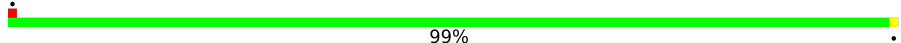
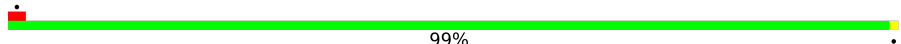
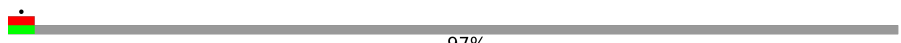
The reported resolution of this entry is 3.02 Å.

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	13913 (2.52 - 3.52)

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	U1	98	 99%
1	u1	98	 99%
2	U2	3634	 97%
2	u2	3634	 97%

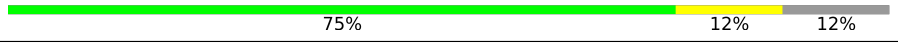
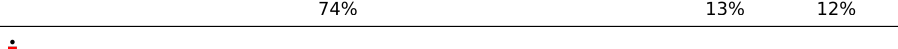
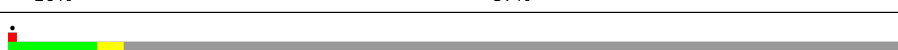
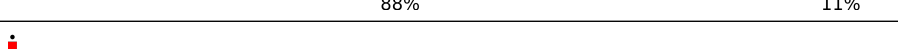
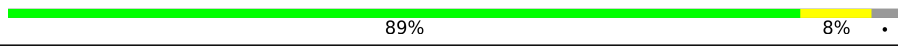
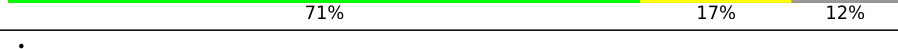
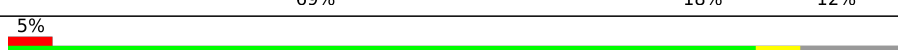
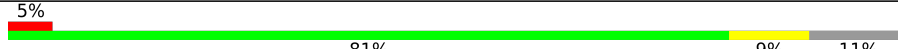
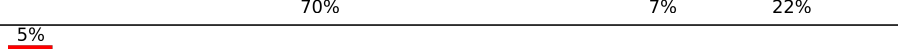
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Mol	Chain	Length	Quality of chain
3	U3	34	85% 100%
3	u3	34	91% 100%
4	U4	30	93% 100%
4	u4	30	100%
5	U5	172	11% 17% 81%
5	u5	172	11% 17% 81%
6	U6	478	8% 91%
6	u6	478	8% 91%
7	C1	688	72% 25%
7	c1	688	75% 23%
8	C2	604	79% 16% 5%
8	c2	604	79% 16% 5%
9	C3	594	10% 76% 18% 5%
9	c3	594	10% 76% 18% 5%
10	5B	637	71% 15% 13%
10	5b	637	72% 14% 13%
11	6A	130	80% 16%
11	6a	130	82% 15%
12	6B	230	81% 14%
12	6b	230	82% 13%
13	6L	88	76% 11% 13%
13	6l	88	76% 11% 13%
14	6C	103	75% 17% 8%
14	6c	103	78% 15% 8%
15	7A	133	70% 30%

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Mol	Chain	Length	Quality of chain
15	7a	133	
16	7C	236	
16	7c	236	
17	7L	990	
17	7l	990	
18	M1	346	
18	m1	346	
19	M2	318	
19	m2	318	
20	M3	330	
20	m3	330	
21	T1	72	
21	t1	72	
22	T2	72	
22	t2	72	
23	T3	93	
23	t3	93	
24	T4	68	
24	t4	68	
25	T5	81	
25	t5	81	
26	T6	72	
26	t6	72	
27	BP	380	
27	bp	380	

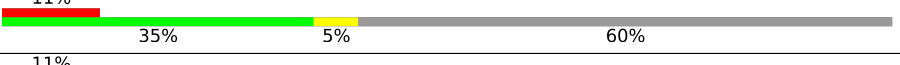
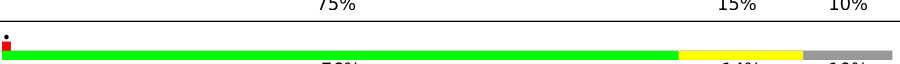
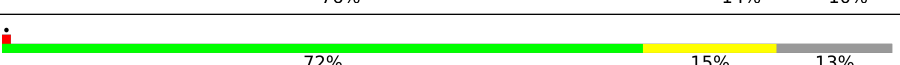
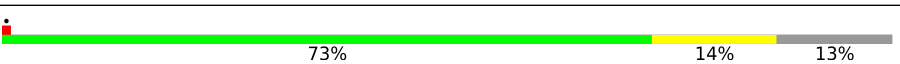
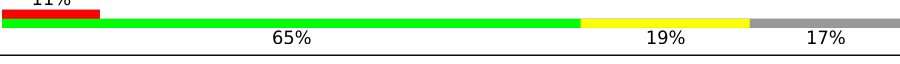
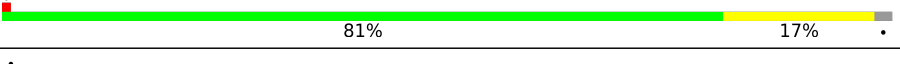
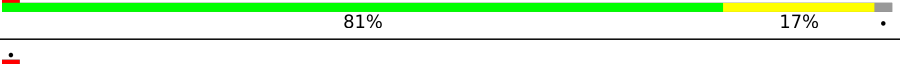
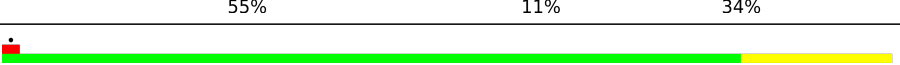
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Mol	Chain	Length	Quality of chain
28	FS	188	
28	fs	188	
29	AC	127	
29	ac	127	
30	Y7	453	
30	y7	453	
31	Y0	89	
31	y0	89	
32	Y5	190	
32	y5	190	
33	A	490	
33	a	490	
34	B	473	
34	b	473	
35	C	1471	
35	c	1471	
36	D	402	
36	d	402	
37	E	385	
37	e	385	
38	F	348	
38	f	348	
39	G	318	
39	g	318	
40	H	318	

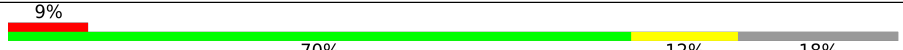
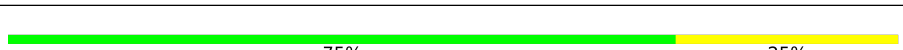
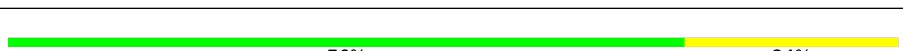
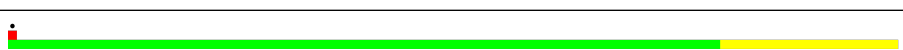
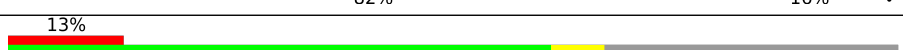
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Mol	Chain	Length	Quality of chain
40	h	318	
41	I	252	
41	i	252	
42	J	234	
42	j	234	
43	K	231	
43	k	231	
44	L	222	
44	l	222	
45	M	220	
45	m	220	
46	N	210	
46	n	210	
47	O	193	
47	o	193	
48	P	175	
48	p	175	
49	Q	173	
49	q	173	
50	R	173	
50	r	173	
51	S	170	
51	s	170	
52	T	158	
52	t	158	

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Mol	Chain	Length	Quality of chain
53	U	154	
53	u	154	
54	V	149	
54	v	149	
55	W	124	
55	w	124	
56	X	122	
56	x	122	
57	Y	105	
57	y	105	
58	Z	90	
58	z	90	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 190448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	U1	98	Total	C	N	O	0	0
			490	294	98	98		
1	u1	98	Total	C	N	O	0	0
			490	294	98	98		

- Molecule 2 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U2	127	Total	C	N	O	S	0	0
			743	456	139	143	5		
2	u2	127	Total	C	N	O	S	0	0
			743	456	139	143	5		

- Molecule 3 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	U3	34	Total	C	N	O	0	0
			170	102	34	34		
3	u3	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 4 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	U4	30	Total	C	N	O	0	0
			150	90	30	30		
4	u4	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 5 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U5	33	Total	C	N	O	0	0
			242	160	40	42		
5	u5	33	Total	C	N	O	0	0
			242	160	40	42		

- Molecule 6 is a protein called Protein transporter Sec61 alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U6	42	Total	C	N	O	S	0	0
			275	178	45	50	2		
6	u6	42	Total	C	N	O	S	0	0
			275	178	45	50	2		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C1	672	Total	C	N	O	S	0	0
			5563	3722	908	897	36		
7	c1	672	Total	C	N	O	S	0	0
			5563	3722	908	897	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C2	576	Total	C	N	O	S	0	0
			4883	3186	841	846	10		
8	c2	576	Total	C	N	O	S	0	0
			4883	3186	841	846	10		

- Molecule 9 is a protein called Ymf68.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C3	563	Total	C	N	O	S	0	0
			4930	3354	763	805	8		
9	c3	563	Total	C	N	O	S	0	0
			4930	3354	763	805	8		

- Molecule 10 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	5B	554	Total	C	N	O	P	S	0	0
			4624	2915	778	912	2	17		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	5b	554	Total	C	N	O	P	S	0	0
			4624	2915	778	912	2	17		

- Molecule 11 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	6A	125	Total	C	N	O	S		0	0
			1074	693	183	196	2			
11	6a	125	Total	C	N	O	S		0	0
			1074	693	183	196	2			

- Molecule 12 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	6B	221	Total	C	N	O	S		0	0
			1904	1234	311	346	13			
12	6b	221	Total	C	N	O	S		0	0
			1904	1234	311	346	13			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 6B-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	6L	77	Total	C	N	O	S		0	0
			638	408	108	116	6			
13	6l	77	Total	C	N	O	S		0	0
			638	408	108	116	6			

- Molecule 14 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	6C	95	Total	C	N	O	S		0	0
			841	545	151	143	2			
14	6c	95	Total	C	N	O	S		0	0
			841	545	151	143	2			

- Molecule 15 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	7A	133	Total	C	N	O	S		0	0
			1168	770	197	200	1			
15	7a	133	Total	C	N	O	S		0	0
			1168	770	197	200	1			

- Molecule 16 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	7C	207	Total	C	N	O	P	S	0	0
			1789	1139	287	353	2	8		
16	7c	207	Total	C	N	O	P	S	0	0
			1789	1139	287	353	2	8		

- Molecule 17 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7L	130	Total	C	N	O	S	0	0
			1070	693	174	195	8		
17	7l	130	Total	C	N	O	S	0	0
			1070	693	174	195	8		

- Molecule 18 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M1	346	Total	C	N	O	S	0	0
			2863	1890	469	491	13		
18	m1	346	Total	C	N	O	S	0	0
			2863	1890	469	491	13		

- Molecule 19 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M2	318	Total	C	N	O	S	0	0
			2560	1666	440	450	4		
19	m2	318	Total	C	N	O	S	0	0
			2560	1666	440	450	4		

- Molecule 20 is a protein called Carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M3	329	Total	C	N	O	S	0	0
			2620	1700	446	470	4		
20	m3	329	Total	C	N	O	S	0	0
			2620	1700	446	470	4		

- Molecule 21 is a protein called Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T1	70	Total	C	N	O	S	0	0
			540	329	98	109	4		
21	t1	70	Total	C	N	O	S	0	0
			540	329	98	109	4		

- Molecule 22 is a protein called Cytochrome c oxidase small TIM subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T2	63	Total	C	N	O	S	0	0
			513	319	90	100	4		
22	t2	63	Total	C	N	O	S	0	0
			513	319	90	100	4		

- Molecule 23 is a protein called Cytochrome c oxidase small TIM subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T3	83	Total	C	N	O	S	0	0
			655	412	109	128	6		
23	t3	83	Total	C	N	O	S	0	0
			655	412	109	128	6		

- Molecule 24 is a protein called Cytochrome c oxidase small TIM subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T4	57	Total	C	N	O	S	0	0
			483	309	80	91	3		
24	t4	57	Total	C	N	O	S	0	0
			483	309	80	91	3		

- Molecule 25 is a protein called Cytochrome c oxidase small TIM subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T5	63	Total	C	N	O	S	0	0
			515	327	90	96	2		
25	t5	63	Total	C	N	O	S	0	0
			515	327	90	96	2		

- Molecule 26 is a protein called Cytochrome c oxidase small TIM subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T6	70	Total	C	N	O	S	0	0
			563	363	90	106	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	t6	70	Total	C	N	O	S	0	0
			563	363	90	106	4		

- Molecule 27 is a protein called Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BP	380	Total	C	N	O	S	0	0
			2916	1856	492	566	2		
27	bp	380	Total	C	N	O	S	0	0
			2916	1856	492	566	2		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BP	413	GLU	-	expression tag	UNP Q22RF2
BP	414	THR	-	expression tag	UNP Q22RF2
BP	415	GLY	-	expression tag	UNP Q22RF2
BP	416	LYS	-	expression tag	UNP Q22RF2
BP	417	ILE	-	expression tag	UNP Q22RF2
BP	418	TYR	-	expression tag	UNP Q22RF2
BP	419	GLN	-	expression tag	UNP Q22RF2
BP	420	PHE	-	expression tag	UNP Q22RF2
BP	421	ASN	-	expression tag	UNP Q22RF2
BP	422	GLU	-	expression tag	UNP Q22RF2
BP	423	PHE	-	expression tag	UNP Q22RF2
BP	424	VAL	-	expression tag	UNP Q22RF2
BP	425	GLY	-	expression tag	UNP Q22RF2
BP	426	VAL	-	expression tag	UNP Q22RF2
BP	427	SER	-	expression tag	UNP Q22RF2
BP	428	THR	-	expression tag	UNP Q22RF2
BP	429	ASN	-	expression tag	UNP Q22RF2
BP	430	GLU	-	expression tag	UNP Q22RF2
BP	431	VAL	-	expression tag	UNP Q22RF2
BP	432	GLY	-	expression tag	UNP Q22RF2
BP	433	ASN	-	expression tag	UNP Q22RF2
BP	434	ASP	-	expression tag	UNP Q22RF2
BP	435	TYR	-	expression tag	UNP Q22RF2
BP	436	ASN	-	expression tag	UNP Q22RF2
BP	437	VAL	-	expression tag	UNP Q22RF2
BP	438	ALA	-	expression tag	UNP Q22RF2
BP	439	ASP	-	expression tag	UNP Q22RF2
BP	440	SER	-	expression tag	UNP Q22RF2

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Chain	Residue	Modelled	Actual	Comment	Reference
BP	441	LYS	-	expression tag	UNP Q22RF2
BP	442	ALA	-	expression tag	UNP Q22RF2
BP	443	PHE	-	expression tag	UNP Q22RF2
BP	444	GLU	-	expression tag	UNP Q22RF2
BP	445	GLY	-	expression tag	UNP Q22RF2
BP	446	LYS	-	expression tag	UNP Q22RF2
BP	447	VAL	-	expression tag	UNP Q22RF2
BP	448	VAL	-	expression tag	UNP Q22RF2
BP	449	ASP	-	expression tag	UNP Q22RF2
BP	450	LEU	-	expression tag	UNP Q22RF2
BP	451	GLY	-	expression tag	UNP Q22RF2
BP	452	GLY	-	expression tag	UNP Q22RF2
BP	453	SER	-	expression tag	UNP Q22RF2
BP	454	TYR	-	expression tag	UNP Q22RF2
BP	455	GLY	-	expression tag	UNP Q22RF2
BP	456	ILE	-	expression tag	UNP Q22RF2
BP	457	ARG	-	expression tag	UNP Q22RF2
BP	458	PHE	-	expression tag	UNP Q22RF2
BP	459	ALA	-	expression tag	UNP Q22RF2
BP	460	ILE	-	expression tag	UNP Q22RF2
BP	461	VAL	-	expression tag	UNP Q22RF2
BP	462	ASN	-	expression tag	UNP Q22RF2
bp	413	GLU	-	expression tag	UNP Q22RF2
bp	414	THR	-	expression tag	UNP Q22RF2
bp	415	GLY	-	expression tag	UNP Q22RF2
bp	416	LYS	-	expression tag	UNP Q22RF2
bp	417	ILE	-	expression tag	UNP Q22RF2
bp	418	TYR	-	expression tag	UNP Q22RF2
bp	419	GLN	-	expression tag	UNP Q22RF2
bp	420	PHE	-	expression tag	UNP Q22RF2
bp	421	ASN	-	expression tag	UNP Q22RF2
bp	422	GLU	-	expression tag	UNP Q22RF2
bp	423	PHE	-	expression tag	UNP Q22RF2
bp	424	VAL	-	expression tag	UNP Q22RF2
bp	425	GLY	-	expression tag	UNP Q22RF2
bp	426	VAL	-	expression tag	UNP Q22RF2
bp	427	SER	-	expression tag	UNP Q22RF2
bp	428	THR	-	expression tag	UNP Q22RF2
bp	429	ASN	-	expression tag	UNP Q22RF2
bp	430	GLU	-	expression tag	UNP Q22RF2
bp	431	VAL	-	expression tag	UNP Q22RF2
bp	432	GLY	-	expression tag	UNP Q22RF2

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Chain	Residue	Modelled	Actual	Comment	Reference
bp	433	ASN	-	expression tag	UNP Q22RF2
bp	434	ASP	-	expression tag	UNP Q22RF2
bp	435	TYR	-	expression tag	UNP Q22RF2
bp	436	ASN	-	expression tag	UNP Q22RF2
bp	437	VAL	-	expression tag	UNP Q22RF2
bp	438	ALA	-	expression tag	UNP Q22RF2
bp	439	ASP	-	expression tag	UNP Q22RF2
bp	440	SER	-	expression tag	UNP Q22RF2
bp	441	LYS	-	expression tag	UNP Q22RF2
bp	442	ALA	-	expression tag	UNP Q22RF2
bp	443	PHE	-	expression tag	UNP Q22RF2
bp	444	GLU	-	expression tag	UNP Q22RF2
bp	445	GLY	-	expression tag	UNP Q22RF2
bp	446	LYS	-	expression tag	UNP Q22RF2
bp	447	VAL	-	expression tag	UNP Q22RF2
bp	448	VAL	-	expression tag	UNP Q22RF2
bp	449	ASP	-	expression tag	UNP Q22RF2
bp	450	LEU	-	expression tag	UNP Q22RF2
bp	451	GLY	-	expression tag	UNP Q22RF2
bp	452	GLY	-	expression tag	UNP Q22RF2
bp	453	SER	-	expression tag	UNP Q22RF2
bp	454	TYR	-	expression tag	UNP Q22RF2
bp	455	GLY	-	expression tag	UNP Q22RF2
bp	456	ILE	-	expression tag	UNP Q22RF2
bp	457	ARG	-	expression tag	UNP Q22RF2
bp	458	PHE	-	expression tag	UNP Q22RF2
bp	459	ALA	-	expression tag	UNP Q22RF2
bp	460	ILE	-	expression tag	UNP Q22RF2
bp	461	VAL	-	expression tag	UNP Q22RF2
bp	462	ASN	-	expression tag	UNP Q22RF2

- Molecule 28 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	FS	188	Total	C	N	O	S	0	0
			1509	978	260	257	14		
28	fs	188	Total	C	N	O	S	0	0
			1509	978	260	257	14		

- Molecule 29 is a protein called Cytochrome c oxidase acyl carrier-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AC	100	Total	C	N	O	S	0	0
			816	519	144	151	2		
29	ac	100	Total	C	N	O	S	0	0
			816	519	144	151	2		

- Molecule 30 is a protein called Ymf67.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y7	338	Total	C	N	O	S	0	0
			2895	1936	459	494	6		
30	y7	338	Total	C	N	O	S	0	0
			2895	1936	459	494	6		

- Molecule 31 is a protein called Ymf70.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y0	89	Total	C	N	O	S	0	0
			777	536	115	124	2		
31	y0	89	Total	C	N	O	S	0	0
			777	536	115	124	2		

- Molecule 32 is a protein called Ymf75.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y5	104	Total	C	N	O		0	0
			924	638	140	146			
32	y5	104	Total	C	N	O		0	0
			924	638	140	146			

- Molecule 33 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A	448	Total	C	N	O	S	0	0
			3746	2402	635	700	9		
33	a	448	Total	C	N	O	S	0	0
			3746	2402	635	700	9		

- Molecule 34 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B	214	Total	C	N	O	S	0	0
			1682	1087	287	307	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	214	Total	C	N	O	S	0	0
			1682	1087	287	307	1		

- Molecule 35 is a protein called Cyclic nucleotide-binding domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	46	Total	C	N	O	S	0	0
			383	261	60	60	2		
35	c	46	Total	C	N	O	S	0	0
			383	261	60	60	2		

- Molecule 36 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D	284	Total	C	N	O	S	0	0
			2331	1504	395	427	5		
36	d	284	Total	C	N	O	S	0	0
			2331	1504	395	427	5		

- Molecule 37 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	E	384	Total	C	N	O	S	0	0
			3178	2046	549	576	7		
37	e	384	Total	C	N	O	S	0	0
			3178	2046	549	576	7		

- Molecule 38 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	F	242	Total	C	N	O	S	0	0
			2014	1298	332	379	5		
38	f	242	Total	C	N	O	S	0	0
			2014	1298	332	379	5		

- Molecule 39 is a protein called Cytochrome c oxidase subunit TT7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	281	Total	C	N	O	S	0	0
			2364	1510	395	447	12		
39	g	281	Total	C	N	O	S	0	0
			2364	1510	395	447	12		

- Molecule 40 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	H	239	Total	C	N	O	S	0	0
			1915	1204	330	372	9		
40	h	239	Total	C	N	O	S	0	0
			1915	1204	330	372	9		

- Molecule 41 is a protein called Cytochrome c oxidase subunit TT9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	I	101	Total	C	N	O		0	0
			852	538	150	164			
41	i	101	Total	C	N	O		0	0
			852	538	150	164			

- Molecule 42 is a protein called Cytochrome c oxidase subunit TT10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	187	Total	C	N	O	S	0	0
			1575	1024	276	274	1		
42	j	187	Total	C	N	O	S	0	0
			1575	1024	276	274	1		

- Molecule 43 is a protein called Cytochrome c oxidase subunit TT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	208	Total	C	N	O	S	0	0
			1714	1090	302	319	3		
43	k	208	Total	C	N	O	S	0	0
			1714	1090	302	319	3		

- Molecule 44 is a protein called Cytochrome c oxidase subunit TT12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	194	Total	C	N	O	S	0	0
			1668	1089	284	293	2		
44	l	194	Total	C	N	O	S	0	0
			1668	1089	284	293	2		

- Molecule 45 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	183	Total	C	N	O	S	0	0
			1581	1030	264	276	11		
45	m	183	Total	C	N	O	S	0	0
			1581	1030	264	276	11		

- Molecule 46 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N	206	Total	C	N	O	S	0	0
			1716	1117	286	306	7		
46	n	206	Total	C	N	O	S	0	0
			1716	1117	286	306	7		

- Molecule 47 is a protein called Cytochrome c oxidase subunit TT15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	128	Total	C	N	O	S	0	0
			1073	671	189	207	6		
47	o	128	Total	C	N	O	S	0	0
			1073	671	189	207	6		

- Molecule 48 is a protein called Cytochrome c oxidase subunit TT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	175	Total	C	N	O	S	0	0
			1412	890	247	274	1		
48	p	175	Total	C	N	O	S	0	0
			1412	890	247	274	1		

- Molecule 49 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	173	Total	C	N	O	S	0	0
			1434	927	243	255	9		
49	q	173	Total	C	N	O	S	0	0
			1434	927	243	255	9		

- Molecule 50 is a protein called Cytochrome c oxidase subunit TT18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	159	Total	C	N	O	S	0	0
			1305	854	217	231	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	159	Total	C	N	O	S	0	0
			1305	854	217	231	3		

- Molecule 51 is a protein called Cytochrome c oxidase subunit TT19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	143	Total	C	N	O	S	0	0
			1165	732	204	224	5		
51	s	143	Total	C	N	O	S	0	0
			1165	732	204	224	5		

- Molecule 52 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	157	Total	C	N	O	S	0	0
			1323	864	231	224	4		
52	t	157	Total	C	N	O	S	0	0
			1323	864	231	224	4		

- Molecule 53 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	153	Total	C	N	O	S	0	0
			1304	848	221	230	5		
53	u	153	Total	C	N	O	S	0	0
			1304	848	221	230	5		

- Molecule 54 is a protein called Cytochrome c oxidase subunit TT22.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	146	Total	C	N	O	S	0	0
			1234	802	217	213	2		
54	v	146	Total	C	N	O	S	0	0
			1234	802	217	213	2		

- Molecule 55 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	102	Total	C	N	O	S	0	0
			902	588	146	164	4		
55	w	102	Total	C	N	O	S	0	0
			902	588	146	164	4		

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	122	Total	C	N	O	S	0	0
			1012	665	171	172	4		
56	x	122	Total	C	N	O	S	0	0
			1012	665	171	172	4		

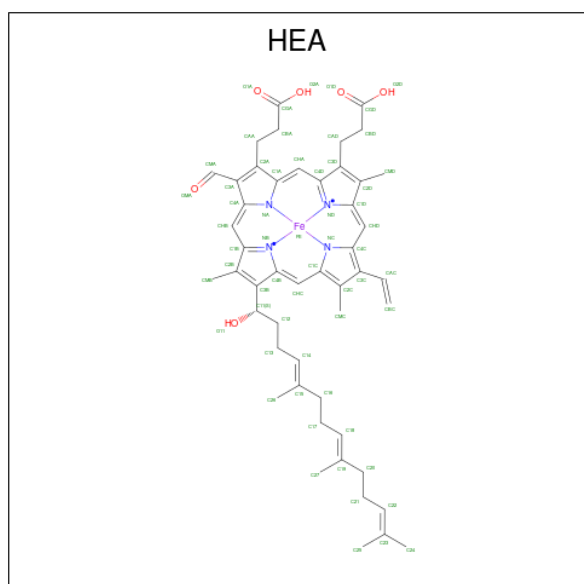
- Molecule 57 is a protein called Cytochrome c oxidase subunit TT25.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y	105	Total	C	N	O	S	0	0
			859	540	157	153	9		
57	y	105	Total	C	N	O	S	0	0
			859	540	157	153	9		

- Molecule 58 is a protein called Cytochrome c oxidase subunit TT26.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Z	60	Total	C	N	O	0	0
			479	310	85	84		
58	z	60	Total	C	N	O	0	0
			479	310	85	84		

- Molecule 59 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
59	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
59	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
59	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
59	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

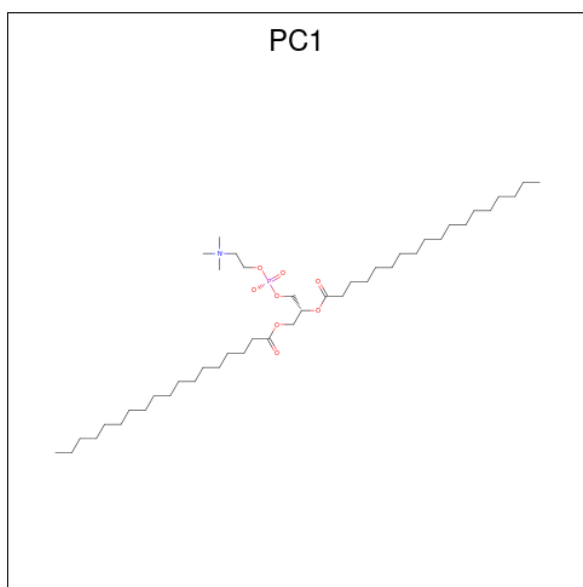
- Molecule 60 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
60	C1	1	Total	Cu	0
			1	1	
60	C2	2	Total	Cu	0
			2	2	
60	c1	1	Total	Cu	0
			1	1	
60	c2	2	Total	Cu	0
			2	2	

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
61	C1	1	Total	Mg	0
			1	1	
61	c1	1	Total	Mg	0
			1	1	

- Molecule 62 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



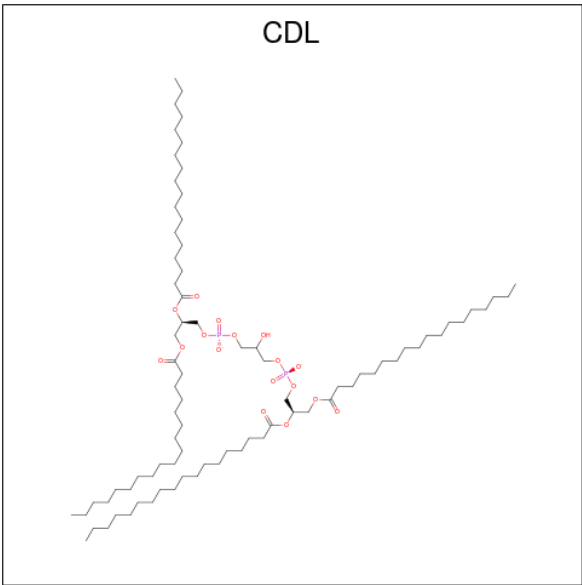
Mol	Chain	Residues	Atoms					AltConf
62	C1	1	Total	C	N	O	P	0
			49	39	1	8	1	
62	C3	1	Total	C	N	O	P	0
			52	42	1	8	1	
62	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
62	C3	1	Total	C	N	O	P	0
			31	21	1	8	1	
62	C3	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	7C	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	7C	1	Total	C	N	O	P	0
			43	33	1	8	1	
62	M1	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	M2	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	M2	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	M2	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
62	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	J	1	Total	C	N	O	P	0
			37	27	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
62	N	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	N	1	Total	C	N	O	P	0
			36	26	1	8	1	
62	V	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	c1	1	Total	C	N	O	P	0
			49	39	1	8	1	
62	c3	1	Total	C	N	O	P	0
			52	42	1	8	1	
62	c3	1	Total	C	N	O	P	0
			39	29	1	8	1	
62	c3	1	Total	C	N	O	P	0
			31	21	1	8	1	
62	c3	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	7c	1	Total	C	N	O	P	0
			43	33	1	8	1	
62	m1	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	m1	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	m2	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	m2	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	m2	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
62	a	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	j	1	Total	C	N	O	P	0
			37	27	1	8	1	
62	n	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	n	1	Total	C	N	O	P	0
			36	26	1	8	1	
62	v	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 63 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
63	C1	1	Total	C	O	P	0
			59	40	17	2	
63	C1	1	Total	C	O	P	0
			65	46	17	2	
63	C3	1	Total	C	O	P	0
			68	49	17	2	
63	5B	1	Total	C	O	P	0
			87	68	17	2	
63	5B	1	Total	C	O	P	0
			62	43	17	2	
63	5B	1	Total	C	O	P	0
			67	48	17	2	
63	7A	1	Total	C	O	P	0
			67	48	17	2	
63	7A	1	Total	C	O	P	0
			100	81	17	2	
63	7C	1	Total	C	O	P	0
			85	66	17	2	
63	7C	1	Total	C	O	P	0
			51	32	17	2	
63	M1	1	Total	C	O	P	0
			95	76	17	2	
63	M1	1	Total	C	O	P	0
			66	47	17	2	
63	M1	1	Total	C	O	P	0
			66	47	17	2	
63	M2	1	Total	C	O	P	0
			54	35	17	2	

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Mol	Chain	Residues	Atoms				AltConf
63	M2	1	Total	C	O	P	0
			66	47	17	2	
63	M2	1	Total	C	O	P	0
			74	55	17	2	
63	M3	1	Total	C	O	P	0
			94	75	17	2	
63	M3	1	Total	C	O	P	0
			51	32	17	2	
63	M3	1	Total	C	O	P	0
			63	44	17	2	
63	Y7	1	Total	C	O	P	0
			65	46	17	2	
63	Y0	1	Total	C	O	P	0
			64	45	17	2	
63	Y5	1	Total	C	O	P	0
			81	62	17	2	
63	A	1	Total	C	O	P	0
			51	32	17	2	
63	B	1	Total	C	O	P	0
			62	43	17	2	
63	E	1	Total	C	O	P	0
			60	41	17	2	
63	E	1	Total	C	O	P	0
			72	53	17	2	
63	F	1	Total	C	O	P	0
			100	81	17	2	
63	J	1	Total	C	O	P	0
			70	51	17	2	
63	L	1	Total	C	O	P	0
			74	55	17	2	
63	N	1	Total	C	O	P	0
			95	76	17	2	
63	T	1	Total	C	O	P	0
			68	49	17	2	
63	T	1	Total	C	O	P	0
			75	56	17	2	
63	U	1	Total	C	O	P	0
			82	63	17	2	
63	V	1	Total	C	O	P	0
			91	72	17	2	
63	c1	1	Total	C	O	P	0
			59	40	17	2	

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Mol	Chain	Residues	Atoms				AltConf
63	c1	1	Total	C	O	P	0
			65	46	17	2	
63	c3	1	Total	C	O	P	0
			68	49	17	2	
63	5b	1	Total	C	O	P	0
			87	68	17	2	
63	5b	1	Total	C	O	P	0
			67	48	17	2	
63	7a	1	Total	C	O	P	0
			67	48	17	2	
63	7a	1	Total	C	O	P	0
			100	81	17	2	
63	7c	1	Total	C	O	P	0
			85	66	17	2	
63	7c	1	Total	C	O	P	0
			51	32	17	2	
63	m1	1	Total	C	O	P	0
			95	76	17	2	
63	m1	1	Total	C	O	P	0
			66	47	17	2	
63	m1	1	Total	C	O	P	0
			66	47	17	2	
63	m2	1	Total	C	O	P	0
			54	35	17	2	
63	m2	1	Total	C	O	P	0
			66	47	17	2	
63	m2	1	Total	C	O	P	0
			74	55	17	2	
63	m3	1	Total	C	O	P	0
			94	75	17	2	
63	m3	1	Total	C	O	P	0
			51	32	17	2	
63	m3	1	Total	C	O	P	0
			63	44	17	2	
63	y7	1	Total	C	O	P	0
			65	46	17	2	
63	y0	1	Total	C	O	P	0
			64	45	17	2	
63	y5	1	Total	C	O	P	0
			81	62	17	2	
63	a	1	Total	C	O	P	0
			51	32	17	2	

Continued on next page...

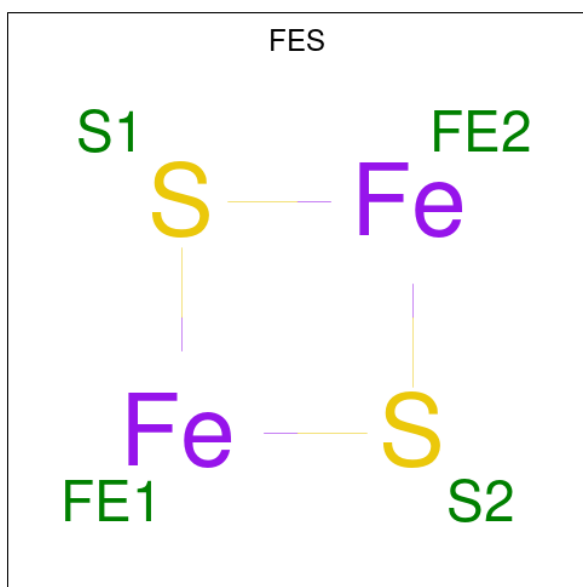
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
63	b	1	Total	C	O	P	0
			62	43	17	2	
63	e	1	Total	C	O	P	0
			60	41	17	2	
63	e	1	Total	C	O	P	0
			72	53	17	2	
63	f	1	Total	C	O	P	0
			100	81	17	2	
63	j	1	Total	C	O	P	0
			70	51	17	2	
63	k	1	Total	C	O	P	0
			62	43	17	2	
63	l	1	Total	C	O	P	0
			74	55	17	2	
63	n	1	Total	C	O	P	0
			95	76	17	2	
63	t	1	Total	C	O	P	0
			68	49	17	2	
63	t	1	Total	C	O	P	0
			75	56	17	2	
63	u	1	Total	C	O	P	0
			82	63	17	2	
63	v	1	Total	C	O	P	0
			91	72	17	2	

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
64	5B	1	Total	Zn	0
			1	1	
64	M	1	Total	Zn	0
			1	1	
64	5b	1	Total	Zn	0
			1	1	
64	m	1	Total	Zn	0
			1	1	

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

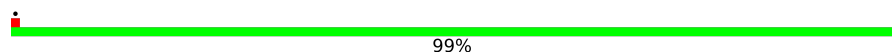


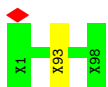
Mol	Chain	Residues	Atoms			AltConf
65	FS	1	Total	Fe	S	0
			4	2	2	
65	FS	1	Total	Fe	S	0
			4	2	2	
65	fs	1	Total	Fe	S	0
			4	2	2	
65	fs	1	Total	Fe	S	0
			4	2	2	

3 Residue-property plots

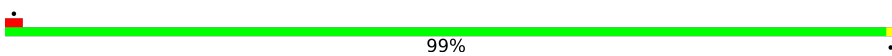
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

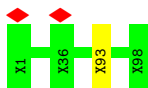
- Molecule 1: Unknown peptide

Chain U1: 

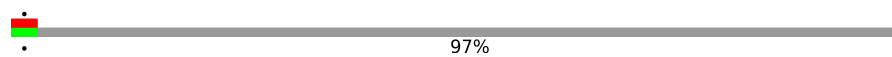


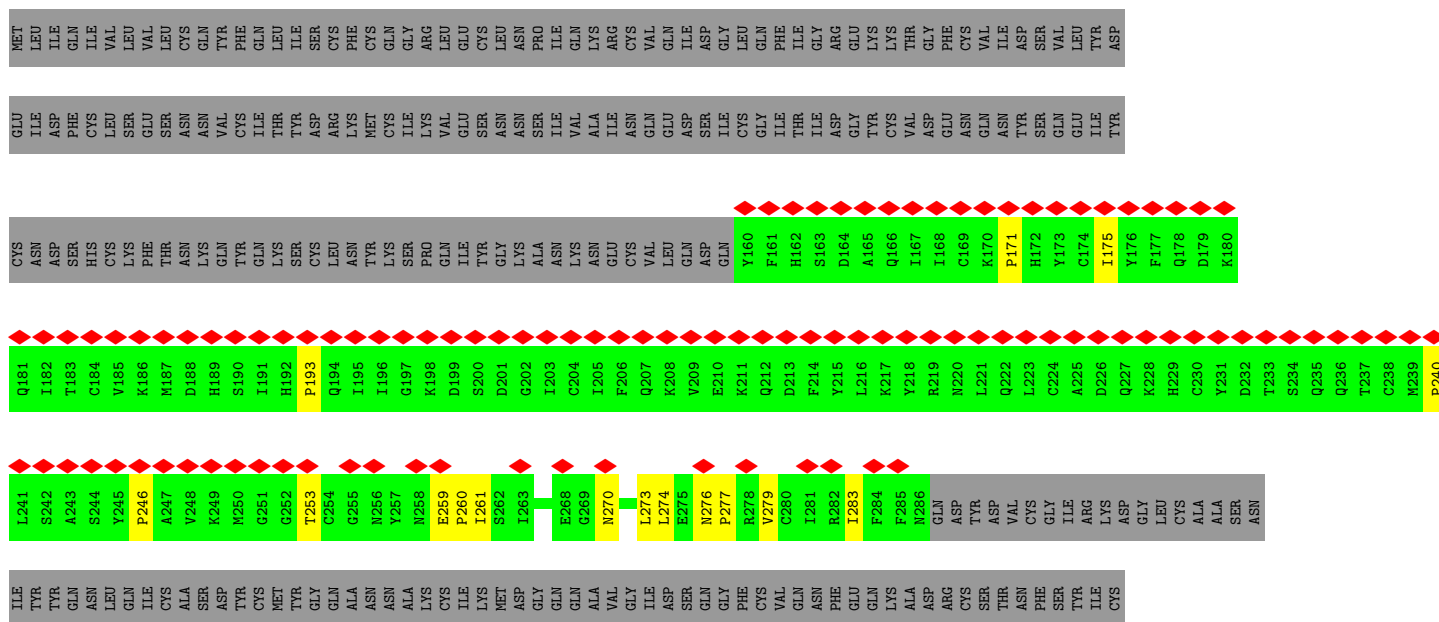
- Molecule 1: Unknown peptide

Chain u1: 



- Molecule 2: Transmembrane protein, putative

Chain U2: 





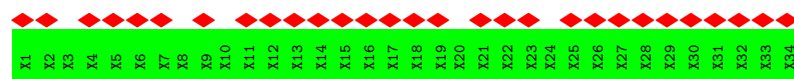




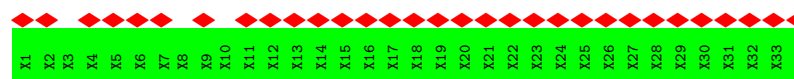
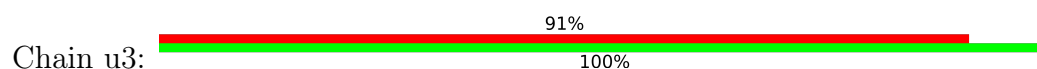




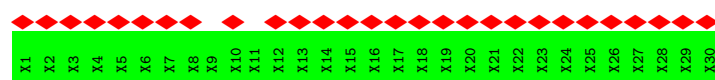




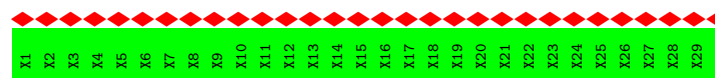
• Molecule 3: Unknown peptide



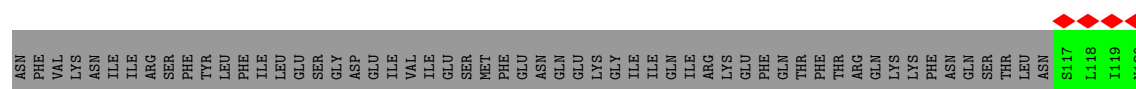
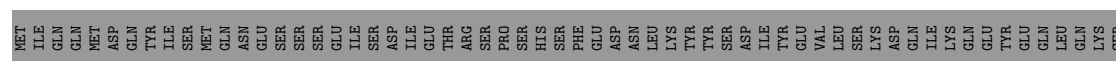
• Molecule 4: Unknown peptide



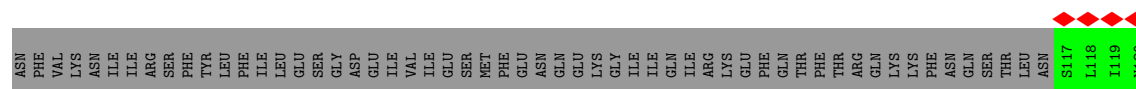
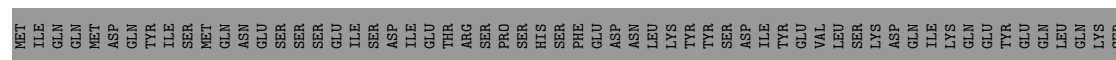
• Molecule 4: Unknown peptide

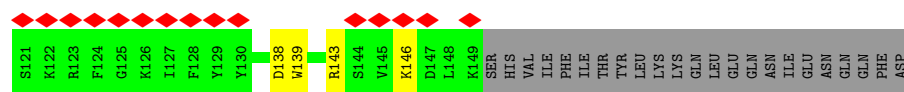


• Molecule 5: Uncharacterized protein



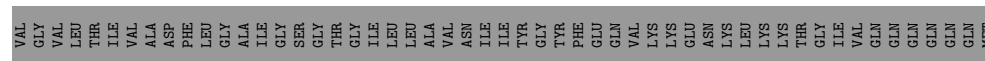
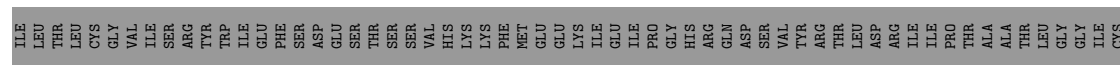
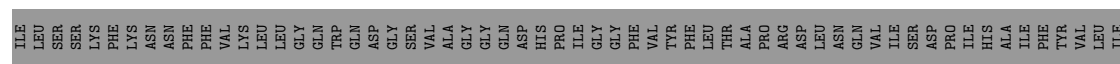
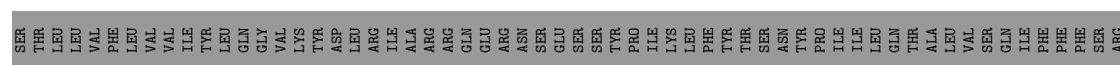
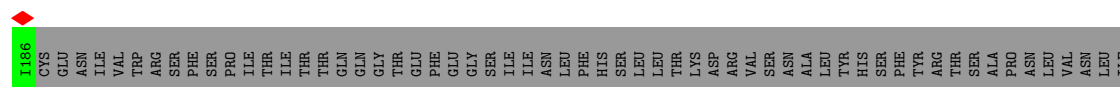
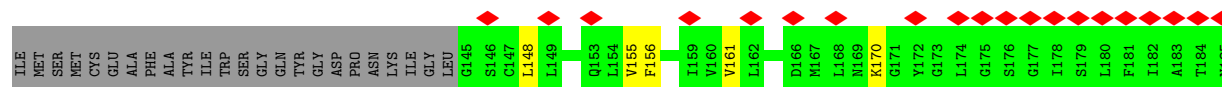
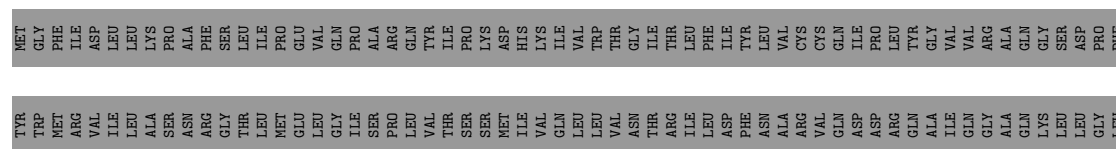
• Molecule 5: Uncharacterized protein





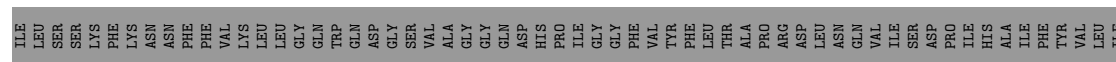
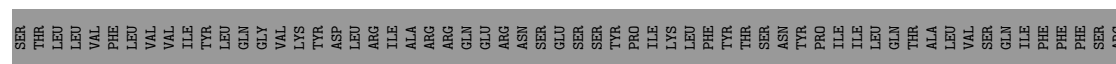
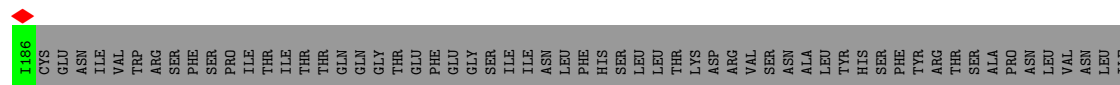
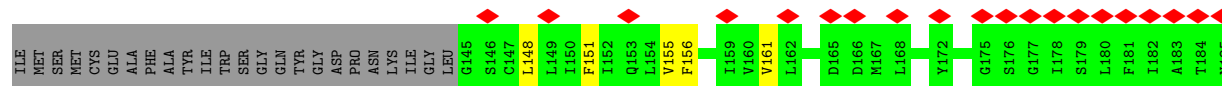
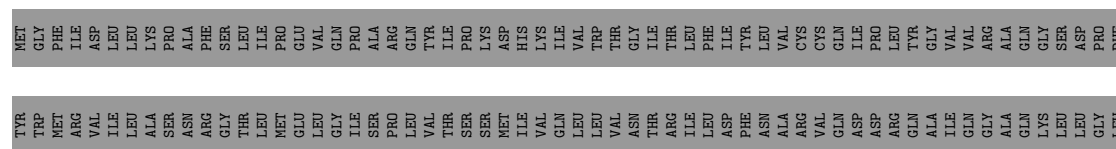
• Molecule 6: Protein transporter Sec61 alpha subunit

Chain U6: 8% . 91%

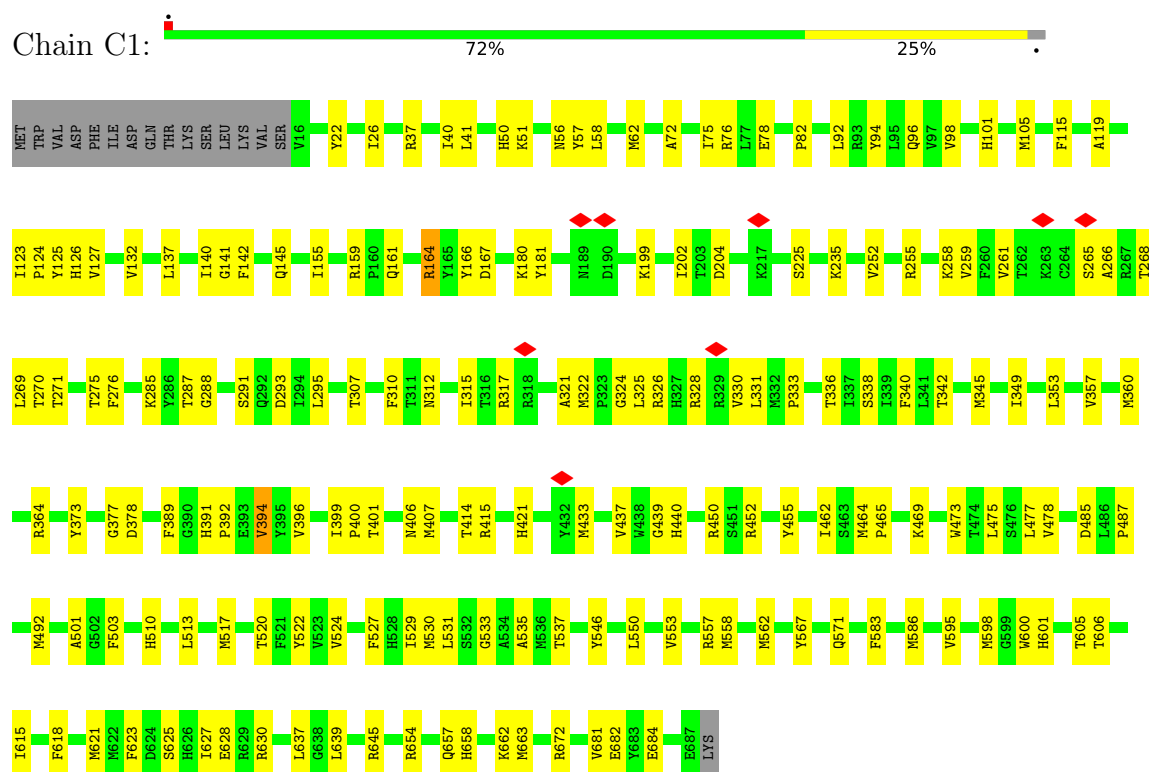


• Molecule 6: Protein transporter Sec61 alpha subunit

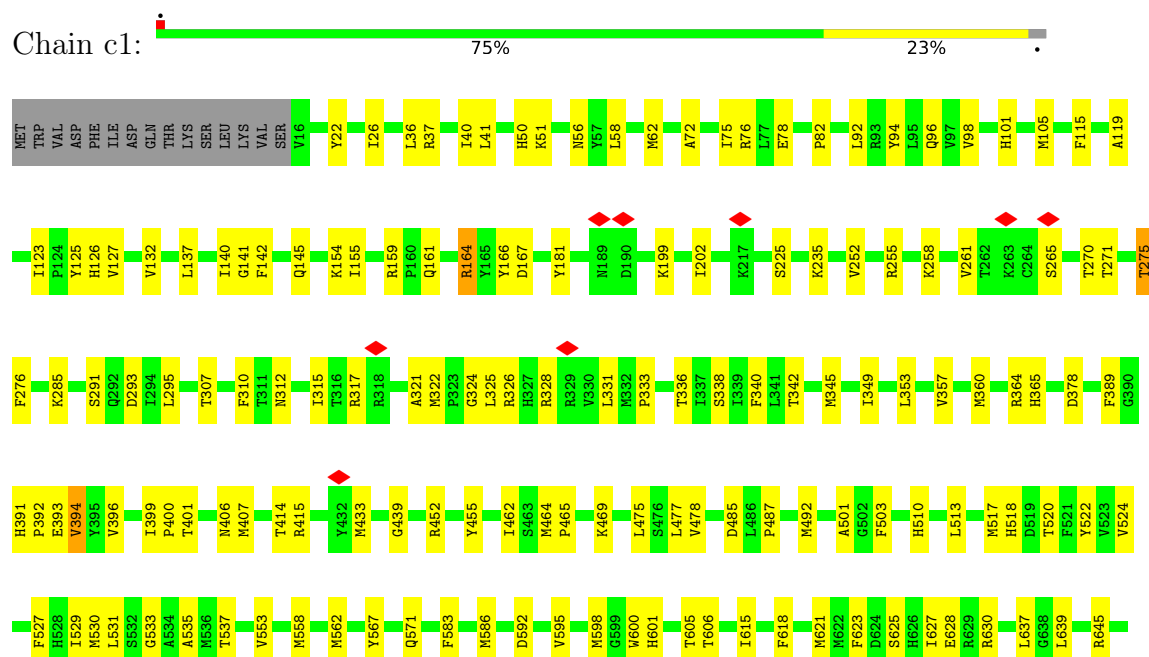
Chain u6: 8% . 91%



- Molecule 7: Cytochrome c oxidase subunit 1



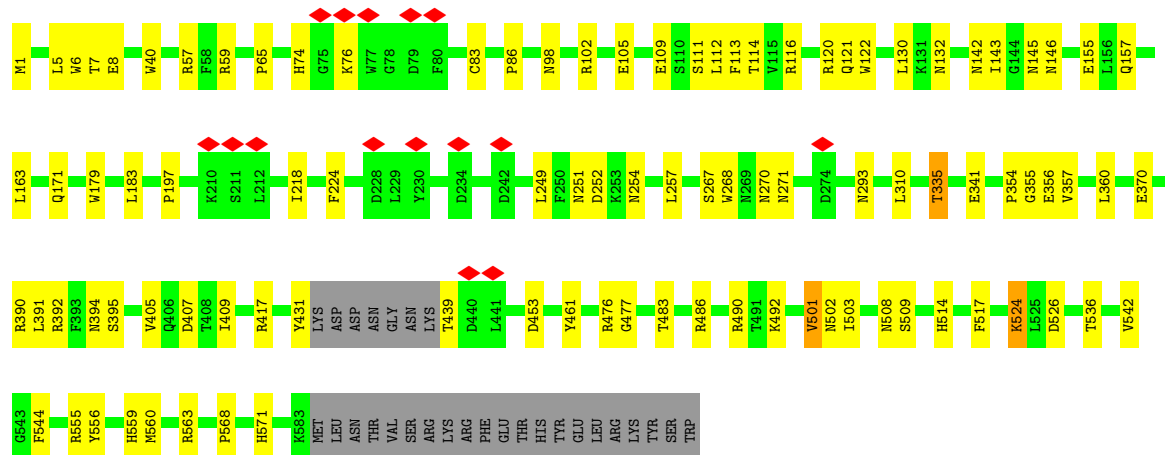
- Molecule 7: Cytochrome c oxidase subunit 1





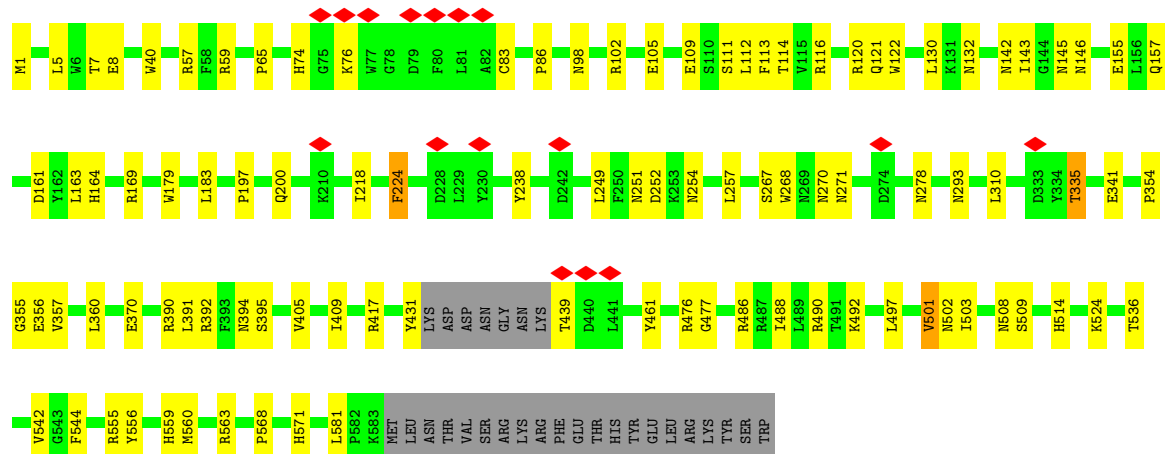
• Molecule 8: Cytochrome c oxidase subunit 2

Chain C2: 79% 16% 5%



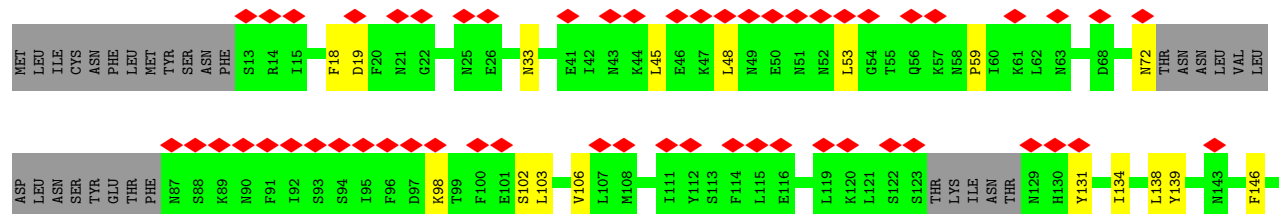
• Molecule 8: Cytochrome c oxidase subunit 2

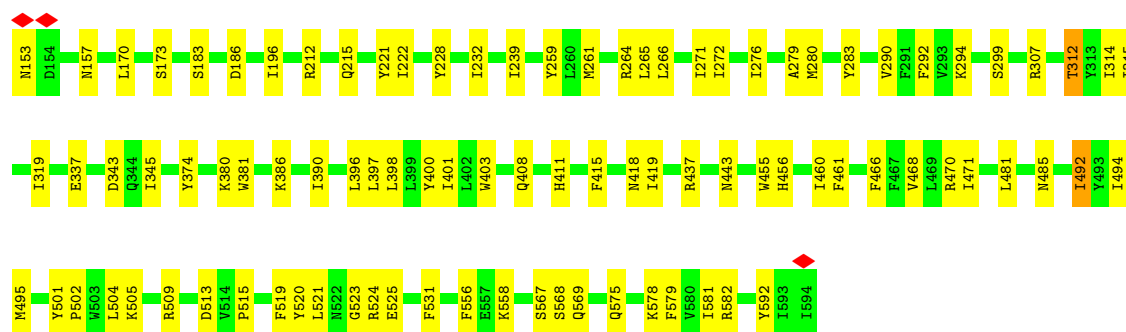
Chain c2: 79% 16% 5%



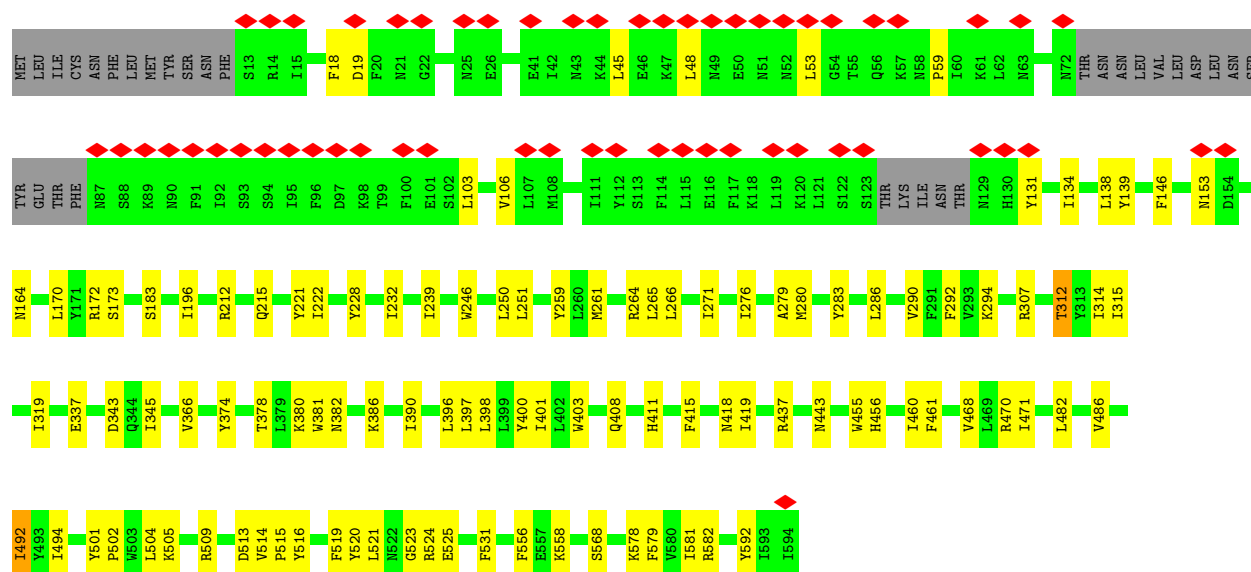
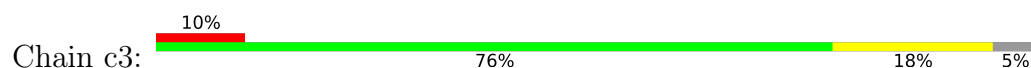
• Molecule 9: Ymf68

Chain C3: 10% 76% 18% 5%

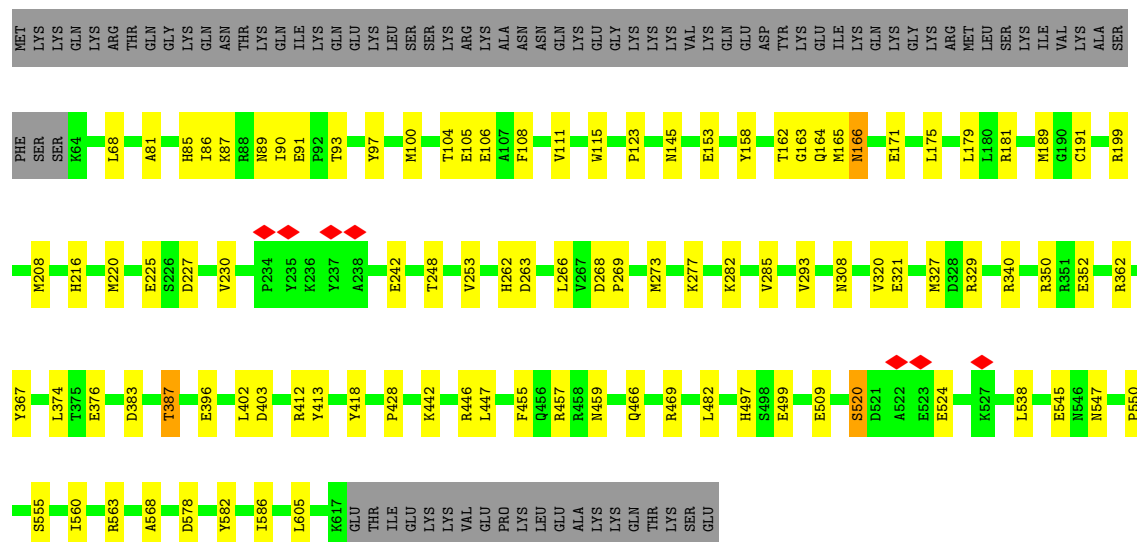




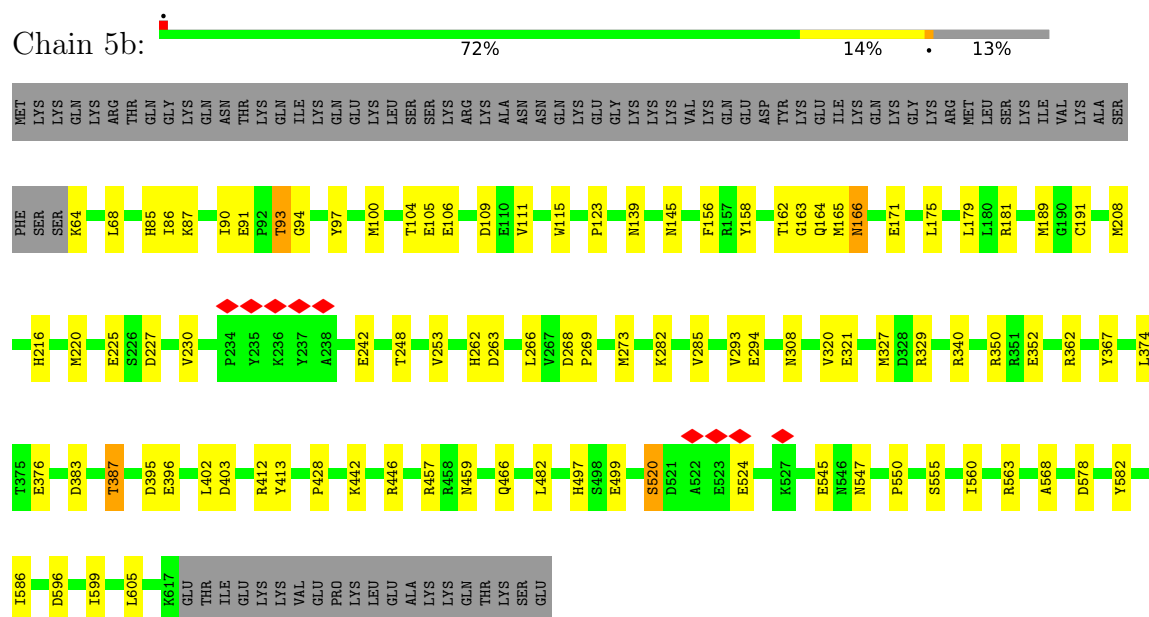
• Molecule 9: Ymf68



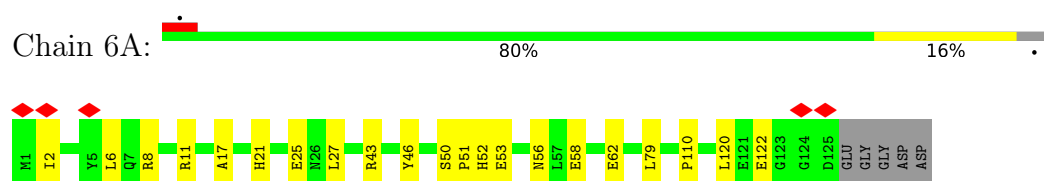
• Molecule 10: Cytochrome C oxidase subunit Vb protein



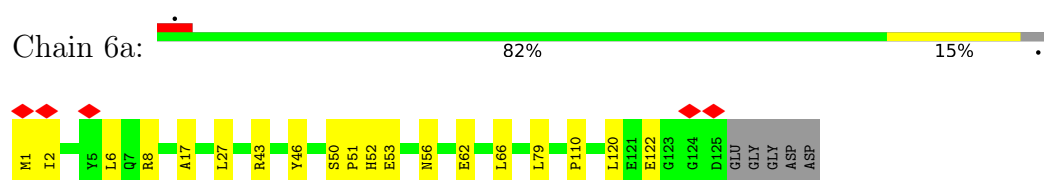
- Molecule 10: Cytochrome C oxidase subunit Vb protein



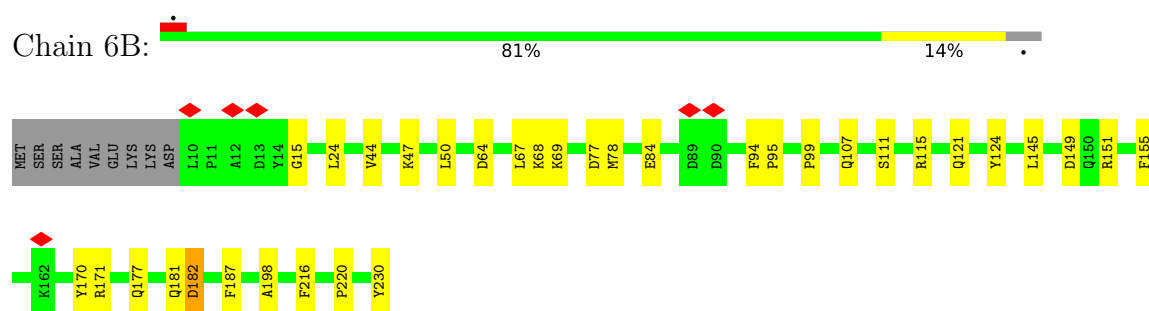
- Molecule 11: Transmembrane protein, putative



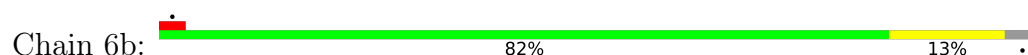
- Molecule 11: Transmembrane protein, putative

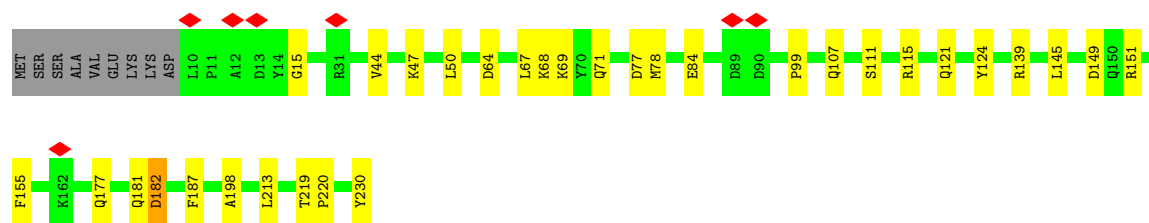


- Molecule 12: Cytochrome c oxidase subunit 6B

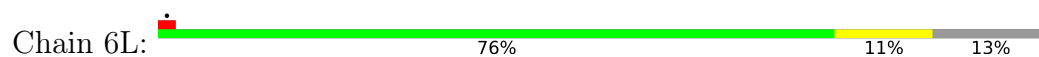


- Molecule 12: Cytochrome c oxidase subunit 6B

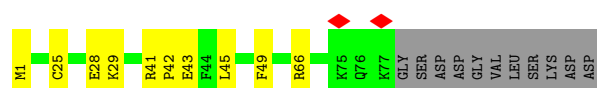
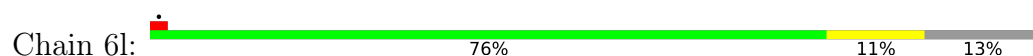




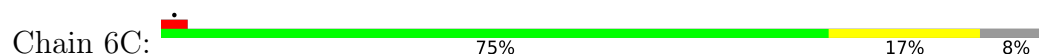
- Molecule 13: Cytochrome c oxidase subunit 6B-like



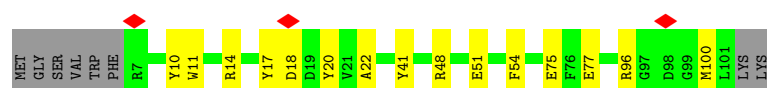
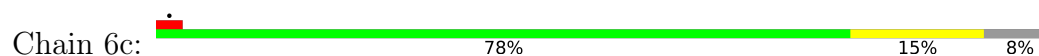
- Molecule 13: Cytochrome c oxidase subunit 6B-like



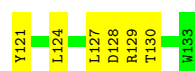
- Molecule 14: Transmembrane protein, putative



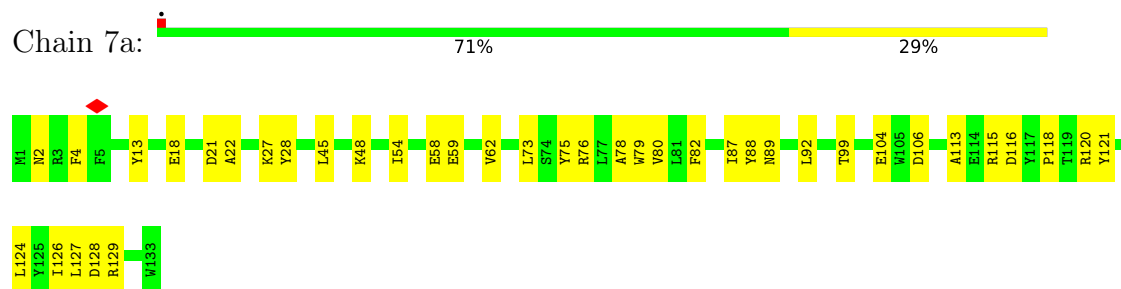
- Molecule 14: Transmembrane protein, putative



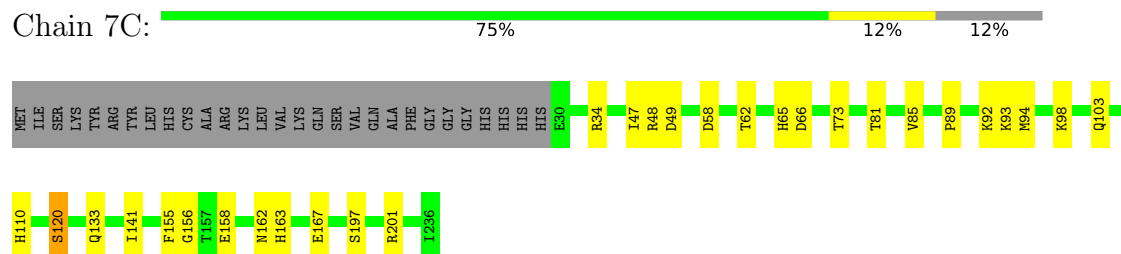
- Molecule 15: Transmembrane protein, putative



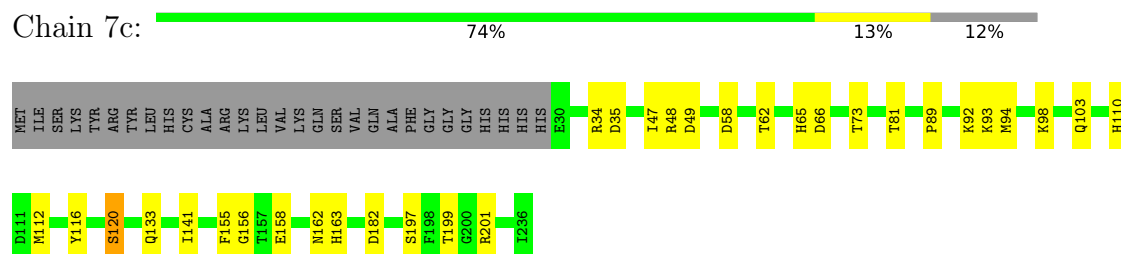
- Molecule 15: Transmembrane protein, putative



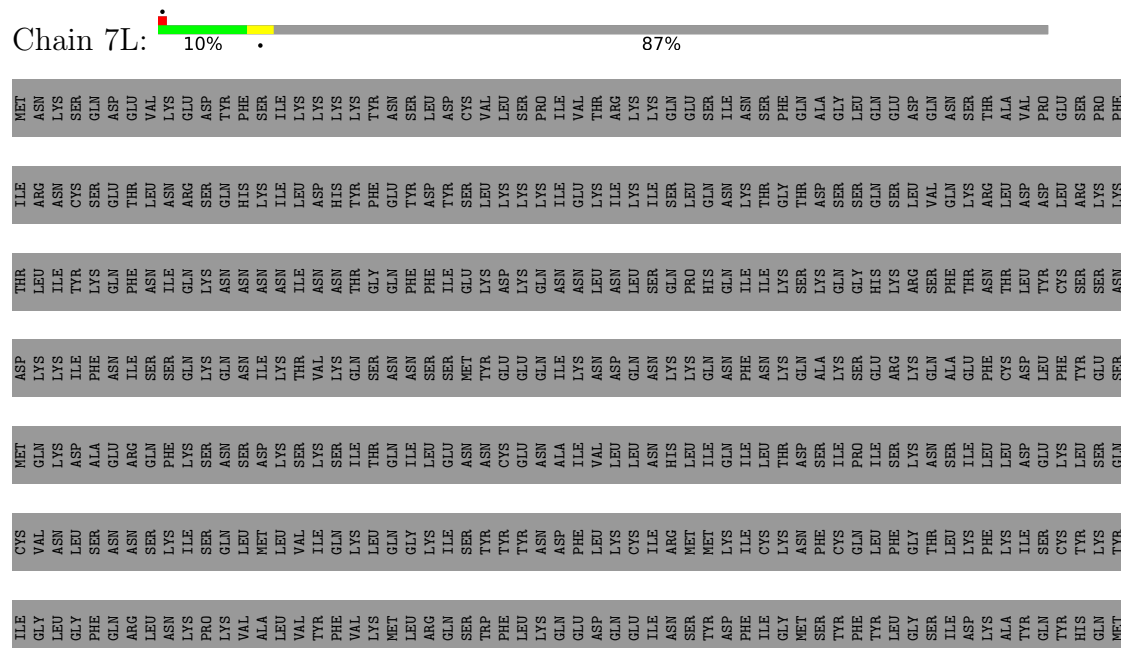
- Molecule 16: Cytochrome c oxidase subunit 7C



- Molecule 16: Cytochrome c oxidase subunit 7C



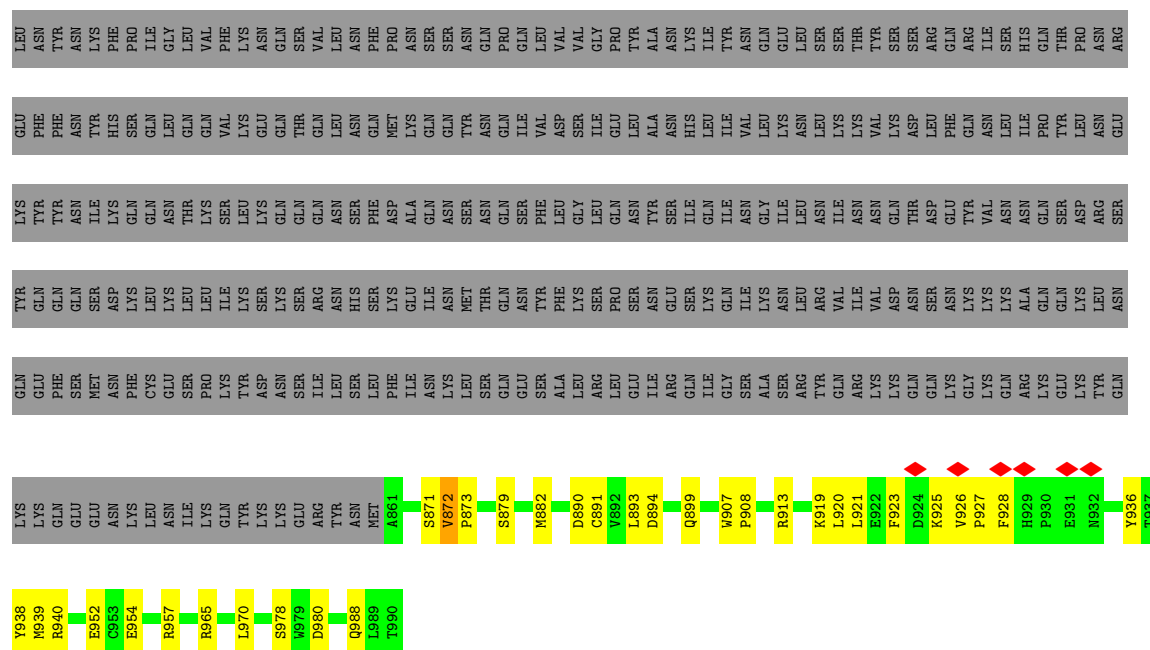
- Molecule 17: CTF/NF-I domain-containing protein



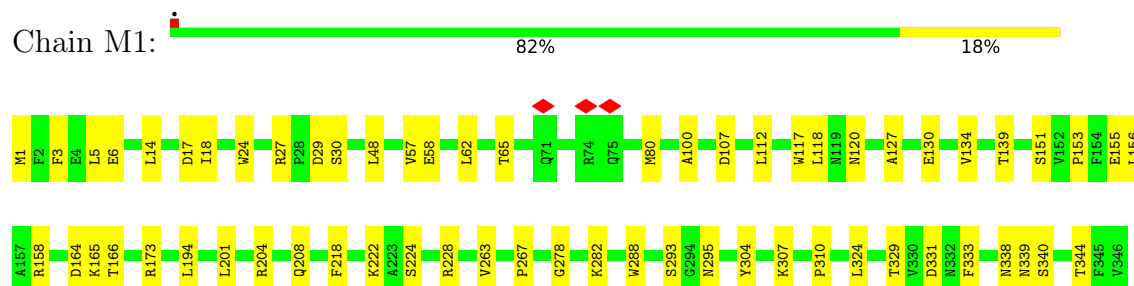
A horizontal timeline of the 1990s. It consists of a series of yellow rectangular blocks, each containing a year. The years are M939, R940, E954, R957, R965, L970, D980, and T990. The blocks are connected by short horizontal lines. The block for T990 is colored green, while the others are yellow.

Chain 71: 10% 87%

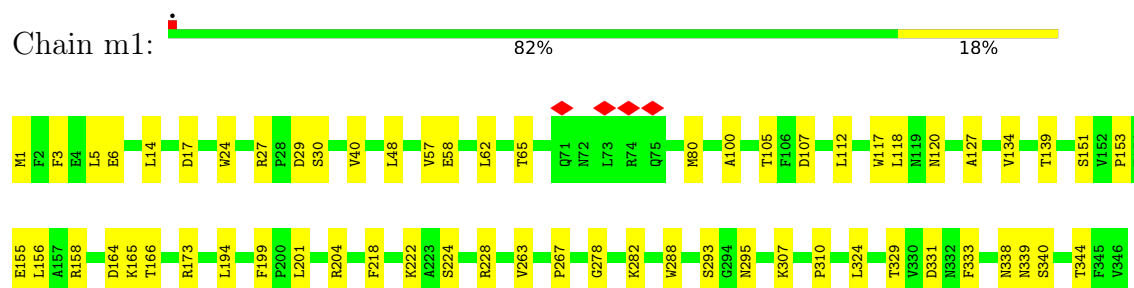




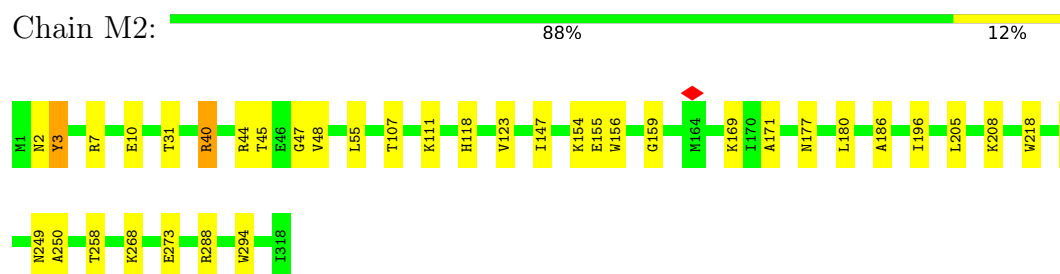
- Molecule 18: Oxoglutarate/malate translocator protein, putative



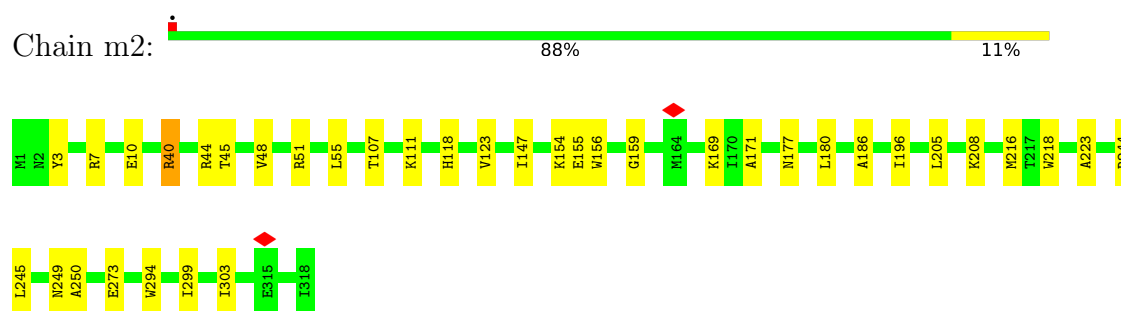
- Molecule 18: Oxoglutarate/malate translocator protein, putative



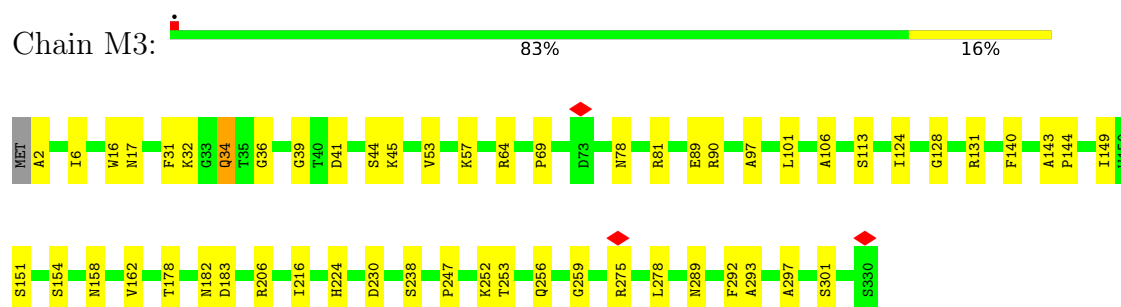
- Molecule 19: 2-oxoglutarate/malate carrier protein



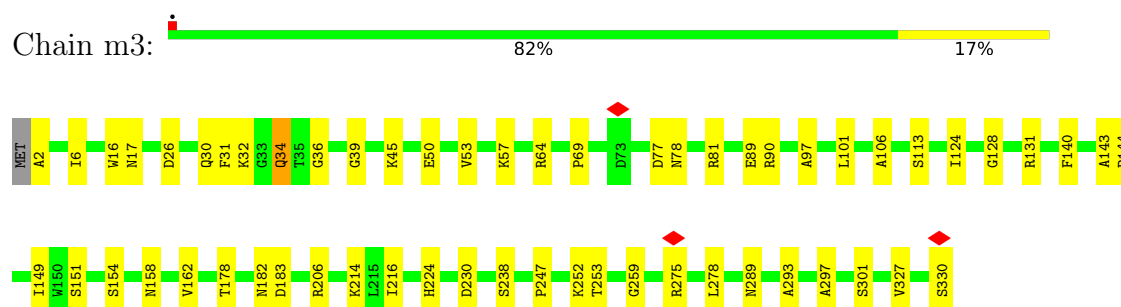
- Molecule 19: 2-oxoglutarate/malate carrier protein



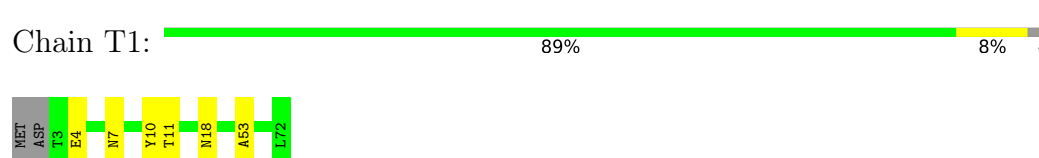
- Molecule 20: Carrier protein



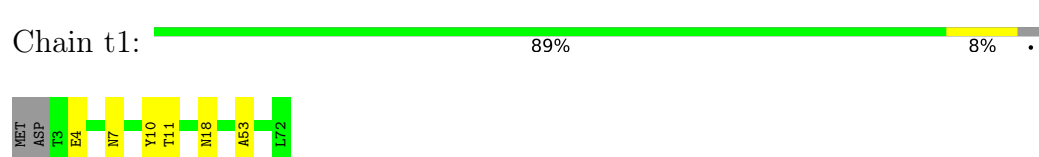
- Molecule 20: Carrier protein



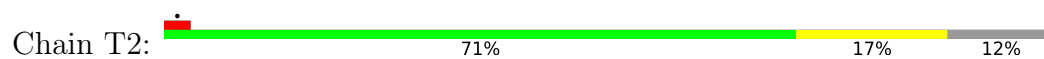
- Molecule 21: Tim10/DDP family zinc finger protein



- Molecule 21: Tim10/DDP family zinc finger protein



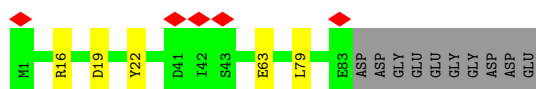
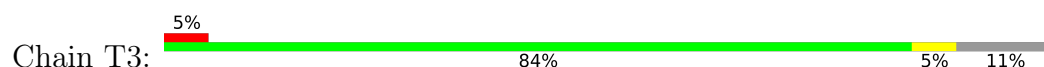
- Molecule 22: Cytochrome c oxidase small TIM subunit 2



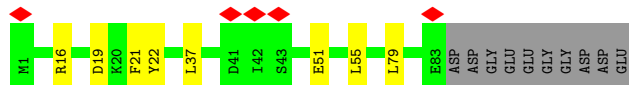
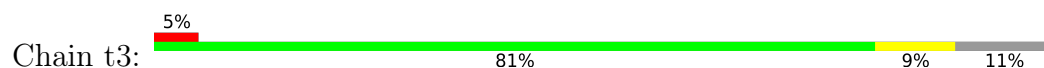
- Molecule 22: Cytochrome c oxidase small TIM subunit 2



- Molecule 23: Cytochrome c oxidase small TIM subunit 3



- Molecule 23: Cytochrome c oxidase small TIM subunit 3



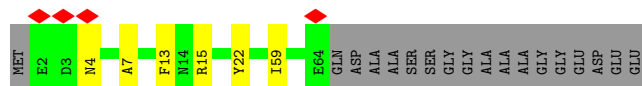
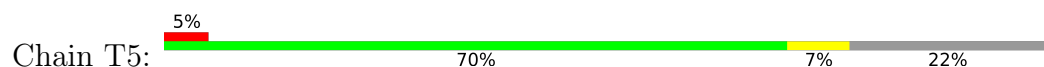
- Molecule 24: Cytochrome c oxidase small TIM subunit 4



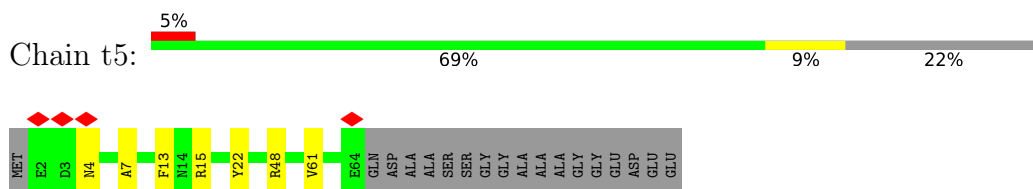
- Molecule 24: Cytochrome c oxidase small TIM subunit 4



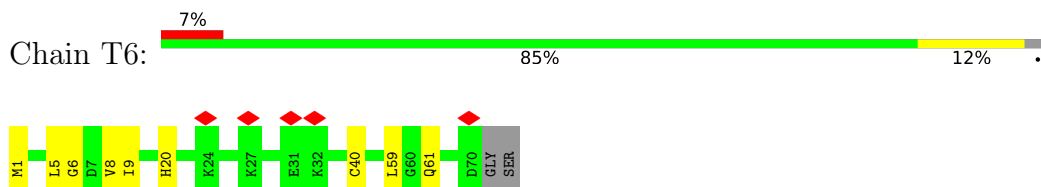
- Molecule 25: Cytochrome c oxidase small TIM subunit 5



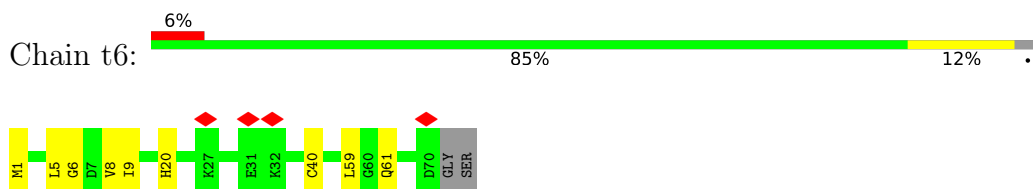
- Molecule 25: Cytochrome c oxidase small TIM subunit 5



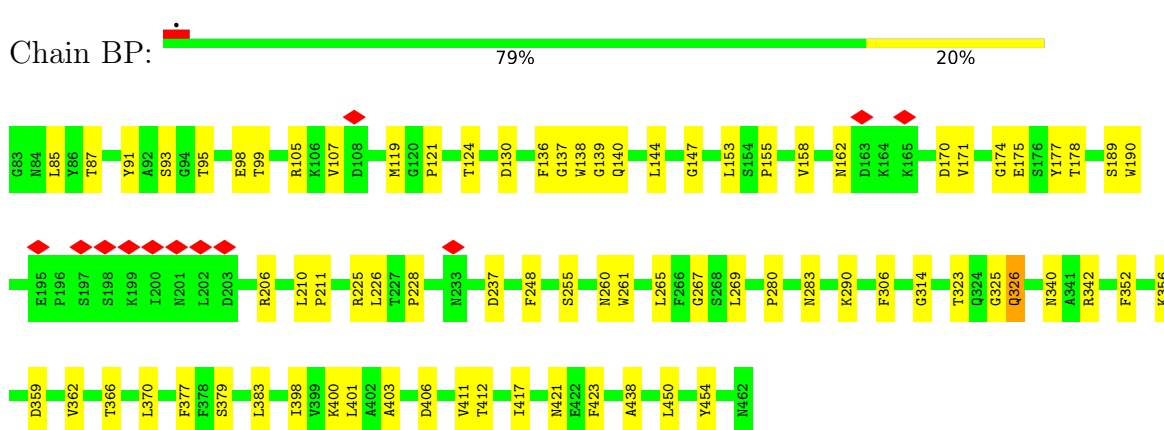
- Molecule 26: Cytochrome c oxidase small TIM subunit 6



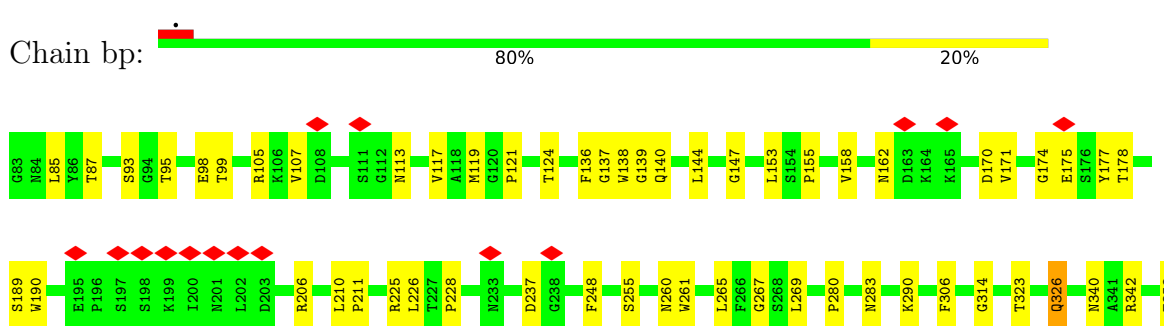
- Molecule 26: Cytochrome c oxidase small TIM subunit 6

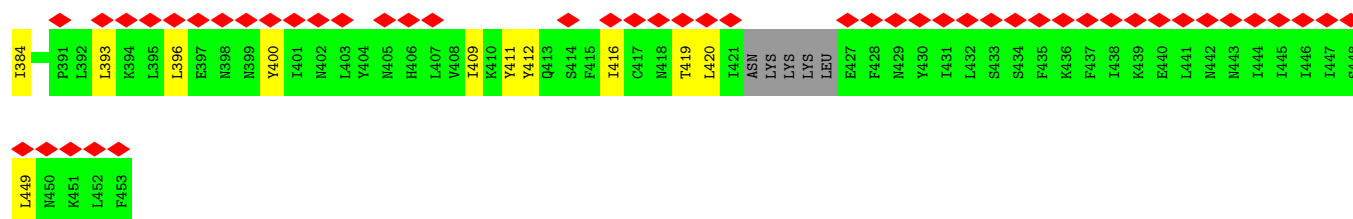


- Molecule 27: Chromosome condensation regulator RCC1 repeat protein

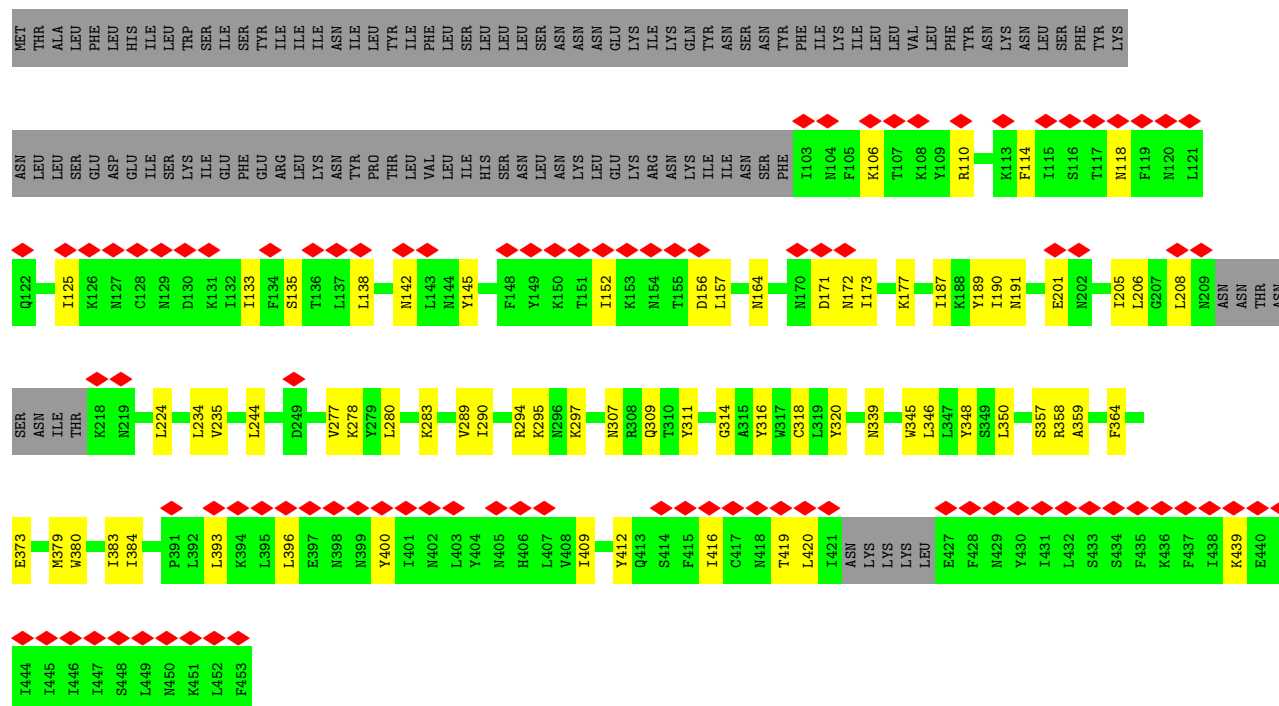


- Molecule 27: Chromosome condensation regulator RCC1 repeat protein

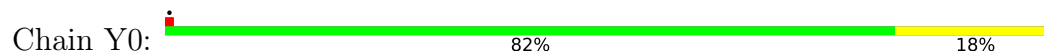




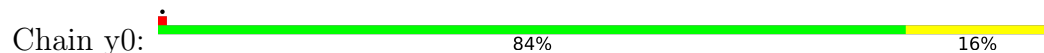
• Molecule 30: Ymf67



• Molecule 31: Ymf70

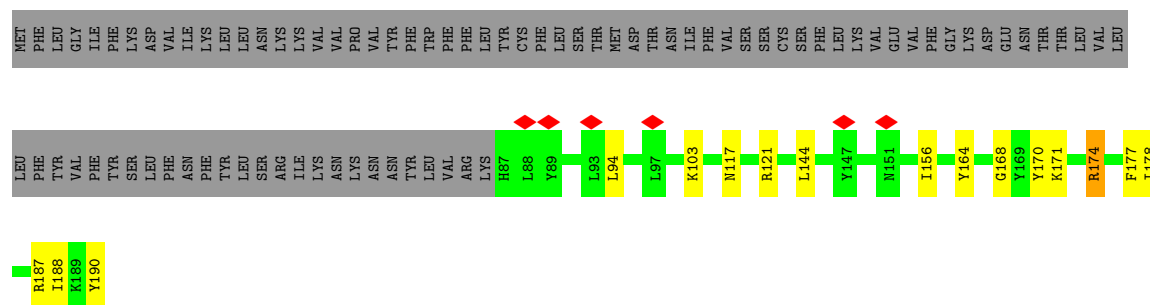


• Molecule 31: Ymf70

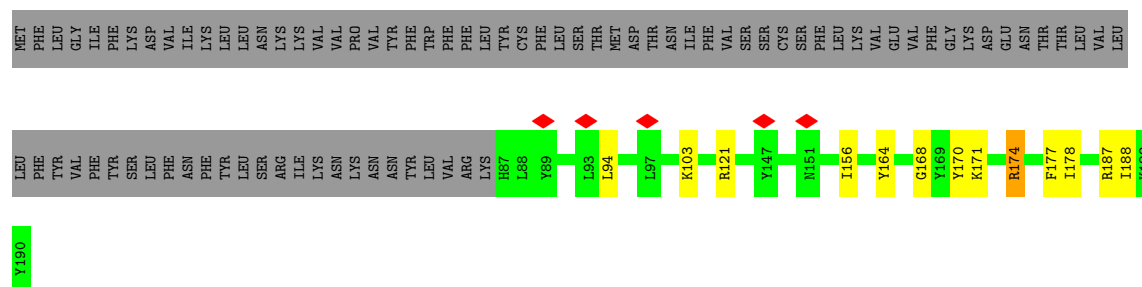


• Molecule 32: Ymf75

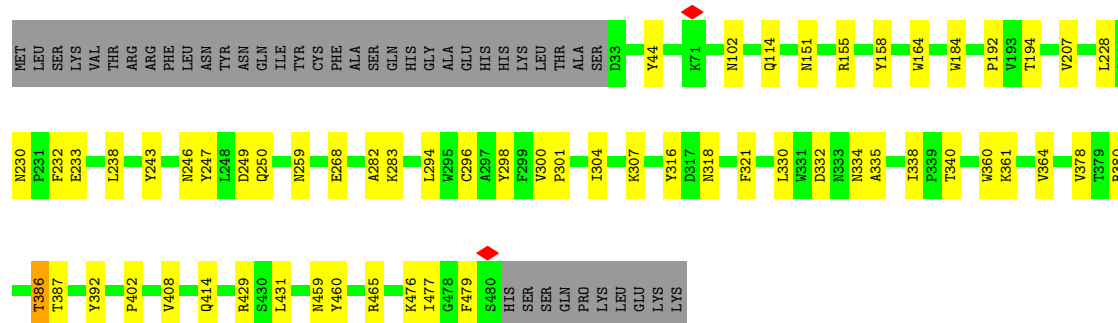
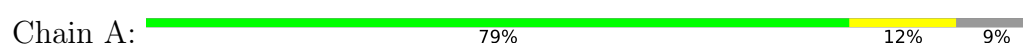




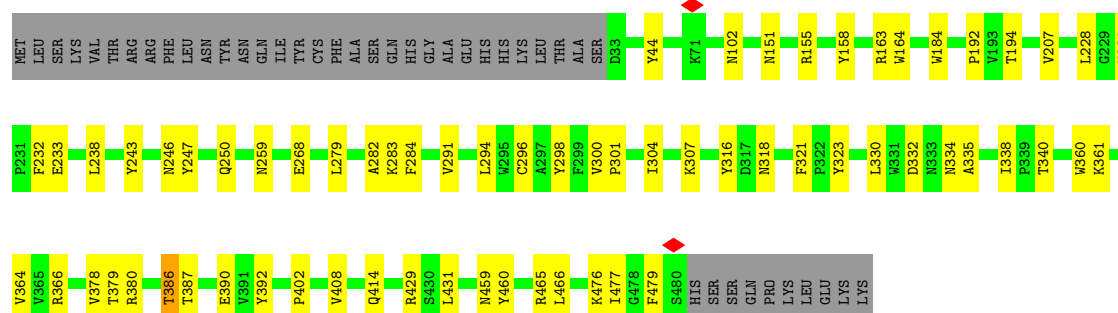
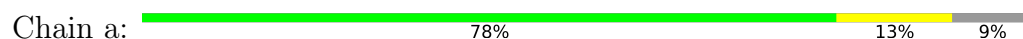
- Molecule 32: Ymf75



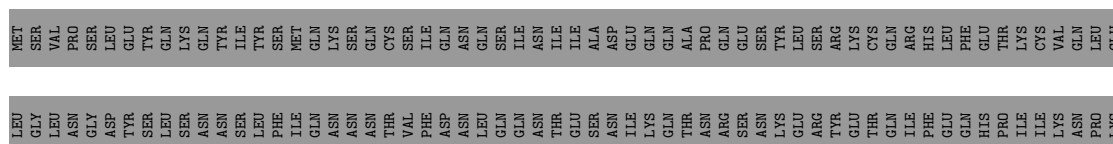
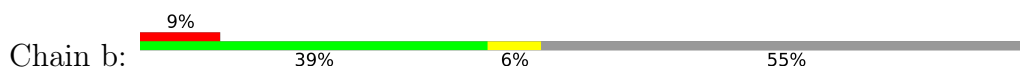
- Molecule 33: Transmembrane protein, putative



- Molecule 33: Transmembrane protein, putative



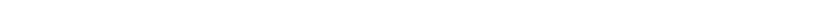
Chain B:





TYR	LEU	SER	TYR	GLY	VAL	SER	LYS	ARG	ARG	GLY	GLN	GLN	PHE	PRO	CYS	ASN	LYS	HIS	ASN	LEU	THR	LEU	TYR	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 35: Cyclic nucleotide-binding domain protein

Chain c:  97%

LEU GLY LEU LEU ASN GLY ASP TYR SER SER LEU LEU SER ASN ASN ASN SER SER LEU PHE ILE ILE GLN ASN ASN ASN THR THR VAL PHE ASP ASN ASN GLN GLN ASN GLN THR THR GLU GLU SER SER ASN ASN ILE ILE LYS LYS GLN THR THR ASN ASN ARG ARG SER SER ASN ASN LYS GLU ARG ARG TYR TYR GLU GLU THR THR GLN ILE PHE GLU GLU HIS GLN HIS PRO PRO ILE ILE LYS ASN ASN PRO PRO

LYS ILE SER ASP CYS ASN LEU ASP ASP GLN PHE ILE LYS GLY ASP ASP SER ARG LEU ASP GLU SER SER LYS ILE PRO SER LYS CYS CYS GLY TRP ILE PHE GLU GLU ASP ILE ILE HIS GLN LEU ASN ASN ILE LYS VAL THR LEU VAL LYS ASN ASN PHE SER ASP

ARG ASP TYR ALA SER ILE ASN ASP LEU SER ASN PHE TYR LYS SER HIS LYS LYS ARG ASN LYS PHE MET LYS PHE ASN PHE VAL ILE LYS LEU SER GLN LYS LEU LYS PRO THR ASP LEU ARG VAL VAL TRP ASP VAL ILE LEU VAL LEU PHE

LYS		F429	F430	I437	V438	L439	G440	I441	K442	V443	I444	K445	R446	S447	T450	V451	Y452	M453	P454	M455	H456	M457	L458	L459	T460	V461	C462	C463	F463	N464	M465	L466	T467	F468	F469	K470	V471	N472	G473	I474	SER	SER	LYS	LYS	GLY	PHE	ASP	TYR	VAL	PHE	THR
-----	--	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

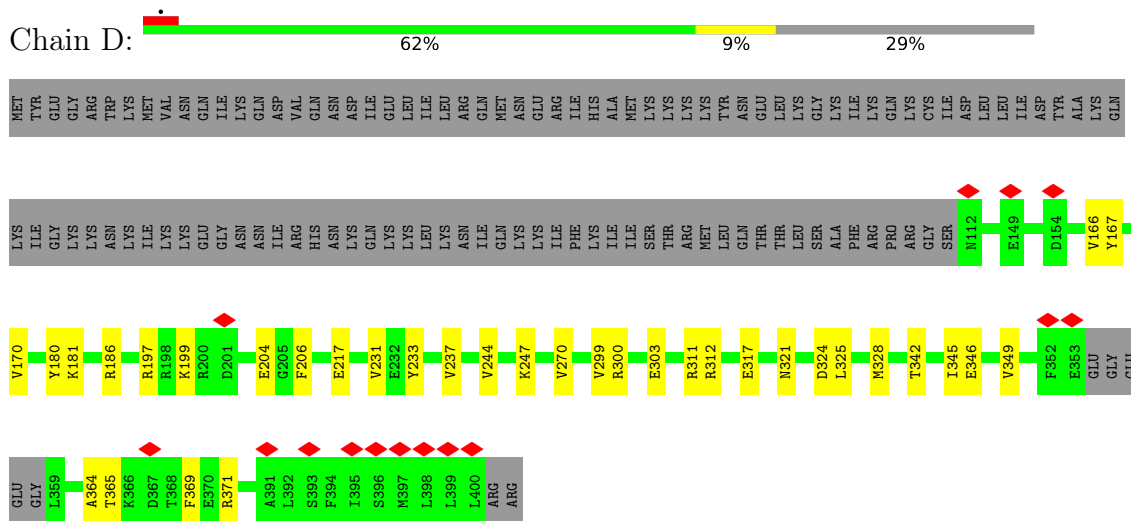
THR	VAL	GLU	GLU	ILE	ASN	ASN	LYS	ILE	LEU	ASN	LYS	PHE	ASN	ILE	PHE	SER	SER	ASN	PHE	SER	GLN	THR	LEU	ASP	LYS	LEU	VAL	PHE	LYS	MET	THR	THR	GLU	VAL	VAL	LEU	ILE	ASN	PRO	ASN	ASN	GLU	GLU	GLN	ASN	ASP	ASP	MET	SER	ILE	TYR	PHE	ILE	GLN	SER	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

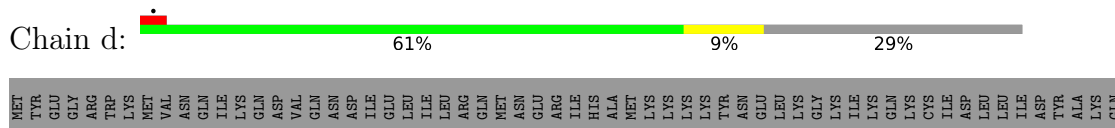
ILE	TYR	SER	SER	PHE	GLN	GLN	ARG	ARG	PHE	PHE	ASP	ARG	THR	ARG	LYS	TYR	ASN	ASN	LEU	LEU	ILE	GLN	ASP	ASN	GLN	ASN	ASN	VAL	CYS	LYS	ILE	LEU	LYS	GLN	ASN	LEU	LEU	ILE	ILE	ASP	ASP	ASP	ASP	ILE	ILE	ILE	GLU	GLU	MET	PHE	ASP	SER	SER	THR	THR	GLY	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

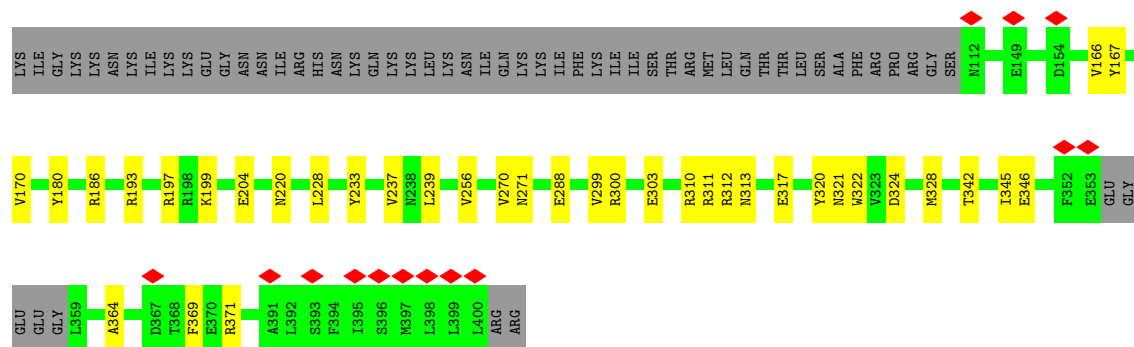
[illegible]

- Molecule 36: SURF1-like protein

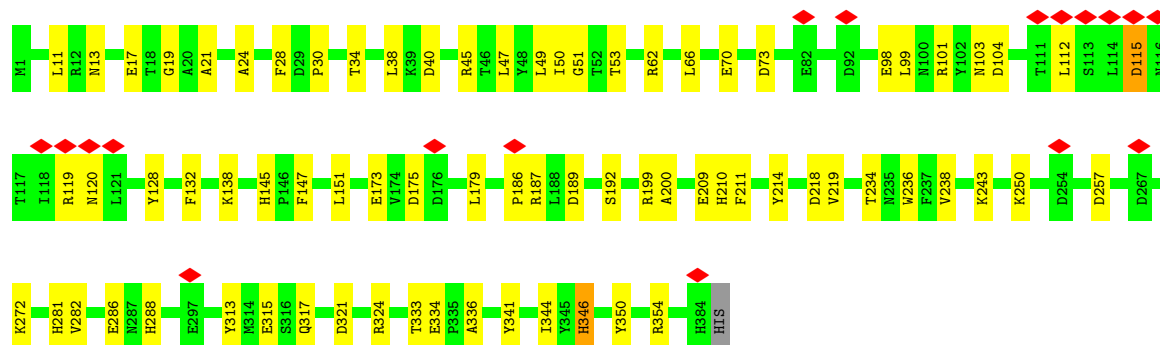
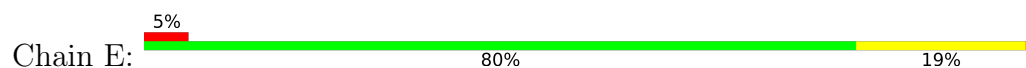


- Molecule 36: SURF1-like protein

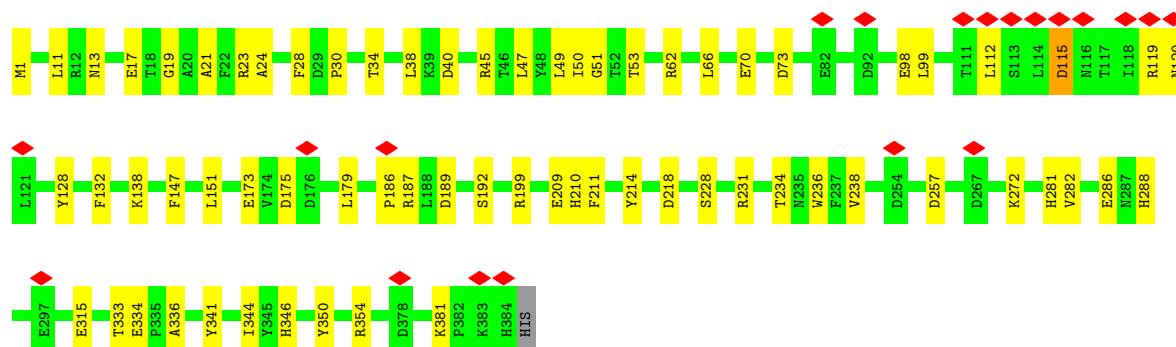
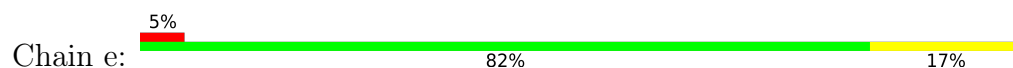




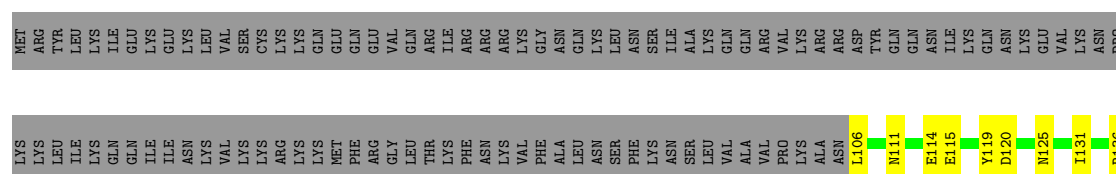
• Molecule 37: TraB family protein

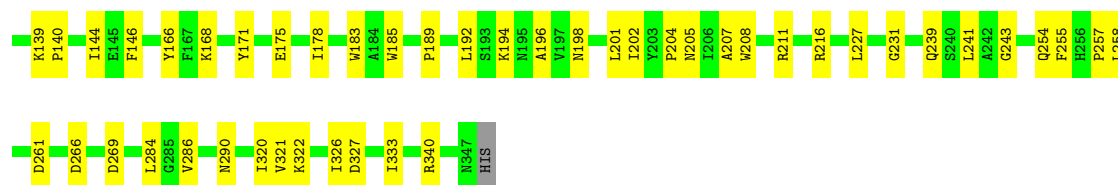


• Molecule 37: TraB family protein



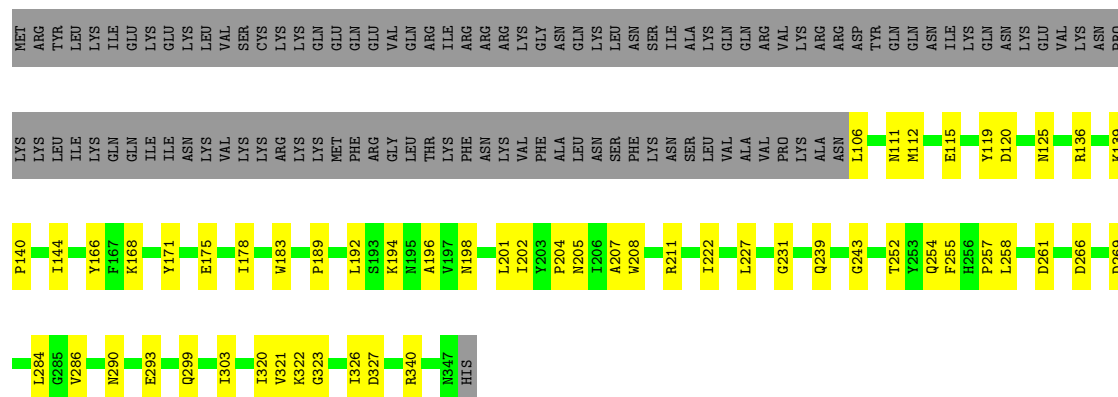
• Molecule 38: Transmembrane protein, putative





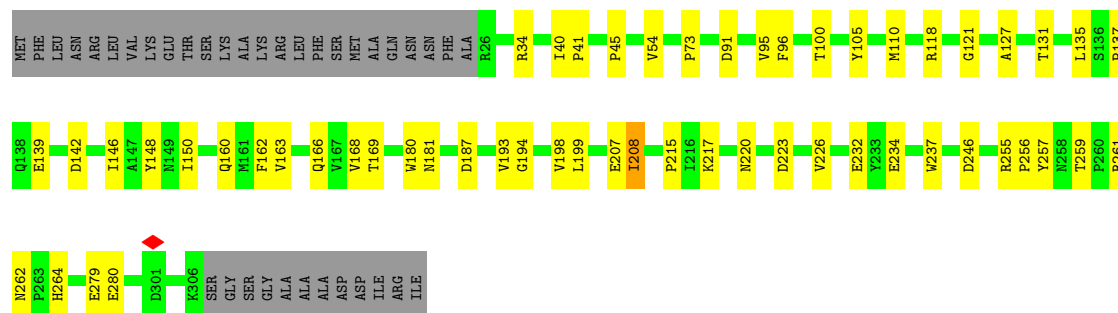
- Molecule 38: Transmembrane protein, putative

Chain f: 54% 16% 30%



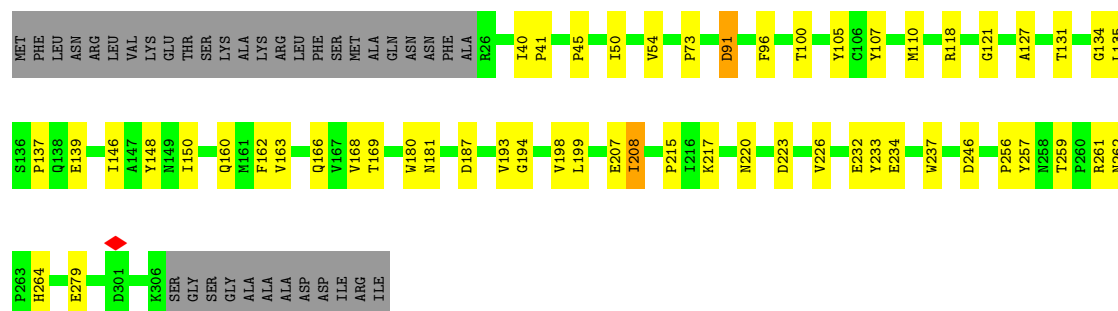
- Molecule 39: Cytochrome c oxidase subunit TT7

Chain G: 71% 17% 12%

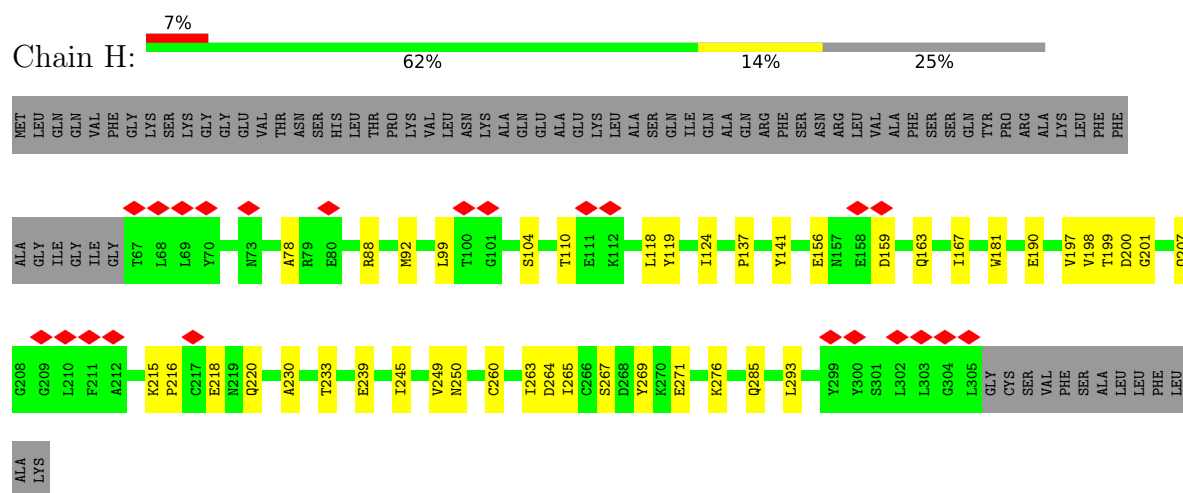


- Molecule 39: Cytochrome c oxidase subunit TT7

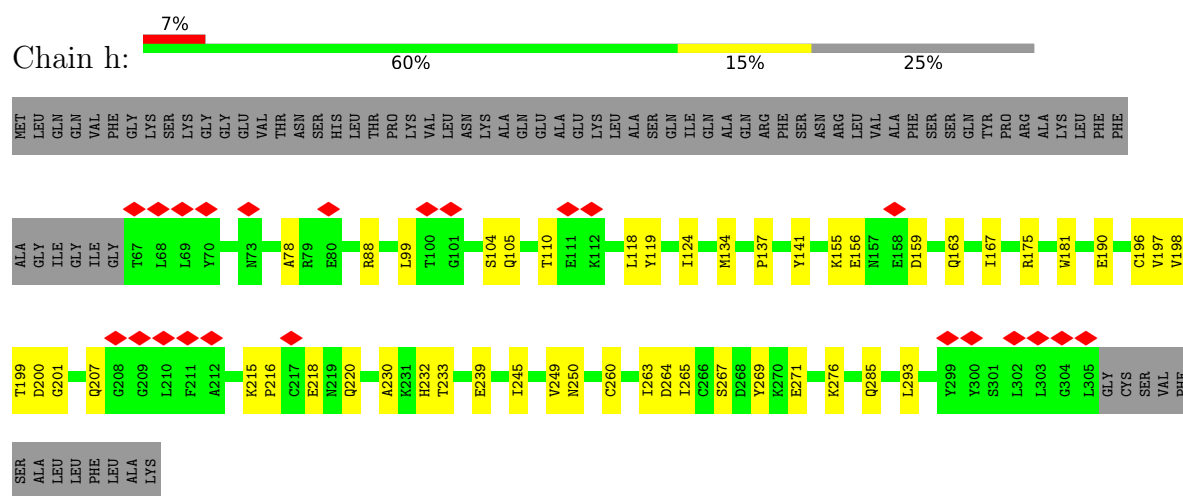
Chain g: 71% 17% 12%



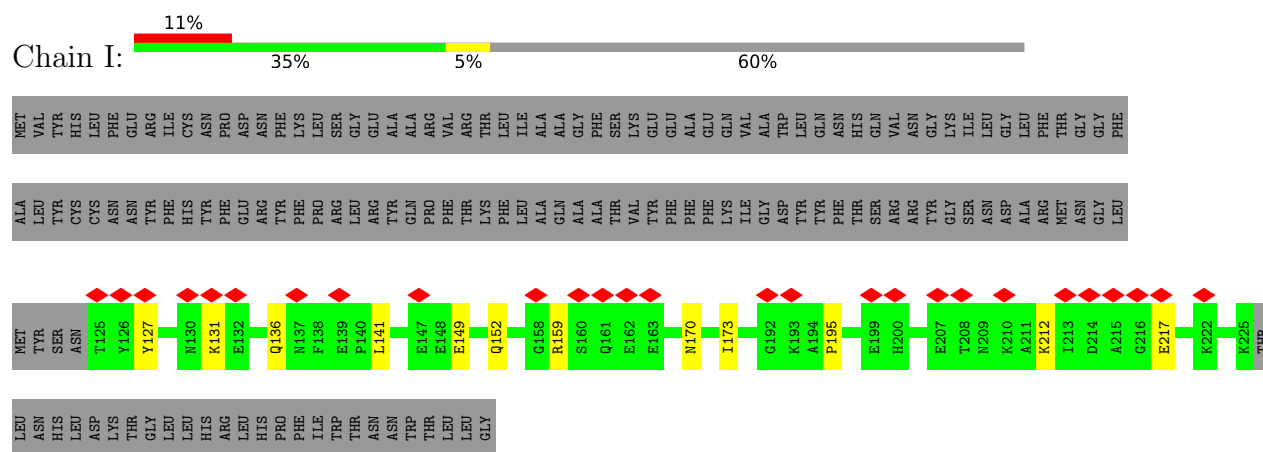
- Molecule 40: SURF1-like protein



- Molecule 40: SURF1-like protein

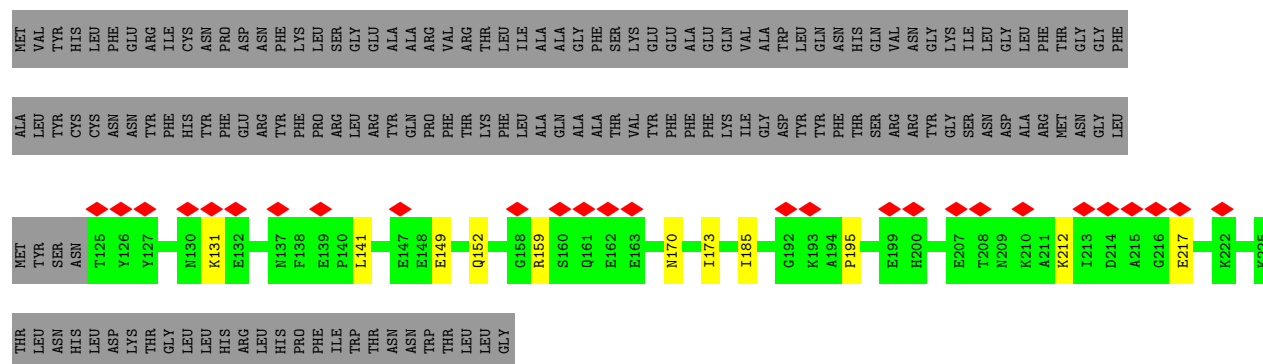


- Molecule 41: Cytochrome c oxidase subunit TT9



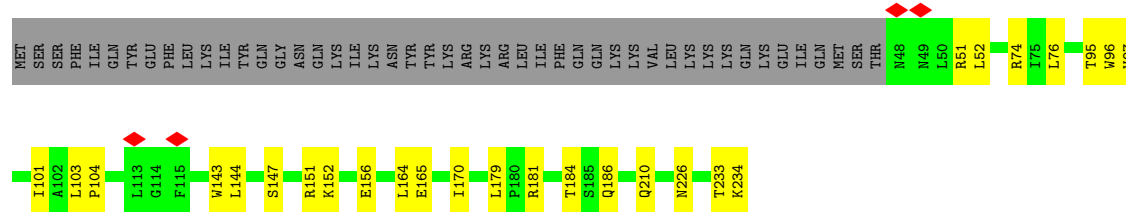
- Molecule 41: Cytochrome c oxidase subunit TT9





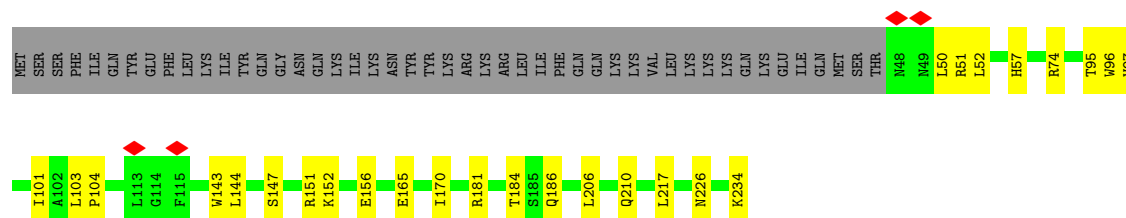
- Molecule 42: Cytochrome c oxidase subunit TT10

Chain J: 68% 12% 20%



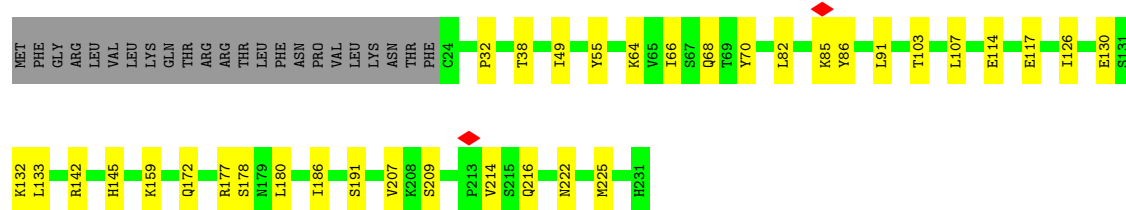
- Molecule 42: Cytochrome c oxidase subunit TT10

Chain j: 68% 12% 20%



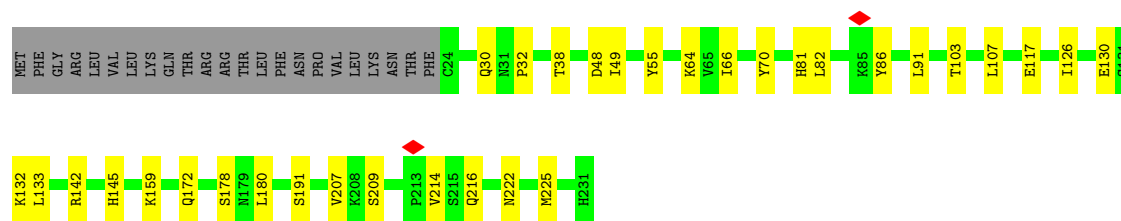
- Molecule 43: Cytochrome c oxidase subunit TT11

Chain K: 75% 15% 10%



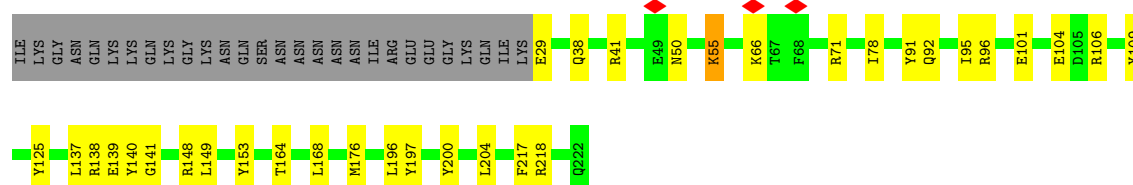
- Molecule 43: Cytochrome c oxidase subunit TT11

Chain k: 76% 14% 10%



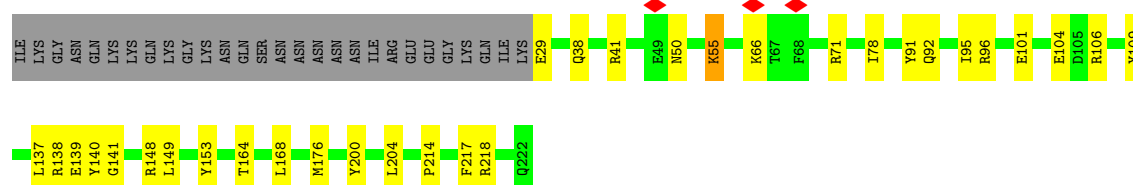
- Molecule 44: Cytochrome c oxidase subunit TT12

Chain L: 72% 15% 13%



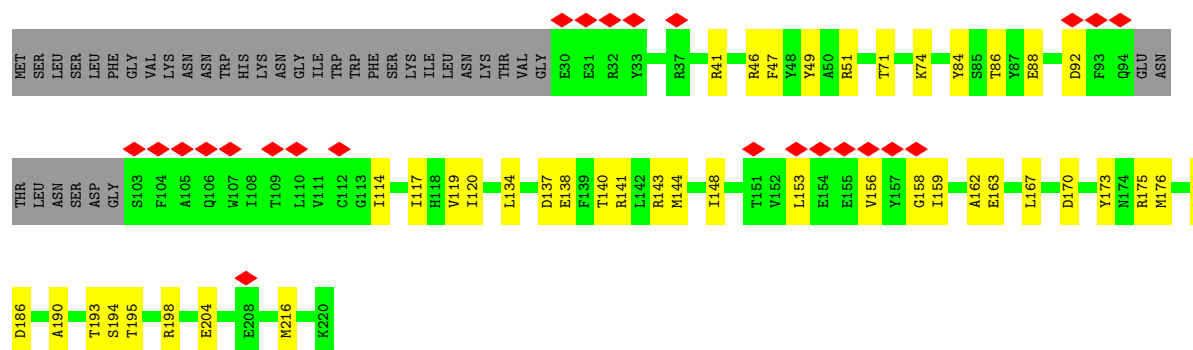
- Molecule 44: Cytochrome c oxidase subunit TT12

Chain l: 73% 14% 13%



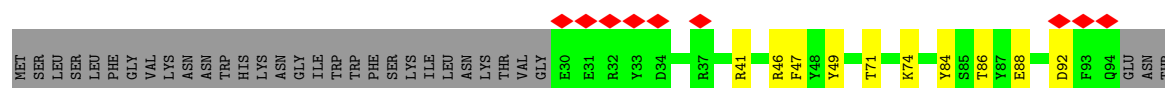
- Molecule 45: Transmembrane protein, putative

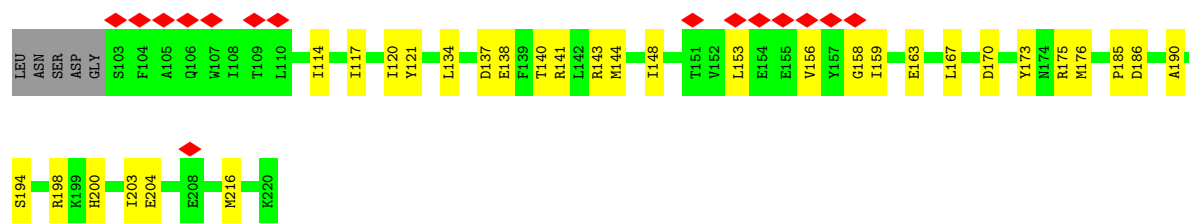
Chain M: 11% 64% 20% 17%



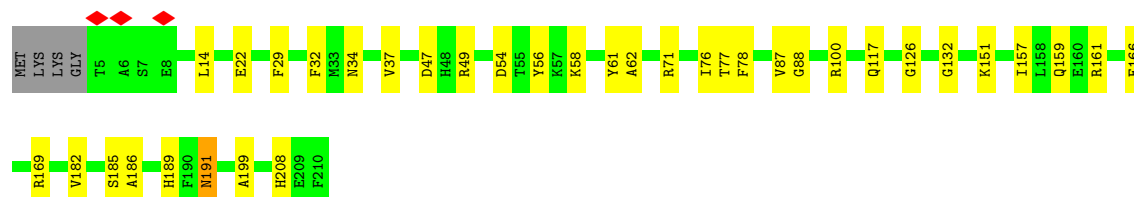
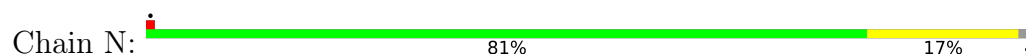
- Molecule 45: Transmembrane protein, putative

Chain m: 11% 65% 19% 17%

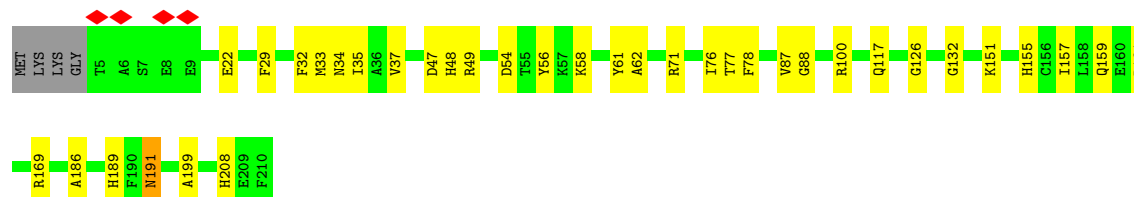
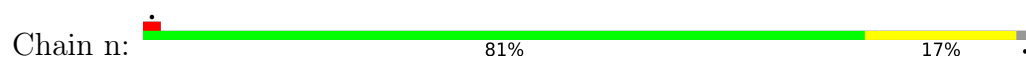




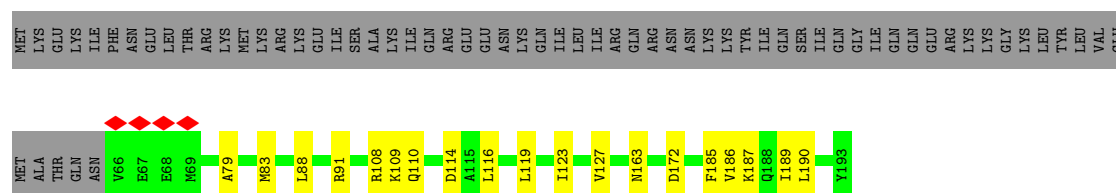
- Molecule 46: Transmembrane protein, putative



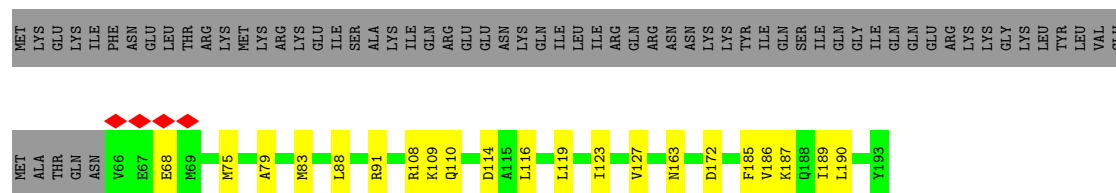
- Molecule 46: Transmembrane protein, putative



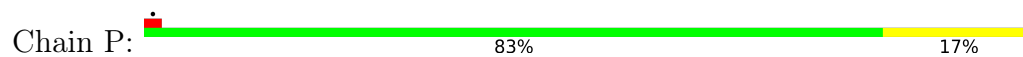
- Molecule 47: Cytochrome c oxidase subunit TT15



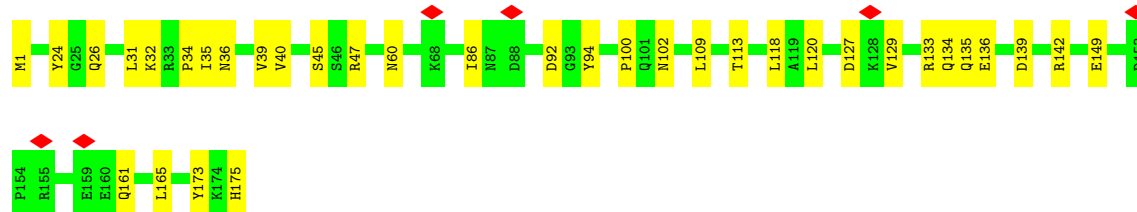
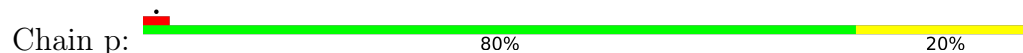
- Molecule 47: Cytochrome c oxidase subunit TT15



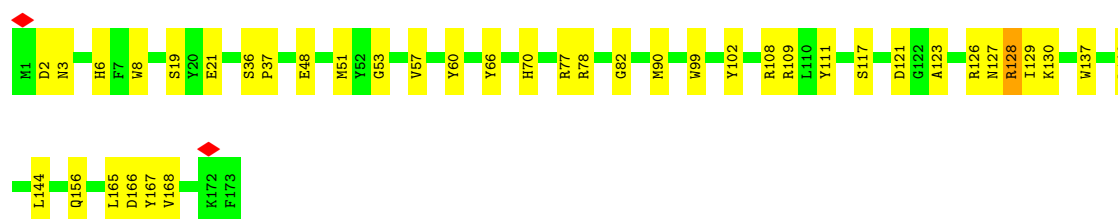
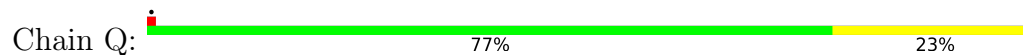
- Molecule 48: Cytochrome c oxidase subunit TT16



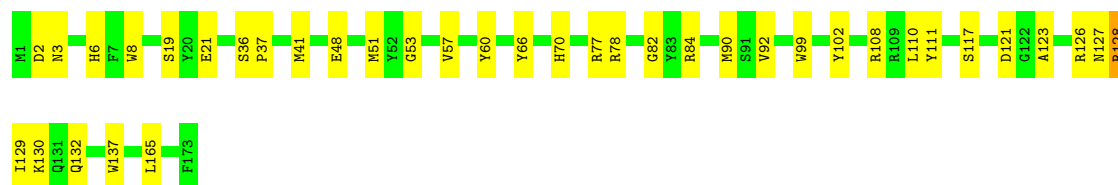
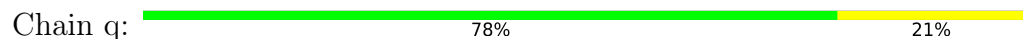
• Molecule 48: Cytochrome c oxidase subunit TT16



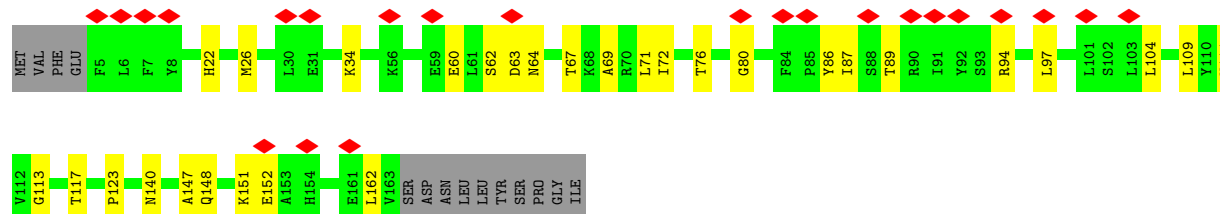
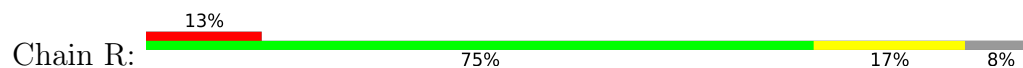
• Molecule 49: Transmembrane protein, putative



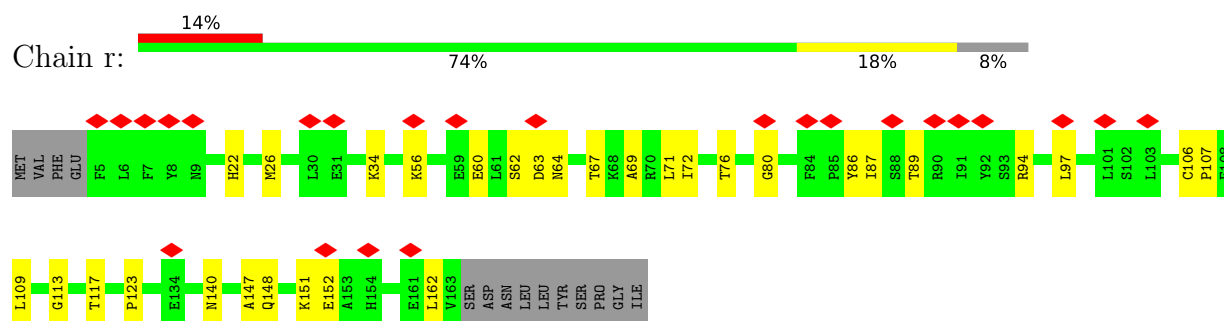
• Molecule 49: Transmembrane protein, putative



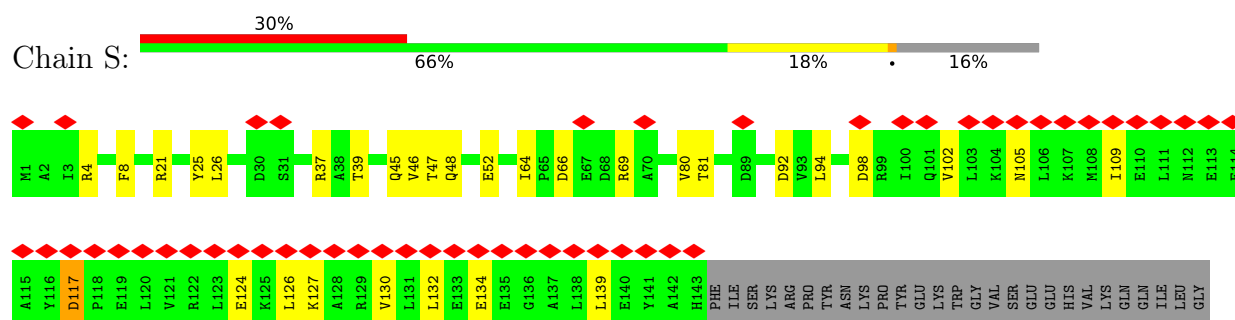
• Molecule 50: Cytochrome c oxidase subunit TT18



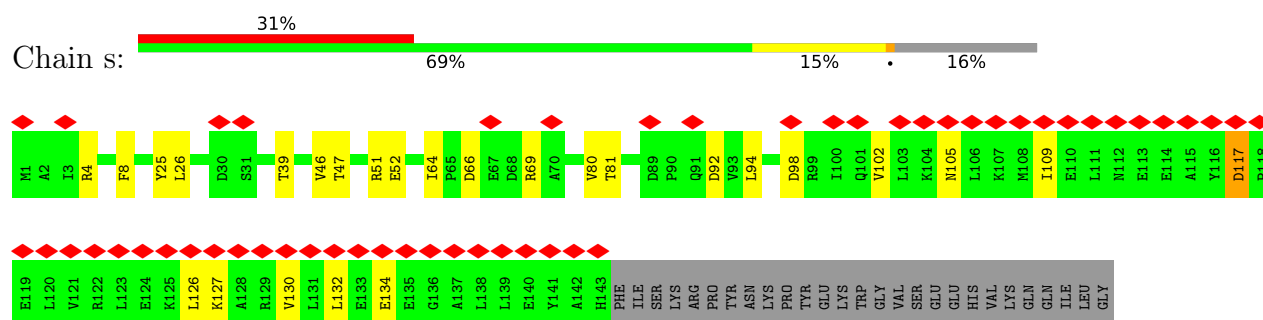
- Molecule 50: Cytochrome c oxidase subunit TT18



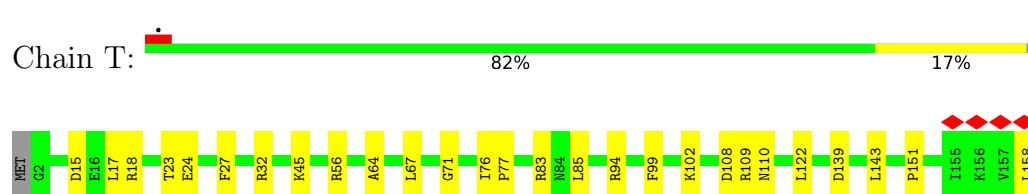
- Molecule 51: Cytochrome c oxidase subunit TT19



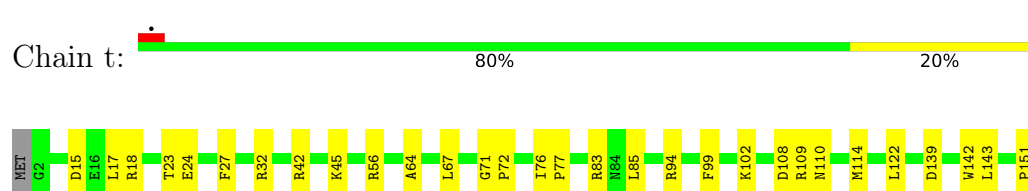
- Molecule 51: Cytochrome c oxidase subunit TT19



- Molecule 52: Transmembrane protein, putative



- Molecule 52: Transmembrane protein, putative



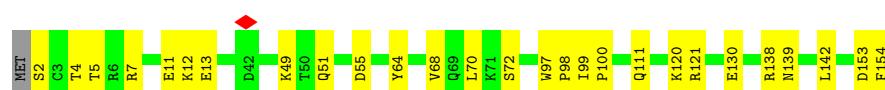
- Molecule 53: Transmembrane protein, putative

Chain U:  82% 17%



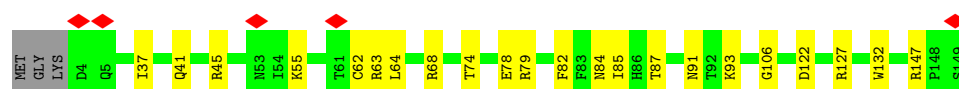
- Molecule 53: Transmembrane protein, putative

Chain u:  82% 18%



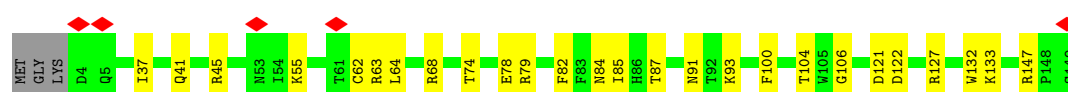
- Molecule 54: Cytochrome c oxidase subunit TT22

Chain V:  83% 15%



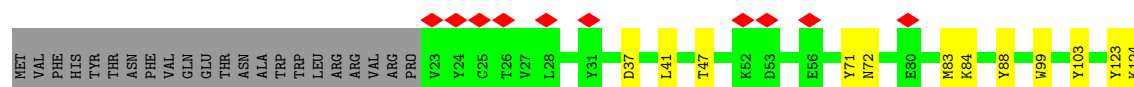
- Molecule 54: Cytochrome c oxidase subunit TT22

Chain v:  81% 17%



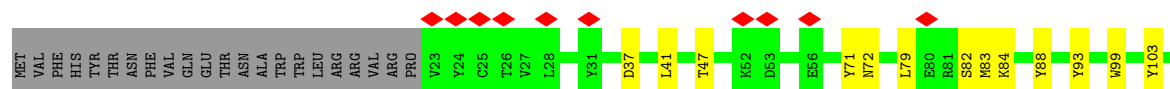
- Molecule 55: Transmembrane protein, putative

Chain W:  8% 73% 10% 18%



- Molecule 55: Transmembrane protein, putative

Chain w:  9% 70% 12% 18%



- Molecule 56: Transmembrane protein, putative

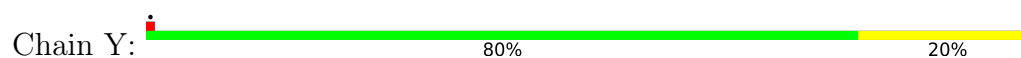
Chain X:  75% 25%



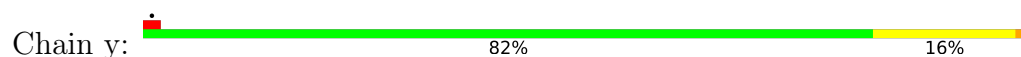
- Molecule 56: Transmembrane protein, putative



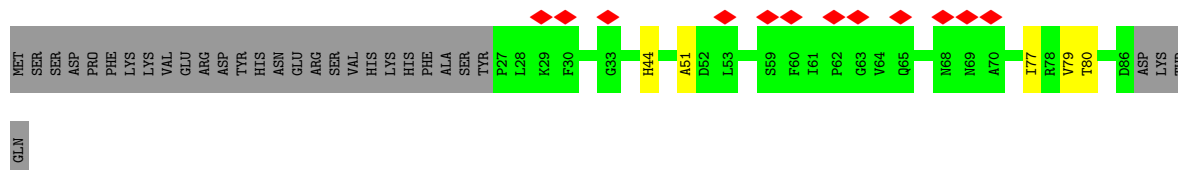
- Molecule 57: Cytochrome c oxidase subunit TT25



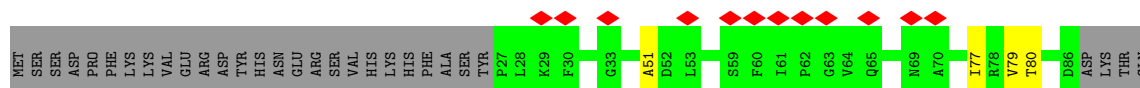
- Molecule 57: Cytochrome c oxidase subunit TT25



- Molecule 58: Cytochrome c oxidase subunit TT26



- Molecule 58: Cytochrome c oxidase subunit TT26



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	394262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	56818	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	33.161	Depositor
Minimum map value	-22.263	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	1.223	Depositor
Recommended contour level	5	Depositor
Map size ($\text{\AA}$)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CDL, CU, FES, MG, PC1, FME, SEP, HEA, TPO

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	$\# Z > 5$
2	U2	0.18	0/749	0.55	4/1031 (0.4%)
2	u2	0.17	0/749	0.55	4/1031 (0.4%)
5	U5	0.14	0/247	0.26	0/335
5	u5	0.12	0/247	0.23	0/335
6	U6	0.15	0/276	0.27	0/373
6	u6	0.14	0/276	0.27	0/373
7	C1	0.17	0/5752	0.31	0/7801
7	c1	0.17	0/5752	0.31	0/7801
8	C2	0.15	0/5027	0.30	0/6818
8	c2	0.16	0/5027	0.30	0/6818
9	C3	0.16	0/5098	0.28	0/6922
9	c3	0.16	0/5098	0.28	0/6922
10	5B	0.14	0/4706	0.23	0/6349
10	5b	0.14	0/4706	0.23	0/6349
11	6A	0.17	0/1107	0.27	0/1500
11	6a	0.16	0/1107	0.26	0/1500
12	6B	0.15	0/1968	0.26	0/2662
12	6b	0.15	0/1968	0.26	0/2662
13	6L	0.13	0/641	0.25	0/861
13	6l	0.13	0/641	0.25	0/861
14	6C	0.15	0/873	0.23	0/1184
14	6c	0.15	0/873	0.23	0/1184
15	7A	0.16	0/1198	0.26	0/1621
15	7a	0.16	0/1198	0.26	0/1621
16	7C	0.15	0/1830	0.24	0/2487
16	7c	0.15	0/1830	0.25	0/2487
17	7L	0.14	0/1099	0.27	0/1495
17	7l	0.15	0/1099	0.28	0/1495
18	M1	0.16	0/2958	0.30	0/4013
18	m1	0.16	0/2958	0.30	0/4013
19	M2	0.15	0/2621	0.26	0/3554
19	m2	0.15	0/2621	0.26	0/3554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	M3	0.14	0/2689	0.26	0/3657
20	m3	0.14	0/2689	0.27	0/3657
21	T1	0.15	0/546	0.22	0/735
21	t1	0.15	0/546	0.21	0/735
22	T2	0.12	0/518	0.23	0/694
22	t2	0.12	0/518	0.23	0/694
23	T3	0.12	0/662	0.24	0/888
23	t3	0.12	0/662	0.24	0/888
24	T4	0.16	0/483	0.29	0/652
24	t4	0.16	0/483	0.28	0/652
25	T5	0.13	0/523	0.25	0/705
25	t5	0.13	0/523	0.24	0/705
26	T6	0.14	0/565	0.26	0/760
26	t6	0.14	0/565	0.26	0/760
27	BP	0.13	0/2984	0.31	0/4047
27	bp	0.13	0/2984	0.31	0/4047
28	FS	0.14	0/1562	0.26	0/2123
28	fs	0.15	0/1562	0.26	0/2123
29	AC	0.14	0/836	0.22	0/1133
29	ac	0.14	0/836	0.23	0/1133
30	Y7	0.13	0/2968	0.23	0/4014
30	y7	0.13	0/2968	0.23	0/4014
31	Y0	0.16	0/793	0.27	0/1077
31	y0	0.16	0/793	0.27	0/1077
32	Y5	0.14	0/951	0.26	0/1284
32	y5	0.14	0/951	0.27	0/1284
33	A	0.16	0/3863	0.27	0/5258
33	a	0.16	0/3863	0.27	0/5258
34	B	0.11	0/1712	0.24	0/2318
34	b	0.11	0/1712	0.23	0/2318
35	C	0.10	0/393	0.26	0/531
35	c	0.10	0/393	0.26	0/531
36	D	0.14	0/2394	0.26	0/3254
36	d	0.14	0/2394	0.26	0/3254
37	E	0.14	0/3258	0.28	0/4425
37	e	0.14	0/3258	0.28	0/4425
38	F	0.15	0/2066	0.28	0/2809
38	f	0.15	0/2066	0.28	0/2809
39	G	0.16	0/2439	0.29	0/3328
39	g	0.16	0/2439	0.29	0/3328
40	H	0.13	0/1960	0.28	0/2656
40	h	0.13	0/1960	0.29	0/2656
41	I	0.09	0/873	0.22	0/1173

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	i	0.09	0/873	0.22	0/1173
42	J	0.14	0/1621	0.27	0/2201
42	j	0.14	0/1621	0.27	0/2201
43	K	0.15	0/1755	0.27	0/2376
43	k	0.14	0/1755	0.27	0/2376
44	L	0.12	0/1718	0.22	0/2333
44	l	0.13	0/1718	0.22	0/2333
45	M	0.14	0/1640	0.27	0/2227
45	m	0.14	0/1640	0.27	0/2227
46	N	0.14	0/1770	0.25	0/2391
46	n	0.14	0/1770	0.25	0/2391
47	O	0.14	0/1090	0.22	0/1466
47	o	0.14	0/1090	0.22	0/1466
48	P	0.13	0/1428	0.25	0/1931
48	p	0.13	0/1428	0.24	0/1931
49	Q	0.17	0/1478	0.31	0/2005
49	q	0.17	0/1478	0.30	0/2005
50	R	0.10	0/1336	0.22	0/1808
50	r	0.10	0/1336	0.22	0/1808
51	S	0.13	0/1178	0.25	0/1588
51	s	0.13	0/1178	0.25	0/1588
52	T	0.16	0/1367	0.29	0/1853
52	t	0.16	0/1367	0.30	0/1853
53	U	0.14	0/1335	0.25	0/1794
53	u	0.15	0/1335	0.25	0/1794
54	V	0.15	0/1277	0.25	0/1735
54	v	0.15	0/1277	0.25	0/1735
55	W	0.12	0/933	0.23	0/1266
55	w	0.12	0/933	0.23	0/1266
56	X	0.16	0/1043	0.25	0/1413
56	x	0.16	0/1043	0.25	0/1413
57	Y	0.15	0/882	0.23	0/1192
57	y	0.15	0/882	0.23	0/1192
58	Z	0.08	0/491	0.19	0/664
58	z	0.09	0/491	0.19	0/664
All	All	0.15	0/187060	0.27	8/253540 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U2	171	PRO	N-CA-CB	7.90	110.34	103.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	u2	171	PRO	N-CA-CB	7.90	110.34	103.31
2	U2	193	PRO	N-CA-CB	6.20	110.15	103.33
2	u2	246	PRO	N-CA-CB	6.17	110.12	103.33
2	U2	240	PRO	N-CA-CB	6.17	110.12	103.33

There are no chirality outliers.

There are no planarity outliers.

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	U1	490	0	102	1	0
1	u1	490	0	103	1	0
2	U2	743	0	482	9	0
2	u2	743	0	482	11	0
3	U3	170	0	36	0	0
3	u3	170	0	36	0	0
4	U4	150	0	32	0	0
4	u4	150	0	32	0	0
5	U5	242	0	206	7	0
5	u5	242	0	206	7	0
6	U6	275	0	258	5	0
6	u6	275	0	258	5	0
7	C1	5563	0	5607	131	0
7	c1	5563	0	5607	126	0
8	C2	4883	0	4861	81	0
8	c2	4883	0	4861	85	0
9	C3	4930	0	4914	94	0
9	c3	4930	0	4914	94	0
10	5B	4624	0	4401	83	0
10	5b	4624	0	4401	80	0
11	6A	1074	0	1014	21	0
11	6a	1074	0	1014	20	0
12	6B	1904	0	1764	32	0
12	6b	1904	0	1764	32	0
13	6L	638	0	638	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	6l	638	0	638	6	0
14	6C	841	0	763	17	0
14	6c	841	0	763	16	0
15	7A	1168	0	1128	33	0
15	7a	1168	0	1128	33	0
16	7C	1789	0	1606	25	0
16	7c	1789	0	1606	28	0
17	7L	1070	0	1062	25	0
17	7l	1070	0	1062	30	0
18	M1	2863	0	2781	46	0
18	m1	2863	0	2781	43	0
19	M2	2560	0	2551	27	0
19	m2	2560	0	2551	26	0
20	M3	2620	0	2584	35	0
20	m3	2620	0	2584	36	0
21	T1	540	0	532	7	0
21	t1	540	0	532	8	0
22	T2	513	0	512	9	0
22	t2	513	0	512	11	0
23	T3	655	0	669	4	0
23	t3	655	0	669	6	0
24	T4	483	0	464	9	0
24	t4	483	0	464	12	0
25	T5	515	0	510	7	0
25	t5	515	0	510	8	0
26	T6	563	0	563	10	0
26	t6	563	0	563	10	0
27	BP	2916	0	2814	46	0
27	bp	2916	0	2814	44	0
28	FS	1509	0	1477	24	0
28	fs	1509	0	1477	25	0
29	AC	816	0	795	9	0
29	ac	816	0	795	8	0
30	Y7	2895	0	2953	51	0
30	y7	2895	0	2953	57	0
31	Y0	777	0	797	14	0
31	y0	777	0	797	12	0
32	Y5	924	0	968	15	0
32	y5	924	0	968	14	0
33	A	3746	0	3550	46	0
33	a	3746	0	3550	52	0
34	B	1682	0	1730	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	b	1682	0	1730	19	0
35	C	383	0	396	8	0
35	c	383	0	396	7	0
36	D	2331	0	2265	22	0
36	d	2331	0	2265	24	0
37	E	3178	0	3107	56	0
37	e	3178	0	3107	52	0
38	F	2014	0	1951	43	0
38	f	2014	0	1951	40	0
39	G	2364	0	2216	48	0
39	g	2364	0	2216	45	0
40	H	1915	0	1845	32	0
40	h	1915	0	1845	34	0
41	I	852	0	816	10	0
41	i	852	0	816	9	0
42	J	1575	0	1567	22	0
42	j	1575	0	1567	23	0
43	K	1714	0	1678	24	0
43	k	1714	0	1678	24	0
44	L	1668	0	1643	24	0
44	l	1668	0	1643	22	0
45	M	1581	0	1476	36	0
45	m	1581	0	1476	34	0
46	N	1716	0	1648	30	0
46	n	1716	0	1648	30	0
47	O	1073	0	1047	16	0
47	o	1073	0	1047	17	0
48	P	1412	0	1390	17	0
48	p	1412	0	1390	21	0
49	Q	1434	0	1393	27	0
49	q	1434	0	1393	29	0
50	R	1305	0	1323	28	0
50	r	1305	0	1323	28	0
51	S	1165	0	1189	24	0
51	s	1165	0	1189	22	0
52	T	1323	0	1297	25	0
52	t	1323	0	1297	29	0
53	U	1304	0	1299	19	0
53	u	1304	0	1299	21	0
54	V	1234	0	1194	21	0
54	v	1234	0	1194	24	0
55	W	902	0	848	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	w	902	0	848	11	0
56	X	1012	0	1000	23	0
56	x	1012	0	1000	23	0
57	Y	859	0	812	17	0
57	y	859	0	812	14	0
58	Z	479	0	475	4	0
58	z	479	0	475	3	0
59	C1	120	0	108	9	0
59	c1	120	0	108	7	0
60	C1	1	0	0	0	0
60	C2	2	0	0	0	0
60	c1	1	0	0	0	0
60	c2	2	0	0	0	0
61	C1	1	0	0	0	0
61	c1	1	0	0	0	0
62	7C	97	0	151	12	0
62	7c	43	0	63	5	0
62	A	86	0	120	4	0
62	C1	49	0	72	4	0
62	C3	163	0	225	6	0
62	J	37	0	48	0	0
62	M1	35	0	44	0	0
62	M2	127	0	182	8	0
62	N	68	0	84	3	0
62	V	54	0	88	3	0
62	a	86	0	120	5	0
62	c1	49	0	72	4	0
62	c3	163	0	225	6	0
62	j	37	0	48	0	0
62	m1	89	0	132	9	0
62	m2	127	0	182	7	0
62	n	68	0	84	4	0
62	v	54	0	88	3	0
63	5B	216	0	276	14	0
63	5b	154	0	205	9	0
63	7A	167	0	234	11	0
63	7C	136	0	166	9	0
63	7a	167	0	234	14	0
63	7c	136	0	166	9	0
63	A	51	0	46	0	0
63	B	62	0	68	0	0
63	C1	124	0	136	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C3	68	0	80	0	0
63	E	132	0	158	7	0
63	F	100	0	156	12	0
63	J	70	0	84	6	0
63	L	74	0	95	3	0
63	M1	227	0	295	16	0
63	M2	194	0	220	9	0
63	M3	208	0	254	9	0
63	N	95	0	143	7	0
63	T	143	0	177	7	0
63	U	82	0	111	4	0
63	V	91	0	132	3	0
63	Y0	64	0	72	4	0
63	Y5	81	0	109	2	0
63	Y7	65	0	74	1	0
63	a	51	0	46	0	0
63	b	62	0	68	0	0
63	c1	124	0	136	6	0
63	c3	68	0	80	0	0
63	e	132	0	158	9	0
63	f	100	0	156	9	0
63	j	70	0	84	7	0
63	k	62	0	71	3	0
63	l	74	0	95	2	0
63	m1	227	0	295	15	0
63	m2	194	0	220	11	0
63	m3	208	0	254	12	0
63	n	95	0	143	9	0
63	t	143	0	177	7	0
63	u	82	0	111	4	0
63	v	91	0	132	3	0
63	y0	64	0	72	3	0
63	y5	81	0	109	1	0
63	y7	65	0	74	1	0
64	5B	1	0	0	0	0
64	5b	1	0	0	0	0
64	M	1	0	0	0	0
64	m	1	0	0	0	0
65	FS	8	0	0	0	0
65	fs	8	0	0	0	0
All	All	190448	0	186415	2493	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 7.

The worst 5 of 2493 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)
34:b:291:PHE:HB3	34:b:357:LEU:HB3	1.61	0.83
34:B:291:PHE:HB3	34:B:357:LEU:HB3	1.62	0.81
17:7L:936:TYR:HB3	17:7L:939:MET:HB2	1.61	0.81
17:7l:936:TYR:HB3	17:7l:939:MET:HB2	1.61	0.80
13:6l:49:PHE:HB2	14:6c:75:GLU:HG3	1.64	0.79

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	
2	U2	125/3634 (3%)	115 (92%)	9 (7%)	1 (1%)	16	48
2	u2	125/3634 (3%)	114 (91%)	10 (8%)	1 (1%)	16	48
5	U5	31/172 (18%)	31 (100%)	0	0	100	100
5	u5	31/172 (18%)	31 (100%)	0	0	100	100
6	U6	40/478 (8%)	39 (98%)	1 (2%)	0	100	100
6	u6	40/478 (8%)	39 (98%)	1 (2%)	0	100	100
7	C1	670/688 (97%)	638 (95%)	32 (5%)	0	100	100
7	c1	670/688 (97%)	638 (95%)	32 (5%)	0	100	100
8	C2	572/604 (95%)	547 (96%)	25 (4%)	0	100	100
8	c2	572/604 (95%)	547 (96%)	25 (4%)	0	100	100
9	C3	557/594 (94%)	542 (97%)	15 (3%)	0	100	100
9	c3	557/594 (94%)	543 (98%)	14 (2%)	0	100	100
10	5B	550/637 (86%)	539 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	5b	550/637 (86%)	540 (98%)	10 (2%)	0	100	100
11	6A	123/130 (95%)	117 (95%)	6 (5%)	0	100	100
11	6a	123/130 (95%)	117 (95%)	6 (5%)	0	100	100
12	6B	219/230 (95%)	215 (98%)	4 (2%)	0	100	100
12	6b	219/230 (95%)	216 (99%)	3 (1%)	0	100	100
13	6L	75/88 (85%)	75 (100%)	0	0	100	100
13	6l	75/88 (85%)	75 (100%)	0	0	100	100
14	6C	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
14	6c	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
15	7A	131/133 (98%)	124 (95%)	7 (5%)	0	100	100
15	7a	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
16	7C	203/236 (86%)	198 (98%)	5 (2%)	0	100	100
16	7c	203/236 (86%)	198 (98%)	5 (2%)	0	100	100
17	7L	128/990 (13%)	120 (94%)	8 (6%)	0	100	100
17	7l	128/990 (13%)	120 (94%)	8 (6%)	0	100	100
18	M1	344/346 (99%)	330 (96%)	14 (4%)	0	100	100
18	m1	344/346 (99%)	330 (96%)	14 (4%)	0	100	100
19	M2	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
19	m2	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
20	M3	327/330 (99%)	312 (95%)	15 (5%)	0	100	100
20	m3	327/330 (99%)	313 (96%)	14 (4%)	0	100	100
21	T1	68/72 (94%)	68 (100%)	0	0	100	100
21	t1	68/72 (94%)	68 (100%)	0	0	100	100
22	T2	61/72 (85%)	61 (100%)	0	0	100	100
22	t2	61/72 (85%)	61 (100%)	0	0	100	100
23	T3	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
23	t3	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
24	T4	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
24	t4	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
25	T5	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
25	t5	61/81 (75%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	T6	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
26	t6	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
27	BP	378/380 (100%)	361 (96%)	17 (4%)	0	100	100
27	bp	378/380 (100%)	359 (95%)	19 (5%)	0	100	100
28	FS	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
28	fs	186/188 (99%)	178 (96%)	8 (4%)	0	100	100
29	AC	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
29	ac	98/127 (77%)	98 (100%)	0	0	100	100
30	Y7	332/453 (73%)	326 (98%)	6 (2%)	0	100	100
30	y7	332/453 (73%)	325 (98%)	7 (2%)	0	100	100
31	Y0	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
31	y0	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
32	Y5	102/190 (54%)	99 (97%)	3 (3%)	0	100	100
32	y5	102/190 (54%)	99 (97%)	3 (3%)	0	100	100
33	A	446/490 (91%)	431 (97%)	15 (3%)	0	100	100
33	a	446/490 (91%)	432 (97%)	14 (3%)	0	100	100
34	B	212/473 (45%)	203 (96%)	9 (4%)	0	100	100
34	b	212/473 (45%)	203 (96%)	9 (4%)	0	100	100
35	C	44/1471 (3%)	43 (98%)	1 (2%)	0	100	100
35	c	44/1471 (3%)	43 (98%)	1 (2%)	0	100	100
36	D	280/402 (70%)	275 (98%)	5 (2%)	0	100	100
36	d	280/402 (70%)	275 (98%)	5 (2%)	0	100	100
37	E	382/385 (99%)	361 (94%)	21 (6%)	0	100	100
37	e	382/385 (99%)	361 (94%)	21 (6%)	0	100	100
38	F	240/348 (69%)	232 (97%)	8 (3%)	0	100	100
38	f	240/348 (69%)	233 (97%)	7 (3%)	0	100	100
39	G	279/318 (88%)	270 (97%)	9 (3%)	0	100	100
39	g	279/318 (88%)	271 (97%)	8 (3%)	0	100	100
40	H	237/318 (74%)	233 (98%)	4 (2%)	0	100	100
40	h	237/318 (74%)	234 (99%)	3 (1%)	0	100	100
41	I	99/252 (39%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	i	99/252 (39%)	98 (99%)	1 (1%)	0	100	100
42	J	185/234 (79%)	182 (98%)	3 (2%)	0	100	100
42	j	185/234 (79%)	182 (98%)	3 (2%)	0	100	100
43	K	206/231 (89%)	194 (94%)	12 (6%)	0	100	100
43	k	206/231 (89%)	195 (95%)	11 (5%)	0	100	100
44	L	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
44	l	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
45	M	179/220 (81%)	176 (98%)	3 (2%)	0	100	100
45	m	179/220 (81%)	176 (98%)	3 (2%)	0	100	100
46	N	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
46	n	204/210 (97%)	198 (97%)	6 (3%)	0	100	100
47	O	126/193 (65%)	125 (99%)	1 (1%)	0	100	100
47	o	126/193 (65%)	126 (100%)	0	0	100	100
48	P	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
48	p	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
49	Q	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
49	q	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
50	R	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
50	r	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
51	S	141/170 (83%)	137 (97%)	4 (3%)	0	100	100
51	s	141/170 (83%)	137 (97%)	4 (3%)	0	100	100
52	T	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
52	t	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
53	U	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
53	u	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
54	V	144/149 (97%)	139 (96%)	5 (4%)	0	100	100
54	v	144/149 (97%)	139 (96%)	5 (4%)	0	100	100
55	W	100/124 (81%)	99 (99%)	1 (1%)	0	100	100
55	w	100/124 (81%)	100 (100%)	0	0	100	100
56	X	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
56	x	120/122 (98%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	Y	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
57	y	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
58	Z	58/90 (64%)	58 (100%)	0	0	100	100
58	z	58/90 (64%)	58 (100%)	0	0	100	100
All	All	21730/37912 (57%)	21056 (97%)	672 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U2	175	ILE
2	u2	175	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U2	35/3358 (1%)	35 (100%)	0	100	100
2	u2	35/3358 (1%)	35 (100%)	0	100	100
5	U5	19/169 (11%)	19 (100%)	0	100	100
5	u5	19/169 (11%)	19 (100%)	0	100	100
6	U6	24/419 (6%)	23 (96%)	1 (4%)	26	59
6	u6	24/419 (6%)	23 (96%)	1 (4%)	26	59
7	C1	597/613 (97%)	590 (99%)	7 (1%)	63	81
7	c1	597/613 (97%)	590 (99%)	7 (1%)	63	81
8	C2	542/569 (95%)	534 (98%)	8 (2%)	57	79
8	c2	542/569 (95%)	534 (98%)	8 (2%)	57	79
9	C3	534/565 (94%)	529 (99%)	5 (1%)	70	84
9	c3	534/565 (94%)	529 (99%)	5 (1%)	70	84
10	5B	502/579 (87%)	498 (99%)	4 (1%)	73	85
10	5b	502/579 (87%)	498 (99%)	4 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	6A	113/116 (97%)	113 (100%)	0	100	100
11	6a	113/116 (97%)	113 (100%)	0	100	100
12	6B	199/207 (96%)	196 (98%)	3 (2%)	57	79
12	6b	199/207 (96%)	197 (99%)	2 (1%)	68	83
13	6L	71/80 (89%)	70 (99%)	1 (1%)	59	79
13	6l	71/80 (89%)	70 (99%)	1 (1%)	59	79
14	6C	81/88 (92%)	80 (99%)	1 (1%)	63	81
14	6c	81/88 (92%)	81 (100%)	0	100	100
15	7A	119/119 (100%)	119 (100%)	0	100	100
15	7a	119/119 (100%)	118 (99%)	1 (1%)	73	85
16	7C	193/217 (89%)	190 (98%)	3 (2%)	55	78
16	7c	193/217 (89%)	191 (99%)	2 (1%)	68	83
17	7L	121/943 (13%)	120 (99%)	1 (1%)	73	85
17	7l	121/943 (13%)	120 (99%)	1 (1%)	73	85
18	M1	294/294 (100%)	292 (99%)	2 (1%)	76	85
18	m1	294/294 (100%)	292 (99%)	2 (1%)	76	85
19	M2	259/259 (100%)	255 (98%)	4 (2%)	57	79
19	m2	259/259 (100%)	256 (99%)	3 (1%)	63	81
20	M3	275/276 (100%)	274 (100%)	1 (0%)	84	89
20	m3	275/276 (100%)	273 (99%)	2 (1%)	76	85
21	T1	61/63 (97%)	61 (100%)	0	100	100
21	t1	61/63 (97%)	61 (100%)	0	100	100
22	T2	58/67 (87%)	58 (100%)	0	100	100
22	t2	58/67 (87%)	58 (100%)	0	100	100
23	T3	76/83 (92%)	76 (100%)	0	100	100
23	t3	76/83 (92%)	76 (100%)	0	100	100
24	T4	53/62 (86%)	53 (100%)	0	100	100
24	t4	53/62 (86%)	53 (100%)	0	100	100
25	T5	57/66 (86%)	57 (100%)	0	100	100
25	t5	57/66 (86%)	57 (100%)	0	100	100
26	T6	61/62 (98%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	t6	61/62 (98%)	61 (100%)	0	100	100
27	BP	308/308 (100%)	307 (100%)	1 (0%)	86	90
27	bp	308/308 (100%)	307 (100%)	1 (0%)	86	90
28	FS	164/164 (100%)	163 (99%)	1 (1%)	78	87
28	fs	164/164 (100%)	162 (99%)	2 (1%)	63	81
29	AC	87/113 (77%)	87 (100%)	0	100	100
29	ac	87/113 (77%)	87 (100%)	0	100	100
30	Y7	328/442 (74%)	325 (99%)	3 (1%)	70	84
30	y7	328/442 (74%)	324 (99%)	4 (1%)	63	81
31	Y0	83/83 (100%)	83 (100%)	0	100	100
31	y0	83/83 (100%)	83 (100%)	0	100	100
32	Y5	101/185 (55%)	99 (98%)	2 (2%)	48	75
32	y5	101/185 (55%)	100 (99%)	1 (1%)	68	83
33	A	409/447 (92%)	407 (100%)	2 (0%)	81	88
33	a	409/447 (92%)	406 (99%)	3 (1%)	76	85
34	B	182/413 (44%)	182 (100%)	0	100	100
34	b	182/413 (44%)	182 (100%)	0	100	100
35	C	44/1405 (3%)	40 (91%)	4 (9%)	9	32
35	c	44/1405 (3%)	40 (91%)	4 (9%)	9	32
36	D	250/358 (70%)	247 (99%)	3 (1%)	63	81
36	d	250/358 (70%)	248 (99%)	2 (1%)	73	85
37	E	341/342 (100%)	338 (99%)	3 (1%)	70	84
37	e	341/342 (100%)	338 (99%)	3 (1%)	70	84
38	F	218/318 (69%)	218 (100%)	0	100	100
38	f	218/318 (69%)	218 (100%)	0	100	100
39	G	260/289 (90%)	257 (99%)	3 (1%)	63	81
39	g	260/289 (90%)	256 (98%)	4 (2%)	57	79
40	H	209/272 (77%)	208 (100%)	1 (0%)	81	88
40	h	209/272 (77%)	207 (99%)	2 (1%)	68	83
41	I	90/219 (41%)	90 (100%)	0	100	100
41	i	90/219 (41%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	J	170/216 (79%)	170 (100%)	0	100	100
42	j	170/216 (79%)	170 (100%)	0	100	100
43	K	191/213 (90%)	190 (100%)	1 (0%)	81	88
43	k	191/213 (90%)	191 (100%)	0	100	100
44	L	181/206 (88%)	180 (99%)	1 (1%)	78	87
44	l	181/206 (88%)	180 (99%)	1 (1%)	78	87
45	M	166/199 (83%)	165 (99%)	1 (1%)	78	87
45	m	166/199 (83%)	165 (99%)	1 (1%)	78	87
46	N	178/181 (98%)	175 (98%)	3 (2%)	53	77
46	n	178/181 (98%)	175 (98%)	3 (2%)	53	77
47	O	119/180 (66%)	118 (99%)	1 (1%)	73	85
47	o	119/180 (66%)	117 (98%)	2 (2%)	53	77
48	P	156/156 (100%)	156 (100%)	0	100	100
48	p	156/156 (100%)	156 (100%)	0	100	100
49	Q	157/157 (100%)	155 (99%)	2 (1%)	61	80
49	q	157/157 (100%)	155 (99%)	2 (1%)	61	80
50	R	144/157 (92%)	144 (100%)	0	100	100
50	r	144/157 (92%)	144 (100%)	0	100	100
51	S	129/154 (84%)	128 (99%)	1 (1%)	73	85
51	s	129/154 (84%)	128 (99%)	1 (1%)	73	85
52	T	138/139 (99%)	138 (100%)	0	100	100
52	t	138/139 (99%)	138 (100%)	0	100	100
53	U	137/138 (99%)	137 (100%)	0	100	100
53	u	137/138 (99%)	137 (100%)	0	100	100
54	V	133/135 (98%)	133 (100%)	0	100	100
54	v	133/135 (98%)	133 (100%)	0	100	100
55	W	92/113 (81%)	91 (99%)	1 (1%)	65	82
55	w	92/113 (81%)	91 (99%)	1 (1%)	65	82
56	X	105/105 (100%)	104 (99%)	1 (1%)	68	83
56	x	105/105 (100%)	104 (99%)	1 (1%)	68	83
57	Y	88/88 (100%)	87 (99%)	1 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	y	88/88 (100%)	85 (97%)	3 (3%)	32	64
58	Z	51/80 (64%)	51 (100%)	0	100	100
58	z	51/80 (64%)	51 (100%)	0	100	100
All	All	19506/34498 (56%)	19349 (99%)	157 (1%)	70	85

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	m3	77	ASP
47	o	68	GLU
30	y7	106	LYS
37	e	115	ASP
57	y	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 203 such sidechains are listed below:

Mol	Chain	Res	Type
8	c2	146	ASN
21	t1	18	ASN
54	v	141	GLN
9	c3	130	HIS
12	6b	163	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	FME	7a	1	15	8,9,10	0.98	0	8,9,11	0.87	0
15	FME	7A	1	15	8,9,10	0.99	0	8,9,11	0.87	0
26	FME	T6	1	26	8,9,10	0.97	0	8,9,11	0.81	0
10	SEP	5B	520	10	8,9,10	1.58	1 (12%)	7,12,14	1.25	1 (14%)
16	SEP	7c	197	16	8,9,10	1.57	1 (12%)	7,12,14	1.81	1 (14%)
16	SEP	7C	120	16	8,9,10	1.55	1 (12%)	7,12,14	1.33	1 (14%)
19	FME	m2	1	19	8,9,10	0.98	0	8,9,11	0.95	0
37	FME	E	1	37	8,9,10	0.98	0	8,9,11	0.95	0
48	FME	P	1	48	8,9,10	0.96	0	8,9,11	1.01	0
31	FME	y0	1	31	8,9,10	0.98	0	8,9,11	0.87	0
19	FME	M2	1	19	8,9,10	0.98	0	8,9,11	0.99	0
10	TPO	5b	387	10	8,10,11	1.60	1 (12%)	10,14,16	2.11	1 (10%)
48	FME	p	1	48	8,9,10	0.95	0	8,9,11	1.03	0
31	FME	Y0	1	31	8,9,10	1.00	0	8,9,11	0.86	0
10	TPO	5B	387	10	8,10,11	1.06	0	10,14,16	2.09	1 (10%)
13	FME	6L	1	13	8,9,10	0.99	0	8,9,11	0.91	0
24	FME	T4	1	24	8,9,10	0.96	0	8,9,11	0.87	0
10	SEP	5b	520	10	8,9,10	1.59	1 (12%)	7,12,14	1.26	1 (14%)
26	FME	t6	1	26	8,9,10	0.97	0	8,9,11	0.79	0
13	FME	6l	1	13	8,9,10	0.97	0	8,9,11	0.93	0
37	FME	e	1	37	8,9,10	0.98	0	8,9,11	0.96	0
24	FME	t4	1	24	8,9,10	0.96	0	8,9,11	0.89	0
16	SEP	7C	197	16	8,9,10	1.59	1 (12%)	7,12,14	1.85	1 (14%)
16	SEP	7c	120	16	8,9,10	1.56	1 (12%)	7,12,14	1.25	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	7a	1	15	-	4/7/9/11	-
15	FME	7A	1	15	-	4/7/9/11	-
26	FME	T6	1	26	-	5/7/9/11	-
10	SEP	5B	520	10	-	3/6/8/10	-
16	SEP	7c	197	16	-	0/6/8/10	-
16	SEP	7C	120	16	-	0/6/8/10	-
19	FME	m2	1	19	-	4/7/9/11	-
37	FME	E	1	37	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FME	P	1	48	-	3/7/9/11	-
31	FME	y0	1	31	-	5/7/9/11	-
19	FME	M2	1	19	-	4/7/9/11	-
10	TPO	5b	387	10	-	1/9/11/13	-
48	FME	p	1	48	-	3/7/9/11	-
31	FME	Y0	1	31	-	5/7/9/11	-
10	TPO	5B	387	10	-	1/9/11/13	-
13	FME	6L	1	13	-	5/7/9/11	-
24	FME	T4	1	24	-	4/7/9/11	-
10	SEP	5b	520	10	-	3/6/8/10	-
26	FME	t6	1	26	-	5/7/9/11	-
13	FME	6l	1	13	-	6/7/9/11	-
37	FME	e	1	37	-	5/7/9/11	-
24	FME	t4	1	24	-	4/7/9/11	-
16	SEP	7C	197	16	-	2/6/8/10	-
16	SEP	7c	120	16	-	0/6/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7C	197	SEP	P-O1P	3.49	1.61	1.50
10	5b	520	SEP	P-O1P	3.47	1.61	1.50
10	5B	520	SEP	P-O1P	3.46	1.61	1.50
16	7c	120	SEP	P-O1P	3.43	1.61	1.50
10	5b	387	TPO	P-O1P	3.41	1.61	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5b	387	TPO	P-OG1-CB	-6.12	106.70	123.33
10	5B	387	TPO	P-OG1-CB	-6.02	106.97	123.33
16	7C	197	SEP	OG-CB-CA	4.32	112.35	108.14
16	7c	197	SEP	OG-CB-CA	4.18	112.21	108.14
16	7C	120	SEP	OG-CB-CA	2.99	111.05	108.14

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	5B	387	TPO	O-C-CA-CB
10	5B	520	SEP	CB-OG-P-O1P
10	5B	520	SEP	CB-OG-P-O2P
10	5B	520	SEP	CB-OG-P-O3P
13	6L	1	FME	O1-CN-N-CA

There are no ring outliers.

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	T6	1	FME	2	0
10	5B	520	SEP	2	0
16	7C	120	SEP	2	0
31	y0	1	FME	1	0
10	5b	387	TPO	1	0
48	p	1	FME	1	0
31	Y0	1	FME	1	0
10	5B	387	TPO	1	0
24	T4	1	FME	1	0
10	5b	520	SEP	2	0
26	t6	1	FME	2	0
13	6l	1	FME	1	0
37	e	1	FME	1	0
24	t4	1	FME	1	0
16	7c	120	SEP	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 122 ligands modelled in this entry, 12 are monoatomic - leaving 110 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
63	CDL	m3	401	-	93,93,99	0.30	0	99,105,111	0.33	0
62	PC1	C3	601	-	51,51,53	0.29	0	57,59,61	0.38	0
63	CDL	e	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	7C	303	-	50,50,99	0.41	0	56,62,111	0.35	0
65	FES	fs	201	28	0,4,4	-	-	-		
62	PC1	M2	405	-	40,40,53	0.33	0	46,48,61	0.34	0
63	CDL	y7	501	-	64,64,99	0.37	0	70,76,111	0.37	0
65	FES	fs	202	28	0,4,4	-	-	-		
63	CDL	t	201	-	67,67,99	0.36	0	73,79,111	0.35	0
59	HEA	c1	702	7	67,67,67	1.23	10 (14%)	81,103,103	1.53	16 (19%)
63	CDL	M3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
62	PC1	c3	602	-	38,38,53	0.33	0	44,46,61	0.34	0
63	CDL	M2	401	-	53,53,99	0.40	0	59,65,111	0.39	0
63	CDL	A	503	-	50,50,99	0.41	0	56,62,111	0.50	0
62	PC1	v	202	-	53,53,53	0.29	0	59,61,61	0.33	0
62	PC1	j	302	-	36,36,53	0.34	0	42,44,61	0.33	0
63	CDL	m2	404	-	73,73,99	0.34	0	79,85,111	0.35	0
63	CDL	7A	202	-	99,99,99	0.30	0	105,111,111	0.29	0
63	CDL	7C	301	-	84,84,99	0.32	0	90,96,111	0.34	0
63	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.32	0
62	PC1	A	501	-	44,44,53	0.31	0	50,52,61	0.36	0
62	PC1	C3	605	-	40,40,53	0.33	0	46,48,61	0.42	0
63	CDL	m3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
62	PC1	n	301	-	31,31,53	0.36	0	37,39,61	0.36	0
63	CDL	C3	604	-	67,67,99	0.36	0	73,79,111	0.30	0
62	PC1	a	502	-	40,40,53	0.34	0	46,48,61	0.40	0
63	CDL	Y7	501	-	64,64,99	0.37	0	70,76,111	0.37	0
62	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.38	0
62	PC1	m2	402	-	31,31,53	0.37	0	37,39,61	0.37	0
63	CDL	E	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	c1	706	-	58,58,99	0.38	0	64,70,111	0.41	0
59	HEA	c1	701	7	67,67,67	1.20	9 (13%)	81,103,103	1.51	16 (19%)
62	PC1	M1	404	-	34,34,53	0.35	0	40,42,61	0.33	0
62	PC1	c1	705	-	48,48,53	0.31	0	54,56,61	0.31	0
63	CDL	M1	403	-	65,65,99	0.36	0	71,77,111	0.30	0
63	CDL	5b	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	5B	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	m2	406	-	53,53,53	0.29	0	59,61,61	0.28	0
59	HEA	C1	702	7	67,67,67	1.23	10 (14%)	81,103,103	1.54	16 (19%)
63	CDL	l	301	-	73,73,99	0.34	0	79,85,111	0.29	0
63	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	CDL	7a	202	-	99,99,99	0.30	0	105,111,111	0.30	0
62	PC1	V	202	-	53,53,53	0.29	0	59,61,61	0.33	0
63	CDL	7c	302	-	50,50,99	0.40	0	56,62,111	0.34	0
63	CDL	7A	201	-	66,66,99	0.36	0	72,78,111	0.38	0
62	PC1	N	302	-	35,35,53	0.36	0	41,43,61	0.35	0
63	CDL	c1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
63	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	a	501	-	44,44,53	0.31	0	50,52,61	0.36	0
63	CDL	u	201	-	81,81,99	0.32	0	87,93,111	0.32	0
63	CDL	v	201	-	90,90,99	0.32	0	96,102,111	0.37	0
63	CDL	C1	706	-	58,58,99	0.38	0	64,70,111	0.40	0
63	CDL	m1	401	-	94,94,99	0.31	0	100,106,111	0.32	0
62	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.39	0
63	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.30	0
59	HEA	C1	701	7	67,67,67	1.20	9 (13%)	81,103,103	1.53	17 (20%)
62	PC1	C1	705	-	48,48,53	0.31	0	54,56,61	0.31	0
63	CDL	m2	401	-	53,53,99	0.40	0	59,65,111	0.40	0
63	CDL	U	201	-	81,81,99	0.32	0	87,93,111	0.32	0
63	CDL	5B	704	-	66,66,99	0.36	0	72,78,111	0.34	0
62	PC1	N	301	-	31,31,53	0.36	0	37,39,61	0.36	0
63	CDL	n	303	-	94,94,99	0.31	0	100,106,111	0.37	0
62	PC1	m2	405	-	40,40,53	0.33	0	46,48,61	0.33	0
62	PC1	7C	304	-	42,42,53	0.32	0	48,50,61	0.30	0
62	PC1	C3	602	-	38,38,53	0.33	0	44,46,61	0.34	0
63	CDL	m1	403	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	f	401	-	99,99,99	0.29	0	105,111,111	0.35	0
65	FES	FS	202	28	0,4,4	-	-	-	-	-
63	CDL	Y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
63	CDL	E	401	-	59,59,99	0.38	0	65,71,111	0.38	0
63	CDL	m3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
63	CDL	N	303	-	94,94,99	0.31	0	100,106,111	0.36	0
63	CDL	7c	301	-	84,84,99	0.32	0	90,96,111	0.34	0
63	CDL	k	301	-	61,61,99	0.37	0	67,73,111	0.33	0
63	CDL	7a	201	-	66,66,99	0.36	0	72,78,111	0.38	0
63	CDL	e	401	-	59,59,99	0.38	0	65,71,111	0.38	0
62	PC1	7c	303	-	42,42,53	0.32	0	48,50,61	0.30	0
63	CDL	M3	401	-	93,93,99	0.30	0	99,105,111	0.34	0
62	PC1	A	502	-	40,40,53	0.33	0	46,48,61	0.39	0
63	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
62	PC1	m1	402	-	53,53,53	0.29	0	59,61,61	0.35	0
63	CDL	V	201	-	90,90,99	0.32	0	96,102,111	0.37	0
65	FES	FS	201	28	0,4,4	-	-	-	-	-
63	CDL	M3	402	-	50,50,99	0.41	0	56,62,111	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	PC1	n	302	-	35,35,53	0.36	0	41,43,61	0.35	0
63	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.35	0
62	PC1	J	302	-	36,36,53	0.34	0	42,44,61	0.33	0
63	CDL	T	201	-	67,67,99	0.36	0	73,79,111	0.35	0
63	CDL	m1	404	-	65,65,99	0.36	0	71,77,111	0.30	0
63	CDL	T	202	-	74,74,99	0.34	0	80,86,111	0.35	0
63	CDL	M1	401	-	94,94,99	0.31	0	100,106,111	0.32	0
63	CDL	5b	703	-	66,66,99	0.36	0	72,78,111	0.33	0
62	PC1	m1	405	-	34,34,53	0.35	0	40,42,61	0.32	0
62	PC1	7C	302	-	53,53,53	0.29	0	59,61,61	0.36	0
63	CDL	a	503	-	50,50,99	0.41	0	56,62,111	0.51	0
63	CDL	5B	703	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	M2	406	-	53,53,53	0.29	0	59,61,61	0.28	0
62	PC1	c3	605	-	40,40,53	0.33	0	46,48,61	0.42	0
62	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.39	0
63	CDL	y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
63	CDL	y0	101	-	63,63,99	0.37	0	69,75,111	0.34	0
63	CDL	c3	604	-	67,67,99	0.36	0	73,79,111	0.31	0
63	CDL	Y0	101	-	63,63,99	0.37	0	69,75,111	0.34	0
63	CDL	t	202	-	74,74,99	0.34	0	80,86,111	0.35	0
62	PC1	M2	402	-	31,31,53	0.37	0	37,39,61	0.37	0
63	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.30	0
63	CDL	F	401	-	99,99,99	0.29	0	105,111,111	0.36	0
63	CDL	M2	403	-	65,65,99	0.36	0	71,77,111	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	CDL	m3	401	-	-	19/104/104/110	-
62	PC1	C3	601	-	-	12/55/55/57	-
63	CDL	e	402	-	-	14/82/82/110	-
63	CDL	7C	303	-	-	15/61/61/110	-
65	FES	fs	201	28	-	-	0/1/1/1
62	PC1	M2	405	-	-	11/44/44/57	-
63	CDL	y7	501	-	-	10/75/75/110	-
65	FES	fs	202	28	-	-	0/1/1/1
63	CDL	t	201	-	-	10/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	HEA	c1	702	7	-	14/36/76/76	-
63	CDL	M3	403	-	-	17/73/73/110	-
62	PC1	c3	602	-	-	9/42/42/57	-
63	CDL	M2	401	-	-	15/64/64/110	-
63	CDL	A	503	-	-	8/61/61/110	-
62	PC1	v	202	-	-	9/57/57/57	-
62	PC1	j	302	-	-	8/40/40/57	-
63	CDL	m2	404	-	-	16/84/84/110	-
63	CDL	7A	202	-	-	19/110/110/110	-
63	CDL	7C	301	-	-	22/95/95/110	-
63	CDL	M1	402	-	-	15/76/76/110	-
62	PC1	A	501	-	-	11/48/48/57	-
62	PC1	C3	605	-	-	10/44/44/57	-
63	CDL	m3	403	-	-	18/73/73/110	-
62	PC1	n	301	-	-	13/35/35/57	-
63	CDL	C3	604	-	-	9/78/78/110	-
62	PC1	a	502	-	-	9/44/44/57	-
63	CDL	Y7	501	-	-	11/75/75/110	-
62	PC1	c3	601	-	-	12/55/55/57	-
62	PC1	m2	402	-	-	3/35/35/57	-
63	CDL	E	402	-	-	14/82/82/110	-
63	CDL	c1	706	-	-	19/69/69/110	-
59	HEA	c1	701	7	-	18/36/76/76	-
62	PC1	M1	404	-	-	8/38/38/57	-
62	PC1	c1	705	-	-	9/52/52/57	-
63	CDL	M1	403	-	-	9/76/76/110	-
63	CDL	5b	702	-	-	23/97/97/110	-
63	CDL	5B	702	-	-	23/97/97/110	-
63	CDL	b	501	-	-	14/72/72/110	-
62	PC1	m2	406	-	-	8/57/57/57	-
59	HEA	C1	702	7	-	14/36/76/76	-
63	CDL	l	301	-	-	21/84/84/110	-
63	CDL	L	301	-	-	21/84/84/110	-
63	CDL	7a	202	-	-	23/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	V	202	-	-	10/57/57/57	-
63	CDL	7c	302	-	-	15/61/61/110	-
63	CDL	7A	201	-	-	12/77/77/110	-
62	PC1	N	302	-	-	4/39/39/57	-
63	CDL	c1	707	-	-	10/75/75/110	-
63	CDL	B	501	-	-	14/72/72/110	-
62	PC1	a	501	-	-	13/48/48/57	-
63	CDL	u	201	-	-	15/92/92/110	-
63	CDL	v	201	-	-	13/101/101/110	-
63	CDL	C1	706	-	-	17/69/69/110	-
63	CDL	m1	401	-	-	26/105/105/110	-
62	PC1	c3	603	-	-	10/34/34/57	-
63	CDL	j	301	-	-	13/80/80/110	-
59	HEA	C1	701	7	-	17/36/76/76	-
62	PC1	C1	705	-	-	12/52/52/57	-
63	CDL	m2	401	-	-	18/64/64/110	-
63	CDL	U	201	-	-	17/92/92/110	-
63	CDL	5B	704	-	-	9/77/77/110	-
62	PC1	N	301	-	-	13/35/35/57	-
63	CDL	n	303	-	-	22/105/105/110	-
62	PC1	m2	405	-	-	6/44/44/57	-
62	PC1	7C	304	-	-	12/46/46/57	-
62	PC1	C3	602	-	-	10/42/42/57	-
63	CDL	m1	403	-	-	15/76/76/110	-
63	CDL	f	401	-	-	17/110/110/110	-
65	FES	FS	202	28	-	-	0/1/1/1
63	CDL	Y5	201	-	-	16/91/91/110	-
63	CDL	E	401	-	-	17/70/70/110	-
63	CDL	m3	402	-	-	13/61/61/110	-
63	CDL	N	303	-	-	22/105/105/110	-
63	CDL	7c	301	-	-	24/95/95/110	-
63	CDL	k	301	-	-	14/72/72/110	-
63	CDL	7a	201	-	-	13/77/77/110	-
63	CDL	e	401	-	-	16/70/70/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	7c	303	-	-	13/46/46/57	-
63	CDL	M3	401	-	-	20/104/104/110	-
62	PC1	A	502	-	-	11/44/44/57	-
63	CDL	C1	707	-	-	11/75/75/110	-
62	PC1	m1	402	-	-	16/57/57/57	-
63	CDL	V	201	-	-	14/101/101/110	-
65	FES	FS	201	28	-	-	0/1/1/1
63	CDL	M3	402	-	-	13/61/61/110	-
62	PC1	n	302	-	-	4/39/39/57	-
63	CDL	m2	403	-	-	15/76/76/110	-
63	CDL	M2	404	-	-	17/84/84/110	-
62	PC1	J	302	-	-	7/40/40/57	-
63	CDL	T	201	-	-	12/78/78/110	-
63	CDL	m1	404	-	-	10/76/76/110	-
63	CDL	T	202	-	-	13/85/85/110	-
63	CDL	M1	401	-	-	27/105/105/110	-
63	CDL	5b	703	-	-	11/77/77/110	-
62	PC1	m1	405	-	-	8/38/38/57	-
62	PC1	7C	302	-	-	17/57/57/57	-
63	CDL	a	503	-	-	12/61/61/110	-
63	CDL	5B	703	-	-	14/72/72/110	-
62	PC1	M2	406	-	-	8/57/57/57	-
62	PC1	c3	605	-	-	9/44/44/57	-
62	PC1	C3	603	-	-	10/34/34/57	-
63	CDL	y5	201	-	-	15/91/91/110	-
63	CDL	y0	101	-	-	21/74/74/110	-
63	CDL	c3	604	-	-	9/78/78/110	-
63	CDL	Y0	101	-	-	17/74/74/110	-
63	CDL	t	202	-	-	14/85/85/110	-
62	PC1	M2	402	-	-	4/35/35/57	-
63	CDL	J	301	-	-	12/80/80/110	-
63	CDL	F	401	-	-	19/110/110/110	-
63	CDL	M2	403	-	-	15/76/76/110	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	702	HEA	C4D-C3D	3.26	1.50	1.45
59	C1	702	HEA	C4D-C3D	3.25	1.50	1.45
59	C1	702	HEA	C3A-C4A	-3.20	1.40	1.46
59	c1	702	HEA	C3A-C4A	-3.17	1.40	1.46
59	C1	702	HEA	FE-NB	3.09	2.04	1.94

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	C1	702	HEA	C13-C12-C11	-4.84	106.65	114.39
59	c1	702	HEA	C13-C12-C11	-4.80	106.73	114.39
59	C1	701	HEA	C13-C12-C11	-3.67	108.53	114.39
59	c1	701	HEA	C13-C12-C11	-3.61	108.63	114.39
59	C1	702	HEA	CHB-C4A-NA	3.61	128.38	124.45

There are no chirality outliers.

5 of 1456 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	C1	701	HEA	C2A-C3A-CMA-OMA
59	C1	701	HEA	C4A-C3A-CMA-OMA
59	C1	701	HEA	C26-C15-C16-C17
59	C1	701	HEA	C15-C16-C17-C18
59	C1	701	HEA	C17-C18-C19-C20

There are no ring outliers.

90 monomers are involved in 344 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	m3	401	CDL	12	0
62	C3	601	PC1	1	0
63	e	402	CDL	6	0
63	7C	303	CDL	1	0
62	M2	405	PC1	4	0
63	y7	501	CDL	1	0
63	t	201	CDL	2	0
59	c1	702	HEA	1	0
63	M2	401	CDL	2	0
62	v	202	PC1	3	0
63	m2	404	CDL	3	0
63	7A	202	CDL	7	0
63	7C	301	CDL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	M1	402	CDL	3	0
62	A	501	PC1	3	0
62	C3	605	PC1	3	0
62	n	301	PC1	3	0
62	a	502	PC1	2	0
63	Y7	501	CDL	1	0
62	c3	601	PC1	1	0
62	m2	402	PC1	2	0
63	E	402	CDL	5	0
63	c1	706	CDL	5	0
59	c1	701	HEA	6	0
62	c1	705	PC1	4	0
63	M1	403	CDL	5	0
63	5b	702	CDL	6	0
63	5B	702	CDL	9	0
62	m2	406	PC1	1	0
59	C1	702	HEA	2	0
63	l	301	CDL	2	0
63	L	301	CDL	3	0
63	7a	202	CDL	8	0
62	V	202	PC1	3	0
63	7c	302	CDL	1	0
63	7A	201	CDL	4	0
62	N	302	PC1	1	0
63	c1	707	CDL	1	0
62	a	501	PC1	3	0
63	u	201	CDL	4	0
63	v	201	CDL	3	0
63	C1	706	CDL	5	0
63	m1	401	CDL	8	0
62	c3	603	PC1	2	0
63	j	301	CDL	7	0
59	C1	701	HEA	7	0
62	C1	705	PC1	4	0
63	m2	401	CDL	3	0
63	U	201	CDL	4	0
63	5B	704	CDL	2	0
62	N	301	PC1	2	0
63	n	303	CDL	9	0
62	m2	405	PC1	4	0
62	7C	304	PC1	5	0
63	m1	403	CDL	3	0

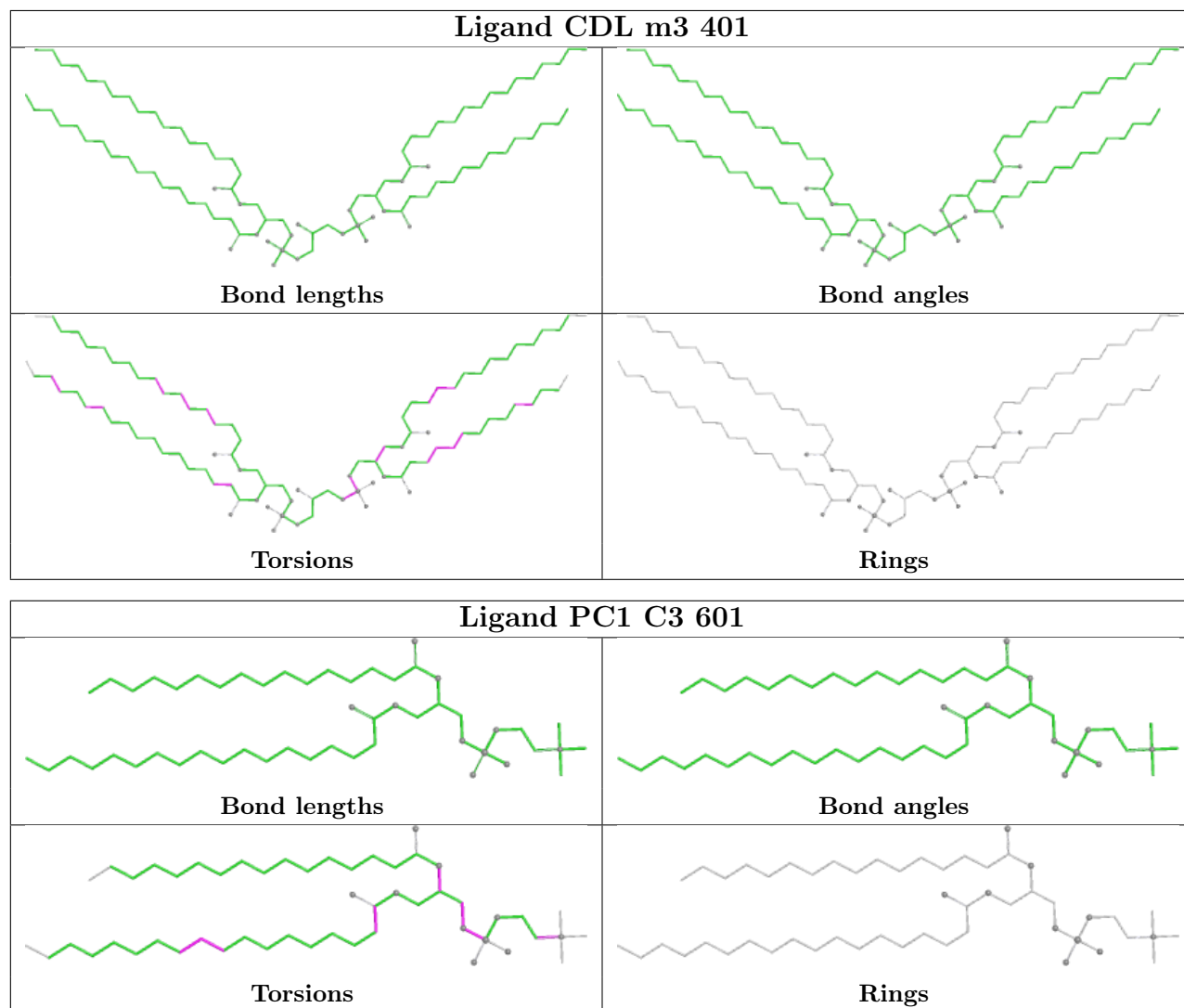
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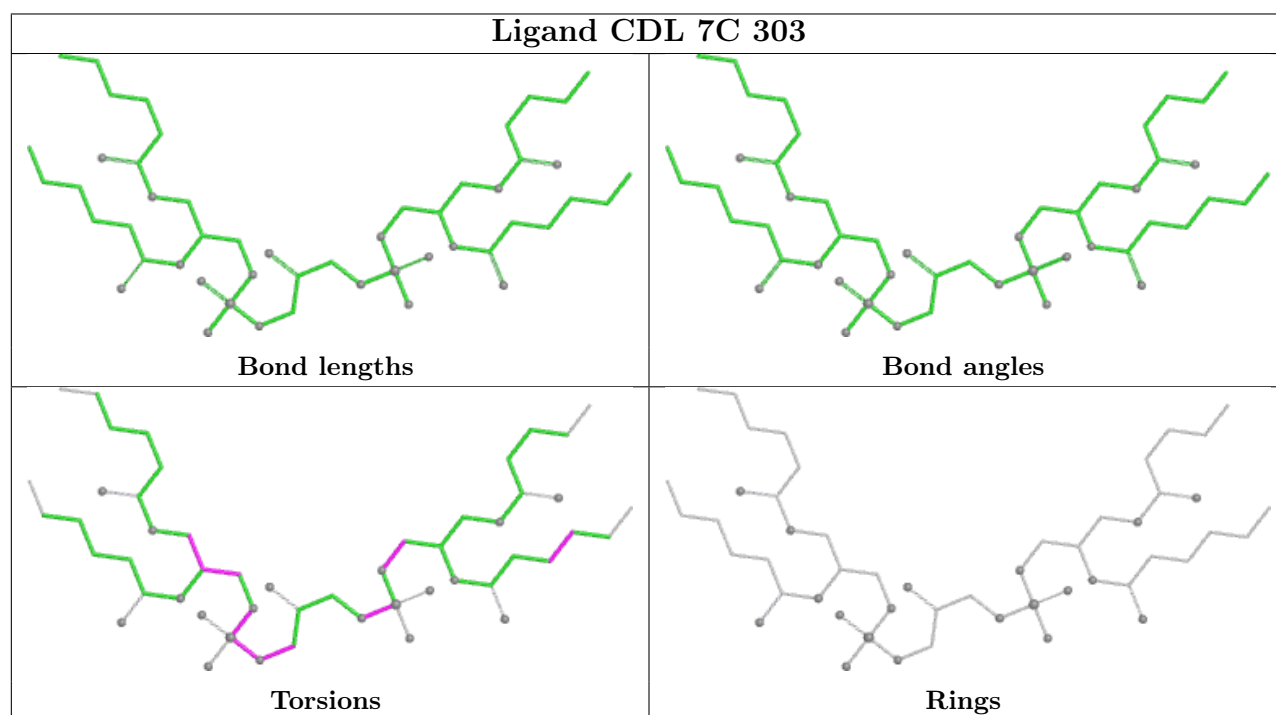
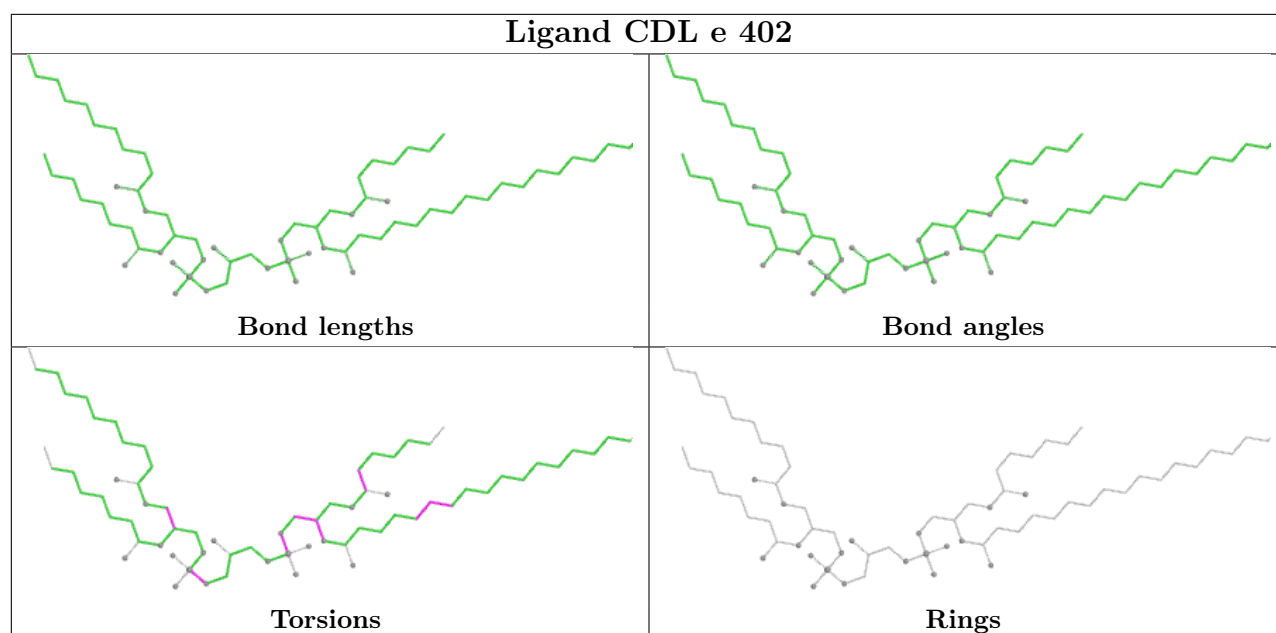
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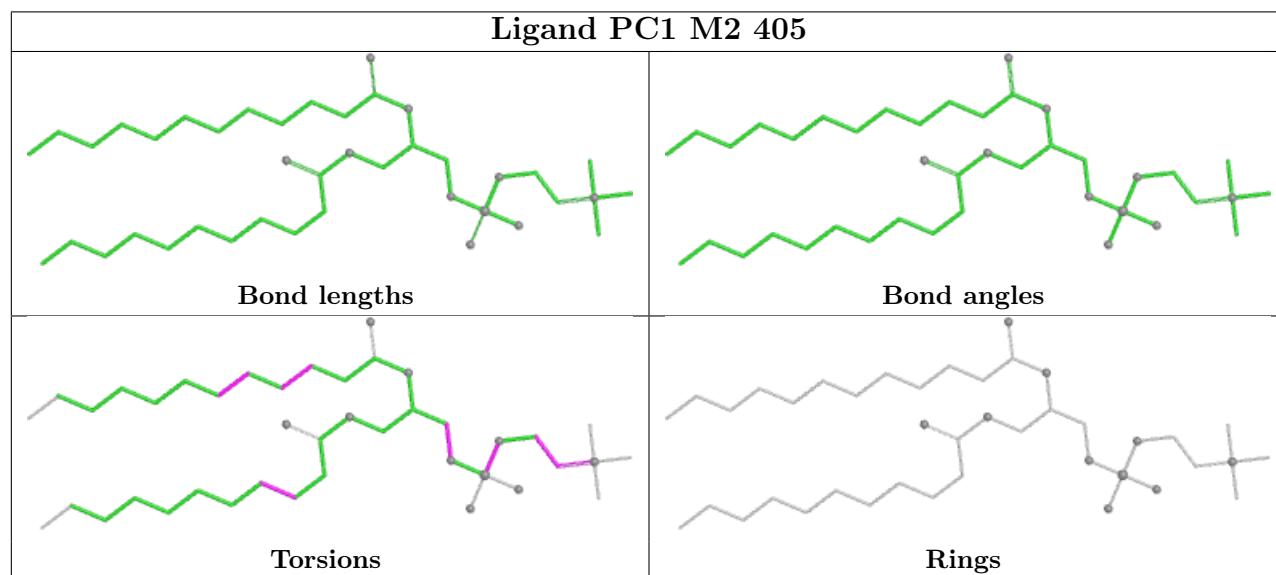
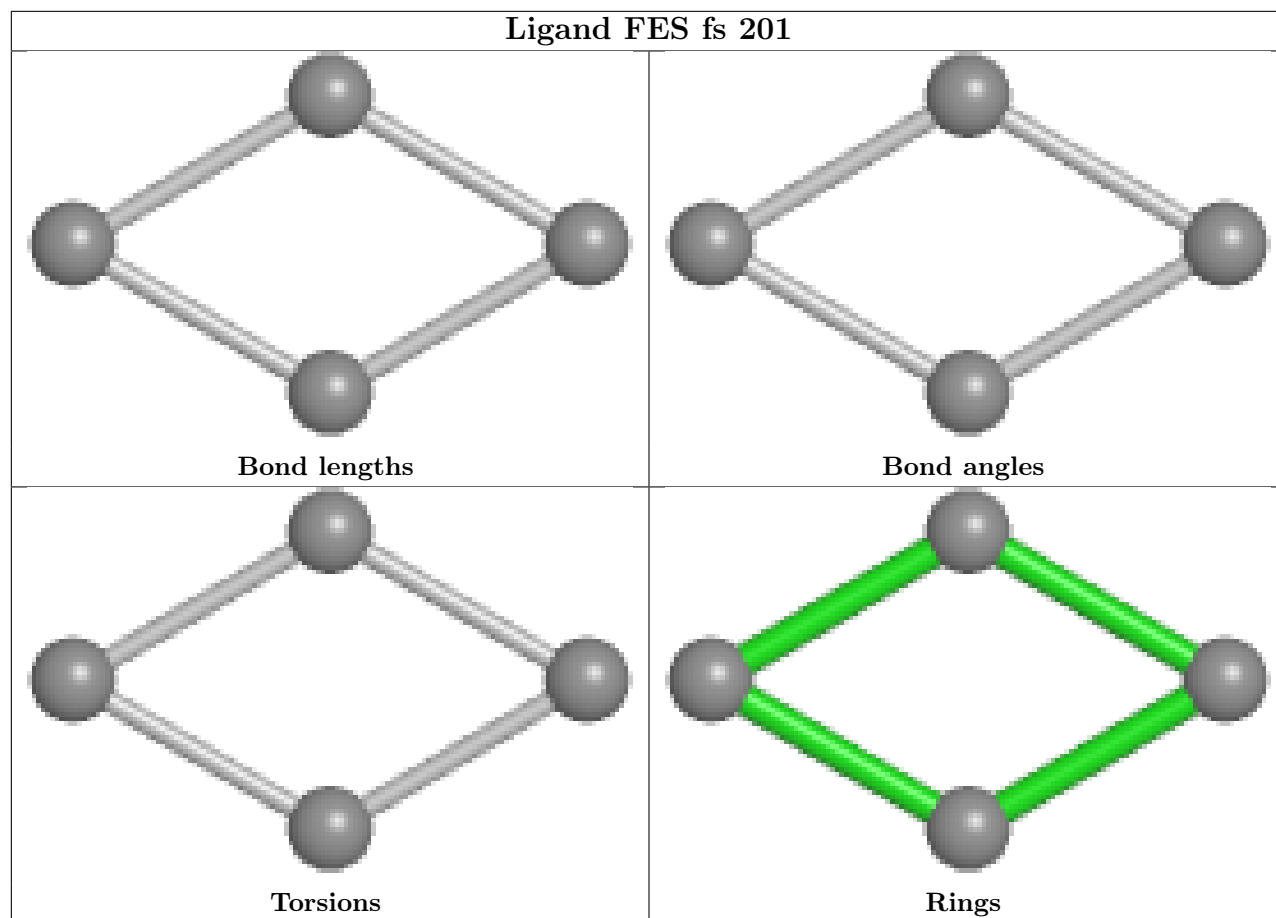
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	f	401	CDL	9	0
63	Y5	201	CDL	2	0
63	E	401	CDL	2	0
63	N	303	CDL	7	0
63	7c	301	CDL	8	0
63	k	301	CDL	3	0
63	7a	201	CDL	6	0
63	e	401	CDL	3	0
62	7c	303	PC1	5	0
63	M3	401	CDL	9	0
62	A	502	PC1	2	0
63	C1	707	CDL	1	0
62	m1	402	PC1	9	0
63	V	201	CDL	3	0
62	n	302	PC1	1	0
63	m2	403	CDL	5	0
63	M2	404	CDL	2	0
63	T	201	CDL	2	0
63	m1	404	CDL	4	0
63	T	202	CDL	5	0
63	M1	401	CDL	8	0
63	5b	703	CDL	3	0
62	7C	302	PC1	8	0
63	5B	703	CDL	3	0
62	M2	406	PC1	1	0
62	c3	605	PC1	3	0
62	C3	603	PC1	2	0
63	y5	201	CDL	1	0
63	y0	101	CDL	3	0
63	Y0	101	CDL	4	0
63	t	202	CDL	5	0
62	M2	402	PC1	3	0
63	J	301	CDL	6	0
63	F	401	CDL	12	0
63	M2	403	CDL	5	0

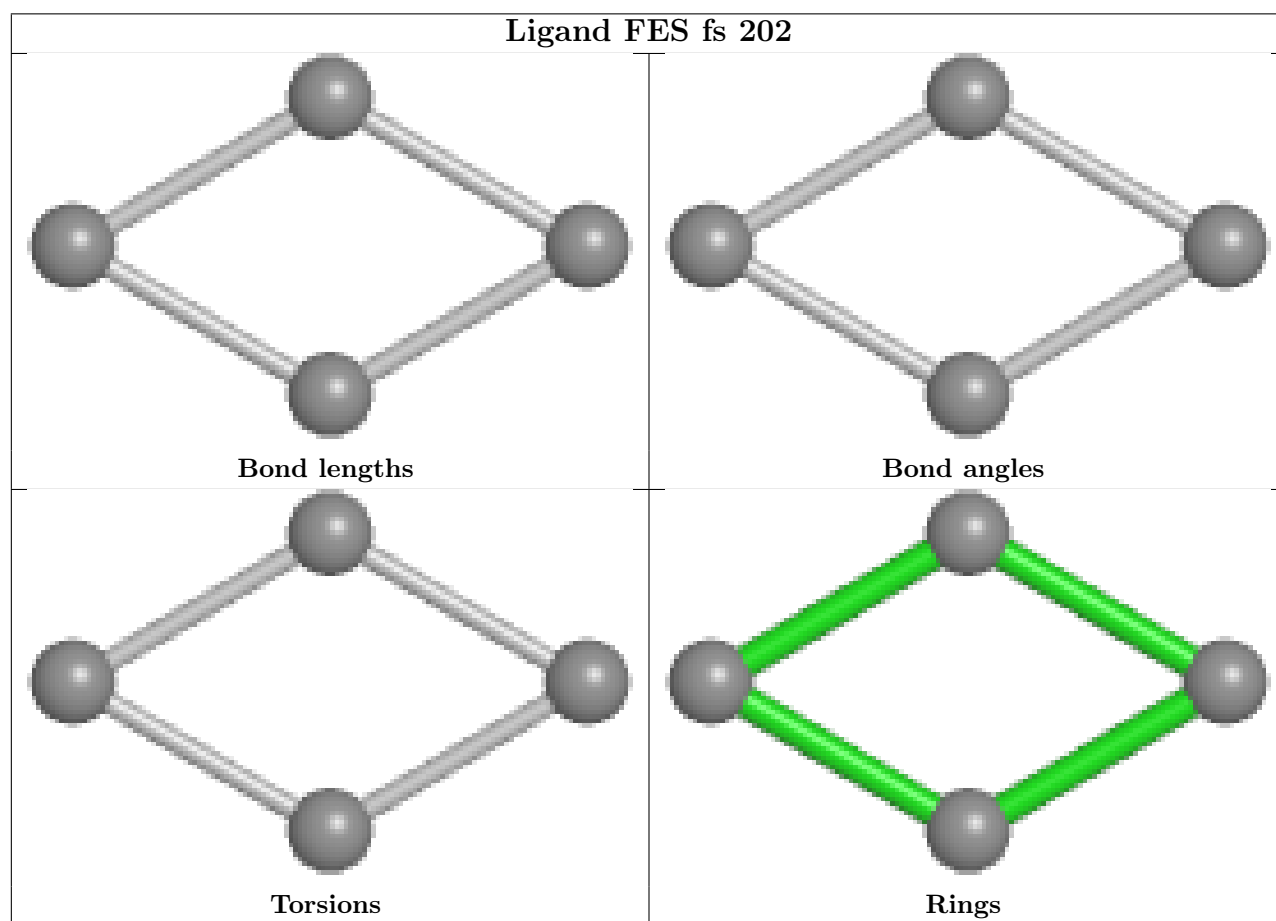
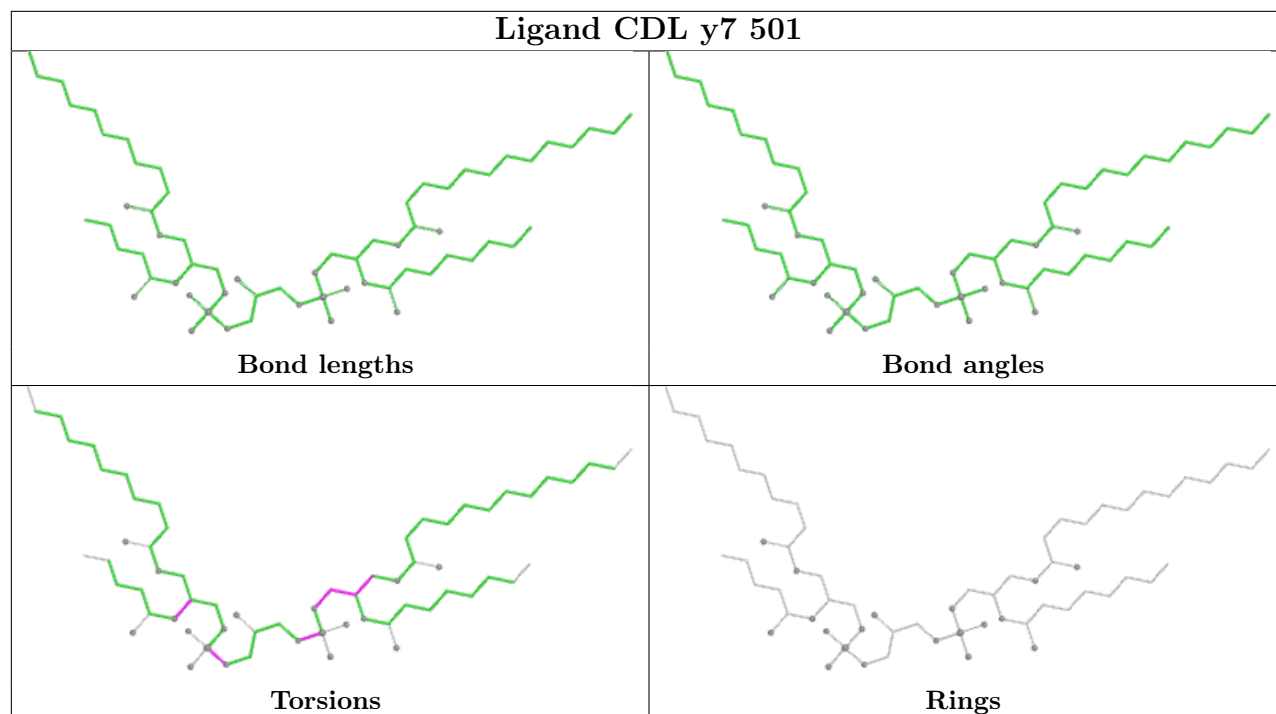
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

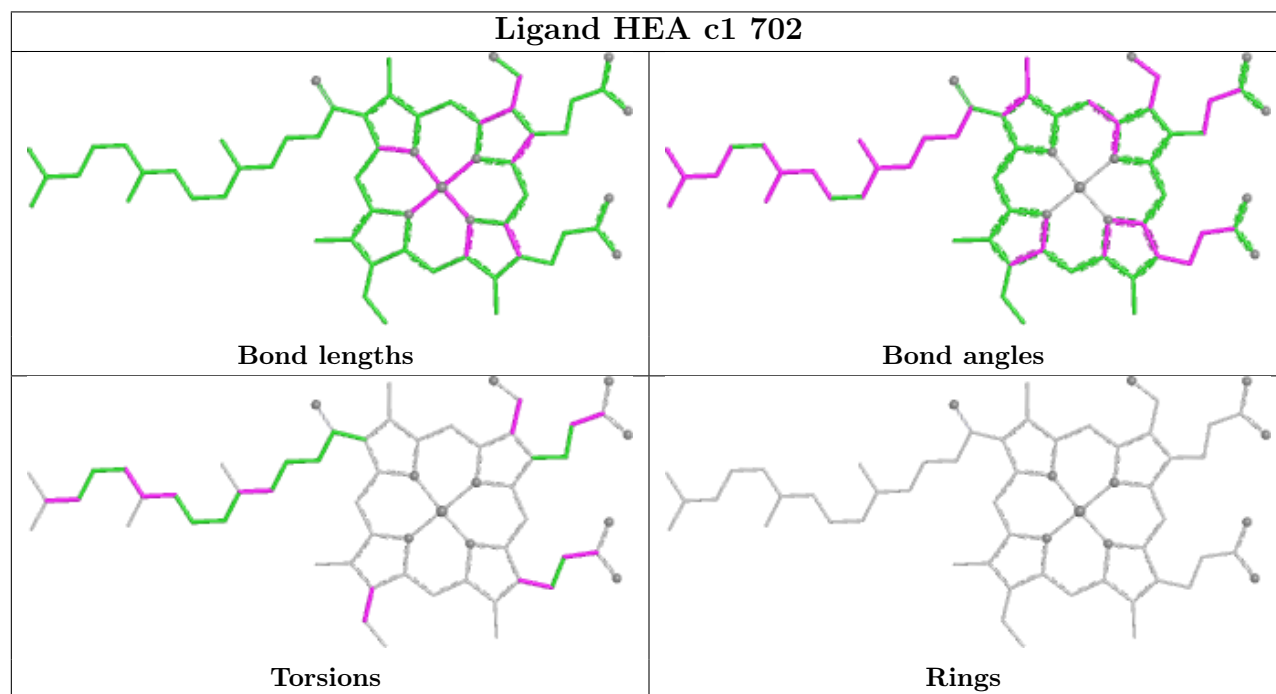
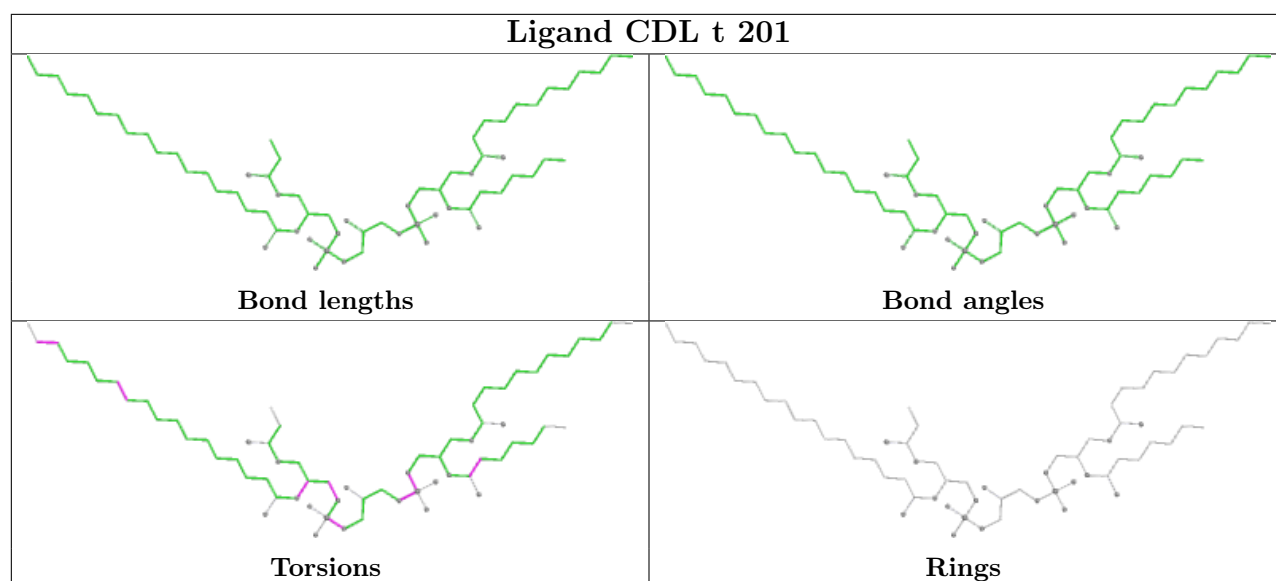
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

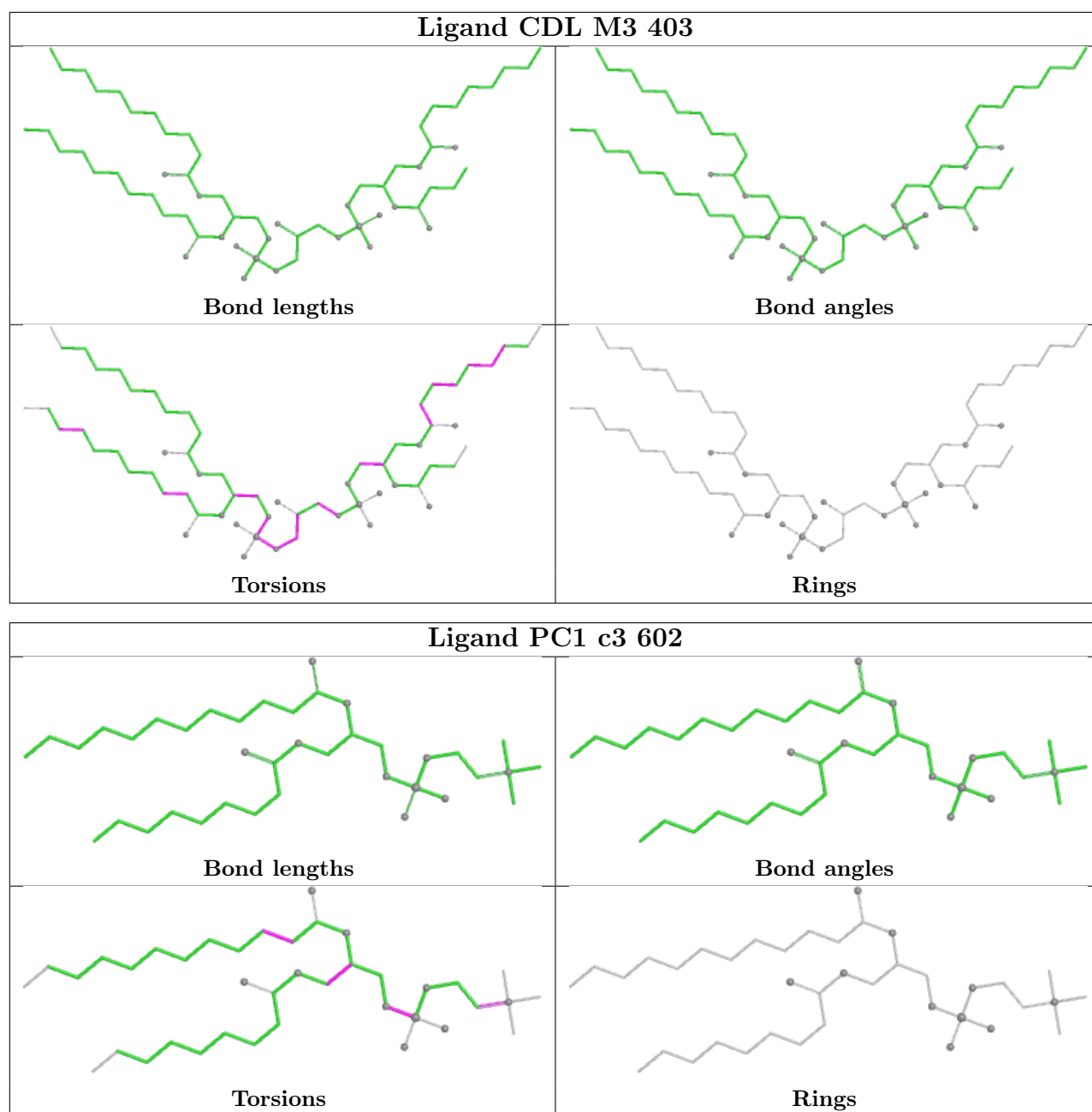


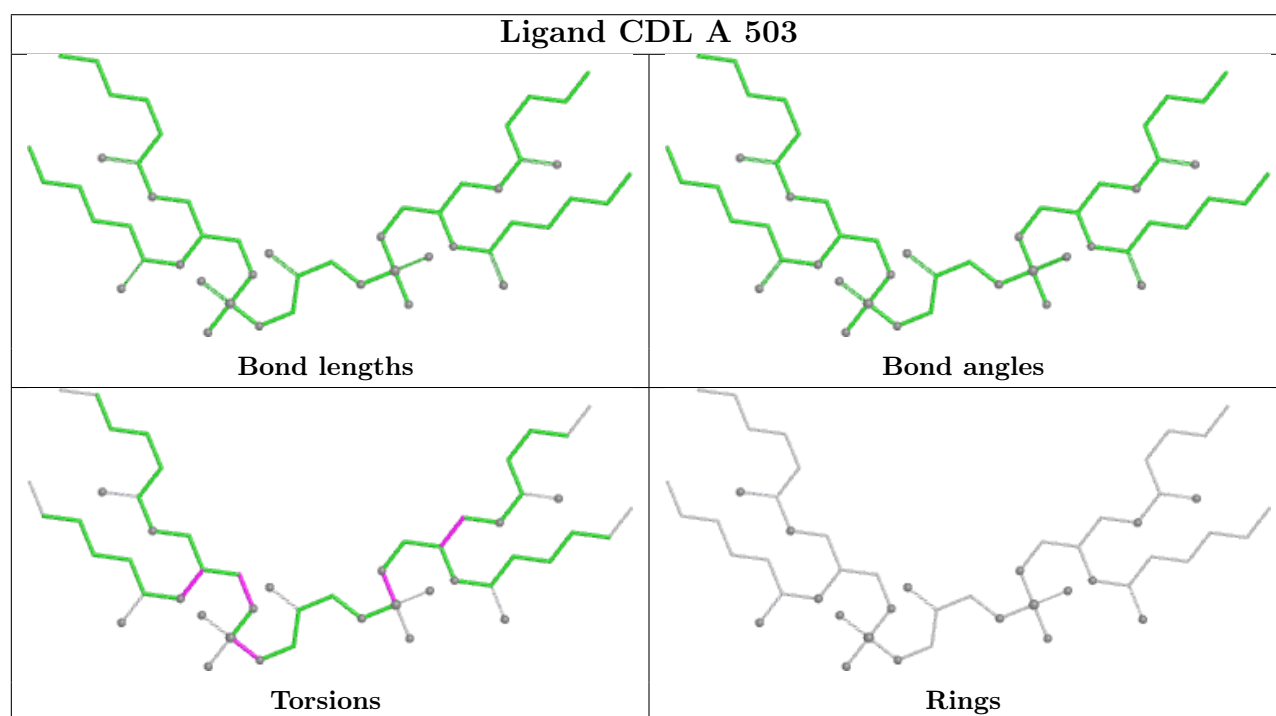
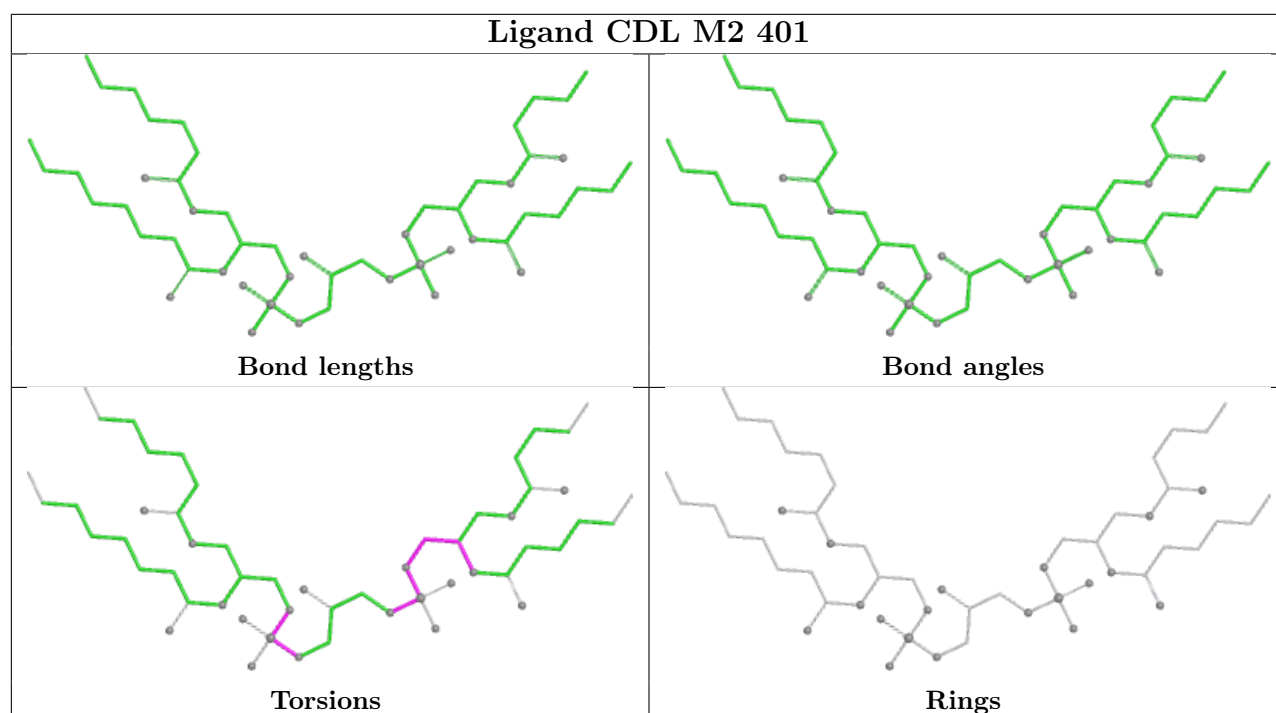


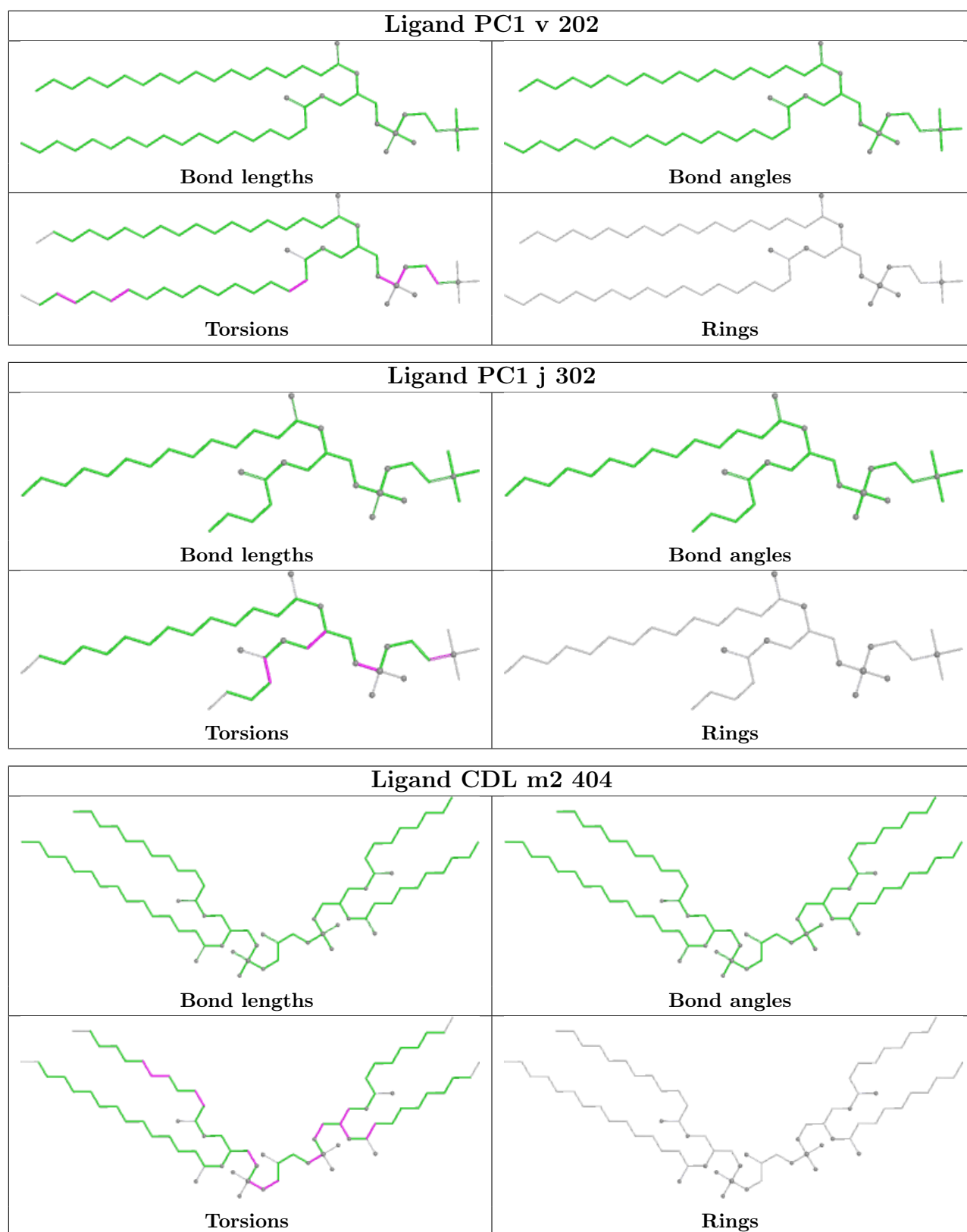


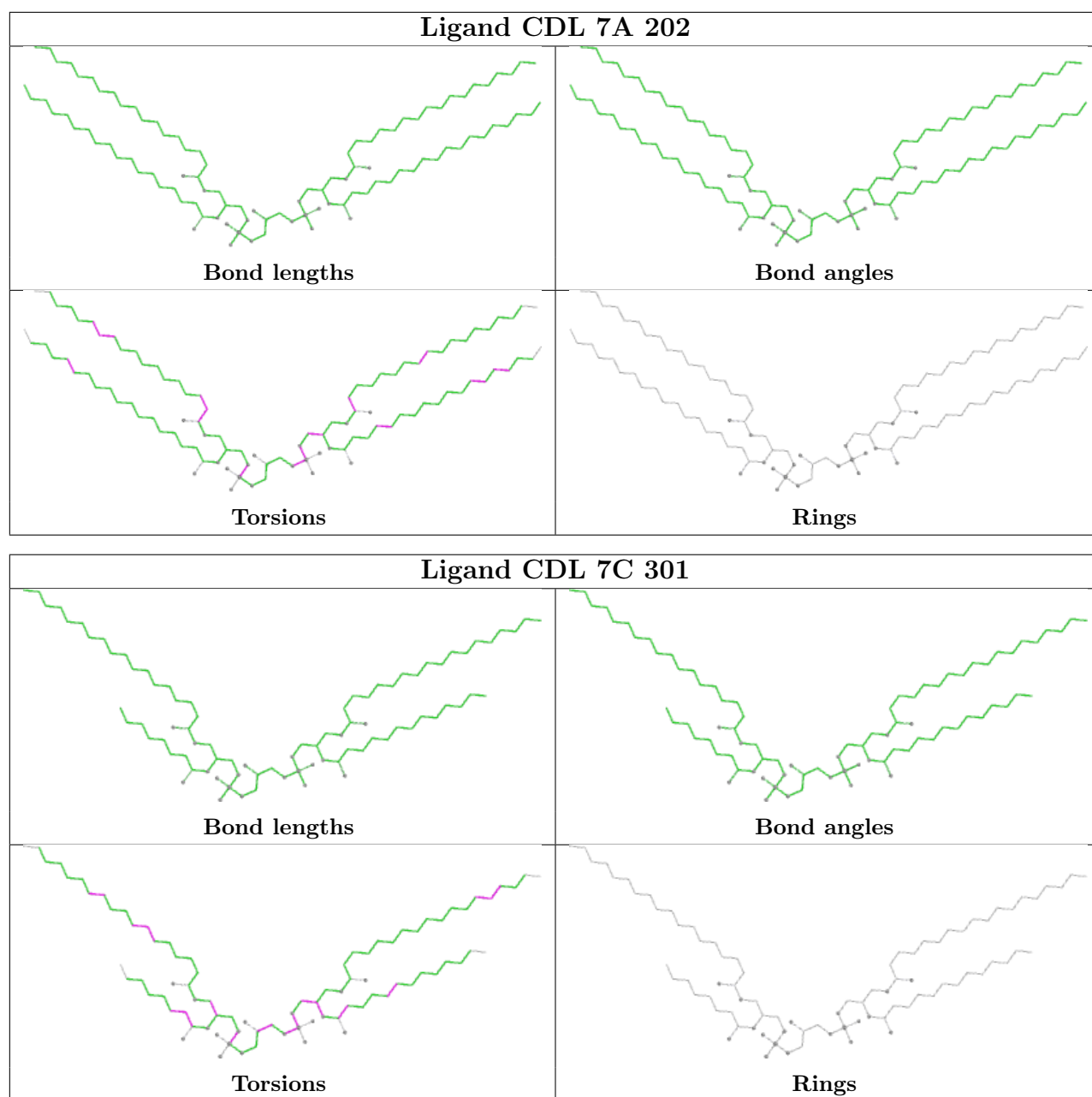


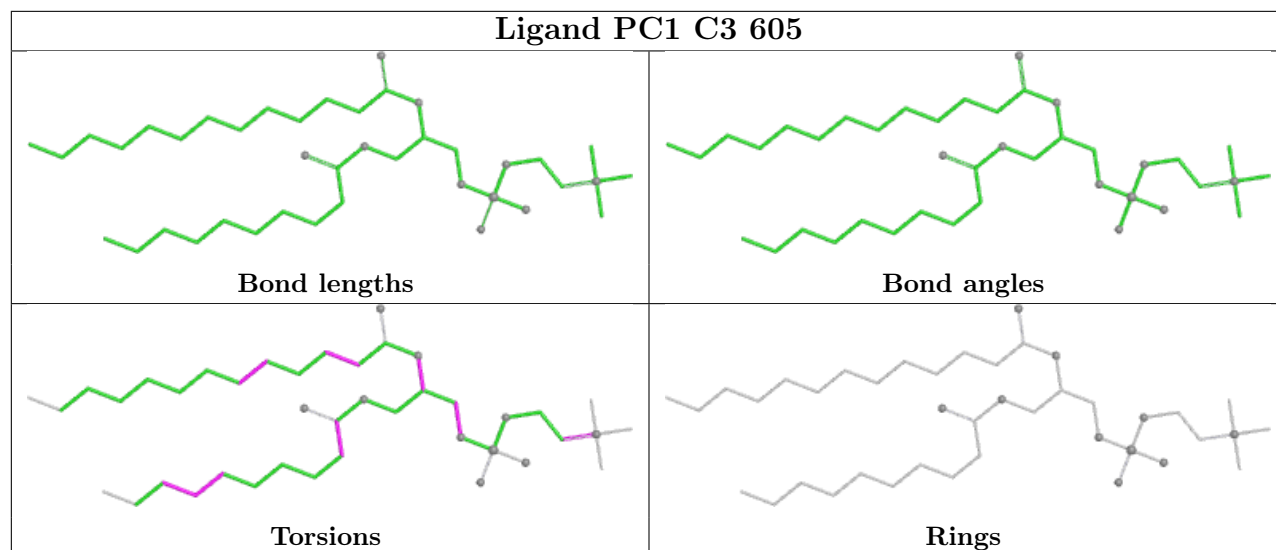
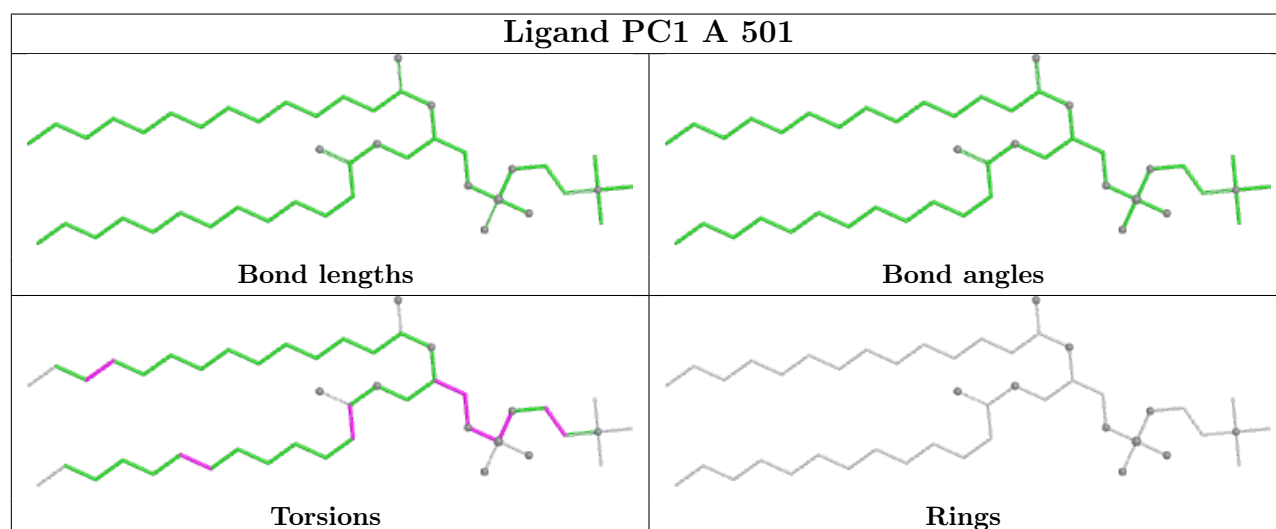
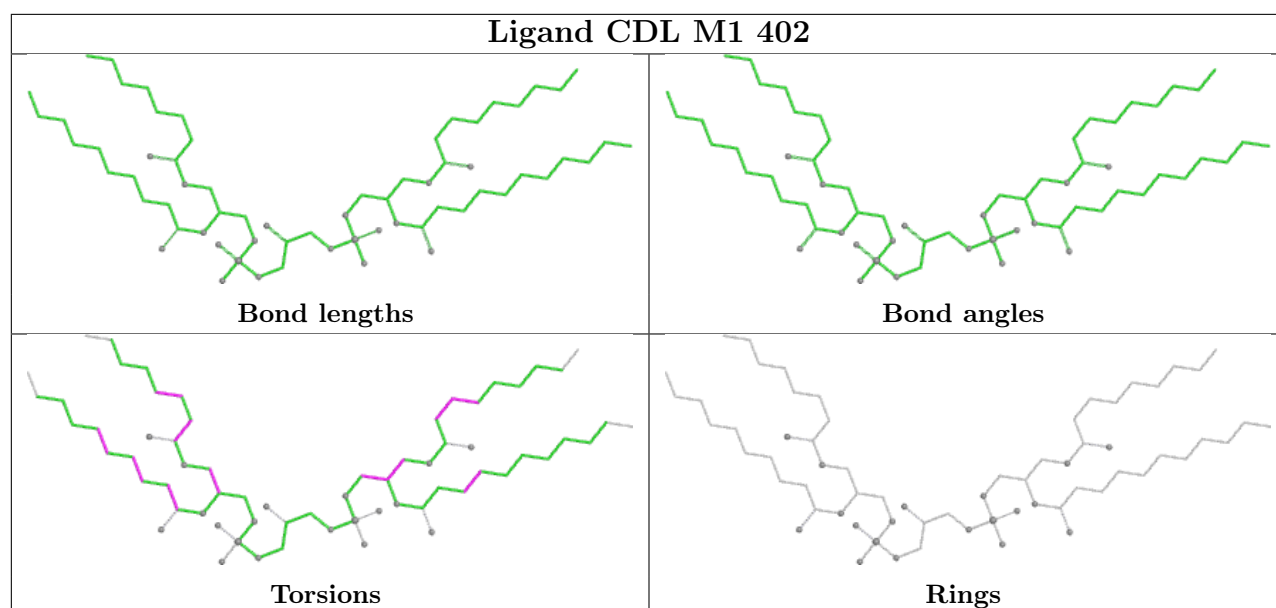


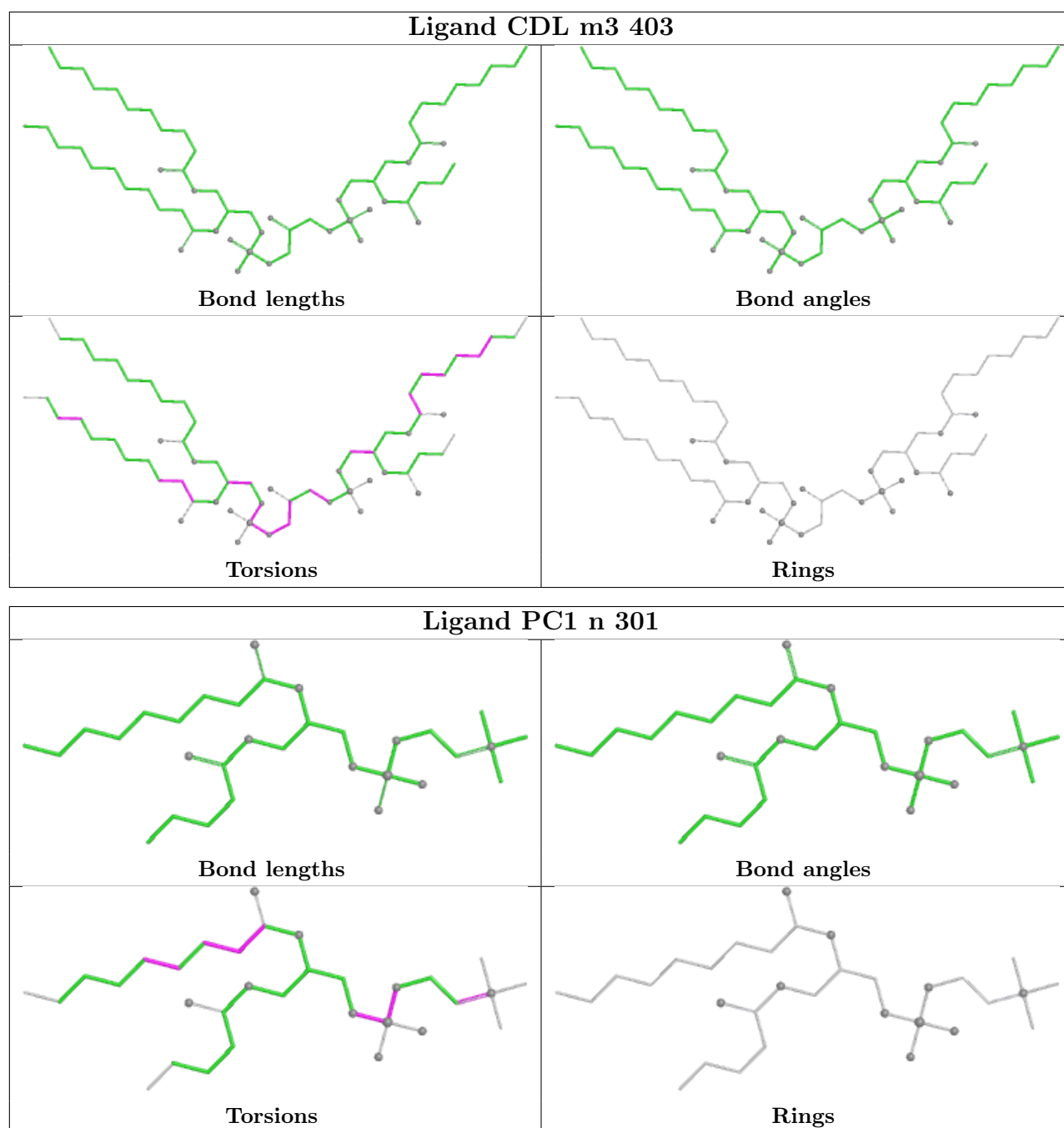


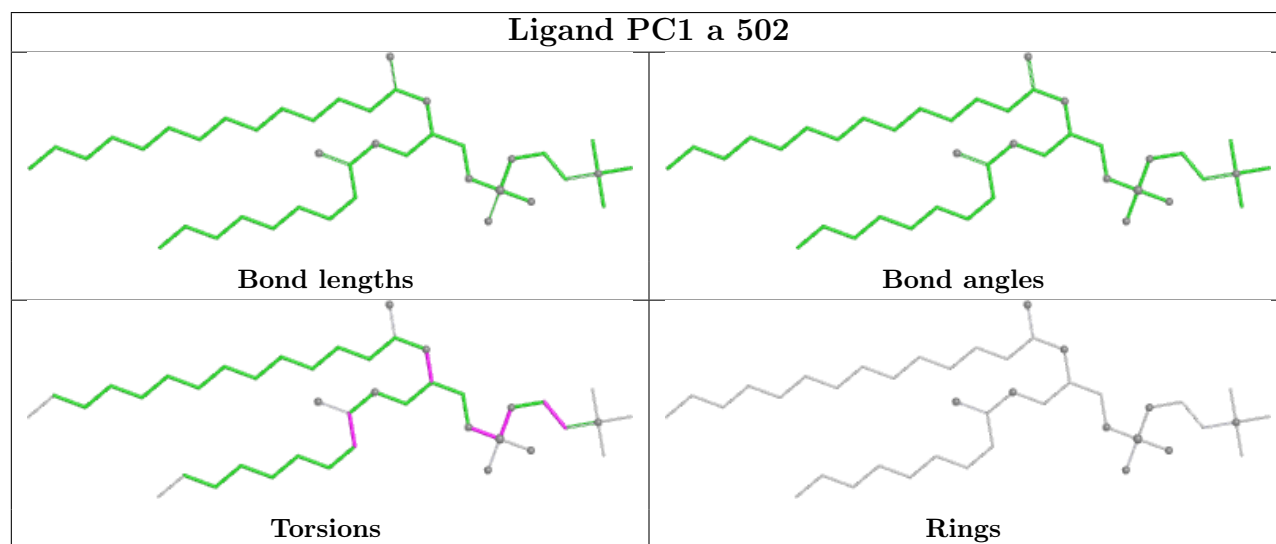
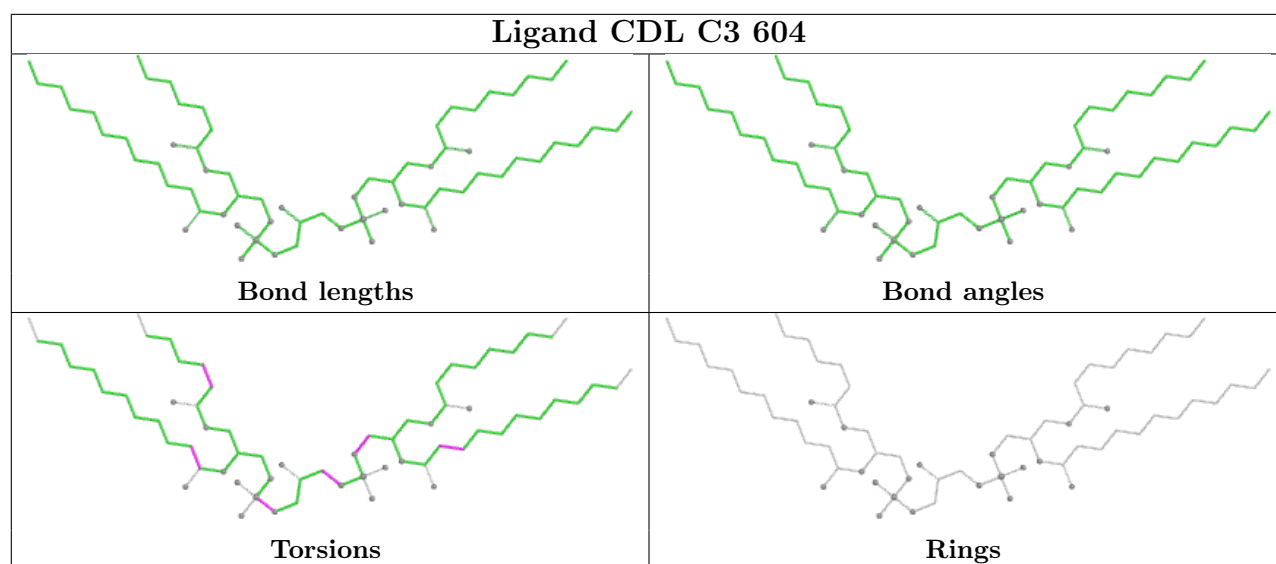


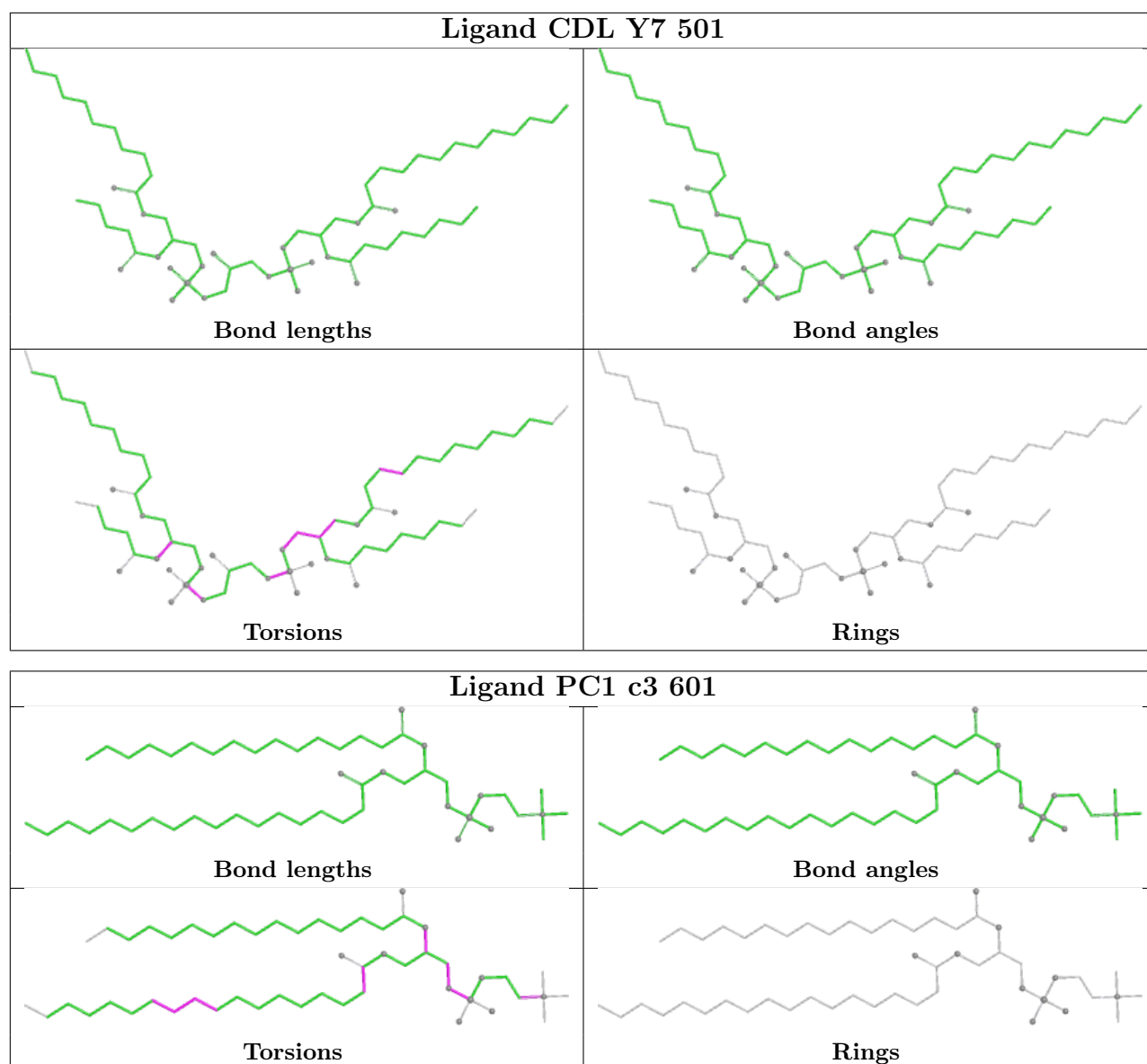


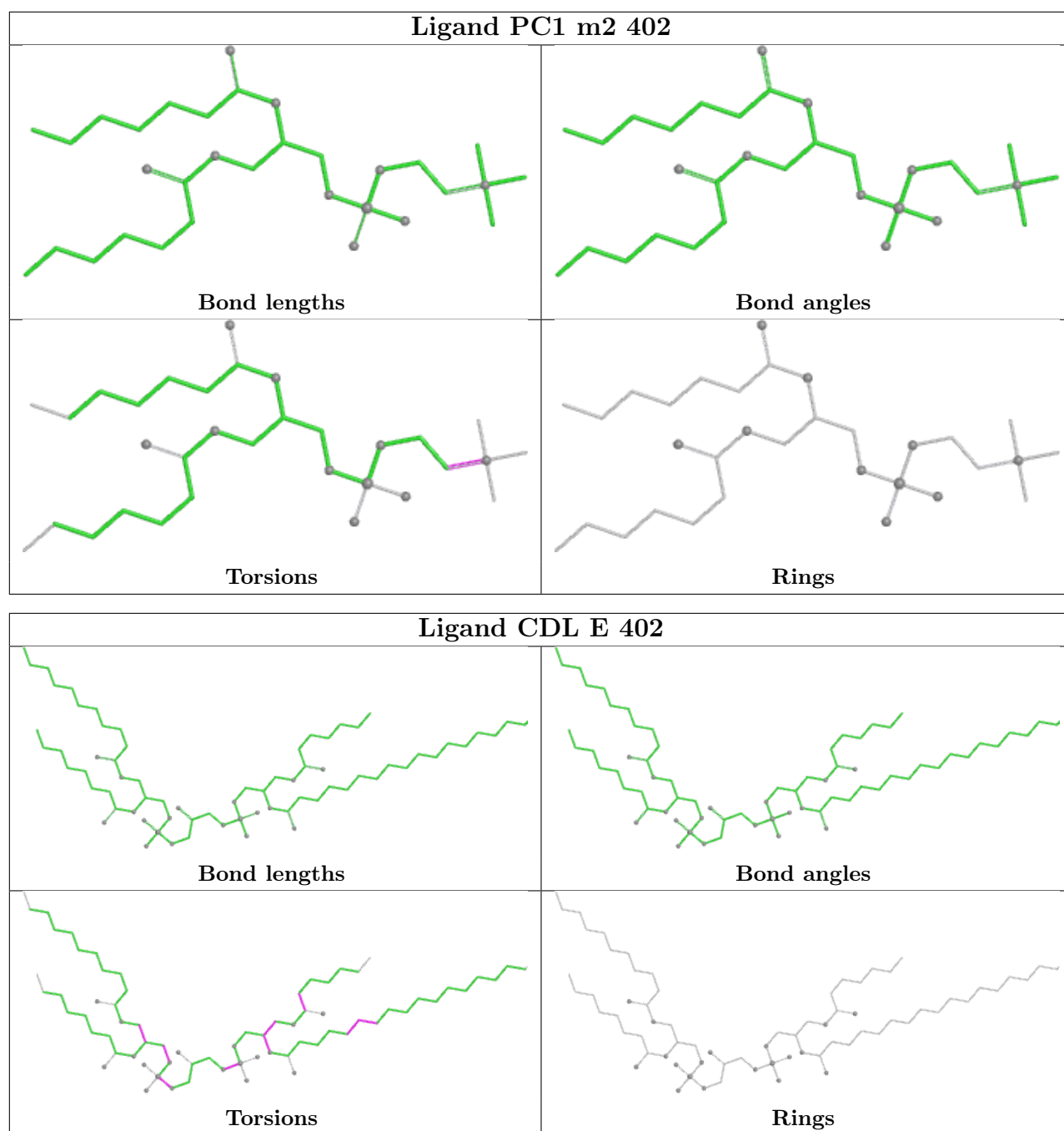


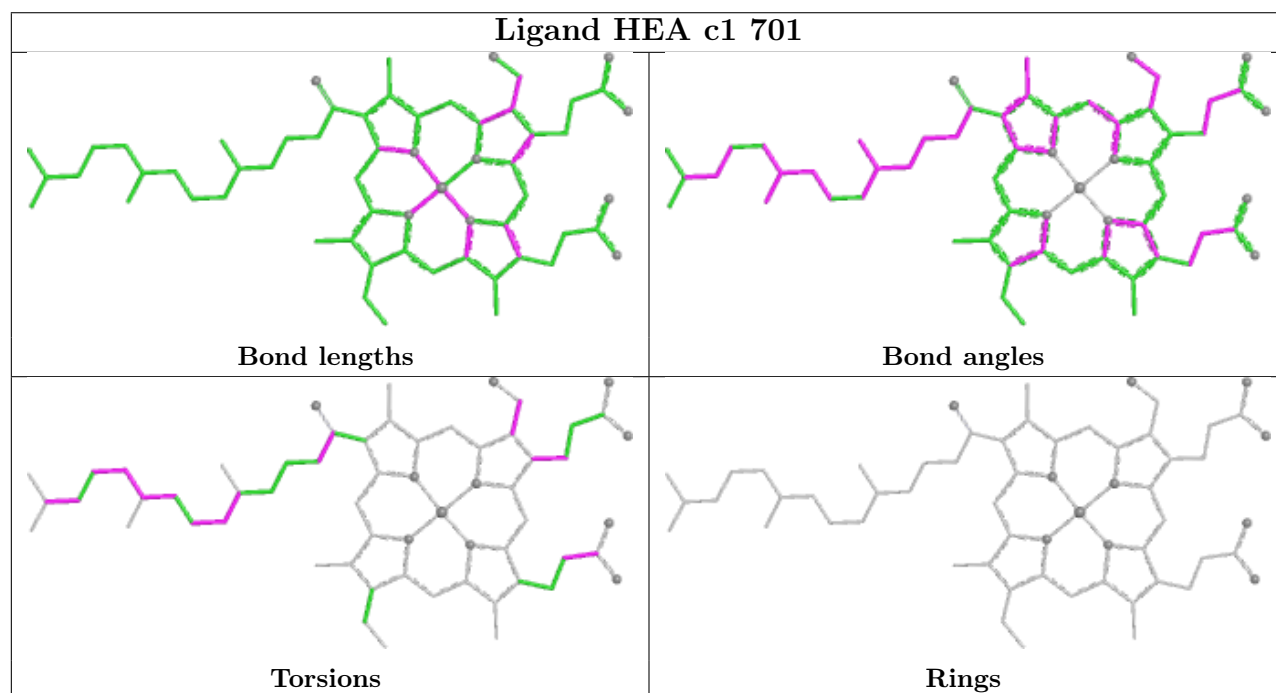
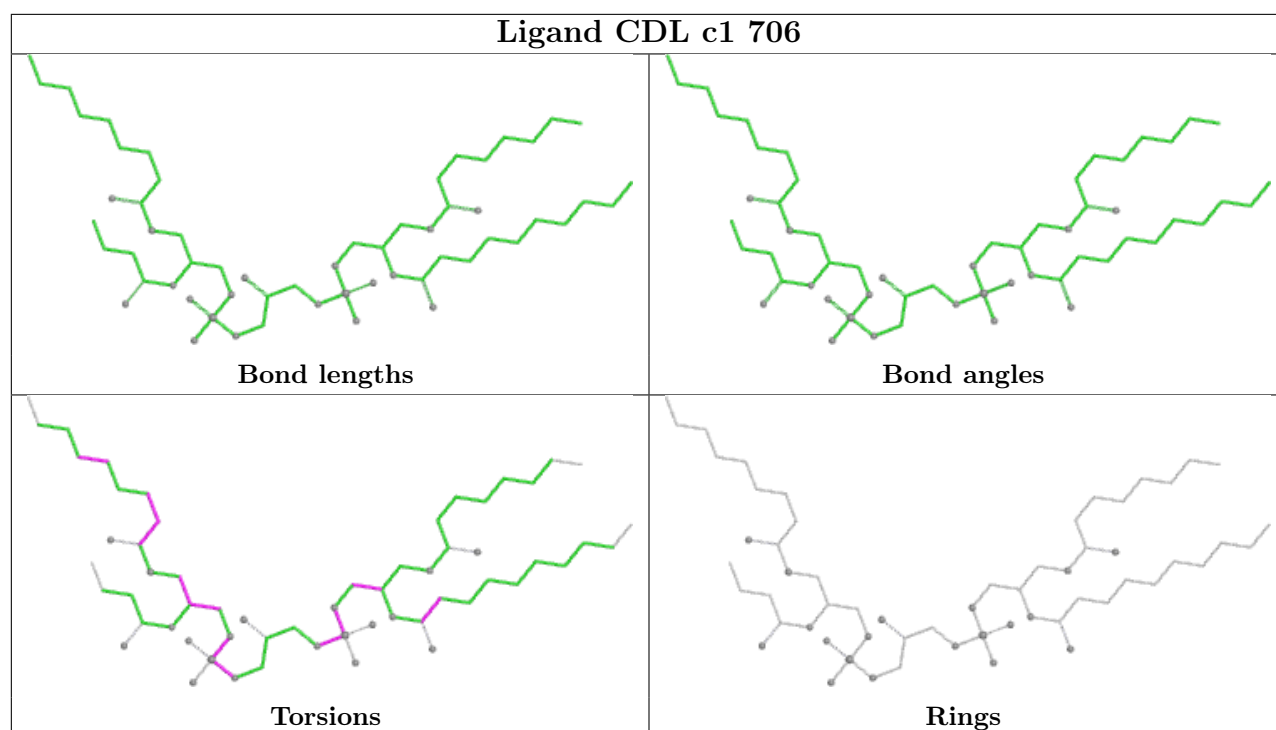


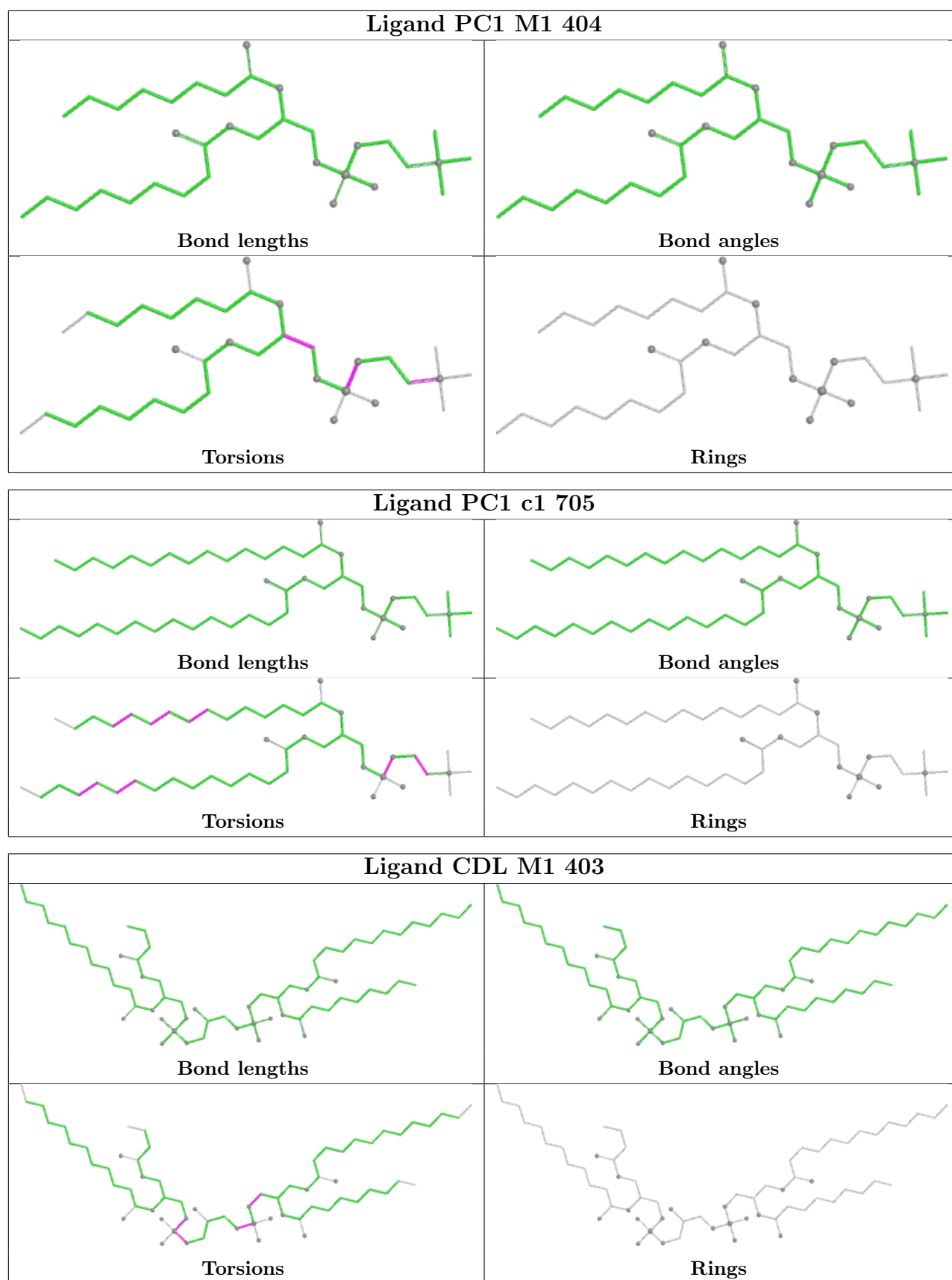


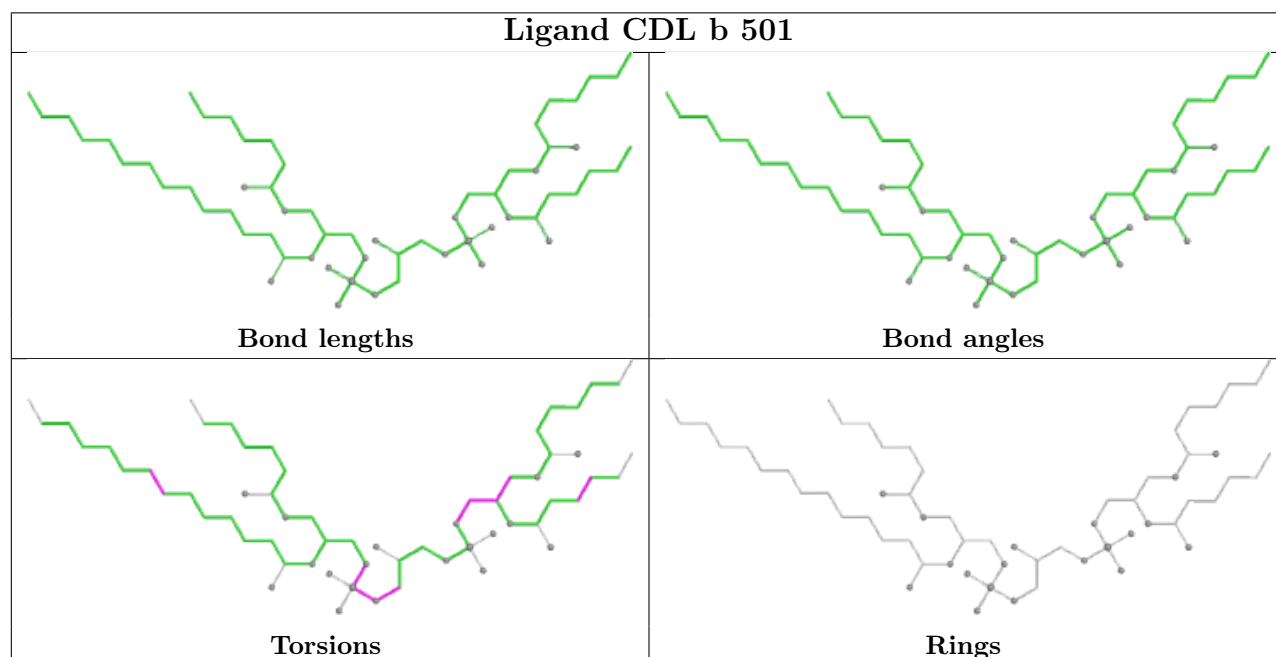
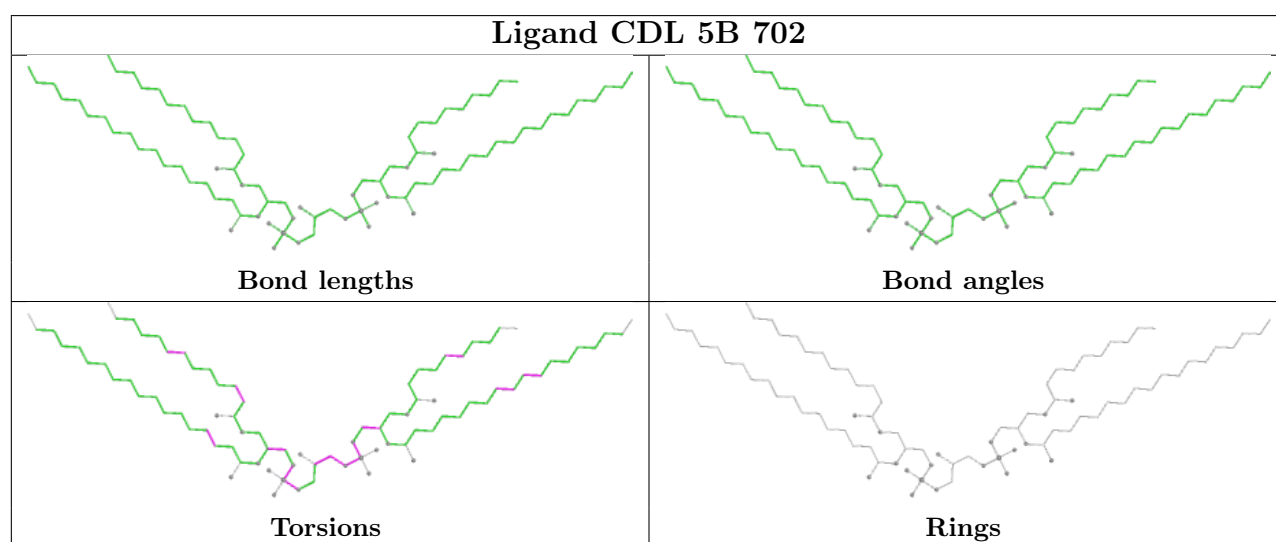
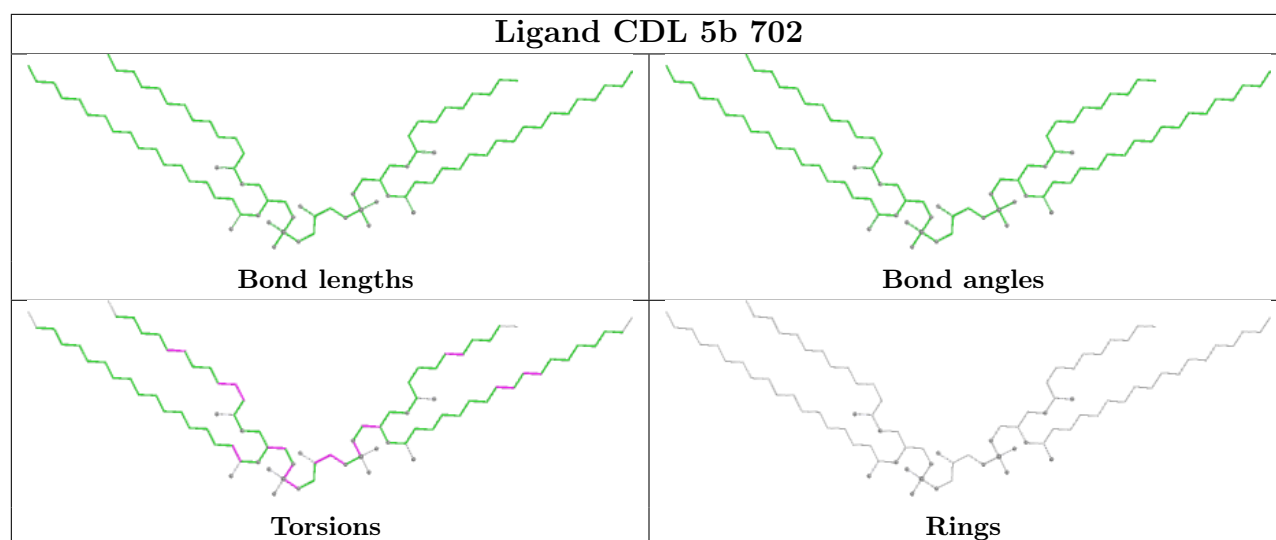


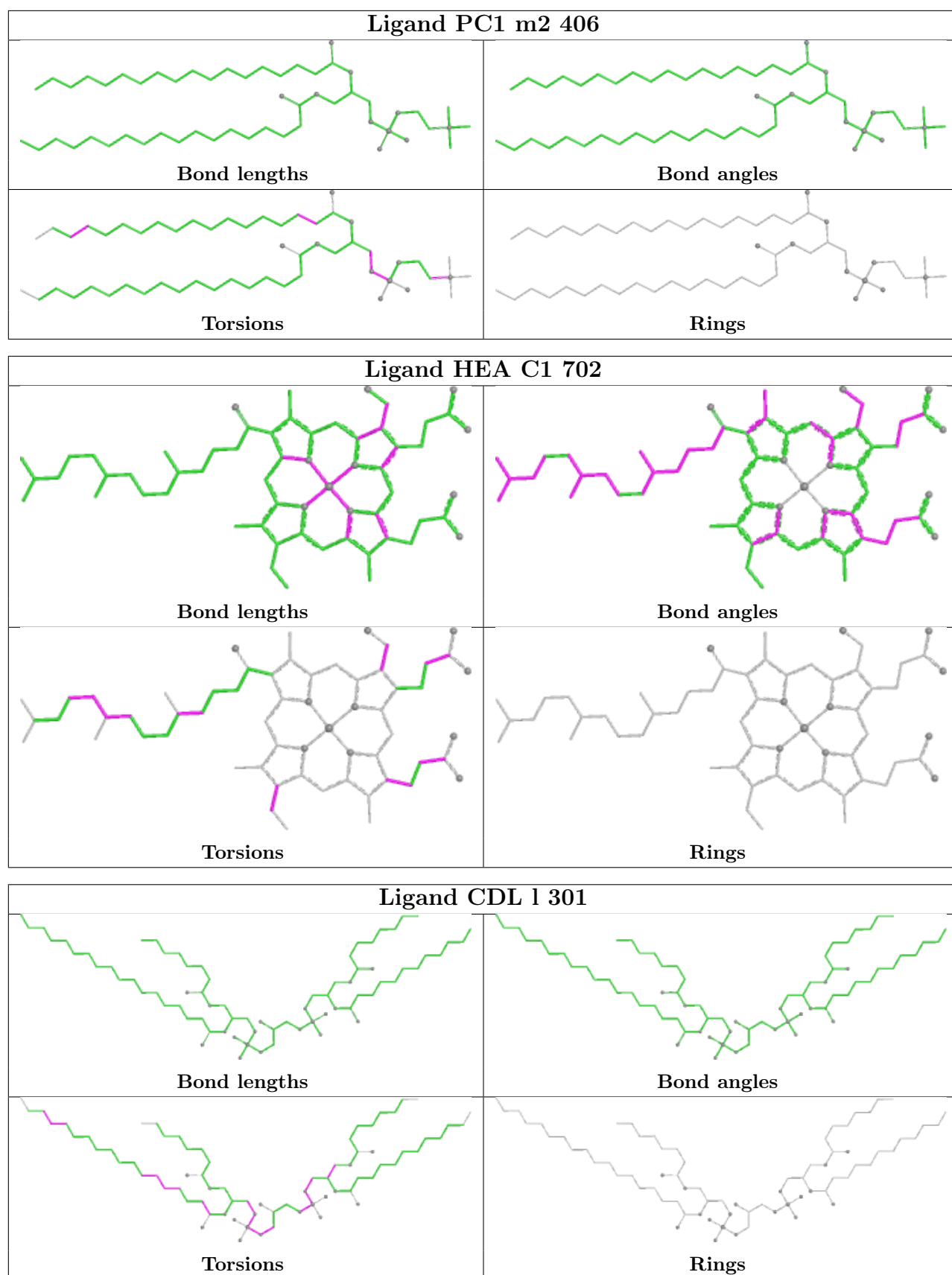


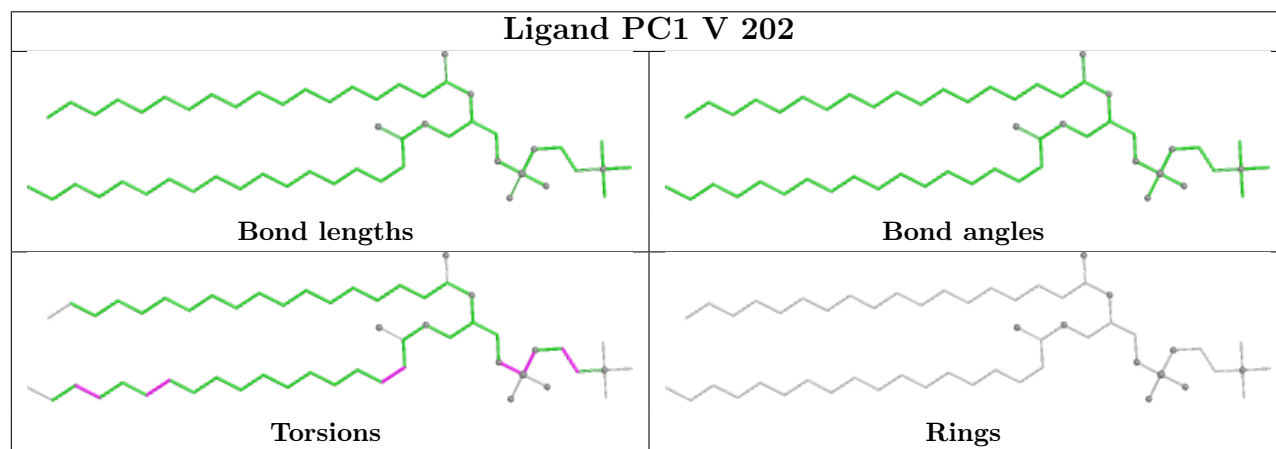
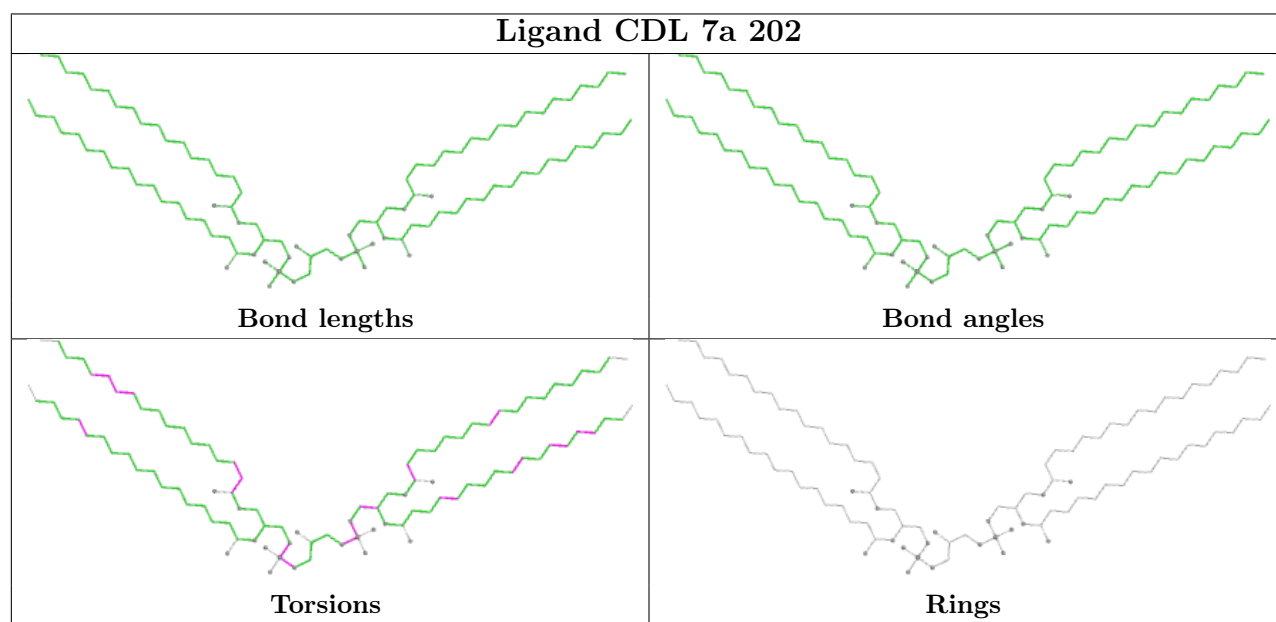
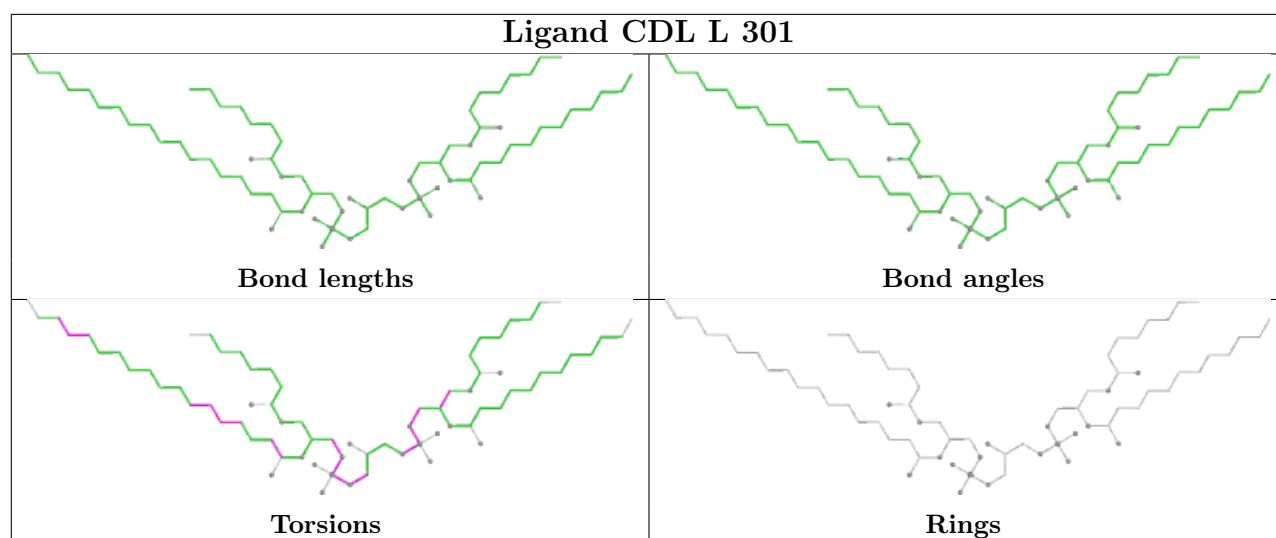


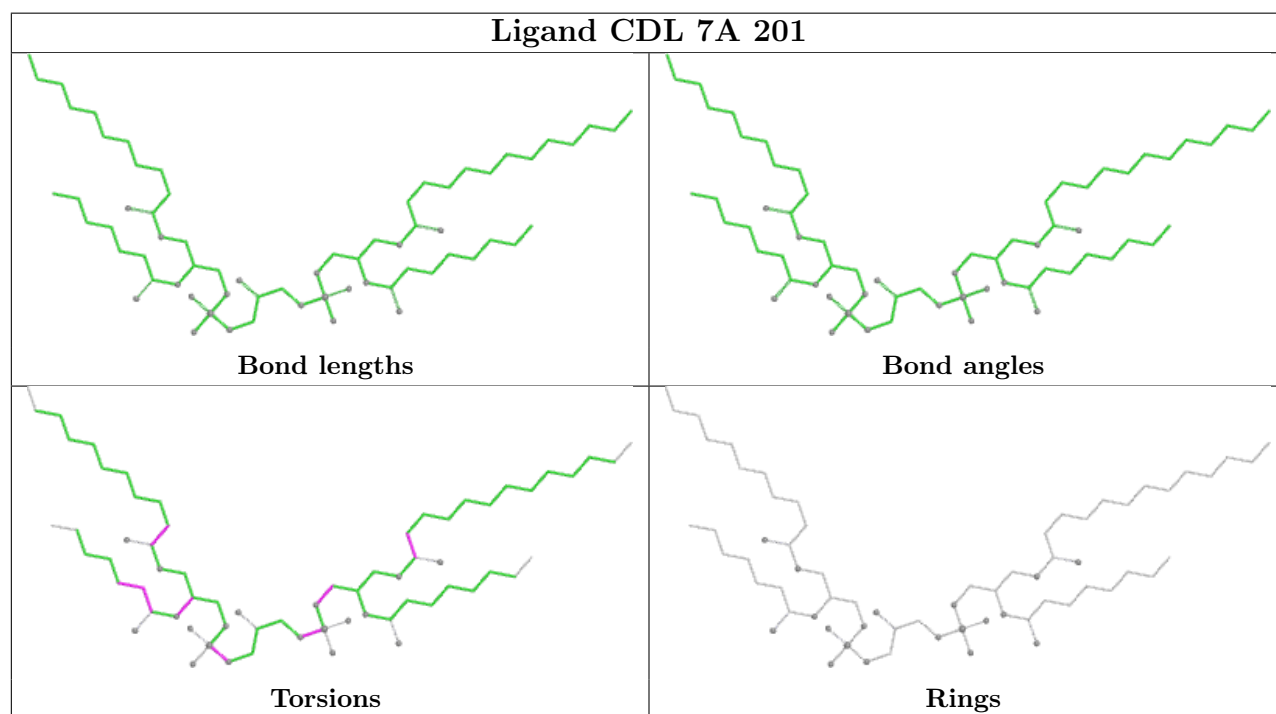
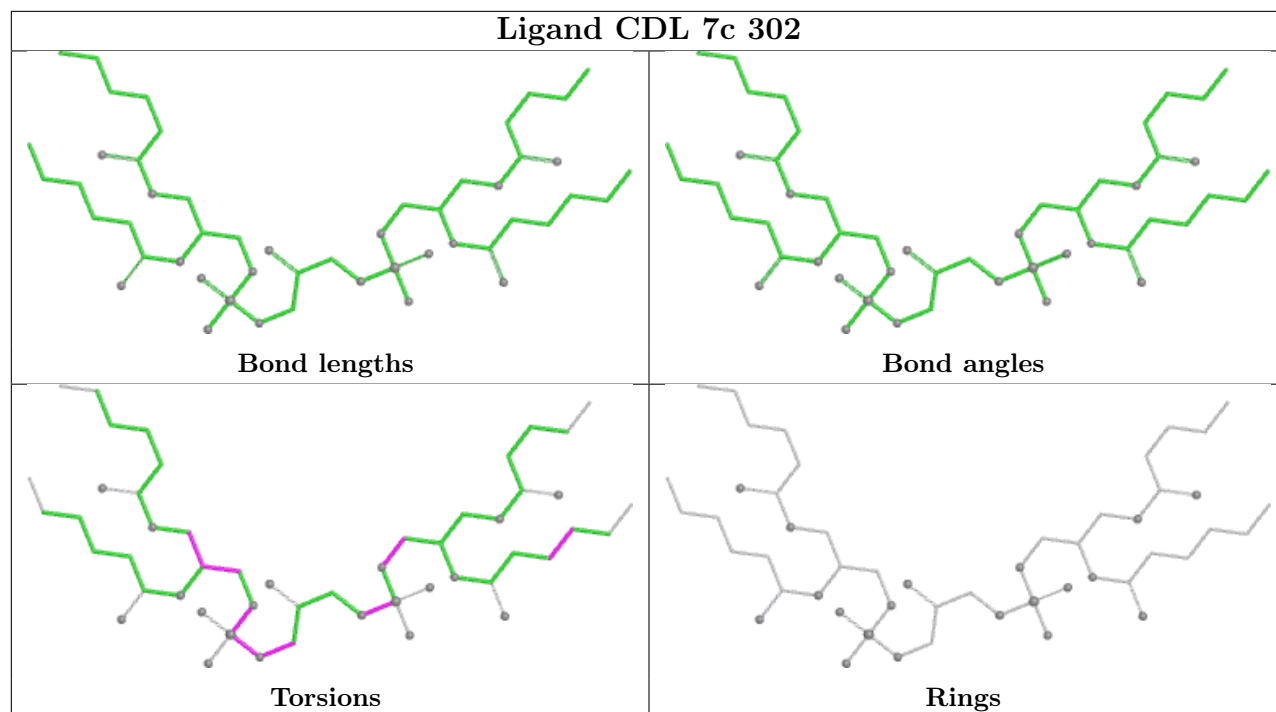


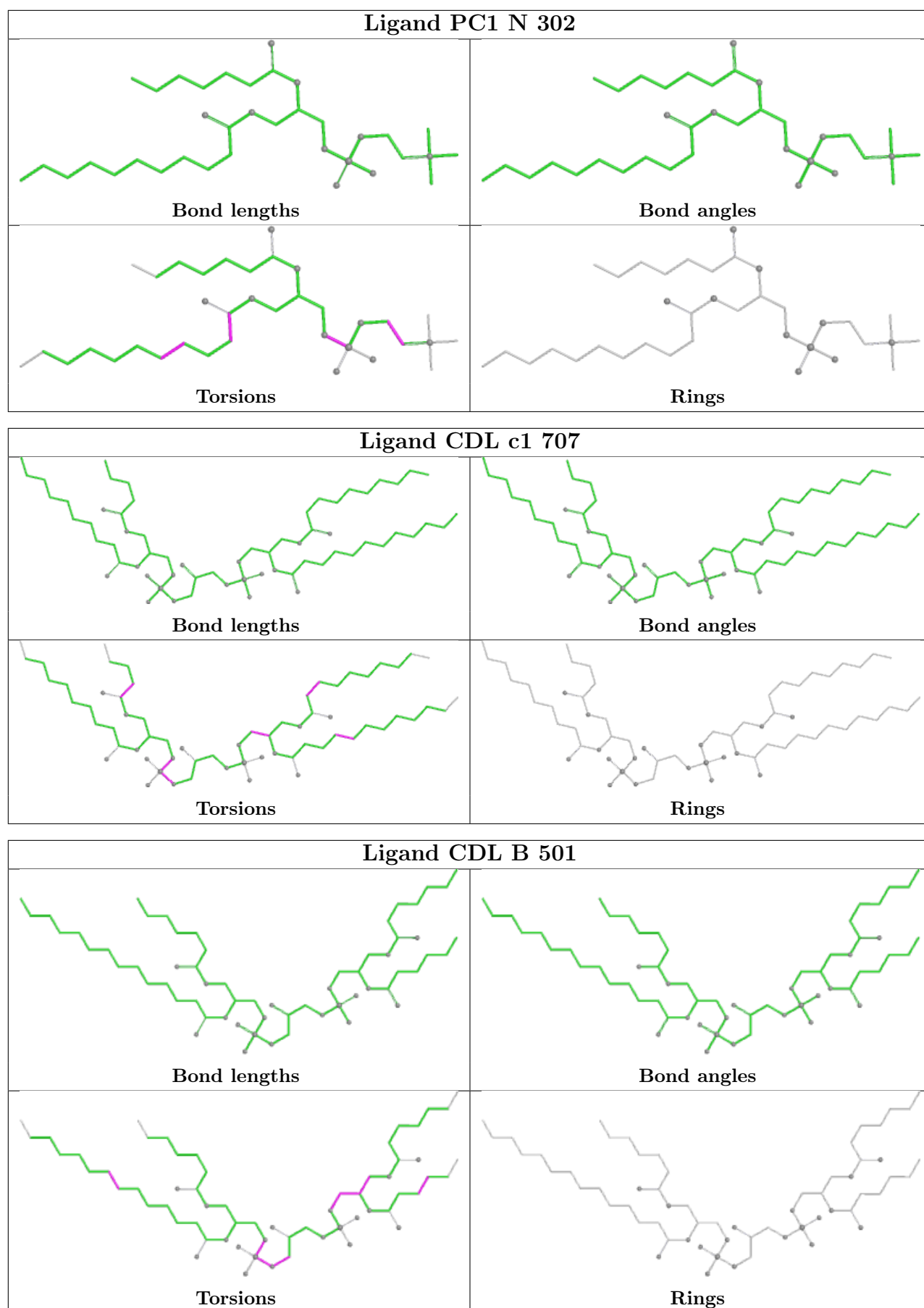


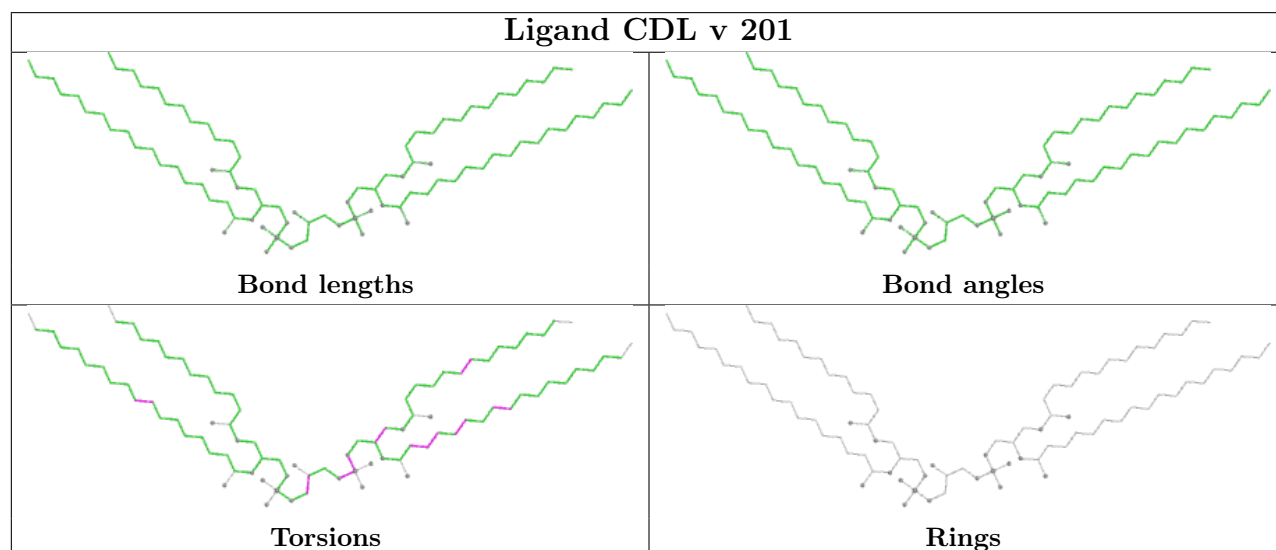
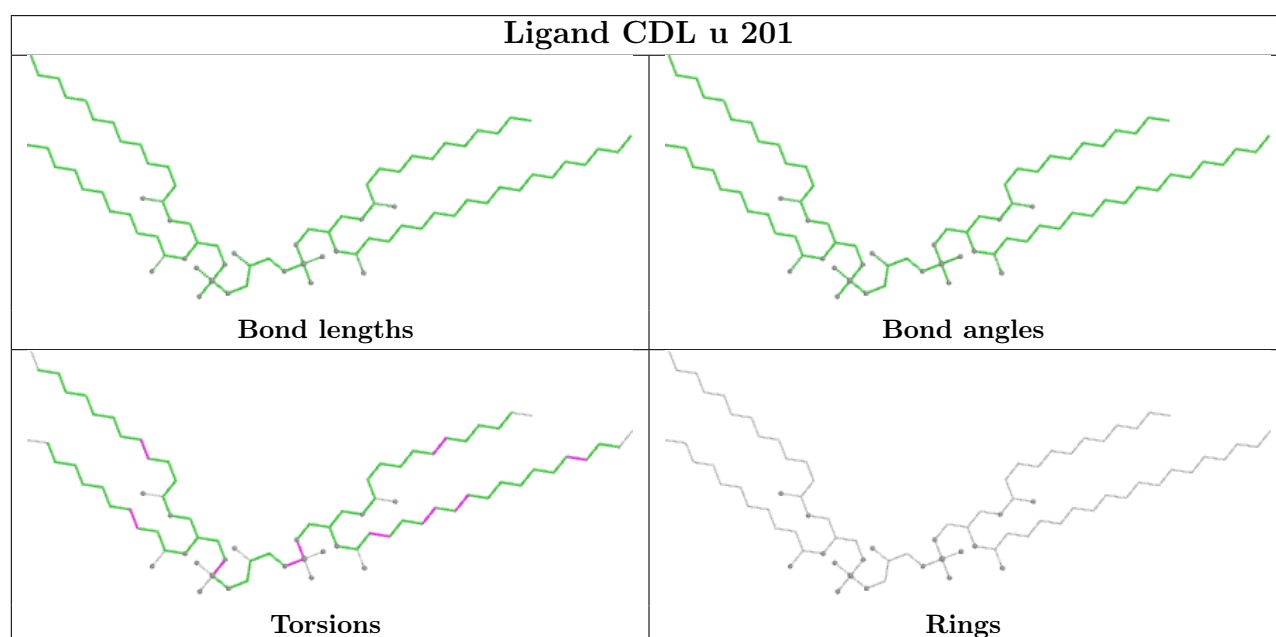
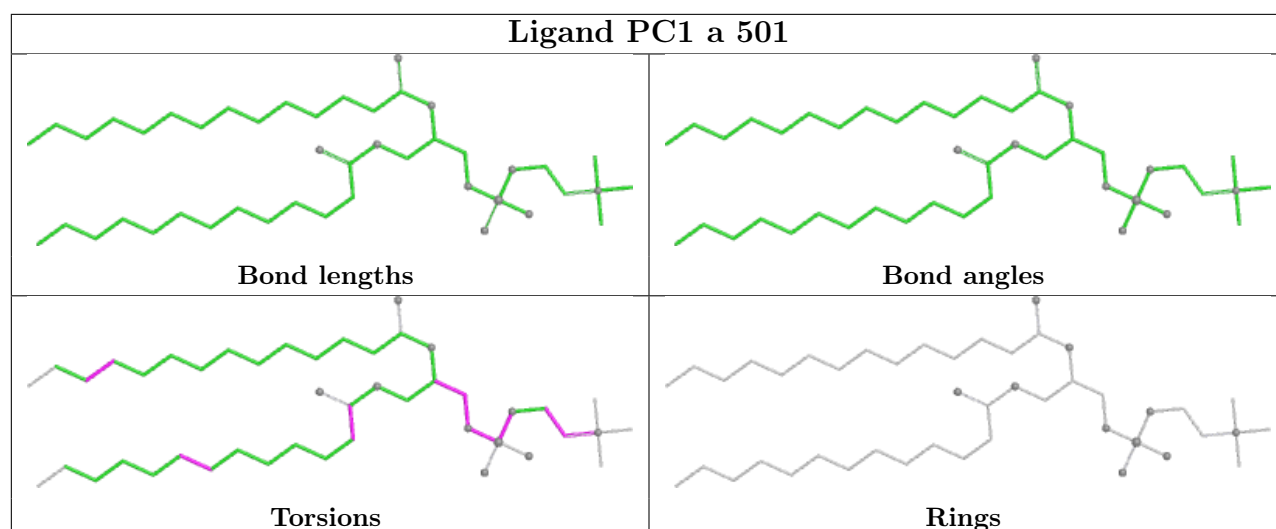


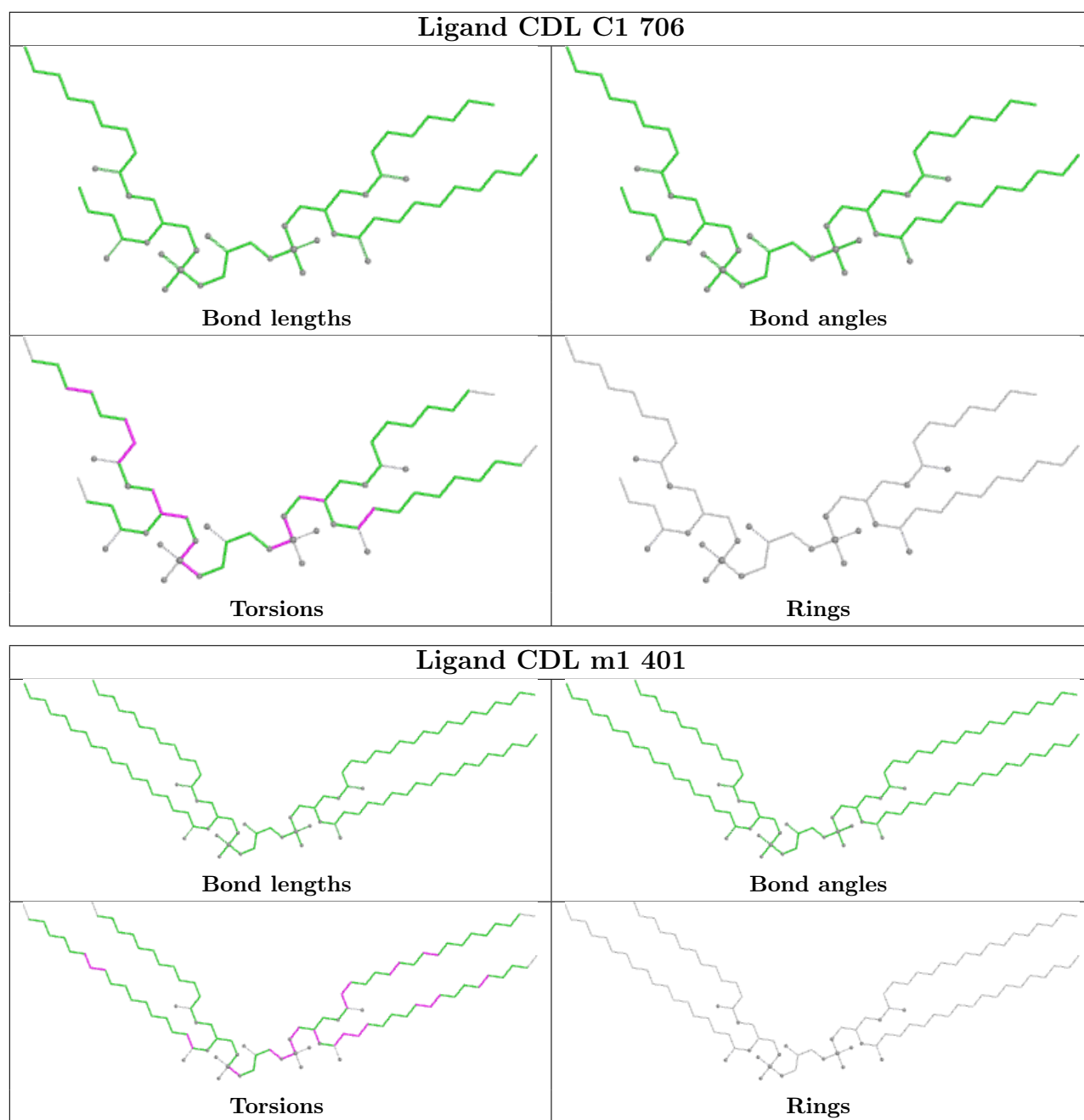


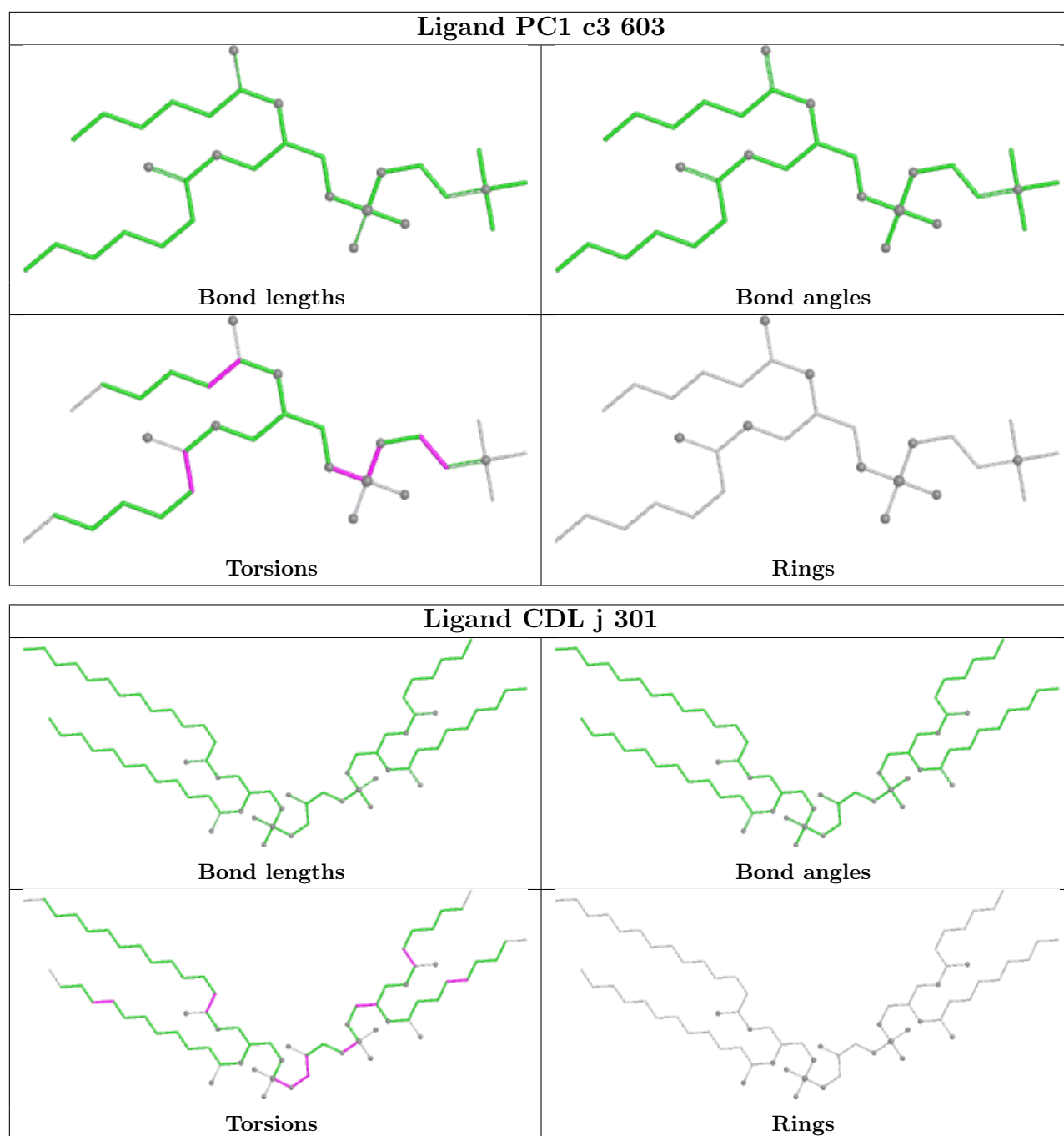


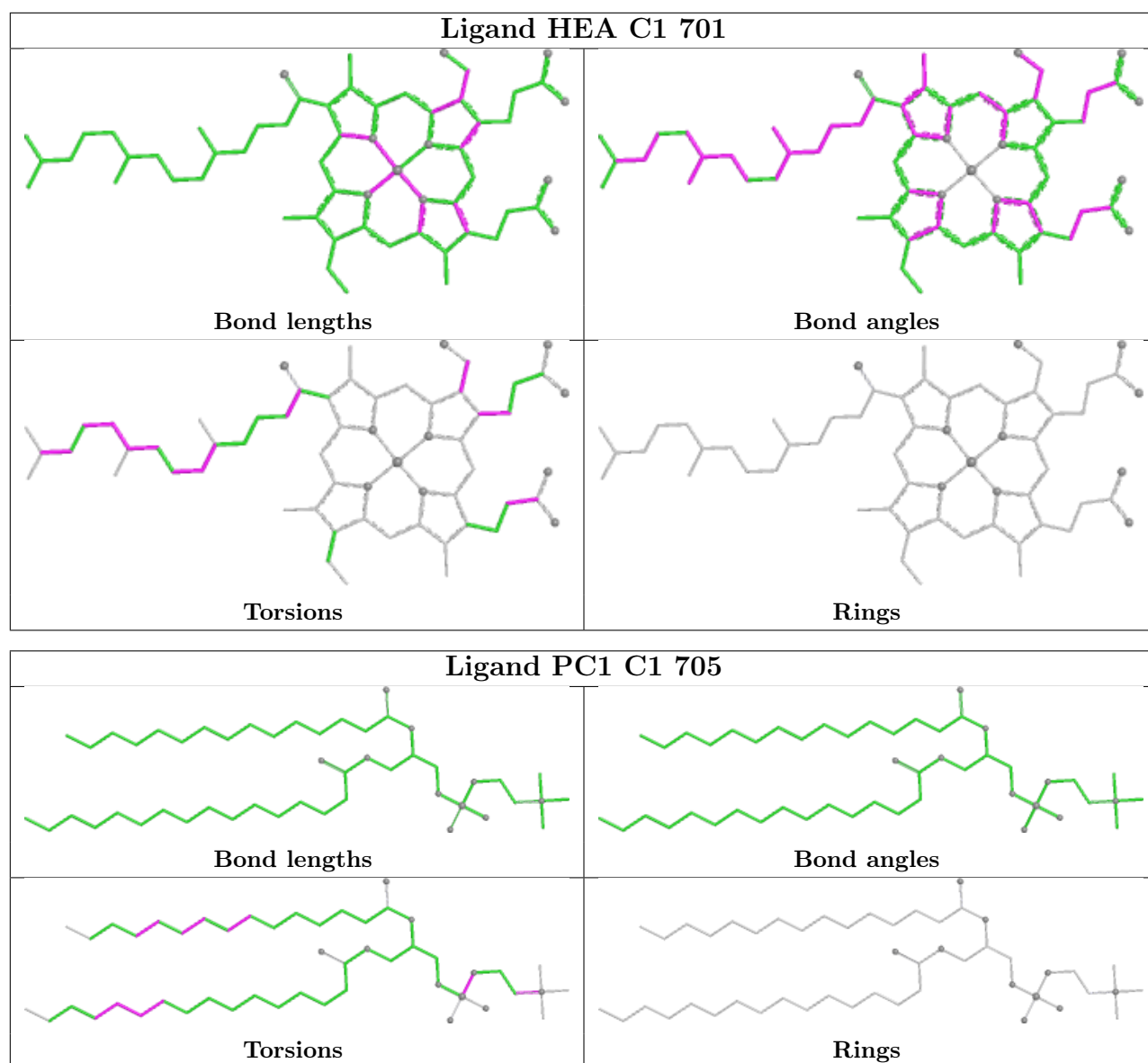


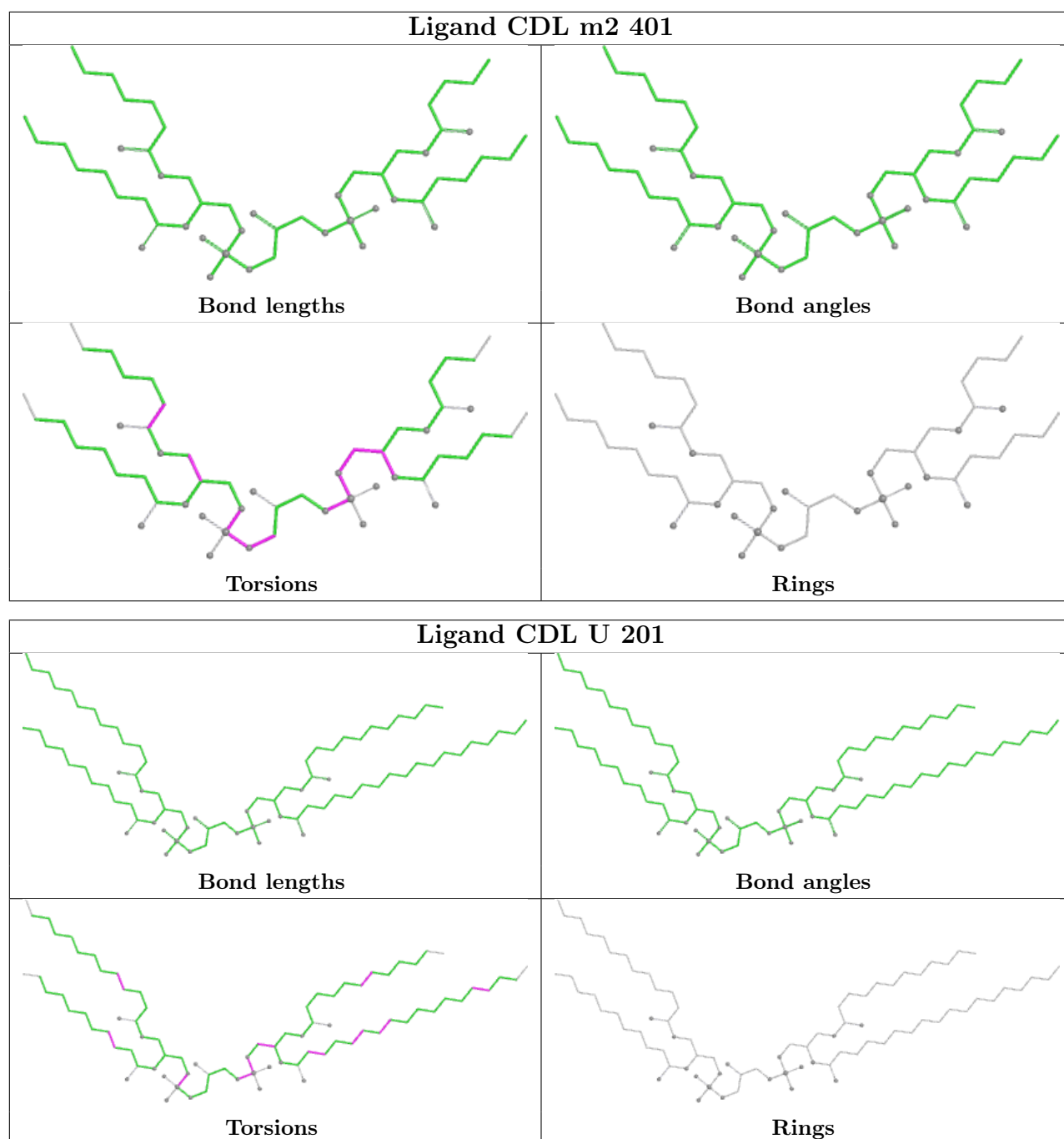


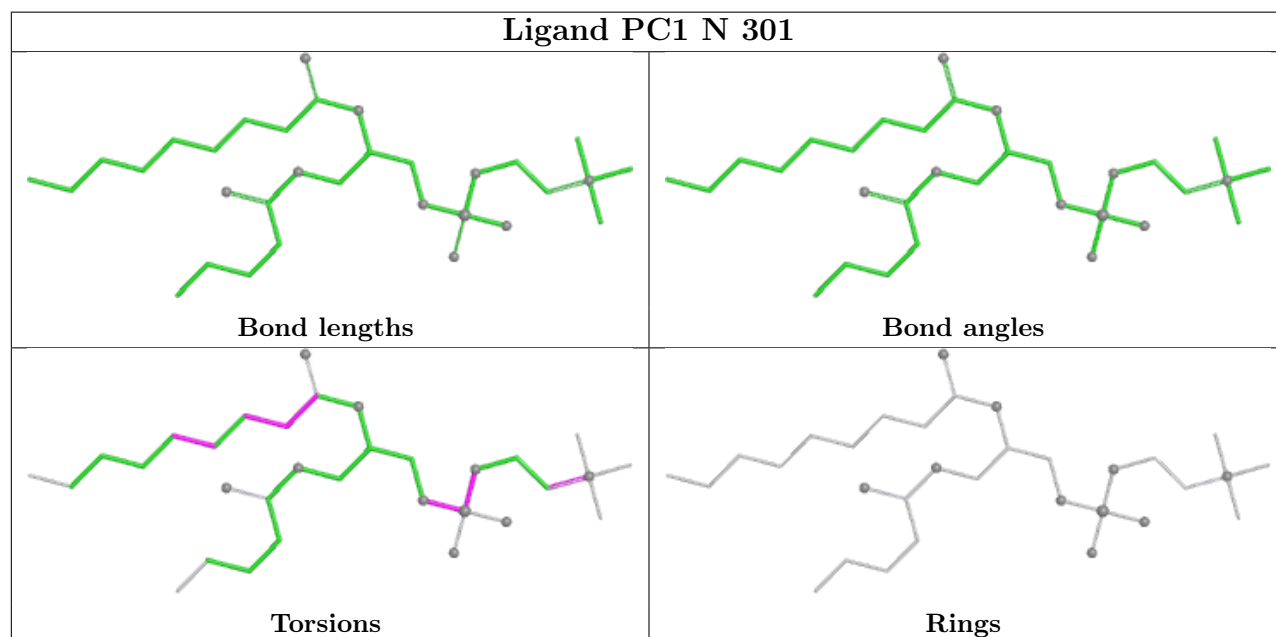
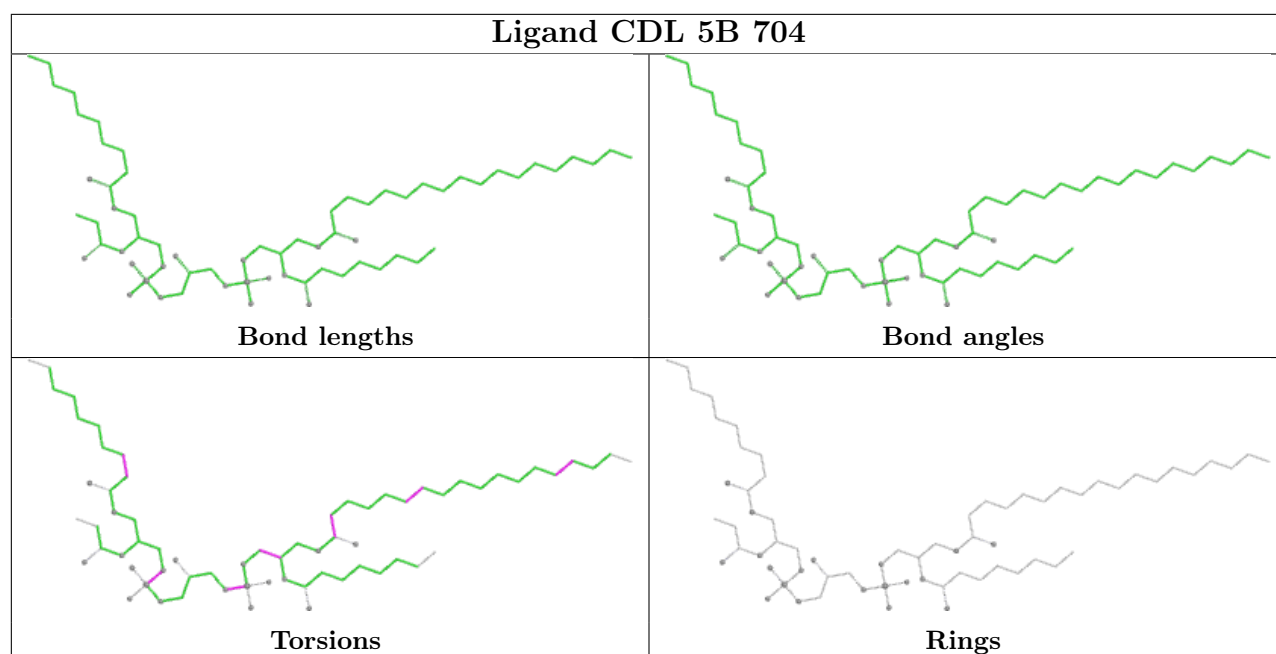


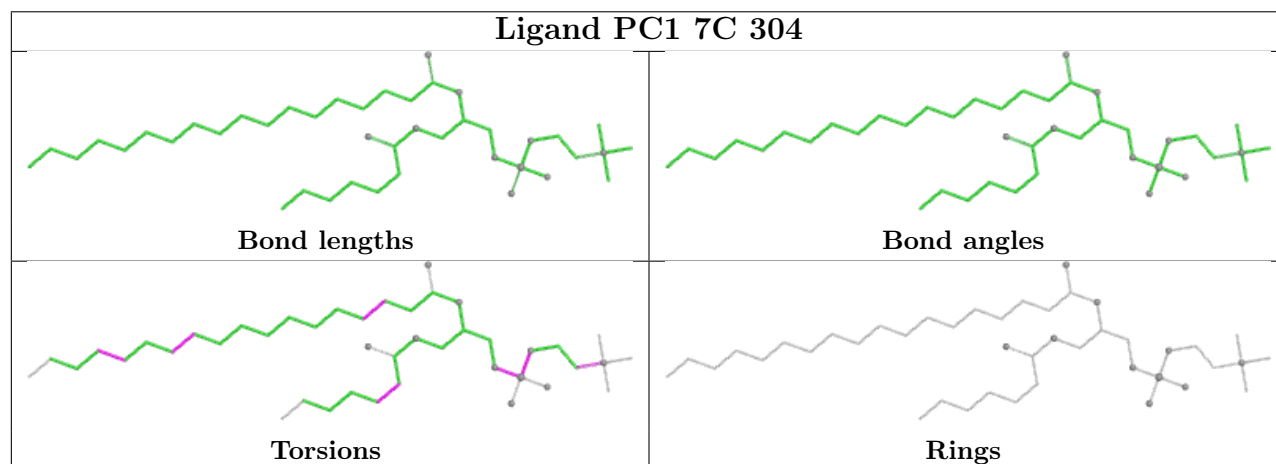
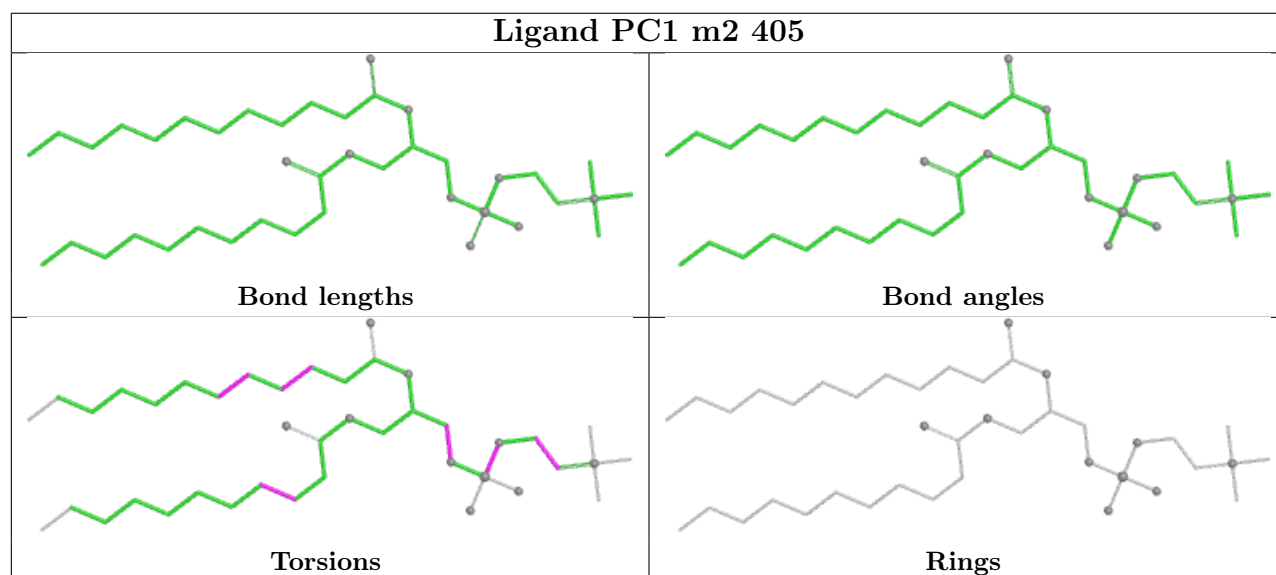
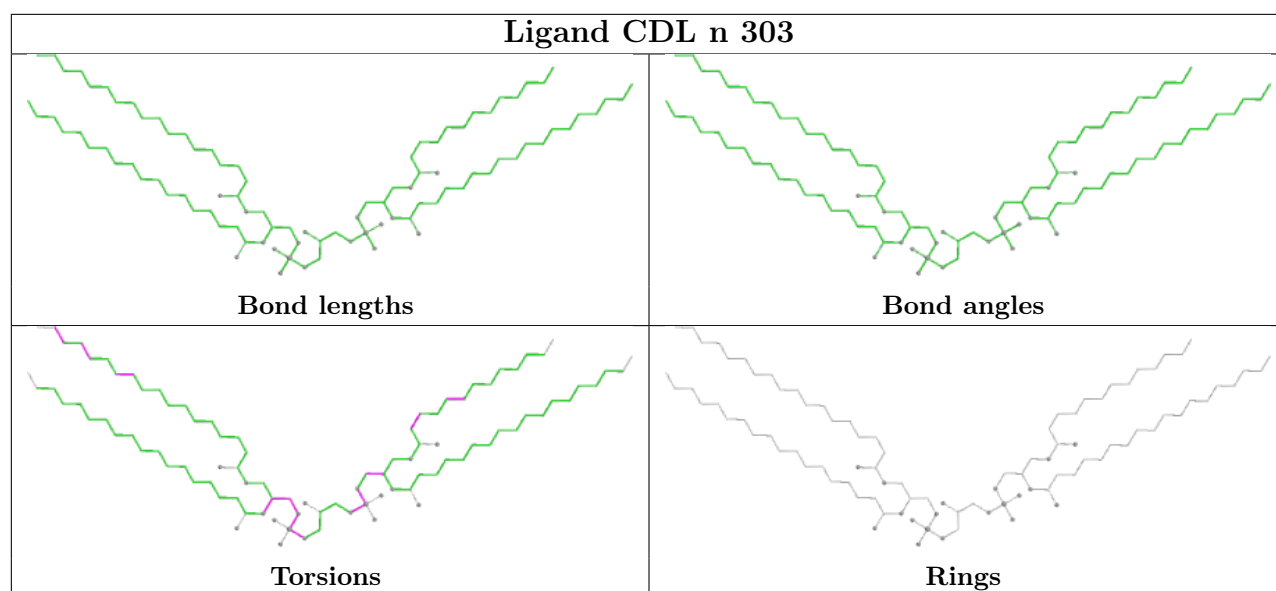


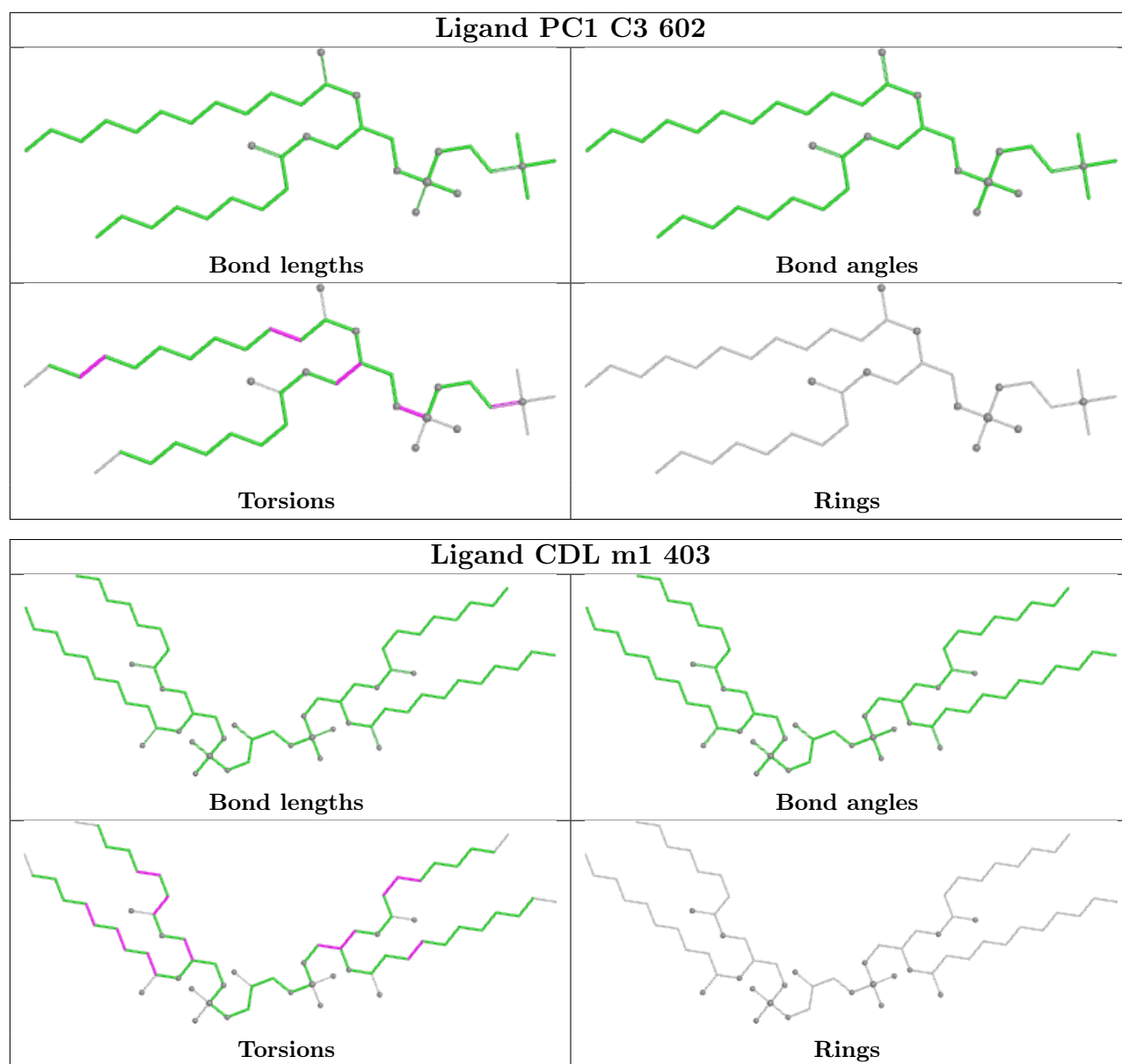


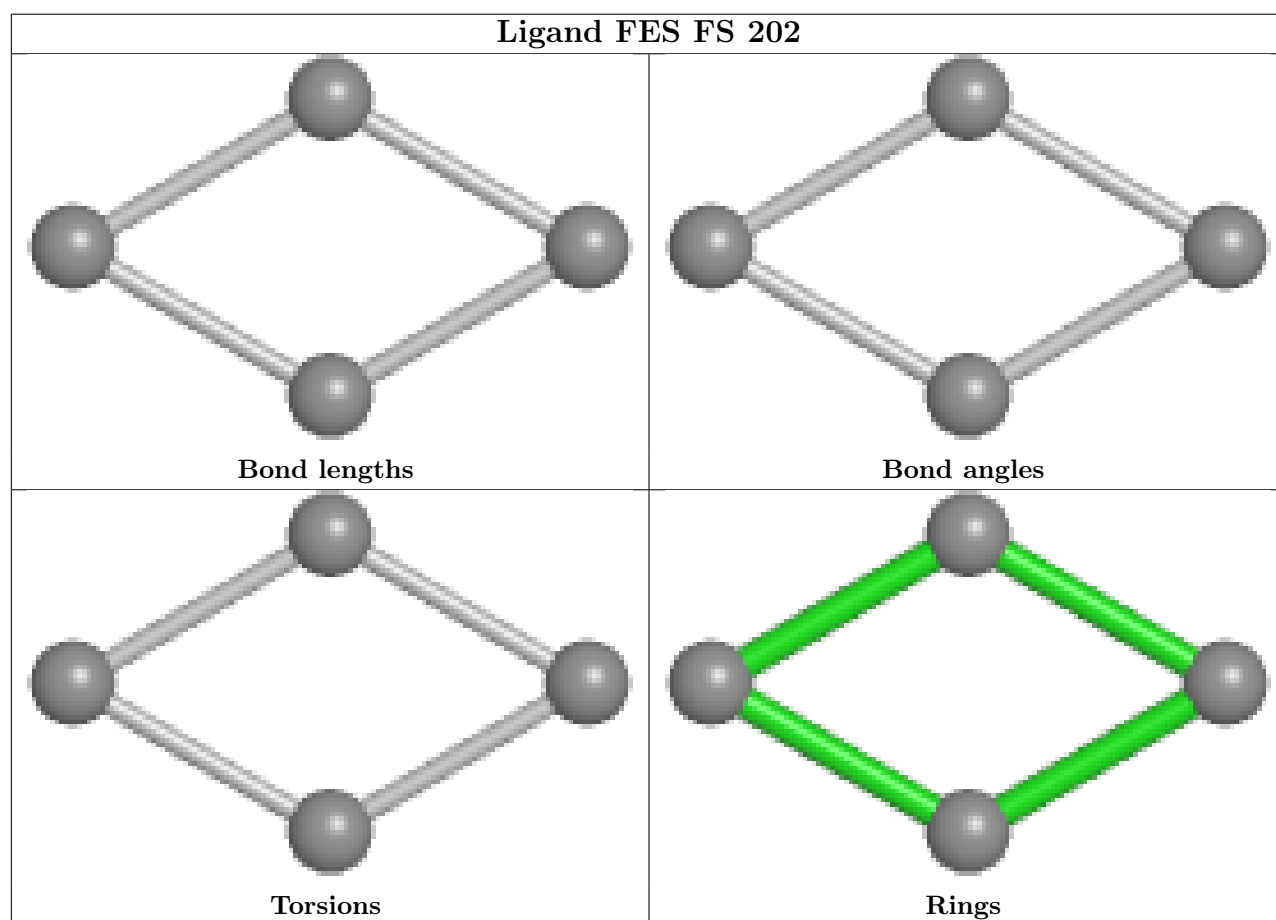
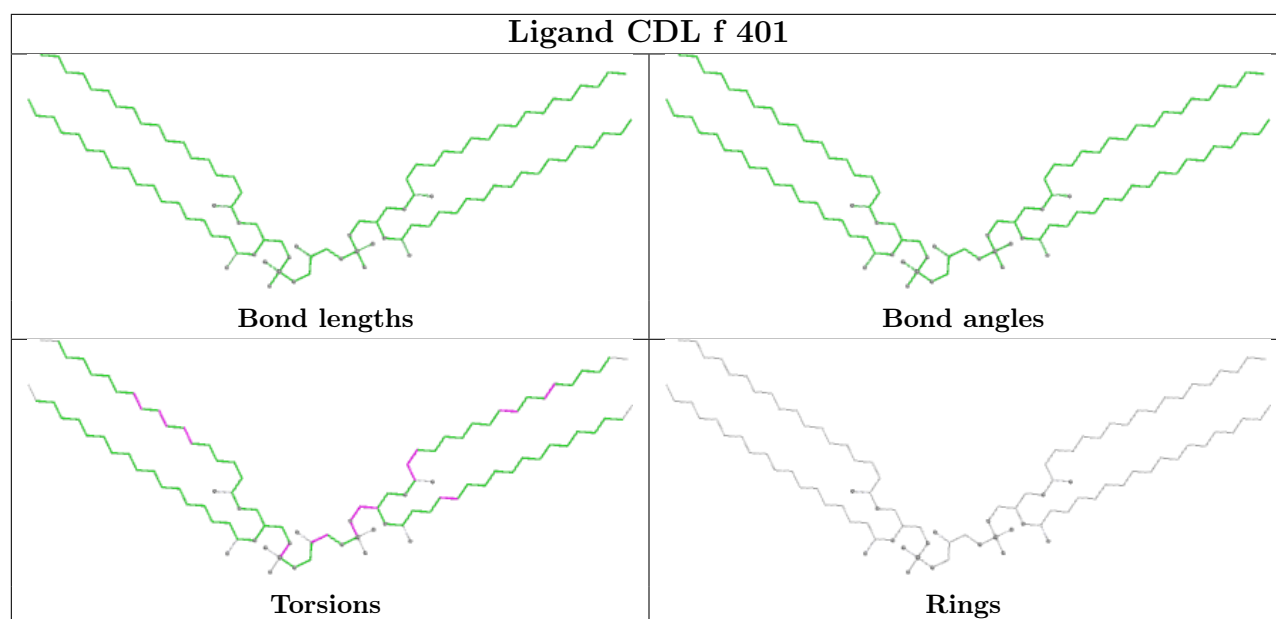


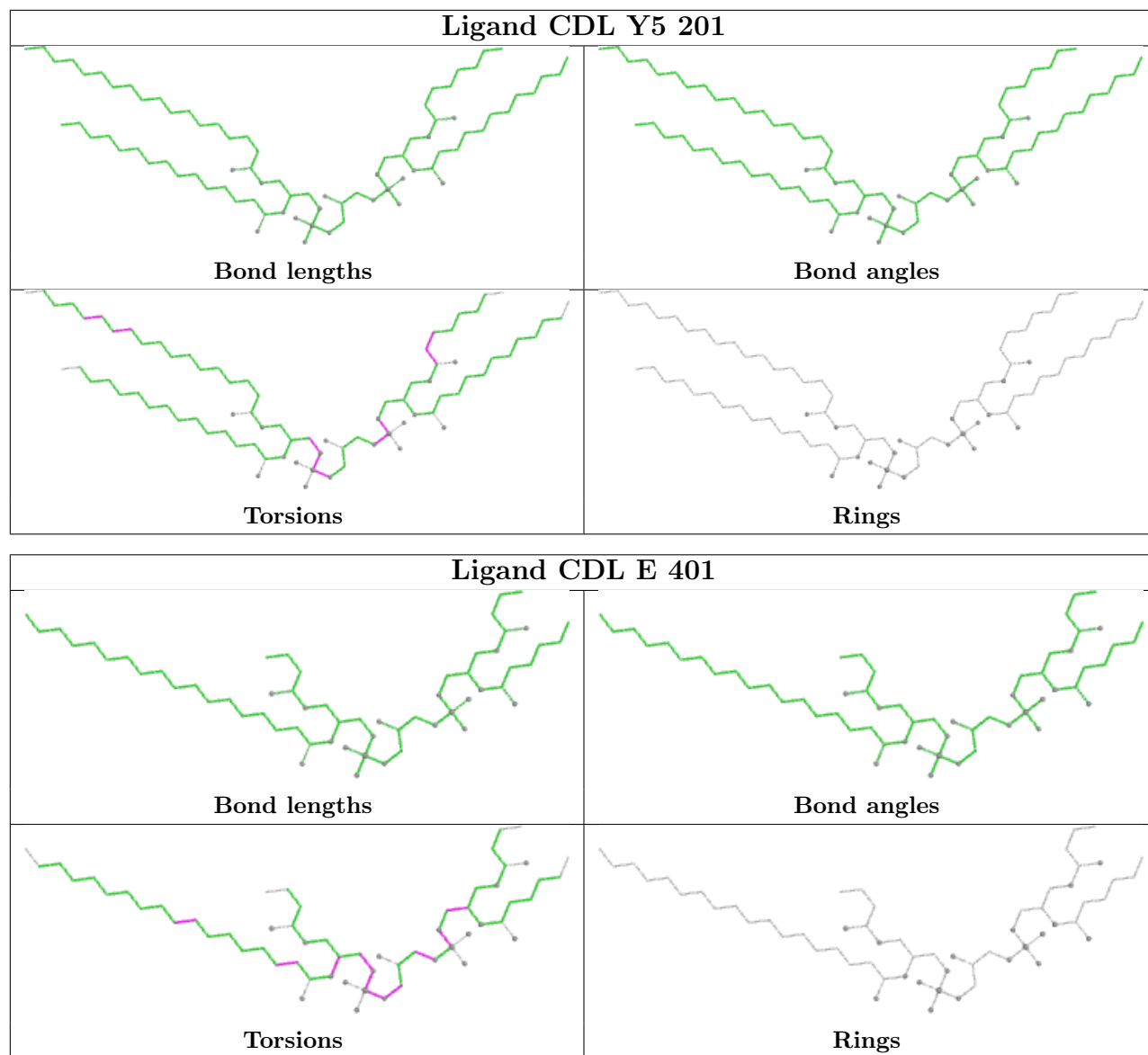


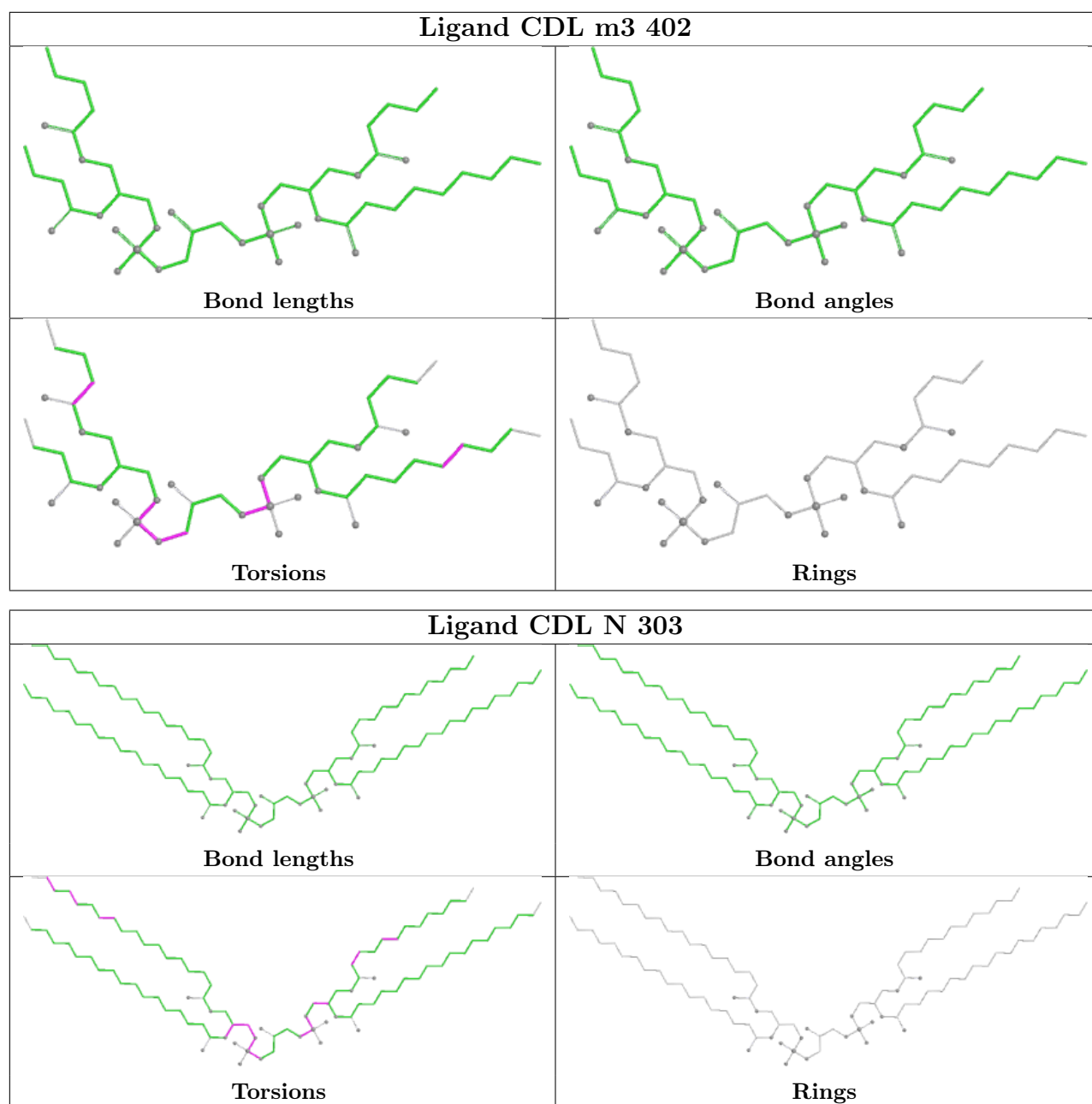


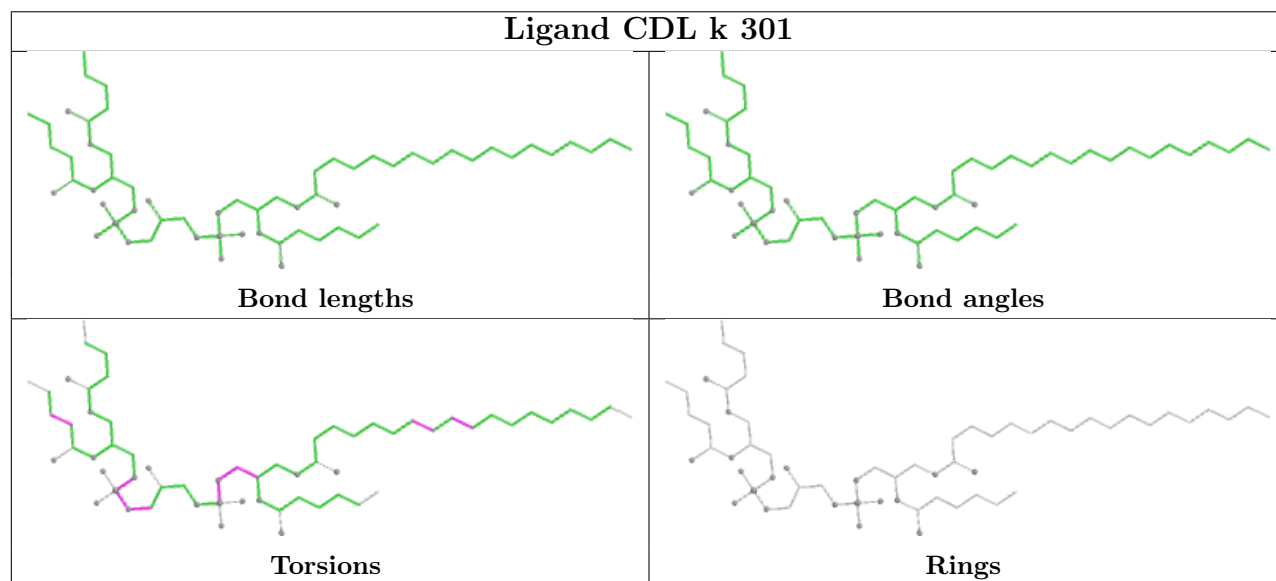
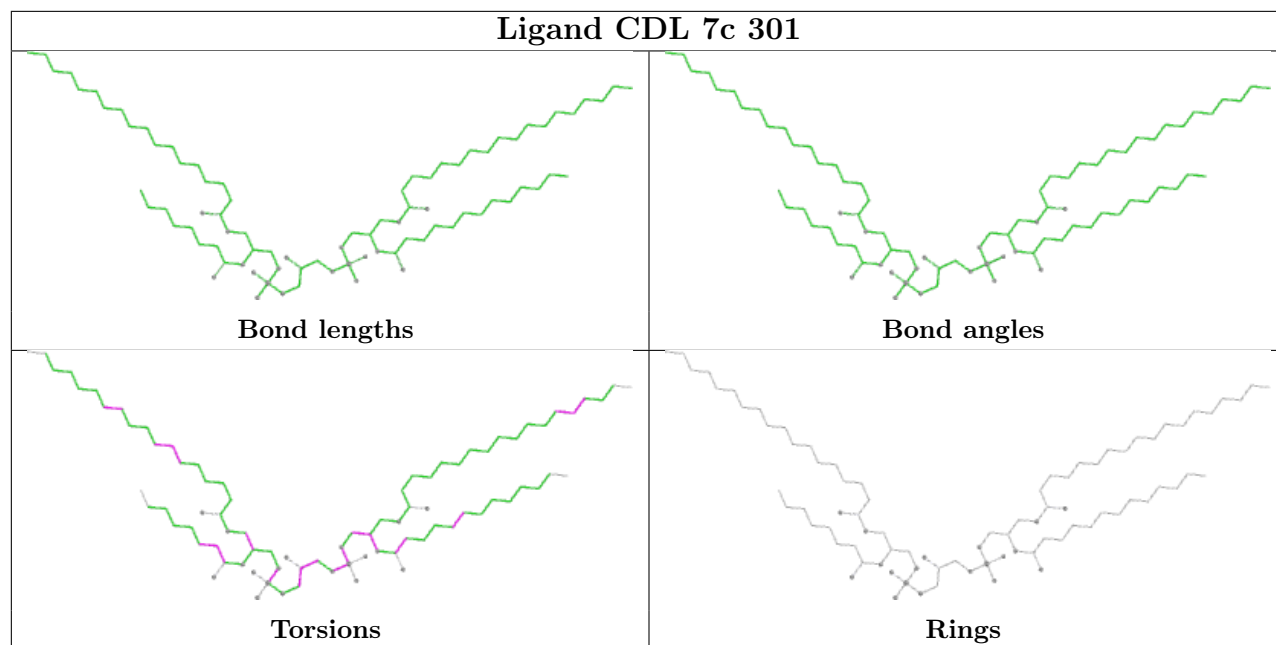


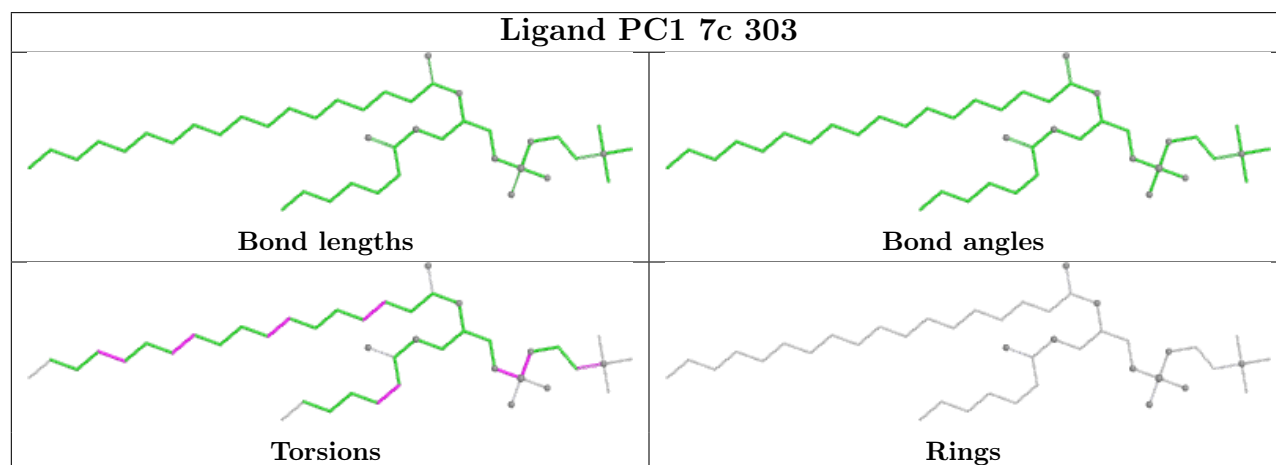
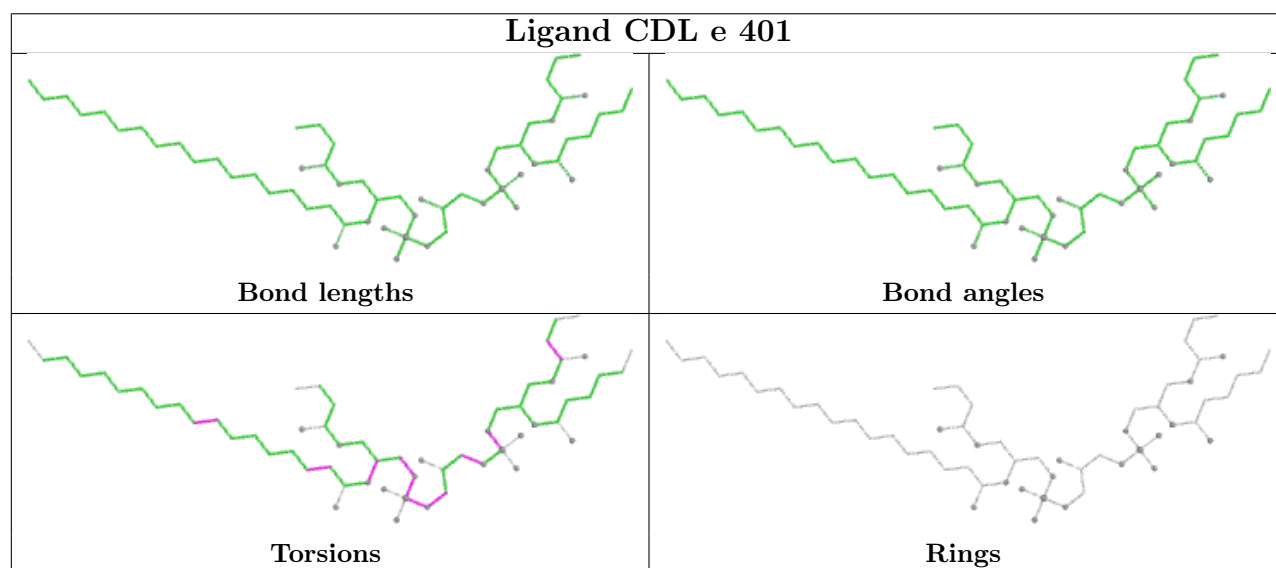
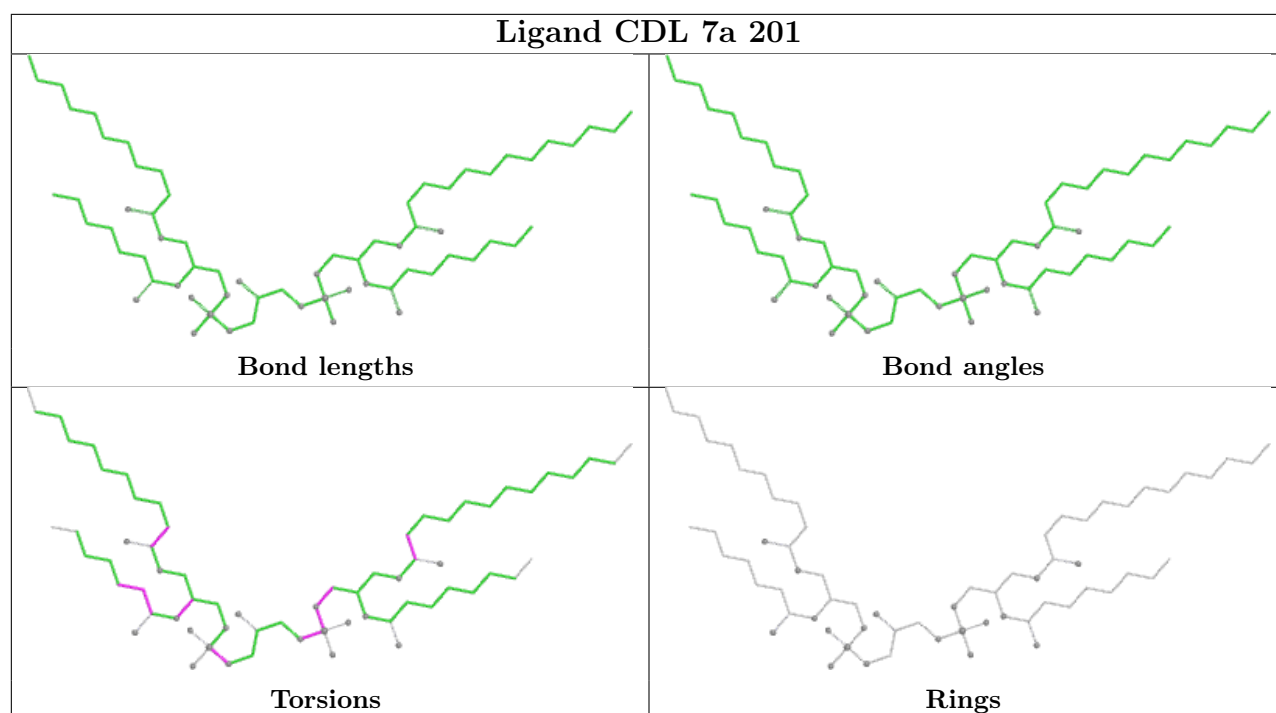


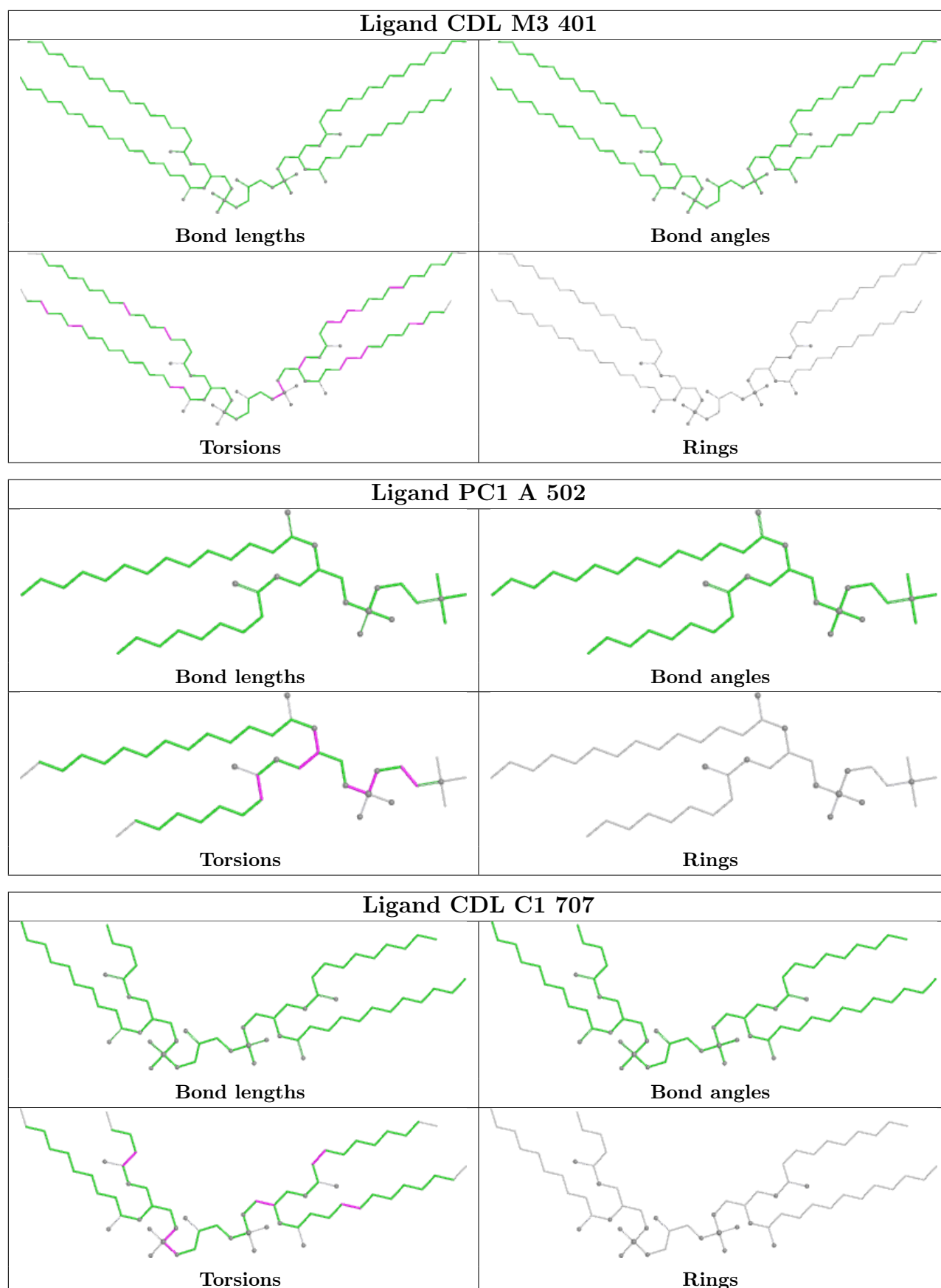


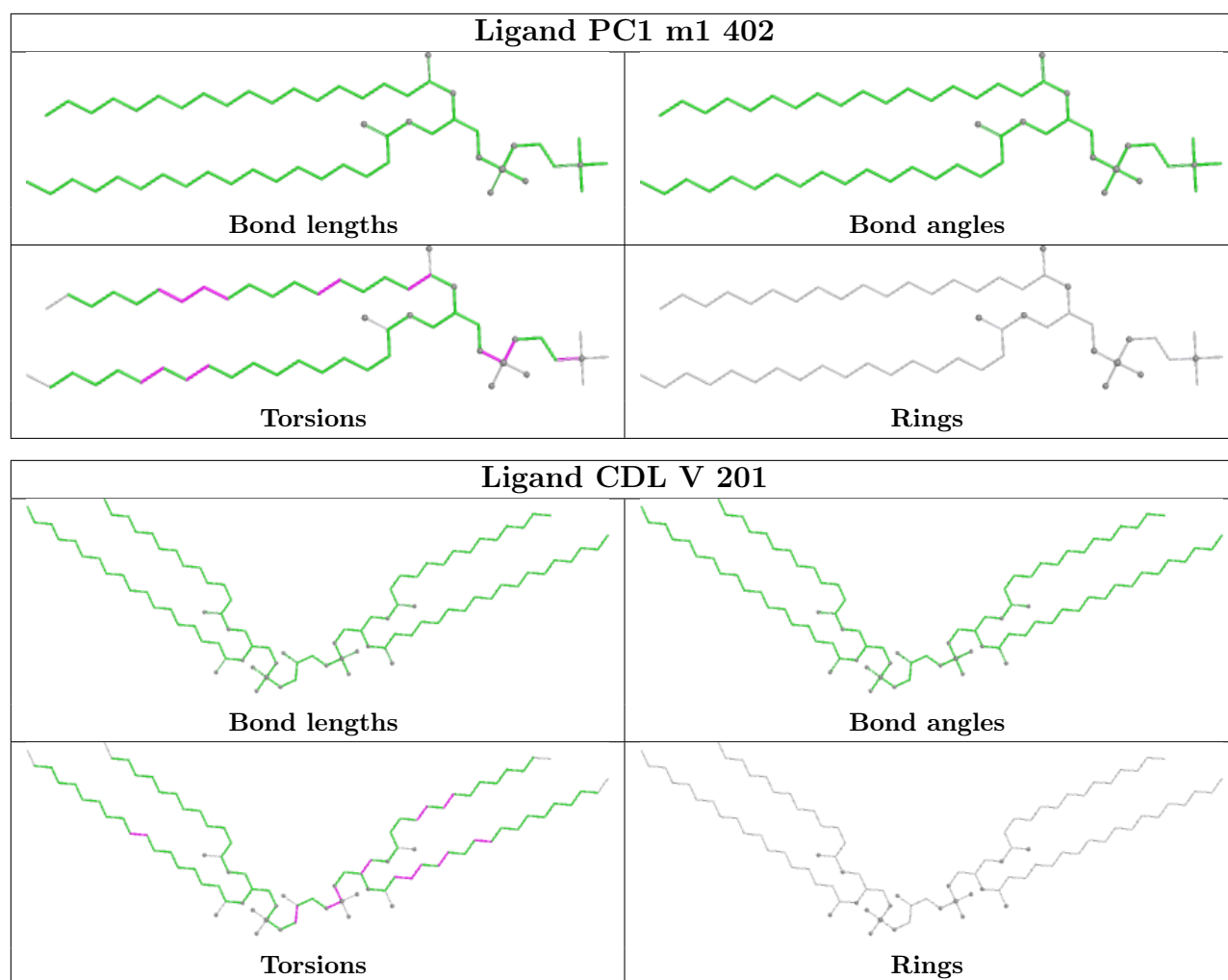


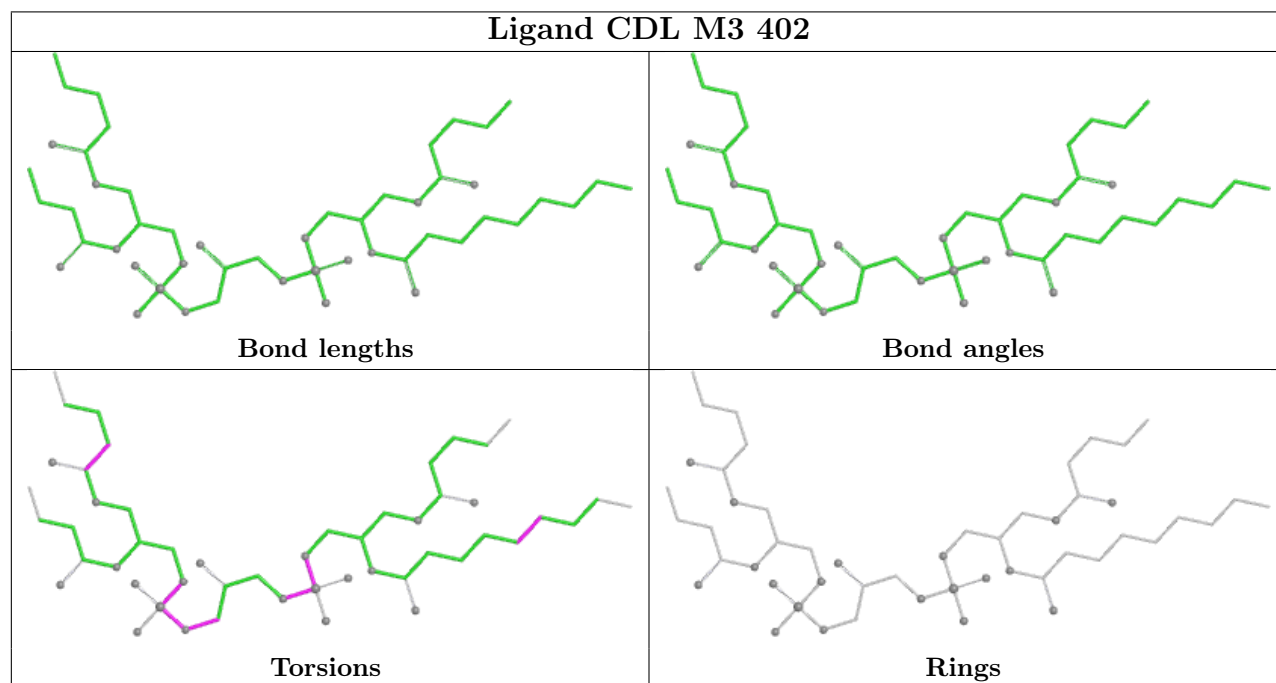
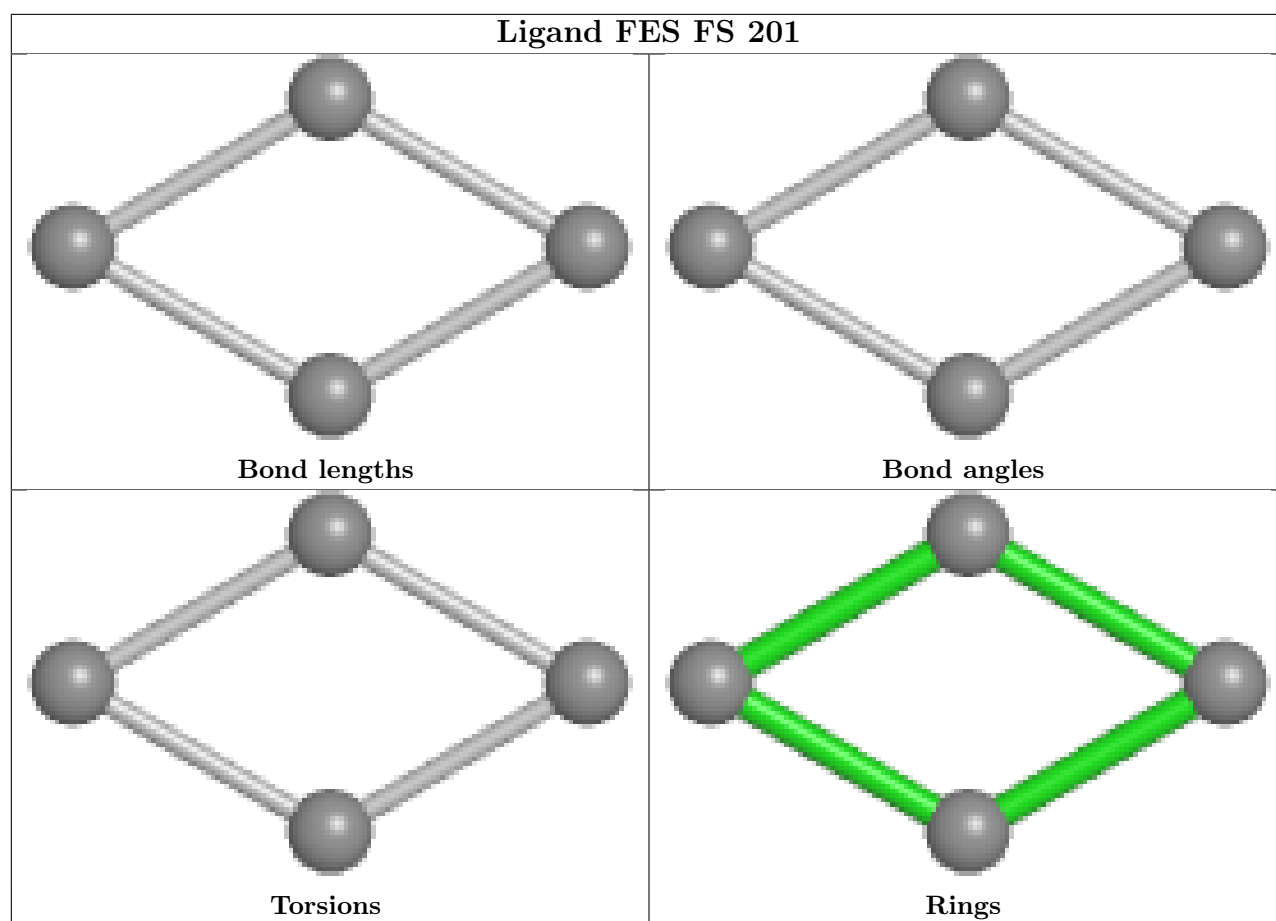


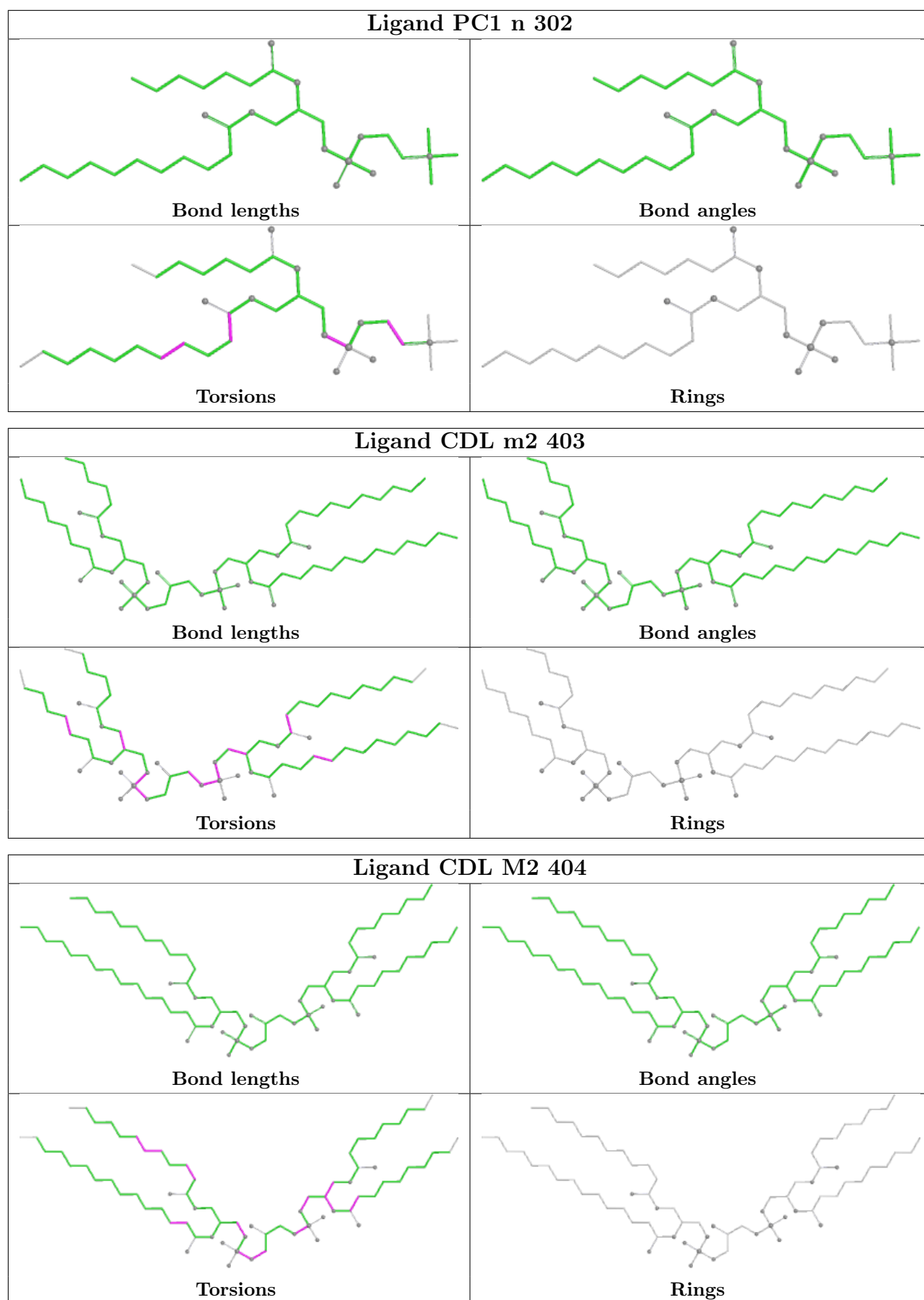


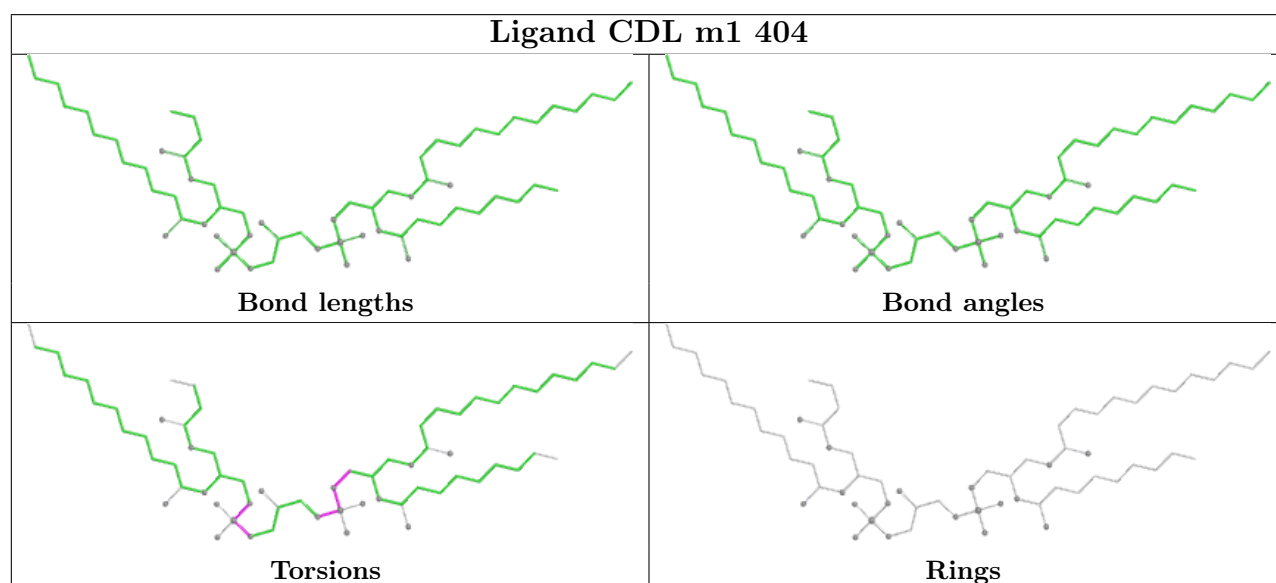
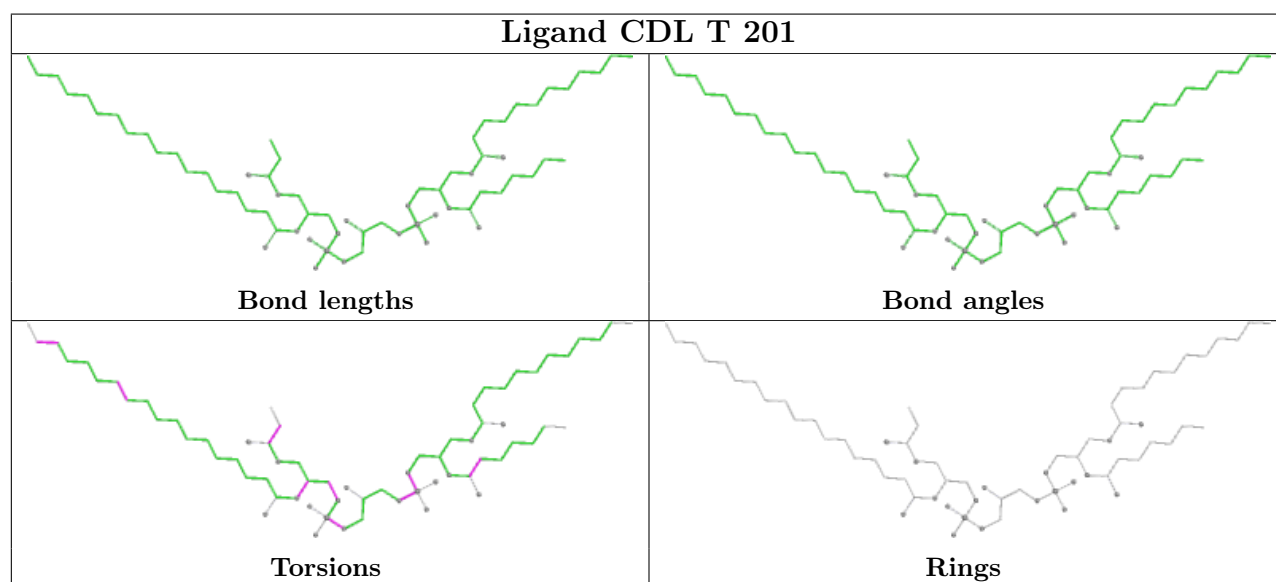
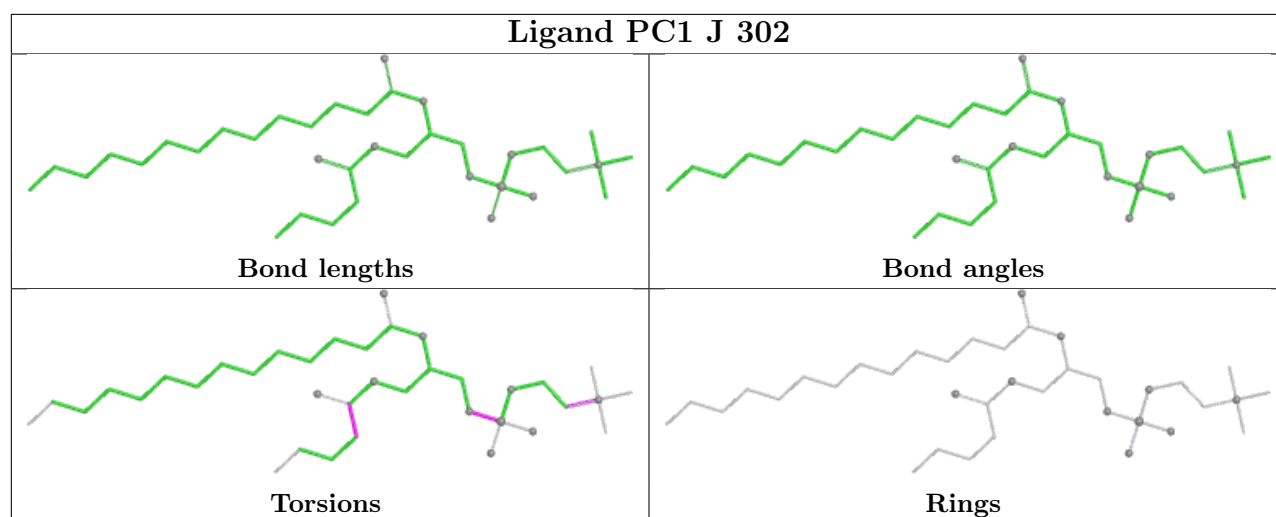


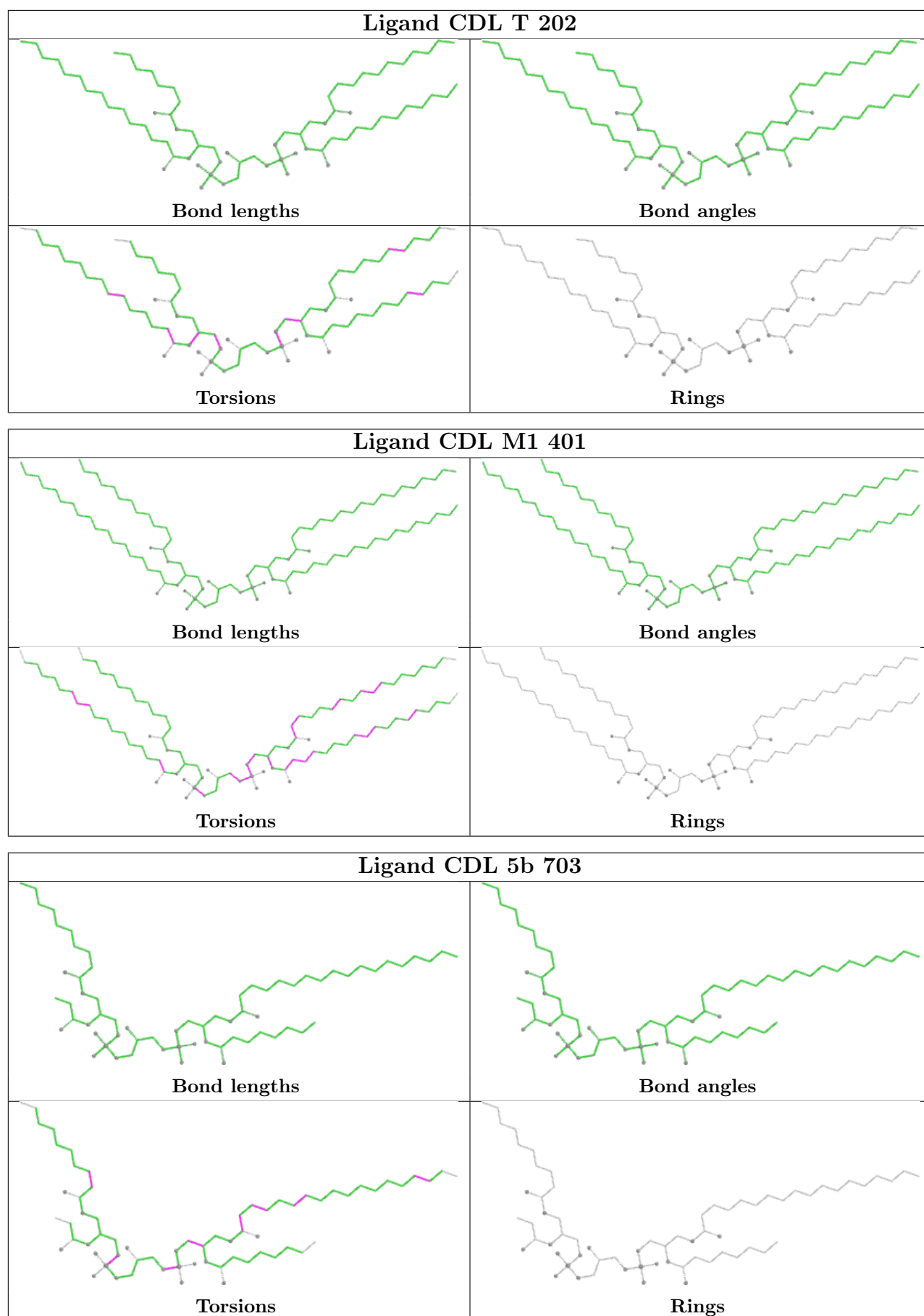


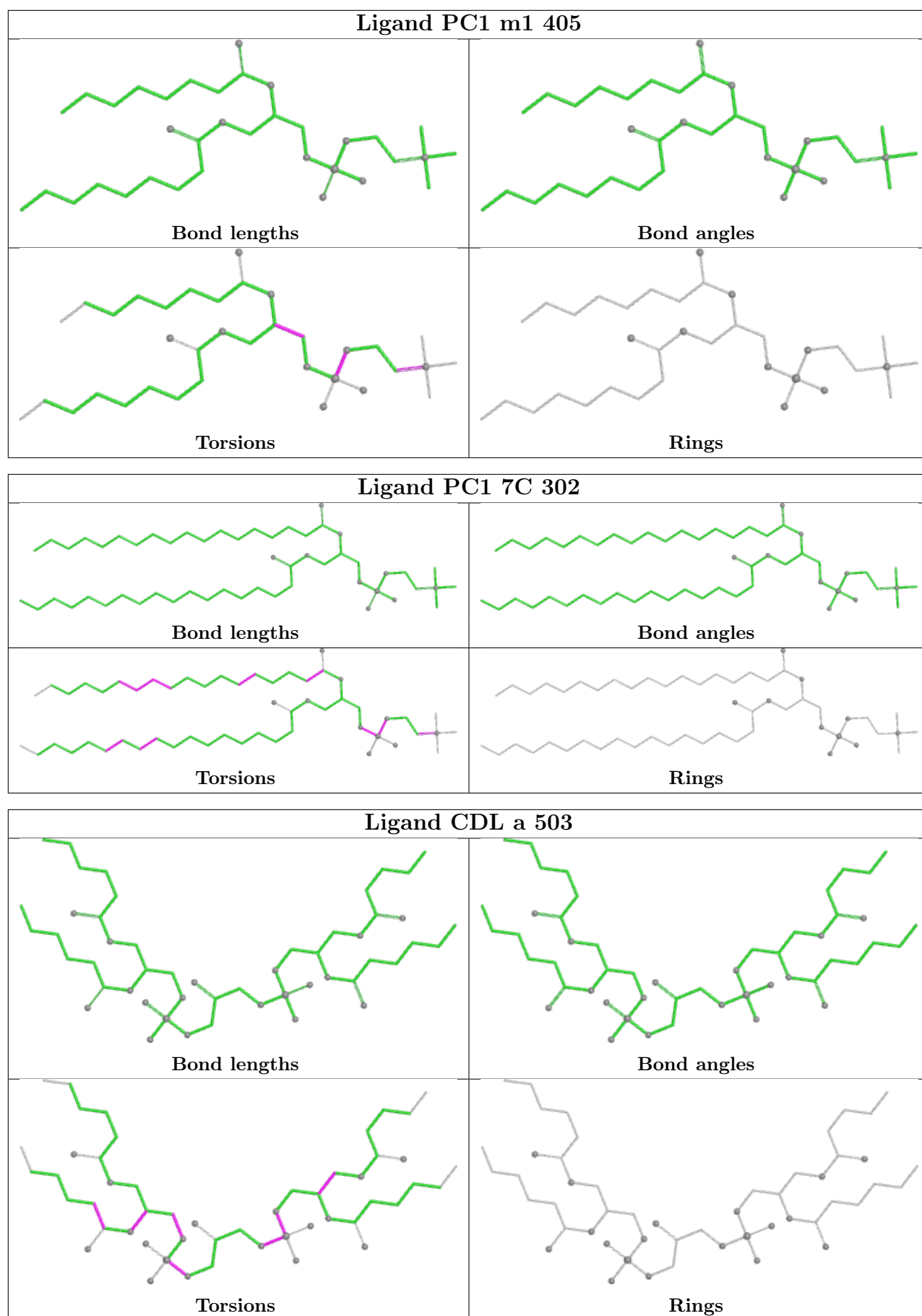


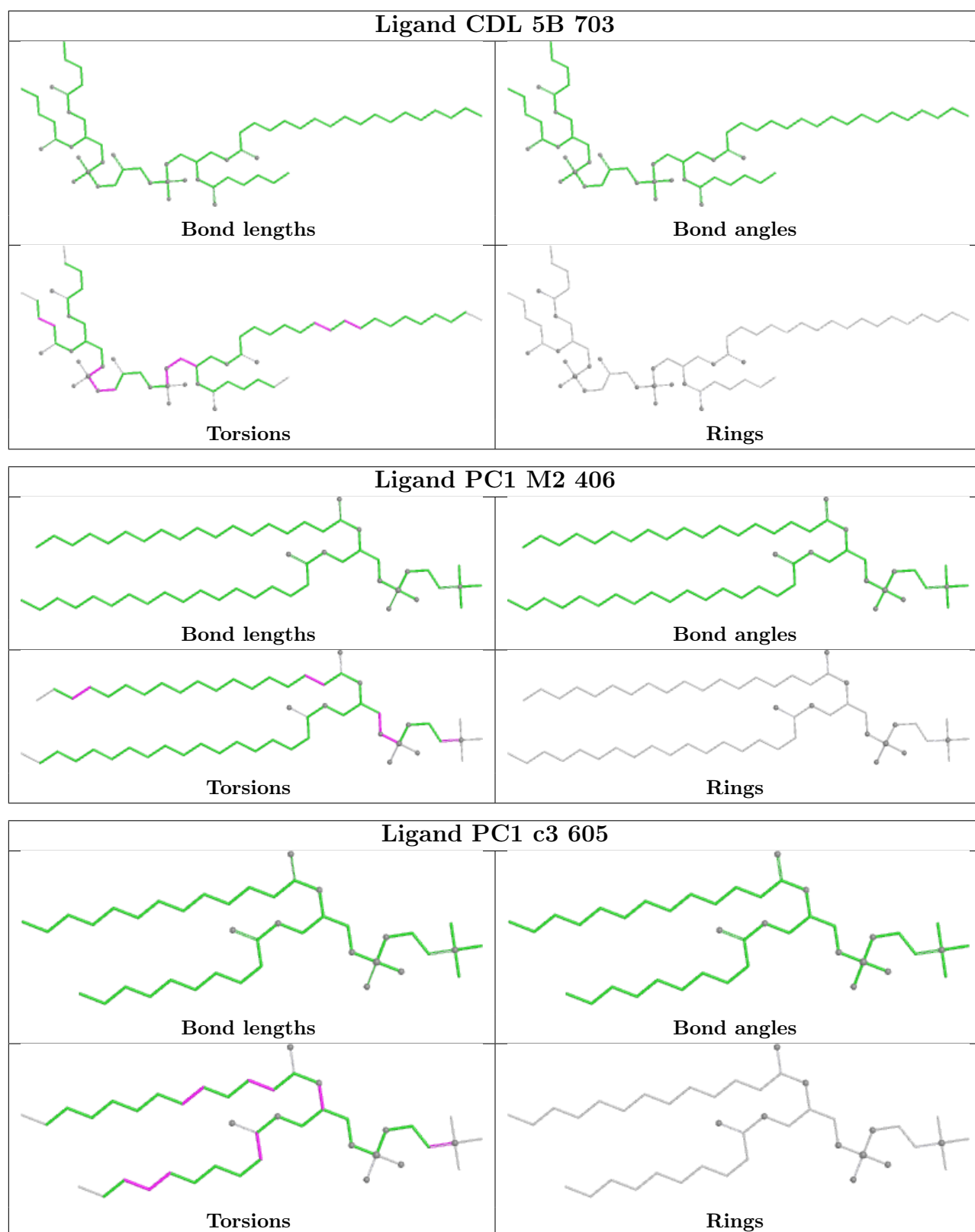


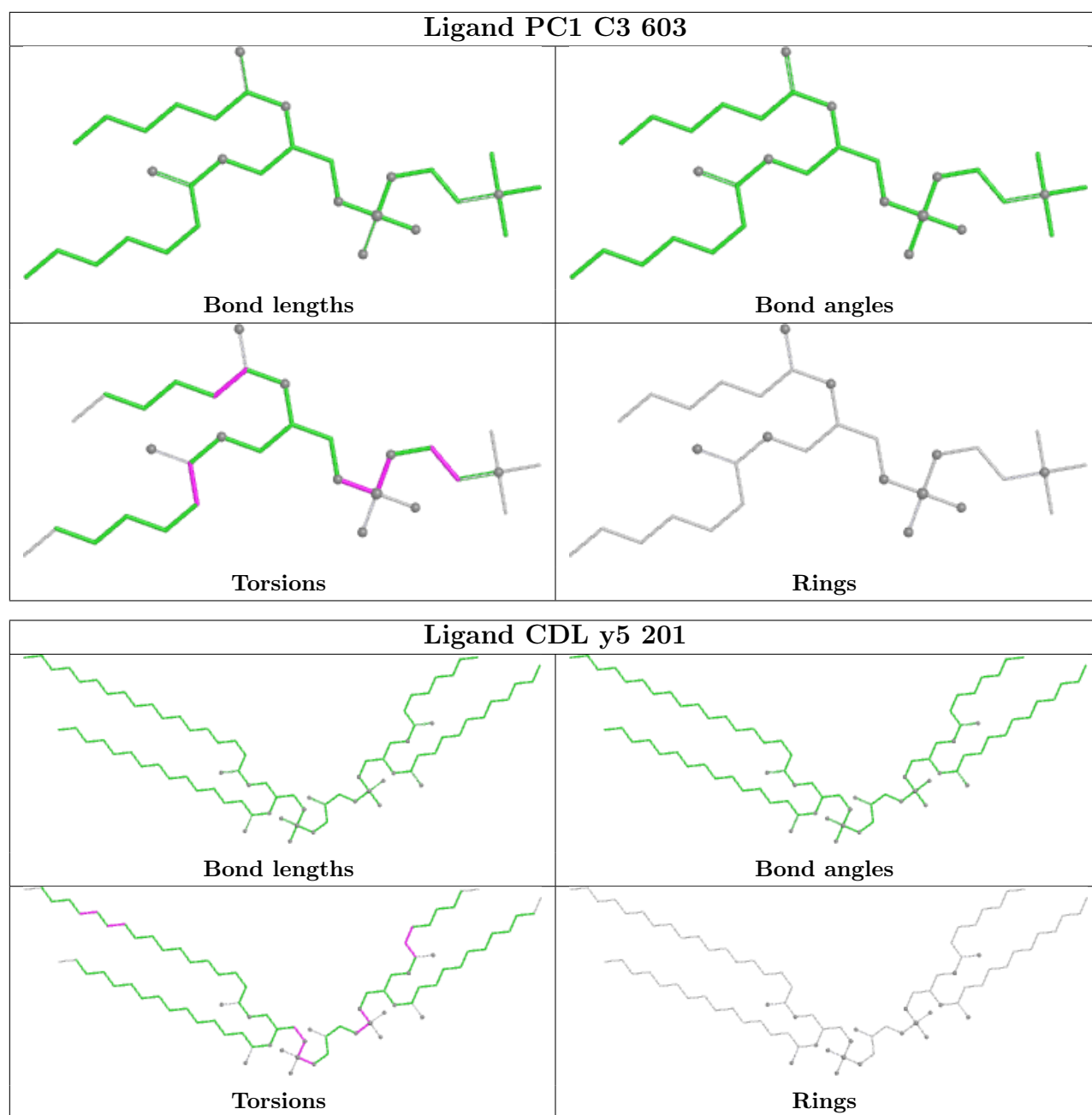


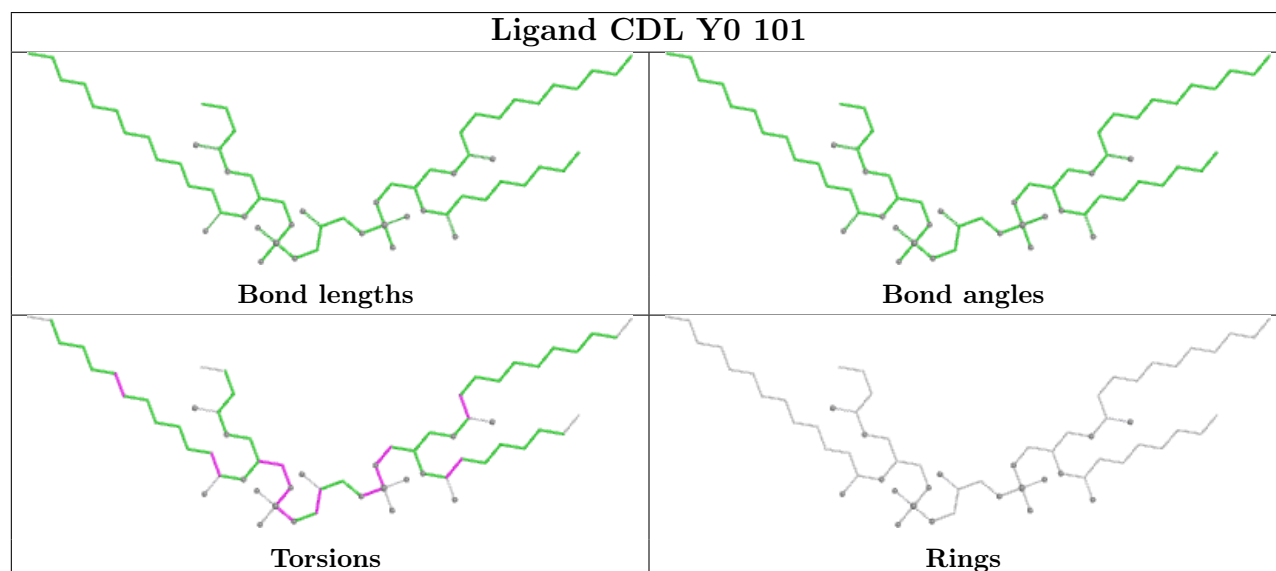
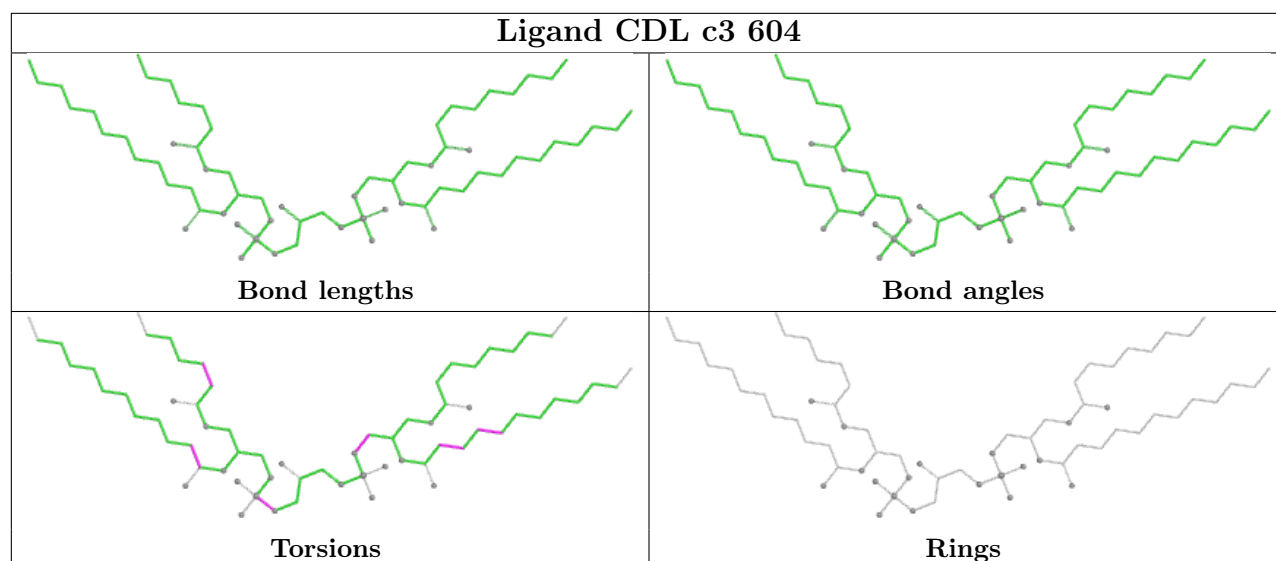
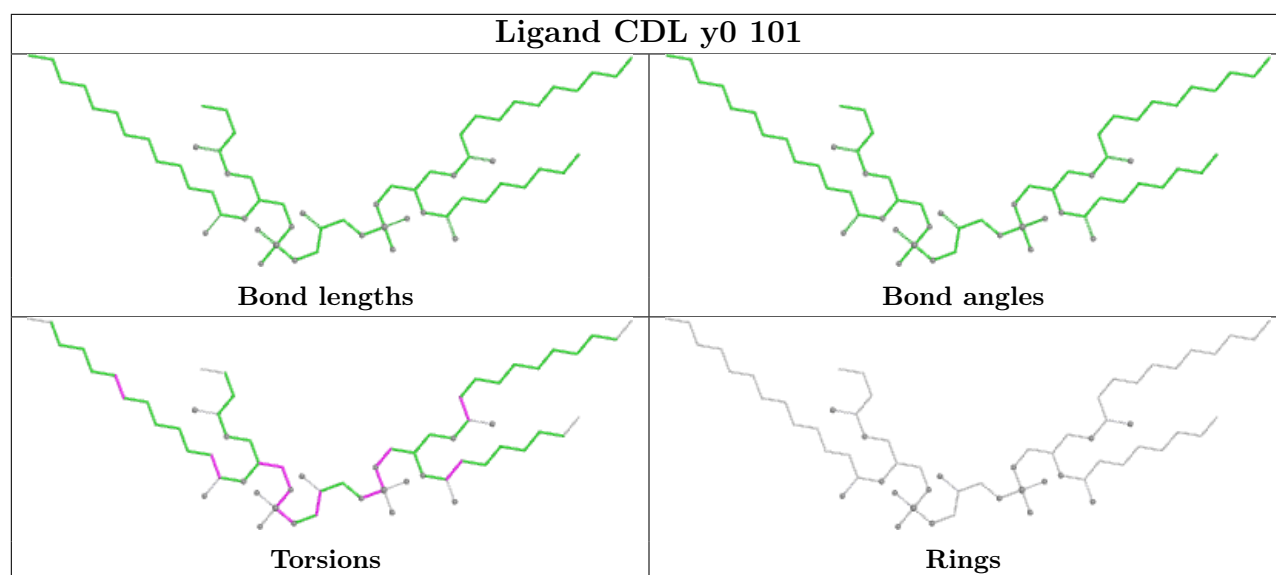


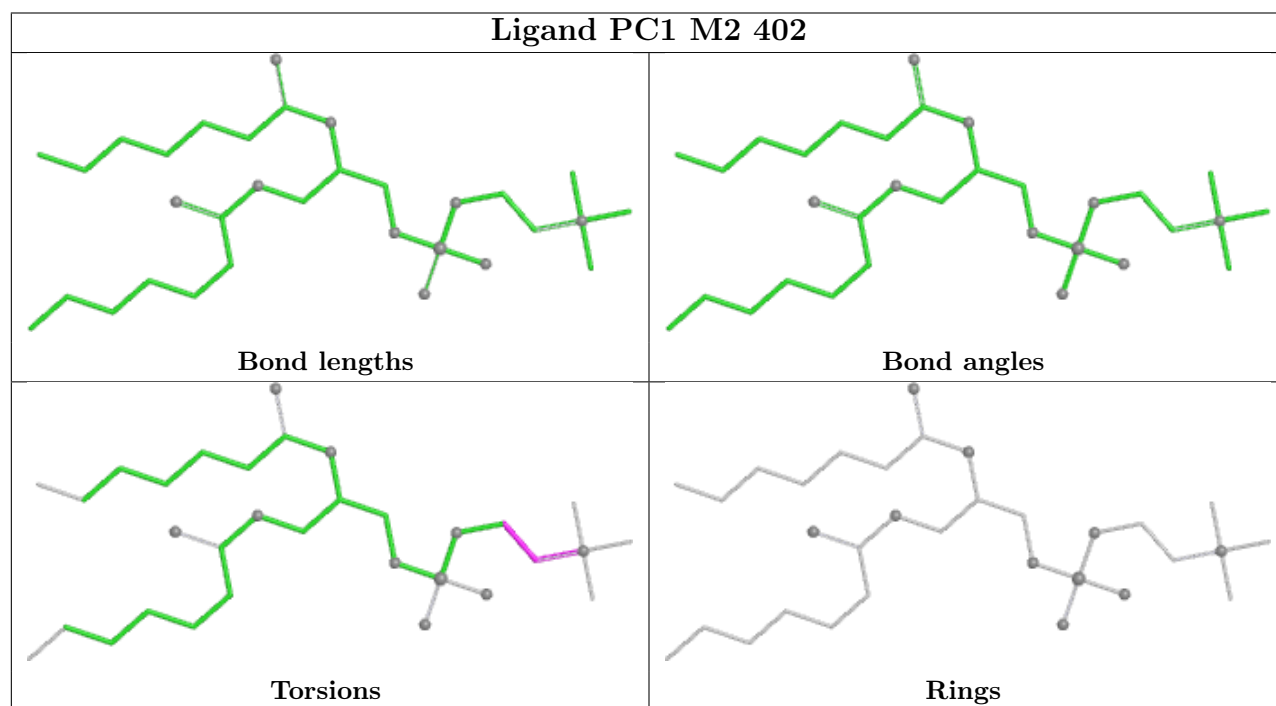
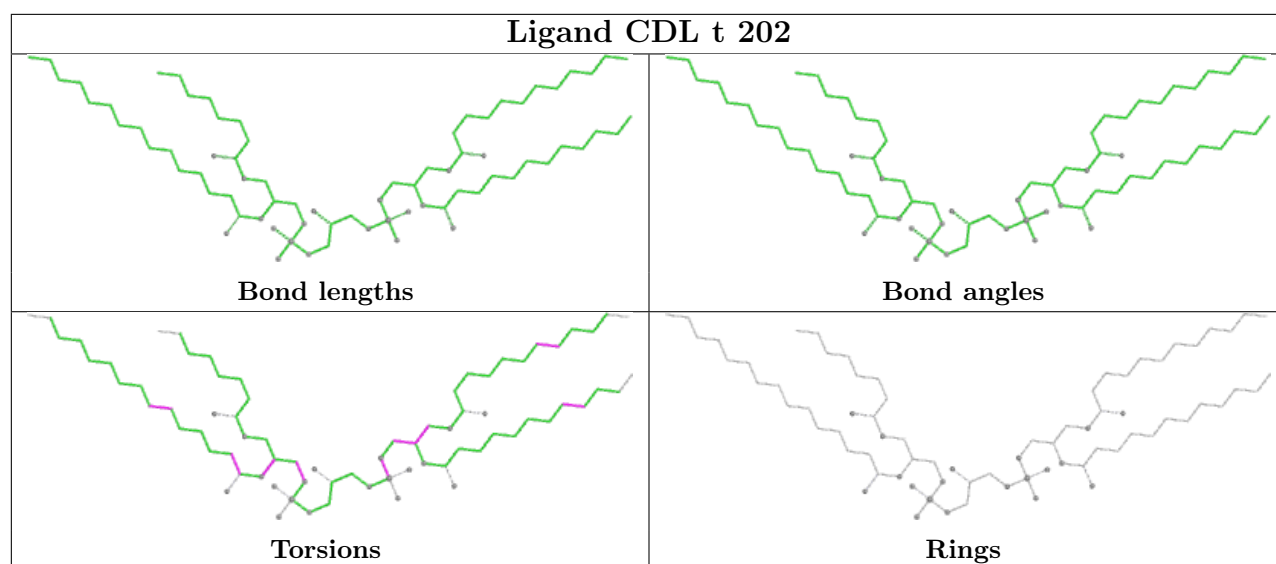


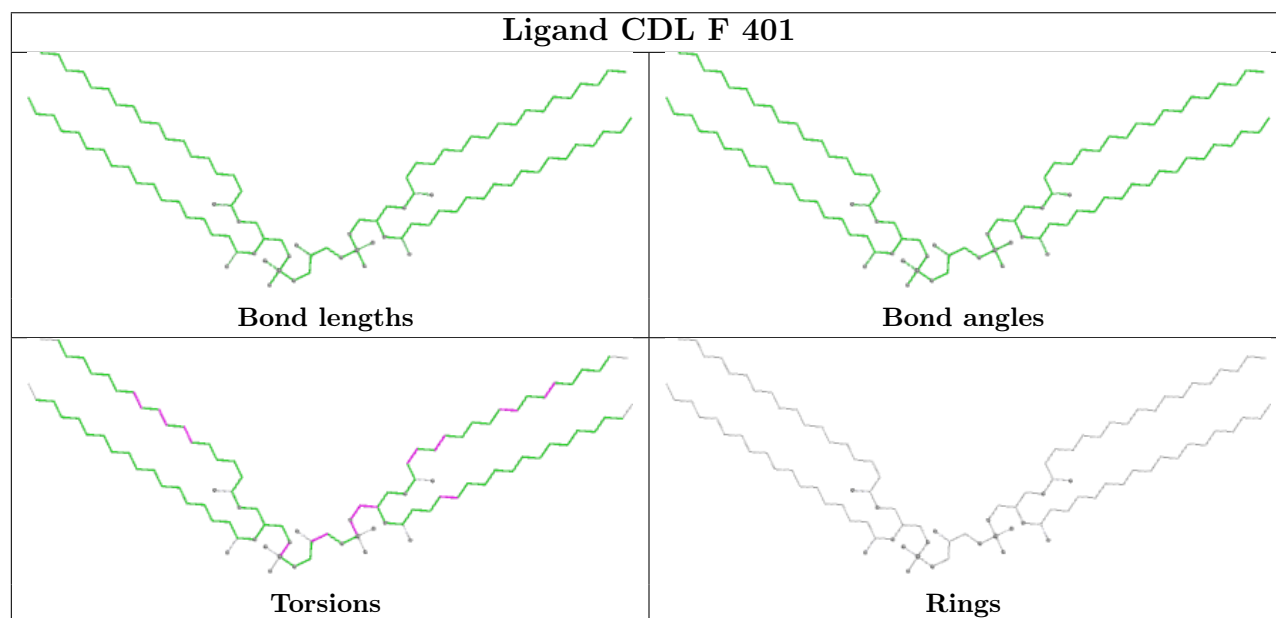
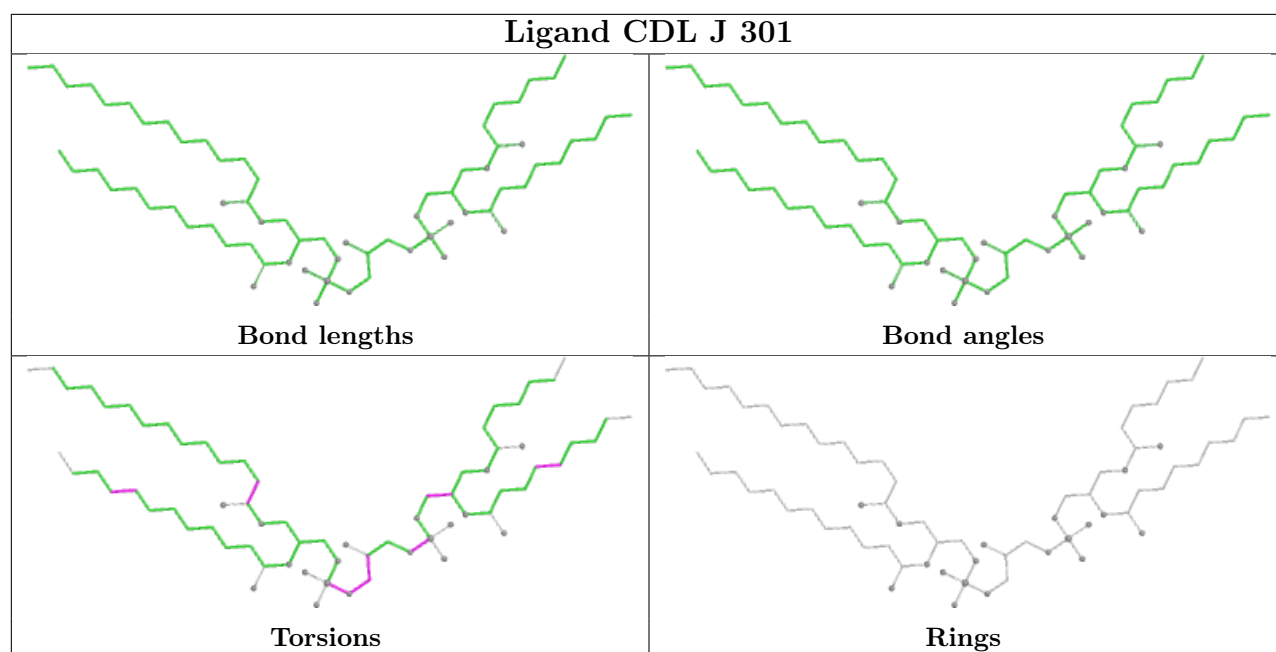


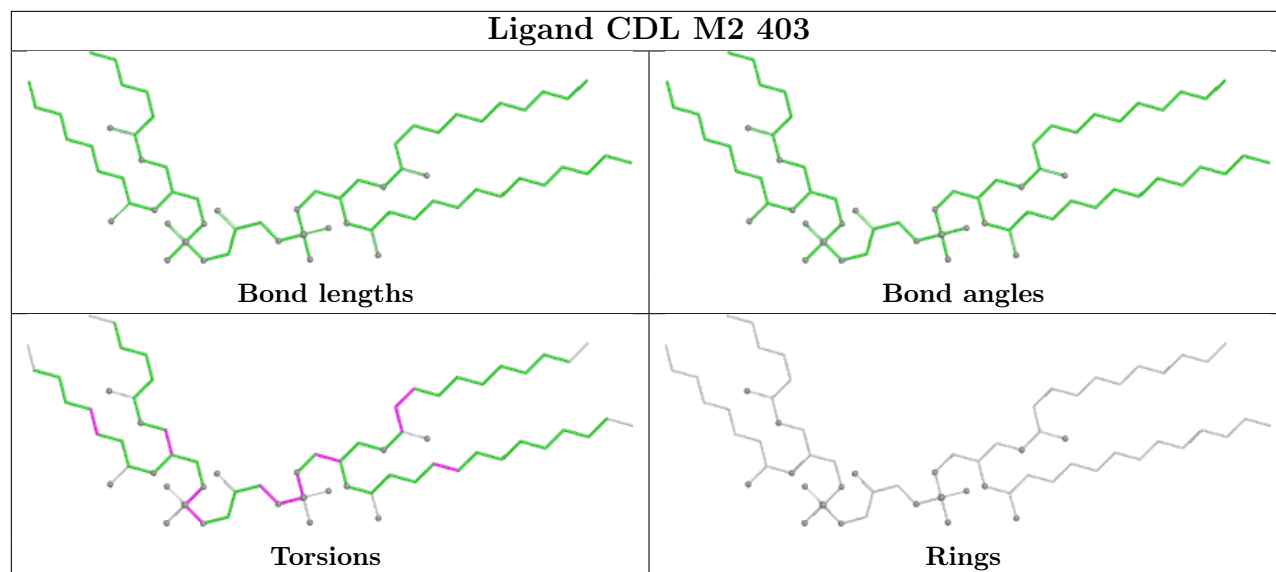












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

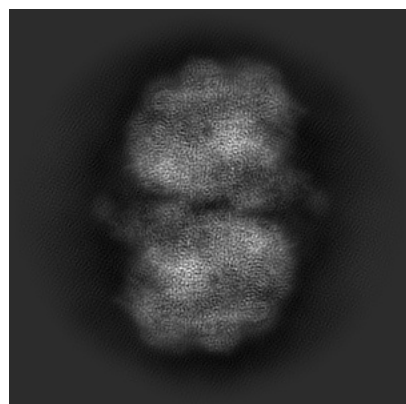
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32325. These allow visual inspection of the internal detail of the map and identification of artifacts.

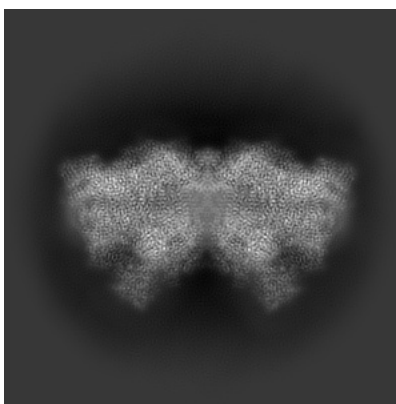
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

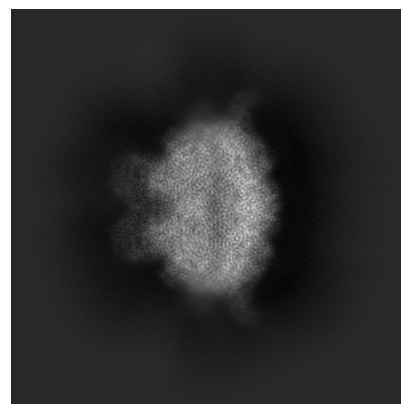
6.1.1 Primary map



X

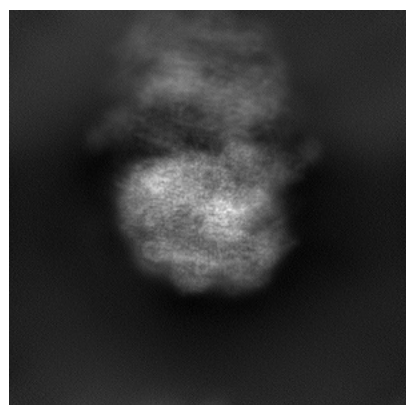


Y

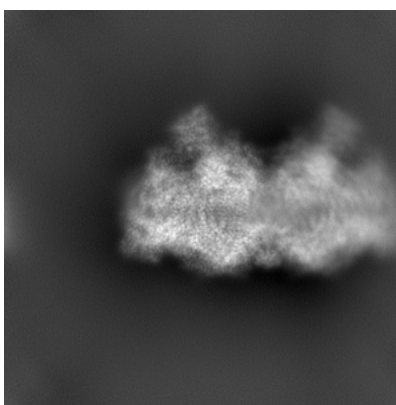


Z

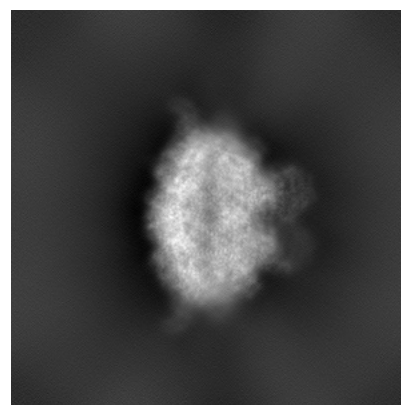
6.1.2 Raw map



X



Y

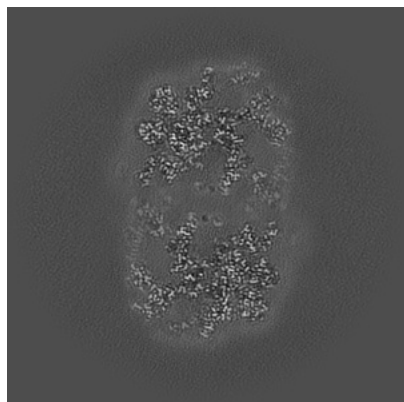


Z

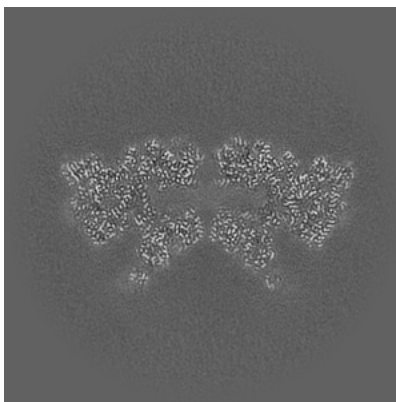
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

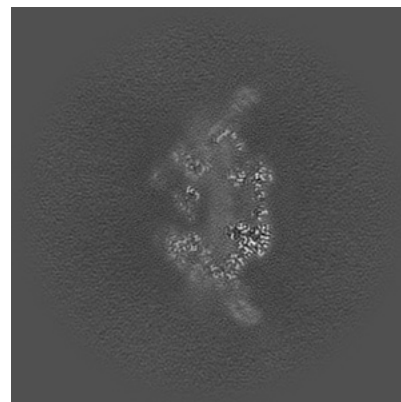
6.2.1 Primary map



X Index: 256

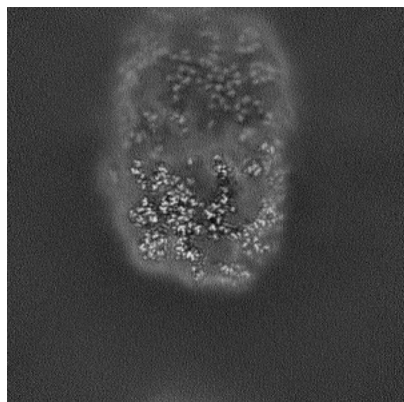


Y Index: 256

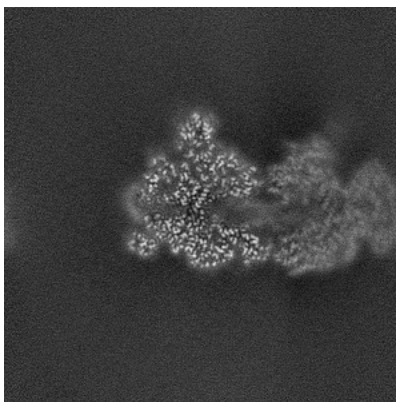


Z Index: 256

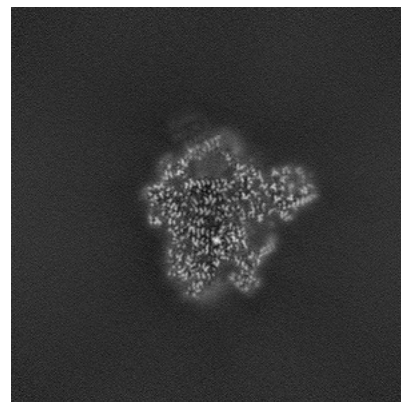
6.2.2 Raw map



X Index: 256



Y Index: 256

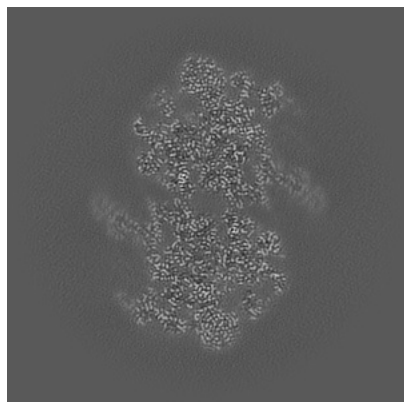


Z Index: 256

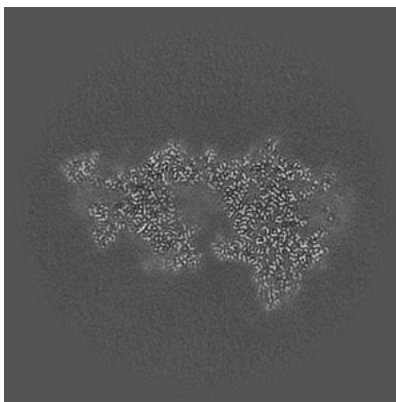
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

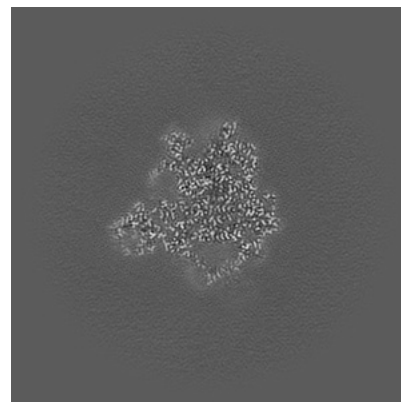
6.3.1 Primary map



X Index: 297

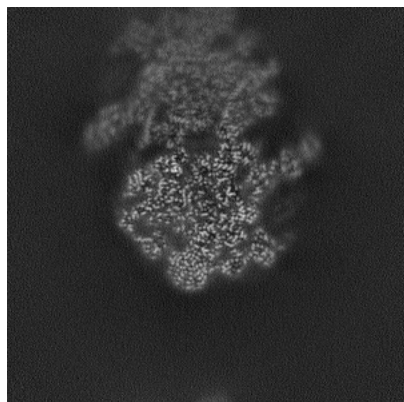


Y Index: 286

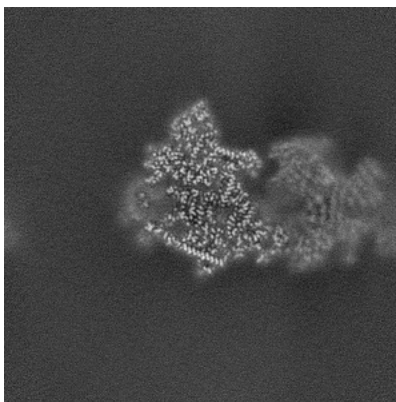


Z Index: 180

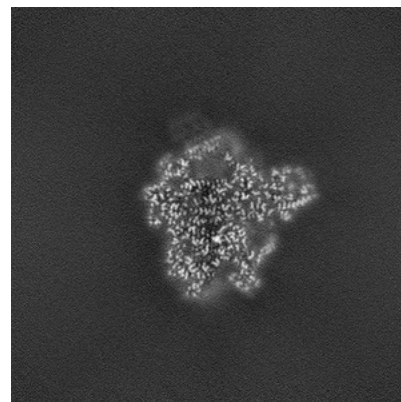
6.3.2 Raw map



X Index: 217



Y Index: 273

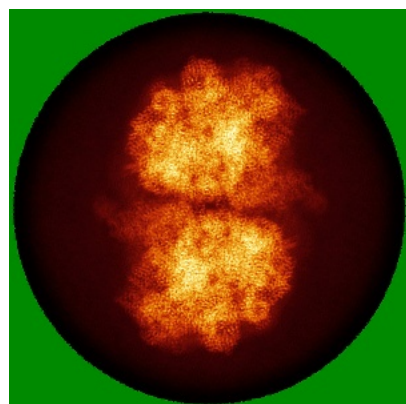


Z Index: 257

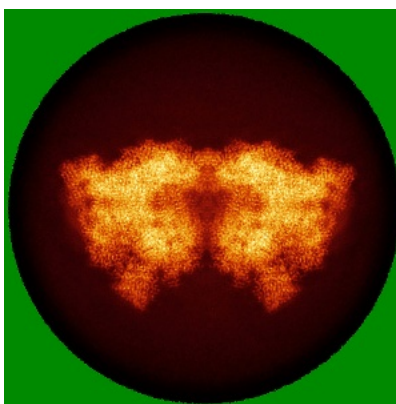
The images above show the largest variance slices of the map in three orthogonal directions.

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

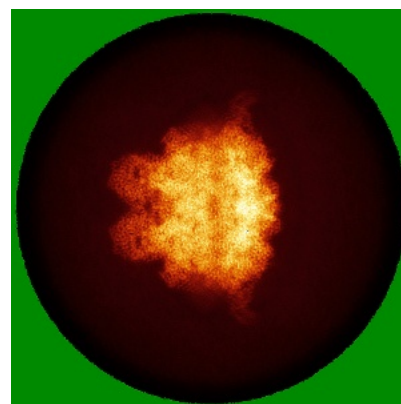
6.4.1 Primary map



X

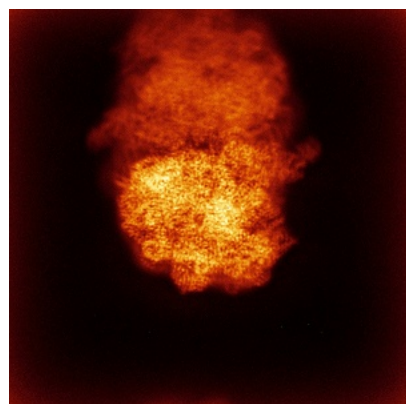


Y

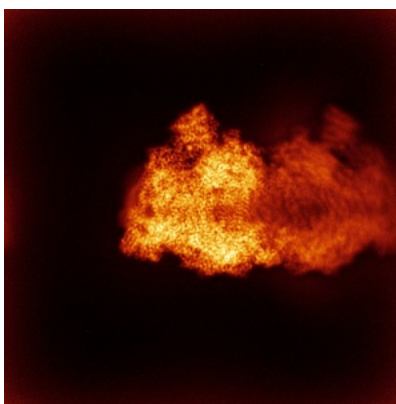


Z

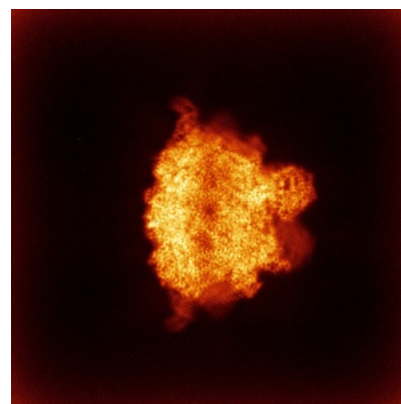
6.4.2 Raw map



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](#)

This section was not generated.

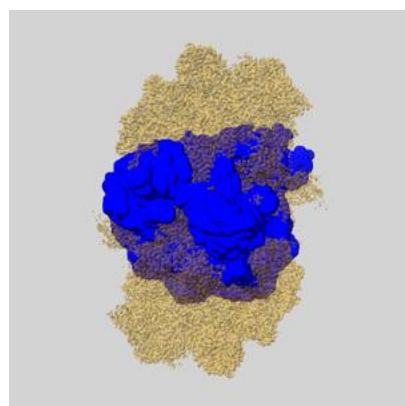
6.6 Mask visualisation [i](#)

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

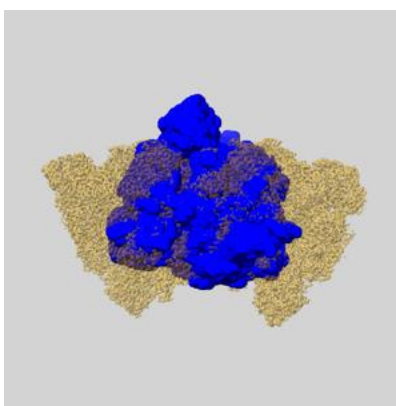
A mask typically either:

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

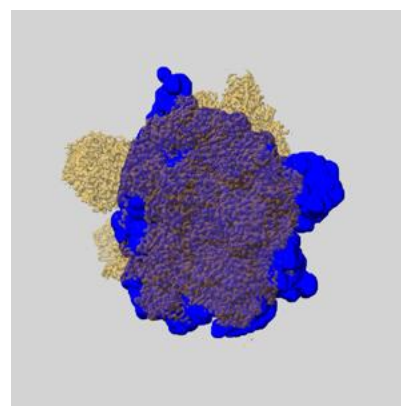
6.6.1 emd_32325_msk_1.map [i](#)



X



Y

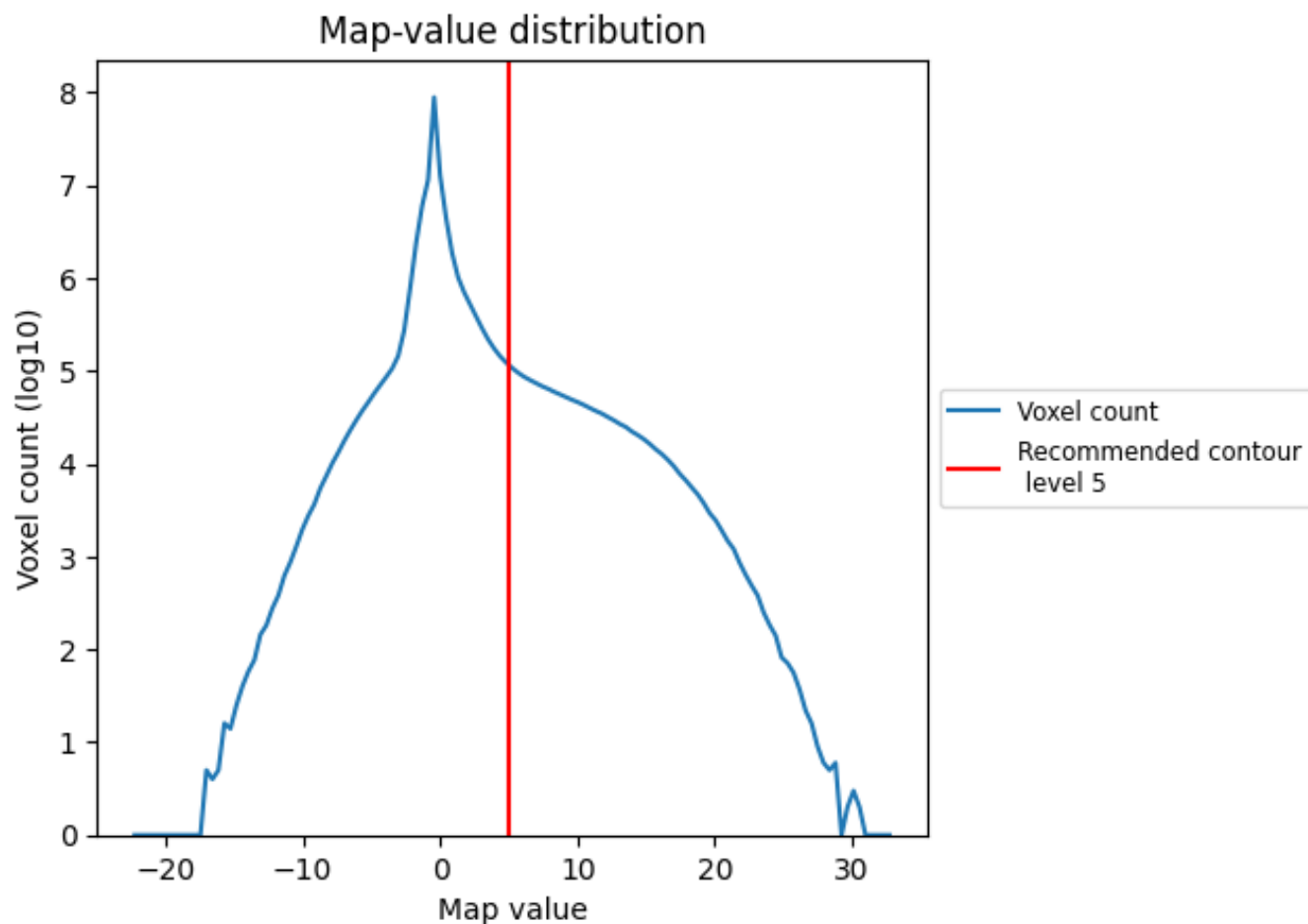


Z

7 Map analysis [i](#)

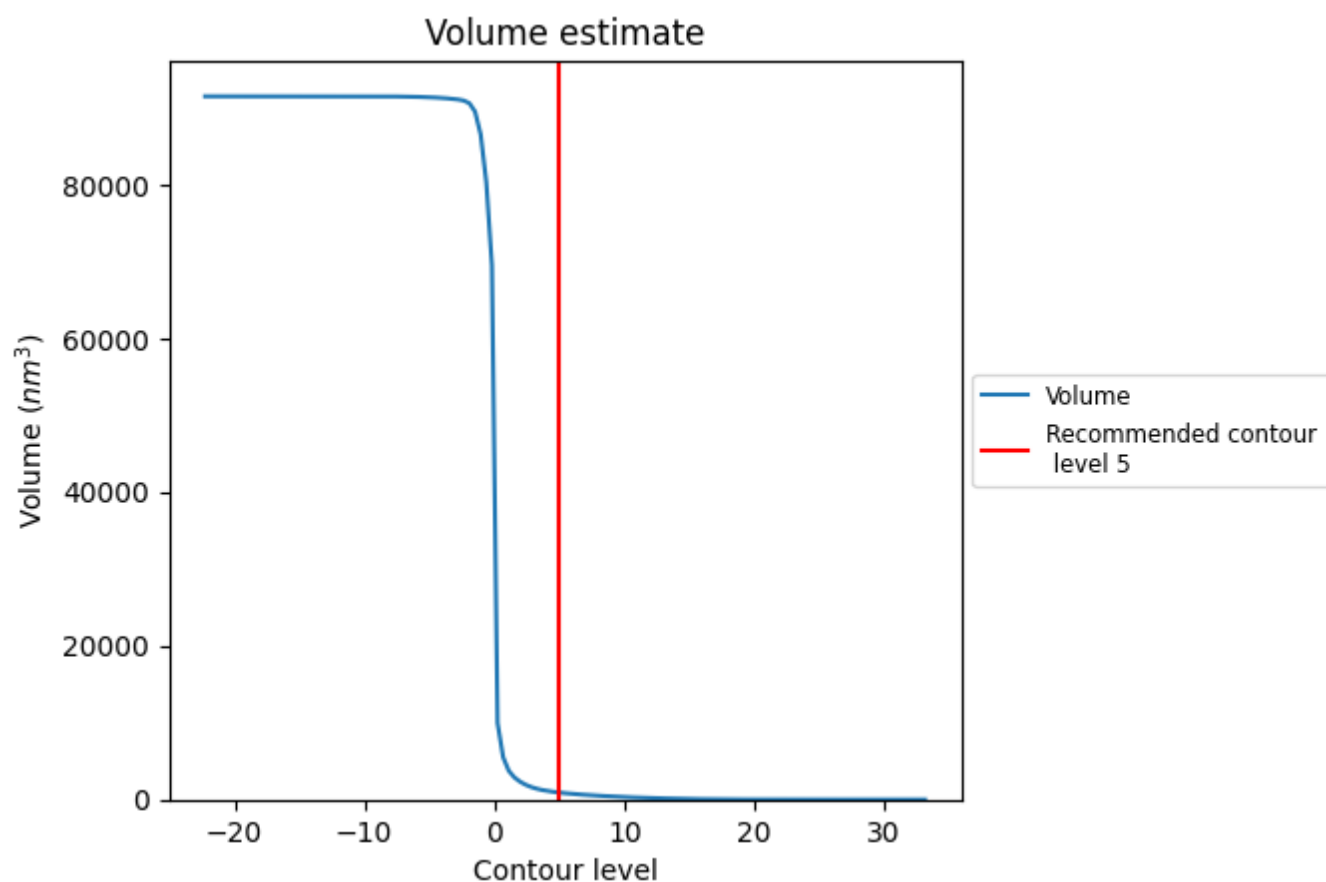
This section contains the results of statistical analysis of the map.

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.

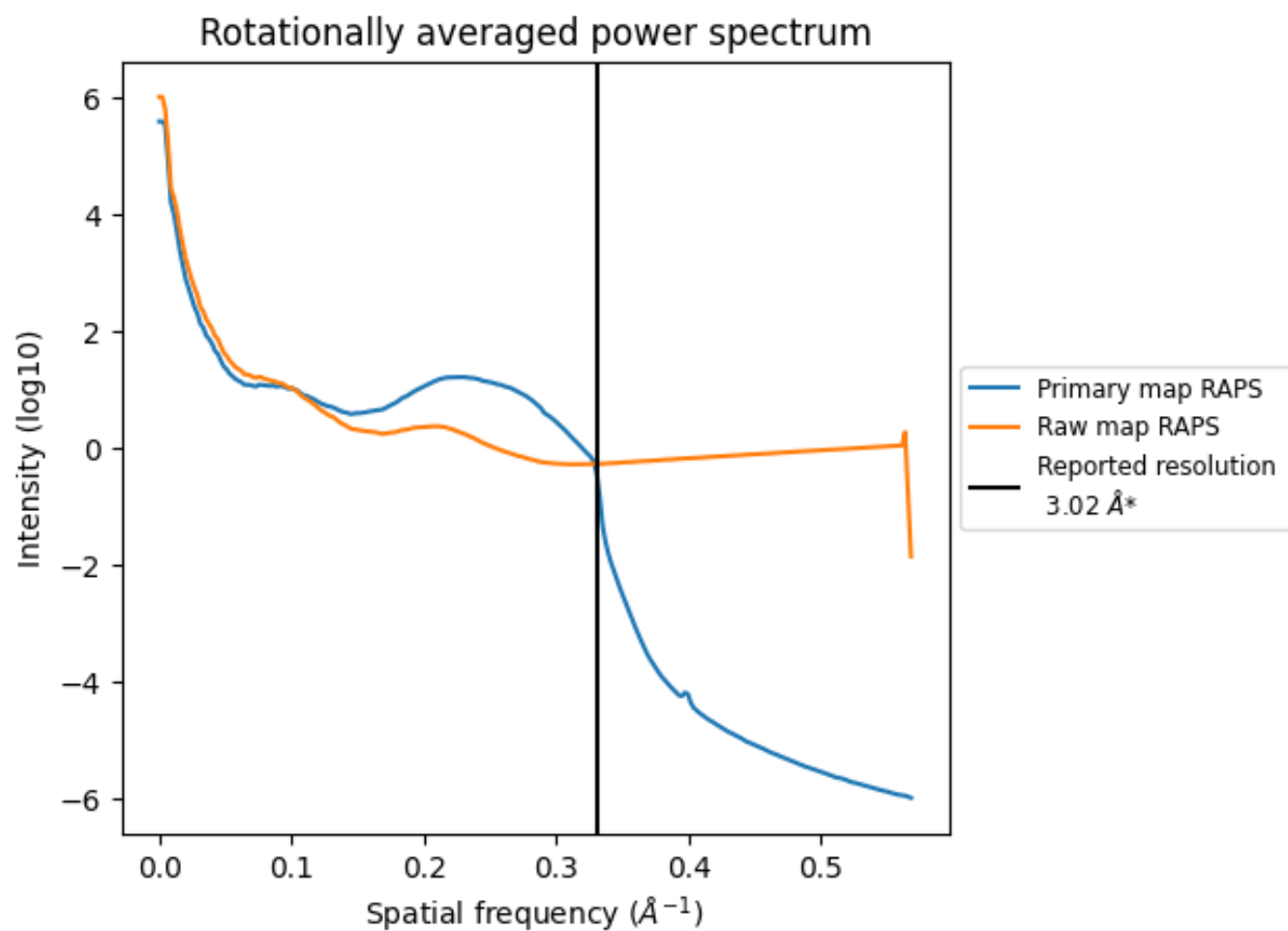
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm³; this corresponds to an approximate mass of 823 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 ⓘ

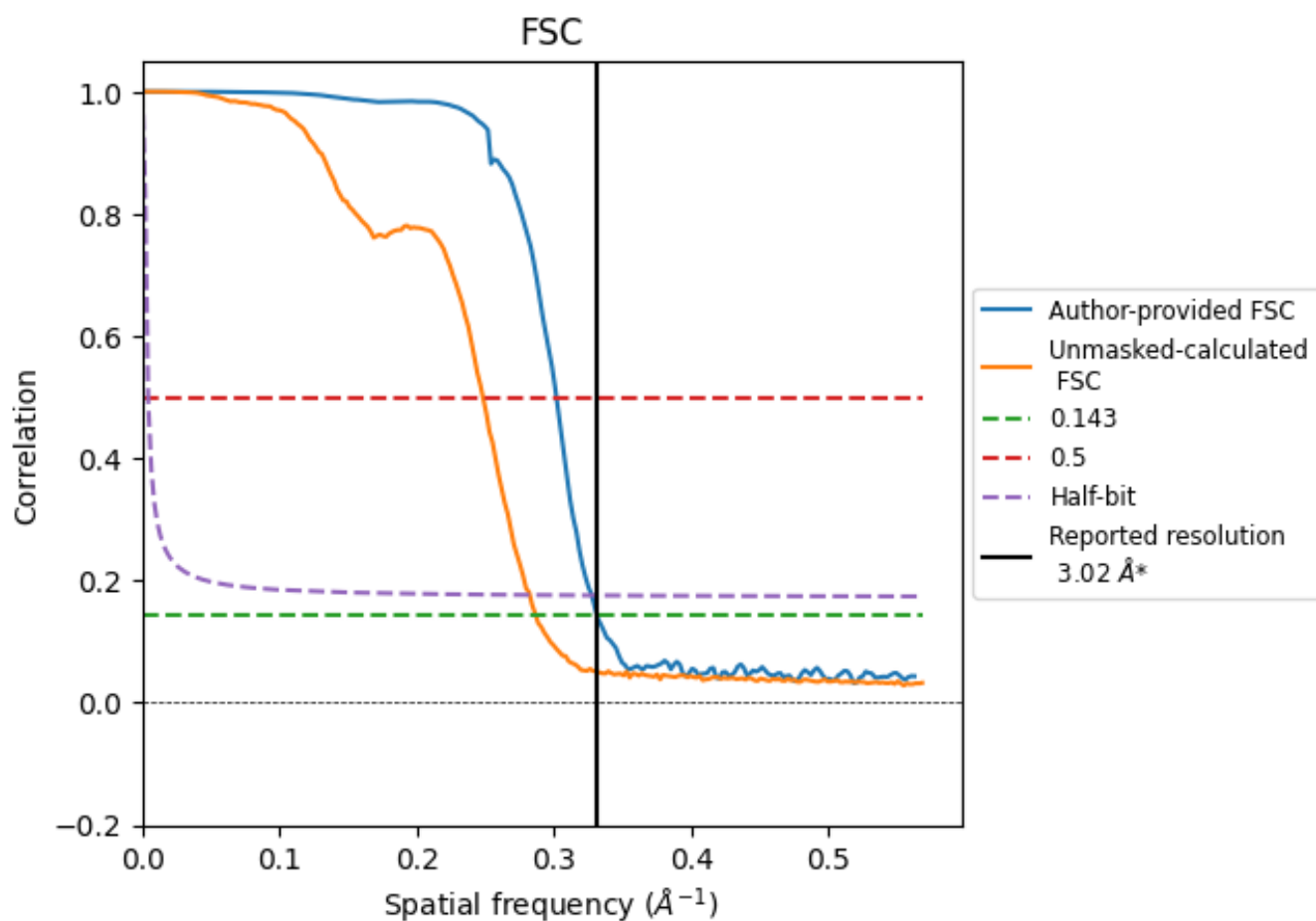


*Reported resolution corresponds to spatial frequency of 0.331 $\text{\AA}^{-1}$

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 0.331 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

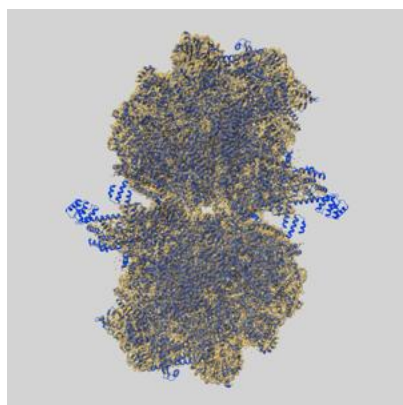
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.31	3.05
Unmasked-calculated*	3.49	4.03	3.54

*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 3.49 differs from the reported value 3.02 by more than 10 %

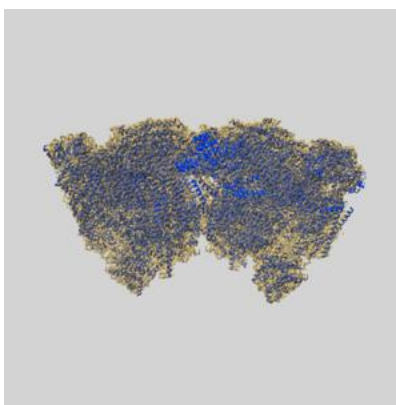
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32325 and PDB model 7W5Z. Per-residue inclusion information can be found in section 3 on page 30.

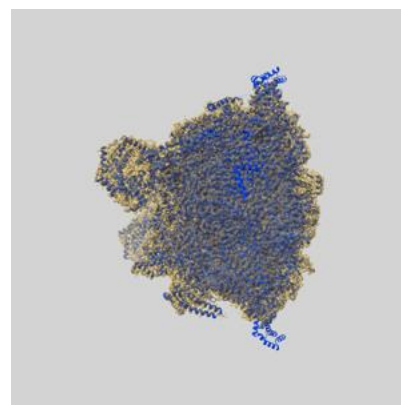
9.1 Map-model overlay [i](#)



X



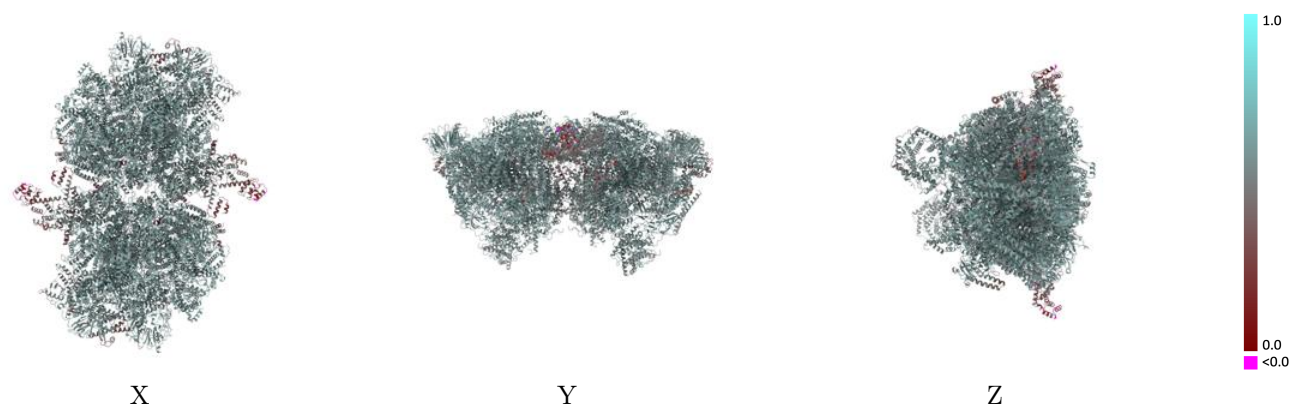
Y



Z

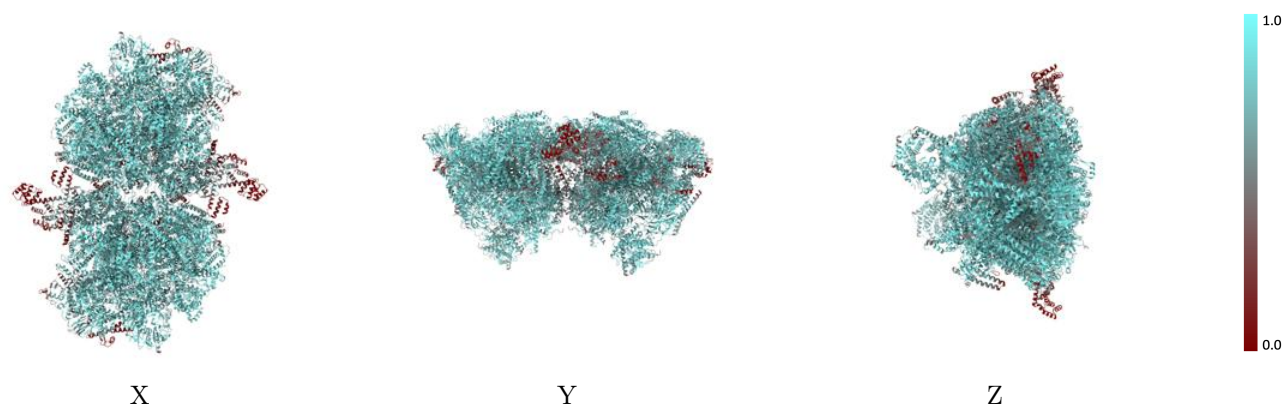
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



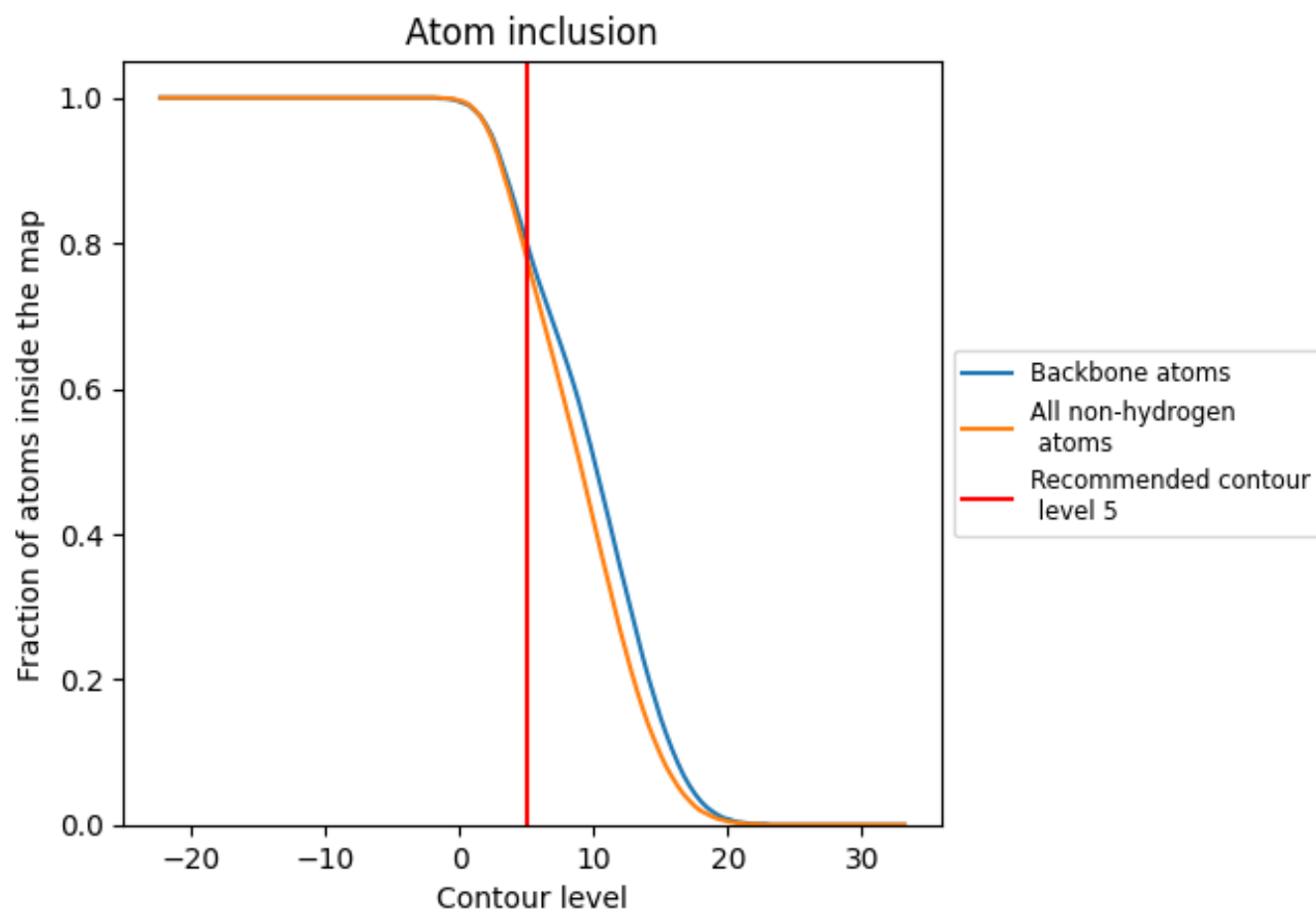
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.5680
5B	 0.8080	 0.5800
5b	 0.8080	 0.5790
6A	 0.8120	 0.5890
6B	 0.8530	 0.5890
6C	 0.8020	 0.5790
6L	 0.8290	 0.5640
6a	 0.8100	 0.5880
6b	 0.8580	 0.5900
6c	 0.8000	 0.5790
6l	 0.8230	 0.5640
7A	 0.8530	 0.6040
7C	 0.8460	 0.5920
7L	 0.8010	 0.5590
7a	 0.8500	 0.6030
7c	 0.8420	 0.5900
7l	 0.8010	 0.5590
A	 0.8400	 0.5910
AC	 0.8350	 0.5970
B	 0.5960	 0.5200
BP	 0.8080	 0.5750
C	 0.2690	 0.4150
C1	 0.8480	 0.5900
C2	 0.8260	 0.5800
C3	 0.7670	 0.5690
D	 0.7750	 0.5640
E	 0.7780	 0.5730
F	 0.8510	 0.5820
FS	 0.8390	 0.5810
G	 0.8750	 0.5890
H	 0.7430	 0.5450
I	 0.5910	 0.5130
J	 0.8190	 0.5820
K	 0.8380	 0.5780
L	 0.7810	 0.5690



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Chain	Atom inclusion	Q-score
M	 0.7180	 0.5520
M1	 0.8400	 0.5800
M2	 0.8440	 0.5870
M3	 0.7890	 0.5770
N	 0.8300	 0.5870
O	 0.8080	 0.5760
P	 0.7950	 0.5670
Q	 0.8470	 0.5900
R	 0.6280	 0.5160
S	 0.4690	 0.4540
T	 0.7560	 0.5810
T1	 0.8120	 0.5690
T2	 0.7560	 0.5490
T3	 0.7430	 0.5210
T4	 0.8170	 0.5560
T5	 0.7710	 0.5390
T6	 0.7910	 0.5410
U	 0.8170	 0.5790
U1	 0.7550	 0.5310
U2	 0.1760	 0.3210
U3	 0.2820	 0.3910
U4	 0.1600	 0.3930
U5	 0.4150	 0.4690
U6	 0.4110	 0.4220
V	 0.8100	 0.5780
W	 0.7220	 0.5520
X	 0.8520	 0.5930
Y	 0.8760	 0.5940
Y0	 0.8460	 0.5900
Y5	 0.7020	 0.5520
Y7	 0.6180	 0.5230
Z	 0.5880	 0.5160
a	 0.8440	 0.5900
ac	 0.8330	 0.5960
b	 0.6000	 0.5200
bp	 0.8060	 0.5740
c	 0.2800	 0.4160
c1	 0.8500	 0.5910
c2	 0.8300	 0.5800
c3	 0.7680	 0.5690
d	 0.7740	 0.5670
e	 0.7800	 0.5730

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Chain	Atom inclusion	Q-score
f	 0.8550	 0.5840
fs	 0.8410	 0.5810
g	 0.8760	 0.5890
h	 0.7450	 0.5470
i	 0.5980	 0.5140
j	 0.8190	 0.5810
k	 0.8340	 0.5780
l	 0.7790	 0.5700
m	 0.7250	 0.5520
m1	 0.8330	 0.5810
m2	 0.8420	 0.5870
m3	 0.7920	 0.5760
n	 0.8300	 0.5870
o	 0.8090	 0.5760
p	 0.7900	 0.5680
q	 0.8470	 0.5880
r	 0.6350	 0.5160
s	 0.4680	 0.4530
t	 0.7560	 0.5810
t1	 0.8180	 0.5640
t2	 0.7680	 0.5500
t3	 0.7380	 0.5210
t4	 0.8100	 0.5580
t5	 0.7790	 0.5430
t6	 0.7870	 0.5420
u	 0.8080	 0.5770
u1	 0.7470	 0.5330
u2	 0.1820	 0.3190
u3	 0.2530	 0.4000
u4	 0.1530	 0.4160
u5	 0.4190	 0.4830
u6	 0.4070	 0.4350
v	 0.8090	 0.5800
w	 0.7230	 0.5530
x	 0.8560	 0.5950
y	 0.8800	 0.5940
y0	 0.8370	 0.5880
y5	 0.7010	 0.5510
y7	 0.6150	 0.5240
z	 0.5940	 0.5200